The Use of Classification Methods for Gross Error Detection in Process Data

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ABSTRACT

All process measurements contain some element of error. Typically, a distinction is made between random errors, with zero expected value, and gross errors with non-zero magnitude. Data Reconciliation (DR) and Gross Error Detection (GED) comprise a collection of techniques designed to attenuate measurement errors in process data in order to reduce the effect of the errors on subsequent use of the data. DR proceeds by finding the optimum adjustments so that reconciled measurement data satisfy imposed process constraints, such as material and energy balances. The DR solution is optimal under the assumed statistical random error model, typically Gaussian with zero mean and known covariance.

The presence of outliers and gross errors in the measurements or imposed process constraints invalidates the assumptions underlying DR, so that the DR solution may become biased. GED is required to detect, identify and remove or otherwise compensate for the gross errors. Typically GED relies on formal hypothesis testing of constraint residuals or measurement adjustment-based statistics derived from the assumed random error statistical model.

Classification methodologies are methods by which observations are classified as belonging to one of several possible groups. For the GED problem, artificial neural networks (ANN's) have been applied historically to resolve the classification of a data set as either containing or not containing a gross error. The hypothesis investigated in this thesis is that classification methodologies, specifically classification trees (CT) and linear or quadratic classification functions (LCF, QCF), may provide an alternative to the classical GED techniques.

This hypothesis is tested via the modelling of a simple steady-state process unit with associated simulated process measurements. DR is performed on the simulated process measurements in order to satisfy one linear and two nonlinear material conservation constraints. Selected features from the DR procedure and process constraints are incorporated into two separate input vectors for classifier construction. The performance of the classification methodologies developed on each input vector is compared with the classical measurement test in order to address the posed hypothesis.

General trends in the results are as follows:

- The power to detect and/or identify a gross error is a strong function of the gross error magnitude as well as location for all the classification methodologies as well as the measurement test.
- For some locations there exist large differences between the power to detect a gross error and the power to identify it correctly. This is consistent over all the classifiers and their associated measurement tests, and indicates significant smearing of gross errors.
- In general, the classification methodologies have higher power for equivalent type I error than the measurement test.
- The measurement test is superior for small magnitude gross errors, and for specific locations, depending on which classification methodology it is compared with.

There is significant scope to extend the work to more complex processes and constraints, including dynamic processes with multiple gross errors in the system. Further investigation into the optimal selection of input vector elements for the classification methodologies is also required.

OPSOMMING

Alle prosesmetings bevat ’n sekere mate van metingsfoute. Die fout-element van ’n prosesmeting word dikwels uitgedruk as bestaande uit ’n ewekansige fout met nul verwagte waarde, asook ’n nie-ewekansige fout met ’n beduidende grootte. Data Rekonsiliasie (DR) en Fout Opsporing (FO) is ’n versameling van tegnieke met die doelwit om die effek van sulke foute in prosesdata op die daaropvolgende aanwending van die data te verminder. DR word uitgevoer deur die optimale veranderinge aan die oorspronklike prosesmetings aan te bring sodat die aangepaste metings sekere prosesmodelle gehoorsaam, tipies massa- en energie-balanse. Die DR-oplossing is optimaal, mits die statistiese aannames rakende die ewekansige fout-element in die prosesdata geldig is. Dit word tipies aanvaar dat die fout-element normaal verdeel is, met nul verwagte waarde, en ’n gegewe kovariansie matriks.

Wanneer nie-ewekansige foute in die data teenwoordig is, kan die resultate van DR sydig wees. FO is daarom nodig om nie-ewekansige foute te vind (Deteksie) en te identifiseer (Identifikasie). FO maak gewoonlik staat op die statistiese eienskappe van die meting aanpassings wat gemaak word deur die DR prosedure, of die afwykingsverskil van die model vergelykings, om formele hipoteses rakende die teenwoordigheid van nie-ewekansige foute te toets.

Klassifikasie tegnieke word gebruik om die klasverwantskap van observasies te bepaal. Rakende die FO probleem, is sintetiese neurale netwerke (SNN) histories aangewend om die Deteksie en Identifikasie probleme op te los. Die hipotese van hierdie tesis is dat klassifikasie tegnieke, spesifiek klassifikasie-bome (CT) en lineêre asook kwadratiese klassifikasie funksies (LCF en QCF), suksesvol aangewend kan word om die FO probleem op te los.

Die hipotese word ondersoek deur middel van ’n simulasie rondom ’n eenvoudige gestadigde toestand proses-eenheid wat aan een lineêre en twee nie-lineêre vergelykings onderhewig is. Kunsmatige prosesmetings word geskep met behulp van lukrake syfers sodat die foutkomponent van elke prosesmeting bekend is. DR word toegepas op die kunsmatige data, en die DR resultate word gebruik om twee verskillende insetvektore vir die klassifikasie tegnieke te skep. Die prestasie van die klassifikasie metodes word vergelyk met die metingstoets van klassieke FO ten einde die gestelde hipotese te beantwoord.

Die onderliggende tendense in die resultate is soos volg:

- Die vermoë om ‘n nie-ewekansige fout op te spoor en te identifiseer is sterk afhanklik van die grootte asook die ligging van die fout vir al die klassifikasie tegnieke sowel as die metingstoets.
- Vir sekere liggings van die nie-ewekansige fout is daar ‘n groot verskil tussen die vermoë om die fout op te spoor, en die vermoë om die fout te identifiseer, wat dui op smering van die fout. Al die klassifikasie tegnieke asook die metingstoets baar hierdie eienskap.
- Oor die algemeen toon die klassifikasie metodes groter sukses as die metingstoets.
- Die metingstoets is meer suksesvol vir relatief klein nie-ewekansige foute, asook vir sekere liggings van die nie-ewekansige fout, afhangende van die klassifikasie tegniek ter sprake.

Daar is verskeie maniere om die bestek van hierdie ondersoek uit te brei. Meer komplekse, nie-gestadigde prosesse met sterk nie-lineêre prosesmodelle en meervuldige nie-ewekansige foute kan ondersoek word. Die moontlikheid bestaan ook om die prestasie van klassifikasie metodes te verbeter deur die gepaste keuse van insetvektor elemente.

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GLOSSARY

Bias	*A systematic deviation from the true value of a measurement that is persistent over time*
Classification	*The process of determining and assigning the group membership of an unknown vector*
Data Reconciliation (DR)	*The process of determining the optimal measurement adjustments required so that the adjusted process measurements satisfy all imposed process constraints*
Discriminant Analysis	*The description of group separation, related to Classification*
Gross Error Detection (GED)	*The process of identifying measurements or constraints inconsistent with the assumed random error model*
Outlier	*A measurement value inconsistent with the bulk of the measurement data, typically occurring infrequently without any assignable cause*
Process Topology	*The structure of an industrial process, usually defined by the number of process units and the interconnections between process units formed by process streams*
Serial Correlation	*The autocorrelation of measurement values in time*
Type I Error	*Related to statistical hypothesis testing, the probability of rejecting the null hypothesis when it is true*
Type II Error	*Related to statistical hypothesis testing, the probability of failing to reject the null hypothesis when it is false*

LIST OF SYMBOLS

The convention for notation followed in this thesis is:

- Upper case letters or symbols refer to matrices
- Lower case bold letters or symbols refer to vectors
- Lower case letters or symbols refer to scalars

English Symbols

A	*Constraint matrix for linear systems, Jacobian matrix for nonlinear systems*
A_j	*Disjoint partitions of the input space* X *related to classifier development*
$\mathbf{a}$	*Vector of measurement adjustments determined through Data Reconciliation procedure, or vector of coefficients related to discriminant analysis*
a_i	*The adjustability of the* i^{th} *measurement*
$b^*, b,$ *or* $\mathbf{b}$	*Relative magnitude of gross error component, or scalar/ vector of gross error magnitude(s)*
B	*Matrix related to gross error magnitude estimation*
$\mathbf{c}$	*Vector of known constants related to constraints applied in linear Data Reconciliation*
C	*A set of classes related to classifier development*
$C(i\|j)$	*Misclassification cost associated with classifying a member of class j as class i*

cov_y	*Common coefficient of variation of the measurement vector* $\mathbf{y}$
$\mathbf{cov}_{\boldsymbol{\varepsilon}}$	*Vector of coefficients of variation of random error components*
$\mathbf{d}$	*Vector of diagonal elements of the measurement error covariance matrix to be estimated via the indirect method*
d_i	*The detectability of the* i^{th} *measurement*
D	*Matrix relating* $\mathbf{d}$ *to* $vec(H)$ *for measurement error covariance estimation via the indirect method*
$D_i^2(\mathbf{x})$	*Mahalanobis distance of vector* $\mathbf{x}$ *from a given class mean vector* $\bar{\mathbf{x}}_i$, *related to classification analysis*
$\mathbf{e}_j$	*A unit vector consisting of the* j^{th} *column of the identity matrix* I
$\mathbf{f}$	*Vector of diagonal and off-diagonal elements of the measurement error covariance matrix to be estimated via the indirect method*
$\mathbf{f}_k$	*Signature vector for the Generalized Likelihood Ratio Test*
$F(\cdot)$	*Set of nonlinear equality constraints related to Data Reconciliation*
F_2	*Diagonal matrix of unmeasured flow rates related to bilinear Data Reconciliation*
$G(\cdot)$	*Set of nonlinear inequality constraints related to Data Reconciliation*
G	*Matrix relating* $\mathbf{f}$ *to* $vec(H)$ *for measurement error covariance estimation via the indirect method*
$G_{\mathbf{x}}$	*Modified constraint matrix after removal of unmeasured variables by matrix projection*

H	*Covariance matrix of* $\mathbf{r}$*, the vector of constraint residuals*
I	*The identity matrix, consisting of ones on the diagonal and zeros elsewhere*
J	*Number of classes in the set* C
$\mathbf{k}$	*Vector of known parameters related to bilinear Data Reconciliation problem, or vector of known bounds related to bounded Data Reconciliation*
$L(\cdot)$	*Likelihood function related to Data Reconciliation with unknown error variance matrix*
L	*Matrix, with columns consisting of unit vectors corresponding to gross error locations, related to gross error magnitude estimation*
$L_i(\mathbf{x})$	*A linear classification function derived from* $D_i^2(\mathbf{x})$
l_i	*Lower bound on the* i^{th} *process variable, related to bounded Data Reconciliation*
M	*Matrix relating* $\mathbf{y}$ *to* $\mathbf{x}$ *when measurements are indirectly related to process states*
$M(\hat{\mathbf{x}})$	*Sum of squares of the vector of adjustments related to Data Reconciliation with unknown error variance matrix*
p	*The number of repeated measurement vectors available for covariance estimation*
$P(\cdot)$	*Probability function related to Data Reconciliation with unknown error variance matrix*

P	*Projection matrix used to remove unmeasured variables from the constraints prior to Data Reconciliation*
Q	*Matrix related to QR decomposition algorithm for finding a projection matrix* P
$Q_i(\mathbf{x})$	*A quadratic classification function derived from* $D_i^2(\mathbf{x})$
$\mathbf{r}$	*Vector of constraint residuals in linear Data Reconciliation*
R_i	*Ratio of variance estimates obtained from exponential filter estimates of the mean square deviation and difference of a process variable, related to steady-state identification*
R	*Matrix related to QR decomposition algorithm for finding a projection matrix* P
$R(T)$	*Estimated rate of misclassification of classification tree* T
S	*Sample estimate of covariance matrix*
$\mathbf{u}$	*Vector of unmeasured process variables*
u_i	*Upper bound on the* i^{th} *process variable, related to bounded Data Reconciliation*
$\mathbf{x}$	*Vector of unknown true process variables or input vector for classifier development*
$\hat{\mathbf{x}}$	*Estimate of* $\mathbf{x}$ *obtained via Data Reconciliation, where* $\mathbf{x}$ *represents a vector of unknown process variables*
$\hat{x}_i$	*The* i^{th} *element of* $\hat{\mathbf{x}}$ *, or an exponential filter estimate at time i*

X	*Input space containing all possible input vectors* $\mathbf{x}$ *for classifier development*
$\mathbf{y}$	*Measurement vector related to* $\mathbf{x}$
z	*Statistic related to the Nodal and Measurement Tests in Gross Error Detection*

Greek Symbols

α	*Level of significance of a statistical hypothesis test*
β	*Modified level of significance for multiple simultaneous statistical hypothesis tests, or constant used as a stop criterion in classification tree development*
$\boldsymbol{\varepsilon}$	*Vector of random measurement error components*
$\hat{\delta}_i^2$	*Exponential filter estimate of the mean square difference of a process variable at time i*
$\phi(\cdot)$	*Impurity function related to classification tree development*
λ *or* $\boldsymbol{\lambda}$	*Filter constant for exponential filter, or vector of Lagrange multipliers related to solving the linear Data Reconciliation problem*
$\hat{\upsilon}_i^2$	*Exponential filter estimate of the mean square deviation of a process variable at time i*
Π	*Permutation matrix*
τ	*Statistic related to the Global Test in Gross Error Detection*
ρ	*Autocorrelation coefficient of a process variable*

$\boldsymbol{\rho}$	*Vector of constraint residuals in the generalized linear Data Reconciliation problem*
Σ_y	*Covariance matrix of measurement vector* $\mathbf{y}$
Σ_ε	*Covariance matrix of random error vector* $\boldsymbol{\varepsilon}$

1 INTRODUCTION

This section introduces the concepts of Data Reconciliation (DR) and Gross Error Detection (GED) as it applies in the chemical and metallurgical process industries.

1.1 THE CONCEPT OF DATA RECONCILIATION AND GROSS ERROR DETECTION

It is hard to imagine an industrial process that does not generate an output of information of some form at regular time intervals. Most modern plants are designed with at least a minimal network of sensors and instruments for process control purposes, and similarly older plants are retrofitted for competitive and safety reasons. Some industrial processes may have thousands of variables that are routinely recorded, such as tank levels, stream flows, densities, compositions, temperatures and pressures, at frequencies of seconds or less. In addition to measurements made by online instrumentation, routine sampling to obtain laboratory assays of selected process stream constituents may be done over time periods corresponding to operations shifts, batches of product etc., where *assays* refer to procedures used to estimate the quantity or concentration of a particular stream component. Non-routine plant sampling campaigns may also be conducted from time to time in order to generate information regarding the process not obtainable from the online instrumentation or routine samples. Collectively all plant measurements are obtained with the objective of improving the efficiency of the process, either by preventing unsafe or hazardous conditions through process interlocks and safeguards, maintaining near optimum operating conditions through advanced control, providing information on the efficiency of unit operations on a regular basis, or aiding product quality control.

Measurements of process variables contain error, i.e. there is a difference between the measured and true value of a variable. The true value of a measurement can never be known in an absolute sense, but at best described statistically. The potential sources of measurement error are numerous, and may be related to online instrumentation (e.g. calibration error, hysteresis, zero and span drift due to fouling or wear), signal processing and transmission (including human error and transcription errors), sampling practice (especially for heterogeneous particulates), and sample analysis (i.e. assay procedures).

Depending on the intended use of a measurement or group of measurements, the measurement error may have significant impact on the usefulness of such measurement(s). There is therefore a need to reduce the impact of measurement errors on subsequent interpretation and use of the process data. Technological advances have led to smart instruments with internal diagnostic checks to ensure data quality. Statistical signal processing can also attenuate some of the variability associated with high frequency measurements and possibly detect outliers.

These techniques focus on each measured variable in isolation. It is, however, possible to exploit the topology of a process to relate the measurements to each other via a process model with implied constraints on the variables, typically the laws of conservation of mass and energy, although kinetic and thermodynamic relations related to mass and heat transfer may also be used (Madron, 1992: 27, 41). Such imposed constraints allow analysis of the measurements as a connected system, and limit the allowable measurement magnitudes, which serve as the basis for gross error detection.

Data Reconciliation (DR) and Gross Error Detection (GED) comprise a collection of techniques that exploit relationships between variables imposed by some process model in order to reduce the effect of errors on the subsequent processing and interpretation of measurements, by attenuating the measurement error present in process measurements in order to find reconciled estimates that are optimal in some way (Narasimhan and Jordache, 2000: 4).

1.2 TOPICS IN DATA RECONCILIATION AND GROSS ERROR DETECTION

A general scheme for the typical DR and GED problem is illustrated below:

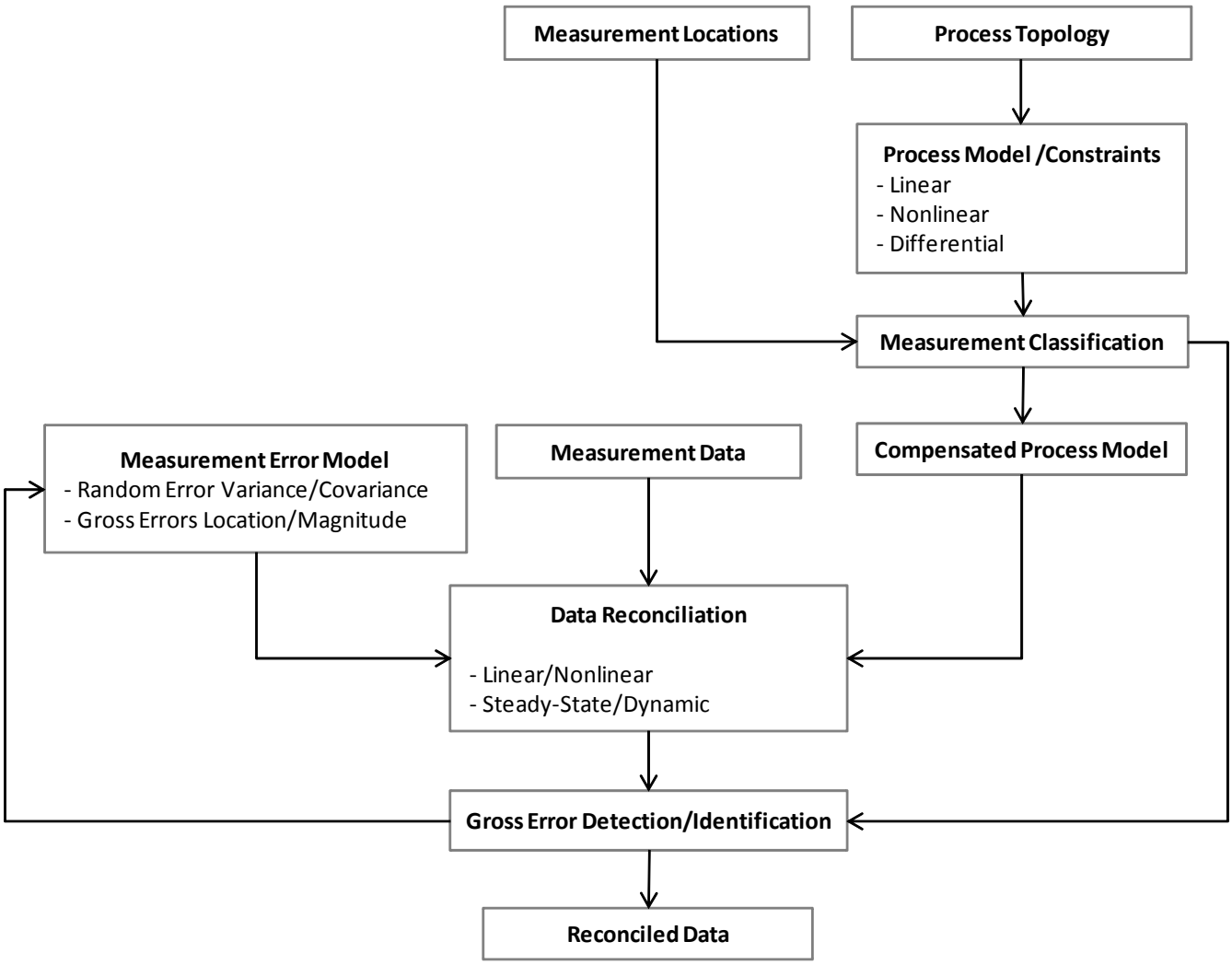

Figure 1-1 - Example of Data Reconciliation and Gross Error Detection Scheme

The scheme illustrated in Figure 1-1 is not unique or comprehensive, but serves to illustrate the relevant topics that will be discussed in more detail below. Some alternative approaches combine the DR and GED steps in a simultaneous strategy (Tjoa and Biegler, 1991).

1.2.1 Concerning Process Measurements and Errors

1.2.1.1 Redundancy and Observability

It may be infeasible or uneconomic to obtain measurements of all the variables in a process plant, so that typically there will be a number of unmeasured variables. Depending on the process topology and measurement locations, measured variables may be redundant or non-redundant, a distinction which is important as only redundant measurements impact on the DR results, and interpretation of GED results for non-redundant measurements are problematic (Albequerque and Biegler, 1996). A measured variable is redundant if, had the variable not been measured, its value could be estimated from the remaining measured variables through the process model (Bagajewicz, 2010: 37).

When unmeasured variables are present in the imposed process constraints, the values of some of these unmeasured variables may be uniquely estimable from the measured variables through the process constraints (Crowe, 1996). Unmeasured variables that may be inferred in this way are observable, while the remaining unmeasured variables are unobservable, i.e. no legitimate estimate of their magnitudes is possible, although the DR procedure may often ascribe magnitudes to unobservable variables.

Variable classification methods are therefore required in order to correctly interpret the results of DR and GED, including estimates of unmeasured variables.

1.2.1.2 Measurement Error

The total error in a measurement can be decomposed depending on the source of each component of the measurement error, and is typically expressed as the sum of a random error (white noise) component and a systematic (or gross) error component:

$$y = x + b + \varepsilon \tag{1.1}$$

Where y is the measured value, x is the unknown true value, and ε and b represent random and gross error components, respectively. The additive error model in (1.1) is not unique; it is possible that measurement errors may be proportional to the measured value, as would be the case for span drift, or that the measurement value and error components are some other (possibly nonlinear) functions of the process state variable x.

The classification and definition of measurement error components is not consistent in the Data Reconciliation and Gross Error Detection literature. A summary of the different components described in the literature, and some of their pertinent properties, is given in Table 1-1 and the paragraphs that follow.

Table 1-1 : Summary of Properties of Measurement error Components

	Random Error	Outliers	Systematic Error	Bias	Gross Error
Distribution	Gaussian	Gaussian?	N/A	N/A	N/A
Expected Value	Zero	Zero/Non-zero	Non-zero	Non-zero	Large Non-zero
Variance	Small	Large	Small	Small	N/A
Spatial Correlation	Yes/No	No	Yes	No	N/A
Serial Correlation	No	No	No	Yes	N/A

Random errors are stochastic in nature, with typically low repeatability and small magnitudes which can be describe by a probability density function (pdf). The expected value of the random error component is assumed to be zero (Crowe, 1996). The most frequently assumed pdf for the random error component is the normal distribution, based on the hypothesis that the realization of any particular random error is the summation of many unknown sources of error, in which case the central limit theorem dictates that the resultant distribution should be Gaussian. However, the nonlinear transformations used by many modern online measurement devices may invalidate this assumption. Crowe (1996) also questions the validity of this assumption since the domain of the normal distribution is $(-\infty,\infty)$, while most process related measurements are bounded, e.g. greater than or equal to zero. Crowe (1996) suggests the log-normal distribution as an alternative to incorporate such bounds.

Bagajewicz (2001:71, 292) discerns *outliers* in measured data, which are data points with magnitudes that does not fit the probability density function used to describe random errors, but does not have the high repeatability of gross errors. Bagajewicz states that the distinction between outliers and gross errors is less clear if the outlier component has a non-zero expected value, which tends to skew the measurement data and has a similar effect as a constant gross error. Albequerque and Biegler (1996) also do not discern between outliers and gross errors, and describe both types of error as having a probability distribution that does not fit the bulk of the data. While it is generally assumed that all measurements contain a random error component that can be compensated for through some simple techniques, the presence of large gross errors in measurements pose a special problem in the process industries.

Systematic errors are generally assumed deterministic in nature, and could possibly have large but unknown magnitudes. Systematic errors are expected to have a similar impact on more than one measurement in a group of measurements at a particular time, e.g. a voltage fluctuation that impact on several flow meters. This implies spatial correlation of systematic errors, but not necessarily time correlation, i.e. high repeatability. Madron (1992:72) divides the deterministic component of measurement error into *systematic* and *gross* errors, the distinction seemingly dependent on the magnitude of the error, although this distinction between systematic and gross errors is not consistent in the literature, and the terms seem to be used interchangeably.

Bias is commonly viewed as errors with non-zero magnitude that affects a specific measurement with high repeatability, i.e. time correlation. Rollins *et al.* (1992) contended that the term *gross error* does not apply to a component of the measurement error, but rather to the interpretation of measurement data, that is gross errors may be caused by bias, systematic error or outliers.

In this thesis all error components with statistical properties different from the random error component is viewed as gross errors.

Since by definition the expected value of the random error component is zero, the impact of these errors may be reduced by repeated measurement, in which case the variance associated with the average of the repeated measurements is reduced according to the central limit theorem of statistics. The cost of repeated measurement may be prohibitive though, as would be the case for large scale plant surveys. The impact of systematic or gross errors with non-zero expected value is not diminished with repeated measurement though, and requires alternative strategies in order to be effectively contained.

1.2.1.3 Error Variance-Covariance

An accurate estimate of the error structure of process measurements is essential for successful resolution of the DR and GED problem. The variance-covariance of the random measurement error component is used directly in the DR objective function, and serves as a statistical framework for the detection and identification of gross errors (Crowe, 1996). However, since the true values of process measurements are unknown, the error in measurements can only be estimated approximately, and the results of DR and GED become conditional on the accuracy of these estimates.

Crowe (1996) provides some examples of causes of correlation (i.e. non-zero covariance terms) between measurements, such as chemical reaction causing correlation between reactant and product species' flow, and bulk flow rates affecting all species flow rates in a stream. Other causes may include common electrical and/or

pneumatic circuits which cause measurement devices to be subjected to the same voltage fluctuations and possibly fail simultaneously. In addition to correlation caused by plant infrastructure and topology as outlined above, auto and cross correlation may also occur in time (Crowe, 1996), collectively referred to as serial correlation. Crowe (1996) states that serial correlation invalidates the application of the central limit theorem to plant data, and consequent assumption of normal distribution for random errors.

Although it is commonly accepted that no process is ever truly at steady-state, constraints based on this assumption are often imposed during DR and GED (Crowe, 1996). The underlying process dynamics can therefore contribute to measurements violating the steady-state constraints. Crowe (1996) suggests that the effect of underlying process dynamics should be incorporated into the estimate of measurement variance, in order to prevent gross errors being erroneously detected in otherwise accurate measurements due to variability in the process. This could be done by simply calculating the sample variance/covariance for a set of measurement vectors collected over a period of interest.

Several authors disagree with this approach [Almasy and Mah (1984), Keller *et al.* (1992), Romagnoli and Sanchez (2000)], and methods have been developed to isolate the measurement error variance from the dynamic process variability. Tamhane and Mah (1985) points out that serial correlation among measurements invalidates the simple direct method of using sample statistics to estimate measurement error variance/covariance.

1.2.2 Concerning Process Constraints

When mass and energy balances are incorporated in the process constraints, it is essential to determine whether the process under consideration is at steady-state, or subject to dynamic fluctuations. Dynamic processes are typically more complicated in a mathematical sense, as the accumulation terms for material in process units cannot be ignored, resulting in a combination of differential and algebraic constraints on the process (Bagajewicz, 2000). Techniques are therefore required to discern between steady-state and dynamic processes.

Besides mass and energy conservation laws, other relations between process variables may also be included in the process model constraints, such as kinetic, thermodynamic, stoichiometric or even empirically derived equations (Madron, 1992: 34). Evidently, not all possible process models are equivalent with regards to theoretical validity, and it is possible to bias the DR procedure by enforcing invalid process constraints, e.g. through enforcing a steady-state mass balance on a dynamic process, or a molar component balance around a chemical reactor. Due consideration and care is thus required in selection of the imposed constraints.

The nature of the measurement error model, and the constraints imposed on the measurements through the process model, have a pronounced effect on the DR and GED procedure, since the applied optimization algorithm is affected. Typically, for systems with only linear constraints and measurement model, analytical solution to the DR problem is possible, although non-negativity and other feasibility constraints cannot be imposed on the adjusted measurement values. When nonlinear process constraints or measurement models are incorporated, nonlinear optimization techniques are required to solve the DR problem, adding computational burden to the resolution of the DR problem. When dynamic systems are considered, the process model may include differential equations, which incorporates additional complexity into the DR problem. Both nonlinear and differential constraints may require iterative numerical methods for resolution of the DR problem. Further, if an iterative GED procedure is also incorporated, the complete data rectification scheme may become so computationally expensive as to inhibit its utility, for instance computational time may prohibit online implementation for process control purposes.

The distinction between steady-state and dynamic process models requires methods to distinguish between these two states in practice.

1.2.3 The Data Reconciliation Procedure

Data Reconciliation requires that a set of adjusted measurements be found that satisfies the constraints imposed by a model of the process under consideration, and that is optimal under the assumed measurement error model, typically by minimizing a weighted sum-of-squares objective function (Crowe, 1996). For a steady-state process subject only to linear constraints, this can be formulated as:

$$\begin{aligned} & J = \min_{\mathbf{x}} (\mathbf{y}-\mathbf{x})^T \Sigma^{-1} (\mathbf{y}-\mathbf{x}) \\ & s.t. \\ & A\mathbf{x} = \mathbf{0} \end{aligned} \tag{1.2}$$

Where $\mathbf{y}$ is a vector of process measurements, $\mathbf{x}$ is a vector of adjusted measurements, the matrix Σ is the variance/covariance matrix of the measurement error, and the matrix A represents a set of linear constraints imposed on the process. The solution to this optimization problem can be found analytically, and is given by:

$$\hat{\mathbf{x}} = \left(I - \Sigma A^T (A\Sigma A^T)^{-1} A\right)\mathbf{y} \tag{1.3}$$

Where I is the identity matrix of appropriate size. The vector $\tilde{\mathbf{y}}$ is a maximum likelihood estimate of the unknown true process states, subject to the following conditions:

1. Only random errors are present.

2. The random errors follow a multivariate normal distribution, with expected value zero.
3. The variance/covariance matrix of the random errors is known and is given by Σ.

Different formulations of the DR problem are possible, depending on the imposed constraints and measurement error model considered. However, the objective is always to find the optimal set of adjusted measurements under the assumed statistical model of the measurement error, so that the constraints imposed by the process model are satisfied.

1.2.4 The Gross Error Detection Procedure

Typically, the formulation of the DR objective function assumes no gross errors are present in the data. Using the example above, if $\mathbf{y}$ contains no gross errors, then the expected value of the adjusted measurement vector is given by:

$$\begin{aligned} E(\hat{\mathbf{x}}) &= \left(I - \Sigma A^T (A\Sigma A^T)^{-1} A\right) \cdot E(\mathbf{y}) \\ &= \left(I - \Sigma A^T (A\Sigma A^T)^{-1} A\right) \cdot E(\mathbf{x} + \boldsymbol{\varepsilon}) \\ &= E(\mathbf{x}) \\ &= \mathbf{x} \end{aligned} \tag{1.4}$$

However, when one or more gross errors are present in the data, the results of DR are corrupted:

$$\begin{aligned} E(\hat{\mathbf{x}}) &= \left(I - \Sigma A^T (A\Sigma A^T)^{-1} A\right) \cdot E(\mathbf{y}) \\ &= \left(I - \Sigma A^T (A\Sigma A^T)^{-1} A\right) \cdot E(\mathbf{x} + \boldsymbol{\varepsilon} + \mathbf{b}) \\ &= E(\mathbf{x}) + \left(I - \Sigma A^T (A\Sigma A^T)^{-1} A\right) \cdot E(\mathbf{b}) \\ &= \mathbf{x} + \left(I - \Sigma A^T (A\Sigma A^T)^{-1} A\right) \cdot \mathbf{b} \end{aligned} \tag{1.5}$$

This example illustrates how all elements of the adjusted measurement vector are impacted by the presence of even a single gross error. This phenomenon is called *smearing* of gross error through the DR procedure, and illustrates the need for effective GED procedures.

Narasimhan and Jordache (2000: 175) identify four components of a GED strategy:

1. Detecting the presence of one or more gross errors in a group of measurements – the Detection problem.
2. Identifying the type and location of a gross error – the Identification problem.
3. Estimating the magnitude of an identified gross error.
4. Determining the presence and/or locations of multiple gross errors.

Both Crowe (1996) and Bagajewicz (2000) highlight the detection and identification of multiple gross errors as a particularly problematic area, and state that most of the statistical methods developed to date are only valid when single gross errors are present in the data. Prior knowledge of the number of gross errors present in a data set is of course not available to the analyst.

Gross error may exist not only in the measurement data, but be imposed through misspecification of the process model, or due to failures that may invalidate an otherwise accurate process model, such as leaks. Once a gross error has been detected and identified, the affected measurement or constraint may either be removed from the DR procedure, or compensated with the estimated magnitude of the gross error (Bagajewicz, 2010: 66).

The scheme of Figure 1-1 implies an iterative, serial strategy, where GED is performed subsequent to DR, and depending on the results of the GED procedure, the measurement model may be updated in order to incorporate information on gross error size and location, and DR repeated. This scheme is not unique, and other approaches exist where the DR and GED problems are solved simultaneously (Tjoa and Biegler, 1991; Soderstorm *et al.*, 2001).

1.3 Motivation for Data Reconciliation and Gross Error Detection

The primary benefit of DR and GED is an increase in the accuracy of reconciled measurements, and that therefore a higher degree of confidence can be placed on the results of the subsequent use the reconciled measurement data. A secondary benefit is that some unmeasured variables may be estimated from the reconciled variables, referred to as the Coaptation Problem (Narasimhan and Jordache, 2000: 77), some of which may be critical to the process but impractical or impossible to measure directly.

Some of the benefits of implementing a DR and GED procedure may include (Narasimhan and Jordache, 2000: 20):

1. Identifying systematic errors in measured variables can assist in maintenance and calibration scheduling for instrumentation.
2. The accuracy of yield and inventory accounting, and to a lesser extent utility consumption, is improved. This is critical for internal business optimization, but may also be required for regulatory oversight.
3. The accuracy of process model parameter estimation is improved. Accurate process model parameters are essential for effective simulation and optimization, with direct economic benefit.

4. Critical performance parameters for unit operations, e.g. fouling in heat exchangers, may be estimated and maintenance scheduled accordingly.
5. In general, process control performance can be improved by more accurate estimates of process variables, which would limit the extent of de-tuning of control loops required to cope with measurement noise. Some advanced control strategies require accurate estimates of the target variables, which may be supplied by data reconciliation.
6. At the design or retrofit stage of projects, data reconciliation methods can be used to optimize the sensor network design.

A typical scheme for process data management is illustrated below (Narasimhan and Jordache, 2001: 5):

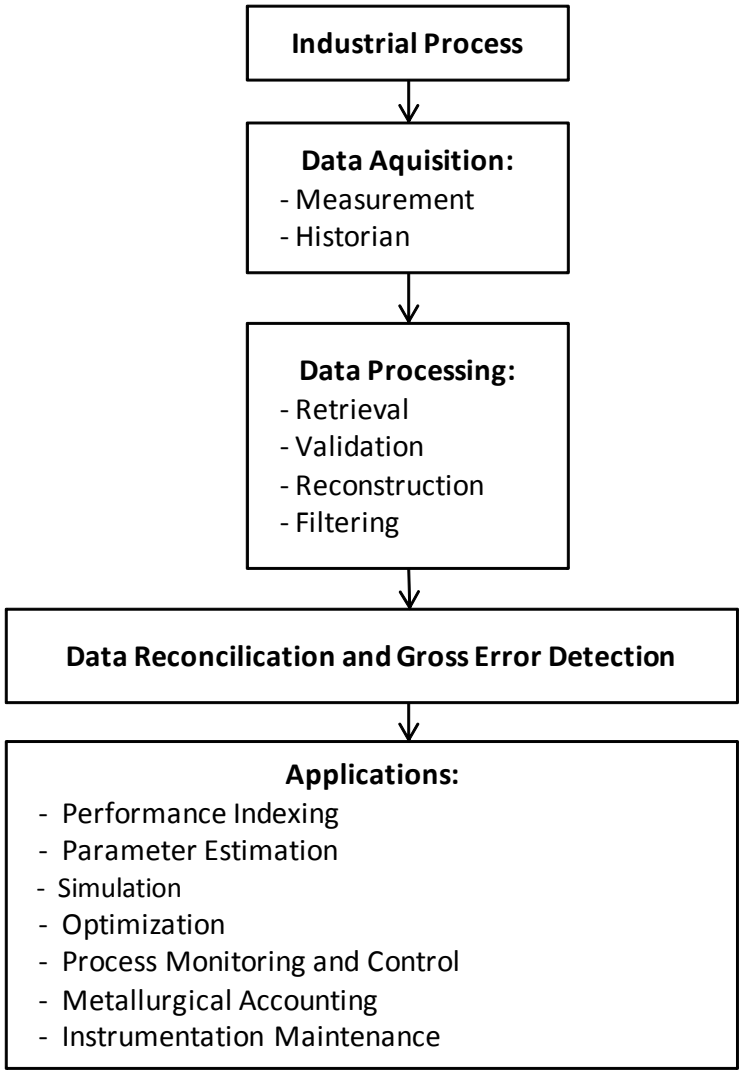

Figure 1-2 - Example of Process Data Management Hierarchy (Narasimhan and Jordache, 2001: 5)

For DR and GED to find widespread acceptance in industry, the improved accuracy and precision of plant data that arise as a result of DR and GED have to be translated into an economic measure of value. Crowe (1996) states that there is not general agreement on the economic value of DR and GED techniques. Bagajewicz, Markowski and Budek (2005) estimated the net present value (NPV) of applying data reconciliation to a crude distillation unit. Bagajewicz (2006) extended this work to consider the presence of gross errors, and NguyenThanh, Siemanond and Bagajewicz (2006) further expanded on the work of Bagajewicz to provide closed form solutions that is amenable to practical implementation.

1.4 The Case for Non-Parametric Methods

The objective of DR and GED is to attenuate random noise and locate and compensate for gross errors in process measurements. The results of DR and GED depend strongly on the variance/covariance structure and assumed pdf of the random noise - which can at best be determined approximately from the unaltered process measurements. The presence of gross errors invalidates the assumptions regarding the error model underlying the classical DR algorithms, which gives rise to the need for GED in order to eliminate or compensate the affected measurements. The DR algorithm typically has to be executed subsequent to such elimination or compensation of measurements, which is the reason for the iterative procedure outlined in Figure 1-1. The GED problem is usually resolved by making statistical inference on the results of the DR procedure in order to identify measurements or model constraints that do not fit the assumed statistical framework of the measurement model. This strong dependence on assumptions that can only be verified only approximately is a significant weakness of classical DR and GED techniques.

There is therefore a need for robust methods, i.e. methods that will give unbiased results when the classical assumptions are in fact true, but that will be insensitive to deviations from the classical assumptions (Albequerque and Biegler, 1996).

Non-parametric statistics does not make explicit assumptions about the statistical distribution of measures on experimental units (Scheffe, 1943 and Siegel, 1957). This is in contrast to classical DR and GED techniques, which makes explicit assumptions about both the distribution form and parameter values of the random error component contained in measurements, which, as outlined above, is difficult to verify. Non-parametric methods therefore seem like an attractive alternative to the classical, parametric tests developed to resolve the DR and GED problems.

The application of DR to steady-state processes and the subsequent resolution of the GED problem through statistical inference using parametric statistics is a relatively mature field. Tamhane and Mah (1985) list several GED techniques, including:

1. The Global Test (Credited to Ripps, 1965)
2. The Nodal Test (Credited to Reilly and Carpani, 1963)
3. The Measurement Test (Mah and Tamhane, 1982)

Crowe (1996) lists the same GED techniques, along with some others:

4. The Maximum Power (MP) Measurement Test (Credited to Almasy and Sztano, 1975)
5. The Generalized Likelihood Ratio (GLR) Test (Narasimhan and Mah, 1987)
6. The Principal Component Analysis (PCA) Test (Tong and Crowe, 1996)

All of the above techniques are strictly valid only when a single gross error is present in the data Crowe (1996).

The use of non-parametric statistics to resolve the GED problem has not received much attention. Aldrich and van Deventer (1993) use back propagation neural networks to solve the Detection problem in a linear as well as nonlinear system. They state that the major advantage of the neural network is its applicability to nonlinear problems, as well as its non-parametric nature. Terry and Himmelblau (1993) use a similar neural network approach to solve the DR problem around a steady-state heat exchanger. Their examples show that the neural network can solve the DR problem more effectively than classical nonlinear programming methods. Gupta and Narasimhan (1993) also solve the Detection problem through the use of neural networks. Aldrich and van Deventer apply neural networks to solve the DR problem (1994a) as well as to solve the Identification problem related to GED (1994b). In their 1995 paper, Aldrich and van Deventer refine the neural network structure in order to optimize the performance on the Identification problem. Du *et al.* (1997) compare two different neural network structures to classical nonlinear programming in resolving the DR problem for a simulated flotation process. They use six different indices of performance for the comparison, with the neural network methodology outperforming the classical approach for some of these indices. They note the utility of the neural network approach for handling missing data and online implementation. Reddy and Mavrovouniotis (1998) compare the neural network methodology to principal component analysis in resolving the Detection and Identification problems related to gross errors, as well as for replacement of missing data due to sensor failure, and conclude the neural network to be superior. Alves and Nascimento (2002) use a combination of neural network and clustering techniques to identify outliers in plant data, which can be viewed as a form of gross error compensation. In general, the researchers above used either the raw measurements, the adjustments made to the measurements through a DR procedure, or the residuals of the constraints as input to the neural network algorithm.

Both the Detection and Identification problems that collectively constitute the GED problem are essentially classification problems. The Detection problem is resolved by either classifying a group of measurements collectively as containing a gross error or being gross error free, and the Identification problem constitutes the same classification for each individual measurement location. The classical GED techniques accomplish this classification by formal hypothesis testing based on the pdf's of the measurement adjustments or model equation residuals, which are conditional on the pdf of the random error component being known, and the measurements being gross error free. The question arises whether traditional classification techniques, such as linear and quadratic discriminant functions or classification trees, could be more effective at resolving this classification problem than the classical GED techniques.

Discriminant functions use distance metrics between an unknown vector that needs to be classified, and the known mean vectors of different classes. The unknown vector is classified as belonging to the class that it is closest to, based on the particular distance metric used. The derivation of the discriminant functions is non-parametric in that it does not assume any particular pdf for the elements of the input vector. However, when prior probabilities for different classes are included in the classification rule, the classification becomes optimal only for a multivariate normal distribution (Rencher, 2002: 302).

Classification trees consist of a collection of logical statements on the elements of the input vector, which is used to classify the input vector. The logical statements collectively comprise the classification rule, and are derived by constructing the classification tree on a training sample of vectors with known class membership. The classification tree attempts to maximally separate the vectors in the training sample. The degree of separation can be defined in different ways, and may impact on the final structure of the classification tree. Since no assumptions regarding the pdf's of elements of the input vector are made, a classification tree is a non-parametric method.

Breiman *et al.* (1984:56) further lists several advantages of the classification tree methodology:

1. The method can be applied to any data structure. This is of particular utility in the process industry, where some plant measurements may be non-numeric (such as the particular feed blend being processed), or numeric but discontinuous (such as alarm states).
2. The classifier has a simple structure than can easily be stored and used to classify new data.
3. It simultaneously provides a classification as well as an estimate of its misclassification rate.
4. It is extremely robust with respect to outliers.

Whereas classical GED techniques compare the residuals generated by DR to an estimated statistical distribution for detection of gross errors, a classification methodology could be applied similarly but without any assumption on the statistical distribution being required. However, a classification methodology would have to be constructed using a sample of process data with known gross error magnitudes and locations, typically obtained through generation of simulated measurement data. This introduces two problems:

1. The simulated data would contain assumptions regarding measurement noise, creating a degree of dependence between the efficacy of the classification tree methodology and the accuracy of the assumptions regarding the random error component.
2. The need for a training sample limits application of a particular tree classifier to the process topology it was developed for.

1.5 RESEARCH STATEMENT AND OBJECTIVES

The hypothesis of this investigation is that a classification methodology, specifically classification trees and discriminant analysis, can be used successfully to detect and locate gross errors in process measurements.

The above hypothesis will be investigated by through the following objectives:

1. A critical review of the relevant literature.
2. Construction of a simulated DR problem.
3. Application of a classical GED technique to the simulated problem.
4. Development of a classifier to solve the GED problem for the simulated DR problem.
5. Comparison of the results of the classical and classification methodology in resolving the GED problem.

1.6 LAYOUT OF REPORT

The first part of this report introduces classical data reconciliation and gross error detection techniques. It is divided into subsections dealing with the major topics of a systematic DR and GED approach. Although not all the topics discussed are subsequently used in the case study, they are presented for the sake of completeness, and to provide a holistic perspective of the DR and GED problem.

Section 2 of this report discusses steady-state detection in industrial processes. This is followed by section 3 discussing methods of estimating the variance/covariance structure of the measurement errors, including robust methods that are resistant to the influence of outliers.

Section 4 contains the topics of classical DR and GED techniques, including:

- Data Reconciliation algorithms for steady-state and dynamic processes
- Variable classification techniques
- Gross error detection and identification in steady-state and dynamic system
- Detection and identification of multiple gross errors

Section 5 discuss alternative approached to the DR and GED problem, including artificial neural networks classification trees, and discriminant functions. Principal component analysis (PCA) is introduced in section 6 as a means of visualizing multivariate data.

Section 7 provides details on the methodology followed in development of the case study used to compare classification methods with classical GED techniques.

Section 8 presents the first results of the case study, specifically the results of PCA used to visualize the presence of gross errors. Sections 9 cover the main results, while section 10 summarizes the conclusions and recommendations of the research.

A list of references is provided in section 11.

1.7 SCOPE AND LIMITATIONS

The investigation will use simulated process data related to a typical process unit. This enables the magnitude and location of gross errors in the system to be exactly known - something that is not feasible with real data.

The investigation will focus on whether the classification tree and discriminant analysis methodologies can successfully detect and locate gross errors in reconciled process data. Estimating the magnitude of the gross error is excluded from this investigation. The performance of the classification methods will be benchmarked with one of the classical gross error detection/identification methods to assess the relative utility of the classification methodologies.

No specially tailored software will be used in the investigation. The MS Excel® and MATLAB® packages will be used for all data generation, reconciliation, as well as classification tree and discriminant function development. These software packages are widely used in the process industries, making a data reconciliation and gross error detection algorithm developed with them accessible to a large audience.

Limitations that arise due to the scope as defined above will be discussed where relevant.

2 STEADY-STATE IDENTIFICATION

Steady-state is an important assumption that determines the type of DR and GED techniques used. Applying steady-state techniques to measurements collected from a dynamic process can lead to erroneous conclusions based on the reconciled data, deteriorating process performance and associated economic loss. As will be illustrated in the following section, the steady-state assumption may have a significant impact on the estimated measurement error model when measurement error variance/covariance is estimated from raw data. There is therefore value in the ability to confirm or reject the steady-state hypothesis.

A process is said to be at steady-state when the process state variable(s) remain unchanged with time (Cao and Rhinehart, 1995). It is commonly accepted that true steady-state conditions can exist only approximately in industrial process, as input disturbances and control action constantly modulate process variables. Notwithstanding this, whether or not a process is assumed at steady-state has a significant impact on the formulation and solution of the DR and GED problem. Successful implementation of a DR and GED strategy therefore requires methods to discern between steady-state and dynamic process behaviour.

The case study presented later in this thesis was simulated as a steady-state process, and no hypothesis testing regarding the steady-state assumption was therefore required. Given the importance of this hypothesis to the general DR and GED formulation, one of the methods for steady-state identification is discussed below.

Cao and Rhinehart (1995) presents a method for detecting steady-state in process variables suitable for online implementation based on the ratio of two different estimates of the process variance:

Step 1: Use an exponential filter to estimate the current value of the process variable:

$$\hat{x}_i = \lambda_1 x_i + (1-\lambda_1)\hat{x}_{i-1} \tag{2.1}$$

Step 2: Estimate the mean square deviation of the measurements through a second exponential filter:

$$\hat{\upsilon}_i^2 = \lambda_2 (x_i - \hat{x}_{i-1})^2 + (1-\lambda_2)\hat{\upsilon}_{i-1}^2 \tag{2.2}$$

Step 3: Obtain a second estimate of the mean square difference between successive measurements from:

$$\hat{\delta}_i^2 = \lambda_3 (x_i - x_{i-1})^2 + (1-\lambda_3)\hat{\delta}_{i-1}^2 \tag{2.3}$$

Step 4: Calculate the ratio:

$$R_i = \frac{(2-\lambda_1)\cdot\hat{\upsilon}_i^2}{\hat{\delta}_i^2} \tag{2.4}$$

Step 5: Compare the value of R_i to a critical value R_α. If $R_i > R_\alpha$, conclude that the process is not at steady state.

Where $0 < \lambda_k < 1, \quad k = 1,2,3$ are filter constants for the respective exponential filters used. The null hypothesis for the above test is that the process is at steady state. Type I error rate is defined as the probability of rejecting the null hypothesis when it is true, and Type II error rate is defined as the probability of failing to reject the null hypothesis when it is false.

In their original paper, Cao & Rhinehart (1995) qualitatively discuss the influence of several factors on the empirically obtained (through Monte Carlo simulation) probability density function of the R-statistic.

They state that process conditions under which the expected value of *R* will be less than 1 is such a rare anomaly (sequential measurements fluctuating between high and low values) that only right-tailed values of *R* need to be considered. Other factors that could influence the pdf of *R* is:

1. The distribution of $\{x_i\}$
2. The choice of the filter constants λ_1, λ_2 and λ_3
3. The autocorrelation between successive $\{x_i\}$

They show that for typical values of the filter parameters, the *R*-statistic is robust with regards to the distribution of $\{x_i\}$. The distribution of $\{x_i\}$ was simulated as being exponential, gamma, uniform and Gaussian for filter values all set at 0.1, and although the resulting distributions of *R* are not identical, the right tailed areas were similar enough to be regarded as equal for practical purposes. The usual assumption of additive Gaussian noise would therefore not have a detrimental impact on the implementation of the *R*-statistic. In later work (Cao & Rhinehart, 1997) they prove that the distribution of the *R*-statistic is independent of the measurement value or variance for additive Gaussian noise.

The effect of the filter constant λ is to reduce the influence of noise on the estimates of the process variance. Cao and Rhinehart (1995) state that very small filter constants can result in the steady-state and non steady-state pdf's of the *R*-statistic separating, so that Type I and Type II errors are drastically reduced. However, this would make the filtered values lag behind the real process to such an extent that the method would have no online application. The values of $\lambda_1 = 0.2$, $\lambda_2 = 0.1$ and $\lambda_3 = 0.1$ are suggested as a compromise between minimizing Type I and Type II errors while retaining sufficient rate of response from the filtered values to allow

online application. The critical values for R using these filter constants are $R_{0.95} = 1.44$, $R_{0.975} = 1.56$, $R_{0.99} = 1.73$ and $R_{0.995} = 1.86$ These values were estimated through computer simulation making use of pseudo-random number generators (Cao and Rhinehart, 1997).

Significant autocorrelation between successive measurements would reduce the variance estimate $s_{2,i}^2 = \hat{\delta}_i^2 / 2$, so that the pdf of R would be shifted to the right. If autocorrelation is present in the process measurements, then a relationship exist between successive measurements:

$$x_i = \rho \cdot x_{i-1} + a_i \tag{2.5}$$

Where: ρ is the autocorrelation coefficient, and a_i is a random noise term. Under these conditions the value of the steady-state identifier is given by (Cao and Rhinehart, 1997):

$$E(R_i) = \frac{(2-\lambda_1) \cdot E(\upsilon^2)}{E(\delta^2)} = \frac{1}{1-(1-\lambda_1) \cdot \rho} \tag{2.6}$$

Hence, the larger the autocorrelation coefficient, the larger the expected value of R_i. Cao and Rhinehart (1995) suggest using a large enough sampling interval to ensure $\rho < 0.05$ in order to reduce the effect of autocorrelation.

