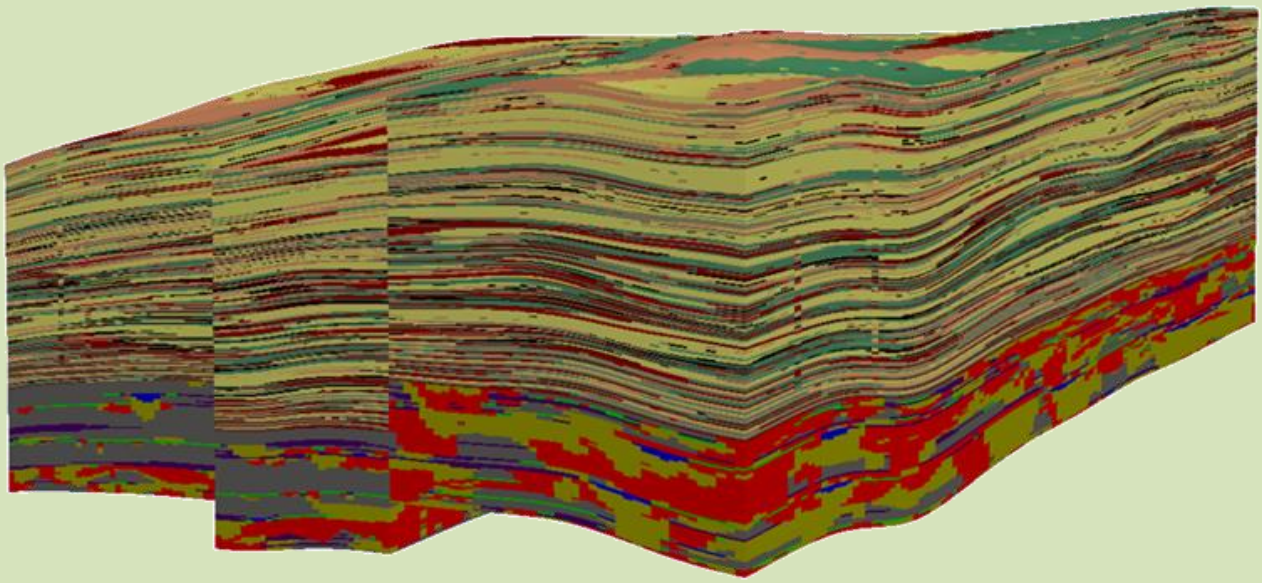
# Calibration and Uncertainty Analysis for Complex Environmental Models



PEST: complete theory and what it means for modelling the real world

John Doherty

# Calibration and Uncertainty Analysis for Complex Environmental Models

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# A Message for Your Conscience

This book is very cheap. But it is not free.

If you are reading this book and have not paid for it, then I urge you to do so. This book is the product of many month's work. The story which it tells is the story of PEST, which is the outcome of a lifetime's work. PEST is free. This book is not - for one very practical reason. It is because the author must, like everyone else, earn a living.

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# Preface

PEST stands for "parameter estimation". When it was originally written in 1994, this is all that PEST did. However over the 20 years that have elapsed since then, the capabilities of the PEST suite of software have expanded enormously. The emphasis has shifted from inversion to inversion-constrained model parameter and predictive uncertainty analysis.

The purpose of this document is to present, in one place, the theory that underpins PEST and that underpins the plethora of utility software that supports and complements PEST. In doing this, it serves the same purpose for the next generation of PEST-like software. This includes PEST++ and pyEMU. As such, it is hoped that this book provides a valuable resource for those who wish to understand inversion and inversion-constrained uncertainty analysis as it pertains to environmental models. These type of models include (but are not limited to) petroleum and geothermal reservoir models, groundwater models and surface water hydraulic and hydrologic models.

As well as presenting theory, an equally important role of this book is to draw some important conclusions from the theory. These conclusions pertain to real world model usage. Some of them question modelling practices that are commonplace today. Others suggest roles for models in environmental management beyond those which they presently play.