2.1.1 Multivariate Steady-State Detection

DR requires that multiple process measurements be linked via a process model. Applying steady-state DR techniques therefore requires that the steady-state hypothesis be satisfied for several measurements simultaneously. Brown and Rhinehart (2000) extend the single variable test described above to a multivariate one. The define the outcome of any single variable test as SS_i, where:

$$SS_i = \begin{cases} 0, R \geq R_{crit} \\ 1, R < R_{crit} \end{cases} \tag{2.7}$$

They further pose that the overall process is not at steady-state if any one of the single variables is not at steady-state, i.e.:

$$SS_{Process} = \prod_{i=1}^{n} SS_i \tag{2.8}$$

The relation in (2.8) can be used to determine the required significance level for individual tests in order to obtain a given overall significance level in accordance with the Sidak correction:

$$\alpha_i = 1 - (1 - \alpha_{Process})^{\frac{1}{n}} \tag{2.9}$$

In addition to the requirement that the autocorrelation between measurements of the same variable be negligible, a further requirement is that there should be no cross correlation between the process variables at steady-state, i.e. that the noise levels in the different variables are independent.

2.1.2 Other Approaches

Cao and Rhinehart (1995) qualitatively critique of some of the other methods for steady-state detection, which include:

- Linear Regression and testing for a zero slope:
- The primitive F-Test:
- Moving Average with Control Limits
- Comparing averages in different time windows

These methods will not be discussed in detail given that steady-state identification is not used in the case study presented later.

3 MEASUREMENT ERROR VARIANCE-COVARIANCE

Once the steady-state assumption is confirmed or rejected using the method described in the previous section, an appropriate DR/GED strategy may be implemented. An integral part of DR techniques is the assumptions regarding the variance and covariance of measurement errors. It is typically assumed that errors follow a Gaussian distribution, and that the covariance matrix of the measurement errors is known. Estimates of the pdf of measurement errors can only be obtained through sample statistics when the process is at steady-state. (Almasy and Mah, 1984).

In practice, the covariance matrix is unknown, or only approximately known. Even when *a priori* information regarding the error covariance is available, such as manufacturer specifications, these still have to be validated in order to have confidence in the DR results. Techniques for estimating the error covariance from process measurements are thus needed.

Several factors complicate the estimation of the error covariance matrix (Romagnoli and Sanchez, 2000:183):

- Industrial processes are never really at strict steady-state, and the true variation of the process variables may be interpreted as, or included in, the error covariance estimates. This is especially true if the process variation is similar or larger in magnitude than the error variances.
- The elements of the error covariance matrix may have different magnitudes depending on the state of the underlying process, as the accuracy and precision of process instrumentation typically vary over the operating range.
- Process measurements can contain outliers, i.e. data points that are not explained by the statistical distribution of the measurement errors or actual process. Such data points can have a significant impact on the magnitude of the statistics calculated from the process data.

Techniques for estimating the error covariance matrix from process measurements can be divided into direct, indirect and robust methods. Figure 3-1 below displays the different approaches that will be discussed:

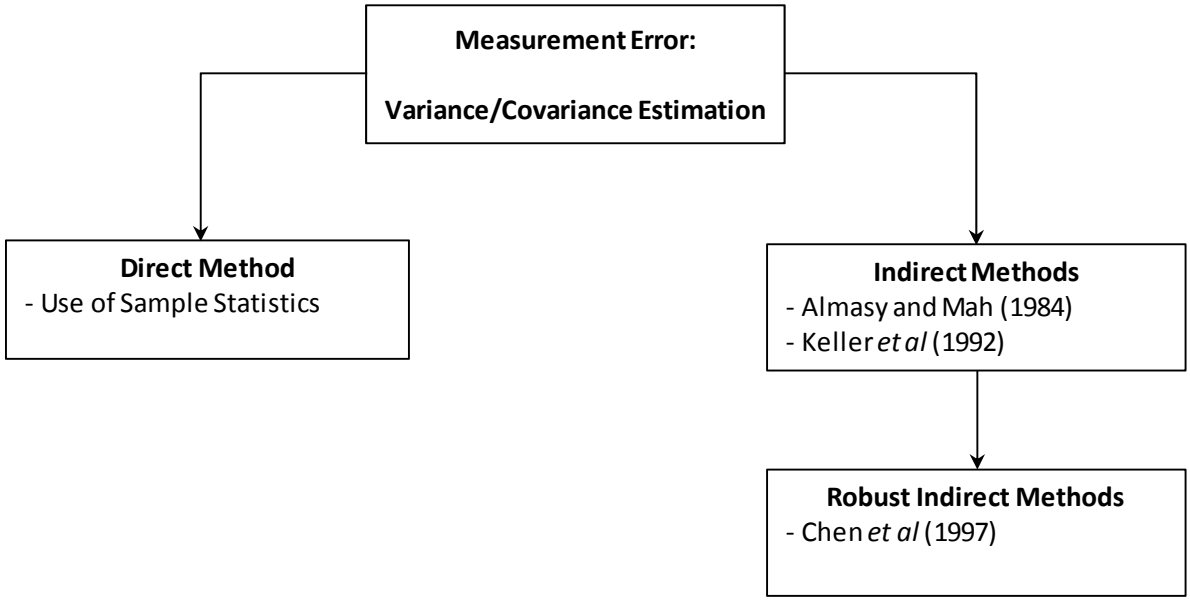

Figure 3-1 : Different Approaches for Estimating Measurement Error Variance/Covariance

3.1 THE DIRECT METHOD

For a process which is truly at steady-state, the sample variance and covariance of the process measurements are sufficient to use (Keller *et al.*., 1992). In general, if p repeated measurement vectors are available, the sample statistics for the i^{th} element of the measurement vector can be calculated as follows:

$$\bar{y}_i = \frac{1}{p}\sum_{k=1}^{p} y_{i,k}$$

$$\mathrm{var}(y_i) = \frac{1}{p-1}\sum_{k=1}^{p}\left(y_{i,k} - \bar{y}_i\right)^2 \qquad (3.1)$$

$$\mathrm{cov}(y_i, y_j) = \frac{1}{p-1}\sum_{k=1}^{p}\left(y_{i,k} - \bar{y}_i\right)\left(y_{j,k} - \bar{y}_j\right)$$

The number of measurement vectors p used for the above calculation depends on the size of the window in which the process is deemed to be at steady-state. The determination of steady-state is not exact. To some degree it is dependent on the amount of variation that can be tolerated by the analyst before the process is classified as being in a dynamic state (Almasy and Mah, 1984). The methods described in the preceding section can be used to more rigorously discern between steady and dynamic processes. The direct method gives unbiased maximum likelihood estimates under the assumption of an independent error distribution with

constant variance. No use is made of the inherent relationship between process variables as established by the process model. This can lead to dynamic process variation being incorporated into the estimated measurement error variance/covariance when the direct method is applied to a process that is not at steady-state (Romagnoli and Sanchez, 2000:184).

Indirect methods make use of the process model to remove the effect of process variation from the error covariance calculation.

3.2 THE INDIRECT METHOD

The simplest form of the *n*-dimensional measurement model, obtained at time increment k, is given by (Romagnoli and Sanchez, 2000: 185):

$$\mathbf{y}_k = \mathbf{x}_k + \boldsymbol{\varepsilon}_k \tag{3.2}$$

where:

- $\mathbf{y}_k$ is the vector of process measurements
- $\mathbf{x}_k$ is the vector of process variables
- $\boldsymbol{\varepsilon}_k$ is the vector of measurement errors

A linear, steady-state process model with *m* model equations is given by:

$$A\mathbf{x}_k = \mathbf{0} \tag{3.3}$$

Where: $A_{m\times n}$ is the system matrix. The residuals of the model equations (3.3) are given by:

$$\mathbf{r}_k = A\mathbf{y}_k = A\mathbf{x}_k + A\boldsymbol{\varepsilon}_k = A\boldsymbol{\varepsilon}_k \tag{3.4}$$

The usual assumptions about the statistical properties of the measurement error vector are made; that is, Gaussian with zero mean and a fixed, positive definite covariance matrix, i.e.:

$$\boldsymbol{\varepsilon}_k \sim N(\mathbf{0}, \Sigma_y) \tag{3.5}$$

Where Σ is the covariance matrix of ε_k. The properties of the residual vector can now be determined as:

$$\begin{aligned} E(\mathbf{r}_k) &= E(A\boldsymbol{\varepsilon}_k) = AE(\boldsymbol{\varepsilon}_k) = A\mathbf{0} = \mathbf{0} \\ H = \mathrm{cov}(\mathbf{r}_k) &= E(\mathbf{r}_k\mathbf{r}_k^T) = E(A\boldsymbol{\varepsilon}_k\boldsymbol{\varepsilon}_k^T A^T) = AE(\boldsymbol{\varepsilon}_k\boldsymbol{\varepsilon}_k^T)A^T = A\Sigma A^T \end{aligned} \tag{3.6}$$

Where H is the covariance matrix of $\mathbf{r}_k$. An implicit assumption in (3.6) is that the measurement errors are unbiased (Alamsy and Mah, 1984). The result obtained in (3.6) can be restated using the Kronecker product of matrices and the $vec(\otimes)$ operator as:

$$vec(H) = (A \otimes A)vec(\Sigma) \tag{3.7}$$

The residual covariance matrix can be estimated from the residual vector obtained in (3.4) over a time horizon containing *p* measurements:

$$H = \frac{1}{p-1}\sum_{i=1}^{p} \mathbf{r}_i \mathbf{r}_i^T \tag{3.8}$$

The estimate of *H* is then used to obtain the measurement error covariance from (3.7). Romagnoli and Sanchez (2000: 185) mention two methods to accomplish this; the method of Almasy and Mah (1984), and the method of Keller *et al.* (1992).

3.2.1 The Method of Almasy and Mah (1984)

Almasy and Mah (1984) argue that measurement errors should be uncorrelated, as measurements are usually made by distinct, independent instruments. Nonetheless, some weak correlation could exist, so that the error covariance matrix should at least be diagonally dominant, if not strictly diagonal. The basis for their method therefore rests on minimizing the sum of squares of the off-diagonal elements in the error covariance estimate.

They accomplish this by relating vectors containing the diagonal and off-diagonal elements of Σ_y to the elements of *H* calculated from (3.8), and minimizing the sum of squares of the vector of off-diagonal elements subject to the relation holding. They performed simulation studies to test their method, and made the following observations:

- The method is sensitive to correlation between measurement errors, and it is recommended that the method should not be used when the correlation coefficient is greater than 10%.
- The method performs best when the variances are comparable in magnitude, and deteriorates as the range of the magnitudes increases.
- The relative error of estimation is negatively correlated with the magnitude of the variance, i.e. small variances have the poorest estimates.

3.2.2 The Method of Keller *et al.* (1992)

The method of Keller, Zasadzinski and Darouach (1992) requires that the measurement errors that are correlated be specified in advance. This requirement obviously has the potential to incorporate significant analyst bias into the results. The specific analytical technique followed depends on whether the measurement covariance matrix is diagonal or not.

For the diagonal case, it is required to find the vector:

$$\mathbf{d} = \left[\Sigma_{11}, \Sigma_{22}, ..., \Sigma_{nn}\right] \tag{3.9}$$

Where: the dimension of the measurement vector is n. Equation (3.7) can then be written as:

$$vec(H) = D\mathbf{d} \tag{3.10}$$

Where:

$$D = \begin{pmatrix} a_{11}A_1 & \cdots & a_{1n}A_n \\ \vdots & \ddots & \vdots \\ a_{m1}A_1 & \cdots & a_{mn}A_n \end{pmatrix} \tag{3.11}$$

and: $A_j = col_j(A)$, the j[th] column of *A*. Given an *m* x *n* system matrix *A*, then:

$$\begin{aligned} \dim\left[vec(H)\right] &= (m^2 \times 1) \\ \dim\left[D\right] &= (m^2 \times n) \\ \dim\left[\mathbf{d}\right] &= (n \times 1) \end{aligned} \tag{3.12}$$

Under the assumption of an independent normal error distribution with constant covariance, the maximum likelihood estimate of **d** is obtained from:

$$\hat{\mathbf{d}} = (D^T D)^{-1} D^T vec(H) \tag{3.13}$$

Keller *et al.* (1992) states that $\hat{\mathbf{d}}$ exist subject to $(D^T D)$ being non-singular, i.e.:

$$rank(D) = n \tag{3.14}$$

When some of the measurement errors are correlated, the covariance matrix is not diagonal. Keller *et al.* (1992) assume that it is possible to know *a priori* which measurement errors are correlated. It is thus possible to determine beforehand the vector of variance-covariance magnitudes to be estimated as:

$$\mathbf{f} = \left[\Sigma_{11}, \Sigma_{22}, ..., \Sigma_{nn}, \Sigma_{ij}, ..., \Sigma_{kl}\right] \tag{3.15}$$

Where Σ_{kl} are the non-zero covariance terms specified *a priori*. Without loss of generality, it may be assumed that it is determined that *s* measurement errors are correlated, so that the vector **f** is of dimension (*n* + *s* x 1). Equation (3.7) can then be written as:

$$vec(H) = G\mathbf{f} \tag{3.16}$$

Where:

$$G = \begin{pmatrix} a_{11}A_1 & \cdots & a_{1n}A_n & a_{1i}A_i + a_{1j}A_j & \cdots & a_{1k}A_k + a_{1l}A_l \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ a_{m1}A_1 & \cdots & a_{nn}A_n & a_{mi}A_i + a_{mj}A_j & \cdots & a_{mk}A_k + a_{ml}A_l \end{pmatrix} \tag{3.17}$$

The maximum likelihood estimator of **f** is then given by:

$$\hat{\mathbf{f}} = (G^T G)^{-1} G^T vec(H) \tag{3.18}$$

Keller *et al.* (1992) stated that $\hat{\mathbf{f}}$ exists subject to $(G^T G)$ being non-singular, i.e.:

$$rank(G) = n + s \tag{3.19}$$

The analytical method of Keller *et al.* (1992) has the advantage that it is not sensitive to correlation between measurement errors.

3.3 Robust Covariance Estimation

According to Chen, Bandoni and Romagnoli (1997), the indirect methods described above are sensitive to outliers in the measurement data. The indirect methods use a direct method to estimate the covariance matrix of the model residuals, and measurement outliers can cause the statistical assumptions about the residuals to be violated. They develop a robust M-estimator, or generalized maximum likelihood estimator, for the measurement error covariance matrix Σ_y, by finding a robust estimate of the residuals covariance matrix *H*, which is then used in the indirect method of Keller *et al.* (1992) to obtain a robust estimate of the measurement error covariance matrix.

The principle of the M-estimator is to assign a weight to each observation in a sample based on its distance from the sample mean, so that extreme observations has less influence on the estimate of sample mean and variance. The robust method proceeds by initializing a location vector and covariance matrix for the constraint residuals. Each vector in the data set is then assigned a weight based on its distance from the location vector, and the procedure is iterated until convergence on the location vector and covariance matrix is achieved. Romagnoli and Sanchez (2000) note that the fraction of outliers that can be present in the measurement data before the algorithm fails to converge, is given by $1/(1+m)$. Details of the algorithm are beyond the scope of this thesis.

Morad, Svrcek and Mackay (1999) note that the indirect method suffers from a weakness in that the matrix *G* in (3.17) may be rank deficient, i.e. (3.19) is not satisfied, depending on which covariance terms are assumed *a priori* to be non-zero. They suggest a direct robust method that also makes use of the M-estimator to determine the mean and covariance of the measurement vectors $\mathbf{y}_k$. They present examples that indicate the robust direct

method compares favourably with the robust indirect method, but it is not clear how process dynamics could influence the accuracy of robust direct method.

Maquin, Narasimhan and Ragot (1999) simultaneously solve the DR problem and estimate the measurement error variance/covariance matrix. They define a joint likelihood function for the reconciled estimates and the covariance matrix, and present an iterative solution technique. Their method makes the usual assumptions of normal, independent random errors with zero expectation, and steady-state process with constraints as in (3.3). They present two examples that indicate good results for their method, when the underlying assumptions are satisfied. It is not clear how outliers, gross errors, dynamic process conditions or non-Gaussian error distributions may affect their results.

It should be noted that the methods in this section apply to linear systems where the relation in (3.3) holds. Determination of measurement error variance/covariance for nonlinear systems is not treated in the literature, although Morad *et al.* mention that it would be computationally expensive to include nonlinear constraints in their method.

4 CLASSICAL DATA RECONCILIATION AND GROSS ERROR DETECTION

4.1 STEADY-STATE DATA RECONCILIATION

The principle of Data Reconciliation rests on finding a set of reconciled measurements that satisfies the imposed process constraints and is optimal in some way – thus it is an optimization sub-problem (Madron, 1992: 136). In order to formulate the reconciliation problem, it is necessary to describe the process constraints and measurements with a mathematical model, and to formulate an objective function based on this model that can be minimized to arrive at an optimal solution.

The general steady-state data reconciliation problem, incorporating nonlinear and inequality constraints can be stated as follows:

$$\begin{aligned} & J = \min_{\mathbf{x}} \ (\mathbf{y}-\mathbf{x})^T \Sigma_{\mathbf{y}}^{-1} (\mathbf{y}-\mathbf{x}) \\ & s.t. \\ & F(\mathbf{x},\mathbf{u}) = \mathbf{0} \\ & G(\mathbf{x},\mathbf{u}) \le \mathbf{0} \end{aligned} \tag{4.1}$$

Where: $\mathbf{y}$ is a vector of measurements of a subset of process variables, $\mathbf{x}$ is the corresponding vector of actual values of the process variables, $\mathbf{u}$ is a vector of unmeasured process variables, $\Sigma_{\mathbf{y}}$ is the variance-covariance matrix of the measurement errors, $F(\mathbf{x},\mathbf{u})$ and $G(\mathbf{x},\mathbf{u})$ are sets of constraints imposed by a model of the process, possibly including lower and upper feasibility bounds for the measured and unmeasured variables where applicable. The objective function is a weighted sum of squares of the measurement adjustments, and under the assumptions listed below, produces maximum likelihood estimates of the process variables.

Assuming no gross errors are present in the data, the measurements of process variables can be modelled as:

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon}_{\mathbf{x}} \tag{4.2}$$

Where: $\mathbf{y}$ and $\mathbf{x}$ are the measured and actual values, as before, and $\boldsymbol{\varepsilon}_{\mathbf{x}}$ is a vector of random errors. Since the actual values of process variables are unknown, it is not possible to calculate the values of the measurement errors directly. The typical assumptions made regarding the vector $\boldsymbol{\varepsilon}_{\mathbf{x}}$ are (Romagnoli and Sanchez, 2000: 76):

1. The process measurements are unbiased, i.e. $E\left[\boldsymbol{\varepsilon}_{\mathbf{x}}\right] = \mathbf{0}$
2. Successive vectors of measurements are independent, i.e. $E\left[\boldsymbol{\varepsilon}_{\mathbf{x},\mathbf{i}} \boldsymbol{\varepsilon}_{\mathbf{x},\mathbf{j}}^{\mathbf{T}}\right] = \mathbf{0}$

3. The covariance matrix of the measurement errors is known and positive definite, i.e. $Cov(\boldsymbol{\varepsilon}_x) = E\left[\boldsymbol{\varepsilon}_x \boldsymbol{\varepsilon}_x^T\right] = \Sigma_y$

The one-to-one correspondence of measurements to variables implied in the above problem formulation does not impose any limitations on the method, since other forms of the measurements model can be converted to the one used above (Narasimhan and Jordache 2000, 60).

Different methods for solving the problem posed in (4.1) have been developed, depending on the nature of the constraints imposed, as will be outlined below.

4.1.1 Linear Systems with all Variables Measured

Linear systems commonly arise when only bulk flow or mass balances are considered in the process constraints. When all the process variables are measured, and ignoring bounds on the variables, the constraints are given by:

$$A\mathbf{x} = \mathbf{0} \tag{4.3}$$

Where: A is a matrix of coefficients describing the linear process model for the system and $\mathbf{x}$ is the vector of process variables. The reconciliation problem for the linear case with all variables measured is then given by:

$$\begin{aligned} & J = \min_{\mathbf{x}} \ (\mathbf{y}-\mathbf{x})^T \Sigma_{\mathbf{y}}^{-1} (\mathbf{y}-\mathbf{x}) \\ & s.t. \\ & A\mathbf{x} = \mathbf{0} \end{aligned} \tag{4.4}$$

The solution to (4.4) is obtained by the method of Lagrange multipliers; the Lagrangian for the system is given by:

$$L = \boldsymbol{\varepsilon}_y^{\mathbf{T}} \Sigma_y^{-\mathbf{1}} \boldsymbol{\varepsilon}_y - 2\boldsymbol{\lambda}^{\mathbf{T}} A(\mathbf{y} - \boldsymbol{\varepsilon}_y) \tag{4.5}$$

Where: $\boldsymbol{\varepsilon}_y = (\mathbf{y}-\mathbf{x})$ and $\boldsymbol{\lambda}$ is a vector of Lagrange multipliers with dimension equal to the number of constraints. The necessary and sufficient conditions for an optimum solution are:

$$\begin{aligned} & \frac{\partial L}{\partial \boldsymbol{\varepsilon}_y} = 2\Sigma_y^{-\mathbf{1}} \boldsymbol{\varepsilon}_y + 2A^T \boldsymbol{\lambda} = \mathbf{0} \\ & \frac{\partial L}{\partial \boldsymbol{\lambda}} = A(\mathbf{y} - \boldsymbol{\varepsilon}_y) = \mathbf{0} \end{aligned} \tag{4.6}$$

From the above, it follows that:

$$\begin{aligned} & \boldsymbol{\varepsilon}_y = -\Sigma_y A^T \boldsymbol{\lambda} \\ & \boldsymbol{\lambda} = -\left(A\Sigma_y A^T\right)^{-1} A\mathbf{y} \end{aligned} \tag{4.7}$$

Using the result from (4.7), the estimates of the process variables can now be obtained as:

$$\hat{\mathbf{x}} = \mathbf{y} - \Sigma_y A^T (A\Sigma_y A^T)^{-1} A\mathbf{y} \tag{4.8}$$

Where: $\hat{\mathbf{x}}$ is the maximum likelihood estimate of $\mathbf{x}$ under the assumptions of unbiased measurements with Gaussian errors (Romagnoli and Sanchez, 2000:77-78).

In general it is possible that the constraints include some non-zero elements on the right-hand-side (RHS) of (4.3), i.e. the constraints are given by:

$$A\mathbf{x} = \mathbf{c} \tag{4.9}$$

Where: $\mathbf{c}$ is a vector containing some non-zero elements. The solution to the DR problem with (4.9) included as constraints in (4.4) instead of (4.3) is then given by (Mah and Tamhane, 1982):

$$\hat{\mathbf{x}} = \mathbf{y} - \Sigma_y A^T (A\Sigma_y A^T)^{-1} (A\mathbf{y} - \mathbf{c}) \tag{4.10}$$

4.1.2 Linear Systems with Indirect Measurements

It is possible that the state variables are not directly measured. If it is desired that an explicit relationship between the process state variables of interest and the measurements be included in the DR procedure, the measurement model would be of the form:

$$\mathbf{y} = M\mathbf{x} + \boldsymbol{\varepsilon}_x \tag{4.11}$$

Where: M is a matrix relating the measurements $\mathbf{y}$ to the state variables $\mathbf{x}$. The solution to the linear DR problem (4.4) in this case is given by (Mah and Tamhane, 1982):

$$\begin{aligned} \hat{\mathbf{x}}_0 &= (M^T \Sigma_y M)^{-1} M^T \Sigma_y^{-1} \mathbf{y} \\ \hat{\mathbf{x}} &= \hat{\mathbf{x}}_0 - (M^T \Sigma_y M)^{-1} A^T \left[A(M^T \Sigma_y M)^{-1} A^T \right]^{-1} (A\hat{\mathbf{x}}_0 - \mathbf{c}) \end{aligned} \tag{4.12}$$

Where: $\hat{\mathbf{x}}_0$ is the unconstrained estimate of $\mathbf{x}$ from equation (4.11).

4.1.3 Linear Systems with Unknown Variance Matrix

The formulation of the DR optimization problem in (4.4) requires knowledge of the measurement error covariance matrix Σ_y. In general the covariance matrix is not known, and has to be estimated from the data. Techniques for estimating the covariance matrix of the measurement errors were presented in section 3 of this review. These estimates are obtained prior to the DR procedure. Maquin *et al.* (1999) presents a method of obtaining simultaneous estimates of reconciled measurements and their associated variance matrix.

The same additive error model applies as in (4.2), with system constraints as in (4.3). They define the probability function of the random error component as:

$$P(\boldsymbol{\varepsilon}_x) = (2\pi)^{-kn/2} \prod_{i=1}^{k} \left|\Sigma_y\right|^{-1/2} \exp\left(-\frac{1}{2}\left[\boldsymbol{\varepsilon}_{x,i}^T \Sigma_y^{-1} \boldsymbol{\varepsilon}_{x,i} \right] \right) \tag{4.13}$$

Where: there are k repeated measurements of the p-dimensional vector $\mathbf{y}$. The likelihood function for the reconciled estimates $\hat{\mathbf{x}}$ is then given by:

$$L(\hat{\mathbf{x}}) = (2\pi)^{-kn/2} \prod_{i=1}^{k} \left|\Sigma_y\right|^{-1/2} \exp\left(-\frac{1}{2} Tr\left(\Sigma_y^{-1} M(\hat{\mathbf{x}}) \right) \right) \tag{4.14}$$

Where *Tr()* indicate the trace operator, and $M(\hat{\mathbf{x}})$ is defined by:

$$M(\hat{\mathbf{x}}) = \sum_{i=1}^{k} \boldsymbol{\varepsilon}_x \boldsymbol{\varepsilon}_x^T = \sum_{i=1}^{k} \left(\mathbf{y}_i - \hat{\mathbf{x}}_i \right) \left(\mathbf{y}_i - \hat{\mathbf{x}}_i \right)^T \tag{4.15}$$

Maquin *et al.* (1999) propose a recursive procedure for maximising the likelihood function in (4.14):

1. Initialize $t = 0,\ \hat{\mathbf{x}}_t = \frac{1}{k} \sum_{i=1}^{k} \mathbf{y}_i = \bar{\mathbf{y}}$
2. Calculate $M(\hat{\mathbf{x}})$ from (4.15)
3. Calculate the estimate covariance matrix from:

$$\Sigma_{y,t} = \frac{1}{k} M(\hat{\mathbf{x}}_t) \tag{4.16}$$

4. Update the estimate of $\hat{\mathbf{x}}$ from:

$$\hat{\mathbf{x}}_{t+1} = \left(I - \Sigma_{y,t} A^T (A \Sigma_{y,t} A^T)^{-1} A \right) \bar{\mathbf{y}} \tag{4.17}$$

5. Check for convergence on $\hat{\mathbf{x}}_t$ and $\Sigma_{y,t}$, and terminate when appropriate

Maquin *et al.* (1999) extends the method to linear systems operating at multiple steady-states over time. They present examples that show good performance for the method when the underlying assumptions regarding the measurement error pdf are valid.

4.1.4 Linear Systems Containing Unmeasured Variables

In general to perform DR on linear systems with unmeasured variables, the problem is decomposed into two sub-problems; one where the redundant measured variables are adjusted (Reconciliation), and one where the observable unmeasured variables are estimated from the reconciled redundant variables (Coaptation) (Narasimhan and Jordache, 2000: 63).

The measurement model is as the direct model of (4.2). Considering that there are unmeasured variables, the process constraints are written in terms of both the measured and unmeasured variables:

$$A_x\mathbf{x} + A_u\mathbf{u} = \mathbf{c} \tag{4.18}$$

In order to eliminate the unmeasured variables from Equation (4.18), a projection matrix P has to be found with the property:

$$PA_u\mathbf{u} = \mathbf{0} \tag{4.19}$$

By pre-multiplying the constraints in (4.18) with *P*, a reduced set of constraints are then obtained:

$$PA_x\mathbf{x} = P\mathbf{c} \tag{4.20}$$

The objective function for maximum likelihood estimates under the assumptions of zero bias and Gaussian errors is again:

$$\begin{aligned} &J = \min_{\mathbf{x}} \ (\mathbf{y}-\mathbf{x})^T\Sigma_{\mathbf{y}}^{-1}(\mathbf{y}-\mathbf{x}) \\ &s.t. \\ &PA_x\mathbf{x} = P\mathbf{c} \end{aligned} \tag{4.21}$$

As before, an analytical solution is possible using the method of Lagrange multipliers:

$$\hat{\mathbf{x}} = \mathbf{y} - \Sigma_y G_x(G_x\Sigma_y G_x^T)^{-1}(G_x\mathbf{y} - P\mathbf{c}) \tag{4.22}$$

Where: $G_{\mathbf{x}} = PA_{\mathbf{x}}$ (Romagnoli and Sanchez, 2000: 80-81)

4.1.4.1 Techniques for finding the Projection Matrix

The projection matrix *P* in (4.19) is not unique (Kelly, 1998). Crowe *et al.* (1983) first introduced the concept of the projection matrix. They state that a partition $\Pi_R A_u \Pi_C = \begin{bmatrix} A_{u,1} & A_{u,3} \\ A_{u,2} & A_{u,4} \end{bmatrix}$ can be found such that $A_{u,1}$ is maximally square and non-singular, where Π_R and Π_C are row and column permutation matrices, respectively. The desired projection matrix is then given by:

$$P = [-A_{u,2}A_{u,1}^{-1} \;\; I] \tag{4.23}$$

Where: I is a unit matrix of appropriate size. Kelly (1998) describes two methods of finding the partition of A_u so that P can be calculated from (4.23). The first method of Kelly (1998) constructs the matrix $A_{u,1}$ by recursively identifying independent columns and rows of A_u. The independent columns of $A_{u,1}$ are identified by checking for non-zero determinant (i.e. non-singularity) of matrix $A_{u,1}^{*T}A_{u,1}^{*}$, where $A_{u,1}^{*}$ is a sub matrix of $A_{u,1}$ formed by recursively adding columns of $A_{u,1}$ to $A_{u,1}^{*}$. Independent rows are identified in an analogous way by testing for non-zero determinant of the matrix $A_{u,1}^{*}A_{u,1}^{*T}$. Kelly (1998) further describes a modified Cholesky factorization that can be used to find independent rows and columns of A_u from $A_u^T A_u$ and $A_u A_u^T$.

Sanchez and Romagnoli (1996) use a QR decomposition to construct a projection matrix with desired properties as required by (4.19). The matrix A_u can be factorized as:

$$A_u\Pi_u = Q_u R_u = [Q_1 \quad Q_2]\begin{bmatrix} R_1 & R_2 \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \tag{4.24}$$

where: Π_u is a permutation matrix. The matrix Q_2^T is the desired projection matrix required in (4.19).

Kelly (1998) compares the recursive matrix inversion and modified Cholesky factorization with QR factorization of Sanchez and Romagnoli (1996) and concludes that, although the QR factorization may be the most computationally efficient method for some examples (but not all), it in general results in lower degree of sparsity in the factor matrices, which he views as detrimental for gross error detection.

4.1.4.2 Solving for the Unmeasured Variables

Sanchez and Romagnoli (1996) state that $rank(A_u) = s = rank(R_1)$ from (4.24). The vector of unmeasured variables can then be partitioned as:

$$\Pi_u^T \mathbf{u} = \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} \tag{4.25}$$

Where Π_u is the permutation matrix from (4.24), $\mathbf{u}_1$ is a (s x 1) vector and $\mathbf{u}_2$ is a ((p-s) x 1)vector, where s is the rank of A_u as defined before, and p is the total number of unmeasured variables.

Substituting (4.24) and (4.25) into (4.18), the system constraints become:

$$A_x\mathbf{x} + \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R_1 & R_2 \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} = \mathbf{c} \tag{4.26}$$

Pre-multiplying (4.26) with Q^T yields:

$$\begin{bmatrix} Q_1^T A_x & R_1 & R_2 \\ Q_2^T A_x & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} = \begin{bmatrix} Q_1^T \mathbf{c} \\ Q_2^T \mathbf{c} \end{bmatrix} \tag{4.27}$$

An estimates of $\mathbf{x}$ is obtained from the DR procedure solving the system (4.21) with $P = Q_2^T$. A relationship between the two parts of the partitioned vector of unmeasured variables can be established from (4.27) as:

$$\mathbf{u}_1 = R_1^{-1} Q_1^T (\mathbf{c} - A_x \hat{\mathbf{x}}) - R_1^{-1} R_2 \mathbf{u}_2 \tag{4.28}$$

Some of the unmeasured variables in $\mathbf{u}_1$ may be determined from the relation in (4.28), provided the rows in the matrix $R_1^{-1}R_2$ corresponding to these variables consist entirely of zero's. The unmeasured variables contained in $\mathbf{u}_2$, and any variables in $\mathbf{u}_1$ corresponding to non-zero rows of $R_1^{-1}R_2$, are indeterminable.

4.1.5 Bilinear and Multi-linear Systems

A special case of nonlinear process constraints arise when the nonlinearity is as a result of the product of two or more measurements. An example of a bilinear term from the chemical industries would be obtaining the component flow rate from the product measurements of the bulk flow and concentration, e.g. $f_{i,j} = F_j \cdot c_{i,j}$, where $f_{i,j}$ is the flow rate of component i in stream j, F_j is the bulk flow of stream j, and $c_{i,j}$ is the concentration of component i in stream j. Multi-linear terms can arise in the minerals industry, e.g. obtaining the species flow rate inside a particle size fraction for a specific stream j: $f_{m,k,j} = F_j \cdot \rho_j \cdot s_j \cdot p_{k,j} \cdot a_{m,k,j}$ where $f_{m,k,j}$ is the flow rate of species m in particle size class k in stream j, F_j is the volumetric bulk flow rate, ρ_j is the density, s_j is the solids concentration, $p_{k,j}$ is the fraction of solids reporting to particle size class k, and $a_{m,k,j}$ is the assay of species m in particle size class k.

Special techniques to deal with multi-linear constraints have been developed, which are typically more computationally efficient than general nonlinear techniques (Narasimhan and Jordache, 2000: 86). In general the techniques exploit the fact that, if all but one of the variables in a multi-linear term is held constant, the resulting constraints are linear, and can be solved analytically using the techniques described in the previous section (Crowe, 1983).

Hodouin and Everell (1980) developed a hierarchical procedure for adjusting bilinear data with application in mineral processing circuits. They classified measurements as either macroscopic (bulk flows and densities) or microscopic (particle size distributions and chemical assays), and formulated the process constraints so that the macroscopic and microscopic material balances could be decoupled. The microscopic balance formulation was linear and could be solved analytically, although a nonlinear programming routine was necessary to solve the DR problem for the macroscopic variables due to the presence of nonlinear constraints in the macroscopic balance. Makni and Hodouin (1994) extended the general hierarchical algorithm to an online implementation, while Makni and Hodouin (1996) improved the online implementation by incorporating models of process dynamics.

Crowe (1986) provides a solution to the general bilinear DR problem. The process streams are divided into 3 categories, depending on the combination of variables measured for each stream, as outlined in Table 4-1 below (categories 3 and 4 are combined in the analysis), where ‘M’ indicates that the variable of interest is measured, and ‘U’ indicates that it is unmeasured:

Table 4-1: Classification of Process Streams for the Bilinear Problem (Crowe, 1986)

Category	Total Flow	Concentrations
1	M	M
2	U	M
3	M	U
4	U	U

The resulting system of bilinear constraints is solved recursively by successive application of the projection matrix from Crowe (1983) in order to first eliminate unmeasured variables in category #3, followed by a second projection to eliminate unmeasured flows in category #2. A recursive procedure is required, as the solution is dependent on initial guesses for the bulk flow rates of category #2. Crowe (1986) describes the process constraints for the bilinear problem as:

$$A_0\mathbf{k} + A_1(\mathbf{y}_1 + \Delta\mathbf{y}_1) + A_2F_2(\mathbf{y}_2 + \Delta\mathbf{y}_2) + A_3\mathbf{u}_3 = \mathbf{0} \tag{4.29}$$

Where: $\mathbf{k}$ is a vector of exactly known parameters (component flows, in Crowe's formulation), $\mathbf{y}_1$ represents component flows of category #1 variables and $\Delta\mathbf{y}_1$ represent the required adjustment to the measured component flow rates in order to satisfy the constraints, $\mathbf{y}_2$ represents measured concentrations from category #2 and $\Delta\mathbf{y}_2$ the required adjustments to these, F_2 is a diagonal matrix with unmeasured flow rates from category 2 variables corresponding to the elements of $(\mathbf{y}_2 + \Delta\mathbf{y}_2)$, $\mathbf{u}_3$ represent all unmeasured variables from category #3 (possibly including extents of reaction), and A_i, $i = 0,1,2,3$ are the respective coefficient matrices. The corresponding objective function for the DR problem is given by:

$$J = \min_{\Delta\mathbf{y}_1, \Delta\mathbf{y}_2, F_2} (\Delta\mathbf{y}_1)^T \Sigma_{y,1} (\Delta\mathbf{y}_1) + (\Delta\mathbf{y}_2)^T \Sigma_{y,2} (\Delta\mathbf{y}_2) \tag{4.30}$$

Where: $\Sigma_{y,i}$, $i = 1,2$ are the respective measurement error covariance matrices. It is desired to use projection matrices in order to remove the unmeasured variables from (4.29). A projection matrix P_1 can be found as described before such that $P_1A_3 = \mathbf{0}$, so that the modified constraints after the first projection are given by:

$$P_1\left[A_0\mathbf{k} + A_1(\mathbf{y}_1 + \Delta\mathbf{y}_1) + A_2F_2(\mathbf{y}_2 + \Delta\mathbf{y}_2)\right] = \mathbf{0} \tag{4.31}$$

In order to eliminate the unmeasured category 2 flow rates in F_2, it is required to find a matrix B_2 such that $B_2\mathbf{f}_2 = P_1A_2F_2\mathbf{y}_2$, where $\mathbf{f}_2$ is the vector of unmeasured category 2 flow rates. The required matrix is given by:

$$B_2^T = [A_{2,1}\mathbf{y}_{2,1} \;\; A_{2,2}\mathbf{y}_{2,2} \;\ldots\ldots\; A_{2,i}\mathbf{y}_{2,i}]P_1^T \tag{4.32}$$

Where: $A_{2,i}$ are the columns of A_2 corresponding to the i^{th} category 2 flow rate, and $\mathbf{y}_{2,i}$ is the vector of corresponding measured concentrations. Using this notation, the process constraints are given by:

$$P_1\left[A_0\mathbf{k} + A_1(\mathbf{y}_1 + \Delta\mathbf{y}_1) + B_2\mathbf{f}_2 + A_2F_2\Delta\mathbf{y}_2\right] = \mathbf{0} \tag{4.33}$$

A second projection matrix P_2 can then be found such that $P_2B_2\mathbf{f}_2 = \mathbf{0}$, so that the process constraints become:

$$P_2P_1\left[A_0\mathbf{k} + A_1(\mathbf{y}_1 + \Delta\mathbf{y}_1) + A_2F_2\Delta\mathbf{y}_2\right] = \mathbf{0} \tag{4.34}$$

The objective function in (4.30) is modified for the new constraints as:

$$J = \min_{\Delta\mathbf{y}_1,(F_2\Delta\mathbf{y}_2)} (\Delta\mathbf{y}_1)^T\Sigma_{y,1}(\Delta\mathbf{y}_1) + (F_2\Delta\mathbf{y}_2)^T\Sigma_{F_2\Delta\mathbf{y}_2}(F_2\Delta\mathbf{y}_2) \tag{4.35}$$

Where: $\Sigma_{F_2\Delta\mathbf{y}_2} = \hat{F}_2\Sigma_{y,2}\hat{F}_2$, $\hat{F}_2$ containing an initial estimate for the unmeasured flow rates in category 2. The optimization problem in (4.35) is linear in the variables $\Delta\mathbf{y}_1$ and $\left(F_2\Delta\mathbf{y}_2\right)$, so an analytical solution can be found. Some of the unmeasured variables may then be solved for using the solution to (4.35) and the process constraints. Since the solution to (4.35) depend on the initial estimates of the flows in F_2, iteration may be required for convergence.

Sanchez and Romagnoli (1996) modify the method of Crowe (1986) by decoupling the unmeasured flow rates from the unmeasured concentrations, and using a QR factorization to find the projection matrix. Kelly (2004) formulates a general solution to the bilinear problem by classifying variables as being extensive (dependent on system mass, e.g. mass or volumetric flow rate)) or intensive (independent of system mass, e.g. concentration, temperature, specific enthalpy) in nature, as opposed to Hodouin and Everell's (1980) classification into macro and microscopic variables.

Given that bilinear and multi-linear problems can be solved by general nonlinear DR methods, these are discussed next in more detail.

4.1.6 Benefits and Problems of Analytical Techniques

The solutions discussed in the preceding sections are all of an analytical nature, i.e. the solution is solved for explicitly from the problem formulation using methods of multivariable calculus.

This has the benefit of guaranteeing that the global minimum of the objective function is obtained, and that problems related to the convergence of iterative methods are avoided.

However, there is no guarantee that the solution will be feasible. It is possible to obtain negative values for some of the process variables at the optimum objection function value, which may be physically meaningless. Typically this problem can be addressed by incorporating bounds on the variables restricting their feasible range. Unfortunately, this result in inequality constraints, and an analytical solution is no longer feasible (Narasimhan and Jordache, 2000: 61& 86).

4.1.7 Data Reconciliation for Nonlinear Systems

The methods used for linear and bilinear data reconciliation has the limitation that inequality constraints, such as those necessary to impose feasibility bounds on process variables, and nonlinear constraints (other than those that are of a bilinear nature) cannot be accommodated. Many processes are subject to nonlinear constraints, such as thermodynamic relationships, kinetic relationships, functions describing physical properties etc. The general data reconciliation problem, incorporating nonlinear constraints and imposing upper and lower bounds on the process variables, was stated in (4.1) as:

$$\begin{aligned} & J = \min_{\mathbf{x}} \ (\mathbf{y}-\mathbf{x})^T \Sigma_{\mathbf{y}}^{-1} (\mathbf{y}-\mathbf{x}) \\ & s.t. \\ & F(\mathbf{x},\mathbf{u}) = \mathbf{0} \\ & G(\mathbf{x},\mathbf{u}) \le \mathbf{0} \end{aligned} \tag{4.1}$$

Madron (1992: 162) states that including nonlinear constraints in the DR problem prevents a rigorous statistical analysis of the DR results. This is primarily due to the propagation of random measurement errors via nonlinear functions. The result is that the statistical distribution of the measurement adjustments made by the DR procedure cannot be derived, which is required by several GED algorithms (Narasimhan and Harikumar, 1993).

Several algorithms have been developed to solve Problem (4.1), and describing all of them in detail is beyond the scope of this report. The two most prevalent methods will be discussed below.

4.1.7.1 Successive Linearization

If no inequality constraints are present in the process model, and initial values of $\mathbf{u}$ are available, then (4.1) can be solved in an iterative procedure by linearizing the constraints and using the techniques for the linear systems discussed in the previous sections. This has the advantage that analytical solutions are obtained at relatively low computational expense.

The linearized constraints are obtained by a first order Taylor series expansion of $F(\mathbf{x},\mathbf{u})$ at each iteration:

$$F(\mathbf{x},\mathbf{u}) \approx F(\hat{\mathbf{x}}^k,\hat{\mathbf{u}}^k) + \frac{\partial F}{\partial \mathbf{x}}\left(\mathbf{x}-\hat{\mathbf{x}}^k\right) + \frac{\partial F}{\partial \mathbf{u}}\left(\mathbf{u}-\hat{\mathbf{u}}^k\right) = \mathbf{0} \tag{4.36}$$

The constraints in (4.1) can be simplified to:

$$A_{\mathbf{x}}^k\mathbf{x} + A_{\mathbf{u}}^k\mathbf{u} = \mathbf{c} \tag{4.37}$$

Where: $A_{\mathbf{x}}^k = \frac{\partial F}{\partial \mathbf{x}}(\hat{\mathbf{x}}^k)$, $A_{\mathbf{u}}^k = \frac{\partial F}{\partial \mathbf{u}}(\hat{\mathbf{u}}^k)$, $\mathbf{c} = A_{\mathbf{x}}^k\hat{\mathbf{x}}^k + A_{\mathbf{u}}^k\hat{\mathbf{u}}^k - F(\hat{\mathbf{x}}^k,\hat{\mathbf{u}}^k)$, and $\hat{\mathbf{x}}^k,\hat{\mathbf{u}}^k$ are the values obtained by the k[th] iteration. The unmeasured variables can be eliminated from (4.37) by QR factorization as described before, to yield an optimization problem at the (k+1)[th] iteration:

$$\begin{aligned} &J = \min_{\mathbf{x}} \ (\mathbf{y}-\mathbf{x})^T\Sigma_{\mathbf{y}}^{-1}(\mathbf{y}-\mathbf{x}) \\ &s.t. \\ &G_x\mathbf{x} = \mathbf{b} \end{aligned} \tag{4.38}$$

Where: $G_{\mathbf{x}} = Q_{\mathbf{u},2}^T A_{\mathbf{x}}^k$ and $\mathbf{b} = Q_{\mathbf{u},2}^T\mathbf{c}$. The solution to (4.38) is obtained by the method of Lagrange multipliers, and is given by:

$$\begin{aligned} \hat{\mathbf{x}}^{(k+1)} &= \mathbf{y} - \Sigma_{\mathbf{x}}G_{\mathbf{x}}^T(G_{\mathbf{x}}\Sigma_{\mathbf{x}}G_{\mathbf{x}}^T)^{-1}(G_{\mathbf{x}}\mathbf{y}-\mathbf{b}) \\ \mathbf{u}_{ru}^{(k+1)} &= R_{\mathbf{u},1}^{-1}Q_{\mathbf{u},1}^{\mathbf{T}}\mathbf{c} - R_{\mathbf{u},1}^{-1}Q_{\mathbf{u},1}^{\mathbf{T}}A_{\mathbf{x}}^k\hat{\mathbf{x}}^{(k+1)} - R_{\mathbf{u},1}^{-1}R_{\mathbf{u},2}\mathbf{u}_{nu-ru} \end{aligned} \tag{4.39}$$

The iterations are continued until a feasible solution satisfying the nonlinear constraints is obtained (Romagnoli and Sanchez, 2000: 84)

Using linearized constraints have several limitations that may hamper the implementation of the method. First, there is no guarantee that either the intermediate solutions or the final solution will satisfy the nonlinear constraints. A method using a penalty function to increase the feasibility of the iterative solutions has been developed (Pai and Fisher, 1984, quoted in Romagnoli and Sanchez, 2000: 85), but this decreases the optimality of the intermediate solution, and may result in slow convergence (Narasimhan and Jordache, 2000: 128). When

large errors are present in the data, more iterations may be required for convergence, and the method may become computationally inefficient, especially for large problems (Narasimhan and Jordache, 2000: 128).

4.1.7.2 Successive Quadratic Programming

For problems that include both equality inequality constraints, the first order necessary conditions for a local extremum are called the Kuhn-Tucker (KT) or the Karush-Kuhn-Tucker (KKT) conditions (Edgar, Himmelblau & Lasdon, 2006: 273). Combining the measured and unmeasured variables in one vector $\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{u} \end{bmatrix}$, the general nonlinear data reconciliation problem given by (4.1), can be written as:

$$\begin{aligned} &\underset{\mathbf{z}}{Min}\ h(\mathbf{z}) = \begin{bmatrix} \tilde{\mathbf{x}} - \mathbf{x} \\ \tilde{\mathbf{u}} - \mathbf{u} \end{bmatrix} \begin{bmatrix} \Sigma_{\mathbf{x}}^{-1} & O \\ O & O \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{x}} - \mathbf{x} \\ \tilde{\mathbf{u}} - \mathbf{u} \end{bmatrix} \\ &s.t. \\ &f_i(\mathbf{z}) = \mathbf{0}\,;\, i = 1,2...,m \\ &g_j(\mathbf{z}) \le \mathbf{0}\,;\ j = 1,2,...,r \end{aligned} \tag{4.40}$$

The Lagrangian of the above problem is given by:

$$L(\mathbf{z},\boldsymbol{\lambda},\boldsymbol{\delta}) = h(\mathbf{z}) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{z}) + \sum_{j=1}^{r} \delta_j g_j(\mathbf{z}) \tag{4.41}$$

Where: λ_i , $i = 1,2,...,m$ and δ_j , $j = 1,2,...,r$ are Lagrangian multipliers associated with the equality and inequality constraints, respectively. The Kuhn-Tucker conditions are then given by:

1. Linear Dependency between the gradients of the objective and various constraint functions:

$$\nabla L(\mathbf{z},\boldsymbol{\lambda},\boldsymbol{\delta}) = \nabla h(\mathbf{z}) + \sum_{i=1}^{m} \lambda_i \nabla f_i(\mathbf{z}) + \sum_{j=1}^{r} \delta_j \nabla g_j(\mathbf{z}) = \mathbf{0} \tag{4.42}$$

2. Feasibility of the Constraints:

$$\begin{aligned} f_i(\mathbf{z}) &= 0\,,\ i = 1,2,.....,m \\ g_j(\mathbf{z}) &\le 0\,,\ j = 1,2,....,r \end{aligned} \tag{4.43}$$

3. Complimentary Slackness of the Lagrange multipliers associated with inequality constraints:

$$\delta_j g_j(\mathbf{z}) = 0\,,\ j = 1,2,.....,r \tag{4.44}$$

4. Non-negativity of the Lagrange multipliers associated with inequality constraints

$$\delta_j \ge 0\,,\ j = 1,2,.....,r \tag{4.45}$$

A fifth condition is listed by Biegler *et al.* (1997), namely that the active constraints at a local solution must be linearly independent.

In order to implement successive quadratic programming (SQP), the optimization problem (4.40) is reformulated as:

$$\begin{aligned} &\underset{\mathbf{z}}{Min}\ h(\mathbf{z}) + \nabla_{\mathbf{z}} h(\mathbf{z})^T \mathbf{p} + \tfrac{1}{2}\mathbf{p}^T \nabla^2_{\mathbf{zz}} L(\mathbf{z})\mathbf{p} \\ &s.t. \\ &f_i(\mathbf{z}) + \nabla_{\mathbf{z}} f_i(\mathbf{z})^T \mathbf{p} = \mathbf{0};\ i = 1,2,...,m \\ &g_j(\mathbf{z}) + \nabla_{\mathbf{z}} g_j(\mathbf{z})^T \mathbf{p} \le \mathbf{0};\ j = 1,2,...,r \end{aligned} \tag{4.46}$$

where: $\mathbf{p}$ is the step vector that is solved for at each iteration.

Several algorithms have been developed to solve problem (4.46), however a detailed discussion of these algorithms is beyond the scope of this review.

4.1.8 Data Reconciliation incorporating Bounds on Variables

The benefit of linear or bilinear constraints in DR is that a rigorous statistical analysis can be conducted on the results of the DR procedure. This is due to fact that an analytical relationship exist between the measurements and the resulting adjustments (Narasimhan and Harikumar, 1993). Linear or bilinear DR does not guarantee feasible adjustments, so that infeasible results such as negative flow rates or concentrations may result from applying only linear/bilinear constraints. Incorporating inequality constraints such as bounds on variables require nonlinear numerical techniques to solve the DR problem, and no analytical solution for the adjustments as function of the measurements can be derived, with a resultant loss of statistical rigour. Narasimhan and Harikumar (1993) and Harikumar and Narasimhan (1993) address this problem as it relates to DR and GED respectively.