Although a basic knowledge of matrix algebra, and of statistical and geostatistical concepts, is required in order to follow the discussion provided herein, mathematical prerequisites are not high. Most readers will have acquired the knowledge to understand the following theory at school or though undergraduate university courses. The early part of the book reminds readers of a few basic linear analysis and statistical concepts that they may have forgotten. Refer to the many good books on these topics for further details.

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# 1. Introduction

## 1.1 PEST: The Past

PEST stands for "parameter estimation".

PEST was released in 1994. Upon its release, the feature that most distinguished it from earlier generations of parameter estimation software was the fact that it is able to communicate with a model through that model's own input and output files. While this feature is convenient, its repercussions are more profound than simply convenience. In fact it can almost be deemed as essential to parameter estimation and uncertainty analysis in the environmental modelling context. It allows "the model" to be a batch or script file which runs one or many actual simulators, together with one or many simulator pre-processors and post-processors. An inversion problem can thus be tailored to suit the individual requirements of any modelling and data context.

Over the years since its original release, the capabilities of PEST have continually expanded. Support was added for highly parameterized inversion through introduction of flexible Tikhonov regularization functionality and subspace methods for solution of ill-posed inverse problems. Efficiency in the face of high model run times was supported through the use of "super parameters" defined through singular value decomposition of the sensitivity matrix linking model parameters to model outputs used in the calibration process. Further gains in efficiency were realized through parallelization of model runs, first through Parallel PEST and then through BEOPEST. Even greater efficiencies have more recently emerged with support for the use of surrogate models and polynomial proxy models for derivatives calculation.

Perhaps the most significant trend in PEST development over the past two decades has been the shift in focus from "model calibration" (a questionable concept, as this document will discuss) to what can be loosely described as "calibration-constrained model predictive uncertainty analysis". This shift in emphasis recognizes the fact that environmental models are built to make predictions that support the making of important management decisions. These predictions are often accompanied by a large amount of uncertainty – uncertainty that must be accommodated in any sensible decision-making strategy. Quantification of uncertainty allows evaluation of the risks associated with different management strategies. This then provides the basis for choosing between them.

The shift in emphasis from calibration to uncertainty analysis prompted the development of a suite of utility programs for calculation of model parameter and predictive uncertainty under the assumption of linear model behaviour. Quantities calculated by these programs are approximate as models, and the systems that they simulate, are often far from linear. Nevertheless, these utilities can provide a great deal of useful information. A particular benefit of linear analysis is that, once the uncertainty of a prediction has been evaluated, the reduction in uncertainty of that prediction that would follow the acquisition of further data can also be calculated. Ease of uncertainty quantification under linear conditions follows from the fact that the values of parameters and model outcomes do not feature in the equations on which linear analysis is based; only their sensitivities feature in these equations. Hence assessments of data worth, and of the contributions that different parameters make to the uncertainties of predictions of management interest, only require the undertaking of as many model runs as those needed for calculation of sensitivities of pertinent model outputs to

parameters employed by the model.

Concurrently with the development of linear analysis tools was the development of means to explore calibration-constrained predictive uncertainty, with nonlinear behaviour of the model taken into account. Where a model employs only a few parameters, the constrained maximization/minimization process undertaken by PEST when run in "prediction" mode provides one means to achieve this. Unfortunately the numerical efficiency of PEST's "predictive analyser" starts to fall as parameter numbers start to rise. However in many real world environmental modelling contexts, integrity of uncertainty analysis requires that a model represent parameterization detail on which predictive uncertainty depends, so that the repercussions of incomplete knowledge of this detail on predictive uncertainty can be properly explored. The use of many parameters in model predictive uncertainty analysis therefore becomes mandatory. Long model run times and large numbers of parameters also present serious challenges to Bayesian methods such as Markov chain Monte Carlo. Fortunately, however, with the sacrifice of some Bayesian purity, the null space Monte Carlo methodology (which, to the author's knowledge, is unique to PEST) allows rapid generation of a suite of high dimensional parameter sets which all calibrate a model, and which can collectively be used to make model predictions of management interest in order to explore the uncertainties that are associated with those predictions.