Narasimhan and Harikumar (1993) specify lower and upper bounds for all elements of the state vector $\mathbf{x}$ so that:

$$l_i \le x_i \le u_i\ ,\ i = 1,2,...,p \tag{4.47}$$

Where: p is the number of state variables. A SQP algorithm is then used to solve the inequality constraint bounded DR problem. Subsequently, the vector of state variables is portioned as $\mathbf{x} = \begin{bmatrix} \mathbf{x}_r \\ \mathbf{x}_n \end{bmatrix}$ so that all variables

determined to be at their bounds by the SQP algorithm is contained in the vector $\mathbf{x}_r$. The DR problem is then formulated with linear constraints as:

$$\begin{aligned} & J = \min_{\mathbf{x}} (\mathbf{y}-\mathbf{x})^T \Sigma_y^{-1} (\mathbf{y}-\mathbf{x}) \\ & s.t. \\ & A_r \mathbf{x}_r + A_n \mathbf{x}_n = \mathbf{0} \\ & \mathbf{x}_r = \mathbf{k} \end{aligned} \tag{4.48}$$

Where: $\mathbf{y}$ is the measurement vector, Σ_y^{-1} is the inverse of the measurement error covariance matrix, $\mathbf{x} = \begin{bmatrix} \mathbf{x}_r \\ \mathbf{x}_n \end{bmatrix}$ is the vector of state variables, and $[A_r \; A_n]$ is the partitioned constraint matrix, and the vector $\mathbf{k}$ contains the lower and upper bound constraints found to be active at the minimum objective function value by the SQP algorithm.

A solution for this linear optimization function is then obtained. The inverse of the covariance matrix
Is portioned as:

$$\Sigma_y^{-1} = \begin{bmatrix} W_{rr} & W_{rn} \\ W_{rn}^T & W_{nn} \end{bmatrix} \tag{4.49}$$

The solution to problem (4.48) is then given by:

$$\begin{aligned} & \hat{\mathbf{x}}_r = \mathbf{k} \\ & \hat{\mathbf{x}}_n = \left[I - W_{nn}^{-1} A_n^T H^{-1} A_n \right] \left[\mathbf{y}_n + W_{nn}^{-1} W_{rn} (\mathbf{y}_r - \mathbf{k}) \right] - W_{nn}^{-1} A_n^T H^{-1} A_r \mathbf{k} \end{aligned} \tag{4.50}$$

Where: $H = A_n W_{nn}^{-1} A_n^T$. As will be shown in the section of GED, the analytical relationships in (4.50) can be used to derive the statistical distributions of the measurement adjustments for the bounded DR problem, which can then be used in the associated GED strategy.

Harikumar and Narasimhan (1993) present case studies that indicate the bounded DR and GED methodology perform better than some alternative approaches, and that the degree of outperformance increase the closer the bounds are specified to the true process state variables. This presents a practical difficulty, as in practice it cannot be known how close the specified bounds are to the true values; the true values are unknown and is precisely what the DR procedure is attempting to estimate. The DR practitioner can therefore bias his results by imposing improper bounds through the bounded DR procedure. The possibility of analyst bias being introduced to the DR procedure is not unique to the bounded DR problem – in general the measurement error covariance

matrix estimate may be biased by the analyst, e.g. by assuming zero covariance terms, or by specifying which covariance terms is non-zero.

This concludes the discussion on stead-state DR. The subject of DR has received much attention in the literature, but since this thesis will discuss a steady-state case study in subsequent sections, an investigation into dynamic DR is not part of its scope. Process variable classification will be discussed in the following section.

4.2 PROCESS VARIABLE CLASSIFICATION

Modern process plants may have thousands of process variables. Even if it was technically feasible to measure all of a plant's process variables, it almost certainly would not be economically feasible to do so (Narasimhan and Jordache, 2000: 69).

Depending on the topology of the process, the measurement locations and the imposed process constraints, it may be possible to estimate some of the unmeasured variables given the values of available measurements. Improving the estimates of measured data through DR and GED therefore also improves the estimates of the unmeasured variables. Kretsovalis and Mah (1987) proves that the addition of a redundant measurement to a linearly constrained, gross error free, and fully observable process can only improve overall estimation accuracy (or at worst leave it unchanged), and vice versa for the removal of a redundant measurement from such a system.

4.2.1 Definitions of Terms

It may be possible to estimate the values of some or all of the unmeasured variables by using (reconciled) measured variables and the process constraints. These concepts give rise to the following definitions:

Observable: A variable is observable if it can be estimated uniquely using the measurements and process constraints (Narasimhan and Jordache, 2000: 70).

Redundant: A measured variable is redundant if it remains observable even when the measurement is removed (Narasimhan and Jordache, 2000: 70).

From the above, it follows that all measured variables are observable, since a measurement provides an estimate of the variable. An unmeasured variable may be observable or unobservable, depending on the sensor network

and process constraints. Also, a measured variable may be redundant or non-redundant depending on the sensor network and process constraints.

Restricting the concept of observability to unmeasured variables give rise to a definition more suited for variable classification:

Determinable: An unmeasured variable is determinable if it can be estimated using the available measurements and the process constraints (Romagnoli and Sanchez, 2000: 28).

Indeterminable: An unmeasured variable is indeterminable if it cannot be estimated using the available measurements and the process constraints (Romagnoli and Sanchez, 2000: 28).

The classification of process variables according to the above definitions is illustrated in Figure 2.1:

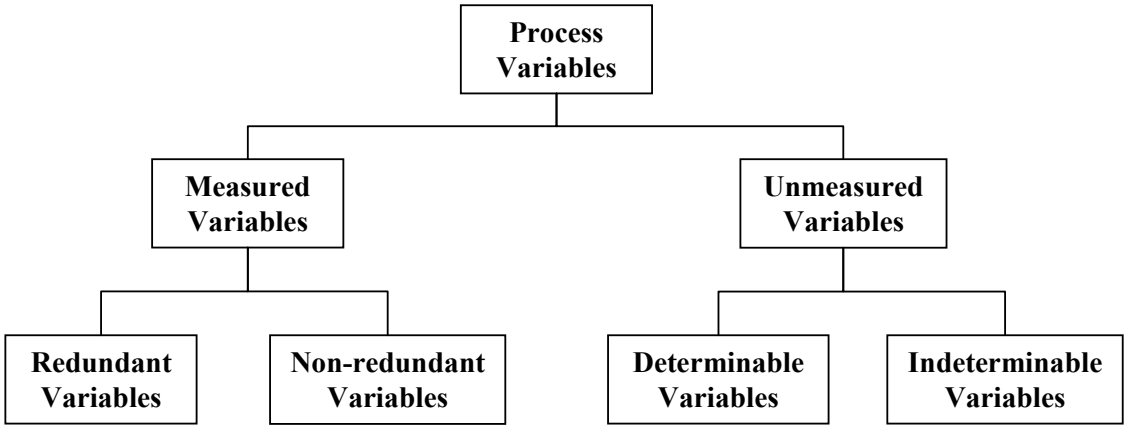

Figure 4-1: Process Variable Classification

It should be noted that some authors do not apply the concept of observability to measured variables, i.e. the distinction between observable/unobservable and determinable/indeterminable is not consistent in the literature.

Variable classification has specific application at the design or retrofit stage for selection of measurement locations and instrument specification, depending on the objective(s) of the control philosophy. Additionally, variable classification impacts on the interpretation of DR and GED results; specifically, identifying a gross error in a non-redundant measurement effectively renders the measurement unobservable (Albequerque and Biegler, 1996).

Several methods exist to accomplish variable classification. Ponzoni *et al.* (1999) gives a brief description of these, which are outlined in the graph below:

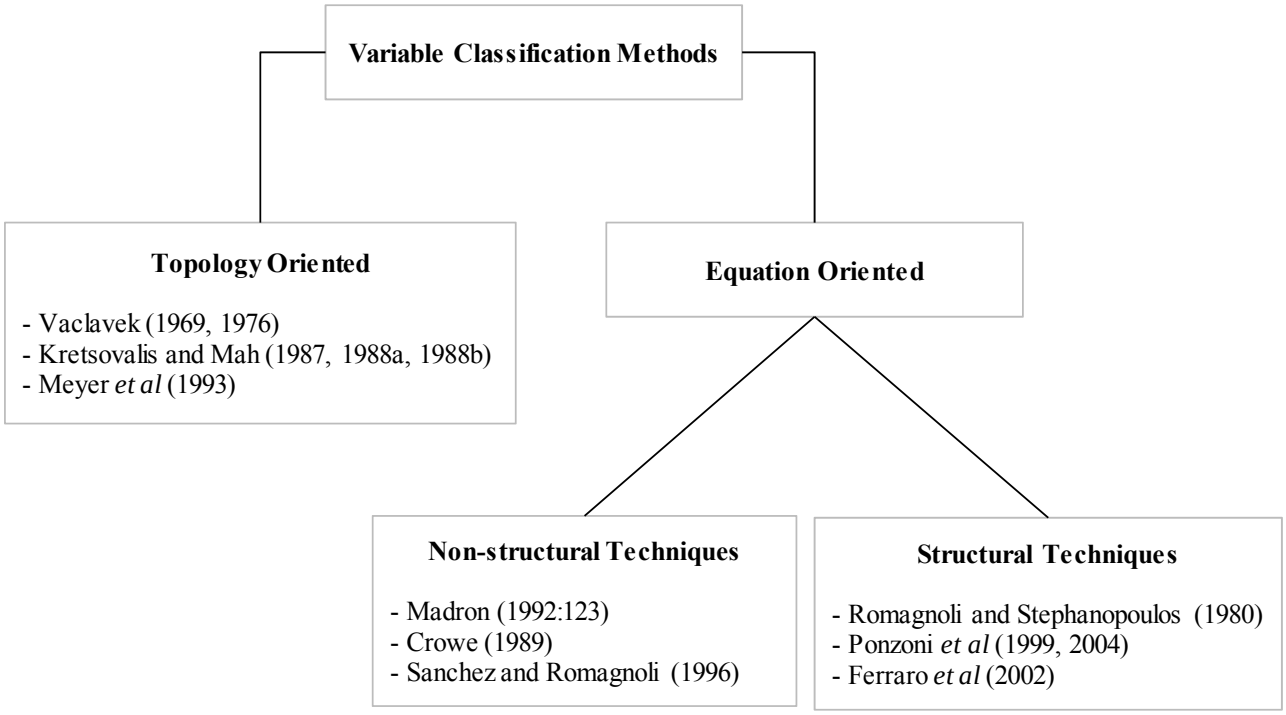

Figure 4-2 : Methods of Process Variable Classification

Topology orientated methods make use of a graph representation of the process, and related graph theoretical arguments to classify variables. Non-structured equation oriented techniques modify the coefficients of the augmented process matrix to achieve the classification. Madron (1992: 123) achieves this through conversion of the augmented system matrix to canonical form for strictly linear systems. Crowe (1989) applies the projection matrix for removing unmeasured variables from the constraints (Crowe, 1986) to solve the classification problem for linear and bilinear systems. Ponzoni *et al.* (1999) mentions that the topology and non-structured equation oriented methods can be applied to linearized systems, although with a loss of classification accuracy. Structured equation oriented techniques can be applied to nonlinear systems, and partially address the problems experienced with the other techniques. Romagnoli and Stephanopoulos (1980) define the occurrence matrix S for a process system as:

$$S_{ij} = \begin{cases} 1, \text{ if variable } j \text{ appears in equation } i \\ 0, \text{ otherwise} \end{cases} \tag{4.51}$$

The structure of the occurrence matrix is then used to assign model equations to unmeasured variables through an output set assignment algorithm. Unmeasured variables not assigned an equation from the model is classified

as indeterminate (unobservable), while measured variables and rules are provided for classifying the measured variables as redundant or non-redundant.

4.2.2 Variable Classification for Steady-State Systems by means of the Projection Matrix

Matrix methods for classifying variables in linearly constrained systems follow directly from the sub-problem of finding a projection matrix to eliminate unmeasured variables from the process constraints. Using the results of matrix projection may convenient in practice as much of the necessary information for classification is obtained as part of the DR solution.

The general solution of the unmeasured variables for a linear system using QR factorization was given in (4.28) as:

$$\mathbf{u}_1 = R_1^{-1} Q_1^T (\mathbf{c} - A_x \hat{\mathbf{x}}) - R_1^{-1} R_2 \mathbf{u}_2 \tag{4.28}$$

Here, $\mathbf{u}_2$ correspond to linearly dependent columns of the system matrix A_u, and is unobservable. A variable contained in $\mathbf{u}_1$ is determinable if the corresponding row in $R_1^{-1} R_2$ contains only zero entries, i.e. if the variable can be calculated uniquely from the reconciled measurements $\hat{\mathbf{x}}$, otherwise it is indeterminable (Sanchez and Romagnoli, 1996). The reduced set of process constraints remaining after matrix projection for the case where the projection is found through QR factorization is given by:

$$Q_2^T A_x \mathbf{x} = Q_2^T \mathbf{c} \tag{4.52}$$

If a column of $Q_2^T A_x$ contains only zeros, the corresponding measurement is non-redundant, otherwise it is redundant. In general, the adjustment made to a non-redundant measurement in the DR procedure will be zero only if the measurement error covariance matrix Σ_y is diagonal, otherwise non-redundant measurements will not be adjusted (Crowe, 1989).

Crowe (1989) provide several lemmas to determine indeterminable and non-redundant variables for the bilinear case. Albequerque and Biegler (1996) extend Crowe's method to linearized dynamic systems.

4.3 GROSS ERROR DETECTION/ IDENTIFICATION IN STEADY-STATE SYSTEMS

4.3.1 Introduction

Bagajewicz (2010: 195) state that the lack of powerful GED methods in commercial software is "*at the core of all problems in Data Reconciliation*". This clearly illustrates the importance of the GED problem.

DR techniques typically rely on the assumption that measurement errors are random and additive in nature, usually with a Gaussian distribution with a zero mean and known covariance matrix. Under this assumption, the measurement model is given by (Romagnoli and Sanchez, 2000: 111):

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon} \tag{4.2}$$

Where: $\mathbf{y}_{n\times 1}$ is a vector of process measurements, $\mathbf{x}_{n\times 1}$ is a vector representing the true values of the measured process variables, and $\boldsymbol{\varepsilon}_{n\times 1} \sim N(\mathbf{0}, \Sigma_y)$ is a vector of random errors. The linear process model is given by:

$$A\mathbf{x} = \mathbf{c} \tag{4.9}$$

Where: $A_{m\times n}$ is a matrix derived from the material and energy balance equations of the process, $\mathbf{x}$ is as above and $\mathbf{c}_{m\times}$ is a vector of known constants, usually the zero vector. The vector of model residuals is then given by:

$$\mathbf{r} = A\mathbf{y} - \mathbf{c} \tag{4.53}$$

The statistical properties of the residuals vector are given by:

$$\begin{aligned} E(\mathbf{r}) &= E(A\mathbf{x} + A\boldsymbol{\varepsilon} - \mathbf{c}) = A \cdot E(\boldsymbol{\varepsilon}) = \mathbf{0} \\ H &= \mathrm{cov}(\mathbf{r}) = E(\mathbf{r}\mathbf{r}^T) = A\Sigma_y A^T \end{aligned} \tag{4.54}$$

Under the assumptions listed above, the DR methods for linear systems discussed in Section 4.1 produce unbiased minimum variance estimates of the true process state variables. The presence of gross errors invalidates the measurement model of (4.2). In the case of a single gross error, assumed to be additive, the measurement model is given by (Bagajewicz, 2010: 66):

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon} + b \cdot \mathbf{e}_i \tag{4.55}$$

Where: b is scalar indicating the gross error magnitude, and $\mathbf{e}_i$ is a unit vector for the i^{th} measurement location. Applying DR techniques from Section 4.1 when gross errors are present leads to biased results, as in general the DR result for bias in the i^{th} measurement will be (Bagajewicz, 2010: 66):

$$\hat{\mathbf{x}}(i) = \hat{\mathbf{x}} + b \cdot \left[I - \Sigma_y A^T (A\Sigma_y A^T)^{-1} A \right] \mathbf{e}_i \tag{4.56}$$

Where: $\hat{\mathbf{x}}$ is the DR result for unbiased measurements. The presence of even a single gross error there results in a biased estimate from DR. Further, inspection of (4.56) reveals that the bias is distributed across all elements of

the DR estimate $\hat{\mathbf{x}}(i)$ due to the matrix $\left[I - \Sigma_y A^T (A\Sigma_y A^T)^{-1} A \right]$ generally being dense. This phenomenon is commonly known as *smearing* of the gross error (Bagajewicz, 2010: 66), and could translate into economic losses or unsafe operating conditions if applied in an industrial setting. As an example, the author is familiar with a coal processing facility where DR and GED are incorporated into the quality control philosophy. Product quality is continuously monitored via an on-stream analyser. The analyser is sensitive to several factors that may vary with time, and is also known to experience calibration drift over time. In order to provide an estimate of analyser accuracy, all shift sample and weightometer data is reconciled via a DR and GED algorithm, and the estimates of quality parameters obtained from the DR/GED procedure compared with those of the analyser. Any undetected bias in the analyser results will result in an economic loss, either by delivery of off-specification product to the customer, with associated penalties for higher than specification product quality, or by loss of yield due to lower than specification product quality. It is therefore necessary to develop a strategy for dealing with gross errors when applying DR.

Bias may be introduced to the results of DR by either the process measurements or the process model. The process model may introduce bias through application of steady-state material and energy conservation constraints to a dynamic process, the presence of unknown leaks or flows, or incorporating process models that was not derived from first principles, e.g. kinetic relations which are in some way dependent on the conditions under which they were derived. In addition, subjective specification of the elements of the measurement error variance/covariance matrix may introduce analyst bias into the DR and GED results. The importance of steady-state detection and measurement error covariance estimation is therefore apparent.

Narasimhan and Jordache (2000:175) identify four functions of a Gross Error Detection strategy:

1. Detect the presence of one or more gross errors (Detection Problem).
2. Identify the type and location of gross errors (Identification Problem).
3. Identify the type and location of multiple gross errors (Multiple Gross Error Detection Problem).
4. Estimate the magnitude of gross errors.

Of these, the Detection and Identification of single gross errors are of primary importance, since detecting and identifying multiple gross errors is secondary to the ability to detect and identify single gross errors, and it's not always necessary to estimate the magnitude of gross errors in order to eliminate their influence.

Romagnoli and Sanchez (2000:109) suggest three possible ways to identify gross errors:

1. Using a theoretical analysis of all the causes of gross errors.

2. Using redundant measurements, i.e. multiple measurement devices for the same variable, with different precision.
3. Checking the extent to which process measurements satisfy the process model or constraints

The third alternative is closely related to DR, and can be used in conjunction with DR in a complete plant data analysis strategy.

The typical methodology for finding gross errors is to derive various test statistics, and using statistical methods to test between H_0: *No Gross Errors are present* and H_1: *At least one Gross Error is present*.

4.3.2 Gross Error Detection in Linear Systems

4.3.2.1 The Global Test

The Global Test uses the statistical properties of the residuals vector derived above to detect the presence of one or more gross errors. The test statistic is given by (Romagnoli and Sanchez, 2000: 112):

$$\tau = \mathbf{r}^T H^{-1} \mathbf{r} \tag{4.57}$$

According to Romagnoli and Sanchez, if the matrix A has full row rank *m*, then τ will have a chi-square distribution with *m* degrees of freedom, i.e.:

$$\tau \sim \chi_m^2 \tag{4.58}$$

The null hypothesis that no gross errors are present in the data can now be tested at a specified level of significance, i.e. the presence of one or more gross errors is detected when:

$$\tau \geq \chi_{1-\alpha}^2(m) \tag{4.59}$$

Where: α is the chosen level of significance, or Type I error rate.

The Global Test has the advantages of simplicity and can be used to test the consistency of the data before any Data Reconciliation has been attempted. However, it cannot identify the location of any gross errors, or discern between single and multiple gross errors.

4.3.2.2 The Nodal/Constraint Test

The vector $\mathbf{r}$ of constraint residuals can be used to derive test statistics (Narasimhan and Jordache, 2000: 180):

$$z_{r,i} = \frac{|r_i|}{\sqrt{H_{ii}}}, i = 1, 2, \ldots m \tag{4.60}$$

Under the null hypothesis that no gross errors are present in the process data or model, $z_{r,i}$ follows a standard normal distribution.

Using (4.60) to test for the presence of gross errors will result in m univariate tests being conducted. It is therefore necessary to modify the level of significance of the individual tests, in order to preserve the overall Type I error probability of the method. According to Narasimhan and Jordache (2000), Mah and Tamhane proposed a modified significance level based on the Sidak inequality:

$$\beta = 1 - (1 - \alpha)^{\frac{1}{m}} \tag{4.61}$$

Where: β is the modified significance level for individual tests, and α is the desired overall Type I error probability. Another method proposed by Rollins and Davis (1992) is to use the Bonferroni confidence interval:

$$\beta = \frac{\alpha}{m} \tag{4.62}$$

Using the modified significance level, a gross error is detected if:

$$z_{r,i} \geq z_{1-\beta/2} \tag{4.63}$$

According to Narasimhan and Jordache, Crowe showed that the power of the Nodal or Constraint Test can be increased by using a linear transformation of the constraint residuals. The test statistics of the maximum power (MP) Nodal/Constraint Test is given by:

$$z^*_{r,i} = \frac{\left|(H^{-1}\mathbf{r})_i\right|}{\sqrt{H^{-1}_{ii}}} \tag{4.64}$$

The test criterion for the MP Nodal/Constraint test is the same as that for the standard Nodal/Constraint Test, given by (4.63).

4.3.2.3 The Measurement Test

The Measurement Test uses the vector of measurement adjustments (Narasimhan and Jordache, 2000: 183):

$$\mathbf{a} = \mathbf{y} - \mathbf{x} = \Sigma_y A^T H^{-1} A\mathbf{y} \tag{4.65}$$

Under the null hypothesis that no gross errors is present in the data, $\mathbf{a}$ follows a multivariate normal distribution, with zero expected value and covariance matrix given by:

$$\Sigma_a = \Sigma_y A^T H^{-1} A \Sigma_y \tag{4.66}$$

Test statistics for the Measurement Test are calculated as:

$$z_{a,i} = \frac{|a_i|}{\sqrt{(\Sigma_a)_{ii}}}, i = 1,2,....,n \tag{4.67}$$

Under H_0, $z_{a,i} \sim N(0,1)$, and the critical values for the test criterion can be chosen according to a desired level of Type I error probability, bearing in mind that n univariate test are being conducted.

Tamhane, as quotes in Narasimhan and Jordache (2000), has shown that for the case where the measurement error covariance matrix Σ is non-diagonal, a maximum power (MP) Measurement Test can be derived by using the following linear transformation:

$$\mathbf{a}^* = \Sigma_y^{-1}\mathbf{a} \tag{4.68}$$

Under H_0 the statistical properties of $\mathbf{a}^*$ are given by:

$$\begin{aligned} \mathbf{a}^* &\sim N(\mathbf{0}, \Sigma_{a^*}) \\ \Sigma_{a^*} &= A^T H^{-1} A \end{aligned} \tag{4.69}$$

The test statistics for the MP Measurement Test are then given by:

$$z_{a^*,i} = \frac{|a^*_i|}{\sqrt{(\Sigma_{a^*})_{ii}}}, i = 1,2,....,n \tag{4.70}$$

4.3.2.4 The Generalized Likelihood Ratio Test

The Generalized Likelihood Ratio (GLR) Test is based on the maximum likelihood ratio principle from statistics (Narasimhan and Jordache, 2000: 185).

Unlike the gross error tests discussed above, the GLR Test requires gross errors to be modelled as part of the measurements model and process constraints. In the presence of a gross error the measurement model linear process constraints become:

$$\mathbf{y} = \mathbf{x} + \boldsymbol{\varepsilon} + b \cdot \mathbf{e}_j \tag{4.71}$$

$$A\mathbf{y} - b \cdot \mathbf{m}_i = \mathbf{c} \tag{4.72}$$

Where: b represents the magnitude of the gross error, $\mathbf{e}_j$ is the unit vector for a bias in the j[th] measurement, and $\mathbf{m}_i$ is a vector representing the loss of mass or energy from the i[th] process node. Narasimhan and Jordache suggest the following rules for assigning values to the elements of $\mathbf{m}_i$:

- If the gross error is modelled as part of the total mass flow through the i[th] process node, then the i[th] element of $\mathbf{m}_i$ should have a magnitude of unity.
- If the gross error is modelled as part of a component balance around node *i*, the i[th] element of $\mathbf{m}_i$ should have a value equal to the average concentration of the relevant component in the streams incident on node *i*.
- If the gross error is modelled as part of the energy balance around the i[th] process node, the i[th] element of $\mathbf{m}_i$ should have a magnitude equal to the average specific enthalpy of the streams incident on node *i*.
- Elements of $\mathbf{m}_i$ not associated with constraints of node *i* are zero.

Given the above gross error models, the statistical properties of the constraint residuals vector can be derived. Under H_0, $\mathbf{r} \sim N(\mathbf{0}, A\Sigma_y A^T)$ from (4.54). If it is assumed that a gross error is present, then the expected value of the residual vector is given by:

$$E[\mathbf{r}] = b\mathbf{f}_k \tag{4.73}$$

Where: $\mathbf{f}_k = A\mathbf{e}_j$ for a gross error in measurement *j*, and $\mathbf{f}_k = \mathbf{m}_i$ for a gross error in node *i*. The covariance matrix of the residuals remains unchanged under H_1, so in the presence of a gross error, $\mathbf{r} \sim \mathbf{N}(b\mathbf{f}_k, A\Sigma_y A^T)$.

Narasimhan and Jordache (2000) refer to the vectors $\mathbf{f}_k$ as *'gross error signature vectors'*, and it follows that there is a signature vector corresponding to each measurement and each constraint in the process model, so that:

$$k = m + n \tag{4.74}$$

The gross error hypothesis can now be restated as:

$$\begin{aligned} H_0 &: \ E[\mathbf{r}] = \mathbf{0} \\ H_1 &: \ E[\mathbf{r}] = b\mathbf{f}_k \end{aligned} \tag{4.75}$$

The test statistic for the GLR Test is the maximum value of the ratio of the probabilities of observing the residual vector $\mathbf{r}$, conditioned on the two hypothesis of (4.75):

$$\lambda = \sup \frac{P(\mathbf{r}|H_1)}{P(\mathbf{r}|H_0)} = \sup_{b,\mathbf{f}_k} \left\{ \frac{\exp\left[-0.5(\mathbf{r} - b\mathbf{f}_k)^T H^{-1}(\mathbf{r} - b\mathbf{f}_k)\right]}{\exp\left[-0.5\mathbf{r}^T H^{-1}\mathbf{r}\right]} \right\} \tag{4.76}$$

Narasimhan and Jordache (2000) simplify the above test statistic to:

$$T = 2\ln\lambda = \sup_{b,\mathbf{f}_k} \left\{ \mathbf{r}^T H^{-1}\mathbf{r} - (\mathbf{r} - b\mathbf{f}_k)^T H^{-1}(\mathbf{r} - b\mathbf{f}_k) \right\} \tag{4.77}$$

The value of b that maximizes the expression in (4.77) is given by:

$$b = \frac{\mathbf{f}_k^T H^{-1} \mathbf{f}_k}{\mathbf{f}_k^T H^{-1} \mathbf{r}} \tag{4.78}$$

For every signature vector $\mathbf{f}_k$ a value of b can be calculated, and substituted back into (4.77) to yield a value of T corresponding to $\mathbf{f}_k$, denoted by T_k:

$$T_k = \frac{(\mathbf{f}_k^T H^{-1} \mathbf{f}_k)^2}{\mathbf{f}_k^T H^{-1} \mathbf{r}} \tag{4.79}$$

The GLR Test statistic is given by:

$$T = \sup_k T_k \tag{4.80}$$

Where: the supremum operator $\sup_k(\cdot)$ selects the maximum from the k arguments. The distribution of T under the null hypothesis is central Chi-square with one degree of freedom, so that a gross error is detected if:

$$T \geq T_{cr} = \chi^2_{1-\beta,1} \tag{4.81}$$

Since the GLR Test selects the maximum among k alternative values of T, it is equivalent to performing $k = m + n$ univariate tests, so that the level of significance β has to be adjusted in order to preserve the overall Type I error probability, as shown before.

4.3.2.5 The Statistical Power of different Gross Error Detection Tests

The tests for Detection of a gross error discussed so far is not an exhaustive list, however discussing all possible variations of the Detection strategy is beyond the scope of this thesis. The case study discussed later utilizes the Measurement Test as a baseline for the classical GED methods discussed here, as this is generally the test applied in commercial software (Bagajewicz, 2010: 82).

Narasimhan and Jordache (2000: 190) state that it is important to apply the gross error detection strategy with the maximum statistical power, in order to obtain optimum performance of the Data Reconciliation/Gross Error Detection strategy.

However, they also state that determining which test has the greatest power is only a partially solved problem. This is in part due to the fact that the power of a test is closely related to its Type I error rate, so in order to compare tests based on power, it has to be ensured that the tests have the same Type I error probability. Some detection strategies use multiple univariate tests, in which case the actual level of significance is difficult to determine, since the modified level of significance given by (4.61) or (4.62) is only an upper bound on the Type I error probability, and the actual significance level has to be determined approximately through simulation. The

result is a semi empirical significance level specific to the problem being simulated, and the results cannot be generalized to all processes in a rigorous manner.

Despite the difficulties described above, Narasimhan and Jordache derive some results based on the following assumptions:

- At most one gross error is present in the problem.
- All possible modes of the gross error are known, so that the signature vectors for the GLR Test are exhaustive.

Under the assumptions stated above, the following holds:

- If gross errors are assumed to only be present in the measurements, then the GLR Test and the Measurement Test is equivalent in power.
- Similarly, if gross errors are only assumed to be present in the process constraints, then the GLR Test and the Nodal Test is equivalent.
- If both types of gross errors are allowed, then the GLR Test is superior to the Measurement Test and Nodal Test.

Due to the univariate nature of the GLR Test, no conclusion can be made about its power relative to that of the Global Test, for the reasons outlined above. However,, Narasimhan and Jordache (2000) recommend using the Global Test for detecting the presence of one or more gross errors for the following reasons:

- Since only a single test statistics have to be computed, the Global Test is computationally more efficient than the GLR Test.
- An exact level of significance can be specified for the Global Test, so that Type I error rate can be controlled more effectively.
- The Global Test does not require prior knowledge of the gross error vectors that can occur in the process, which is an advantage because it may not be possible to have complete knowledge of the gross errors that can occur.

4.3.3 Gross Error Detection in Generalized Linear Systems

4.3.3.1 Unmeasured Variables

In general, not all variables are measured, so that the linear process constraints are given by:

$$A_x \mathbf{x} + A_u \mathbf{u} = \mathbf{c} \tag{4.82}$$

The unmeasured variables can be removed from the constraints by using a projection matrix:

$$PA_x\mathbf{x} = P\mathbf{c} \tag{4.83}$$

The constraint residuals are then given by:

$$\rho = P(A_x\mathbf{y} - \mathbf{c}) \tag{4.84}$$

The covariance matrix of the residuals of the modified constraints is given by:

$$H_\rho = (PA_x)\Sigma_y(PA_x)^T \tag{4.85}$$

For the GLR Test, the gross error signature vectors are given by:

$$\mathbf{f}_{\rho,k} = P\mathbf{f}_k \tag{4.86}$$

These modified values of the system matrix, residuals vector, residuals covariance matrix and gross error signature vectors can be used in the Global Test, Nodal/Constraint Test, Measurement Test and GLR Test as described before (Narasimhan and Mah, 1989).

4.3.3.2 Indirect Measurement Model

In general, variables may not be directly measured. For the linear case, the relationship between the process variable and measurement is given by:

$$\mathbf{y} = M\mathbf{x} + \boldsymbol{\varepsilon}_\mathbf{x} \tag{4.11}$$

The indirect model defined above can be converted into the direct measurement model by defining artificial process variables, that can be directly 'measured', and including the relationship between these variables and the actual process variables in the process constraints:

$$\mathbf{x}_a = M\mathbf{x} \tag{4.87}$$

$$\mathbf{y} = \mathbf{x}_a + \boldsymbol{\varepsilon} \tag{4.88}$$

$$\begin{bmatrix}\mathbf{0}\\ I\end{bmatrix}\mathbf{x}_a + \begin{bmatrix}A\\ M\end{bmatrix}\mathbf{x} = \begin{bmatrix}\mathbf{c}\\ \mathbf{0}\end{bmatrix} \tag{4.89}$$

The DR/GED procedure can then be implemented as usual (Narasimhan and Mah, 1989).

4.3.4 Gross Error Identification in Linear Systems

Narasimhan and Jordache (2000: 203) describe the Identification problem as distinct from the Detection problem. They define the Identification problem as the process of determining the type and location of a gross error, after it was established that a gross error is present in the Detection problem.

In general, the methods used to solve the Detection problem may be applied to the Identification problem as well. Romagnoli and Stephanopoulos (1981) apply the Global Test to solve the Identification problem, while

Mah, Stanley and Downing (1976) apply the Nodal Test similarly. Recursive schemes are required to determine the measurement(s) or constraint(s) in error when using either of these tests. Bagajewicz (2010: 76) describes one such serial elimination strategy that recursively eliminate measurements or groups of measurements until the reduced DR problem does not violate the Global Test. He states that these strategies are not effective in identifying gross errors.

Mah and Tamhane (1982) apply the MP Measurement Test to solve the Identification problem, by eliminating all measurements for which the test statistic exceeds the critical value. Bagajewicz (2010: 77) states that there are several difficulties with using the Measurement Test for identification:

- Due to smearing, gross errors may be identified in the wrong location
- Cancellation or interaction between multiple gross errors can cause poor performance
- The Measurement Test cannot detect leaks or other model error, but are sensitive to their presence

Bagajewicz (2010: 77) describes an alternative serial elimination strategy (as opposed to the collective elimination of Mah and Tamhane (1982)), in which either the measurement with largest test statistic, or the measurement resulting in the greatest reduction in objective function value is eliminated at each iteration.

Narasimhan and Jordache (2000: 204) apply the GLR test for identification of single gross errors in either a measurement or constraint equation based on the maximum test statistic.

For nonlinear DR problems, the methods described so far for linear systems can be applied to a linearized model of the process, where linearization is performed around the final DR estimate. Romagnoli and Stephanopoulos (1981) point out that the process model needs to be well approximated by the linearized model in the region around the point of linearization, and that strictly speaking the statistical properties derived from the linearized model apply to the increments of the variables in the DR problem as opposed to the variables themselves.

There is a large body of literature dealing with detecting and identification of multiple gross errors, and only some of these strategies are mentioned above in regards to the global and constraint tests. Since the case study presented later in this thesis contain only single gross errors, a more detailed discussion of multiple gross error algorithms is outside the scope of this thesis.

The final element of the GED strategy, gross error magnitude estimation, will be discussed in the following section.

4.3.5 Gross Error Magnitude Estimation

Estimates of gross error magnitude can be used to compensate the measurement or process model in a recursive manner to obtain improved DR estimates. DR estimates may also be improved after GED by elimination of the measurement(s) in which a gross error was identified.

When only a single gross error is considered (or a serial strategy for multiple gross errors), an estimate of the magnitude of the measurement or constraint bias can be obtained from the GLR test as described previously.

When several gross measurement errors are considered simultaneously, the measurement model may be written as (Jiang and Bagajewicz, 1998):

$$\mathbf{y} = \mathbf{x} + L\mathbf{b} + \boldsymbol{\varepsilon} \tag{4.90}$$

Where: the columns of $L = \left[\mathbf{e}_1\ \mathbf{e}_2\ .....\mathbf{e}_{nb}\right]$ consist of unit vectors corresponding to the measurement locations considered to be biased, and $\mathbf{b} = \left[b_1\ b_2\ .....\ b_{nb}\right]^T$ is the vector of corresponding magnitudes. The solution to the DR problem incorporating this measurement model is given by:

$$\hat{\mathbf{x}} = \hat{\mathbf{x}}_0 + B\hat{\mathbf{b}} \tag{4.91}$$

Where: $\hat{\mathbf{x}}_0$ is the solution to the DR problem without considering the gross errors in measurements. The matrix B is given by:

$$B = \left[\Sigma_y A^T (A\Sigma_y A^T)^{-1} A - I\right] L \tag{4.92}$$

And the estimate of gross error magnitudes is given by:

$$\hat{\mathbf{b}} = \left[(B+L)^T \Sigma_y^{-1} (B+L)\right]^{-1} (B+L)^T \Sigma_y^{-1} (\mathbf{y} - \hat{\mathbf{x}}_0) \tag{4.93}$$

Jiang and Bagajewicz (1998) point out that the inverse in (4.93) may not exist, depending on the selected gross error locations. Sanchez, Romagnoli, Jiang and Bagajewicz (1999) extend the above method to include gross errors in the constraints.

4.3.6 Detectability and Identifiability of Gross Errors

4.3.6.1 Detectability of Gross Errors

The observability and redundancy analysis of a process system and its associated sensor network leads to a theoretical classification based on the mathematical solvability of the unmeasured variables through the process

constraints given reconciled estimates of the measurements. DR attempts to find a set of estimates of the process variables that satisfy the process constraints, while minimizing the weighted sum of squares of the measurement adjustments. The covariance matrix of the measurement adjustments is not the same as that of the measurement errors, since the measurement adjustments are correlated with each other due to the interrelationships imposed by the process constraints. The results of Data Reconciliation can be used to estimate the values of observable unmeasured process variables (the coaptation problem). The covariance matrix of the observable variables can thus be calculated through knowledge of the covariance of the redundant measurements.

The end result of Data Reconciliation is thus a set of measurement estimates and calculated observable variables, and their respective covariance matrices. In general, the standard deviation of the estimate of a redundant variable is smaller than that of the associated measurement. In practice, it may be found that some redundant measurements behave as non-redundant measurements, referred to as *practically non-redundant measurements*, and similarly some observable variables become *practically unobservable*. If a gross error is present in a practically non-redundant measurement, a large adjustment will not be made to the measurement. Instead, the effect of the gross error will be absorbed in the adjustments made to other measurements in order to satisfy the process constraints, a phenomenon known as *smearing.* (Narasimhan and Jordache, 2000: 210).

Madron (1992: 141) defined the *adjustability* of a measurement as:

$$a_i = 1 - \frac{\sigma_{\hat{x}_i}}{\sigma_{y_i}} \tag{4.94}$$

Where: $\sigma_{\hat{x}_i}$ is the standard deviation of the estimate and σ_{y_i} is the standard deviation of the i^{th} measurement. The adjustability of a measurement thus increases as the standard deviation of its estimate decreases, so that *adjustability* is a measure of the improvement in accuracy obtained through DR. Narasimhan and Jordache suggests that a measurement can be classified as *practically redundant* if its adjustability is greater than a selected threshold, say 0.1, which would imply the ratio of the standard deviations is less than 0.9.

Charpentier, as quoted in Narasimhan and Jordache (2000: 211) suggested an alternative formulation, given by:

$$d_i = \sqrt{\left(1 - \frac{\sigma^2_{\hat{x}_i}}{\sigma^2_{y_i}}\right)} \tag{4.95}$$

Where: d_i is the *detectability* of an error in measurement y_i. Gross errors are more likely to be detected in measurements with a large detectability and Narasimhan and Jordache (2000:211) suggests that it may be possible to detect gross errors of smaller magnitude in these measurements. They suggest that a complete practical redundancy analysis of a system may be very useful, in addition to the theoretical redundancy and observability analysis discussed before.

4.3.6.2 Identifiability of Gross Errors

Bagajewicz (2010: 87) define *equivalent sets of gross errors.* If two distinct sets of gross errors cannot be distinguished from each other, they are said to be equivalent. According to Narasimhan and Jordache, Bagajewicz and Jiang proved that, for any set of *k* measurements that form a cycle on the process graph, no combination of *k-1* gross errors in this cycle can be distinguished from any other. It is also not possible to distinguish gross errors in the measurements of all *k* variables form the measurements of any *k-1* variables in the cycle. In addition, if there are *m* linearly independent constraints imposed on the system, the all sets of *m* linearly independent gross errors are equivalent. Narasimhan and Jordache (2000) state that sets of equivalent gross errors belong to an *equivalency class*. They extend the ideas of Bagajewicz and Jiang to gross error signature vectors, and derive the following result:

> *If the set of signature vectors for a set of k gross errors is linearly dependent with rank k-1, then no set of k-1 gross errors can be distinguished from any other set of k-1 gross errors, and it is impossible to determine if k or k-1 gross errors are present in the system. Also, if the maximum number of independent signature vectors is m, then all sets containing m gross errors with linearly independent signature vectors are indistinguishable from each other.*

5 ALTERNATIVE APPROACHES TO THE DATA RECONCILIATION AND GROSS ERROR DETECTION PROBLEM

The fundamental concept of classical GED techniques is to derive statistical distributions of the constraint residuals and/or measurement adjustments based on the null hypothesis that no gross errors are present. An alternative approach to the GED problem is the application of Artificial Neural Networks (ANN's) to perform a classification based on the information contained in the constraint residuals and/or measurement adjustments.

5.1 APPLICATION OF ARTIFICIAL NEURAL NETWORKS

ANN's consist of multiple simple processing units, such as the one illustrated in Figure 5-1:

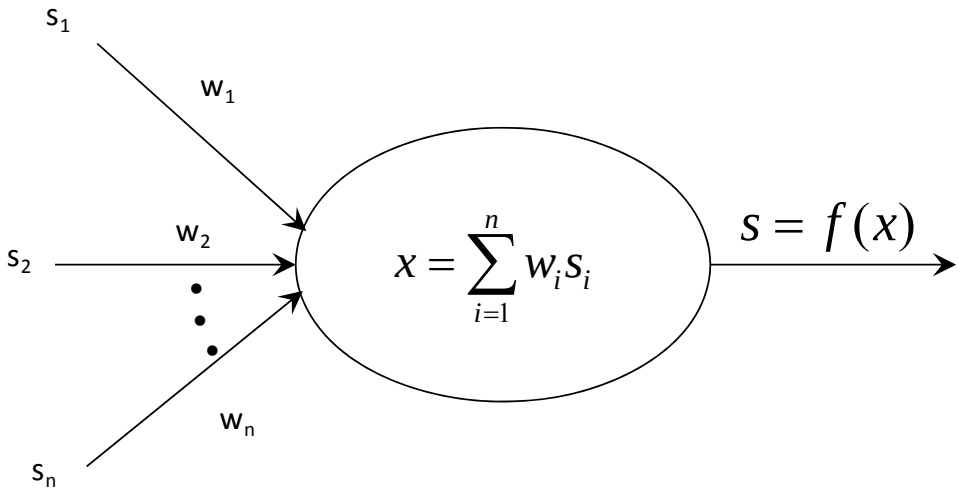

Figure 5-1 : Example of a Simple Neuron

A single neuron generates an output from several weighted inputs. The activation function $f(\cdot)$ may take several possible forms, and the sigmoidal function is often used, that is:

$$s = \frac{1}{1+e^{-x}} \tag{4.96}$$

The ANN is constructed from an arbitrary number of such simple neurons, and the connectivity between neurons may be arbitrarily complex. The structure of a network, i.e. the number of neurons and their connectivity, as well as the activation function(s) employed, are optimization parameters that depend on the specific problem at hand. ANN's are popular due to their versatility, flexibility, and ability to approximate complex relationships between variables while filtering out noise in the data.

ANN's have been applied to resolve the DR problem, as well as the Detection problem of the GED problem.

5.1.1 ANN's applied to the DR problem

Terry *et al.* (1993) applied ANN's to solve the DR problem for a simulated non-linear steady-state process around heat exchanger. Their motivation was that the assumptions underlying the process constraints of steady-state DR is often violated in practice, so that the constraints do not strictly apply. They thus use the ANN primarily as a non-exact approximation for the constraint equations. The input vector to the ANN consisted of the measurement vector, and reconciliation was achieved by training the ANN to reproduce the input vector, i.e. for a steady-state process it would be expected for the network to converge to the average measurement value of the data set. Their results indicated that the ANN performed better than traditional non-linear programming solution for the DR problem, both when random error only and single or multiple gross errors were present in the measurements, as well as when measurement errors were autocorrelated in time.

Aldrich *et al.* (1994a) applied three different ANN structures to resolve the DR problem. They viewed ANN's as an attractive alternative to nonlinear programming due to the parallel processing capability of the ANN, which they expected to decrease computational time. They applied the ANN's to two problems, one with bilinear constraints and one with highly nonlinear constraints, and find the ANN's to be superior for high dimensional problems, and comparable to conventional methods for the simpler problem.

5.1.2 ANN's applied to the Detection problem of GED

Aldrich *et al.* (1993) used back propagation ANN's to solve the Detection problem. Training of the ANN's was achieved by presenting the ANN's with input vectors consisting of the process measurements and associated constraint residuals. The ANN's were developed for two different circuits; a flotation circuit subject to linear total flow constraints only, and a hydrocyclone circuit subject to multiple bilinear constraints. They found that the ANN's misclassified very few random error vectors as gross error vectors, and could successfully classify gross error vectors. The proportion of correctly detected gross errors increased with gross error magnitude. The results of this work are limited due to the fact that no benchmark for ANN performance was implemented, such as a classical GED technique to compare the ANN results with. Also, only positive gross errors were simulated, which would result in a skewed distribution of measurements and constraint residuals for gross error vectors, which may be exploited by the ANN to achieve classification. It is possible that symmetric distributions resulting from including both positive and negative gross errors could result in a more problematic classification problem.

Aldrich *et al.* (1994b) applied ANN's to a two-product splitter subject to one linear and two bilinear material balance constraints, as well as a ball mill with hydrocyclone circuit subject to 8 bilinear constraints. The input vectors to the ANN's consisted of the absolute normalized constraint residuals, the absolute normalized measurement adjustments, and the measurement vector itself, respectively. For the first example, the measurement residuals were calculated as the difference between the measurements and the true values, which is impossible for practical situations. For the second example the measurement residuals consisted of the difference between the measurement and the reconciled value, which would be implementable in practice. Multiple gross errors were simulated, although again only positive gross errors were considered. A modification of the Measurement Test for multiple gross errors, discussed by Serth *et al.* (1986), was used as a benchmark for ANN performance. It was found that the ANN's performed better than the Measurement Test. It was also found that the performance of the ANN's using the constraint and measurement residuals as input vectors were robust for changes in steady-state, which is important for practical applications.

Gupta *et al.* (1993) applied ANN's to detect gross errors in a linear steam metering system first discussed by Serth *et al.* (1986). They employed different gross error magnitudes, ANN training regimes and two different strategies for handling multiple gross errors. The input vector for the ANN's consisted of normalized constraint residuals. They stated that although the detection of gross errors with both positive and negative sign is important, only positive gross errors could be used for training the ANN, as predicting the sign of a gross error is not an objective of ANN training. This logic seems questionable considering the asymmetry, with possible positive effect on classification accuracy, it introduces in the data as discussed in the previous paragraph. The GLR Test was used as a benchmark for ANN performance, and it was found that the ANN performance was slightly inferior to that of the GLR Test. The significance of this conclusion is not clear, as performance measures for multiple gross error detection was compared to each other without consideration for possible correlation between the performance measures.

5.1.3 Summary of ANN applications

ANN's have been shown to be a feasible alternative to classical DR and GED techniques. They have several desirable properties, such as fast processing or large complex systems, no assumption regarding the covariance structure of the measurement errors are required, and higher power to detect gross errors on some examples.
The structure of an ANN may be difficult to interpret though, and it can be argued that some of the simulations discussed are biased towards accurate Detection through the use of positive gross errors only. The statistical

properties of the ANN methodology are impossible to determine *a priori*, and have to be approximated through simulation. This is not necessarily a major drawback compared to classical techniques; the classical techniques rely on hypothesis testing, and the level of significance of these tests rely on accurate estimates of the covariance structure of the measurement errors, which may not be readily available and can only be determined approximately. In addition, the power of the classical techniques may be difficult to calculate for single gross errors, and even more so for multiple gross errors, so that simulation on the process under investigation in order to determine statistical power may be required for these methods as well.

Where the performance of the ANN's were compared to classical GED techniques, it is difficult to formulate a rigorous statistical interpretation of the results. It is generally assumed that differences in powers between the methodologies are statistically significant when the Type I error rates are similar but not necessarily equal, and this assumption is never verified in a rigorous manner according to the author's knowledge. Rigorous statistical inference on the difference in power between two methodologies on the same test set may be problematic. This is due to the fact that the results of two methods on the same test data can be expected to exhibit some correlation, e.g. both methods may exhibit increasing power with increasing gross error magnitude. A solution to the case where only single gross errors are present is presented later in this thesis, although it is not clear how statistical rigour can be achieved for multiple gross errors.

The relative success of ANN's in solving the Detection problem raises the question regarding the applicability of other classification methodologies to the Detection and Identification problems. The methods may use the constraint residuals and measurement adjustments resulting from DR in a similar manner to ANN's in solving the Detection and Identification problems, although they may not be applicable in resolving the DR problem itself. The methods investigated in this study, i.e. Classification Trees and Linear and Quadratic Classification Functions, are discussed in the sections that follow.

5.2 CLASSIFICATION TREES

5.2.1 Introduction to Classification Trees

As an introduction to the general classification problem, a hypothetical, illustrative example is presented. Figure 5-2 presents hypothetical data for two classes in two-dimensional (2D) space:

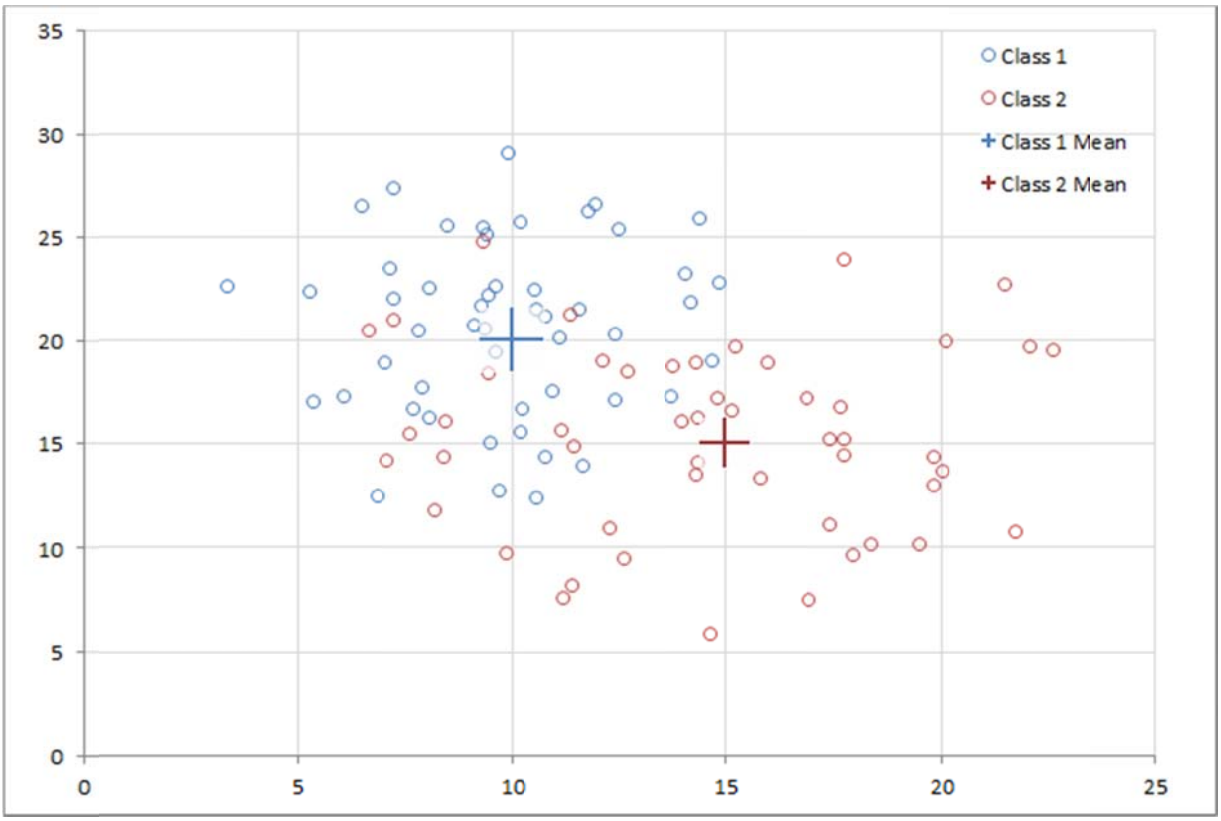

Figure 5-2 : Hypothetical Classification Problem – Raw Data

The crosses represent means for the two classes, and the blue and red dots are randomly generated points around the respective means. The task of a classifier is to assign a new observation to one of the classes based on its position in 2D space. The classification rule must be inferred from the data with known class membership. In general, class separation is not distinct on the input space. This may be due to measurement error in the observations, or due to true overlap in some variables between classes. Therefore, perfect classification is in general not feasible.