Numerical models are imperfect simulators of real world behaviour; they have defects. Hence uncertainties in model predictions often include substantial quantities of "model-generated uncertainty" which is difficult or impossible to analyse, and may be invisible to the calibration process. To make matters worse, for some predictions, contributions to model predictive error arising from model defects may actually be enhanced by the calibration process, while for other predictions these contributions can be "calibrated out". Recent additions to PEST's linear analysis capabilities include the capacity to explore this issue. Meanwhile, the flexibility that PEST provides for defining the calibration objective function in innovative ways, and for running batch or script file models that include pre- and post-processors that can "orthogonalize out" the most damaging components of so-called "structural noise", allows modellers to reduce this source of predictive uncertainty to some extent at least.

Characteristics of some models which make their use with PEST difficult are long run times, and lack of continuity of model outputs with respect to adjustable parameters. There can be many reasons for the latter. Model output numerical granularity can arise from many sources, these including incomplete solver convergence, slight differences in calculation of system state that emerge from differences in time step lengths chosen by a model's adaptive time-stepping scheme, and artificial thresholds and discontinuities built into a model's algorithm. Finite-difference calculation of derivatives of model outputs with respect to adjustable parameters becomes difficult or impossible under these circumstances. Sometimes this problem can be overcome if a simpler, faster, numerically stable surrogate for the complex model is used in its stead for calculation of at least some model derivatives; meanwhile the original model is used only for testing parameter upgrades. "Observation re-referencing" functionality was introduced to PEST in order to allow such replacement of the complex model by one or more simpler models, or even by a polynomial proxy model, for the purpose of derivatives calculation. In the latter case, the building of polynomial proxies linking each model output used in the calibration process to all model parameters estimated through that process is completed under PEST's supervision.

## 1.2 PEST: The Future

Development of PEST in its present form will not continue into the indefinite future. However the ideas and algorithms on which PEST and its supporting utilities rest will continue. The future of environmental model-based decision-making depends on this. At the time of writing, two packages which can claim direct PEST heritage, and which are carrying on the PEST tradition, are PEST++ (Welter et al, 2015) and PyEMU (White et al, 2015). Readers are referred to the manuals of these packages if they wish to become fully acquainted with their capabilities.

## 1.3 The Present Document

Part of the purpose of the present document is to present the theory on which PEST and its utility support software is based. In doing so, it simultaneously presents the theory on which PEST++ and PyEMU rest. However it refers to PEST, and to PEST utilities, to only a limited extent. Instead, future versions of documentation written for PEST, for PEST-related software, and hopefully even for software that is not directly descended from PEST, can refer back to this document for an explanation of its theoretical foundations. The present document is thus software-independent.

The primary purpose of this document is to provide a comprehensive theoretical background for parameter estimation and uncertainty analysis as it pertains to environmental modelling. While the theory and concepts presented herein require software for their implementation, much of these are valuable in their own right, for they provides an understanding of what modelling can and cannot achieve when used as a basis for environmental decision-making. In the author's view, a great deal of modern-day model usage is based more on wishful thinking than on science and mathematics. With a greater understanding of the capacity that a model possesses (or does not possess) for providing receptacles for expert knowledge on the one hand, and for the historical behaviour of a real world environmental system on the other hand, model usage in the decision-making context can be improved.

## 1.4 A Philosophical Note

Let us suppose that a particular numerical simulator possesses enough algorithmic complexity to represent all nuances of real world environmental behaviour at a particular study site. Imagine the complexity of the real world at any study site; then translate that complexity to a model. A valid representation of process complexity, and of the spatial heterogeneity of system properties which govern complex environmental process, would require that a simulator be endowed with many parameters. Sadly, however, most of these parameters will be unknown, except perhaps at a handful of locations where they have been directly measured. This is especially the case where the environmental system of interest is a groundwater or subsurface reservoir system. To some extent, broad scale averages of system properties, or perhaps details of system properties at a small number of locations, may be inferable from measurements of the historical behaviour of the system through solution of an appropriately-posed inverse problem. If a prediction of management interest is sensitive only to thus-inferred properties, then it is possible that the prediction can be made with a moderate to high degree of certainty.

Predictions that are well informed by historical measurements of system state, and can be made with relative certainty because of this, tend to be those which resemble those historical measurements in type, location, and in the stress regime to which the system was subjected. In most instances of environmental management however, predictions are required under an

altered stress regime; often it is this new stress regime which is the focus of management interest. Furthermore, in many decision-making contexts, predictions of interest pertain to a different aspect of the system's behaviour from those which comprise the calibration dataset. Such predictions are likely to be uncertain. This is because they are likely to be sensitive to non-inferable parameters, or (more likely) to non-inferable *combinations* of parameters. If the uncertainties of predictions of this type are to be quantified, then the parameters on which they depend must be represented in the model – not because these parameters can be inferred through the calibration process, but precisely because they *cannot* be inferred through the calibration process. The capacity of these parameters to vary, subject to the constraints that

1. the model is still able to replicate the historical behaviour of the system, and
2. values taken by these parameters are in accordance with expert knowledge

must then be explored. In doing this, uncertainties of predictions which are sensitive to these parameters can also be explored.

If an environmental model is not "calibrated" (a somewhat meaningless word whose significance will be extensively explored in the present document), then few would argue that its parameters are therefore uncertain. However their uncertainty has bounds, for a modeller can usually place limits on the range of values that he/she will allow parameters to take. This says something important about expert knowledge, and indeed about the nature of scientific knowledge itself, particularly as it applies to the environmental sciences. Rarely does an expert know the values that system properties, and the parameters that represent them in a model, must take; however he/she knows what values they must *not* take.

The uncertainty of a model's prediction is a function of two things, both of which are represented in Bayes equation (which will be described in detail herein). The first of these is the innate variability of parameters to which the prediction is sensitive. As stated above, this variability is determined by limits imposed by expert knowledge. The second thing is the extent to which this variability is constrained by the necessity for model outputs to respect historical measurements of system state. Given that there is noise associated with such measurements, this latter requirement is better expressed as the requirement that model outputs are not demonstrably incompatible with historical observations of system state.

Bayes equation states unequivocally that a model prediction must therefore be considered as probabilistic in nature. This means that it cannot be made with certainty, regardless of whether or not a model has been calibrated. In fact it will be shown in the theory that follows that the uncertainties of some predictions made by a "well-calibrated" model are not reduced at all by the calibration process. Their post-calibration uncertainties are therefore just as high as their pre-calibration uncertainties. The uncertainty ranges of these predictions are therefore determined by expert knowledge rather than by history-matching constraints.

*It therefore follows that a model cannot predict what will happen in the future. However, following proper uncertainty analysis, it may be able to predict what will NOT happen in the future.*

This is an important statement with important implications.

Most environmental modelling is undertaken to support environmental management. Environmental management is undertaken to prevent the outcomes of human activity from having unwanted consequences. To put it another way, the purpose of environmental management is to prevent the occurrence of "bad things".

So can environmental modelling support environmental management given that model

predictions are necessarily probabilistic in nature? The answer is a most definite "yes". However before this can happen a change in the philosophy of model usage away from the "crystal ball" mentality which pervades a great deal of modern-day modelling practice is required. Environmental managers must refrain from asking "what will happen if we do this or that?" Instead they should ask "if we implement this particular management strategy, can it be demonstrated that that particular costly bad thing will *not* happen?"