A binary classification tree accomplishes this task by iteratively partitioning the 2D space into disjoint regions so that with each partition the class membership of each region becomes more 'pure', where different definitions of purity can be employed, as will be discussed later in this section. The final structure of the

classification tree depends on several factors as will be discussed later in this section – the optimal tree for this example grown with default settings in Matlab ® is presented in Figure 5-3:

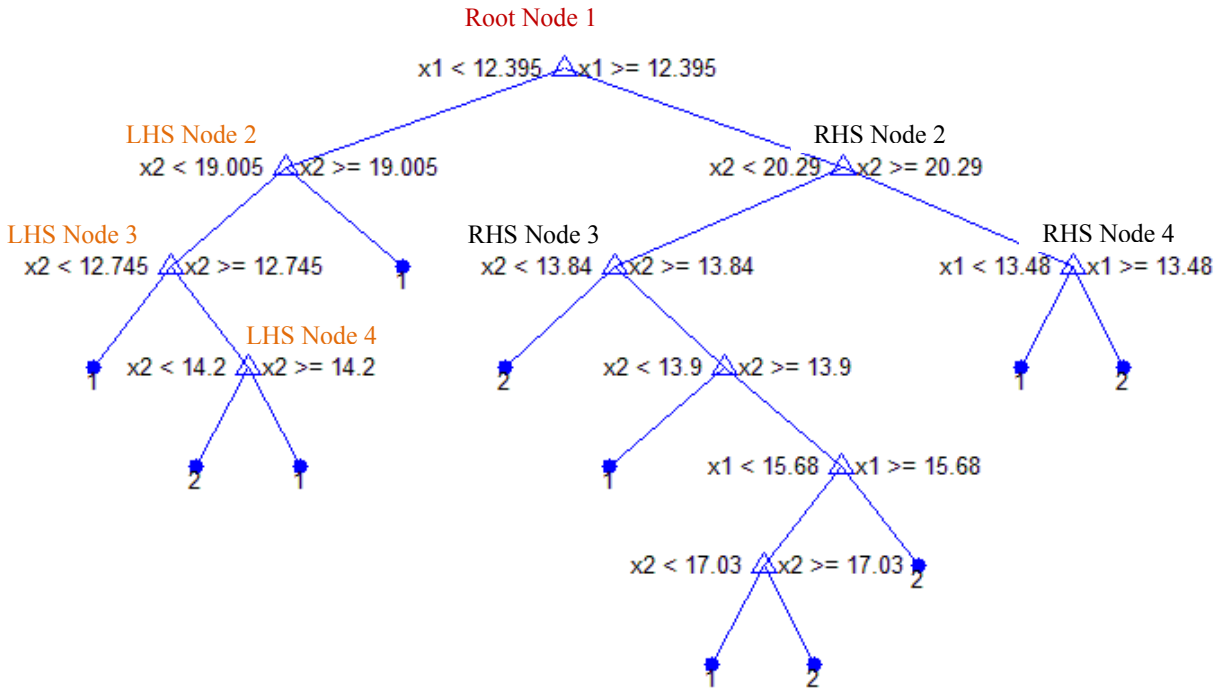

Figure 5-3 : Example - Binary Classification Tree

The classification tree consists of several nodes; the first node is called the 'root' node, nodes where subsequent partitions are defined are called 'branch' nodes, and the terminal nodes where classification is defined are called 'leaf' nodes. Each branch node contains a splitting rule on one of the variables of the input space so that an input vector is uniquely assigned by the branch node to subsequent nodes of the tree. The determination of the split variable and split value for each branch node, the termination and pruning criteria used to determine when splitting should cease, and subsequent class assignment rules for leaf nodes will all be discussed in this section.

The first 4 splits for each side (left hand side: LHS and vice versa for RHS) of the tree in Figure 5-3 is presented on the input space in Figure 5-4:

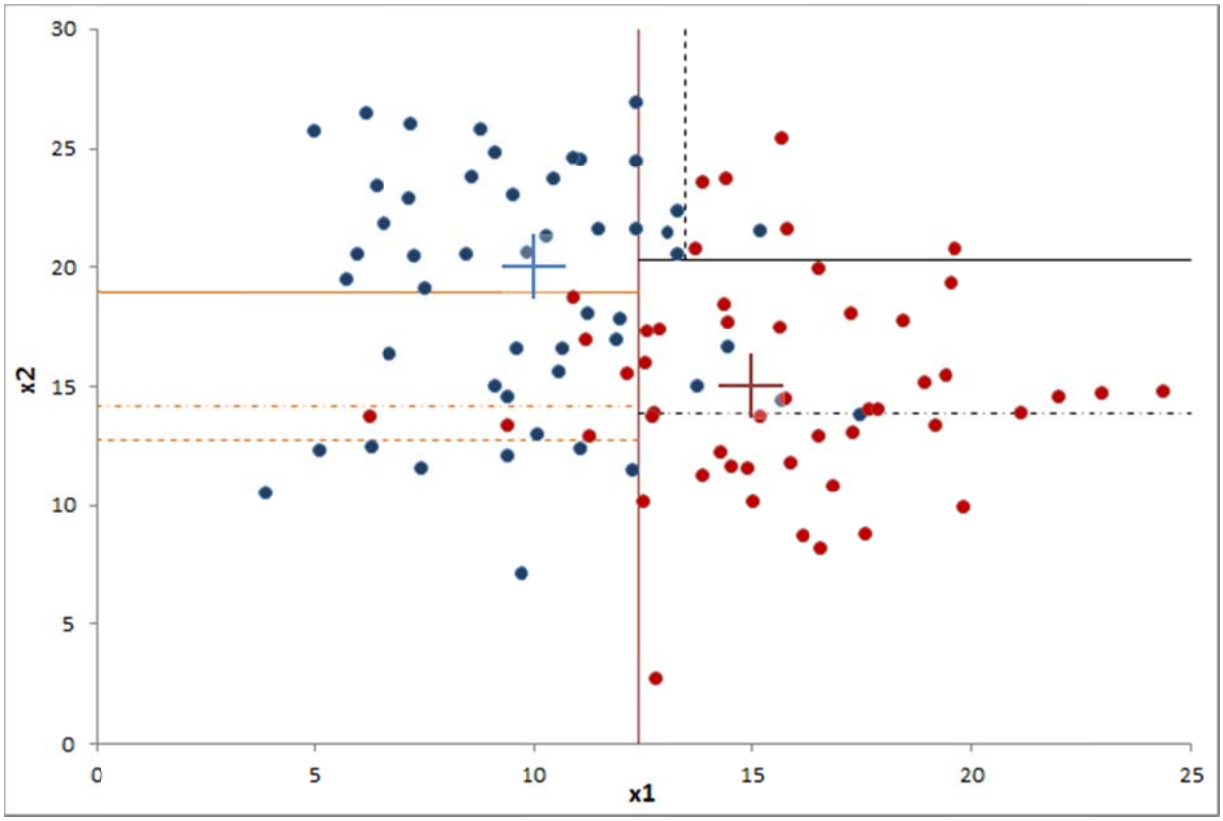

Figure 5-4 : Classification Example - Selected Partitions for Classification Tree Example

The rectangular nature of the partitioning achieved by a binary classification tree is obvious. The red line represents the partition of the root node, the orange lines successive partitions down the LHS of the tree, and black lines some successive partitions down the RHS of the tree.

Inspection of the class membership data in Figure 5-2 leads to an intuitive conclusion that the classes may be well-separated by a linear diagonal boundary. This illustrates one of the weaknesses of the binary classification tree: when the class boundaries are not rectangular with respect to the input space, complicated tree structures with many rectangular splits may arise.

The relevant theory regarding classification tree construction will be presented in the sections that follow.

5.2.2 Background to Classification Trees

Breiman *et al.* (1984) develop their discussion of Classification Trees as being one of a subset of statistical methods called *classifiers*.

They start by defining a measurement space *X*, a set of J classes $C = \{1, 2, ..., J\}$, and defines the classification problem as that of finding a function *d*(***x***) that assign a class J to each measurement vector **x** in *X*, i.e. $\forall \mathbf{x} \in X$, $d(\mathbf{x}) \in C$. The classifier partitions the measurement space into J disjoint subsets A_j, so that $X = \bigcup_j A_j$, where each A_j is associated with a particular class J. Construction of a classifier is typically based on a learning sample *L* containing N vectors or cases from *X*, where the class of each **x** in *L* is known *a priori*.

The notation for classification trees depicts the tree classifier as *T*, with *t* depicting an individual node of the tree. Every *t* in *T* represents a subset of *X*, with the root node $t_1 = X$.

Breiman *et al.* [1984: 56) lists several advantageous properties of classification trees over other classification methods:

1. It can be applied to any data structure.
2. It is easy to store, use and interpret.
3. It makes use of conditional information in handling non-homogenous relationships, where the form of the classifier may be different on different partitions of the measurement space.
4. It does automatic stepwise variable selection and complexity reduction
5. It gives an estimate of misclassification rate without any additional analytical effort
6. For standard data structure, where all vectors in the measurement space have the same dimension, the classification tree is invariant under all monotone variable transformations
7. It is robust with respect to outliers and misclassified learning samples

5.2.3 Constructing Binary Classification Trees

According to the terminology Breiman *et al.* (1984) uses for describing classification tree structure, a node of the tree is equivalent to or associated with a subset of the measurement space *X*. The first, or root node, of the tree is equivalent to *X*.

Breiman *et al.* (1984: 28) define the basic classification tree construction algorithm to consist of 4 elements:

1. A set *S* of candidate splits.
2. A goodness of split criterion
3. A rule to stop splitting
4. A rule for assigning a class to each terminal node of the tree

They later report that the stop-splitting rule alone is insufficient, and has to be augmented with a pruning algorithm to find optimal trees (Breiman *et al.*, 1984: 37).

5.2.3.1 Candidate Splits

Breiman *et al.* (1984) describe the elements in *X* as vectors $\mathbf{x} = (x_1, x_2, ..., x_M)$, where the x_m can be ordered variables taking on any real value, or categorical variables that take on values from some finite set $\{b_1, b_2, ..., b_L\}$.

Candidate splits for a node in the classification tree are of the form [Breiman *et al.*, 1984: 29):

1. $x_m \leq c;\ c \in (-\infty, \infty)$ for ordered variables
2. $x_m \in P;\ P \subseteq \{b_1, b_2, ..., b_L\}$ for categorical variables

The above splits result in a rectangular division of the learning space. Breiman *et al.* (1984: 132) points out that in some problems classes may be separated by hyperplanes not perpendicular to the axis, in which case the basic splits will result in large, difficult to interpret trees. A possible improvement is incorporating linear combinations of variables as candidate splits:

3. $\sum_m a_m x_m < c, c \in (-\infty, \infty)$

The coefficients a_m have the property $\|\mathbf{a}\|^2 = \sum_m a_m^2 = 1$. A search algorithm for finding the best candidate split of linear combinations is described. Breiman *et al.* (1984: 134) note two problems with using splits based on linear combinations of the ordered variables:

- The tree topology is no longer invariant under monotone transformations of the variables
- The resulting tree topology is difficult to interpret

It is also possible to construct splits based on Boolean combinations of variables (Breiman *et al.*, 1984: 136). To reduce computational burden and tree complexity, only splits of the following form is considered:

4. $(s_{m_1} \cap s_{m_2} \cap .... \cap s_{m_h}) = \{Is\, x_{m_1} \in P_1\, and\, x_{m_2} \in P_2\, and\, ...and\, x_{m_h} \in P_{m_h}\}$

Breiman *et al.* (1984: 138) also describe the use of *features*, or real valued functions of the original variables, in construction of candidate splits. They note that this has most utility when:

- The original data is high dimensional with little useable information in the individual coordinates
- Inspection of the learning sample points to the utility of using features.

Breiman *et al.* (1984: 140) describe the use of surrogate splits for handling missing data. A surrogate split is a non-optimal split that best predicts the action of the optimal split for a node in the tree. Surrogate splits can also be used to determine the relative importance of variables to tree topology (Breiman *et al.*, 1984: 144).

5.2.3.2 Goodness of Split Criteria

Breiman *et al.* (1984: 32) describe the purity of a node in the classification tree as being a function of the proportions $p(j|t)$ of the different classes associated with the subspace of *X* present in the node. They state that this impurity function $\phi(\cdot)$ should have the following properties:

1. $\phi(\cdot)$ is nonnegative
2. $\phi(\cdot)$ reaches its maximum when all the node proportions are equal to $1/J$
3. $\phi(\cdot)$ is zero when any node proportions equals unity, i.e. when only one class is present in the node.
4. $\phi(\cdot)$ is symmetric

Breiman *et al.* (1984: 100) describes another desirable property of the impurity function, which is that it should have a continuous second derivative, and be concave, that is:

5. $\phi''(\cdot)$ exists, and $\phi''(\cdot) < 0$

The impurity of a node $i(t)$ is then equivalent to the value that the impurity function assumes, given the proportion of classes in the node. The goodness of split for a given split *s* from the set of all candidate splits *S* is then defined as the weighted decrease in impurity of the descendant nodes relative to the parent node:

$$\Delta i(s,t) = i(t) - p_L \cdot i(t_R) - p_R \cdot i(t_L) \tag{5.1}$$

where: p_L and p_R are the proportion of cases in *t* reporting to the descendant nodes t_L and t_R respectively.

One candidate impurity function is the Gini Index of Diversity, where:

$$i(t) = \sum_{i \neq j} p(i|t) \cdot p(j|t) \tag{5.2}$$

Another candidate 'goodness of split' criterion is the Twoing Rule; the best split is selected based on maximising the expression given by:

$$\frac{p_L \cdot p_R}{4} \left[\sum_j \left| p(j|t_L) - p(j|t_R) \right| \right]^2 \tag{5.3}$$

Where: p_L indicate the proportion of vectors in *t* reporting to the left descendant node t_L, and vice versa for p_R .

Breiman *et al.* (1984: 103-111) discuss various aspects of the Gini Index and Twoing Rule. They note that trees constructed using the two rules have very similar structure, and is often identical. They do state a preference for the Gini Index, based on empirical observation regarding the splits selected.

Breiman *et al.* (1984: 35) also describes the use of a misclassification cost function for evaluating the goodness of split. The misclassification cost $C(i|j)$ is defined as the cost of classifying a vector as class *i*, given that its true class category is *j*. The misclassification cost has the following properties:

1. $C(i|j) \geq 0$, $i \neq j$
2. $C(i|j) = 0$, $i = j$

5.2.3.3 Stop-Splitting Rules and Pruning Algorithms

Breiman *et al.* (1984: 33) describes a naive termination rule that would declare a node terminal if some threshold for decrease in node impurity was not achieved, i.e for some constant β, declare a node *t* terminal if:

$$\max_{s \in S} \Delta i(s,t) < \beta \tag{5.4}$$

Breiman *et al.* (1984: 61) report that termination rules alone, such as the one above, produce unsatisfactory results in general. Too small a value for β will lead to large, over-fitted trees, and too large a value will result in smaller tress that does not make use of all the information in the learning sample *L*.

A different approach to the termination rule is to grow a large tree, and prune it upwards in order to find the tree that minimizes the estimated misclassification cost (Breiman *et al.*, 1984, 62).

5.2.4 Class Assignment Rules

The plurality rule assigns the class of a terminal node to the class with the highest proportion of cases in that terminal node:

$$j^*(t) = j_0;\ if\ \ p(j_0|t) = \max_j p(j|t) \tag{5.5}$$

The misclassification cost function $C(i|j)$ can also be used. In this case, a node is assigned a class $j^*(t) = i_0$ if i_0 minimizes the expression:

$$\sum_j C(i|j) \cdot p(j|t) \tag{5.6}$$

5.2.5 Estimating Classification Accuracy

Breiman *et al.* (1984) denote the true misclassification rate of a classifier *d*(***x***) as R*(*d*). For an input-output pair $(\mathbf{x}, y)$ on the space $X \times C$ they define the probability $P(A, j) = P(\mathbf{x} \in A, y = j);\ A \subset X,\ j \in C$, so that the misclassification rate becomes formally:

$$R^*(T) = P(T(\mathbf{x}) \neq y) \tag{5.7}$$

The misclassification rate is therefore the probability that a particular element drawn from the measurement space *X* will be assigned to the wrong class by the classifier.

They also note that since the structure of a classifier *T* depends on the learning sample *L* used to construct it, the misclassification rate is dependent on the learning sample used.

5.2.5.1 Re-substitution Estimate

The re-substitution estimate is obtained by running all the elements of the learning sample through the classifier after it has been constructed, and taking the proportion of elements misclassified as an estimate of R*(*d*).

Breiman *et al.* (1984) defines an indicator function in order to express the above formally:

$$i(\cdot) = \begin{cases} 1 \ ; \ \text{if the function argument is True} \\ 0 \ ; \ \textit{otherwise} \end{cases} \tag{5.8}$$

The re-substitution estimate is then:

$$R(T) = \frac{1}{N} \sum_{n=1}^{N} i(T(\mathbf{x}_n) \neq j_n) \tag{5.9}$$

They note that the re-substitution estimate may be seriously biased, as it is estimated from the same data used to construct the classifier. Since the classification algorithm inherently tries to minimize the misclassification of elements in the learning sample, the re-substitution estimate could be overly optimistic when used to estimate the true misclassification rate.

5.2.5.2 Test Sample Estimate

Breiman *et al.* (1984) describes a method of dividing the elements of the learning sample randomly into two sub-samples, L_1 and L_2, often with a 2/3, 1/3 split, so that N_1 of the samples in *L* report to L_1 and N_2 of the cases in *L* to L_2. The L_1 sub-sample is used for construction of the classifier, while the smaller sub-sample is used to estimate the misclassification rate in the usual way:

$$R^{ts}(T) = \frac{1}{N_2} \cdot \sum_{(\mathbf{x}_n, j_n) \in L_2} i(T(\mathbf{x}_n) \neq j_n) \tag{5.10}$$

The benefit of this method is that the estimate of R*(*d*) obtained is independent of the learning sample used for construction of the classifier. The method has the drawback that not all available data is used to construct the classifier, which could impact on the structure of the classifier.

5.2.5.3 Cross Validation Estimate

Cross validation takes the concept of a test sample and applies it to multiple subsets of the learning sample. The learning sample L is divided into a number of v disjoint subsets of approximately equal size L_1, L_2, ..., L_v. For each L_k, containing N_k learning samples, a classifier is constructed on L-L_k, and an estimate of the misclassification rate is obtained:

$$R^{(k)}(T^{(k)}) = \frac{1}{N_k} \sum_{(\mathbf{x}_n, j_n) \in L_k} i(T^{(k)}(\mathbf{x}_n) \neq j_n) \tag{5.11}$$

The average misclassification rate over all v sets is use as an estimate for R*(d):

$$R^{CV}(T) = \frac{1}{v} \sum_{k=1}^{v} R^{(k)}(T) \tag{5.12}$$

Breiman *et al.* (1984) state that the assumption behind this method is that the classifier is stable over the learning space, meaning the classifiers $d^{(k)}(\cdot)$ all have misclassification rates approximately equal to R*(d).

Breiman *et al.* (1984: 114) describe the impact of the misclassification cost function $C(i|j)$ and the assumed prior probabilities π_j on the estimated classification accuracy. The prior probabilities π_j can be interpreted as the probability that a case from the learning sample belonging to class j will be presented to the classifier (Breiman *et al.*, 1984: 28). The priors can be estimated from the data as $\pi_j = N_j / N$ or be supplied by the analyst to manipulate the misclassification rate of individual classes as desired (Breiman *et al.*, 1984: 112).

The assumed priors combined with the misclassification cost function impacts on the estimated misclassification cost:

$$R(T) = \sum_{i,j} C(i|j) \cdot Q(i|j) \cdot \pi_j \tag{5.13}$$

Where $Q(i|j)$ is the probability that a case belonging to class j will be classified as class i.

5.2.6 Finding the Optimal Tree

Breiman *et al.* (1984:63) describes the first step of finding the optimal tree as growing a very large tree in which all terminal nodes are either:

- Small, with few, or possibly only one, learning vectors falling in the node
- Pure, with all learning vectors in the node having the same assigned class
- Have identical learning vectors, so that no further partioning of the node is possible

To guarantee a sufficiently large initial tree T_{max}, a number N_{min} is specified, so that all terminal nodes in T_{max} must contain terminal nodes with $N(t) \leq N_{\max}$.

Breiman *et al.* (1984: 65) state that a selective pruning procedure is necessary, due to the large number of possible pruning paths to the root node in a large classification tree. The pruning algorithm starts with the initial tree T_{max}, and prune upwards until the root node t_1 is reached, so that at each stage of pruning R(T) is minimized, where R(T) is the re-substitution estimate for the misclassification cost for the resultant tree. Breiman *et al.* states that the re-substitution estimate is a poor estimate for the true misclassification rate, but that it is sufficient for use in the pruning algorithm.

Breiman *et al.* (1984:65) uses the following objective function for their pruning algorithm:

$$R_\alpha(T) = R(T) + \alpha \cdot \left|\tilde{T}\right| \tag{5.14}$$

Where: $\left|\tilde{T}\right|$ is the number of terminal nodes in T, and α is a positive real number they call the 'complexity cost per terminal node'. The pruning procedure consists of finding the sub-tree of T_{max} that minimizes $R_\alpha(T)$ for every value of α:

$$R_\alpha(T(\alpha)) = \min_{T \prec T_{\max}} R_\alpha(T) \tag{5.15}$$

Breiman *et al.* (1984: 67) state that although α is a continuous variable, there are at most a finite number of sub-trees of T_{max}. For small values of α, the optimal sub-trees will be large, and will decrease with increasing α due to the higher cost associated with the number of terminal nodes, until the root node t_1 is reached. Breiman *et al.* (1984: 70) provides a proof that the sequence of minimal sub-trees constructed by the above method forms a nested sequence, i.e.:

$$T_1 \succ T_2 \succ .... \succ \{t_1\} \tag{5.16}$$

The Test Sample or Cross Validation methods are then used on the sequence of sub-trees $T_1 \succ T_2 \succ .... \succ \{t_1\}$ to get improved estimates of the true misclassification cost of each tree.

A natural choice for the optimal sub-tree would be that tree in the sequence $T_1 \succ T_2 \succ .... \succ \{t_1\}$ that has minimum estimated misclassification cost. Breiman *et al.* (1984: 79) states that typically the optimal level of pruning is ill defined, and that tree selection based on the above method would be sensitive to small changes in the learning sample.

They suggest choosing the smallest sub-tree that has a misclassification cost within one standard error of the minimum estimated misclassification cost. For the Test Sample method, with priors estimated from the learning sample proportions, and unit cost of misclassification, the standard error of the estimated misclassification cost is derived from the binomial distribution:

$$SE(R^{ts}(T)) = \sqrt{\frac{R^{ts}(T) \cdot (1 - R^{ts}(T))}{N_2}} \qquad (5.17)$$

Where: N_2 is the number of vectors in the test sample.

Breiman *et al.* (1984: 78) state that standard statistics can be derived for the Test Sample method, but that the probabilistic formulation of the Cross Validation estimate of R*(T) is complex, and the standard error for Cross Validation estimates are therefore heuristic in nature.

5.3 DISCRIMINANT ANALYSIS AND CLASSIFICATION FUNCTIONS

Rencher (2002: 270) describes two possible objectives for discriminant analysis:

1. Characterizing separation between distinct groups
2. Classifying observations into distinct groups

The role of discriminant analysis in gross error detection and identification relates primarily to the second objective.

5.3.1 Introduction to Discriminant and Classification Functions

As an illustration of the differences between discriminant analysis and classification trees, a linear and quadratic classification rule was developed for the same hypothetical data presented in Section 5 for the classification tree methodology. The classification boundaries are presented in Figure 5-5

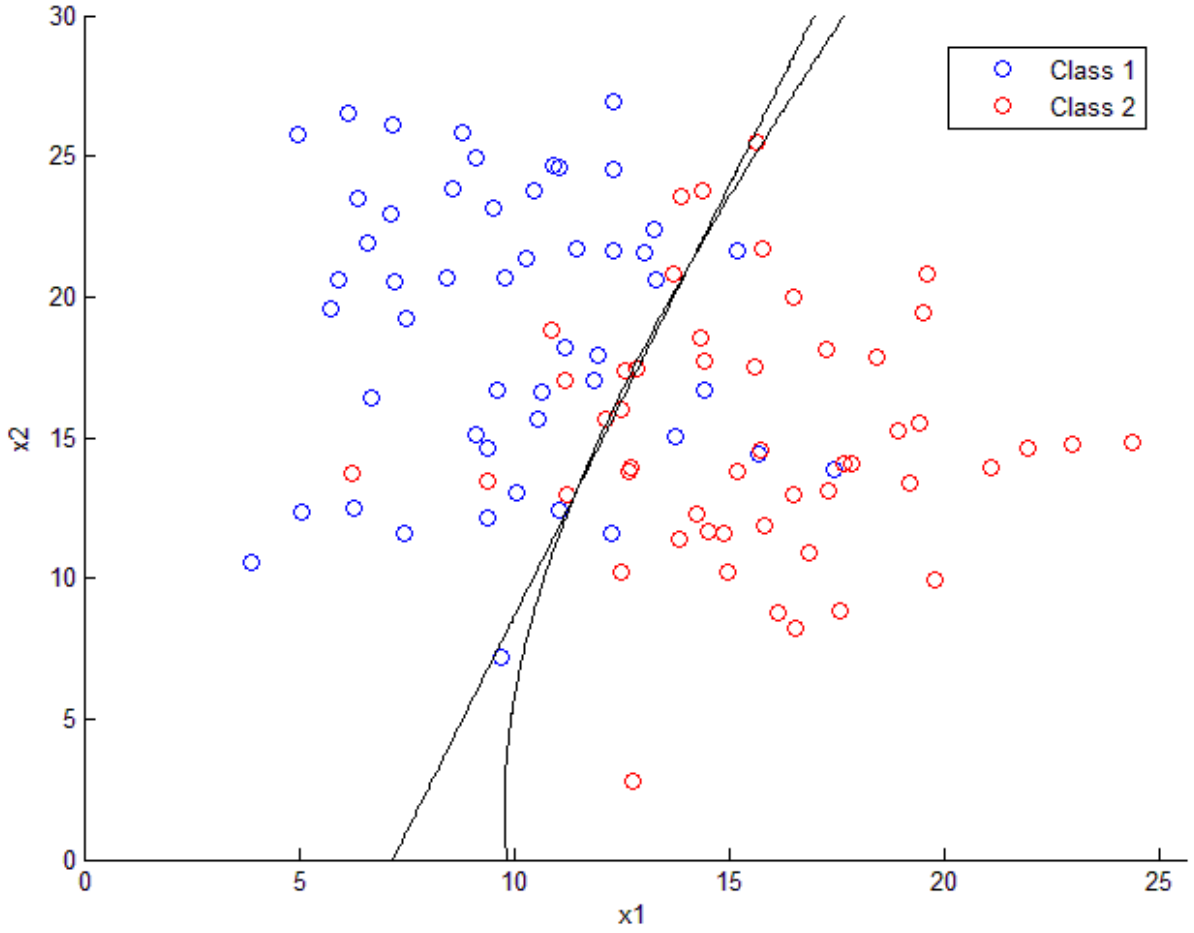

Figure 5-5 : Classification Example – Partition of Linear and Quadratic Classification Functions

The straight line represents the classification boundary for a linear classification function, and the curved black line represents the same for a quadratic classification function. The boundaries represent the location where an

observation would be equally far from the sample means, based on the measures of distance employed by the classification functions. The classification functions resulted in a different type of partitioning of the input space in order to affect classification as opposed to the tree methodology. The relevant theory with regards to classification functions will be presented in the following sections.

5.3.2 Classification for Two Groups

Given two sets of sample vectors with known group membership, i.e. $\mathbf{x}_{1,i}$, $i = 1, 2, ..., n_1$ from G_1 and $\mathbf{x}_{2,j}$, $j = 1, 2, ..., n_2$ from G_2, where G_1 and G_2 correspond to two distinct groups or populations, the objective is to find a vector of coefficients $\mathbf{a}$ such that the standardized separation between the mean vectors are maximised, i.e.:

$$\max_{\mathbf{a}} \frac{[\mathbf{a}^T(\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2)]^2}{\mathbf{a}^T S\, \mathbf{a}} \tag{5.18}$$

Where: $\bar{\mathbf{x}}_1 = {}^{1}\!/_{n_1} \cdot \sum_{i=1}^{n_1} \mathbf{x}_{1,i}$, $\bar{\mathbf{x}}_2 = {}^{1}\!/_{n_2} \cdot \sum_{i=1}^{n_2} \mathbf{x}_{2,i}$, and S is the pooled covariance matrix. The pooled covariance matrix S is calculated from the two sample covariance matrices S_1 and S_2:

$$S = \frac{[(n_1 - 1) \cdot S_1 + (n_2 - 1) \cdot S_2]}{n_1 + n_2 - 2} \tag{5.19}$$

The sample covariance for each group is given by:

$$S_k = \frac{1}{n_k - 1} \sum_{i=1}^{n_k} (\mathbf{x}_{k,i} - \bar{\mathbf{x}}_k)^T (\mathbf{x}_{k,i} - \bar{\mathbf{x}}_k); \quad k = 1, 2 \tag{5.20}$$

Rencher (2002: 271) states that (5.18) is maximised when:

$$\mathbf{a} = S^{-1}(\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2) \tag{5.21}$$

It is important to note that the coefficient matrix $\mathbf{a}$ is obtained from sample vectors with known group affiliation, i.e. a training set. Once the coefficient matrix has been obtained in this way, a classification rule can be constructed for classifying vectors with unknown group affiliation. Assuming prior probabilities p_1 and p_2 can be associated with the two populations corresponding to Group 1 and Group 2 respectively, a classification rule for two groups can be formulated as (Rencher, 2002: 302):

$$\begin{aligned} \mathbf{a}^T \cdot \mathbf{x} &> \frac{1}{2}(\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2)^T S^{-1}(\bar{\mathbf{x}}_1 + \bar{\mathbf{x}}_2) + \ln\left(\frac{p_2}{p_1}\right) \Rightarrow \mathbf{x} \in G_1 \\ \mathbf{a}^T \cdot \mathbf{x} &< \frac{1}{2}(\bar{\mathbf{x}}_1 - \bar{\mathbf{x}}_2)^T S^{-1}(\bar{\mathbf{x}}_1 + \bar{\mathbf{x}}_2) + \ln\left(\frac{p_2}{p_1}\right) \Rightarrow \mathbf{x} \in G_2 \end{aligned} \tag{5.22}$$

This rule ensures that the weighted distance between $\mathbf{x}$ and the mean vector of the group it is assigned to is a minimum.

5.3.3 Classification for Multiple Groups

5.3.3.1 Linear Classification Functions

When *k* population G_k are considered simultaneously, the classification principle remains that a vector $\mathbf{x}$ with unknown group membership is assigned to the group that has a mean vector closest to $\mathbf{x}$ (Rencher, 2002: 304)

A training sample of vectors with known group affiliation $\mathbf{x}_{i,j};\ i=1,2,...,k;\ j=1,2,....,n_k$ is required so that estimates of the mean group vectors $\bar{\mathbf{x}}_i;\ i=1,2,....,k$ can be obtained. The pooled covariance estimate S is estimated from:

$$S=\frac{1}{N-k}\sum_{i=1}^{k}(n_i-1)S_k \tag{5.23}$$

The pooled covariance S is an estimate of the population covariance matrix, and its use in the classification function implies that all groups have a common covariance matrix, that is:

$$E(S)=E(S_1)=E(S_2)=....=E(S_k) \tag{5.24}$$

Where: $N=\sum_{i=1}^{k}n_i$ and S_k is the sample covariance matrix from (5.20). The distance from $\mathbf{x}$ to each $\bar{\mathbf{x}}_i$ is estimated with a distance function:

$$D_i^2(\mathbf{x})=(\mathbf{x}-\bar{\mathbf{x}}_i)^T S^{-1}(\mathbf{x}-\bar{\mathbf{x}}_i) \tag{5.25}$$

Rencher (2002: 304) shows with simple algebra that selecting the minimum of (5.25) is equivalent to selecting the maximum of a linear classification function of the form:

$$L_i(\mathbf{x})=\mathbf{c}_i^T\cdot\mathbf{x}+c_{i,0} \tag{5.26}$$

Where: $\mathbf{c}_i=\bar{\mathbf{x}}_i^T S^{-1}$ and $c_{i,0}=-\frac{1}{2}\bar{\mathbf{x}}_i^T S^{-1}\bar{\mathbf{x}}_i$. When prior probabilities $p_i;\ i=1,2,....,k$ are associated with each group, the classification rule in (5.26) becomes:

$$L_i(\mathbf{x})=\mathbf{c}_i^T\cdot\mathbf{x}+c_{i,0}+\ln(p_i) \tag{5.27}$$

Rencher (2002: 305) distinguishes between a linear classification function and a linear discriminant function. Where the first uses a measure of distance to allocate a vector to a group or class, the second describes the separation of classes on the input space. For the two-class case, the two approaches are equivalent, however for more than two classes, it is necessary to distinguish between a discriminant and a classification function.

5.3.3.2 Quadratic Classification Functions

The use of a linear classification function implies that the groups all have the same covariance matrix. When this is not true, the distance function in (5.25) can be modified by replacing the pooled estimate of the covariance matrix with the sample estimate of the group covariance matrix:

$$D_i^2(\mathbf{x}) = (\mathbf{x} - \overline{\mathbf{x}}_i)^T S_i^{-1} (\mathbf{x} - \overline{\mathbf{x}}_i) \tag{5.28}$$

The classification rule remains to assign a vector **x** with unknown group affiliation to that group for which (5.28) is a minimum. This classification rule is a quadratic function in **x**, and hence is called a quadratic classification function (Rencher, 2002: 306).

If it is assumed that the $\mathbf{x}_{i,j}$ follow multivariate normal distributions, and that each group has a known prior probability p_i, $i = 1, 2, ..., k$, the optimum classification rule is to assign **x** to the group that maximises:

$$Q_i = \ln(p_i) - \frac{1}{2}\ln|S_i| - \frac{1}{2}(\mathbf{x} - \overline{\mathbf{x}}_i)^T S_i^{-1} (\mathbf{x} - \overline{\mathbf{x}}_i) \tag{5.29}$$

6 PRINCIPAL COMPONENT ANALYSIS

The objective of discriminant analysis as discussed in the previous section is to find a linear combination of the variables $\mathbf{x}_{i,j}$ that maximize the separation between the mean vectors $\bar{\mathbf{x}}_i$ of different groups.

Principal component analysis (PCA) differs from discriminant analysis in that no grouping is assumed in the variables, i.e. $k = 1$. The objective of principal component analysis is to find a new set of orthogonal coordinate axis, centred at the location of the mean sample vector in the original coordinate system, such that the maximum variance possible is contained on each axis of the new coordinates. The first principle component is the linear combination of the variables with maximum variance, i.e. the dimension that maximally separate the individual variables; the second principal component is the dimension with maximal variance in a direction perpendicular to the first principal component, and so on (Rencher, 2002: 380).

PCA may be useful as a visualization tool. PCA was performed on the input space of the hypothetical classification example used in the sections on classification trees and discriminant analysis. The PCA scores are presented in Figure 6-1:

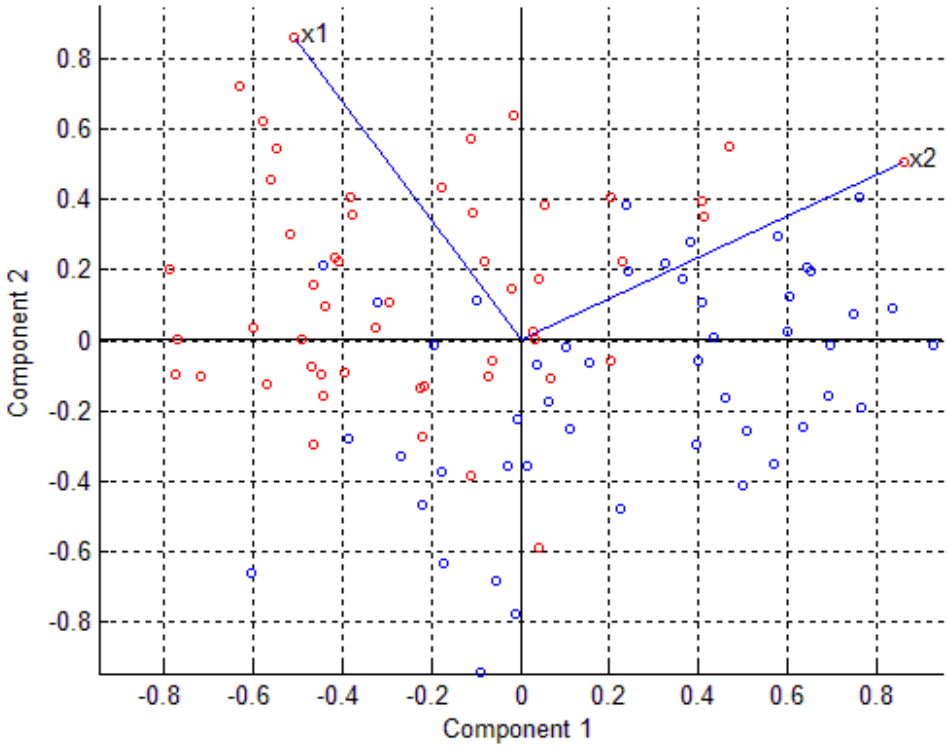

Figure 6-1 : Classification Example - PCA Scores and Coefficients

The PCA scores are plotted separately for the two classes (blue and red circles). The separation between the two classes can be seen in the principle component space. In addition, the contribution of each of the original variables to the respective principle components is visualized by plotting of the PCA coefficients (blue lines).

The directions of the new set of coordinate axis are obtained from the eigenvectors of the sample covariance matrix given by Equation (5.20) for a single group:

$$S = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{x}_i - \overline{\mathbf{x}})^T(\mathbf{x}_i - \overline{\mathbf{x}}) \tag{6.1}$$

The coefficient vectors $\mathbf{a}_j$ are then all the non-zero vectors such that:

$$(S - \lambda_j I)\mathbf{a}_j = \mathbf{0} \tag{6.2}$$

Each coefficient vector $\mathbf{a}_j$ has associated with it an eigenvalue λ_j of the covariance matrix *S*. The covariance matrix *S* may be singular, in which case some of the eigenvalues will be zero. In general, if the dimensionality of the original variables is *p*, then *s* nonzero eigenvalues with associated eigenvectors may be found, where $s \leq p$. The original (centred) variables $\mathbf{x}_i;\ i = 1,2,...,n$ can be transformed to variables $\mathbf{z}_i,\ i = 1,2,....,n$ in the new coordinate system through multiplication with an orthonormal matrix (Rencher, 2002: 381):

$$\mathbf{z}_i = A \cdot \mathbf{x}_i;\ i = 1,2,...,n \tag{6.3}$$

Where:

$$A = \begin{bmatrix} \mathbf{a}_1^T \\ \mathbf{a}_2^T \\ \vdots \\ \mathbf{a}_s^T \end{bmatrix} \tag{6.4}$$

And the coefficient vectors $\mathbf{a}_i$ have been normalized such that:

$$\mathbf{a}_j^T \cdot \mathbf{a}_j = 1;\ j = 1,2,...,s \tag{6.5}$$

Since the coefficient matrix *A* is orthonormal, the distances between observations in the new coordinate system is preserved. For instance, the distance to the origin (Rencher, 2002: 381):

$$\mathbf{z}_i^T\mathbf{z}_i = (A\mathbf{x}_i)^T(A\mathbf{x}_i) = \mathbf{x}_i^T A^T A\mathbf{x}_i = \mathbf{x}_i^T\mathbf{x}_i \tag{6.6}$$

The covariance matrix of the transformed variables $\mathbf{z}_i$ is given by (Rencher, 2002: 382):

$$S^z = ASA^T = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_s \end{bmatrix} \tag{6.7}$$

That is, the variances of the components of the transformed variables are given by the eigenvalues of the covariance matrix of the original variables, and the transformed variables are uncorrelated. The eigenvalues and associated eigenvectors are usually arranged such that $\lambda_1 > \lambda_2 > ... > \lambda_s$. This allow the principal components to be used as a device to reduce dimensionality of the original sample, by retaining only k principal components instead of p original dimensions, where $k < p$. The proportion of the original sample variance contained in the k retained principal components is given by Rencher, 2002: 383):

$$tr(S^{z,k}) = \frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{s} \lambda_i} \tag{6.8}$$

Principal components may have a variety of applications; in this thesis principal components are used as an aid to visualizing the distribution of the input variables, by reducing the high dimensional input space into subspaces that contains the maximum variance possible, without distorting the distances between individual data points. As mentioned before, the distance between individual observations is preserved in the principal component space. Therefore, if data points appear dispersed when projected onto a subspace formed by principal components, they truly are dispersed, however observations that appear to be close together may be separated in a higher dimension that is not apparent in the projection onto the principal component subspace.

7 CASE STUDY METHODOLOGY

7.1 OVERVIEW

In order to compare the Classification approach with a classical GED method, it is necessary to test the performance of both methods on a common data set. It is desirable that this common data set be generated through simulation so that the true process values, as well as properties of the random error, and location and magnitude of any gross errors are exactly known. This is impossible for data obtained from real process systems, hence the need for a simulated data set.

The basic outline of the case study methodology is presented in Figure 7-1:

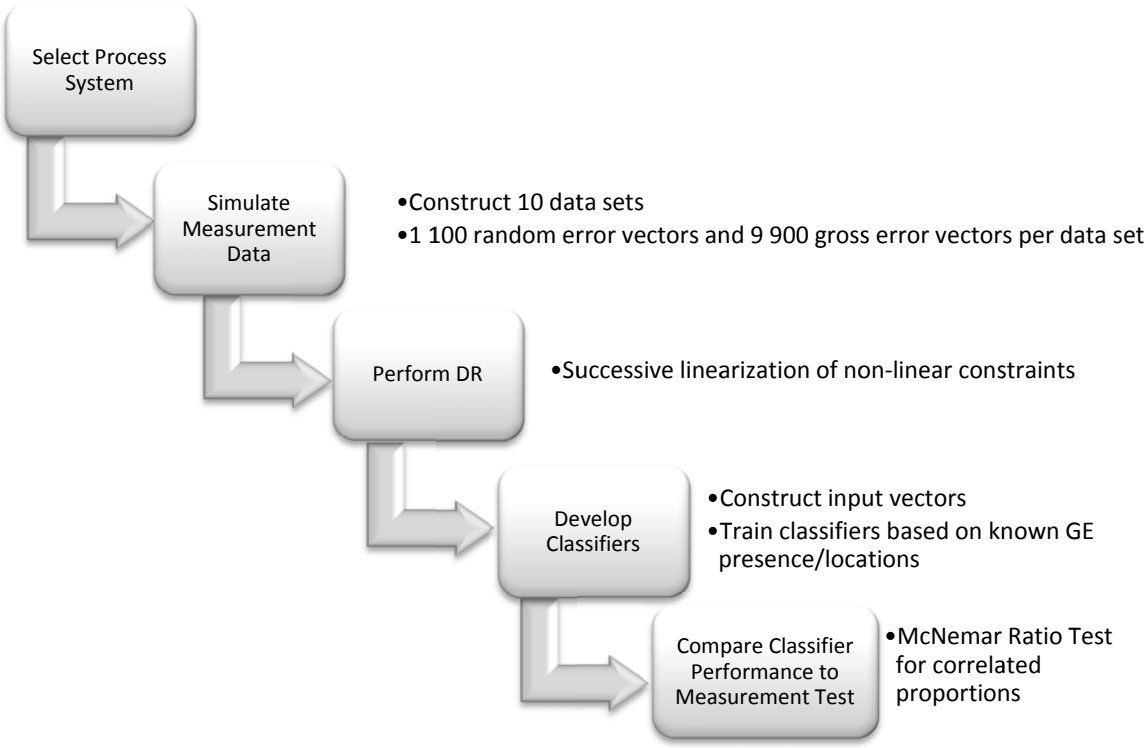

Figure 7-1 : Overview of Case Study Methodology

The sections that follow will discuss and provide details on the elements of the case study methodology outlined in Figure 7-1.

7.2 THE PROCESS SYSTEM

The system used in this study is a generic two-product splitter, as shown in Figure 7-2:

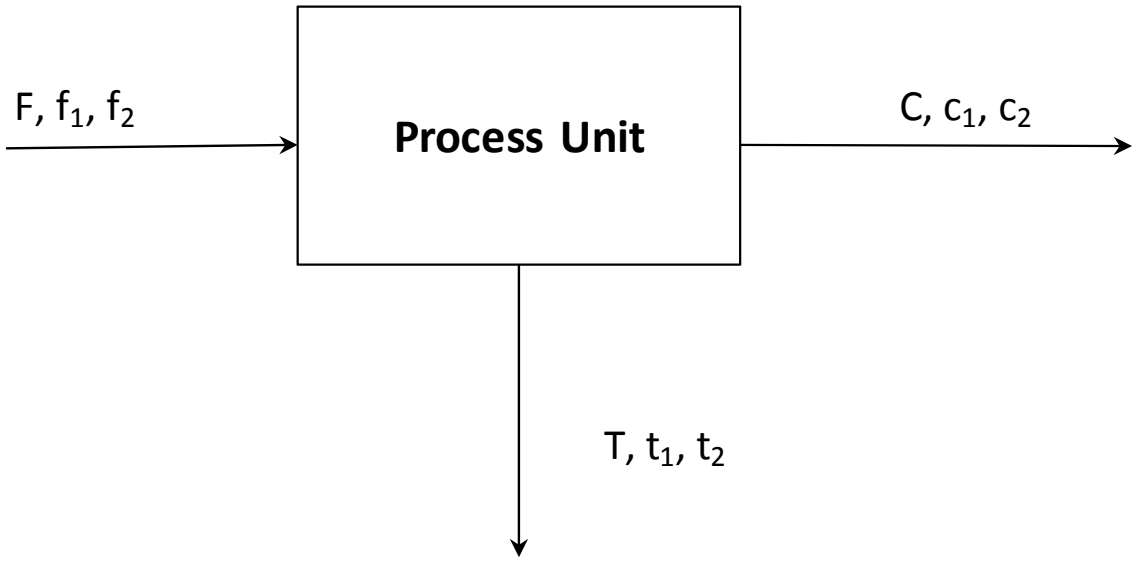

Figure 7-2 : Process Unit Schematic for Case Study

The following material balances apply:

$$\begin{aligned} F - C - T &= 0 \\ F \cdot f_1 - C \cdot c_1 - T \cdot t_1 &= 0 \\ F \cdot f_1 \cdot f_2 - C \cdot c_1 \cdot c_2 - T \cdot t_1 \cdot t_2 &= 0 \end{aligned} \tag{7.1}$$

Where: F, C and T represent bulk mass flows, f_1, c_1 and t_1 represents size or bulk flow assays, and f_2, c_2 and t_2 represent assays in size class, or sub assays of f_1, c_1 and t_1. All variables are treated as measured for the purposes of the data reconciliation exercise. This process unit is conceptually very similar to the one used by Aldrich *et al.* (1994b). Aldrich's system consisted of a two-product splitter subjected to one linear and two bilinear constraints, whereas the system in Figure 7-2 is subjected to one linear, one bilinear and one trilinear constraint. The steady-state values selected for generation of the simulated data also differs between the two systems.

A wide variety of unit operations in the process industry can be modelled as 2-product splitters, such as flotation cells, cyclones, distillation columns and more. What is less common is the tri-linear material balance constraint in (7.1). One example of this would be magnetic separators or cyclones, where the magnetic medium is a component of the solids in the slurry, which in turn is a component of the overall flow, i.e. the magnetite

assay is represented by f_2 , the total solids concentration is represented by f_1, and the total flow rate is represented by F for the feed stream to the unit.

7.3 GENERATING SIMULATED DATA SETS

Simulated measurement data was created for the system described above by using the following hypothetical true steady-state values and coefficients of variation ($\mathbf{cov}_\varepsilon$) for the random error component:

Table 7-1 : Nominal Steady-State Values and cov's for Measurements

	F	C	T	f_1	c_1	t_1	f_2	c_2	t_2
True Value	100	75	25	10.00%	5.00%	25.00%	10.00%	0.10%	15.94%
$\mathbf{cov}_\varepsilon$	2.0%	5.0%	5.0%	2.0%	2.0%	2.0%	1.0%	1.0%	1.0%

Measurement vectors were generated through the following equation:

$$\mathbf{y} = \mathbf{x}_0 + b^* \cdot \mathbf{cov}_\varepsilon(j) \cdot \mathbf{x}_0(j) \cdot \mathbf{e}_j + \boldsymbol{\varepsilon} \tag{7.2}$$

Where: $\mathbf{x}_0$ is the vector of true values contained in Table 7-1, $\mathbf{cov}_\varepsilon$ is the vector of coefficients of variation of the random error components contained in Table 7-1, $b^* \in [-5.0 : 0.5 : 5.0]$ is a scalar controlling the magnitude of the gross error relative to the random error, $\mathbf{e}_j = col_j(I)$ is the j^{th} column of the identity matrix assigning the gross error to a specific measurement location, and $\boldsymbol{\varepsilon}$ is a vector of random error components. The index $j \in [1, 2, ..., 9]$ was uniformly randomly selected, but given the large number of measurements simulated (9 900 gross error vectors per data set), each measurement location has approximately equal number of gross errors. The random error in each measurement was assumed to be normally distributed and both mutually and serially uncorrelated, with the variance of each random error component given by:

$$\text{var}(\varepsilon_i) = \left(\text{cov}_\varepsilon(i) \cdot x_i\right)^2, \quad i = 1, 2, ..., 9 \tag{7.3}$$

The random number generator in MS Excel® was used to generate random numbers that could be converted to random error components for each measurement set via the internal MS Excel® functions for inverting the normal distribution. As is apparent, only single gross errors were considered.

The inclusion of both positive and negative gross error magnitudes represents a change from the typical procedure followed by Aldrich *et al.* (1993, 1994b) and Gupta *et al.* (1993), and is expected to result in a more challenging classification problem due to symmetry of the distributions of the constraint residuals and measurement adjustments.

Ten (10) separate data sets were generated, each containing 11 000 measurement vectors, 1 100 of contained random error components only.