How can such a demonstration be made? The unlikelihood of occurrence of a bad thing can be demonstrated by showing that its occurrence is incompatible with either or both of expert knowledge and/or with the historical behaviour of the system whose management is being considered. A model is unique in its ability to do this. However it cannot do it alone; to achieve this, a model must be used in conjunction with software such as PEST which, through its inversion and uncertainty analysis capabilities, can expose such incompatibilities.

It may be argued that too rigorous an application of such a philosophy in the environmental decision-making context would halt human progress altogether. After all, predictive uncertainty margins are often large - especially predictions of system response to vastly altered stresses regimes such as the excavation of a new mine or the extraction of large amounts of unconventional gas from subsurface water domains. This argument can be countered by noting that application of the above philosophy can be made as complex and as flexible as the situation demands. For example, a proposed development plan may be allowed to proceed if it is accompanied by a well-designed monitoring network. Let us suppose that this monitoring network is comprised of a set of groundwater wells. If modelling can show that a bad thing will not happen if development is curtailed immediately upon drawdowns or contaminant concentrations in specified wells exceeding certain thresholds, then this may constitute sufficient grounds to allow development to provisionally proceed. Meanwhile the task of modelling becomes that of defining monitoring thresholds in such a way that consequential development curtailment does indeed prevent the occurrence of the bad thing while, at the same time, does not present an unnecessarily harsh restriction to development.

# 2. Vectors and Matrices

## 2.1 Introduction

This chapter and the following chapter provide a brief overview of mathematical concepts on which theory covered in later chapters is based. For some, these two chapters may serve as reminders of long-forgotten wisdom that was acquired at school and has since been lost in the mists of time. There are some topics, however, which a reader may not have previously encountered, for example the concepts of null space and the generalized inverse of a matrix. It is not essential that matters such as these be understood in depth. It is only important that their existence be acknowledged, and that patterns of thought that are so elegantly expressed through mathematical symbolism be retained. It is their meanings that are important, and not their details.

The reader is therefore urged to review this and the following chapters with a light heart, to be grateful for the gentle reminders of childhood days that they contain, and to wonder at the glimpses of mathematical beauty which they reveal. The going is not meant to be tough. It is meant to be nothing more than a series of rapid visitations of concepts that are important to the field of inverse problem-solving and post-calibration uncertainty analysis.

## 2.2 Definitions

A scalar is a single real number, such as the value of a parameter or a number that constitutes a predictive model outcome. In the present document it is represented by a lower-case, italicized character, such as *x*.

A vector is a collection of scalars arranged in a column. The individual scalars are its elements. They are indexed according to their place in the column. In the present text (and in most texts) a vector is denoted using a bold, lower-case letter. The vector **x** with three elements can be written as

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \tag{2.2.1}$$

No-one who is reading this text has not heard of vectors. When taught at school vectors were often pictured as having 2 or 3 elements, these representing coordinates in two- or three-dimensional space. The vector "points" from the coordinate system origin (which has coordinates of zero) to the point in space which is designated by its elements. A vector thus has direction as well as size. Its size is its length.

The norm of a vector is another name for its size. The norm of vector **x** is symbolized as $\|\mathbf{x}\|$. Its square is computed as

$$\|\mathbf{x}\|^2 = \sum_{i=1}^{n} x_i^2 \tag{2.2.2}$$

where *n* is the number of elements in the vector.

A vector whose elements are all zero is denoted as **0**.

A matrix is a two-dimensional array of scalars. Matrices are represented using a bold

capitalized letter such as **A**. The elements of a matrix are denoted by their row and column indices. Thus the scalar $a_{ij}$ denotes the element which occupies the $i$'th row and $j$'th column of the matrix **A**. A 2×3 matrix (i.e. a matrix with two rows and three columns) named **A** can be written as

$$\mathbf{A}=\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \tag{2.2.3}$$

An $n$-dimensional vector can be considered to be an $n$×1 matrix. A scalar can be considered to be a one-dimensional vector and a 1×1 matrix.