7.4 PERFORMING DR THROUGH SUCCESSIVE LINEARIZATION

The simulated measurements were reconciled with the method of successive linearization described in Section 4.1.7.1 of this thesis using a MS Excel® spreadsheet programmed for this purpose. A naive objective function for reconciliation was given by:

$$\begin{aligned} & J = \min_{\mathbf{x}} (\mathbf{y}-\mathbf{x})^T \Sigma_y^{-1} (\mathbf{y}-\mathbf{x}) \\ & s.t. \\ & F(\mathbf{x}) = \mathbf{0} \end{aligned} \tag{7.4}$$

Where:

$$F(\mathbf{x}) = \begin{bmatrix} F - C - T \\ F \cdot f_1 - C \cdot c_1 - T \cdot t_1 \\ F \cdot f_1 \cdot f_2 - C \cdot c_1 \cdot c_2 - T \cdot t_1 \cdot t_2 \end{bmatrix} \tag{7.5}$$

The covariance matrix of the measurements was assumed to be diagonal with:

$$\left(\Sigma_y\right)_{i,i} = \left(\mathrm{cov}_y \cdot \mathbf{y}(i)\right)^2, i = 1,2,...,9 \tag{7.6}$$

It should be noted that the covariance matrix assumed for the purposes of DR (Σ_y) is distinct from the covariance matrix of the random error component used for generating the simulated data (Σ_ε). The simulated data have different $\mathbf{cov}_\varepsilon$ magnitudes, but this apparent discrepancy makes the study more realistic, as in practice the true variance/covariance of the measurements is unknown, and can only be assumed or determined approximately by methods described in Section 3 of this thesis. The naïve assumed cov_y in (7.6) was taken as 0.05. The assumption that all measurements have the same cov_y is an unlikely occurrence in real data. The particular magnitude selected for the common cov_y would not change the solution to (7.4) above, as will be shown below, provided unrealistic magnitudes that could impact on numerical accuracy are not selected.

The Jacobian matrix of (7.5) is given by:

$$A = \frac{\partial F(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ f_1 & -c_1 & -t_1 & F & -C & -T & 0 & 0 & 0 \\ f_1 \cdot f_2 & -c_1 \cdot c_2 & -t_1 \cdot t_2 & F \cdot f_2 & -C \cdot c_2 & -T \cdot t_2 & F \cdot f_1 & -C \cdot c_1 & -T \cdot t_1 \end{bmatrix} \tag{7.7}$$

A first order Taylor expansion can be used to obtain linearized constraints from (7.5):

$$F(\mathbf{x}) \approx F(\mathbf{x}_0) + A \cdot (\mathbf{x} - \mathbf{x}_0) = 0$$
$$\Downarrow \tag{7.8}$$
$$A\mathbf{x} = A\mathbf{x}_0 - F(\mathbf{x}_0) = \mathbf{c}$$

The solution to the problem defined by (7.4) and (7.5) can be obtained iteratively through the methods described in Section 4.1.7.1 of this thesis. An iterative scheme for successive linearization is presented in Figure 7-3:

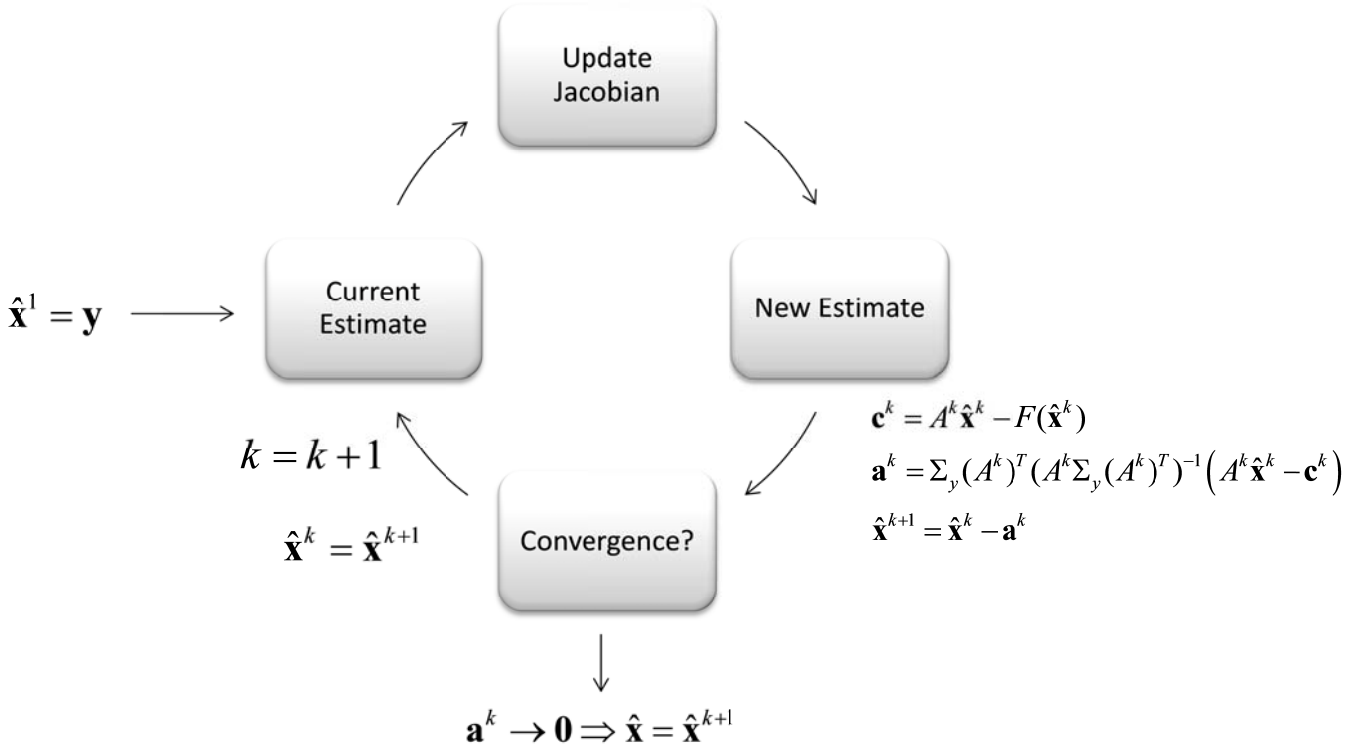

Figure 7-3 : Data Reconciliation through Successive Linearization

The scheme for successive linearization illustrated in Figure 7-3 was implemented in MS Excel® by programming a VBA macro to perform the following sequence of steps:

1. Initialize the procedure by copying a measurement vector $\mathbf{y}$ into the position for the current estimate $\hat{\mathbf{x}}^k$ where the step increment $k = 1$ initially.
2. The Jacobian matrix $A^k = \left.\frac{\partial F(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^k}$ was programmed into the spreadsheet, as well as the calculations for $\mathbf{a}^k$ and $\hat{\mathbf{x}}^{k+1}$, using internal MS Excel® function for matrix inversion and multiplication.
3. If the maximum absolute value of the elements of the adjustment vector $\mathbf{a}^k$ was larger than a preselected tolerance $\left(10^{-7}\right)$, the new estimate $\hat{\mathbf{x}}^{k+1}$ was copied to the position of the original estimate $\hat{\mathbf{x}}^k$, and the procedure repeated.

4. If the maximum absolute value of the elements of the adjustment vector $\mathbf{a}^k$ was smaller than a preselected tolerance $\left(10^{-7}\right)$, the procedure terminated with $\hat{\mathbf{x}}^{k+1}$ as the final reconciled estimate.

For each data set, steps 1 to 4 above would be repeated for each of the 11 000 simulated measurement vectors. After termination of the successive linearization procedure for a specific measurement vector, the residuals $\mathbf{r} = F(\mathbf{y})$, the normalized relative adjustments $\mathbf{a}^* = 100 \cdot diag(\mathbf{y})^{-1} \cdot \mathbf{a}$, and the maximum MT test statistic and location of this test statistic was copied and retained for further use.

The naive object function, assuming a common cov_y, and the successive linearization DR programmed into MS Excel® would commonly be applied in practice. A detailed example of the required iterative calculations to achieve successive linearization DR is provided in the appendix to this thesis.

7.5 Formulation of the Measurement Test

After the successive linearization scheme of Figure 7-3 converged, the Measurement Test (MT) was constructed as described in Section 4.3.2.3 of this thesis from the linearized constraints around the final estimate of the adjusted measurement vector. The vector of measurement adjustments is calculated as:

$$\mathbf{a} = \mathbf{y} - \hat{\mathbf{x}} \tag{7.9}$$

The covariance matrix of $\mathbf{a}$ is calculated from:

$$\Sigma_a = \Sigma_y A^T (A \Sigma_y A^T)^{-1} A \Sigma_y \tag{7.10}$$

Where: $A = \left.\dfrac{\partial F(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\hat{\mathbf{x}}}$ from (7.7) is evaluated at the final reconciled estimates. The MT test statistics are constructed as:

$$z_{a,i} = \frac{|a_i|}{\sqrt{(\Sigma_a)_{ii}}}, i = 1, 2, ..., 9 \tag{7.11}$$

A serendipitous consequence of the assumption of a common cov_y for all measurements was that the Type I error rate of the MT could be manipulated to match the Type I error rate of any classifier developed. The measurement covariance matrix Σ_y assumed for the purposes of DR in (7.6) can be written as:

$$\Sigma_y = \left(\text{cov}_y\right)^2 \cdot D_y \tag{7.12}$$

Where D_y is a diagonal matrix such that:

$$\left(D_y\right)_{i,i} = \mathbf{y}(i)^2, i = 1, 2, ..., 9 \tag{7.13}$$

The covariance matrix Σ_a of the measurement adjustments $\mathbf{a}$ therefore becomes:

$$\begin{aligned}\Sigma_a &= \left(\text{cov}_y\right)^2 \left(D_y A^T\right)\left(\frac{1}{\text{cov}_y}\right)^2 \left(AD_y A^T\right)^{-1}\left(\text{cov}_y\right)^2 \left(AD_y\right) \\ &= \left(\text{cov}_y\right)^2 \left(D_y A^T\right)\left(AD_y A^T\right)^{-1}\left(AD_y\right) \\ &= \left(\text{cov}_y\right)^2 \Sigma_a^*\end{aligned} \tag{7.14}$$

Where $\Sigma_a^* = \left(D_y A^T\right)\left(AD_y A^T\right)^{-1}\left(AD_y\right)$.The MT test statistic in (7.11) therefore implies that:

$$z_{a,i} = \frac{|a_i|}{\left(\text{cov}_y\right)\sqrt{(\Sigma_a^*)_{ii}}},\ i = 1,2,....,9 \tag{7.15}$$

The vector of adjustments $\mathbf{a}^k$ is not impacted by the particular choice of cov_y, as can be seen from:

$$\begin{aligned}\mathbf{a}^k &= \Sigma_y (A^k)^T \left[A^k \Sigma_y (A^k)^T\right]^{-1}\left(A^k \hat{\mathbf{x}}^k - \mathbf{c}^k\right) \\ &= \text{cov}_y^2 \cdot D_y (A^k)^T \cdot \left(\frac{1}{\text{cov}_y^2}\right) \cdot \left[A^k D_y (A^k)^T\right]^{-1}\left(A^k \hat{\mathbf{x}}^k - \mathbf{c}^k\right) \\ &= D_y (A^k)^T \left[A^k D_y (A^k)^T\right]^{-1}\left(A^k \hat{\mathbf{x}}^k - \mathbf{c}^k\right)\end{aligned} \tag{7.16}$$

The implication of (7.16) is that the DR solution is independent of cov_y. Therefore, for a given data set, the proportion of the $z_{a,i}$ statistics that exceeded the critical value could be modified, without impacting the DR results, by changing the value of cov_y, as can be seen from (7.15). For each classifier on each data set, a cov_y could thus be found so that the MT Type I error would match the Type I error of the classifier.

7.6 Construction of Classification Trees and Classification Functions

The MATLAB® suite was used to train the classifiers. The internal MATLAB functions available for classification and regression tree development were used, and no customized code had to be generated.

Two sets of classifiers were constructed for each data set:

1. A set of classifiers to solve the Detection Problem
2. A set of classifiers to solve the Identification Problem

The input data for classifier development consisted of the residuals of (7.1), i.e. $\mathbf{r} = F(\mathbf{y})$, as well as the vector of normalized relative adjustments $\mathbf{a}^* = 100 \cdot diag(\mathbf{y})^{-1} \cdot \mathbf{a}$. Additionally, the Euclidian distance from the origin

for both the vector of residuals $\mathbf{r}$ and the vector of relative adjustments $\mathbf{a}^*$ was included in the input data for classifier construction. The input vector for classifier training is given by:

$$\mathbf{v}_j \in V^i = \begin{bmatrix} \left(\mathbf{r}_j\right)_{3\times 1} \\ \left(\sqrt{\mathbf{r}_j^T \mathbf{r}_j}\right)_{1\times 1} \\ \left(\mathbf{a}_j^*\right)_{9\times 1} \\ \left(\sqrt{(\mathbf{a}_j^*)^T \mathbf{a}_j^*}\right)_{1\times 1} \end{bmatrix}_{14\times 1} \tag{7.17}$$

Where: j indicate the j^{th} vector in the i^{th} data set. The set of class variables for the Detection problem consisted of a scalar $Z_{DET}^i \in \{0,1\}$ where 0 corresponds to a random error vector and 1 to a gross error vector. The set of class variables for the Identification problem consisted of a scalar $Z_{ID}^i \in \{0,1,2,...,9\}$ assuming values of 0 corresponding to each random error vector, or the index ranging from 1 to 9 corresponding to the measurement location containing a gross error. The elements of the input vector are similar to those employed by Aldrich *et al.* (1993, 1994b) and Gupta *et al.* (1993). The fact that the constraint residuals are not scaled by their respective standard deviations as was done for the ANN's would not impact on the Classification Tree methodology, as it is invariant under linear transformations. The Linear and Quadratic Classification Functions could be impacted by the lack of scaling though. Inclusion of the norms of the vectors of residuals and measurement adjustments was an attempt to counteract the effect of symmetrical distributions due to the inclusion of both positive and negative gross errors. The strictly positive norms may have skewed distributions that can be exploited by the classification methodologies. This represents a conceptual change from the work regarding ANN's discussed previously, as the importance of sign of the gross error component is recognized, and an attempt is being made to find a way to counter the undesirable symmetry of distributions resulting from simulating both positive and negative gross errors.

For each of the Detection and Identification problems, a classifier was developed on each data set and evaluated on all the remaining data sets, as illustrated in Figure 7-4:

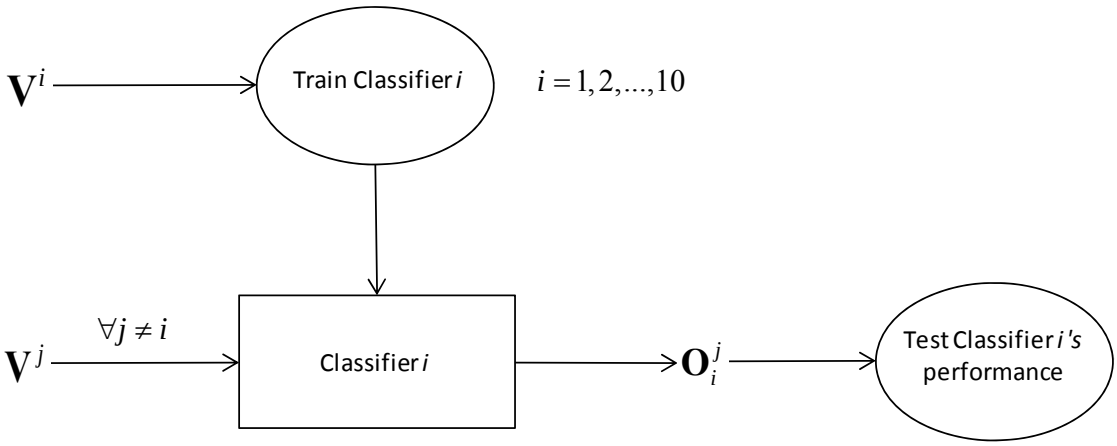

Figure 7-4 : Scheme for Classifier Development and Evaluation

The default MATLAB® settings for growing classification trees were used, that is:

- Misclassification cost $C(m,n) = \begin{cases} 1, & m \neq n \\ 0, & m = n \end{cases}$, where $C(m,n)$ is the cost of classifying a vector in class m into class n.
- Minimum number of observations per leaf = 1.
- Minimum number of observations in a parent node = 10.
- *Prior* probabilities determined empirically from input matrix.
- Split criterion was the Gini diversity index.
- Surrogate splits not determined.
- Observation vector weights set to unity.

The optimal tree in each case was chosen to be the smallest sub-tree with an error rate within one standard error of the minimum error rate. Error rates were estimated through 10-fold cross validation.

In addition to the classification trees constructed, the detection and identification problems were solved by constructing linear discriminant classifiers for each data set using the same input and output variables.

The linear and quadratic discriminant classifiers were constructed using the ClassificationDiscriminant.fit function in MATLAB® with the default settings, that is:

- The pdf of each class was modelled as multivariate normal
- The *prior* probabilities of each class were estimated empirically from the frequencies in the dependent variable.

7.7 BENCHMARKING CLASSIFIER PERFORMANCE

With ten (10) data sets, each with a corresponding tree and linear and quadratic classification function, as well as a Measurement Test detection/identification strategy, the question regarding the performance of classification methods relative to classical gross error detection methods can be addressed.

7.7.1 Achieving Equivalency of Type I Error

The definition of Type I and Type II errors as it applies to statistical hypothesis testing is illustrated in Table 7-2:

Table 7-2 : Type I and Type II Error Rates associated with Hypothesis Testing

		H_0	
		TRUE	FALSE
Test	Fail to Reject H_0	Correct	Type II Error
	Reject H_0	Type I Error	Correct

The power of a method is:

$$1 - \beta \tag{7.18}$$

Where β is the Type II error of the method. Any statistical test has a trade-off between Ttype I and Type II error rates, with typically an increasing Type II error rate for decreasing Type I error rate. Obtaining a meaningful comparison between two methodologies can therefore be a challenge.

For a given test sample, the total number of correctly classified vectors would be determined by the Type I and Type II error rates of the methods under investigation, and the relative proportion of random error/gross error vectors in the sample, so comparing the total number of correctly classified vectors would bias any conclusions based on the composition of the test sample.

Further, if the Type I and Type II error rates are estimated separately and determined to be different on a test sample, it is not clear which method can be said to be 'better' from a theoretical perspective; in practice the 'best' method may be selected based on the cost and/or risk of committing a Type I error vs. a Type II error, and would be specific to the application of the test.

In this particular case study, the naïve formulation of the objection function allowed the above problems to be circumvented: as a common cov_y is assumed for all measurements, the Type I vs. Type II error rate trade-off for the Measurement Test could be manipulated as desired. For a given data set, the Type I error rate of the classification methods was determined, the common measurement cov_y assumed for the DR problem in (7.4) set to achieve a statistically identical Type I error rate on the Measurement Test, and the resultant power to detect/identify gross errors between the methods compared through use of the McNemar statistic for correlated proportions.

The ability to match Type I error rates of the MT with each classifier therefore enables a convenient comparison of the Type II error rates, or power of the methods. When the difference in power between the two methods is statistically significant, as can be determined with the McNemar Test discussed in the following section, the method with the highest power for the same Type I error rate is superior.

7.7.2 Testing for significance differences in Power with the McNemar Ratio Test

A rigorous method is necessary to describe the differences in performance between the classification methodologies and the Measurement Test. It is expected that there would be correlation between the proportions of vectors correctly classified in each data set by the respective methodologies. Given the expectation of dependence between the different methods, McNemar's test (McNemar, 1947) for correlated proportions was selected to test for differences in the marginal probabilities between the classification methods and the Measurement Test.

A univariate McNemar test is based on a 2x2 contingency table as outlined in Table 7-3:

Table 7-3 : Example of a 2x2 Table for McNemar's Test

		MT		
		Success	Failure	Total
Classifier	Success	a	b	a + b
	Failure	c	d	c + d
Total		a + c	b + d	n

For a set of vectors, the output of the classifier or MT for each vector can be classified as a 'success' if a Type I or Type II error did not occur, and a "failure" otherwise. In order to compare the relative performance of say the tree classifier vs. its associated Measurement Test, a contingency table such as in Table 7-3 can be constructed

where the letters *a, b, c* and *d* represent counts of the number of vectors in the set that falls into the categories as defined by the rows and columns of the table. The McNemar test assumes that the distribution of the numbers in Table 7-3 is multinomial with associated (unknown) probabilities π_a , π_b, π_c and π_d.

The objective of the analysis is to determine whether the marginal probabilities of "success" are equal for the two methods in question, i.e. the null hypothesis can be stated as (May and Johnson, 1997):

$$H_0 : \pi_{a+b} = \pi_{a+c} \Rightarrow H_0 : \pi_b = \pi_c \tag{7.19}$$

When comparing a classification method with the Measurement Test, the objective is to test whether the classification method has a higher marginal probability of success than the Measurement Test, which implies an alternative hypothesis:

$$H_1 : \pi_b > \pi_c \tag{7.20}$$

The McNemar statistic is constructed as (McNemar, 1947):

$$T_M = \frac{(b-c)^2}{(b+c)} \tag{7.21}$$

Under the null hypothesis, T_M asymptotically follows a chi-square distribution with one degree of freedom. McNemar (1947) recommends that the chi-square distribution should only be used for inference on T_M when $(b+c) \geq 10$. When $(b+c) < 10$, inference can be made based on the fact that under the null hypothesis the number of discordant pairs follows a binomial distribution, i.e. $b \sim B(b+c, 0.5)$ (Westfall *et al.*., 2010). However, Park (2002) found that the asymptotic test provides good results even for small sample sizes.

7.7.3 Correcting for Multiple Tests

When multiple statistical tests are performed, each at a level of significance α , the probability that at least one null hypothesis among all the tests is rejected erroneously (i.e. a type I error occurs) increase with the number n of tests performed. It is therefore necessary to adjust the level of significance for each individual test, in order to preserve the overall level of significance. One method of achieving this is the Bonferroni inequality (Wackerly *et al.*, 2002: 666). If *k* tests are performed simultaneously, the type I error rate for the *k* hypothesis tested can be maintained at a maximum of α by choosing the confidence limit for the individual tests to be at most α/k , i.e:

$$\alpha_k = \frac{\alpha}{k} \tag{7.22}$$

Where: α_k is the confidence level for each individual test.

8 VISUALIZING GROSS ERRORS

It is expected that the presence of gross errors will cause some discernible features in the input data that can be used to distinguish the input vectors where gross errors are present from the ones containing only random errors. It is these distinguishing features that may be exploited by the classification methods to solve the Detection and Identification problems.

The first method used to investigate the manifestation of gross errors in the input vectors is parallel coordinate plots, where selected percentiles of the elements of the input vectors given by (7.17) are plotted for different gross error magnitudes and locations. If the presence of a gross error causes a distortion in the data, the gross error vectors may have more extreme values relative to the random error vectors, which should be detectable through a parallel coordinate plot. Given the number of gross error magnitudes and locations simulated over multiple data sets, the parallel coordinate plots were simplified by using gross error magnitudes 2.5 and 5, and gross error locations 1, 5 and 9 from data set 1. Since the objective is to look for differences in the extreme values of the input vectors, the 5^{th}, 50^{th} and 95^{th} percentiles was selected for comparison. The same percentiles for the random error input vectors were plotted concurrently for comparison.

The second method used for visualizing gross errors is principal component (PCA) plots. If the presence of a gross error causes a systematic shift in the data, this should be observable as clustering in the PCA plots, i.e. a discernible grouping of the gross error vectors relative to the random error vectors. Also, since the PCA views the distribution of the variables on coordinates of maximum dispersion, extreme values resulting from the presence of gross errors should be readily observable. The same magnitudes and locations of gross errors that were selected for the parallel coordinate plots were used for the PCA plots. However, in order to facilitate interpretation of the resulting scatter plots, only 100 data points corresponding to each magnitude/location is plotted, as well as 100 random error input vectors. The 100 data points for each type of vector were selected randomly from the input vectors to data set 1.

8.1 PARALLEL COORDINATE PLOTS

The parallel coordinate plots for the normalized input vectors, where the elements $v_i, i = 1,2,...,14$ are as described in (7.17), for random error vectors and gross error magnitudes 2.5 and 5.0 are presented in Figure 8-1:

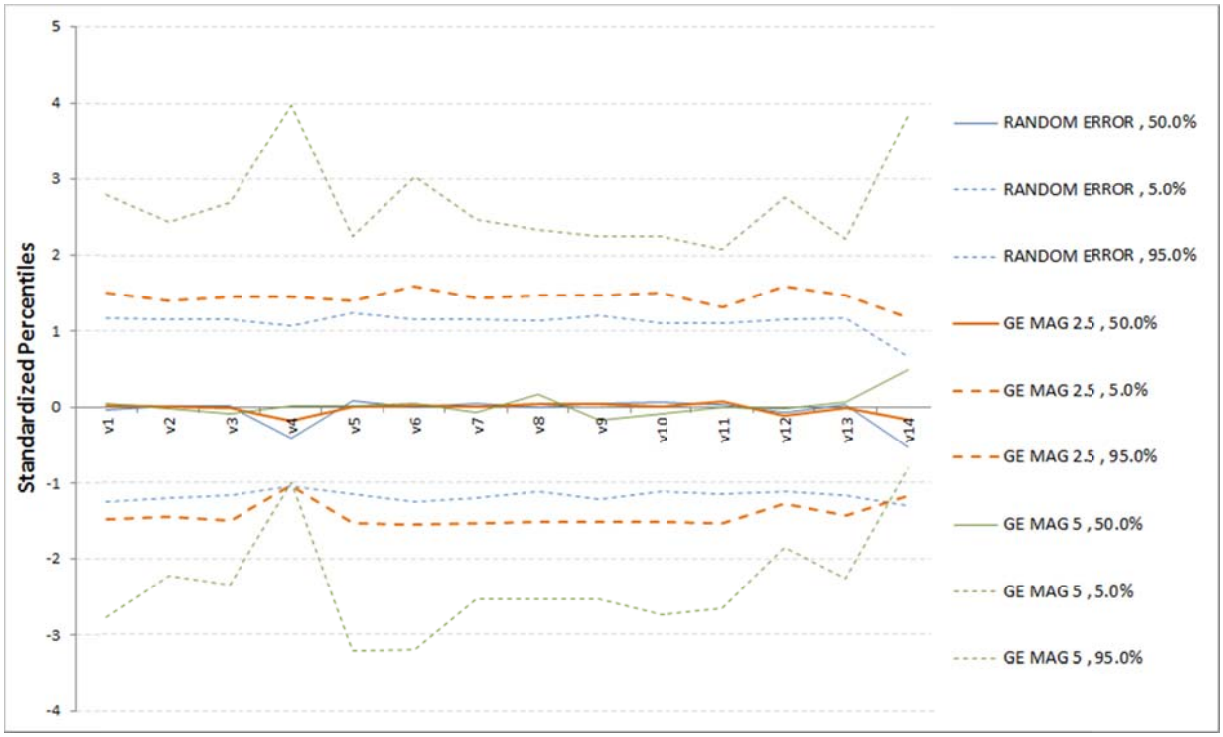

Figure 8-1 : Parallel Coordinates Plot for Input Vectors with different Gross Error Magnitudes on Data Set 1

With the exception of the two strictly positive elements of the input vector (the radii of the residuals v_4 and relative adjustments v_{14}), the medians of the random error vectors and gross error vectors are near identical, and almost equal to zero, i.e. the distribution of all of the input variables seems to be centred on zero. This is due to the incorporation of both positive and negative gross errors of each magnitude in nearly equal proportions. For the two strictly positive elements, the medians of the gross error vectors exceed that of the random error vectors.

The 5^{th} and 95^{th} percentiles of the gross error vectors have larger absolute magnitude than that of the random error vectors, the exceptions again being the strictly positive elements, where the 5^{th} percentiles of the gross error vectors exceed that of the random error vectors. In general the larger magnitude gross errors produce more extreme percentile values, suggesting that they may be easier to detect accurately.

For both random and gross error vectors, the 5^{th} and 95^{th} percentiles are approximately the same distance from the median, i.e. the distributions appear to be symmetrical, with the exception being the strictly positive

elements, where the 5th percentile is closer to the median than the 95th percentile, i.e. the distributions for the strictly positive elements are positively skewed.

The corresponding results for different gross error locations are presented Figure 8-2:

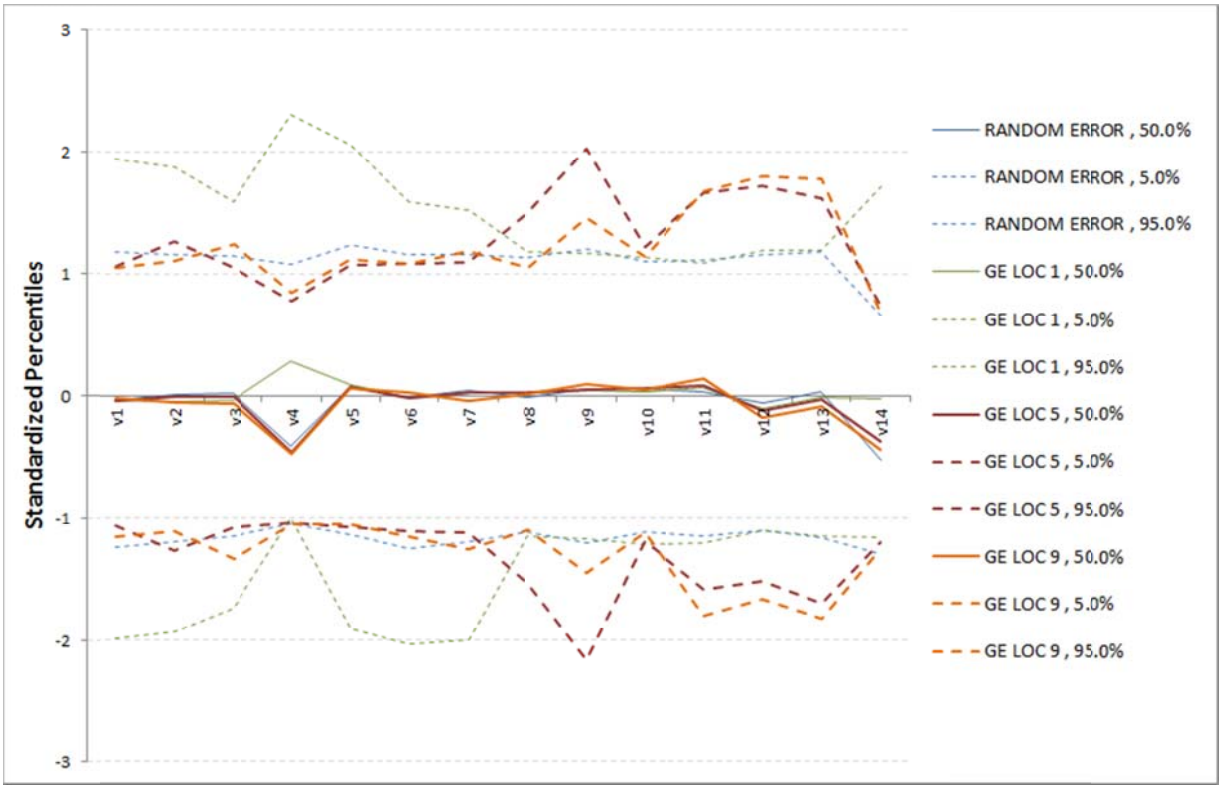

Figure 8-2 : Parallel Coordinates Plot for Input Vectors with different Gross Locations on Data Set 1

The parallel coordinates for different gross error locations display the similar trends as that for gross error magnitude, i.e.:

- The distributions are centred on zero, with exception of the two strictly positive elements.
- The 5th and 95th percentiles of the gross error vectors exceed that of the random error vectors, with exception of the two strictly positive elements.
- The percentiles of gross error vectors for locations 5 and 9 are nearly equal to that of the random error vectors, suggesting that the Identification problem may be difficult to resolve for some gross error locations.
- The distribution of elements of the input vectors of both random error and gross error vectors seems to be symmetrical, with exception of the two strictly positive elements.

This concludes the discussion of parallel coordinate plots. PCA plots are discussed in the next section.

8.2 VISUALIZATION THROUGH PRINCIPAL COMPONENT ANALYSIS

Principal components were extracted from the complete set of vectors comprising data set 1. The proportion of total variance contained in each principal component is displayed in Figure 8-3:

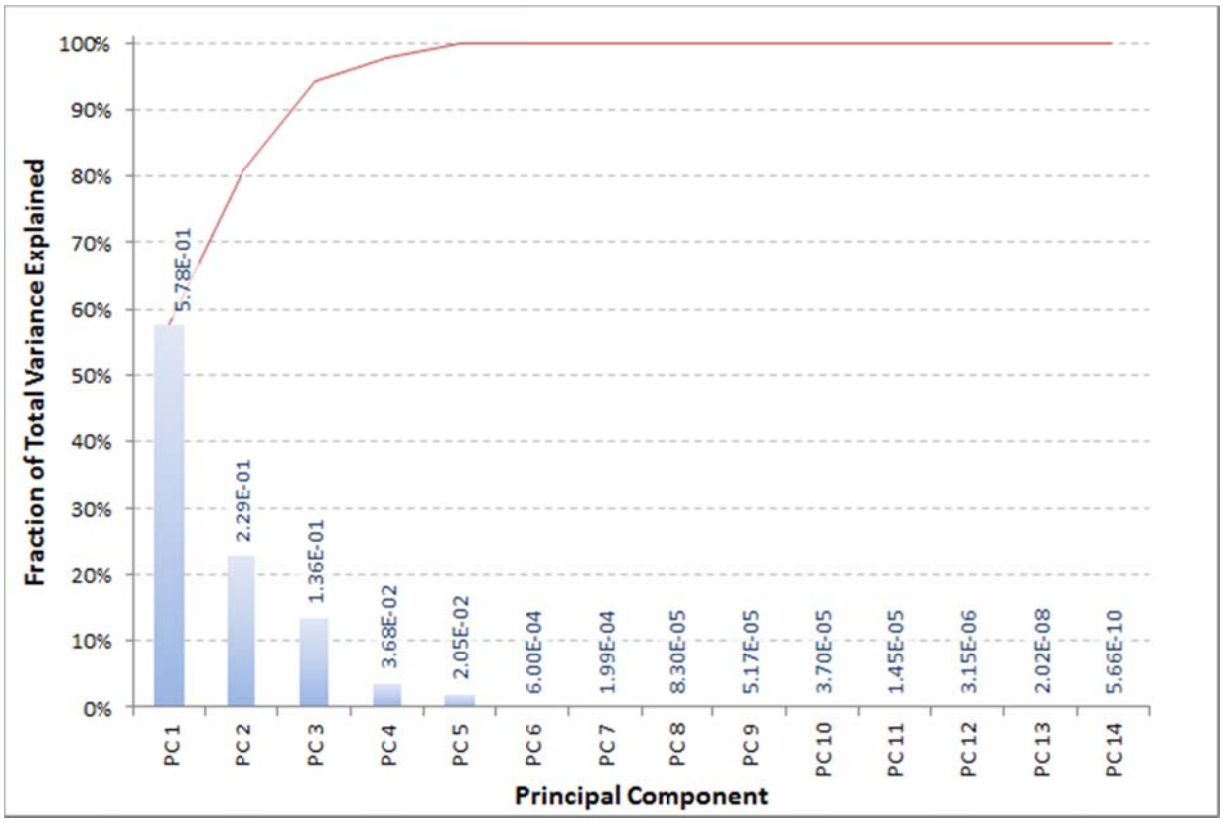

Figure 8-3 : Distribution of Variance on Principal Components – Data Set 1

The blue bars indicate the proportion of total variance contained in each principal component, while the red line indicates the cumulative proportion.

The first three principal components explain more than 90% of the total variance, and are thus viewed as sufficient to describe the data set. As explained before, 100 vectors each corresponding to gross error magnitudes of 0, 2.5 and 5.0 were randomly selected to be plotted on the first three principal components.

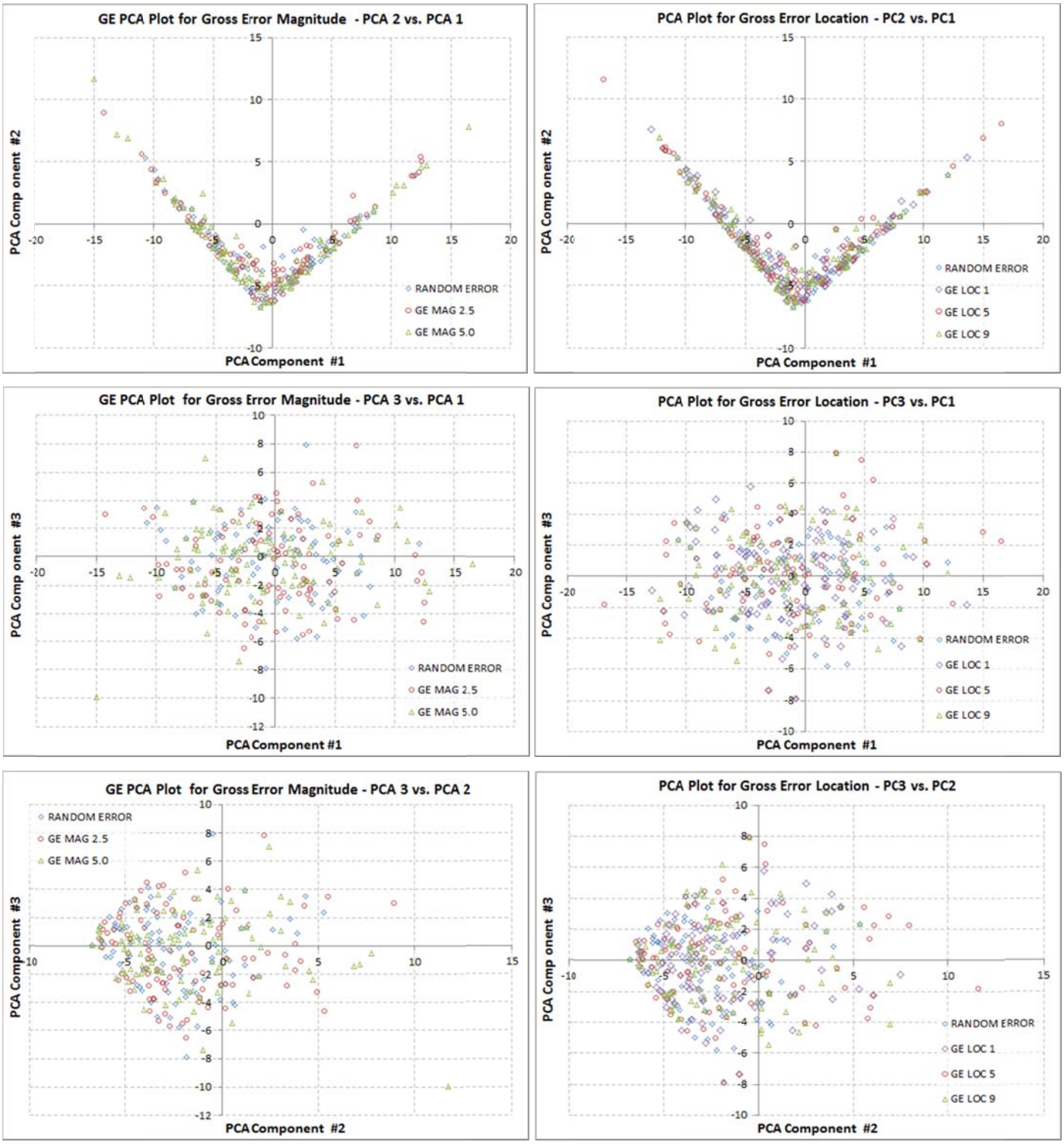

Figure 8-4 : PCA Plots for Different Gross Error Magnitudes and Locations

The PCA plots for different gross error magnitudes and locations do not indicate any clustering in the data, i.e the observations are dispersed fairly symmetrical on the principal component axis.

The observations containing gross errors result in more extreme values than those corresponding to random error vectors only, however, the bulk of the observations show no discernible separation. This confirms in a broad sense the conclusions made from the parallel coordinate plots.

9 RESULTS AND DISCUSSION

The results are discussed under three main sections:

The first section covers the contribution of the input variables to classifier structure. Since the classification tree and linear discriminant classifiers are constructed with different algorithms using different measures of class separation, different measures of variable importance arise for the two methods. For the classification tree methodology variable importance is rated based on the average reduction in node risk associated with each split selected in the tree, and for the linear discriminant classifier variable importance is based on the standardized coefficients for each variable in the classification function. The variable importance is ranked for the two methods in order to have a means of comparing variable importance based on different measures of importance.

The objective of the thesis is to compare the performance of the two classification methods with the benchmark Measurement Test. Following the section on variable importance, the results for the Detection and Identification problem will be discussed in two separate sections. Each of these sections will treat the results of the classification tree, and linear and quadratic classification functions separately, and compares the performance of the classification methods to that of the Measurement Test for different gross error magnitudes and locations.

For both the Detection and Identification problem, 10 individual classifiers were constructed for each classification methodology, corresponding to the 10 data sets developed. The classification accuracy of each classifier was determined on each of the 9 remaining data set, i.e. there are 90 sets of results corresponding to the classification tree methodology for the Detection problem, etc. For each classifier, a Measurement Test was constructed that matched the Type I error rate of the classifier on each data set, so that the power of the classifier could be compared directly to that of the Measurement Test, for the same type I error rate.

For a given classification method, its performance for a given gross error magnitude or location is summarized as the average proportion of vectors corresponding to that magnitude or location that the method classified correctly. The average is calculated over the 9 data sets that were not used in training the classification method, i.e. the ‘test’ sets as opposed to the ‘training’ set. The performance of the Measurement Test corresponding to the classification method is expressed similarly. The McNemar statistic is used to determine where differences in power are significant or not, and the average of significant differences in power are calculated over the 10 data sets. This is used as the basis for inference on performance of the classification methods relative to the Measurement Test.

A general layout of the results section is presented in Figure 9-1:

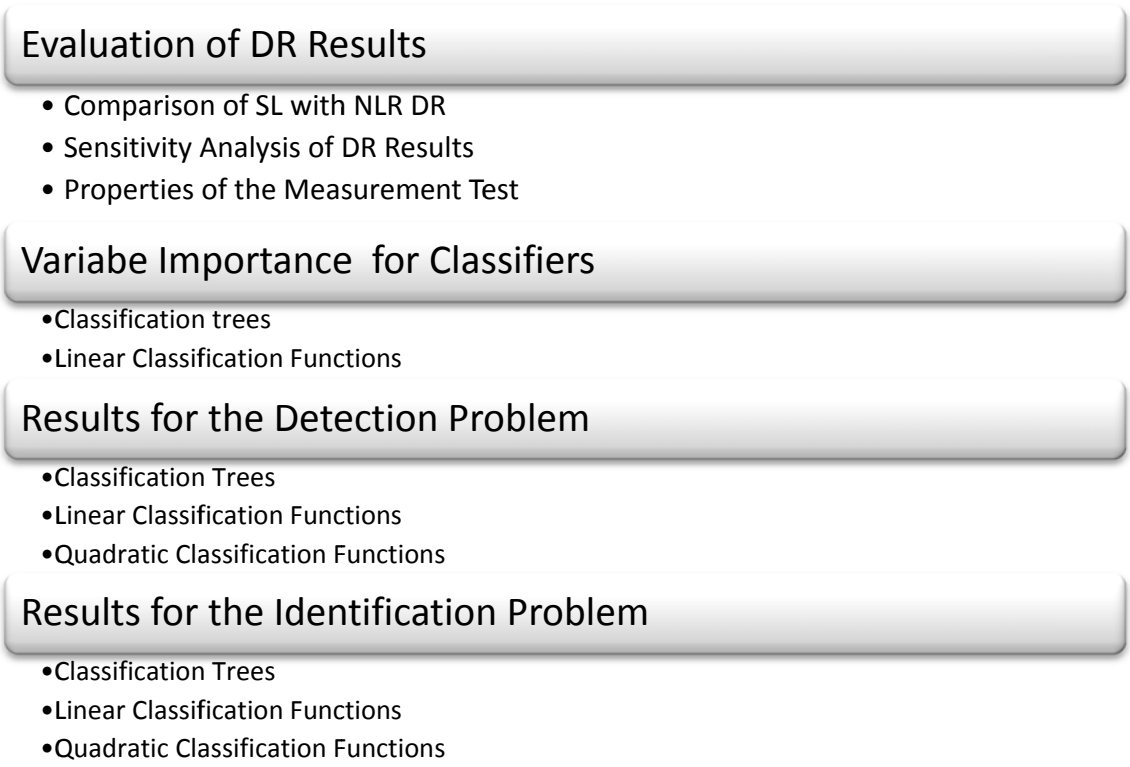

Figure 9-1 : Layout of the Results Section

9.1 EVALUATION OF DATA RECONCILIATION RESULTS

9.1.1 Comparison of Successive Linearization with Nonlinear Data Reconciliation

In this case study the detection and identification of gross errors occurs subsequent to data reconciliation. This is a requirement for the Measurement Test, as measurement adjustments do not exist prior to the reconciliation exercise. The classification methodologies also incorporated the results of the reconciliation step, as well as information contained in the balance equations' residuals prior to the reconciliation step.

The reconciliation algorithm used is successive linearization. It was hypothesized that, given the nonlinear constraints of the problem, a nonlinear programming algorithm may result in a lower objective function, i.e. better estimates of the true values of the measurements, in which case improved performance would be expected from the gross error detection/identification procedures, as smearing of gross errors would be reduced through the improved reconciliation method.

In order to investigate the effect of nonlinear programming on the DR solution, , 200 input vectors were selected from each of the 10 data sets, of which 100 corresponded to vectors that contained a simulated gross error (biased) and 100 were unbiased. The selection was based on objective function value, i.e. the 100 largest objective function values from each category were selected from each data set to construct a subset containing 2000 vectors. The Solver® package available in Microsoft Excel® was used to solve the nonlinear reconciliation problem for each of the 2000 vectors. The relative percentage change in objective function value was calculated, and is displayed below for biased and unbiased vectors:

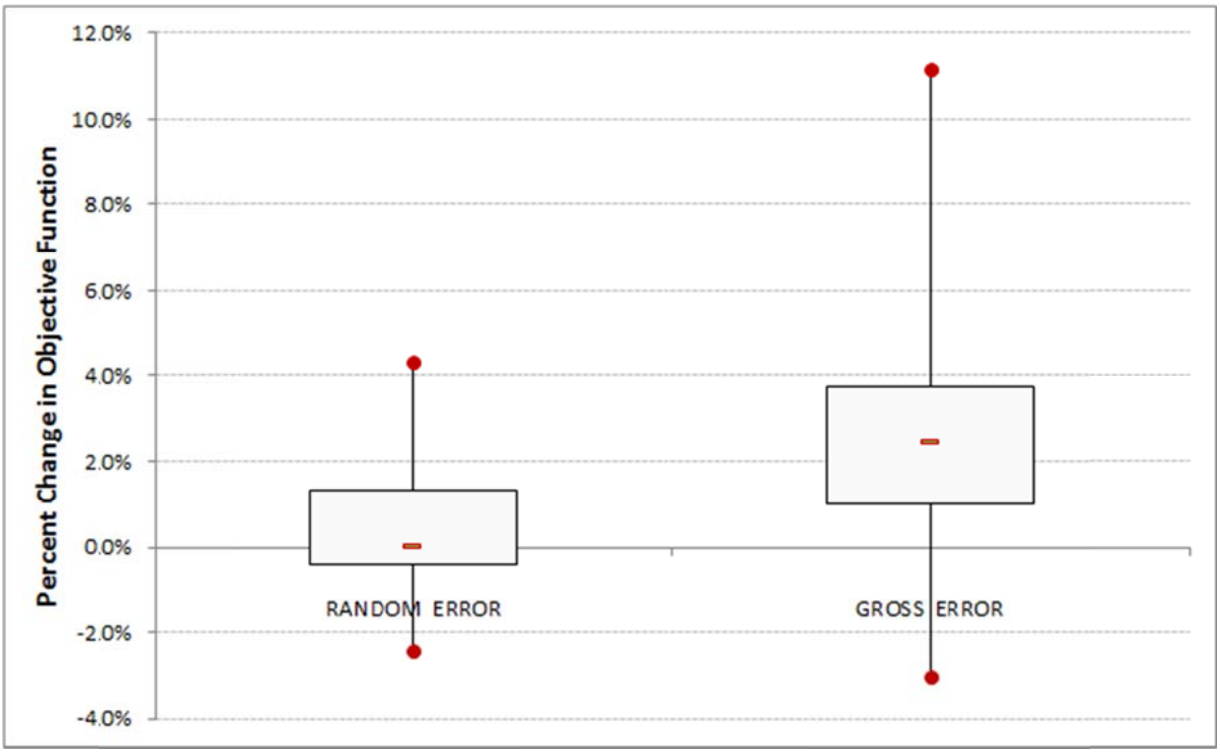

Figure 9-2 : Boxplots for percentage change in Objective Function value after nonlinear optimization

The outer red dots represent minimum and maximum values, the box represent 1st and 3rd quartiles, and the red dash represents the median for the two plots.

The variance of the percentage change in objective function value is larger for the biased vectors than for the unbiased vectors, with a range of 14.14% vs. 6.72%. Both the biased and unbiased vectors have positive average percentage change in objective function; 0.37% for unbiased vectors and 2.31% for biased vectors, suggesting that nonlinear programming results in an increase in the objective function. A student's t-test was performed on the mean percentage adjustment for each class of vector to test the null hypothesis that the true percentage change in objective function value is zero. The results are displayed below:

Table 9-1 : t-Test on Mean Percentage

	RANDOM ERROR	GROSS ERROR
Mean	0.37%	2.31%
SD	1.32%	2.19%
Count	1000	1000
t	8.79	33.38
t-crit	2.245	2.245

Both test statistics are highly significant. Given that nonlinear programming resulted in a deterioration of the objective function value, no further investigations on the effect of nonlinear optimization were carried out. It would normally be expected that a nonlinear optimization algorithm would perform better on a problem with

nonlinear constraints. The objective function defined in (7.4) is quadratic in the measurement adjustments. The anomaly observed in this case implies that the feasible region defined by the constraints must be strictly convex, allowing the successive linearization algorithm employed to converge to the global minimum. A convex feasible region is not guaranteed in general when resolving the Data Reconciliation problem. The increase in objective function values observed for the nonlinear algorithm is likely a numerical anomaly caused by the optional settings of the algorithm selected, e.g. the value of the convergence, tolerance for constraint violation, method of estimating the tangent, and algorithm to select step direction and magnitude can all impact on the final objective function value reached by a nonlinear optimization method. These settings are readily available in MS Excel® Solver®, and won't be discussed in detail, as a detailed discussion of optimization theory is beyond the scope of this thesis.

9.1.2 Sensitivity Analysis of DR Results

Errors in measurements are compensated for through Data Reconciliation by calculating the vector of measurement adjustments that is optimal given the measurement vector, error model and process constraints. Not all measurement locations are affected equally by an error in a given location, and significant 'smearing' of errors can occur from one location to another. For linear systems the sensitivity of the final reconciled estimate for a specific location on the magnitudes and variances of all other measurement locations can be determined directly (Heyen *et al.*, 1996). A direct approach is not possible for nonlinear systems, but an approximate solution may be found from the linearized system model. The tendency for smearing to occur in the selected process system was investigated as outlined in Figure 9-3:

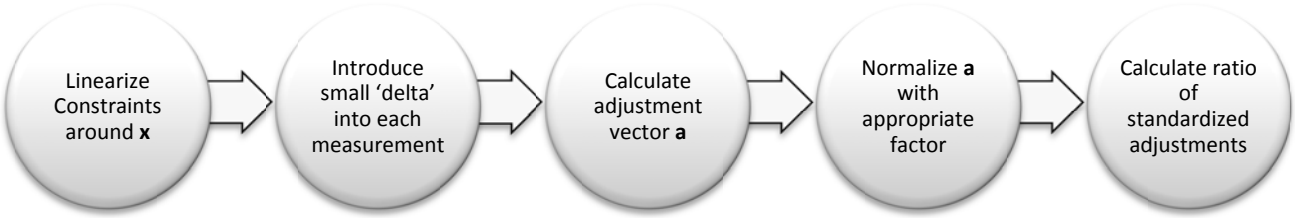

Figure 9-3 : Methodology of Sensitivity Analysis

Since the true values of the process variables used to generate the simulated data sets are available and were presented in Table 7-1, the nonlinear constraints in (7.1) can be linearized around the true values by calculating the Jacobian matrix at the point defined by the true values. This can be accomplished by substituting the true values $\mathbf{x}_0$ into the Jacobian matrix defined in (7.7).

For each respective measurement location, a small delta $\delta_i = 10^{-6}$ was added to the true values:

$$\mathbf{y}_i = \mathbf{x}_0 + \delta_i \cdot \mathbf{e}_i, i = 1,2,...,9 \tag{9.1}$$

The vector of measurement adjustments corresponding to this δ_i for each location could then be calculated:

$$\mathbf{a}_i = \Sigma_y A^T (A\Sigma_y A^T)^{-1} A\mathbf{y}_i, i = 1,2,...,9 \tag{9.2}$$

The same $\text{cov}_y = 0.05$ was used for the assumed Σ_y in (9.2) as was for done for the DR procedure. The small value of δ_i was chosen to ensure that the linearized process model remains representative of process behaviour around the true steady-state values. To estimate the impact of δ_i, it is required that each element of $\mathbf{a}_i$ be normalized with an appropriate factor:

$$(Z_a)_{i,j} = \frac{\mathbf{a}_i(j)}{s_{i,j}}; i = 1,2,...,9,\ j = 1,2,...,9 \tag{9.3}$$

For the MT, the appropriate scaling factor is $s_{i,j} = \sqrt{(\Sigma_a)_{j,j}}$, where Σ_a is the covariance matrix of the measurement adjustments evaluated at the true steady-state process values given in Table 7-1, as this would yield the real value of the MT test statistic when applied in (9.3). The values of $(Z_a)_{i,j}$ from (9.3) for each measurement location *j* corresponding to a $\delta_i = 10^{-6}$ in measurement location *i*, where *i* is the row index and *j* is the column index, is presented in Table 9-2:

Table 9-2 : Normalized Measurement Adjustments

$Z_{i,j}$		Location of Adjustment								
		F	*C*	*T*	f_1	c_1	t_1	f_2	c_2	t_2
Location of Error	F	-1.58E-07	1.35E-07	9.27E-08	-1.51E-08	3.79E-09	2.01E-08	-1.17E-08	1.17E-08	1.17E-08
	C	1.46E-07	-1.72E-07	-1.31E-08	-5.03E-08	1.26E-08	6.70E-08	-3.90E-08	3.90E-08	3.90E-08
	T	1.94E-07	-2.53E-08	-3.31E-07	2.11E-07	-5.30E-08	-2.81E-07	1.64E-07	-1.64E-07	-1.64E-07
	f_1	-1.44E-05	-4.44E-05	9.66E-05	-1.52E-04	1.23E-04	1.33E-04	2.49E-05	-2.49E-05	-2.49E-05
	c_1	3.82E-06	1.17E-05	-2.55E-05	1.29E-04	-1.60E-04	-6.95E-05	-1.13E-04	1.13E-04	1.13E-04
	t_1	5.01E-06	1.54E-05	-3.35E-05	3.48E-05	-1.72E-05	-3.95E-05	1.27E-05	-1.27E-05	-1.27E-05
	f_2	-9.44E-06	-2.90E-05	6.32E-05	2.10E-05	-9.08E-05	4.12E-05	-1.28E-04	1.28E-04	1.28E-04
	c_2	3.54E-06	1.09E-05	-2.37E-05	-7.88E-06	3.41E-05	-1.54E-05	4.79E-05	-4.79E-05	-4.79E-05
	t_2	5.90E-06	1.81E-05	-3.95E-05	-1.31E-05	5.68E-05	-2.57E-05	7.98E-05	-7.98E-05	-7.98E-05

The effect of an error in each location on the other locations can then be estimated by calculating the ratio:

$$P_{i,j} = \frac{(Z_a)_{i,j}}{(Z_a)_{i,i}}, i = 1,2,...,9 \quad j = 1,2,...,9 \tag{9.4}$$

The ratios $P_{i,j}$ represent the number of standard deviations a measurement in location *j* is adjusted when a small error occurs in measurement location *i*, relative to the number of standard deviation measurement *i* itself is adjusted. These ratios are presented in Table 9-3, where again *i* is the row index and *j* is the column index:

Table 9-3 : Sensitivity Analysis for Measurement Test

$P_{i,j}$		Location of Adjustment								
		F	*C*	*T*	f_1	c_1	t_1	f_2	c_2	t_2
Location of Error	F	1.00	-0.85	-0.59	0.10	-0.02	-0.13	0.07	-0.07	-0.07
	C	-0.85	1.00	0.08	0.29	-0.07	-0.39	0.23	-0.23	-0.23
	T	-0.59	0.08	1.00	-0.64	0.16	0.85	-0.49	0.49	0.49
	f_1	0.10	0.29	-0.64	1.00	-0.81	-0.88	-0.16	0.16	0.16
	c_1	-0.02	-0.07	0.16	-0.81	1.00	0.44	0.71	-0.71	-0.71
	t_1	-0.13	-0.39	0.85	-0.88	0.44	1.00	-0.32	0.32	0.32
	f_2	0.07	0.23	-0.49	-0.16	0.71	-0.32	1.00	-1.00	-1.00
	c_2	-0.07	-0.23	0.49	0.16	-0.71	0.32	-1.00	1.00	1.00
	t_2	-0.07	-0.23	0.49	0.16	-0.71	0.32	-1.00	1.00	1.00

A detailed example of the required calculations to derive the numbers in Table 9-3 is provided in the appendix to this thesis.

The larger absolute magnitude ratios in Table 9-3 are highlighted red for ease of reference, as these indicate how a small error in the row measurement locations affects the column measurement locations, i.e. large off-diagonal elements are indicative of smearing.

Table 9-3 indicate that all measurement location experience smearing to some extent. The least affected location is *C*, with smearing of errors in this location occurring to location *F* only. All other locations smear onto 2 or more locations. It is notable that errors in f_2, c_2 and t_2 seem indistinguishable from each other by the MT. Bagajewicz [2010: 80] describes this phenomenon of the MT, which occurs when linear dependencies exist between the columns of the constraint matrix. The columns of the Jacobian matrix are not linearly dependent, and numeric anomaly in Table 9-3 occurred because the Jacobian matrix was assumed fixed for the purposes of the sensitivity analysis. If the Jacobian is allowed to vary for each δ_i of (9.1), the ratios in Table 9-3 would be altered slightly so that locations f_2, c_2 and t_2 would not appear identical, although the differences would only arise from the 4th decimal place onwards, and thus would not impact on the conclusions made regarding the sensitivity of the different measurement locations.

It is expected that the tendency for smearing to occur would impact adversely on the ability of the MT to resolve the Identification problem. The adjustability (from (4.94)) and detectability (from (4.95)) for each measurement location was calculated for the linearized system, and is presented in Table 9-4:

Table 9-4 : Adjustability and Detectability of Linearized System

	ADJUSTABILITY	DETECTABILITY
F	38.9%	79.1%
C	23.5%	64.3%
T	9.0%	41.4%
f_1	34.7%	75.8%
c_1	8.3%	39.9%
t_1	13.0%	49.3%
f_2	23.0%	63.8%
c_2	0.0%	0.2%
t_2	22.8%	63.6%

If 10% adjustability is chosen as a threshold level, then locations T, c_1 and c_2 are practically non-redundant, with t_1 being barely redundant. The detectability numbers confirm that c_2 can be expected to have very poor detection and identification, but the detectability of f_2 and t_2 compares well with that of the other locations, suggesting that reasonable detection/identification for gross errors in these locations should be expected. This is contrary to the conclusion drawn from Table 9-3. The apparent contradiction is due to the fact that the numbers in Table 9-3 is a measure of sensitivity based on the ratio of standardized adjustments, while the adjustability/detectability measures depend on the ratios of the adjustment standard deviation to the measurement standard deviation.

9.1.3 Properties of the Measurement Test

A key part of the methodology in this thesis is the equivalency of the Type I error rates between the MT and each of the classifiers. No attempt was made to modify or control the Type I error rates of the classifiers developed. The Type I error of the MT could be matched to each classifier by changing the cov_y from (7.6) associated with that classifier. It was verified that this manipulation would neither impact the DR solution or the location of the maximum MT statistic, i.e. only the Type I error of the MT would be modified. To illustrate this, the desired vs. actual Type I error rate of the MT for three different values of cov_y is presented in Figure 9-4:

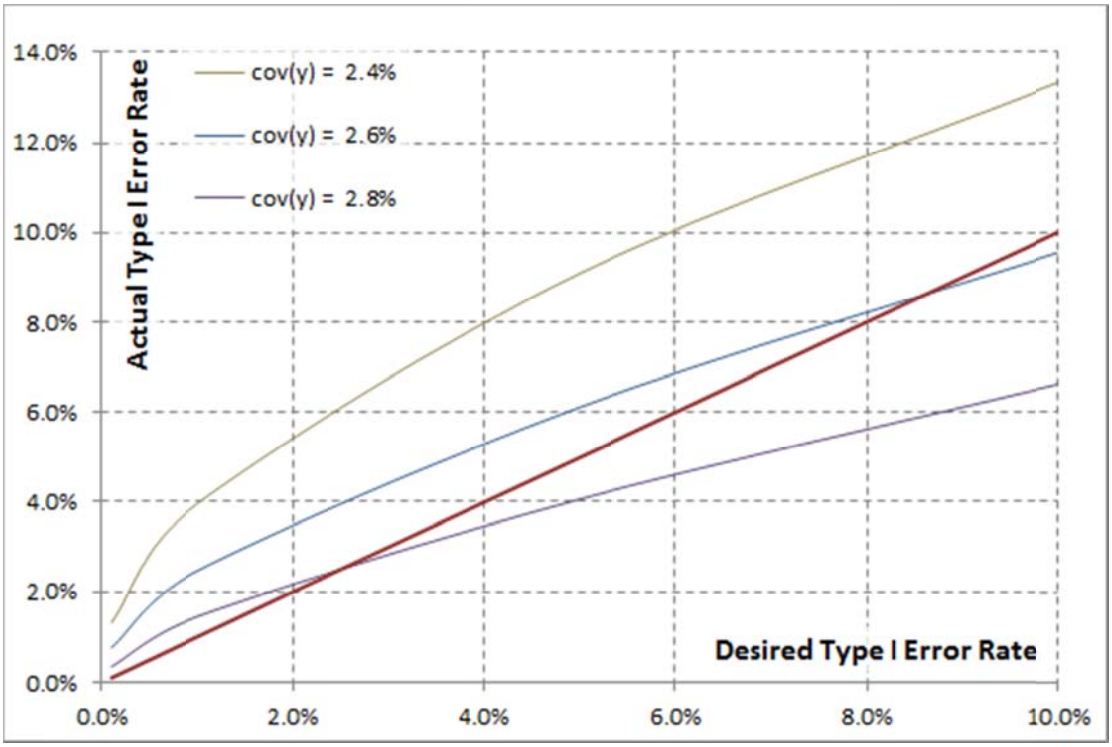

Figure 9-4 : Relationship between Type II and Type I Error for the Measurement Test

The red line indicates where the ordinate value equals that of the abscissa. The variation in Type I error for different cov_y is obvious. It is notable that the actual Type I error rate is non-linearly related to the desired Type I error for a given cov_y, i.e. in practice the real Type I error may be very different from the desired Type I error for this problem, and the magnitude of the difference is strongly dependent on the covariance of the measurements. This illustrates the importance of covariance estimation discussed in section 3 of this thesis.

9.2 THE CONTRIBUTION OF INDEPENDENT VARIABLES TO CLASSIFIER STRUCTURE

The elements of the independent variable used as input to the classification tree and discriminant methodologies were described before. The ability of a classification method to successfully detect and/or identify a gross error depends on the extent to which a gross error attenuates the elements of the independent variable, and the ability of the classification method to exploit this attenuation.

Understanding how the individual elements in the independent variable contribute to the structure of the classification method can help interpret classifier performance.

For the classification tree methodology, a measure of variable importance was obtained from the *predictorImportance* function in Matlab®. This function calculates the mean reduction in risk associated with each input variable, i.e. the larger the reduction in risk associated with a variable, the more important that variable is for classification tree performance. Matlab ® calculates the risk of a node as:

$$r(i) = p(i) \cdot e(i) \tag{9.5}$$

Where: $p(i)$ is the probability of the node (the proportion of training vectors that report to the node) and $e(i)$ is the node error, or probability of misclassification at the node.

Various methods exist to evaluate variable importance for linear discriminant classifiers. The method favoured by Rencher (1992) is to rank variables based on the absolute value of the standardized coefficient associated with each variable in the discriminant function.

Given that the measure of variable importance is different for the two classification methodologies, the variable importance for each method is ranked so that ranks of the different variables may be compared between the classification tree and linear discriminant classifiers.

9.2.1 Variable Importance for the Classification Tree Classifiers

Only considering the ranked contribution of each input variable to reduction in risk may be deceptive for classification trees, as a specific tree may split on few variables but still have complex structure. Ten trees were constructed for each of the detection problem and identification problem, i.e. 2 trees for each of 10 data sets. A summary of the number of input variables used, as well as the number of branch and leaf nodes in each tree is therefore given in Table 9-5:

Table 9-5 : Summary of Classification Tree Structure

Data Set	Detection Tree			Identification Tree		
	Split Var's	Branch Nodes	Leaf Nodes	Split Var's	Branch Nodes	Leaf Nodes
1	2	3	4	9	17	18
2	6	7	8	10	29	30
3	3	6	7	8	24	25
4	2	4	5	12	28	29
5	2	3	4	12	29	30
6	4	8	9	11	43	44
7	2	3	4	12	43	44
8	4	4	5	12	43	44
9	6	7	8	8	20	21
10	8	12	13	12	27	28

A variety of tree structures arise in both the detection and the identification problem. In general there is an increase in tree complexity, as measured by total number of nodes, when a larger number of elements of the input vector are utilized in the tree. The classification trees, where the problem contains 10 classes as opposed to the 2 of the detection trees, resulted in larger, more complex tree structures.

The rank for each variable based on this total reduction in risk is presented in Table 9-6:

Table 9-6 : Ranks based on Total Reduction in Risk by Independent Variable for Classification Trees solving the Detection Problem

Variable	Classification Tree 1	2	3	4	5	6	7	8	9	10	Mean
res_1											
res_2									5	4	4.5
res_3											
d(res)	2									3	2.5
ra_1		5									5.0
ra_2		6									6.0
ra_3											
ra_4									6	8	7.0
ra_5		2	2	2	2	3	2	3	2	2	2.2
ra_6											
ra_7		4				4		4	3	5	4.0
ra_8		3						2	4	6	3.8
ra_9			3			2				7	4.0
d(ra)	1	1	1	1	1	1	1	1	1	1	1.0

Only one variable, *d(ra),* is present in all classification trees used to solve the detection problem. This variable is the norm of the vector of measurement adjustments, and would be particularly sensitive to larger adjustments due to the presence of gross errors, which explains its importance to the Detection problem. It was verified that this variable was selected as the split variable on the root node of every detection tree developed, i.e. it was most valuable in separating the two classes for the Detection problem. The classification trees display a variety of structures, from simple trees that only employ 2 variables (trees # 1, 4, 5 and 7) to more complex tree that employ many variables (trees # 2, 9 and 10).

Qualitatively, as indicated by the mean ranks and frequency of occurrence in the tree structure, the relative adjustment of measurements was more important in solving the detection problem than the residuals of the balance equations in this case study. The diversity of the tree structures and degree dependence on the input variables is large when it is considered that the 10 data sets each contained 11 000 training vectors, generated using identical error variance assumptions, i.e. the only cause of the tree diversity is random fluctuations.

The rank for each variable based on this total reduction in risk is presented in Table 9-7:

Table 9-7 : Ranks based on Total Reduction in Risk by Independent Variable for Classification Trees solving the Identification Problem

Variable	Tree 1	2	3	4	5	6	7	8	9	10	Mean
res_1							10	11			10.5
res_2		8			8				8	11	8.8
res_3	4	4	4	5	4	4	4	3	5	4	4.1
d(res)	1	1	1	1	1	1	1	1	1	1	1.0
ra_1				12	9	10		8		12	10.2
ra_2	9	9		7	12		8	9		9	9.0
ra_3	3	5	5	4	5	5	5	5	4	5	4.6
ra_4			7	11		8	11	12			9.8
ra_5	2	3	2	2	2	3	2	2	2	2	2.2
ra_6	8	7		8	10	11	7			7	8.3
ra_7		6		10	7	7	12	7		10	8.4
ra_8	6		8	9	6	6	6	6	7	8	6.9
ra_9	7	10	6	6	11	9	9	10	6	6	8.0
d(ra)	5	2	3	3	3	2	3	4	3	3	3.1

For the identification problem, most of the input variables contributed to some extent to the tree structures. Variables that consistently played an important role are *d(res)*, ra_5, *d(ra)*, res_3 and ra_3. The contribution of variables res_1 and res_2 was marginal. It was observed that *d(res)* was selected as the split variable for the root node in all identification trees, and that in general smaller values of *d(res)* were associated with either random error vectors or gross errors in measurements locations 4 to 9, while larger values were associated with locations 1 to 3. It seems that *d(res)* is important in distinguishing between random and gross error vectors, as well as gross errors in larger and smaller magnitude measurements. Interpreting the relative importance of the other variables is difficult from such a casual study due to the conditional probabilistic nature of the classification tree methodology.

9.2.2 Variable Importance for the Linear Classification Function

The measure of variable importance used for the linear classification function (LCF) is absolute value of the standardized coefficient associated with each input variable. Although there are statistical procedures that can be used to select only the most important input variables for inclusion in the classification model, such a detailed analysis did not fit in the scope of this study. The ranks based on absolute value of the coefficients in the LCF, are presented in Table 9-8:

Table 9-8 : Ranks based on Standardized Coefficients of Linear Classification Functions solving the Detection Problem

	Linear Classification Function										
Variable	1	2	3	4	5	6	7	8	9	10	Mean
res_1	1	2	1	2	3	2	1	2	5	7	2.6
res_2	13	1	6	1	8	7	3	3	2	10	5.4
res_3	3	4	9	4	14	13	6	5	3	14	7.5
d(res)	12	13	11	10	10	9	11	11	13	9	10.9
ra_1	6	11	3	5	2	3	9	7	4	3	5.3
ra_2	5	12	8	12	11	8	7	13	6	8	9.0
ra_3	8	7	13	14	9	11	10	9	10	13	10.4
ra_4	14	10	12	11	7	14	14	10	12	12	11.6
ra_5	4	6	4	8	5	4	5	8	9	2	5.5
ra_6	2	3	2	3	1	1	2	1	1	1	1.7
ra_7	11	14	14	13	12	12	12	14	11	11	12.4
ra_8	7	9	10	9	13	10	13	12	14	4	10.1
ra_9	10	5	5	6	4	6	4	4	8	6	5.8
d(ra)	9	8	7	7	6	5	8	6	7	5	6.8

From the mean ranks it is clear that the residuals of the balance equations played a larger role in resolving the detection problem with the linear discriminant classifier than it did with the classification tree. It is noteworthy that ra_6 and res_1 are the most important variables for the LCF, whereas these variables did not feature in any of the classification trees solving the Detection problem.

It is difficult to interpret the reasons for the differences in relative variable importance between the CT and LCF for the Detection problem, although the underlying reason must be rooted in the difference in classification rules for the methods, i.e. the use of a measure of class purity as opposed the use of a measure of distance.

Whereas the Detection problem has 2 classes corresponding to whether a gross error is present or not, the Identification problem has 10 classes – corresponding to each of the 9 possible measurement locations, and one class for the case where no gross error is present. The coefficients of the linear classification function for the identification problem is obtained by multiplying the mean vector for each class with the within-class covariance matrix, as per (5.27), resulting in 10 sets of coefficients for each of the 10 linear classification functions constructed for each data set. For each data set, the coefficients as well as their ranks based on absolute value were averaged. The ranks based on absolute value, are presented in Table 9-9:

Table 9-9 : Ranks based on Standardized Coefficients for Linear Classification Functions solving the Identification Problem

	Linear Classification Function										
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**Mean**
res_1	4.0	2.0	2.0	5.0	3.0	9.0	11.0	12.0	4.0	3.0	5.5
res_2	8.0	11.0	10.0	10.0	1.0	1.0	4.0	4.0	9.0	7.0	6.5
res_3	11.0	5.0	6.0	2.0	6.0	5.0	10.0	5.0	10.0	9.0	6.9
d(res)	12.0	14.0	14.0	13.0	13.0	14.0	14.0	14.0	12.0	13.0	13.3
ra_1	2.0	1.0	4.0	4.0	4.0	2.0	2.0	2.0	2.0	2.0	2.5
ra_2	1.0	6.0	1.0	1.0	2.0	3.0	1.0	1.0	1.0	1.0	1.8
ra_3	3.0	4.0	3.0	6.0	10.0	4.0	5.0	3.0	3.0	4.0	4.5
ra_4	5.0	3.0	5.0	11.0	5.0	12.0	6.0	11.0	5.0	5.0	6.8
ra_5	9.0	7.0	9.0	12.0	12.0	8.0	8.0	13.0	8.0	11.0	9.7
ra_6	6.0	12.0	13.0	3.0	7.0	6.0	3.0	10.0	6.0	6.0	7.2
ra_7	14.0	13.0	12.0	8.0	11.0	13.0	9.0	9.0	14.0	10.0	11.3
ra_8	13.0	10.0	11.0	14.0	14.0	11.0	12.0	7.0	13.0	14.0	11.9
ra_9	10.0	9.0	8.0	9.0	9.0	7.0	13.0	6.0	11.0	12.0	9.4
d(ra)	7.0	8.0	7.0	7.0	8.0	10.0	7.0	8.0	7.0	8.0	7.7

The relative adjustments of measurements F_1 and F_2 were consistently the most important input variables for resolving the Identification problem through the LCF. This is markedly different from the corresponding classification tree classifier, where these variables played a minor role.

As for the Detection problem, this difference in variable importance between the two classification methods is not just attributable to the different measures of variable importance used between the two methodologies, but points to the fundamentally different way the input variables are used to construct classification rules.

9.2.3 Summary of Variable Importance

The average ranks of the input variables for all classifiers are presented in Figure 9-5:

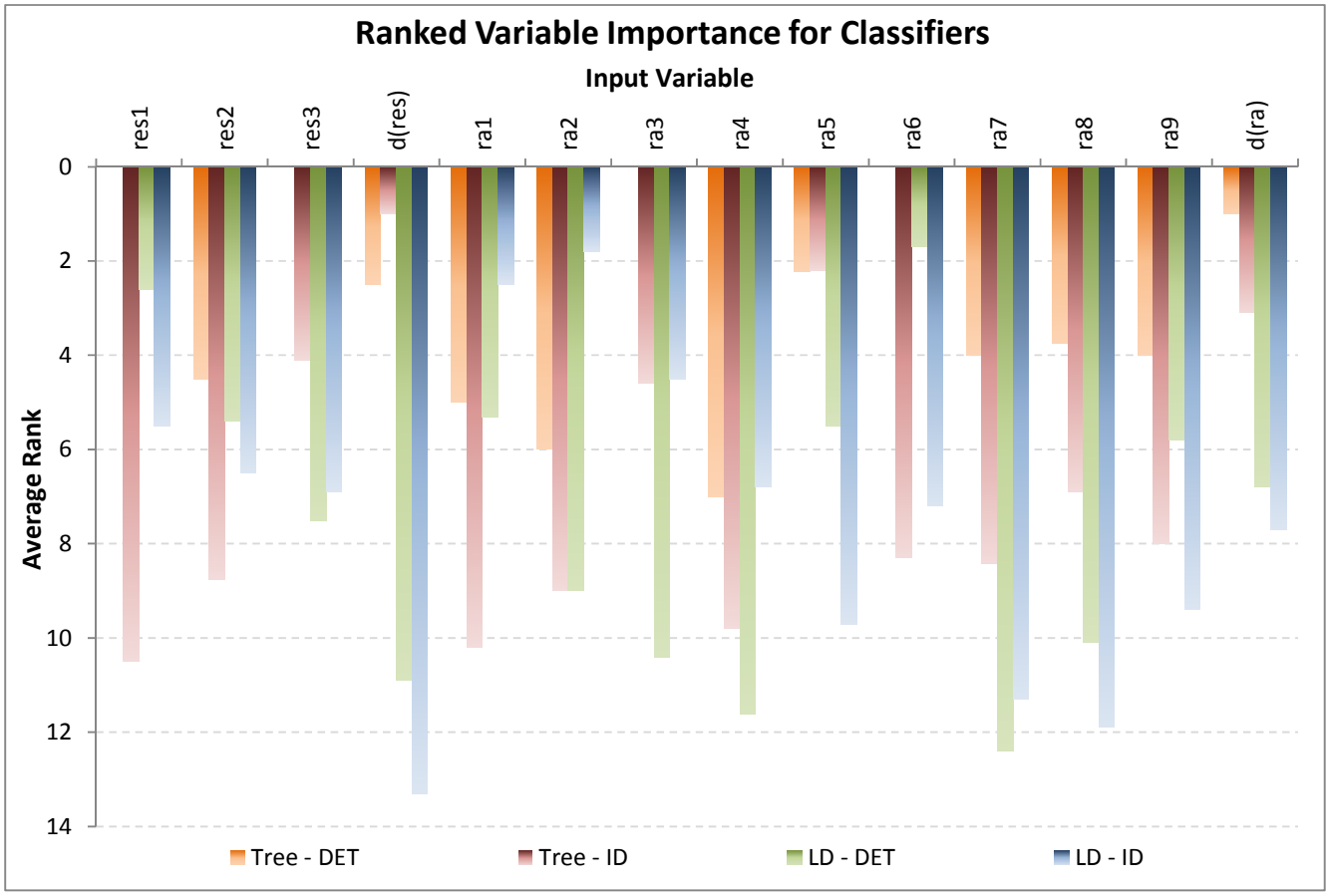

Figure 9-5 : Mean Ranks of Input Variables for all Classifiers

The diverse nature of the classifiers, and the two classification problems, is illustrated through the relative variable importance:

The Detection trees did not make use of several of the input variables, res_1, res_3, ra_3 and ra_6. The importance of these variables to the Identification trees ranged from relatively unimportant (res_1 and ra_6) with mean ranks of 10.5 and 8.3 respectively, to ranking on average 4.1 and 4.6 for res_3 and ra_3. The norm of the vector of balance residuals *d(res)*, as well as the norm for the vector of measurement adjustments *d(ra)*, played an important role in both the classification trees. For the Detection problem, it is hypothesized that these variables are important due to their sensitivity to larger errors in the measurements. Inspection of the tree structures revealed that these variables were always the split variable on the root nodes for the Identification and Detection problems respectively.

For the linear discriminant/classification functions, the residuals of the balance equations played a larger role in the Detection problem, while the relative adjustments, specifically ra_1, ra_2, ra_3, and ra_4 were more important for the Identification problem, although ra_6 was the highest ranked variable for the Detection problem. Intuitively it would be expected for Identification to be more reliant on features of the measurement adjustment vector, whereas the balance residuals are not directly related to the location of a gross error, but a function of all the measurement errors in the measurements relevant to the particular balance equation.

Since not all variables are present in the structure of the classification trees, not all variables were ranked for the classification tree methodology. This introduces a bias when analysing the ranks, and the ranks for the classification trees should not be compared with those of the linear classification functions.

9.3 Results for the Detection Problem

The results pertaining to the performance of the classification methodologies relative to the Measurement Test in resolving the detection problem is presented in the following sections. The results will be displayed as the proportion of vectors correctly detected or identified for different gross error magnitudes and locations. Gross error magnitudes and locations of zero correspond to random error vectors. Therefore, the Type I error rate can be deduced from the proportion of correctly detected/identified vectors for this magnitude/location, as the sum of Type I error and correctly identified vectors must equal 100%. For all other magnitudes and locations, the reported proportion correctly detected/identified vectors is identical to the statistical power of the method.

9.3.1 Detection Results for the Classification Tree Classifier

The mean proportion of vectors correctly classified over the 9 test sets by the classification tree method and its corresponding Measurement Test is presented in Table 9-10 for different gross error magnitudes:

Table 9-10 : Proportion of Vectors Correctly Detected by Classification Tree Classifier vs. Gross Error Magnitude

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	80.8%	82.6%	84.9%	67.4%	70.4%	79.7%	87.5%	80.5%	79.0%	72.3%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	2.3%	1.4%	0.4%	5.0%	2.9%	1.2%	0.3%	1.0%	1.5%	5.2%
	1.5	12.1%	9.8%	6.2%	24.0%	21.3%	11.7%	4.4%	10.0%	11.6%	19.7%
	2.0	25.4%	23.0%	21.3%	42.6%	40.4%	27.2%	17.3%	26.1%	28.7%	34.3%
	2.5	37.5%	36.3%	35.5%	54.6%	50.5%	40.4%	30.4%	39.0%	42.0%	46.9%
	3.0	45.9%	44.8%	45.0%	61.3%	57.6%	50.0%	39.7%	47.9%	50.9%	56.1%
	3.5	51.8%	52.1%	52.7%	66.5%	63.2%	56.3%	47.3%	54.7%	57.7%	63.0%
	4.0	57.1%	56.6%	58.0%	70.2%	66.8%	62.4%	52.0%	60.3%	63.5%	68.4%
	4.5	60.6%	61.6%	63.0%	74.1%	69.8%	68.0%	57.6%	65.3%	66.8%	72.3%
	5.0	65.5%	67.2%	68.7%	77.9%	73.9%	72.1%	62.0%	70.3%	72.4%	76.9%
		Measurement Test for Classification Tree									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	80.8%	82.6%	84.9%	67.5%	70.4%	79.7%	87.5%	80.5%	79.0%	72.3%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	0.9%	0.6%	0.2%	6.3%	4.3%	0.9%	0.0%	1.0%	1.0%	3.3%
	1.5	11.1%	9.9%	7.7%	26.4%	22.9%	11.7%	5.6%	11.3%	12.8%	20.1%
	2.0	26.2%	24.3%	21.3%	42.4%	39.7%	26.9%	17.4%	26.7%	28.0%	36.6%
	2.5	36.0%	34.8%	31.2%	52.1%	48.7%	37.3%	27.6%	36.4%	38.4%	46.2%
	3.0	42.6%	41.3%	37.6%	57.1%	54.4%	43.6%	34.9%	43.0%	44.6%	51.8%
	3.5	47.6%	46.4%	43.4%	61.4%	59.1%	48.5%	39.9%	48.1%	49.7%	57.0%
	4.0	51.6%	50.1%	47.0%	65.4%	63.1%	52.4%	43.8%	51.8%	53.3%	60.8%
	4.5	56.0%	54.0%	51.3%	68.5%	66.0%	56.8%	47.8%	55.8%	57.1%	63.0%
	5.0	59.4%	58.2%	54.8%	72.2%	69.7%	60.3%	51.8%	59.3%	61.2%	67.9%

The results for zero magnitude indicate relative poor type I error rates ranging from ~12.5% to ~32.6%. The power to detect a gross error ranged from 0.0% for the smallest gross error magnitudes, to 77.9% for the largest magnitudes for the classification tree, and between 0.0% and 72.2% for the Measurement Test. It is noteworthy that gross errors with magnitudes of 0.5 and 1.0 were almost undetectable.

It is expected that larger gross error magnitudes will create a greater distortion in the elements of the independent vector, and therefore will be easier to detect. The strength of the linear relationship between power to detect and gross error magnitude was tested through regression analysis, the results of which are displayed in Table 9-11, where the degrees of freedom associated with the numerator and denominator of each F-statistic is respectively 1 and 9:

Table 9-11 : Linear Regression of Power to Detect vs. Gross Error Magnitude for Classification Tree

Tree #		1	2	3	4	5	6	7	8	9	10
CT	Slope	15.873%	16.438%	17.200%	18.110%	17.399%	17.785%	15.707%	17.326%	17.741%	18.194%
	F	226.28	278.15	246.37	87.11	87.19	237.34	258.00	233.61	188.61	185.81
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
MT	Slope	14.476%	14.193%	13.586%	16.272%	16.045%	14.651%	12.923%	14.429%	14.748%	15.747%
	F	160.47	165.75	198.62	73.99	82.28	149.97	231.96	148.37	136.87	92.86
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

All the regressions are significant at the modified 0.25% level of significance for 20 simultaneous tests, indicating a strong linear relationship between power to detect and gross error magnitude.

The proportion of correctly detected gross errors reported in Table 9-10 suggest that the classification tree was superior in resolving the detection problem. In order to better quantify the difference in performance between the classification tree and Measurement Test, the difference between the proportions correctly classified, where such difference was determined as significant by the McNemar statistic, was averaged over the 9 test sets for each classification tree. The results for the average significant differences are displayed in Table 9-12:

Table 9-12 : Mean Magnitude of Outperformance vs. Gross Error Magnitude of Classification Tree solving the Detection Problem

GE Magnitude	Classification Tree 1	2	3	4	5	6	7	8	9	10
	Mean Underperformance									
0.0										
0.5										
1.0					-2.85%					
1.5			-2.69%	-4.61%	-2.60%				-3.91%	
2.0		-5.61%								-6.26%
2.5										
3.0										
3.5										
4.0										
4.5										
5.0										
	Mean Outperformance									
0.0										
0.5										
1.0										
1.5	3.74%									
2.0				3.33%	2.19%					
2.5	4.10%	4.03%	4.60%	4.43%	4.25%	4.93%	3.75%	4.68%	4.92%	
3.0	5.00%	6.41%	7.40%	5.08%	3.83%	6.75%	5.03%	5.60%	6.69%	6.00%
3.5	5.93%	6.80%	9.35%	5.23%	4.63%	7.79%	7.45%	7.07%	8.00%	6.72%
4.0	6.30%	8.21%	10.98%	5.50%	4.25%	9.98%	8.99%	8.52%	10.20%	7.59%
4.5	5.84%	8.17%	11.71%	5.62%	4.08%	11.16%	9.77%	9.49%	9.75%	9.33%
5.0	7.25%	9.59%	13.86%	6.25%	5.14%	11.87%	10.16%	11.04%	11.19%	9.83%

The classification tree had lower power on some data sets for small gross error magnitudes, and consistently displays higher power for larger gross error magnitudes. The magnitude of the significant differences in power between the two methods seems related to gross error magnitude. The section on variable importance showed that the norm of the vector of relative adjustments was consistently the most important input variable for detection tree performance. The norm would be sensitive to adjustments in all of the measurements, whereas the Measurement Test only considers the largest of the measurement adjustments. Further, the magnitude of the norm would increase more than 1:1 for a corresponding increase in one of the measurement adjustments, the measurement adjustments being a function of the magnitude of the error in the measurements. This could explain the outperformance of the tree methodology and the dependence of this outperformance on gross error magnitude.

The counts associated with the mean significant differences in Table 9-12 are presented in Table 9-13:

Table 9-13 : Counts for Data Sets with Significant McNemar Statistics by Magnitude for the Classification Tree solving the Detection Problem

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0					1					
	1.5			1	2	2				1	
	2.0		1								2
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Count of Significant Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5	1									
	2.0				1	2					
	2.5	2	1	8	4	2	4	5	4	5	
	3.0	4	3	9	7	7	8	8	8	8	4
	3.5	5	6	9	8	7	9	9	8	9	7
	4.0	7	6	9	7	7	9	8	9	9	9
	4.5	4	8	9	9	8	9	9	9	9	9
	5.0	6	8	9	7	6	9	9	9	9	8

The Measurement Test has superior performance on only 1 or 2 data sets for small gross error magnitudes, while the classification tree has superior performance on almost all the data sets for larger magnitudes.

This concludes the results and discussion on detection power relative to gross error magnitude for the classification tree classifier. The effect of gross error location is discussed next. Gross error locations were indexed numerically from 1 through 9, where the numerical indexes correspond to measurement locations as per Table 9-14:

Table 9-14 : Gross Error Location Indices

Measurement	F	C	T	f_1	c_1	t_1	f_2	c_2	t_2
Index	1	2	3	4	5	6	7	8	9

The mean proportion of vectors correctly classified by the classification tree method and its corresponding Measurement Test is presented in Table 9-15 for different gross error locations:

Table 9-15 : Proportion of Vectors Correctly Detected by Classification Tree vs. Gross Error Location

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	80.8%	82.6%	84.9%	67.4%	70.4%	79.7%	87.5%	80.5%	79.0%	72.3%
	1	36.9%	35.2%	37.0%	56.8%	56.7%	39.1%	35.5%	42.8%	41.6%	42.2%
	2	74.3%	69.8%	75.8%	87.6%	89.3%	76.8%	73.8%	79.1%	78.0%	67.4%
	3	68.0%	59.1%	62.2%	72.2%	72.9%	64.6%	51.5%	66.8%	70.5%	73.8%
	4	57.5%	53.3%	52.9%	73.8%	66.0%	59.1%	57.1%	50.3%	62.1%	73.0%
	5	32.0%	43.1%	37.1%	53.4%	44.2%	43.5%	33.3%	37.5%	41.4%	53.1%
	6	36.6%	25.9%	25.4%	46.0%	43.0%	31.6%	23.2%	28.3%	36.0%	44.0%
	7	26.9%	34.6%	32.2%	42.2%	38.2%	38.8%	20.6%	36.8%	33.4%	43.2%
	8	15.5%	14.4%	11.8%	27.7%	25.0%	16.1%	9.7%	15.7%	16.9%	23.5%
	9	26.2%	33.6%	31.1%	41.6%	36.8%	37.3%	19.0%	35.3%	33.4%	42.3%
		Measurement Test for Classification Tree									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	80.8%	82.6%	84.9%	67.5%	70.4%	79.7%	87.5%	80.5%	79.0%	72.3%
	1	48.2%	46.5%	43.3%	60.8%	58.6%	48.6%	40.5%	47.9%	49.8%	56.7%
	2	84.0%	83.1%	81.2%	92.2%	90.8%	85.0%	78.8%	84.5%	85.4%	89.6%
	3	64.1%	62.8%	59.8%	77.5%	75.2%	65.2%	56.3%	64.7%	66.5%	73.0%
	4	46.2%	44.3%	40.7%	61.8%	59.0%	47.1%	36.9%	46.5%	48.2%	56.1%
	5	22.1%	20.7%	17.7%	39.4%	35.8%	23.1%	13.9%	22.5%	24.0%	32.8%
	6	30.7%	29.0%	25.4%	46.1%	43.1%	32.0%	22.1%	30.8%	32.8%	40.9%
	7	19.2%	17.7%	14.9%	35.8%	32.6%	20.4%	12.7%	19.7%	21.5%	29.3%
	8	15.3%	14.5%	11.9%	28.2%	25.6%	15.7%	9.7%	15.7%	16.7%	23.2%
	9	19.0%	17.6%	14.3%	35.0%	31.6%	19.6%	11.5%	19.2%	20.7%	28.6%

The power to detect ranges between 9.7% and 92.2% for different locations and classification trees. It appears as if there is a definitive relationship between location and power. This was tested with an ANOVA on the data for the classification tree:

Table 9-16 : ANOVA for Detection – Classification Tree and Location

ANOVA - Proportion Correctly Classified vs. GE Location - Classification Tree						
Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
GE Location	3.83610	9	4.26E-01	134.488	0.0000%	1.998
Classification Tree	0.21593	9	2.40E-02	7.570	0.0000%	1.998
Error	0.25671	81	3.17E-03			
Total	4.30874	99				

The ANOVA indicates that both the classification tree and location has a significant impact on power to detect. The proportions of correctly detected vectors presented in Table 9-15 suggest that the classification tree has greater power than the Measurement Test for some locations, and vice versa for other locations. As was done for the comparison on gross error magnitudes, the average of positive and negative differences that were determined to be significant by the McNemar statistic over the 9 test data sets were calculated:

Table 9-17 : Mean Magnitude of Outperformance vs. Gross Error Location of Classification Tree solving the Detection Problem

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Location	0										
	1	-11.27%	-11.33%	-6.33%	-4.27%	-2.59%	-9.47%	-5.00%	-5.14%	-8.21%	-14.49%
	2	-9.66%	-13.33%	-5.36%	-4.64%	-1.86%	-8.16%	-4.94%	-5.41%	-7.38%	-22.22%
	3		-5.15%		-5.31%	-2.74%		-4.81%			
	4										
	5										
	6		-6.08%						-4.09%		
	7										
	8										
	9										
		Mean Outperformance									
GE Location	0										
	1										
	2										
	3	4.74%		6.15%					4.03%	4.26%	
	4	11.28%	9.08%	12.14%	11.94%	7.03%	12.06%	20.20%	4.77%	13.83%	16.94%
	5	9.91%	22.32%	19.45%	14.01%	8.35%	20.43%	19.39%	15.05%	17.49%	20.28%
	6	6.72%						2.59%		4.57%	4.83%
	7	7.65%	16.95%	17.37%	6.76%	5.61%	18.38%	7.94%	17.06%	11.97%	13.86%
	8										
	9	7.20%	15.92%	16.75%	7.56%	5.65%	17.73%	7.43%	16.11%	12.70%	13.64%

The results of Table 9-17 indicate that the Measurement Test is significantly better for location 1 and 2, while the classification tree is better for locations 4, 5, 7 and 9. Locations 3 and 6 produce conflicting results, while no significant differences existed for location 8.

The counts associated with the averages presented in Table 9-17 are presented in Table 9-18:

Table 9-18 : Counts for Data Sets with Significant McNemar Statistics by Location for the Classification Tree solving the Detection Problem

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Location	0										
	1	9	9	9	8	5	9	9	9	9	9
	2	9	9	9	9	7	9	9	9	9	9
	3		3		9	7		9			
	4										
	5										
	6		2						2		
	7										
	8										
	9										
		Count of Significant Outperformance									
GE Location	0										
	1										
	2										
	3	6		1					2	8	
	4	9	9	9	9	9	9	9	5	9	9
	5	9	9	9	9	9	9	9	9	9	9
	6	7						1		5	3
	7	9	9	9	8	9	9	9	9	9	9
	8										
	9	9	9	9	7	8	9	9	9	9	9

The counts of significant differences confirm the conclusions drawn on relative performance by location.

The results of this section indicate that the classification tree methodology may be an attractive alternative to the Measurement Test to solve the Detection problem. Practical implementation may be problematic due to several factors:

- The reproducibility of the methodology is poor as indicated by the ANOVA on power vs. location. This is despite large training samples being used.
- The methodology will always depend on the representativeness of the training sample.
- It is not clear how the trade-off between type I and type II error may be optimized for the methodology, although the trade-off may be manipulated by changing training parameters.

This concludes the discussion of the results for the classification tree methodology solving the Detection problem. The results for the linear classification methodology will be presented in the following section.

9.3.2 Detection Results for the Linear Classification Function

The second classification methodology employed was the linear classification function (LCF). The mean proportions of vectors correctly classified by the LCF classifier and its associated Measurement Test for different gross error magnitudes are displayed in Table 9-19:

Table 9-19 : Proportion of Vectors Correctly Detected by Linear Classification Function vs. Gross Error Magnitude

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	67.3%	69.6%	68.6%	64.8%	67.9%	64.6%	68.6%	67.3%	64.2%	65.9%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	3.6%	2.4%	3.5%	5.1%	3.6%	4.3%	4.0%	3.5%	4.3%	4.0%
	1.5	24.2%	20.9%	22.4%	26.0%	23.5%	26.7%	23.0%	23.3%	26.7%	24.8%
	2.0	44.1%	41.0%	42.6%	45.2%	43.3%	46.6%	41.7%	43.7%	46.8%	45.1%
	2.5	55.9%	53.9%	54.9%	57.7%	55.4%	58.3%	55.1%	55.7%	58.4%	57.0%
	3.0	63.2%	61.7%	61.7%	64.4%	62.3%	64.6%	62.3%	62.3%	64.8%	63.4%
	3.5	68.4%	67.4%	67.9%	69.4%	68.2%	69.7%	67.7%	68.2%	70.0%	68.9%
	4.0	72.6%	71.7%	71.8%	73.8%	71.8%	74.0%	72.2%	72.2%	74.3%	72.9%
	4.5	75.4%	74.4%	74.8%	77.0%	75.0%	76.8%	75.3%	75.4%	77.0%	75.9%
	5.0	79.9%	79.0%	78.9%	81.0%	79.0%	79.9%	78.8%	79.4%	80.6%	79.8%
		Measurement Test for Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	67.3%	69.6%	68.5%	64.8%	67.9%	64.6%	68.6%	67.3%	64.2%	65.9%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	6.3%	4.7%	5.5%	7.9%	5.6%	7.3%	5.4%	5.8%	7.7%	7.0%
	1.5	26.3%	23.9%	24.7%	29.1%	25.5%	28.9%	25.0%	26.1%	29.6%	27.7%
	2.0	42.6%	40.6%	41.7%	45.1%	42.5%	45.4%	41.4%	42.9%	45.8%	44.2%
	2.5	51.9%	50.3%	50.9%	54.7%	51.5%	55.0%	50.8%	52.0%	55.1%	53.4%
	3.0	57.2%	55.6%	55.7%	59.5%	56.5%	59.8%	56.4%	57.0%	60.0%	58.2%
	3.5	61.8%	60.4%	61.2%	63.7%	61.6%	64.3%	60.9%	61.9%	64.7%	63.3%
	4.0	65.8%	63.8%	64.5%	67.6%	65.0%	68.0%	64.7%	65.5%	68.3%	66.8%
	4.5	68.8%	66.8%	67.6%	70.5%	68.5%	71.5%	67.8%	68.6%	71.4%	69.8%
	5.0	72.4%	71.0%	71.3%	74.2%	71.5%	74.0%	71.2%	72.1%	74.8%	73.4%

The type I error rate ranged from 30.4% to 35.8%. The power of the LCF ranged from 0.0% to 81.0% for different magnitudes. Magnitudes of 0.5 were undetectable, but some errors with magnitude 1.0 could be detected, in contrast with the classification tree methodology.

As before, the strength of the linear relationship between power and gross error magnitude was tested through regression analysis, the results of which are displayed in Table 9-20:

Table 9-20 : Linear Regression of Power to Detect vs. Gross Error Magnitude for Linear Classification Function

LCF #		1	2	3	4	5	6	7	8	9	10
LDA	Slope	18.716%	18.855%	18.659%	18.801%	18.598%	18.640%	18.661%	18.694%	18.767%	18.671%
	F	81.04	91.06	86.64	80.06	82.57	69.43	89.11	83.25	70.87	76.56
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
MT	Slope	16.366%	16.217%	16.220%	16.479%	16.282%	16.626%	16.249%	16.328%	16.648%	16.457%
	F	75.63	78.25	76.53	66.52	73.05	64.87	76.26	71.82	65.27	69.52
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

All the regressions are significant at the modified 0.25% level of significance for 20 simultaneous tests, indicating a strong linear relationship between power to detect and gross error magnitude.

The proportions of correctly classified vectors in Table 9-19 suggest that the LCF method achieved higher power to detect a gross error than the Measurement Test. The average value of the difference in power between the LCF and the Measurement Test for data sets where the McNemar statistic indicates significance is presented in Table 9-21:

Table 9-21 : Mean Magnitude of Significant Outperformance vs. Gross Error Magnitude of Linear Classification Function solving the Detection Problem

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0	-4.6%	-4.7%	-4.3%	-4.8%	-3.7%	-4.3%		-4.3%	-5.1%	-4.9%
	1.5	-5.0%	-4.5%	-3.4%	-4.3%	-3.9%	-4.2%	-3.5%	-3.3%	-3.7%	-3.8%
	2.0		-4.3%		-6.0%		-4.0%			-3.9%	
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Mean Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0	3.5%	3.3%	3.3%	3.3%	3.2%	3.6%	3.8%	3.1%	3.3%	3.0%
	2.5	5.0%	4.5%	5.3%	4.5%	5.2%	3.8%	5.1%	5.1%	4.4%	4.6%
	3.0	6.4%	6.3%	5.9%	5.7%	5.9%	5.1%	6.0%	5.7%	6.1%	6.1%
	3.5	6.6%	7.5%	7.1%	6.0%	6.8%	5.7%	7.4%	6.5%	5.6%	5.8%
	4.0	6.8%	7.9%	7.3%	6.7%	6.7%	6.4%	7.6%	6.7%	6.3%	6.1%
	4.5	6.6%	7.8%	7.2%	6.5%	6.6%	5.5%	7.5%	7.1%	5.9%	6.2%
	5.0	7.4%	8.0%	7.6%	7.2%	7.5%	6.2%	7.5%	7.6%	6.6%	7.3%

The Measurement Test was superior for smaller magnitudes, while the LCF was superior for larger magnitudes. As with the classification tree, the magnitude of the difference in power seems to be a function of gross error magnitude. Since the norms of the residuals and adjustments vectors were included in the input vector of the LCF, a similar argument can be made as was done for the classification tree to explain the dependence of outperformance on gross error magnitude.

The counts associated with the averages presented in Table 9-21 are presented in Table 9-22:

Table 9-22 : Counts of Data Sets with Significant McNemar Statistics by Magnitude for the Linear Classification Function solving the Detection Problem

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0	1	1	2	1	1	3		2	3	2
	1.5	1	4	2	5	1	2	1	4	5	6
	2.0		1		1		1			1	
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Count of Significant Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0	2	2	1	1	1	1	1	1	1	1
	2.5	6	7	7	5	6	8	8	5	6	6
	3.0	8	8	9	7	8	8	8	8	6	7
	3.5	9	8	8	8	8	8	8	8	8	8
	4.0	9	9	9	8	9	8	9	9	8	9
	4.5	9	8	9	9	9	8	9	8	8	8
	5.0	9	9	9	8	9	8	9	8	7	7

The outperformance of the Measurement Test for smaller magnitudes occurred on relatively few data sets, while that for the LCF at larger magnitudes is consistent on most data sets.

The results for the LCF classifier with respect to gross error location are discussed next. For convenience, the location indices for the measurements are repeated in Table 9-23:

Table 9-23 : Gross Error Location Indices

Measurement	F	C	T	f_1	c_1	t_1	f_2	c_2	t_2
Index	1	2	3	4	5	6	7	8	9

The mean proportions of vectors correctly classified by the LCF for different gross error locations are displayed in Table 9-24:

Table 9-24 : Proportion of Vectors Correctly Detected by Linear Classification Function vs. Gross Error Location

	Linear Classification Function									
	1	2	3	4	5	6	7	8	9	10
GE Location 0	67.3%	69.6%	68.6%	64.8%	67.9%	64.6%	68.6%	67.3%	64.2%	65.9%
1	59.0%	59.6%	60.0%	60.4%	60.8%	62.0%	60.7%	59.1%	61.5%	58.1%
2	83.2%	81.8%	83.5%	84.6%	84.1%	87.7%	81.2%	84.5%	87.2%	86.1%
3	80.3%	76.7%	77.9%	79.7%	78.1%	80.6%	77.8%	79.4%	80.4%	79.6%
4	72.7%	70.7%	72.1%	72.7%	73.2%	73.2%	72.2%	71.7%	74.1%	74.0%
5	55.2%	56.0%	55.5%	57.3%	54.4%	57.6%	56.9%	54.6%	57.3%	55.7%
6	49.4%	46.6%	47.0%	51.4%	47.6%	51.1%	48.0%	49.0%	51.8%	49.6%
7	43.6%	42.2%	42.3%	47.8%	42.1%	44.6%	42.1%	43.6%	45.5%	45.5%
8	28.0%	25.6%	26.7%	29.8%	27.3%	29.9%	26.9%	27.9%	30.5%	29.0%
9	41.3%	38.5%	39.4%	43.0%	41.2%	42.1%	39.8%	40.8%	43.6%	42.2%
	Measurement Test for Linear Classification Function									
	1	2	3	4	5	6	7	8	9	10
GE Location 0	67.3%	69.6%	68.5%	64.8%	67.9%	64.6%	68.6%	67.3%	64.2%	65.9%
1	60.9%	59.4%	59.9%	62.6%	60.6%	62.9%	60.1%	60.8%	63.3%	62.1%
2	92.1%	91.2%	91.7%	92.9%	92.0%	93.0%	91.7%	92.1%	93.1%	92.6%
3	77.3%	76.2%	76.7%	79.6%	77.1%	79.9%	76.6%	77.6%	80.0%	78.6%
4	62.2%	60.0%	60.8%	64.7%	61.6%	64.8%	61.0%	61.9%	65.5%	63.3%
5	39.7%	37.2%	38.7%	42.3%	38.9%	42.8%	38.4%	39.4%	43.5%	41.3%
6	46.0%	44.3%	44.6%	48.4%	45.5%	49.2%	45.0%	46.1%	49.1%	47.7%
7	35.7%	33.8%	34.5%	38.7%	35.5%	38.7%	35.0%	35.9%	39.4%	37.3%
8	28.3%	26.4%	27.0%	30.8%	28.0%	30.7%	27.1%	28.5%	31.6%	30.1%
9	35.2%	33.4%	33.9%	38.0%	34.8%	38.3%	34.3%	35.3%	38.9%	37.1%

The power to detect varies between 25.6% and 87.7% for the LCF at different locations, and between 26.4% and 93.1% for the Measurement Test. As for the classification tree, an ANOVA was performed to test for significant differences in power:

Table 9-25 : ANOVA for Detection – Linear Classification Function and Location

ANOVA - Proportion Correctly Classified vs. GE Location - Linear Classification Function						
Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
GE Location	2.89106	9	3.21E-01	1715.834	0.0000%	1.998
LCF	0.00836	9	9.29E-04	4.962	0.0026%	1.998
Error	0.01516	81	1.87E-04			
Total	2.91459	99				

The ANOVA indicates that both the LCF and the location have a significant impact on power to detect. While it is somewhat expected that detection power may vary by location, the significance of LCF is surprising. The LCF achieves classification by comparing a distance measure based on sample mean vector and covariance matrix calculated on the training set. This result seems to indicate that despite the large training samples, enough variation in the sample statistics exist so that the LCF performance exhibits poor reproducibility.