The transpose of a matrix is obtained by interchanging its rows and columns. The transpose of a matrix is indicated by a "t" superscript herein. For **x** and **A** defined above, $\mathbf{x}^t$ and $\mathbf{A}^t$ are given by

$$\mathbf{x}^t=\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \tag{2.2.4}$$

$$\mathbf{A}^t=\begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \\ a_{13} & a_{23} \end{bmatrix} \tag{2.2.5}$$

Note that in the second of the above equations the subscripts on the $a$'s denote the original row/column positions of these scalars in the **A** matrix prior to transposition.

Transposing a matrix twice yields the original matrix. Thus

$$[\mathbf{A}^t]^t = \mathbf{A} \tag{2.2.6}$$

A matrix is symmetric if

$$\mathbf{A}^t = \mathbf{A} \tag{2.2.7}$$

It is obvious that a symmetric matrix must be a square matrix; as such it has an equal number of rows and columns.

The diagonal elements of a matrix are those whose row and column indices are equal. A diagonal matrix is one whose off-diagonal elements are zero. The identity matrix is a square, diagonal matrix whose diagonal elements are all 1 and whose off-diagonal elements are all 0. It is represented by **I**. The 3×3 identity matrix is

$$\mathbf{I}=\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.2.8}$$

The trace of a matrix **A**, denoted as tr(**A**), is the sum of its diagonal elements.

A triangular matrix is one for which all elements above the diagonal are zero (this is a lower triangular matrix), or for which all elements below the diagonal are zero (this is an upper triangular matrix).

## 2.3 Addition and Scalar Multiplication of Matrices

Let $s$ be a scalar. For the matrix **A** defined in (2.2.3), the matrix $s$**A** is

$$s\mathbf{A} = \mathbf{A}s = \begin{bmatrix} sa_{11} & sa_{12} & sa_{13} \\ sa_{21} & sa_{22} & sa_{23} \end{bmatrix} \tag{2.3.1}$$

Matrices are added by adding their respective elements. Suppose that **A** and **B** are each 2×3 matrices. Then the matrix **C** is their sum if

$$\mathbf{C} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \end{bmatrix} = \begin{bmatrix} a_{11}+b_{11} & a_{12}+b_{12} & a_{12}+b_{13} \\ a_{21}+b_{21} & a_{22}+b_{22} & a_{23}+b_{23} \end{bmatrix} \tag{2.3.2}$$

Obviously, associative and commutative rules apply, so that

$$\mathbf{A} + (\mathbf{B} + \mathbf{C}) = (\mathbf{A} + \mathbf{B}) + \mathbf{C} \tag{2.3.3}$$

and

$$\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A} \tag{2.3.4}$$

## 2.4 Multiplication of Matrices

Let **x** be the three-dimensional vector defined in equation (2.2.1) and **A** be the 2×3 matrix defined in (2.2.3). Let the two-dimensional vector **y** be the outcome of multiplication of the vector **x** by the matrix **A**. This is written as

$$\mathbf{y} = \mathbf{A}\mathbf{x} \tag{2.4.1}$$

The vector **y** has as many rows as there are rows of **A**. Multiplication of **x** by **A** can only occur if **A** has as many columns as there are rows in **x**. The elements of **y**, namely $y_1$ and $y_2$, are calculated as follows

$$y_i = \sum_{j=1}^{3} a_{ij} x_j \tag{2.4.2}$$

where *i* can be 1 or 2 in this equation.

Matrix multiplication can be viewed in two different ways. As written in (2.4.2), the *i*'th element of **y** is calculated by travelling along the *i*'th row of the matrix **A**, and multiplying every element encountered in this journey by the element encountered in a simultaneous journey down the single column of **x**.