The average magnitude of the differences in power between the LCF and Measurement Test that were determined to be significant by the McNemar statistic are displayed in Table 9-26:

Table 9-26 : Mean Magnitude of Outperformance vs. Gross Error Location for the Linear Classification Function solving the Detection Problem.

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Location	0										
	1	-2.65%	-2.70%		-3.60%		-3.23%		-3.77%	-3.73%	-3.96%
	2	-8.85%	-9.34%	-8.16%	-8.38%	-7.94%	-5.30%	-10.51%	-7.63%	-5.88%	-6.48%
	3										
	4										
	5										
	6										
	7										
	8				-3.47%						-3.02%
	9										
		Mean Outperformance									
GE Location	0										
	1							3.47%			
	2										
	3	3.75%		2.82%		3.10%		3.44%	2.98%	2.48%	3.53%
	4	10.53%	10.65%	11.30%	8.02%	11.60%	8.47%	11.20%	9.81%	8.62%	10.72%
	5	15.51%	18.80%	16.81%	15.02%	15.55%	14.82%	18.50%	15.21%	13.78%	14.43%
	6	4.14%	3.95%	4.13%	5.38%	4.31%	4.05%	4.30%	4.88%	5.84%	3.80%
	7	7.87%	9.07%	7.74%	9.14%	6.62%	6.32%	7.01%	7.68%	6.54%	8.20%
	8										
	9	6.15%	6.12%	6.41%	6.04%	6.82%	5.03%	5.94%	6.58%	5.85%	6.62%

The results of Table 9-26 indicate that the Measurement Test was superior on locations 1 and 2, while the LCF performed better on location 4,5,6,7and 9. In general then, it appears that the LCF is more successful in detecting gross errors in measurements with smaller magnitudes. The section on variable importance indicated that the adjustments to measurements 5, 6 and 9 played an important role in the LCF for the Detection problem, but adjustments to measurements 4 and 7 was unimportant, so there is not a one-to-one correspondence between variable importance and outperformance. The norm of the vector of relative adjustments is also fairly highly ranked for the LCF, and would be sensitive to adjustments in any of the measurements, which is likely the reason for outperformance on smaller magnitude measurements.

The counts associated with these averages are presented in Table 9-27:

Table 9-27 : Counts of Data Sets with Significant McNemar Statistics by Location for the Linear Classification Function solving the Detection Problem

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Location	0										
	1	3	1		3		1		1	2	9
	2	9	9	9	9	9	9	9	9	9	9
	3										
	4										
	5										
	6										
	7										
	8				1						1
	9										
		Count of Significant Outperformance									
GE Location	0										
	1							1			
	2										
	3	6		2		2		1	4	1	1
	4	9	9	9	9	9	9	9	9	9	9
	5	9	9	9	9	9	9	9	9	9	9
	6	5	3	3	3	2	1	5	3	2	3
	7	9	8	9	9	9	8	9	9	8	9
	8										
	9	9	7	7	7	8	6	8	7	7	6

The count data indicates that the significance of the Measurement Test's outperformance on location 1 is questionable, but that for location 2 it is consistently superior. The LCF's superiority on location 6 is not as consistent as for the other locations.

The results of this section showed that the LCF methodology may be an attractive alternative to the Measurement Test to solve the Detection problem. The same comments regarding the possible problems with practical implementation that was made with regards to the classification tree methodology applies to the LCF, which are:

- The reproducibility of the methodology is poor as indicated by the ANOVA on power vs. location. This is despite large training samples being used.
- The methodology will always depend on the representativeness of the training sample.
- It is not clear how the trade-off between type I and type II error may be optimized for the methodology, although the trade-off may be manipulated by changing training parameters.

This concludes the discussion of results for the Detection problem for the LCF classifier. The results for the Quadratic Classification Function (QCF) will be discussed in the following section.

9.3.3 Detection Results for the Quadratic Classification Function

The mean proportions of vectors correctly classified by each QCF and its associated Measurement Test (MT) over the 9 test data sets are presented in Table 9-28 for different gross error magnitudes:

Table 9-28 : Proportion of Vectors Correctly Detected by Quadratic Classification Function vs. Gross Error Magnitude

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	87.4%	89.1%	88.6%	88.0%	88.5%	86.4%	88.2%	88.4%	87.8%	88.1%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.5	2.4%	1.3%	1.5%	1.8%	1.3%	2.2%	1.3%	1.3%	1.7%	1.4%
	2.0	15.7%	13.1%	14.3%	14.9%	13.8%	17.4%	14.2%	14.0%	15.4%	14.5%
	2.5	36.1%	33.9%	34.3%	35.1%	34.3%	37.6%	34.9%	34.5%	35.8%	35.3%
	3.0	50.3%	47.9%	48.6%	49.9%	49.4%	51.5%	49.4%	48.7%	49.1%	49.5%
	3.5	58.2%	57.2%	57.9%	58.5%	57.8%	59.4%	58.1%	57.5%	58.1%	57.9%
	4.0	64.3%	62.6%	63.8%	64.7%	63.7%	65.6%	63.9%	63.8%	64.5%	63.7%
	4.5	68.8%	67.9%	68.7%	69.1%	68.6%	70.8%	69.0%	68.5%	68.6%	68.3%
	5.0	74.0%	72.9%	73.1%	74.1%	72.9%	74.5%	73.3%	73.2%	73.9%	73.5%
		Measurement Test for Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	87.4%	89.1%	88.6%	88.0%	88.5%	86.4%	88.2%	88.3%	87.8%	88.1%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	0.1%	0.0%	0.0%	0.1%	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%
	1.5	5.7%	4.4%	4.7%	5.3%	4.9%	6.2%	4.9%	4.7%	5.1%	5.0%
	2.0	17.8%	15.5%	16.5%	16.8%	16.5%	18.6%	16.5%	16.3%	16.8%	16.9%
	2.5	27.6%	25.4%	26.1%	26.9%	26.0%	28.5%	26.6%	26.0%	27.0%	26.6%
	3.0	34.7%	32.6%	33.0%	33.8%	33.5%	35.6%	33.5%	33.0%	33.7%	33.8%
	3.5	39.8%	38.0%	38.4%	38.8%	38.7%	40.6%	38.8%	38.4%	39.0%	39.2%
	4.0	43.9%	41.7%	42.4%	43.1%	42.6%	44.7%	42.8%	42.5%	43.2%	43.1%
	4.5	48.2%	45.4%	46.4%	46.6%	46.5%	49.1%	46.9%	46.5%	47.4%	46.9%
	5.0	52.0%	50.2%	50.5%	51.2%	50.3%	52.4%	51.0%	50.3%	51.2%	50.9%

The QCF achieved type I error rates between 10.9% and 12.6%. The power to detect a gross error ranged between 0.0% and 74.5% for the QCF, compared to 0.0% and 52.4% for the Measurement Test. This compares with type I error rates of 30.4% to 35.8% and power between 0.0% and 81.0% for the LCF, i.e. the use of a quadratic classification function decreased type I error rates and power, relative to the LCF.

The power to detect a gross error seems to be related to the magnitude of the gross error. The strength of the linear relationship between power to detect and gross error magnitude was tested through regression analysis:

Table 9-29 : Linear Regression of Power to Detect vs. Gross Error Magnitude for the Quadratic Classification Function

QCF #		1	2	3	4	5	6	7	8	9	10
QCF	Slope	19.38%	19.21%	19.34%	19.53%	19.34%	19.68%	19.41%	19.34%	19.40%	19.34%
	F	156.70	153.32	153.87	153.56	146.06	151.33	147.70	152.99	157.83	149.22
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
MT	Slope	12.95%	12.48%	12.61%	12.71%	12.62%	13.10%	12.74%	12.61%	12.81%	12.73%
	F	244.23	257.48	255.09	249.37	241.39	228.10	252.04	253.05	250.69	237.18
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

All of the regressions are significant at the modified level of 0.25% for 20 simultaneous tests, confirming that power of detection increases with increasing gross error magnitude.

The mean proportions of vectors correctly detected presented in Table 9-28 seems to indicate that the QCF has higher power for the same type I error rate than the MT. The McNemar statistic was used to determine where significant differences between the QCF and the MT arose. The mean values of the significant differences are displayed in Table 9-30 for different gross error magnitudes:

Table 9-30 : Mean Magnitude of Outperformance vs. Gross Error Magnitude Quadratic Classification Function solving the Detection Problem

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5	-3.31%	-3.15%	-3.27%	-3.52%	-3.52%	-4.05%	-3.59%	-3.42%	-3.40%	-3.57%
	2.0	-3.66%	-3.83%	-3.51%	-3.54%	-3.99%		-3.92%	-3.30%	-3.25%	-3.70%
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Mean Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0										
	2.5	8.5%	8.5%	8.2%	8.2%	8.2%	9.1%	8.3%	8.5%	8.8%	8.7%
	3.0	15.5%	15.3%	15.6%	16.1%	15.9%	15.9%	15.9%	15.7%	15.4%	15.7%
	3.5	18.5%	19.2%	19.5%	19.7%	19.1%	18.7%	19.2%	19.0%	19.0%	18.7%
	4.0	20.4%	21.0%	21.5%	21.6%	21.1%	20.9%	21.2%	21.3%	21.2%	20.7%
	4.5	20.6%	22.5%	22.3%	22.4%	22.1%	21.6%	22.0%	22.0%	21.2%	21.4%
	5.0	22.0%	22.8%	22.5%	22.9%	22.6%	22.1%	22.3%	22.9%	22.6%	22.7%

The MT is superior for smaller gross error magnitudes, while the QCF is superior for larger gross errors. The magnitude of the outperformance seems to be related to gross error magnitude.

The counts associated with the average significant differences presented in Table 9-30 are presented in Table 9-31:

Table 9-31 : Counts of Data Sets with Significant McNemar Statistics by Magnitude for the Quadratic Classification Function solving the Detection Problem

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5	9	9	9	9	9	9	9	9	9	9
	2.0	3	5	3	4	6		4	6	2	4
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Count of Significant Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0										
	2.5	9	9	9	9	9	9	9	9	9	9
	3.0	9	9	9	9	9	9	9	9	9	9
	3.5	9	9	9	9	9	9	9	9	9	9
	4.0	9	9	9	9	9	9	9	9	9	9
	4.5	9	9	9	9	9	9	9	9	9	9
	5.0	9	9	9	9	9	9	9	9	9	9

The counts indicate that the significant differences are consistent over all the test sets, with the exception of magnitude 2.0, where some inconsistency arises. This concludes the results for different gross error magnitudes. The results for different gross error locations will be discussed next.

The average proportions of correctly detected gross errors over the 9 test sets for each QCF are presented in Table 9-32 for different gross error locations:

Table 9-32 : Proportion of Vectors correctly Detected by Quadratic Classification Function vs. Gross Error Location

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	87.4%	89.1%	88.6%	88.0%	88.5%	86.4%	88.2%	88.4%	87.8%	88.1%
	1	55.8%	54.6%	53.2%	55.4%	54.8%	55.5%	53.6%	52.9%	53.6%	52.9%
	2	68.5%	69.2%	68.1%	67.5%	68.3%	71.1%	69.5%	69.5%	72.0%	69.9%
	3	67.2%	63.4%	64.4%	64.9%	64.3%	67.8%	63.9%	65.7%	64.9%	65.1%
	4	57.2%	53.1%	55.7%	56.4%	56.1%	56.7%	55.8%	53.6%	54.7%	57.7%
	5	38.2%	38.8%	40.4%	40.2%	40.5%	41.5%	41.6%	39.0%	40.7%	39.3%
	6	29.3%	26.5%	28.3%	29.6%	27.5%	30.6%	27.7%	27.8%	28.8%	29.2%
	7	29.7%	27.9%	27.5%	28.5%	26.6%	30.1%	27.6%	28.7%	27.8%	26.9%
	8	10.1%	8.9%	9.8%	10.2%	9.5%	10.9%	9.8%	9.3%	10.3%	9.7%
	9	21.2%	20.0%	20.9%	22.4%	21.3%	23.3%	22.3%	21.4%	22.0%	21.2%
		Measurement Test for Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	87.4%	89.1%	88.6%	88.0%	88.5%	86.4%	88.2%	88.3%	87.8%	88.1%
	1	40.5%	38.3%	38.8%	39.6%	39.1%	41.3%	39.5%	38.9%	39.8%	39.7%
	2	78.6%	77.2%	77.7%	78.1%	77.9%	79.9%	77.9%	77.4%	78.1%	78.2%
	3	55.7%	53.9%	54.5%	55.1%	54.4%	57.0%	55.2%	54.7%	55.4%	55.0%
	4	36.8%	33.7%	34.8%	35.7%	35.0%	37.6%	35.5%	34.8%	36.1%	35.5%
	5	14.0%	12.1%	13.0%	13.3%	12.8%	14.8%	13.1%	12.8%	13.2%	13.3%
	6	22.1%	20.1%	20.6%	21.3%	20.8%	23.5%	21.1%	20.6%	21.6%	21.5%
	7	12.4%	10.5%	11.2%	11.7%	11.5%	13.0%	11.7%	11.4%	11.9%	11.7%
	8	9.7%	8.4%	8.8%	9.1%	9.0%	10.0%	8.9%	8.9%	9.4%	9.3%
	9	11.6%	10.1%	10.5%	10.8%	10.7%	12.2%	10.7%	10.4%	10.9%	10.8%

The power to detect for the QCF varied between 8.9% and 72.0%, compared to 8.4% and 79.9% for the MT.

The power to detect seems to depend on the location of the gross error. This was tested using an ANOVA:

Table 9-33 : ANOVA for Detection – Quadratic Classification Function and Location

ANOVA - Proportion Correctly Classified vs. GE Location - Quadratic Classification Function						
Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
GE Location	5.40687	9	6.01E-01	5718.033	0.0000%	1.998
QCF	0.00330	9	3.66E-04	3.485	0.1107%	1.998
Error	0.00851	81	1.05E-04			
Total	5.41867	99				

The ANOVA indicates that both the QCF and the location have a significant impact on the power to detect a gross error.

The significant differences in power between the QCF and MT, as determined by the McNemar statistic, were averaged over the 9 data sets, and are presented in Table 9-34:

Table 9-34 : Mean Magnitude of Outperformance vs. Gross Error Location for the Quadratic Classification Function solving the Detection Problem.

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Location	0										
	1										
	2	-10.08%	-7.97%	-9.61%	-10.60%	-9.66%	-8.82%	-8.40%	-7.92%	-6.13%	-8.24%
	3										
	4										
	5										
	6										
	7										
	8										
	9										
		Mean Outperformance									
GE Location	0										
	1	15.3%	16.3%	14.3%	15.9%	15.8%	14.2%	14.0%	14.1%	13.8%	13.2%
	2										
	3	11.5%	9.5%	9.8%	9.9%	9.9%	10.8%	8.6%	10.9%	9.4%	10.1%
	4	20.5%	19.5%	20.9%	20.7%	21.1%	19.1%	20.3%	18.8%	18.6%	22.2%
	5	24.2%	26.7%	27.4%	26.8%	27.7%	26.7%	28.4%	26.2%	27.5%	26.0%
	6	7.1%	6.5%	7.7%	8.3%	6.7%	7.2%	6.6%	7.2%	7.2%	7.7%
	7	17.3%	17.4%	16.4%	16.8%	15.1%	17.1%	15.9%	17.3%	15.9%	15.2%
	8										
	9	9.6%	9.9%	10.4%	11.6%	10.6%	11.1%	11.6%	11.0%	11.1%	10.4%

The MT is superior on location 2, while the QCF is superior on all other locations with the exception of location 8, where no significant results were obtained.

The counts associated with the averages presented in Table 9-34 are presented in Table 9-35:

Table 9-35 : Counts of Data Sets with Significant McNemar Statistics by Location for the Quadratic Classification Function solving the Detection Problem

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Location	0										
	1										
	2	9	9	9	9	9	9	9	9	9	9
	3										
	4										
	5										
	6										
	7										
	8										
	9										
		Count of Significant Outperformance									
GE Location	0										
	1	9	9	9	9	9	9	9	9	9	9
	2										
	3	9	9	9	9	9	9	9	9	9	9
	4	9	9	9	9	9	9	9	9	9	9
	5	9	9	9	9	9	9	9	9	9	9
	6	9	9	9	9	9	9	9	9	9	9
	7	9	9	9	9	9	9	9	9	9	9
	8										
	9	9	9	9	9	9	9	9	9	9	9

The count data indicate that the conclusion on relative performance drawn from Table 9-34 is consistent across all test data sets.

9.3.4 Summary of Detection Results

In order to obtain a qualitative indication of how the different classification methods compared to each other, the average type I and type II error rate for each method was calculated over all 9 test data sets. The average type I and type II error rates for the Measurement Test were calculated for data set 1. It was found that the relationship between Type II and Type I error did not change, whether it was manipulated by specifying different levels of significance for the test, or by manipulating the assumed measurement cov_y. The results are plotted in Figure 9-6:

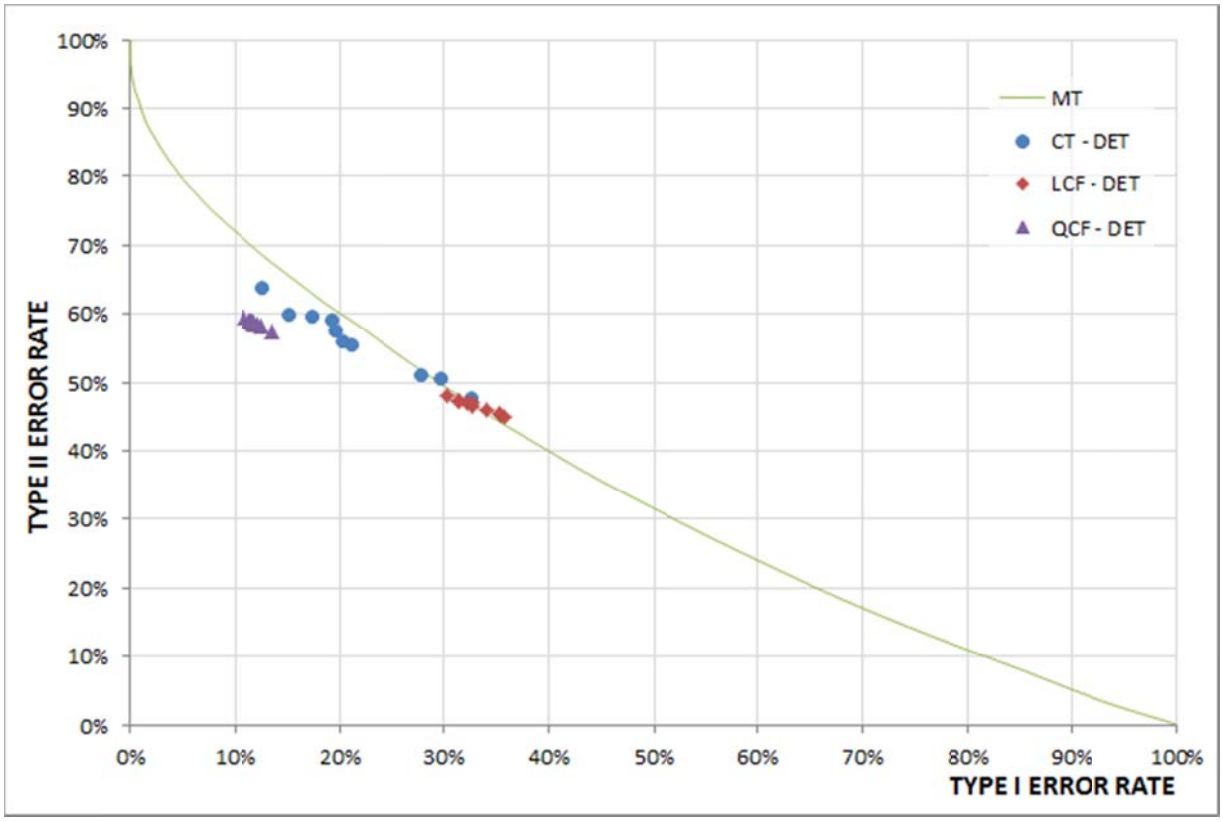

Figure 9-6 : Empirical Type II vs. Type I Error Rates for CT, LCF and QCF vs. MT for the Detection Problem

This differs from the results presented before in that the type II error rate is averaged over all data sets, as well as gross error magnitudes and locations, for each classifier as well as its benchmark Measurement Test.

The results for the CT (blue dots) and LCF (red triangles) seem to lie on a common curve, and to converge with the Measurement Test (solid green line) at higher Type I error rates. It should be noted that although the LCF showed superior performance to the Measurement Test for selected gross error magnitudes and locations, this is not apparent when the results are analyzed collectively, highlighting the need for a detailed analysis.

The QCF results, presented as dark purple triangles, seem to form a distinct pattern that is not part of the common curve formed by the CT and LCF methodologies, with the QCF methodology having a more favourable trade-off between type and type II error, i.e. smaller type II error for similar type I error compared to the other methodologies. The difference between the QCF and LCF methodologies is that the QCF calculates a separate estimate of the covariance matrix for each class, i.e. for the detection problem it estimates the covariance of the gross error vectors independently from the random error vectors from the known training samples. The difference in performance between the two methods indicates the importance of accurate covariance estimation in the detection problem.

This concludes the discussion of the results for the Detection problem. The results for the Identification problem will be discussed in the sections that follow.

9.4 RESULTS FOR THE IDENTIFICATION PROBLEM

The previous section discussed the difference in power observed between the classification methodologies and the Measurement Test in resolving the Detection problem. Results were summarized based on gross error magnitude and location. This section will present the results in a similar fashion for the Identification problem. The results will be displayed as the proportion of vectors correctly detected or identified for different gross error magnitudes and locations. Gross error magnitudes and locations of zero correspond to random error vectors. Therefore, the Type I error rate can be deduced from the proportion of correctly detected/identified vectors for this magnitude/location, as the sum of Type I error and correctly identified vectors must equal 100%. For all other magnitudes and locations, the reported proportion correctly detected/identified vectors is identical to the statistical power of the method.

9.4.1 Identification Results for the Classification Tree Classifier

The mean proportions of vectors correctly identified by the classification tree and Measurement Test over the 9 test sets are presented in Table 9-36 for different gross error magnitudes:

Table 9-36 : Proportion of Vectors Correctly Identified by Classification Tree Classifier vs. Gross Error Magnitude

GE Magnitude	Classification Tree 1	2	3	4	5	6	7	8	9	10
0.0	84.1%	84.1%	83.3%	79.5%	86.0%	77.4%	73.8%	78.6%	80.2%	87.3%
0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
1.0	0.1%	0.1%	0.1%	0.4%	0.1%	0.2%	0.7%	0.1%	0.2%	0.1%
1.5	2.2%	2.1%	2.5%	3.4%	1.6%	3.2%	5.2%	3.4%	3.3%	1.7%
2.0	7.4%	7.3%	8.6%	8.6%	5.9%	10.5%	11.6%	10.2%	9.9%	4.6%
2.5	15.7%	14.0%	15.8%	16.1%	12.8%	18.5%	18.7%	16.9%	17.2%	10.4%
3.0	23.8%	21.5%	23.2%	24.0%	21.7%	25.6%	25.7%	24.0%	23.9%	19.5%
3.5	28.9%	28.1%	29.2%	29.4%	28.9%	31.9%	32.4%	30.1%	28.8%	25.9%
4.0	33.2%	33.3%	33.0%	33.4%	34.8%	36.3%	36.6%	35.6%	33.8%	31.5%
4.5	35.6%	37.1%	37.1%	36.0%	38.1%	40.7%	40.4%	38.6%	36.8%	35.5%
5.0	37.9%	41.0%	40.4%	40.5%	40.9%	43.1%	43.6%	42.5%	39.5%	39.1%

GE Magnitude	Measurement Test for Classification Tree 1	2	3	4	5	6	7	8	9	10
0.0	83.9%	84.1%	83.3%	79.6%	86.0%	98.6%	73.8%	78.6%	80.2%	87.3%
0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
1.0	0.1%	0.1%	0.1%	0.4%	0.0%	0.0%	0.8%	0.4%	0.3%	0.0%
1.5	2.9%	2.9%	3.0%	4.1%	2.4%	0.0%	5.9%	4.2%	4.0%	2.0%
2.0	8.0%	8.0%	8.2%	9.7%	7.4%	0.3%	11.6%	10.2%	9.3%	6.9%
2.5	13.0%	13.1%	13.2%	14.7%	12.0%	2.5%	15.8%	14.6%	14.3%	11.7%
3.0	17.8%	18.1%	18.0%	19.2%	17.0%	6.3%	20.7%	19.0%	18.9%	16.3%
3.5	22.2%	22.5%	22.7%	23.4%	21.8%	10.5%	25.2%	23.7%	23.7%	20.9%
4.0	26.6%	26.6%	26.7%	27.8%	26.1%	14.1%	29.6%	28.0%	28.2%	25.5%
4.5	30.5%	30.5%	30.6%	31.4%	30.0%	18.0%	33.2%	31.7%	31.7%	29.2%
5.0	34.9%	35.0%	35.1%	36.2%	34.0%	21.5%	37.4%	36.1%	36.1%	33.1%

The classification trees achieved type I error rates between ~12.7% and 26.2%, which is a larger range than for the Detection problem. The power to correctly identify gross errors rang from ~0.0% to 43.6% for the classification trees, and between 0.0% and 37.4% for the Measurement Test. As for the Detection problem, smaller gross error magnitudes exhibit smaller power to be identified correctly.

The strength of the linear relationship between power to identify and gross error magnitude was tested through regression analysis, the results of which are presented in Table 9-37, where the degrees of freedom associated with the numerator and denominator of each F-statistic is respectively 1 and 8:

Table 9-37 : Linear Regression of Power to Identify vs. Gross Error Magnitude for the Classification Tree

Tree #		1	2	3	4	5	6	7	8	9	10
CT	Slope	9.917%	10.355%	10.232%	10.117%	10.646%	11.008%	10.869%	10.670%	10.039%	9.961%
	F	215.36	302.54	335.18	330.28	202.23	345.00	490.58	417.87	356.24	190.70
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
MT	Slope	8.403%	8.425%	8.436%	8.575%	8.277%	5.138%	8.820%	8.586%	8.650%	8.085%
	F	623.67	603.76	642.27	934.22	503.82	73.93	1407.06	1004.64	855.03	450.75
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

All of the regressions are significant at the modified 0.25% confidence level for 20 simultaneous tests, indicating a strong linear relationship between power to detect and gross error magnitude.

The lower power of identification relative to detection indicates smearing of gross errors when it is considered that the Measurement Test simultaneously resolves the Detection/Identification problem by identifying a gross error in the measurement with maximum standardized adjustment, provided the adjustment is statistically significant. Therefore, high power to detect coupled with low power to identify implies that a gross error is likely to cause a large adjustment in a measurement other than the one it is located in. The significant regression results can be explained by a conditional argument: there is a positive relationship between power to identify and gross error magnitude, conditional on the Measurement Test having made a correct identification.

The averages of the significant differences in power between the classification tree and Measurement Test, as determined by the McNemar statistic, for different gross error magnitudes are presented in Table 9-38:

Table 9-38 : Mean Magnitude of Differences in Power vs. Gross Error Magnitude of Classification Tree solving the Identification Problem

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5				-2.18%	-1.69%	-2.29%	-2.36%			
	2.0				-2.66%	-2.55%					-2.97%
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Mean Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0								2.24%		
	2.5	3.60%		3.06%	3.18%		3.80%	3.81%	3.73%	3.51%	
	3.0	6.09%	4.21%	5.37%	5.91%	4.66%	5.80%	5.39%	5.27%	5.44%	4.31%
	3.5	6.73%	5.91%	6.53%	6.05%	7.07%	7.64%	7.44%	6.41%	5.42%	5.10%
	4.0	6.61%	6.72%	6.31%	5.98%	8.70%	7.91%	7.30%	7.62%	6.18%	6.25%
	4.5	6.25%	6.99%	6.65%	5.58%	8.37%	8.31%	7.83%	7.18%	6.63%	6.88%
	5.0	5.03%	6.45%	6.17%	7.07%	7.69%	7.63%	6.81%	7.51%	7.92%	6.22%

As for the Detection problem, the Measurement Test performed better at smaller magnitudes, while the classification tree is superior at larger magnitudes. The counts associated with the mean significant differences presented in Table 9-38 are presented in Table 9-39:

Table 9-39 : Counts of Data Sets with Significant McNemar Statistics by Magnitude for the Classification Tree solving the Identification Problem

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5				1	1	2	1			
	2.0				1	3					5
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Count of Significant Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0								1		
	2.5	4		6	2		7	5	3	4	
	3.0	9	6	8	6	9	9	8	8	8	5
	3.5	9	8	9	9	9	9	8	9	8	8
	4.0	9	9	9	8	9	9	8	9	7	8
	4.5	5	8	8	5	8	9	8	8	5	7
	5.0	1	7	6	2	6	6	8	6	1	8

The consistency of the Measurement Test's outperformance at small magnitudes is poor compared to that of the classification tree's outperformance at larger magnitudes.

This concludes the discussion on the identification results relative to gross error magnitude for the classification tree methodology. The results relative to gross error location will be discussed next.

The proportions of vectors correctly classified by the classification tree and its associated Measurement Test for different locations are displayed in Table 9-40:

Table 9-40 : Proportion Vectors Correctly Identified by Classification Tree vs. Gross Error Location

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	84.1%	84.1%	83.3%	79.5%	86.0%	77.4%	73.8%	78.6%	80.2%	87.3%
	1	8.5%	12.5%	14.6%	8.9%	16.4%	17.6%	23.7%	17.4%	15.3%	16.6%
	2	60.0%	59.0%	66.2%	63.0%	55.6%	67.6%	66.9%	69.6%	68.7%	53.1%
	3	49.0%	50.1%	47.7%	52.3%	43.3%	52.6%	50.9%	48.3%	51.1%	36.8%
	4	49.2%	36.5%	38.3%	45.2%	46.0%	40.6%	48.6%	38.5%	37.8%	46.8%
	5	11.0%	21.7%	13.8%	3.7%	5.8%	15.2%	13.3%	16.6%	18.9%	7.0%
	6	0.0%	2.0%	6.0%	5.6%	5.3%	2.7%	4.2%	4.4%	0.0%	1.6%
	7	7.7%	0.0%	0.0%	7.5%	11.4%	6.5%	7.0%	6.9%	5.6%	5.5%
	8	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	9	0.0%	4.1%	5.6%	9.4%	1.9%	10.2%	6.7%	4.4%	0.0%	2.0%
		Measurement Test for Classification Tree									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	83.9%	84.1%	83.3%	79.6%	86.0%	98.6%	73.8%	78.6%	80.2%	87.3%
	1	27.3%	27.2%	27.6%	29.3%	26.2%	9.5%	32.3%	29.4%	29.3%	25.3%
	2	68.7%	68.8%	69.1%	71.2%	67.8%	46.6%	73.6%	71.6%	71.0%	66.9%
	3	33.5%	33.8%	33.9%	35.6%	32.3%	14.3%	38.5%	35.9%	35.7%	31.5%
	4	20.3%	19.9%	20.2%	21.8%	18.9%	4.8%	24.6%	22.2%	21.9%	17.7%
	5	1.8%	1.9%	2.0%	2.6%	1.5%	0.0%	3.9%	2.8%	2.5%	1.1%
	6	9.9%	10.1%	10.2%	11.7%	9.1%	1.3%	13.5%	11.7%	11.6%	8.4%
	7	0.4%	0.4%	0.4%	0.4%	0.3%	0.0%	0.9%	0.6%	0.5%	0.2%
	8	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%	0.1%	0.1%	0.1%	0.0%
	9	0.3%	0.3%	0.3%	0.4%	0.2%	0.0%	0.9%	0.6%	0.4%	0.2%

The power to identify ranged between 0.0% and 69.6% for the classification tree, and between 0.0% and 73.6% for the Measurement Test. There is an obvious effect of location on power to identify; some locations (#'s 6 and 8 for the classification tree, and 5, 7, 8 and 9 for the Measurement Test) display almost no power to identify. For the classification tree this implies that gross errors in these locations did not have a discernible effect on the features of the input vector used for training. The results for the Measurement Test imply significant smearing of gross errors in these locations.

The power of locations 7 and 9 for the classification tree indicates poor reproducibility, likely due to variation in tree structure. This represents a problem for practical implementation, as discussed before.

The averages of the significant differences in power between the classification tree and Measurement Test, as determined by the McNemar statistic, for different gross error locations, are presented in Table 9-41:

Table 9-41 : Mean Magnitude of Differences in Power vs. Gross Error Location of Classification Tree solving the Identification Problem

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Location	0										
	1	-18.77%	-14.65%	-13.01%	-20.31%	-9.74%	-12.50%	-8.58%	-11.99%	-13.95%	-8.64%
	2	-8.66%	-9.75%	-3.70%	-8.21%	-12.16%	-5.28%	-6.69%	-3.56%		-13.82%
	3										
	4										
	5										
	6	-9.93%	-8.10%	-4.27%	-6.12%	-3.83%	-9.61%	-9.30%	-7.30%	-11.55%	-6.88%
	7		-0.91%	-1.00%							
	8										
	9										
		Mean Outperformance									
GE Location	0										
	1										
	2										
	3	15.56%	16.25%	13.81%	16.71%	11.02%	16.02%	12.45%	12.35%	15.40%	5.63%
	4	28.95%	16.68%	18.01%	23.39%	27.04%	17.88%	24.03%	16.35%	15.89%	29.18%
	5	9.15%	19.83%	11.80%	2.20%	4.29%	12.22%	9.38%	13.73%	16.36%	5.84%
	6										
	7	7.29%			7.00%	11.07%	5.87%	6.11%	6.39%	5.07%	5.28%
	8										
	9		3.78%	5.35%	8.95%	1.80%	9.50%	5.79%	3.78%		1.86%

The Measurement Test performed better on locations 1, 2 and 6, while the classification tree was better on locations 3, 4, 5, 7 and 9. This closely resembles the results for the Detection problem presented in Table 9-17.

The counts associated with the average significant differences of Table 9-41 are displayed in Table 9-42:

Table 9-42 : Counts for Data Sets with Significant McNemar Statistics by Location for the Classification Tree solving the Identification Problem

		Classification Tree									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Location	0										
	1	9	9	9	9	9	9	9	9	9	9
	2	9	9	4	9	9	7	9	1		9
	3										
	4										
	5										
	6	9	9	9	9	9	9	9	9	9	9
	7		1	1							
	8										
	9										
		Count of Significant Outperformance									
GE Location	0										
	1										
	2										
	3	9	9	9	9	9	9	9	9	9	8
	4	9	9	9	9	9	9	9	9	9	9
	5	9	9	9	1	9	9	9	9	9	9
	6										
	7	9			9	9	9	9	9	9	9
	8										
	9		9	9	9	8	9	9	9		9

Table 9-42 shows that the majority of the differences in power were significant on all 9 data sets.

The results of this section indicate that the classification tree methodology may be an attractive alternative to the Measurement Test to solve the Identification problem. Practical implementation may be problematic due to several factors stated before for the Detection problem:

- The reproducibility of the methodology is poor as indicated by the ANOVA on power vs. location. This is despite large training samples being used.
- The methodology will always depend on the representativeness of the training sample.
- It is not clear how the trade-off between type I and type II error may be optimized for the methodology, although the trade-off may be manipulated by changing training parameters.

This concludes the discussion for results of the classification tree methodology applied to the Identification problem. The corresponding results for the linear classification methodology are discussed in the following section.

9.4.2 Identification Results for the Linear Classification Function

The mean proportions of vectors correctly identified by the linear classification function (LCF) and Measurement Test over the 9 data sets are displayed in Table 9-43 for different gross error magnitudes:

Table 9-43 : Proportion of Vectors Correctly Identified by Linear Classification Function vs. Gross Error Magnitude

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	88.4%	89.7%	89.0%	87.5%	88.9%	87.5%	87.8%	88.3%	87.6%	88.1%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.5	0.7%	0.5%	0.6%	1.0%	0.7%	0.6%	0.8%	0.7%	0.7%	0.9%
	2.0	5.6%	4.9%	5.2%	5.7%	5.2%	6.2%	5.7%	5.4%	6.1%	5.7%
	2.5	22.0%	21.6%	21.6%	22.3%	21.6%	23.4%	22.9%	21.5%	23.0%	22.4%
	3.0	36.5%	35.7%	35.4%	36.5%	35.7%	36.1%	36.5%	35.7%	36.5%	35.9%
	3.5	46.1%	46.3%	46.2%	47.0%	46.5%	46.5%	46.9%	46.3%	46.8%	46.2%
	4.0	53.7%	52.8%	53.1%	54.3%	53.4%	53.6%	53.6%	53.5%	53.3%	53.2%
	4.5	57.6%	56.7%	57.1%	58.0%	57.5%	58.0%	57.4%	57.4%	57.6%	57.8%
	5.0	62.0%	61.1%	61.5%	61.9%	61.3%	61.3%	61.2%	61.5%	61.6%	61.7%
		Measurement Test for Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	88.4%	89.7%	89.0%	87.5%	88.9%	87.5%	87.8%	88.3%	87.7%	88.1%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.5	1.8%	1.4%	1.6%	2.1%	1.6%	1.9%	1.9%	1.6%	1.9%	1.8%
	2.0	6.2%	5.6%	6.0%	6.7%	6.1%	6.6%	6.5%	6.3%	6.5%	6.5%
	2.5	11.2%	10.7%	10.9%	11.7%	10.9%	11.5%	11.4%	11.2%	11.5%	11.3%
	3.0	16.0%	15.6%	15.7%	16.5%	15.7%	16.1%	16.1%	15.5%	16.1%	16.0%
	3.5	20.3%	19.9%	20.1%	20.7%	20.3%	20.7%	20.7%	20.1%	20.7%	20.5%
	4.0	24.7%	24.1%	24.4%	25.0%	24.7%	25.0%	24.9%	24.5%	25.3%	25.0%
	4.5	29.1%	28.7%	29.0%	29.2%	29.0%	29.6%	29.3%	28.9%	29.6%	29.0%
	5.0	32.9%	32.3%	32.6%	33.4%	32.6%	32.8%	33.1%	32.4%	33.1%	32.9%

The type I error rates for the LCF ranged between ~10.3% and ~12.5%, compared to ~30.4% to ~35.8% for the corresponding Detection problem. Compared with Detection, it seems Identification of smaller magnitude gross errors (<2.5) was especially problematic. As for the classification tree, the power to correctly identify a gross error is lower than for the corresponding Detection problem, ranging between ~0.0% and ~62.0% for the LCF compared to ~0.0% to ~33.4% for the Measurement Test

The strength of the linear relationship between power to identify a gross error and gross error magnitude was tested through regression analysis for both the LCF and the Measurement Test:

Table 9-44 : Linear Regression of Power to Identify vs. Gross Error Magnitude for the Linear Classification Function

LCF #		1	2	3	4	5	6	7	8	9	10
LCF	Slope	16.517%	16.317%	16.394%	16.578%	16.434%	16.440%	16.413%	16.441%	16.437%	16.439%
	F	140.80	132.62	137.55	137.87	135.04	144.76	136.22	137.26	143.30	144.99
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
MT	Slope	8.023%	7.925%	7.965%	8.074%	7.982%	8.060%	8.061%	7.927%	8.106%	8.020%
	F	391.60	335.13	365.72	454.57	372.07	421.22	417.43	392.03	409.69	410.35
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

All of the regressions displayed a significant increase in power with increasing gross error magnitude.

The averages of the significant differences in power between the LCF and Measurement Test, as determined by the McNemar statistic, for different gross error magnitudes are presented in Table 9-45:

Table 9-45 : Mean Magnitude of Differences in Power vs. Gross Error Magnitude of Linear Classification Function solving the Identification Problem

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5	-1.5%	-1.3%	-1.4%	-1.6%	-1.4%	-1.8%	-1.4%	-1.5%	-1.4%	-1.5%
	2.0										
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Mean Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0										
	2.5	10.8%	10.9%	10.7%	10.6%	10.7%	12.0%	11.5%	10.3%	11.6%	11.1%
	3.0	20.5%	20.1%	19.8%	20.1%	20.0%	20.0%	20.5%	20.1%	20.4%	19.9%
	3.5	25.8%	26.3%	26.1%	26.3%	26.2%	25.7%	26.3%	26.1%	26.1%	25.7%
	4.0	29.0%	28.7%	28.7%	29.2%	28.7%	28.6%	28.8%	29.0%	28.1%	28.2%
	4.5	28.5%	28.0%	28.1%	28.8%	28.6%	28.4%	28.2%	28.5%	28.0%	28.8%
	5.0	29.1%	28.7%	28.9%	28.6%	28.7%	28.5%	28.1%	29.1%	28.6%	28.9%

The Measurement Test was marginally superior for magnitudes of 1.5. The LCF proved significantly superior for all magnitudes of 2.5 and greater, with the magnitude of outperformance increasing with gross error

magnitude. This mirror results obtained for the Detection problem. The section on variable importance indicated that the relative adjustments of especially measurements 1, 2, 3 and 4 are important for LCF for the Identification problem. In addition, the residuals of the three balance equations were ranked more important than the remainder of the relative adjustments. In contrast, the Measurement Test only operates on the relative adjustments. It therefore seems that the inclusion of information regarding the residuals resulted in significant outperformance by the LCF methodology.

The counts associated with the averages in Table 9-45 are presented in Table 9-46:

Table 9-46 : Counts of Data Sets with Significant McNemar Statistics by Magnitude for the Linear Classification Function Solving the Identification Problem

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5	4	3	4	3	3	4	3	3	6	2
	2.0										
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
		Count of Significant Outperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0										
	2.5	9	9	9	9	9	9	9	9	9	9
	3.0	9	9	9	9	9	9	9	9	9	9
	3.5	9	9	9	9	9	9	9	9	9	9
	4.0	9	9	9	9	9	9	9	9	9	9
	4.5	9	9	9	9	9	9	9	9	9	9
	5.0	9	9	9	9	9	9	9	9	9	9

The outperformance of the Measurement Test for magnitude 1.5 occurred on about half the test sets, while the LCF outperformance occurred on all the data sets.

The results for Identification problem relative to gross error location are presented in Table 9-47:

Table 9-47 : Proportion of Vectors Correctly Identified by Linear Classification Function vs. Gross Error Location

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	88.4%	89.7%	89.0%	87.5%	88.9%	87.5%	87.8%	88.3%	87.6%	88.1%
	1	48.7%	49.7%	49.6%	51.2%	49.6%	49.4%	50.6%	48.3%	50.5%	48.9%
	2	63.5%	63.5%	63.0%	62.4%	63.6%	66.3%	64.5%	63.3%	64.6%	64.0%
	3	51.3%	52.1%	52.2%	50.9%	50.2%	52.0%	51.6%	51.7%	52.0%	52.2%
	4	50.2%	48.0%	47.6%	48.7%	49.7%	49.6%	49.8%	48.4%	50.2%	49.7%
	5	31.9%	32.3%	32.1%	33.2%	31.9%	32.7%	32.9%	32.3%	33.0%	32.6%
	6	14.6%	11.6%	14.5%	16.2%	14.2%	14.5%	15.8%	16.2%	15.3%	13.3%
	7	20.5%	21.6%	20.4%	21.6%	21.7%	19.5%	21.0%	20.6%	20.3%	22.4%
	8	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	9	2.3%	0.2%	1.6%	3.0%	0.9%	3.0%	0.6%	1.6%	0.6%	1.2%
		Measurement Test for Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	88.4%	89.7%	89.0%	87.5%	88.9%	87.5%	87.8%	88.3%	87.7%	88.1%
	1	24.4%	23.3%	23.9%	25.0%	24.0%	24.8%	25.0%	24.1%	25.0%	24.7%
	2	65.5%	64.6%	65.1%	66.6%	65.4%	66.7%	66.1%	65.5%	66.3%	66.1%
	3	30.6%	30.0%	30.4%	31.3%	30.3%	31.1%	31.3%	30.7%	31.4%	30.8%
	4	17.2%	16.0%	16.5%	17.4%	16.7%	17.2%	17.3%	16.6%	17.4%	17.1%
	5	1.1%	0.9%	1.0%	1.1%	1.0%	1.1%	1.2%	1.0%	1.0%	1.0%
	6	7.9%	7.5%	7.7%	8.3%	7.7%	8.3%	8.1%	7.7%	8.3%	8.1%
	7	0.2%	0.1%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%	0.2%
	8	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	9	0.1%	0.1%	0.1%	0.2%	0.1%	0.2%	0.2%	0.1%	0.2%	0.1%

The power of the LCF ranged from 0.0% to 66.3%, compared to 0.0% to 66.7% for the Measurement Test. The power for both methods is related to location; the LCF could not identify any gross errors in location 8, and only few in location 9. The Measurement Test performed poorly on locations 5, 7, 8 and 9. For the LCF this implies that gross errors in these locations did not have a discernible effect on the features of the input vector used for training, while the results for the Measurement Test imply significant smearing of gross errors, as stated before.

The averages of differences in power that were determined to be significant by the McNemar statistic are displayed Table 9-48:

Table 9-48 : Mean Magnitude of Differences in Power vs. Gross Error Location of Linear Discriminant Function solving the Identification Problem

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Location	0										
	1										
	2	-4.32%		-4.19%	-4.39%	-3.91%			-4.09%		-3.72%
	3										
	4										
	5										
	6										
	7										
	8										
	9										
		Mean Outperformance									
GE Location	0										
	1	24.21%	26.37%	25.73%	26.11%	25.51%	24.60%	25.58%	24.18%	25.46%	24.19%
	2										
	3	20.72%	22.14%	21.75%	19.68%	19.86%	20.89%	20.32%	21.00%	20.65%	21.41%
	4	33.04%	31.95%	31.08%	31.27%	32.96%	32.40%	32.48%	31.82%	32.79%	32.61%
	5	30.84%	31.43%	31.19%	32.13%	30.83%	31.59%	31.68%	31.26%	32.01%	31.60%
	6	6.76%	4.64%	6.88%	7.84%	6.58%	6.13%	7.68%	8.51%	7.06%	5.18%
	7	20.34%	21.49%	20.18%	21.46%	21.55%	19.31%	20.76%	20.46%	20.10%	22.18%
	8										
	9	2.28%		1.79%	2.87%	1.16%	2.80%		1.50%	1.06%	1.38%

The Measurement Test is superior for location 2, while the LCF is superior for all other locations except location 8, where no significant differences occurred.

The counts associated with the mean differences in Table 9-48 is presented in Table 9-49:

Table 9-49 : Counts of Data Sets with Significant McNemar Statistics by Location for the Linear Classification Function Solving the Identification Problem

		Linear Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Location	0										
	1										
	2	2		2	8	2			2		2
	3										
	4										
	5										
	6										
	7										
	8										
	9										
		Count of Significant Outperformance									
GE Location	0										
	1	9	9	9	9	9	9	9	9	9	9
	2										
	3	9	9	9	9	9	9	9	9	9	9
	4	9	9	9	9	9	9	9	9	9	9
	5	9	9	9	9	9	9	9	9	9	9
	6	9	7	9	9	9	9	9	9	9	9
	7	9	9	9	9	9	9	9	9	9	9
	8										
	9	8		7	9	5	9		8	2	6

The count data indicates that the outperformance of the Measurement Test was less consistent than that of the LCF.

The results of this section showed that the LCF methodology may be an attractive alternative to the Measurement Test to solve the Identification problem. The same comments regarding the possible problems with practical implementation that was made with regards to the classification tree methodology applies to the LCF, which are:

- The reproducibility of the methodology is poor as indicated by the ANOVA on power vs. location. This is despite large training samples being used.
- The methodology will always depend on the representativeness of the training sample.
- It is not clear how the trade-off between type I and type II error may be optimized for the methodology, although the trade-off may be manipulated by changing training parameters.

9.4.3 Identification Results for the Quadratic Classification Function

The average proportion of correctly identified vectors over the 9 test data sets are presented in Table 9-50 for different gross error magnitudes:

Table 9-50 : Proportion of Vectors Correctly Identified by Quadratic Classification Function

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	72.6%	47.5%	63.5%	62.5%	46.2%	73.1%	66.9%	48.8%	74.2%	70.4%
	0.5	0.0%	9.0%	7.0%	4.4%	12.8%	0.0%	8.0%	12.7%	0.0%	3.2%
	1.0	0.3%	8.4%	3.8%	2.8%	9.0%	0.0%	3.2%	8.4%	0.2%	1.1%
	1.5	3.5%	7.5%	4.8%	4.9%	8.4%	2.6%	3.9%	7.0%	2.7%	3.2%
	2.0	14.2%	17.0%	15.3%	15.7%	17.9%	13.8%	14.8%	16.8%	13.8%	14.3%
	2.5	32.6%	36.1%	33.8%	34.2%	36.8%	33.3%	34.1%	35.7%	33.3%	33.6%
	3.0	46.5%	48.8%	47.5%	48.1%	50.0%	45.7%	47.5%	48.9%	46.3%	47.0%
	3.5	56.5%	59.6%	58.5%	58.8%	60.6%	56.3%	58.1%	59.2%	56.8%	57.7%
	4.0	65.0%	67.6%	65.7%	66.1%	68.2%	63.8%	65.8%	67.1%	64.0%	65.0%
	4.5	68.9%	72.3%	71.1%	70.5%	72.3%	68.9%	70.2%	71.0%	69.0%	70.2%
	5.0	73.2%	76.3%	75.0%	74.5%	76.2%	72.1%	73.7%	74.8%	72.9%	73.6%
		Measurement Test for Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Magnitude	0.0	72.6%	47.5%	63.5%	62.5%	46.2%	73.1%	66.8%	48.9%	74.1%	70.4%
	0.5	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	0.9%	6.5%	2.6%	2.7%	6.7%	0.6%	1.9%	5.7%	0.8%	1.2%
	1.5	6.1%	12.5%	8.8%	9.1%	12.7%	5.8%	8.0%	12.2%	5.7%	6.7%
	2.0	11.8%	17.6%	14.3%	14.6%	17.8%	11.7%	13.6%	17.3%	11.3%	12.7%
	2.5	16.1%	21.1%	18.2%	18.6%	20.8%	16.2%	17.5%	20.7%	15.8%	16.6%
	3.0	21.1%	25.6%	22.7%	23.2%	25.3%	21.1%	22.2%	24.8%	20.7%	21.4%
	3.5	25.5%	30.4%	27.8%	27.5%	30.3%	25.4%	27.0%	29.6%	25.3%	26.1%
	4.0	30.1%	33.7%	31.9%	31.8%	33.9%	29.8%	31.4%	33.6%	29.8%	30.8%
	4.5	33.3%	37.2%	35.0%	34.8%	37.3%	33.5%	34.6%	36.9%	33.1%	33.7%
	5.0	37.8%	41.6%	39.4%	39.7%	41.5%	37.3%	38.8%	40.9%	37.5%	38.3%

The QCF achieved type I error rates between 25.8% and 53.8%. The power to identify for the QCF varied between 0.0% and 76.3% compared to 0.0% and 41.6% for the MT. This compares with type I error rates of 10.3% to 12.5% and powers between 0.0% and 62.0% for the LCF, i.e. the use of a quadratic classification function increased type I error rates, but increased power to identify as well. The poor power to identify of the QCF and MT for gross error magnitudes of 0.5 and 1.0 should be noted.