There is another way to look at matrix multiplication. Let us write the matrix **A** as

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \end{bmatrix} \tag{2.4.3}$$

The vectors $\mathbf{a}_1$ $\mathbf{a}_2$ and $\mathbf{a}_3$ are so-called "column vectors" of the matrix **A** defined as

$$\mathbf{a}_1 = \begin{bmatrix} a_{11} \\ a_{21} \end{bmatrix}; \quad \mathbf{a}_2 = \begin{bmatrix} a_{12} \\ a_{22} \end{bmatrix}; \quad \mathbf{a}_3 = \begin{bmatrix} a_{13} \\ a_{23} \end{bmatrix} \tag{2.4.4}$$

Then multiplication of the vector **x** by the matrix **A** can be represented in the following way

$$\mathbf{y} = \mathbf{A}\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3 \tag{2.4.5}$$

The scalar product of two vectors can be represented as a matrix multiplication. Suppose that *s* (a scalar) is the scalar product of the vectors **x** and **y**. Then

$$s = \mathbf{y}^{\mathrm{t}}\mathbf{x} = \sum_{i=1}^{n} y_i x_i \tag{2.4.6}$$

where $n$ is the number of elements in each of **x** and **y**.

The norm of a vector (see equation 2.2.2) can be calculated as the square root of the scalar product of a vector with itself. That is

$$\|\mathbf{x}\| = (\mathbf{x}^t\mathbf{x})^{1/2} \tag{2.4.7}$$

Matrix multiplication readily demonstrates that

$$\mathbf{x} = \mathbf{I}\mathbf{x} \tag{2.4.8}$$

That is, multiplication of a vector by the identify matrix leaves the vector unchanged.

Matrix-by-matrix multiplication is defined as a simple extension of vector-by-matrix multiplication. Suppose that the matrix **A** is multiplied by the matrix **B**. This leads to another matrix **C**. It is written as

$$\mathbf{C} = \mathbf{B}\mathbf{A} \tag{2.4.9}$$

For the matrix product to exist, the number of rows of **A** must be the same as the number of columns of **B**. The number of rows of the product matrix **C** is the same as that of **B** while the number of columns of the product matrix **C** is the same as that of **A**. This can be written as

$$\underset{n\times m}{\mathbf{C}} = \underset{n\times r}{\mathbf{B}}\ \underset{r\times m}{\mathbf{A}} \tag{2.4.10}$$

where the number of rows and columns in each matrix is written under the matrix. Each element $c_{ij}$ of **C** is calculated as

$$c_{ij} = \sum_{k=1}^{r} b_{ik}\, a_{kj} \tag{2.4.11}$$

Where more than two matrices are multiplied, this is done in pairwise sequence. It is easily shown that matrix multiplication is associative. Thus

$$\mathbf{D} = \mathbf{C}\mathbf{B}\mathbf{A} = (\mathbf{C}\mathbf{B})\mathbf{A} + \mathbf{C}(\mathbf{B}\mathbf{A}) \tag{2.4.12}$$

where the brackets in the above equation indicate the order in which the operations are carried out. Note, however, that matrix multiplication is *not* commutative. In fact, unless matrices are square, the order of matrix multiplication cannot be reversed. Suppose that equation (2.4.9) holds true. Even if **A** and **B** are square, it does *not* therefore follow that

$$\mathbf{C} = \mathbf{A}\mathbf{B} \tag{2.4.13}$$

The following relationships are easy to prove.

$$(\mathbf{A}\mathbf{B})^t = \mathbf{B}^t\mathbf{A}^t \tag{2.4.14}$$

$$\mathbf{A} = \mathbf{A}\mathbf{I} = \mathbf{I}\mathbf{A} \tag{2.4.15}$$

In the second of the above formulas the number of rows/columns of **I** may differ, depending on whether it pre- or post-multiplies **A**. Suppose that **A** is an $m\times n$ matrix. Then the **I** matrix which pre-multiplies it is necessarily $m\times m$ and the **I** matrix which post-multiplies it is necessarily $n\times n$. The former is thus the $m$-dimensional **I** matrix whereas the latter is the $n$-dimensional **I** matrix.