The strength of the linear relationship between power to identify a gross error and gross error magnitude was tested through regression analysis for both the QCF and its corresponding MT:

Table 9-51 : Linear Regression of Power to Identify vs. Gross Error Magnitude for the Quadratic Classification Function

QCF #		1	2	3	4	5	6	7	8	9	10
QCF	Slope	19.24%	18.10%	18.57%	18.83%	17.63%	19.11%	18.34%	17.43%	19.22%	19.03%
	F	193.35	142.34	140.72	158.34	114.61	179.68	119.18	105.20	181.21	155.15
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
MT	Slope	8.88%	8.95%	9.00%	8.96%	8.92%	8.88%	8.98%	8.89%	8.87%	8.95%
	F	1438.80	883.38	1901.37	1766.75	851.30	1192.65	1798.77	923.59	1322.81	1506.47
	p(F)	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

All of the regressions displayed a significant increase in power with increasing gross error magnitude at the modified level of significance of 0.25% for 20 simultaneous tests.

The averages of the significant differences in power between the QCF and MT, as determined by the McNemar statistic, for different gross error magnitudes are presented below:

Table 9-52 : Mean Magnitude of Differences in Power vs. Gross Error Magnitude of Quadratic Classification Function solving the Identification Problem

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5	-3.11%	-5.48%	-4.67%	-4.58%	-4.80%	-3.24%	-4.34%	-5.45%	-2.98%	-3.64%
	2.0										
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
Mean Outperformance											
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0	3.2%					3.5%	4.0%		3.1%	3.4%
	2.5	16.6%	15.1%	15.6%	15.7%	15.9%	17.1%	16.5%	15.0%	17.5%	17.0%
	3.0	25.4%	23.2%	24.7%	25.0%	24.6%	24.6%	25.3%	24.1%	25.6%	25.6%
	3.5	31.0%	29.2%	30.7%	31.2%	30.3%	30.9%	31.1%	29.6%	31.6%	31.6%
	4.0	34.9%	33.8%	33.8%	34.3%	34.2%	33.9%	34.4%	33.5%	34.1%	34.2%
	4.5	35.5%	35.1%	36.1%	35.7%	35.0%	35.4%	35.5%	34.1%	35.9%	36.4%
	5.0	35.5%	34.7%	35.6%	34.8%	34.8%	34.7%	34.9%	34.0%	35.4%	35.3%

The MT was superior for a magnitude of 1.5, while the QCF is superior for all magnitudes of 2.5 and greater. As for the other classification methodologies, the magnitude of the outperformance is correlated with the magnitude of the gross errors.

The counts associated with the average significant differences in Table 9-52 are presented in Table 9-53:

Table 9-53 : Counts of Data Sets with Significant McNemar Statistics by Magnitude for the Quadratic Classification Function solving the Identification Problem

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5	5	7	6	7	7	9	7	8	8	8
	2.0										
	2.5										
	3.0										
	3.5										
	4.0										
	4.5										
	5.0										
Count of Significant Outperformance											
GE Magnitude	0.0										
	0.5										
	1.0										
	1.5										
	2.0	3					2	1		5	3
	2.5	9	9	9	9	9	9	9	9	9	9
	3.0	9	9	9	9	9	9	9	9	9	9
	3.5	9	9	9	9	9	9	9	9	9	9
	4.0	9	9	9	9	9	9	9	9	9	9
	4.5	9	9	9	9	9	9	9	9	9	9
	5.0	9	9	9	9	9	9	9	9	9	9

The counts indicate that the conclusions regarding relative performance drawn from the differences in Table 9-34 is consistent across most of the training data sets.

The results for the Identification problem relative to gross error location are discussed next:

Table 9-54 : Proportion of Vectors Correctly Identified by Quadratic Classification Function vs. Gross Error Location

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	72.6%	47.5%	63.5%	62.5%	46.2%	73.1%	66.9%	48.8%	74.2%	70.4%
	1	53.4%	54.1%	53.1%	55.1%	54.9%	53.7%	53.6%	53.0%	54.1%	52.1%
	2	68.8%	69.4%	68.9%	68.5%	69.0%	70.6%	69.5%	69.7%	70.8%	69.9%
	3	56.7%	57.9%	58.0%	57.2%	56.8%	58.4%	58.4%	59.5%	57.6%	59.8%
	4	55.2%	53.1%	52.4%	53.7%	54.1%	52.2%	54.0%	51.0%	53.3%	53.2%
	5	40.4%	40.6%	42.7%	41.5%	42.6%	40.6%	42.8%	42.5%	42.5%	40.8%
	6	26.5%	23.6%	25.4%	27.0%	25.5%	25.6%	24.8%	25.7%	24.9%	26.1%
	7	32.4%	30.8%	31.4%	31.4%	34.0%	30.3%	32.0%	32.3%	30.7%	31.4%
	8	7.4%	38.9%	21.8%	20.2%	39.4%	5.7%	14.8%	33.8%	6.7%	12.2%
	9	24.5%	26.6%	24.0%	25.7%	24.1%	24.4%	25.8%	23.9%	23.9%	25.6%
		Measurement Test for Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
GE Location	0	72.6%	47.5%	63.5%	62.5%	46.2%	73.1%	66.8%	48.9%	74.1%	70.4%
	1	32.4%	39.8%	35.5%	35.9%	39.9%	32.2%	34.8%	39.1%	32.1%	33.4%
	2	74.2%	79.9%	76.9%	77.3%	79.9%	74.2%	76.1%	79.6%	73.6%	75.0%
	3	38.6%	45.6%	41.8%	42.1%	45.2%	38.6%	41.1%	44.8%	38.4%	39.4%
	4	25.3%	32.0%	28.4%	28.1%	32.5%	24.6%	27.6%	31.4%	24.3%	25.9%
	5	4.2%	9.7%	6.2%	6.4%	10.0%	4.1%	5.6%	9.4%	3.7%	4.6%
	6	14.0%	20.1%	16.2%	16.6%	19.8%	13.9%	15.3%	19.3%	13.4%	14.6%
	7	0.9%	2.5%	1.4%	1.4%	2.6%	0.9%	1.2%	2.4%	0.8%	1.0%
	8	0.1%	0.6%	0.3%	0.3%	0.7%	0.1%	0.2%	0.6%	0.1%	0.1%
	9	0.9%	2.8%	1.6%	1.6%	2.8%	0.9%	1.4%	2.8%	0.8%	1.1%

The QCF's power to identify ranged between 5.7% and 70.8%, compared to 0.1% and 79.9% for the MT.

The averages of differences in power that were determined to be significant by the McNemar statistic are presented in Table 9-55:

Table 9-55 : Mean Magnitude of Difference in Power vs. Gross Error Location for Quadratic Classification Function solving the Identification Problem

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Mean Underperformance									
GE Location	0										
	1										
	2	-5.39%	-10.53%	-7.99%	-8.77%	-10.95%	-4.48%	-6.58%	-9.96%	-4.31%	-5.30%
	3										
	4										
	5										
	6										
	7										
	8										
	9										
		Mean Outperformance									
GE Location	0										
	1	21.02%	14.32%	17.57%	19.21%	14.96%	21.49%	18.75%	13.85%	21.98%	18.69%
	2										
	3	18.06%	12.32%	16.20%	15.10%	11.59%	19.89%	17.35%	14.65%	19.18%	20.32%
	4	29.97%	21.05%	24.07%	25.59%	21.57%	27.63%	26.41%	19.57%	29.02%	27.30%
	5	36.23%	30.85%	36.44%	35.12%	32.68%	36.52%	37.20%	33.12%	38.75%	36.21%
	6	12.49%	4.01%	9.23%	10.46%	5.89%	11.65%	9.53%	6.36%	11.42%	11.56%
	7	31.48%	28.33%	30.08%	30.03%	31.48%	29.43%	30.75%	29.93%	29.88%	30.42%
	8	7.27%	38.28%	21.57%	19.88%	38.78%	5.63%	14.59%	33.22%	6.60%	12.14%
	9	23.61%	23.83%	22.49%	24.02%	21.35%	23.50%	24.41%	21.17%	23.09%	24.55%

The MT is superior on location 2, while the QCF is superior on all other locations. This result is very similar to the results for the Detection problem.

The counts of number of test data sets that generated significant McNemar statistics associated with the averages in Table 9-55 are displayed in Table 9-56:

Table 9-56 : Counts of Data Sets with Significant McNemar Statistics for the Quadratic Classification Function solving the Identification Problem

		Quadratic Classification Function									
		1	2	3	4	5	6	7	8	9	10
		Count of Significant Underperformance									
GE Location	0										
	1										
	2	9	9	9	9	9	4	9	9	1	8
	3										
	4										
	5										
	6										
	7										
	8										
	9										
		Count of Significant Outperformance									
GE Location	0										
	1	9	9	9	9	9	9	9	9	9	9
	2										
	3	9	9	9	9	9	9	9	9	9	9
	4	9	9	9	9	9	9	9	9	9	9
	5	9	9	9	9	9	9	9	9	9	9
	6	9	4	9	9	8	9	9	9	9	9
	7	9	9	9	9	9	9	9	9	9	9
	8	9	9	9	9	9	9	9	9	9	9
	9	9	9	9	9	9	9	9	9	9	9

The counts in Table 9-56 indicate that the conclusions drawn from the results of Table 9-55 are consistent across all test data sets.

9.4.4 Summary of Identification Results

As for the Detection problem, the average type I and type II error rates over all 9 test data sets, for all gross error magnitudes and locations, were calculated. These are presented in Figure 9-7:

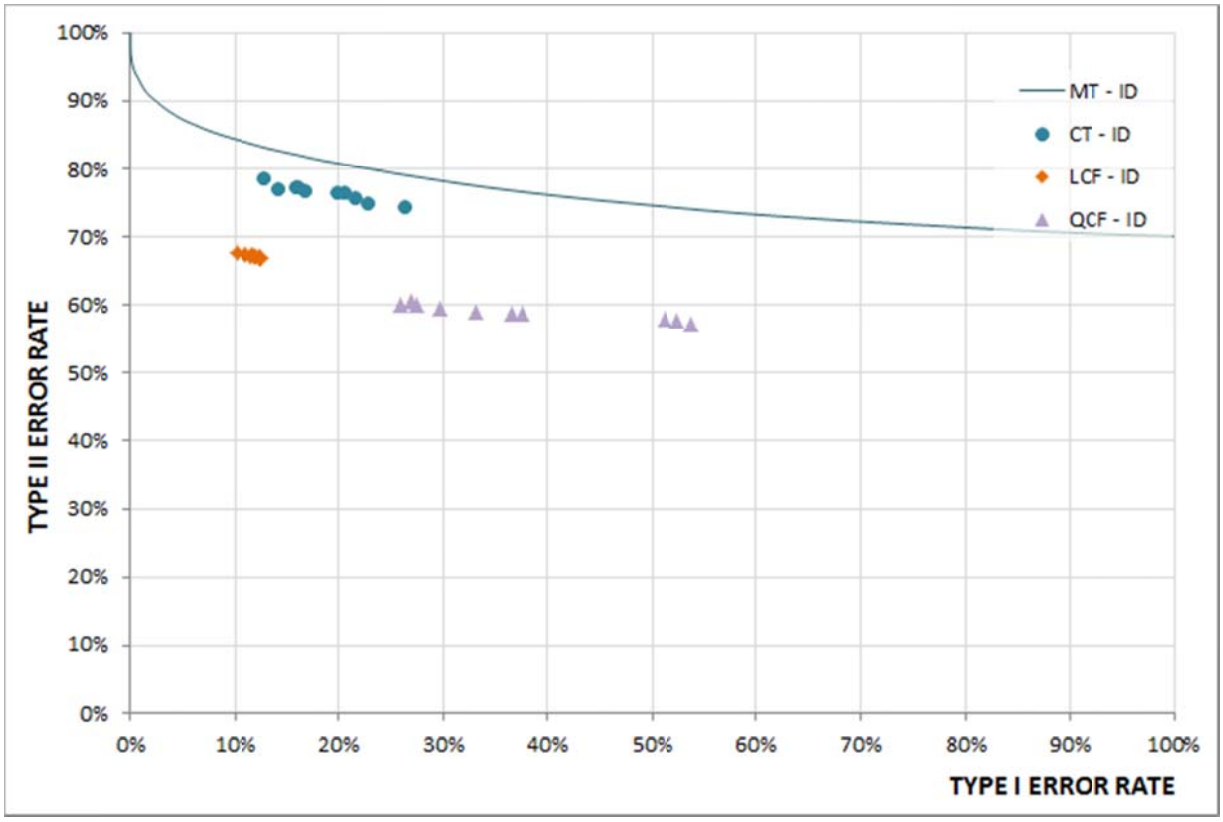

Figure 9-7 : Empirical Type II vs. Type I Error Rates for CT, LCF and QCF vs. MT for the Identification Problem

In contrast with the Detection problem, the CT (light blue dots) and LCF (orange triangles) have distinct curves of Type II vs. Type error.

The QCF (light purple triangles) results form a distinct pattern relative to the CT and LCF methodologies as it did for the Detection problem. The spread in Type I error rates for the QCF is significantly larger than for the Detection problem. The general poor performance for the Identification problem is evident from the consistently high type II error rates.

The QCF results seem to be superior to both the CT and LCF results in terms of outperformance of the benchmark Measurement Test. However, the QCF clearly illustrates one of the difficulties mentioned previously with regards to practical implementation of classification methodologies to solve the Identification problem, which is type I error rate control. The larger Type I error rate of the QCF may simply not be acceptable in practice, despite the fact that it achieves lower type II error rate than what any other methodology would have achieved if it operated at the same type I error rate.

This concludes the discussion on the results for the Identification problem.

9.5 ADDRESSING HIGH TYPE I AND TYPE II ERROR RATES WITH EXPANDED INPUT VECTOR

It was hypothesized that adding additional elements to the input vector of the classification methods could improve classification accuracy.

The input vectors to the classification methodologies were modified by incorporating two additional elements: the maximum absolute value of the relative adjustments made to each vector, and the Mahalanobis distance of each original input vector from the origin, based on the covariance estimate obtained from the unbiased vectors:

$$\mathbf{w}_j \in W^i = \begin{bmatrix} \left(\mathbf{v}_j\right)_{14\times 1} \\ \left(\sup_k \left|a^*_{j,k}\right|\right)_{1\times 1} \\ \left((\mathbf{v}_j - \overline{\mathbf{v}}_j)^T \Sigma^{-1}_{V^i} (\mathbf{v}_j - \overline{\mathbf{v}}_j)\right)_{1\times 1} \end{bmatrix}_{16\times 1} \tag{9.6}$$

Where: $\mathbf{v}_j$ is the j^{th} original input vector for data set i, $a^*_{j,k}$ is the k^{th} element of the vector $\mathbf{a}^*_j$ of standardized relative adjustments, and Σ_{V^i} is the covariance matrix of the $\mathbf{v}_j$ in data set I associated with random error vectors only.

The modified input vectors for each data set were used to grow 10 additional classification trees, linear and quadratic classifiers, as was done for the original input data. The empirical relationship between type II and type I error rates for the new classifiers for the Detection problem is presented in Figure 9-8:

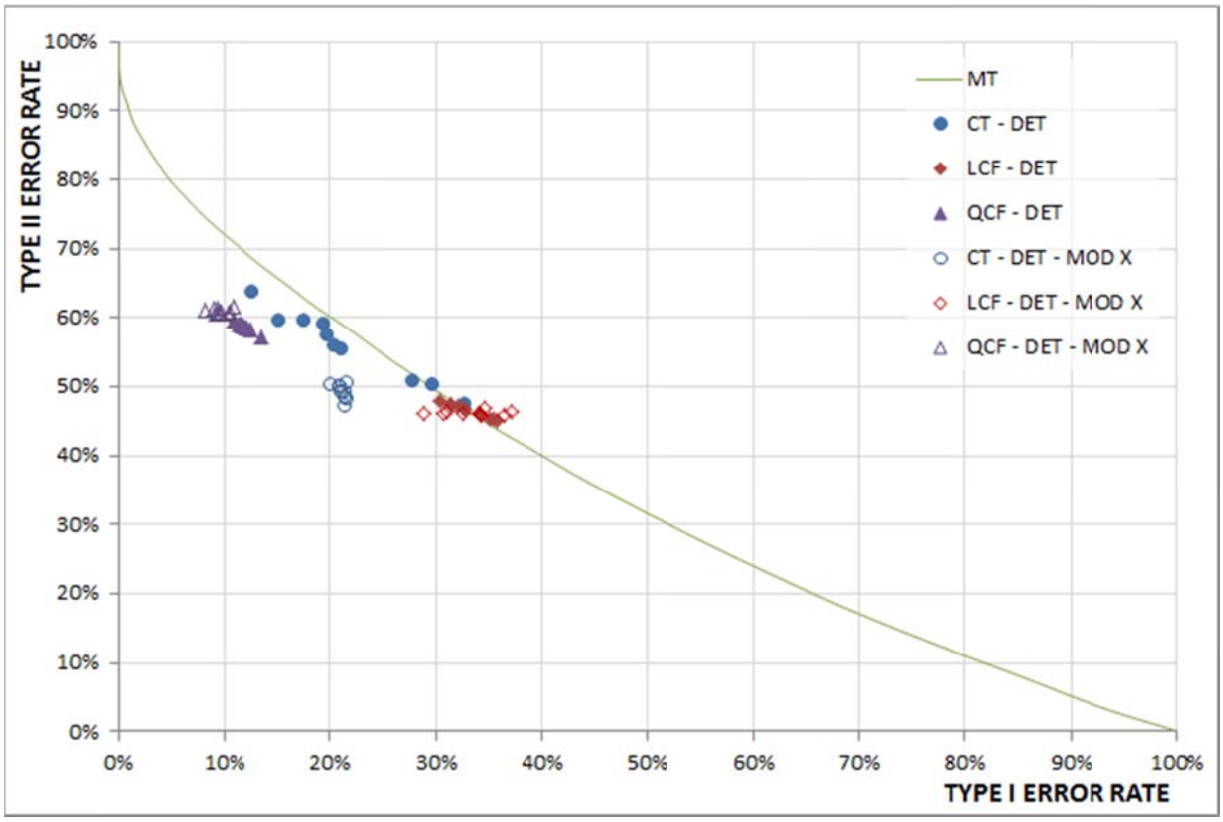

Figure 9-8 : Empirical Type II vs. Type I Error Rates for the Detection Problem with Expanded Input Vector

The results for both the LCFs and QCFs constructed using the modified input vector were very similar to that of the original classifiers. The results for the CT improved using the new input vector so that lower Type II error rates were achieved for similar Type I error rates. The range of Type I error rates for the CT using the new input vector was also much smaller, indicating improved reproducibility of the classifier.

The results for the new CT and QCF, as well as the original QCF, seems to form a common curve nearly parallel to the results of the MT. The similarity of the type II vs. type I error rate trade-off between the CT and QCF is probably related to the choice of Mahalanobis distance as an added input parameter; the QCF inherently makes use of the Mahalanobis distance to classify vectors, and including this distance measure in the CT training data resulted in similar classification efficiencies between the two methods.

The enhanced performance achieved by modifying the input vector is possibly due to the fact that the additional elements would be weakly correlated with the original elements, and especially the Mahalanobis distance measure would be very sensitive to even small disturbances caused by the presence of gross errors.

The results for the Identification problem are presented in Figure 9-9:

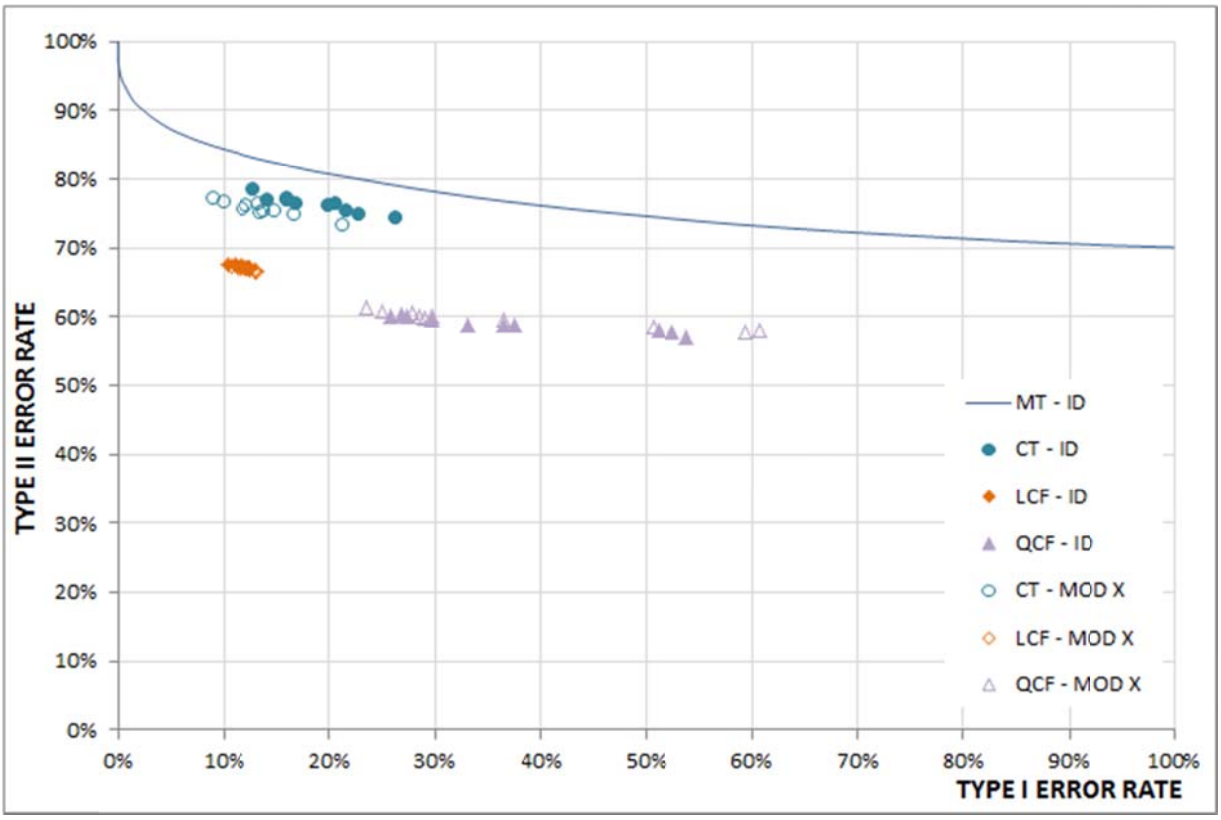

Figure 9-9 : Empirical Type II vs. Type I Error Rates for the Identification Problem with Expanded Input Vector

The LCF results with the new input vector are virtually unchanged. The CT results improved somewhat, while the QCF results seem to be unchanged, although the range of type I error rate increased.

Although both Detection and Identification improved somewhat with use of the new input vector, especially for the CT methodology, the improvement for the Identification problem seems less pronounced. This may be due to the choice of added elements; the maximum absolute relative adjustment may help to detect a gross error, but would contribute little to identifying it without information on the location of the maximum relative adjustment. A similar argument holds for the Mahalanobis distance.

The average performance for each classification methodology over the 9 test data sets using for the expanded input vector is presented in Table 9-57:

Table 9-57 : Average Classification Performance with Expanded Input Vector

		DETECTION			IDENTIFICATION		
		CT	LCF	QCF	CT	LCF	QCF
GE MAGNITUDE	0.0	79.0%	66.6%	90.4%	86.5%	87.8%	62.9%
	0.5	2.1%	0.0%	0.0%	0.0%	0.0%	5.7%
	1.0	1.2%	4.1%	0.0%	0.0%	0.0%	4.3%
	1.5	9.0%	24.4%	1.0%	1.0%	0.9%	4.5%
	2.0	29.0%	44.3%	10.9%	5.6%	6.0%	12.4%
	2.5	49.8%	56.4%	29.1%	13.9%	22.2%	30.5%
	3.0	62.6%	63.6%	45.4%	23.0%	36.5%	45.8%
	3.5	69.7%	69.1%	55.3%	31.3%	47.0%	58.1%
	4.0	74.7%	73.3%	61.9%	37.4%	54.1%	66.4%
	4.5	78.5%	76.3%	67.2%	41.3%	58.1%	71.6%
	5.0	82.2%	80.2%	72.1%	44.9%	61.9%	75.5%
GE LOCATION	F	63.4%	59.7%	51.9%	28.4%	49.9%	52.0%
	C	73.3%	84.2%	66.4%	59.1%	63.0%	65.9%
	T	72.7%	79.0%	61.5%	46.5%	51.6%	54.0%
	f_1	65.8%	73.2%	52.1%	35.4%	49.4%	51.5%
	c_1	54.7%	56.6%	36.4%	17.3%	32.7%	39.8%
	t_1	41.0%	49.7%	25.0%	2.1%	15.5%	25.4%
	f_2	44.3%	45.4%	26.6%	7.6%	23.0%	31.3%
	c_2	19.9%	28.5%	7.8%	0.0%	0.0%	24.1%
	t_2	37.7%	42.4%	18.9%	1.5%	1.9%	25.0%

In order to help visualize the impact of expanding the input vector, the differences between the mean performance for the original and expanded input vector is presented in Table 9-58:

Table 9-58 : Differences in Average Classification Performance between Expanded and Original Input Vector

		DETECTION			IDENTIFICATION		
		CT	LCF	QCF	CT	LCF	QCF
GE MAGNITUDE	0.0	0.5%	-0.3%	2.4%	5.1%	-0.5%	0.4%
	0.5	2.1%	0.0%	0.0%	0.0%	0.0%	0.0%
	1.0	-0.9%	0.2%	0.0%	-0.2%	0.0%	0.5%
	1.5	-4.1%	0.2%	-0.6%	-1.8%	0.1%	-0.4%
	2.0	0.4%	0.3%	-3.8%	-2.8%	0.4%	-2.9%
	2.5	8.5%	0.2%	-6.1%	-1.7%	0.0%	-3.9%
	3.0	12.7%	0.5%	-4.0%	-0.3%	0.4%	-1.8%
	3.5	13.1%	0.6%	-2.7%	1.9%	0.5%	-0.1%
	4.0	13.2%	0.6%	-2.2%	3.2%	0.7%	0.6%
	4.5	12.6%	0.6%	-1.7%	3.7%	0.6%	1.2%
	5.0	11.5%	0.6%	-1.5%	4.0%	0.3%	1.3%
GE LOCATION	0	0.5%	-0.3%	2.4%	5.1%	-0.5%	0.4%
	1	21.0%	-0.5%	-2.3%	13.2%	0.3%	-1.7%
	2	-3.9%	-0.2%	-3.0%	-3.9%	-0.9%	-3.6%
	3	6.5%	-0.1%	-3.7%	-1.7%	0.0%	-4.1%
	4	5.3%	0.5%	-3.6%	-7.3%	0.2%	-1.7%
	5	12.8%	0.5%	-3.6%	4.6%	0.2%	-1.9%
	6	7.0%	0.5%	-3.5%	-1.1%	0.9%	-0.1%
	7	9.6%	1.5%	-1.5%	1.8%	2.1%	-0.4%
	8	2.3%	0.3%	-2.0%	0.0%	0.0%	4.0%
	9	4.0%	1.2%	-2.7%	-2.9%	0.4%	0.1%

The results of Table 9-58 indicate that the classification tree methodology was impacted most by the additional input features, specifically with regards to the Detection problem. The detection of larger magnitude gross errors improved significantly, probably due to the sensitivity of the Mahalanobis distance to gross error magnitude. The detection for gross error locations 1 and 5 also improved significantly. The identification results did not improve much on the whole, as the additional features did not contain information on gross error location.

This section has shown that improvement in classifier performance may be obtained through the choice of input vector elements, however it remains an open question as to what the element should be to improve specifically the Identification problem.

10 CONCLUSIONS AND RECOMMENDATIONS

The hypothesis investigated in this thesis is that classification methodologies can successfully resolve the GED problem.

The research objectives stated in the introduction to this thesis are re-stated here for convenience:

1. A critical review of the relevant literature.
2. Construction of a simulated DR problem.
3. Application of a classical GED technique to the simulated problem.
4. Development of a classifier to solve the GED problem for the simulated DR problem.
5. Comparison of the results of the classical and classification methodology in resolving the GED problem.

10.1 CONCLUSIONS

The body of literature covering DR and GED is vast, spanning a period of roughly 40 years. Sufficient background information was reviewed to provide a holistic view of the DR and GED problem. In general the DR and GED problem has been addressed through the use of parametric statistics with the underlying assumption of Gaussian error distributions being pervasive. Relatively few researchers have attempted to apply nonparametric or classical classification techniques to a problem that ultimately amounts to performing a classification. Investigations of nonparametric methods have focussed on applying artificial neural networks (ANNs) to the DR and GED problem, with some success. The success of ANNs indicates that there is scope for other non-parametric methods, such as the ones investigated in this study, to be applied to the GED problem as well. Whereas the structure of an ANN is typically difficult to interpret, the structure of other methods are directly interpretable (e.g. classification trees) and the relative importance of elements of the input vector can be estimated.

The process unit selected for the simulated DR and GED problem is the simple two-product splitter. Similar units can be found in many real processes. One linear, one bilinear and one tri-linear steady-state material conservation constraints were imposed on the unit. A set of hypothetical 'true' process variable values satisfying these constraints were selected and random and gross error components added to the true values to simulate real, steady-state process measurements, so that ten data sets with 11 000 randomly generated measurement vectors each could be constructed. Only single gross errors were simulated. A naïve objective function assuming a common cov_y for all measurements was selected for the DR problem, and the DR problem subsequently resolved through successive linearization.

The classical GED technique selected as a benchmark for the classification methodologies was the measurement test, due to its wide application in commercial software. A convenient consequence of the naïve objective function was that the type I error rate for the measurement test could be manipulated at will to match the type I error rate of all the classifiers on all the data sets, so that a direct comparison of the resulting statistical power of the methods could be made.

The classification methodologies selected to test the main hypothesis of this thesis was classification trees, linear classification functions, and quadratic classification functions. A classifier from each methodology was constructed on each of the ten data sets, using as input vector a combination of balance equation residual vectors, measurement adjustment vectors and the norms of the residual and adjustment vectors.

Due to the simplifying assumption of a common coefficient of variation for all measurements in the DR procedure, it is possible to calibrate a unique measurement test with an equivalent type I error rate for each classifier. By comparing the statistical power of the classification methodologies to that of the measurement test with equivalent type I error rate, deductions can be made regarding relative efficiency of the methods

For the Detection problem, all classifiers consistently perform better than the equivalent measurement test for gross errors of magnitude 2.5 times the standard deviation of the measurement error and greater. The measurement test perform better for a gross error magnitude of 1.5, while gross errors smaller or equal to 1.0 are undetectable by any method. The performance difference was also strongly influenced by gross error location, with the measurement test in general being superior on locations # 1 and 2, while the classification methods performed better on locations #4, 5, 6, 7, and 9.

An ANOVA analysis for all classifiers on the Detection problem indicates that classifiers themselves are significant factors in determining performance, that is, the classifier structure and performance exhibits poor reproducibility. This is a significant consideration for practical implementation.

The results for the Identification problem for different gross error magnitudes follow the same pattern as that for the Detection problem, with the measurement test being superior for smaller magnitudes, and the classification methods being superior for larger magnitudes. The results for different gross error locations also follow much the same pattern, except that the linear and quadratic classification functions is consistently superior in

identifying gross errors in location #1, while the measurement test is superior to the classification tree for this location.

In general he power to identify a gross error for a given location was much lower than the power to detect it. This indicates significant smearing of gross errors. An analysis of the Jacobian of the constraints at the nominal steady-state values of the measurements indicated that the problem is prone to smearing, confirming the conclusion drawn from analysis of the Detection and Identification results.

10.2 RECOMMENDATIONS

The use of statistical classification methodologies to resolve the GED problem shows promising results when compared to the most widely applied classical GED technique. Some issues with practical implementation of classification methodologies arise though:

- The reproducibility of the methodology is poor as indicated by the ANOVA on power vs. location. This is despite large training samples being used.
- The methodology will always depend on the representativeness of the training sample.
- It is not clear how the trade-off between type I and type II error may be optimized for the methodology, although the trade-off may be manipulated by changing training parameters.

The starting point for implementation of a classification methodology is the training sample. Every effort must be made to ensure that it is representative of the process under consideration. The methods described in section 3 of this thesis may be used to derive best estimates for the true variance/covariance structure of the measurement error, which should be used to generate simulated training data. The economics of the particular situation will dictate which gross errors are important to detect and identify, and what the optimum trade-off between type I and type II error rate is.

Investigating factors that impact on and methods to manipulate type I and II error rates for the classification methodologies may be a very productive extension of this work. It is expected that this may also solve the problem of poor reproducibility experienced in this work, that is, it is expected that for a particular classification methodology the power will be statistically identical between different classifiers if their type I error rates are similarly identical.

The scope of the investigation of this thesis is fairly limited. Only a single process was considered, only single gross errors were considered, only gross error in the measurements (as opposed to the process constraints themselves) and only steady-state conditions were considered. Although the process constraints were nonlinear, the degree of nonlinearity was not severe. There is therefore scope to expand the investigation to more complex and possibly dynamic processes, incorporating strongly nonlinear constraints and possibly gross modelling error in the constraints.

Only two facets of the GED problem were addressed in this study: the Detection and Identification of single gross errors. The treatment of multiple gross errors, and gross error magnitude estimation, was not investigated. The classification tree methodology seems especially suitable to the estimation of gross error magnitude, as the Matlab® package can readily extend the tree methodology to incorporate regression functionality for gross error magnitude estimation.

The development of the classification methodologies was not investigated in detail. The initial results for the Detection and Identification problem were disappointing, leading to some investigation into improving classifier performance. This was accomplished by incorporating additional information into the input vector of the classifiers. There is scope to investigate the effect on classifier performance of different elements and manipulations of the input vector.

Finally, the measurement test was selected due to its common application. More powerful GED methods are described in the literature though, and incorporating some of these methods into a comparison with classification methodologies may provide a broader perspective on the applicability of the methods.

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A. Appendix A: Sample Calculations – Successive Linearization DR

The results of this appendix present a set of sample calculations for the successive linearization algorithm for the measurement vector:

Table A-1 : Measurement Vector for Successive Linearization Sample Calculations

$$\begin{bmatrix} F \\ C \\ T \\ f_1 \\ c_1 \\ t_1 \\ f_2 \\ c_2 \\ t_2 \end{bmatrix} = \begin{bmatrix} 109.689 \\ 74.140 \\ 23.460 \\ 9.767\% \\ 4.988\% \\ 25.402\% \\ 10.187\% \\ 0.099\% \\ 15.764\% \end{bmatrix}$$

The SL algorithm was presented in Figure 7-3:

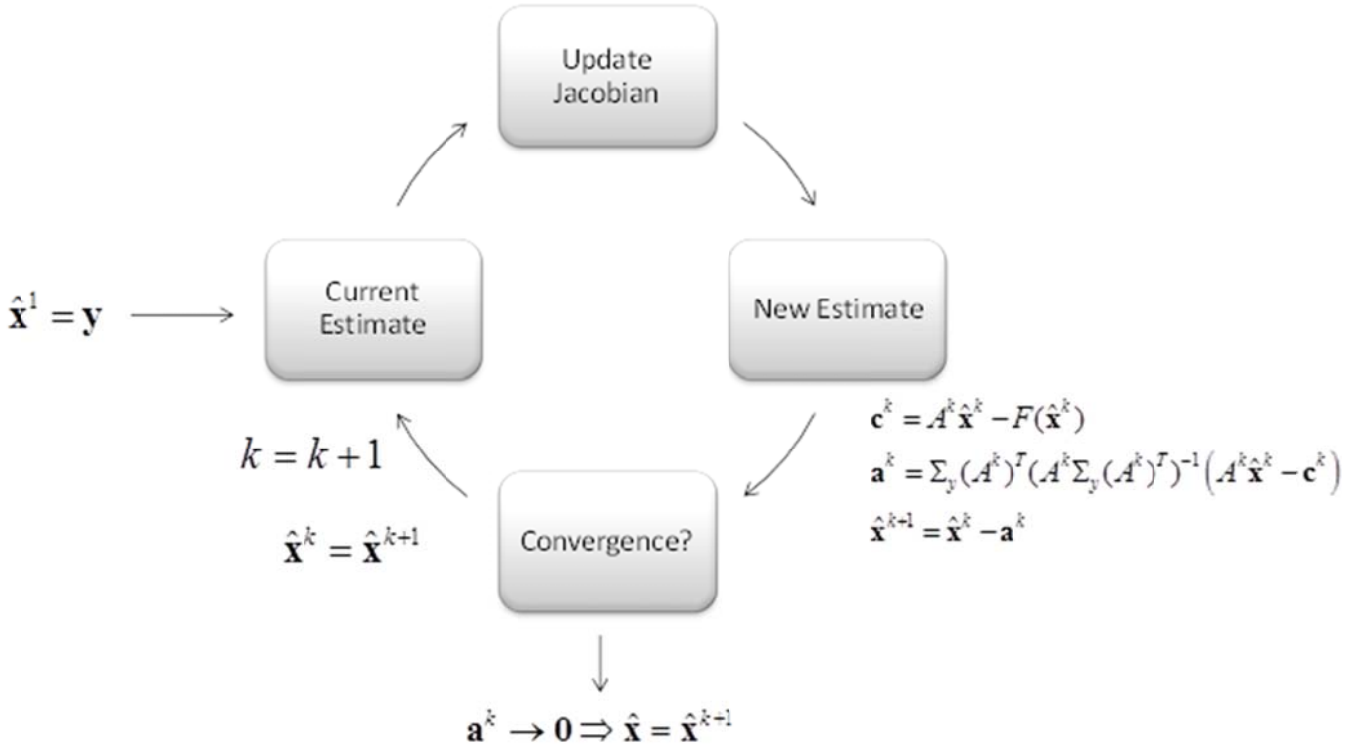

Figure 7-3 : Data Reconciliation through Successive Linearization

The covariance matrix of the measurements was calculated from:

$$\left(\Sigma_y\right)_{i,i} = \left(\text{cov}_y \cdot \mathbf{y}(i)\right)^2, i = 1,2,...,9 \qquad (7.6)$$

Where $\text{cov}_y = 0.05$ was assumed. The resulting measurement error covariance matrix is presented in Table A-2:

Table A-2 : Measurement Error Covariance Matrix for Successive Linearization Sample Calculations

$\Sigma_y =$

3.008E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	1.374E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	1.376E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	2.385E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	6.219E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	1.613E-04	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.594E-05	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.452E-09	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	6.213E-05

The set of constraint equations that need to be satisfied by the reconciled estimates is given by:

$$F(\mathbf{x}) = \begin{bmatrix} F - C - T \\ F \cdot f_1 - C \cdot c_1 - T \cdot t_1 \\ F \cdot f_1 \cdot f_2 - C \cdot c_1 \cdot c_2 - T \cdot t_1 \cdot t_2 \end{bmatrix} \tag{7.5}$$

At each iteration *k* of the SL algorithm, a new estimate of the reconciled measurements can be obtained by solving the following set of equations:

1. Calculate the Jacobian of the constraint equations given in (7.5):

$$A = \frac{\partial F(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ f_1 & -c_1 & -t_1 & F & -C & -T & 0 & 0 & 0 \\ f_1 \cdot f_2 & -c_1 \cdot c_2 & -t_1 \cdot t_2 & F \cdot f_2 & -C \cdot c_2 & -T \cdot t_2 & F \cdot f_1 & -C \cdot c_1 & -T \cdot t_1 \end{bmatrix} \tag{7.7}$$

2. Calculate the vector of linearization constants:

$$\mathbf{c}^k = A\mathbf{x}^k - F(\mathbf{x}^k) \tag{7.8}$$

3. Calculate the vector of measurement adjustments:

$$\mathbf{a}^k = \Sigma_y (A^k)^T \left(A^k \Sigma_y (A^k)^T \right)^{-1} \left(A^k \mathbf{x}^k - \mathbf{c}^k \right) \tag{A.1}$$

   The form of the adjustment vector in (A.1) is required due to the nonlinear nature of the reconciliation problem, as described in section 4.1.7 of this thesis.

4. Calculate the new reconciled estimate:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \mathbf{a}^k \tag{A.2}$$

Results are presented with scientific number formatting so that small incremental changes, which are still large relative to the convergence tolerance of 10^{-7} may be apparent.

k = 1

x^k	$(A^k)^T$			a^k	x^{k+1}
1.097E+02	1.000E+00	9.767E-02	9.950E-03	-8.287E+00	1.014E+02
7.414E+01	-1.000E+00	-4.988E-02	-4.939E-05	3.286E+00	7.743E+01
2.346E+01	-1.000E+00	-2.540E-01	-4.004E-02	5.155E-01	2.398E+01
9.767E-02	0.000E+00	1.097E+02	1.117E+01	3.874E-04	9.806E-02
4.988E-02	0.000E+00	-7.414E+01	-7.342E-02	-4.697E-04	4.941E-02
2.540E-01	0.000E+00	-2.346E+01	-3.698E+00	1.261E-03	2.553E-01
1.019E-01	0.000E+00	0.000E+00	1.071E+01	-2.399E-03	9.947E-02
9.903E-04	0.000E+00	0.000E+00	-3.698E+00	7.825E-08	9.904E-04
1.576E-01	0.000E+00	0.000E+00	-5.959E+00	3.196E-03	1.608E-01

k = 2

x^k	$(A^k)^T$			a^k	x^{k+1}
1.014E+02	1.000E+00	9.806E-02	9.754E-03	-3.165E-03	1.014E+02
7.743E+01	-1.000E+00	-4.941E-02	-4.893E-05	-5.562E-03	7.742E+01
2.398E+01	-1.000E+00	-2.553E-01	-4.106E-02	2.397E-03	2.398E+01
9.806E-02	0.000E+00	1.014E+02	1.009E+01	2.163E-05	9.808E-02
4.941E-02	0.000E+00	-7.743E+01	-7.668E-02	-1.352E-05	4.939E-02
2.553E-01	0.000E+00	-2.398E+01	-3.856E+00	1.151E-05	2.553E-01
9.947E-02	0.000E+00	0.000E+00	9.943E+00	-5.011E-05	9.942E-02
9.904E-04	0.000E+00	0.000E+00	-3.825E+00	1.822E-09	9.904E-04
1.608E-01	0.000E+00	0.000E+00	-6.120E+00	7.386E-05	1.609E-01

k = 3

x^k	$(A^k)^T$			a^k	x^{k+1}
1.014E+02	1.000E+00	9.808E-02	9.751E-03	7.255E-07	1.014E+02
7.742E+01	-1.000E+00	-4.939E-02	-4.892E-05	1.279E-06	7.742E+01
2.398E+01	-1.000E+00	-2.553E-01	-4.108E-02	-5.540E-07	2.398E+01
9.808E-02	0.000E+00	1.014E+02	1.008E+01	-1.853E-10	9.808E-02
4.939E-02	0.000E+00	-7.742E+01	-7.667E-02	1.216E-09	4.939E-02
2.553E-01	0.000E+00	-2.398E+01	-3.858E+00	-5.621E-09	2.553E-01
9.942E-02	0.000E+00	0.000E+00	9.945E+00	6.419E-09	9.942E-02
9.904E-04	0.000E+00	0.000E+00	-3.824E+00	-2.332E-13	9.904E-04
1.609E-01	0.000E+00	0.000E+00	-6.121E+00	-9.462E-09	1.609E-01

k = 4

$\mathbf{x}^k$

1.014E+02
7.742E+01
2.398E+01
9.808E-02
4.939E-02
2.553E-01
9.942E-02
9.904E-04
1.609E-01

$(\mathbf{A}^k)^T$

1.000E+00	9.808E-02	9.751E-03
-1.000E+00	-4.939E-02	-4.892E-05
-1.000E+00	-2.553E-01	-4.108E-02
0.000E+00	1.014E+02	1.008E+01
0.000E+00	-7.742E+01	-7.667E-02
0.000E+00	-2.398E+01	-3.858E+00
0.000E+00	0.000E+00	9.945E+00
0.000E+00	0.000E+00	-3.824E+00
0.000E+00	0.000E+00	-6.121E+00

$\mathbf{a}^k$

1.117E-14
1.969E-14
-8.526E-15
-2.081E-17
2.582E-17
-7.547E-17
1.180E-16
-4.287E-21
-1.739E-16

$\mathbf{x}^{k+1}$

1.014E+02
7.742E+01
2.398E+01
9.808E-02
4.939E-02
2.553E-01
9.942E-02
9.904E-04
1.609E-01

After 4 iterations, the maximum absolute value of the adjustment vector $\mathbf{a}^k$ is smaller than the tolerance of 10^{-7}, so the procedure would terminate with $\mathbf{x}^{k+1}$ as the final DR estimate.

B. Appendix B: Sample Calculations – Sensitivity Analysis

This appendix provides detailed results for the calculations involved in determining the sensitivity of different measurement locations to a small error in location F, that is, corresponding to $i = 1$ according to the notation of Section 7.5 of this thesis. The measurement vector resulting from the introduction of this error is:

Table B-1 : Measurement Vector for Sensitivity Analysis

		y
F	=	1.00000001E+02
C		7.50000000E+01
T		2.50000000E+01
f_1		1.00000000E-01
c_1		5.00000000E-02
t_1		2.50000000E-01
f_2		1.00000000E-03
c_2		1.00000000E-03
t_2		1.59400000E-01

The covariance matrix of the measurements was calculated from:

$$\left(\Sigma_y\right)_{i,i} = \left(\text{cov}_y \cdot \mathbf{y}(i)\right)^2, i = 1,2,...,9 \tag{7.6}$$

Where $\text{cov}_y = 0.05$ was assumed. The resulting measurement error covariance matrix is presented Table B-2:

Table B-2 : Measurement Error Covariance Matrix for Sensitivity Sample Calculations

$\Sigma_y =$

2.500E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	1.406E+01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	1.563E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	2.500E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	6.250E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	1.563E-04	0.000E+00	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E-05	0.000E+00	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	2.500E-09	0.000E+00
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	6.352E-05

The Jacobian of the constraint equations given in (7.5) is:

$$A = \frac{\partial F(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ f_1 & -c_1 & -t_1 & F & -C & -T & 0 & 0 & 0 \\ f_1 \cdot f_2 & -c_1 \cdot c_2 & -t_1 \cdot t_2 & F \cdot f_2 & -C \cdot c_2 & -T \cdot t_2 & F \cdot f_1 & -C \cdot c_1 & -T \cdot t_1 \end{bmatrix} \tag{7.7}$$

The transpose of the Jacobian matrix evaluated at the steady-state values of Table 7-1 is:

Table B-3 : Jacobian Matrix for Sensitivity Sample Calculations

$\mathbf{A^T}$

1.000	0.100	0.010
-1.000	-0.050	0.000
-1.000	-0.250	-0.040
0.000	100.000	10.000
0.000	-75.000	-0.075
0.000	-25.000	-3.985
0.000	0.000	10.000
0.000	0.000	-3.750
0.000	0.000	-6.250

The vector of adjustments is calculated by:

$$\mathbf{a} = \Sigma_y A^T (A\Sigma_y A^T)^{-1} A\mathbf{y} \tag{9.2}$$

The form of the adjustment vector in (9.2) is due to the fact that the nonlinear problem is approximated as a linear reconciliation problem when the true process values, with the exception of a small δ_i in the i^{th} position, are substituted as measurement values.

The vector of adjustments is given in Table B-4:

Table B-4 : Vector of Adjustments for Sensitivity Sample Calculations

$\mathbf{a_1}$

-6.262E-07
3.258E-07
4.796E-08
-5.713E-11
3.777E-12
1.239E-10
-3.736E-11
1.401E-15
5.933E-11

The covariance matrix of the adjustments is calculated from:

$$\Sigma_a = \Sigma_y A^T \left(A\Sigma_y A^T \right)^{-1} A\Sigma_y \tag{4.66}$$

The covariance matrix of the adjustments calculated from the Jacobian is given in Table B-5:

Table B-5 : Covariance Matrix of Adjustments for Sensitivity Sample Calculations

$\Sigma_a =$

1.566E+01	-8.145E+00	-1.199E+00	1.428E-03	-9.443E-05	-3.099E-03	9.340E-04	-3.502E-08	-1.483E-03
-8.145E+00	5.822E+00	9.545E-02	2.678E-03	-1.771E-04	-5.810E-03	1.751E-03	-6.567E-08	-2.781E-03
-1.199E+00	9.545E-02	2.680E-01	-1.250E-03	8.263E-05	2.711E-03	-8.172E-04	3.065E-08	1.298E-03
1.428E-03	2.678E-03	-1.250E-03	1.435E-05	-3.060E-06	-2.057E-05	-1.990E-06	7.462E-11	3.160E-06
-9.443E-05	-1.771E-04	8.263E-05	-3.060E-06	9.939E-07	2.680E-06	2.264E-06	-8.490E-11	-3.595E-06
-3.099E-03	-5.810E-03	2.711E-03	-2.057E-05	2.680E-06	3.803E-05	-6.345E-06	2.379E-10	1.008E-05
9.340E-04	1.751E-03	-8.172E-04	-1.990E-06	2.264E-06	-6.345E-06	1.019E-05	-3.820E-10	-1.618E-05
-3.502E-08	-6.567E-08	3.065E-08	7.462E-11	-8.490E-11	2.379E-10	-3.820E-10	1.432E-14	6.066E-10
-1.483E-03	-2.781E-03	1.298E-03	3.160E-06	-3.595E-06	1.008E-05	-1.618E-05	6.066E-10	2.569E-05

The standardized adjustments are calculated from:

$$\left(Z_a\right)_{i,j} = \frac{\mathbf{a}_i(j)}{s_{i,j}}; i = 1,2,...,9,\ j = 1,2,...,9 \tag{9.3}$$

Where $s_{i,j} = \sqrt{\left(\Sigma_a\right)_{j,j}}$ and $i = 1$ for the sample calculations. The first row of $\left(Z_a\right)_{i,j}$, corresponding to $i = 1$, is presented in Table B-6:

Table B-6 : Row 1 of the Standardized Adjustments Matrix for Sensitivity Calculations

$(Z_a)^T_{row\,1}$
-1.583E-07
1.350E-07
9.266E-08
-1.508E-08
3.789E-09
2.010E-08
-1.171E-08
1.171E-08
1.171E-08

The ratios of standardized adjustments are calculated from:

$$P_{i,j} = \frac{\left(Z_a\right)_{i,j}}{\left(Z_a\right)_{i,i}}, i = 1,2,...,9 \quad j = 1,2,...,9 \tag{9.4}$$

Where $i = 1$ for the sample calculations. The first row of $P_{i,j}$, corresponding to $i = 1$, is presented in Table B-7:

Table B-7 : Row 1 of the Ratios of Standardized Adjustments Matrix for Sensitivity Calculations

$$P^{T}_{row\,1} = \begin{bmatrix} 1.000 \\ -0.853 \\ -0.585 \\ 0.095 \\ -0.024 \\ -0.127 \\ 0.074 \\ -0.074 \\ -0.074 \end{bmatrix}$$