## 2.5 Partitioning of a Matrix

It is often convenient to partition a matrix into submatrices. For example the matrix **A** may be represented as follows.

$$\mathbf{A}=\begin{bmatrix}\mathbf{A}_{11} & \mathbf{A}_{12}\\ \mathbf{A}_{21} & \mathbf{A}_{22}\end{bmatrix} \tag{2.5.1}$$

For such partitioning to occur, $\mathbf{A}_{11}$ and $\mathbf{A}_{12}$ on the one hand, and $\mathbf{A}_{21}$ and $\mathbf{A}_{22}$ on the other hand, must have the same number of rows. Meanwhile $\mathbf{A}_{11}$ and $\mathbf{A}_{21}$ on the one hand, and $\mathbf{A}_{12}$ and $\mathbf{A}_{22}$ on the other hand, must have the same number of columns.

Similarly, the matrix B may be partitioned as

$$\mathbf{B}=\begin{bmatrix}\mathbf{B}_{11} & \mathbf{B}_{12}\\ \mathbf{B}_{21} & \mathbf{B}_{22}\end{bmatrix} \tag{2.5.2}$$

If rows and columns of respective submatrices are compatible, then the matrix product **AB** can be computed as

$$\mathbf{AB}=\begin{bmatrix}\mathbf{A}_{11}\mathbf{B}_{11}+\mathbf{A}_{12}\mathbf{B}_{21} & \mathbf{A}_{11}\mathbf{B}_{12}+\mathbf{A}_{12}\mathbf{B}_{22}\\ \mathbf{A}_{21}\mathbf{B}_{11}+\mathbf{A}_{22}\mathbf{B}_{21} & \mathbf{A}_{21}\mathbf{B}_{12}+\mathbf{A}_{22}\mathbf{B}_{22}\end{bmatrix} \tag{2.5.3}$$

Matrices can be partitioned to suit the occasion. Instead of partitioning a matrix four ways (i.e. by row and by column) as expressed by equation (2.5.1), a matrix can be partitioned by column only. Thus, for example

$$\mathbf{A}=\begin{bmatrix}\mathbf{A}_{11} & \mathbf{A}_{12}\end{bmatrix};\ \mathbf{B}=\begin{bmatrix}\mathbf{B}_{11} & \mathbf{B}_{12}\end{bmatrix} \tag{2.5.4}$$

so that

$$\mathbf{AB}^t = \mathbf{A}_{11}\mathbf{B}^t{}_{11} + \mathbf{A}_{12}\mathbf{B}^t{}_{12} \tag{2.5.5}$$

## 2.6 The Inverse of a Matrix

Suppose that the following holds

$$\mathbf{y} = \mathbf{Ax} \tag{2.6.1}$$

Is it possible to compute **x** from **y**? If **A** is a square matrix then this may indeed be possible. Suppose that **A** is an $n\times n$ matrix. Then calculation of **x** from **y** is a problem that requires solution of $n$ linear equations (these being defined by the rows of **A**) for $n$ unknowns (the number of elements of **x**). It is possible to solve these equations for **x** provided that no row of **A** duplicates the information contained in one or a number of the other rows of **A**. If such duplication does indeed occur, then **A** is said to be "rank-deficient"; this means that at least one of its rows can be expressed as a linear combination of its other rows. However if the rank of **A** is equal to the number of its rows (which is equal to the number of its columns, $n$ in this case), then calculation of **x** from **y** is possible. Details of how this is best achieved can be found elsewhere. The fact that it is possible infers that a matrix exists from which **x** can be calculated from **y**. This matrix is referred to as the inverse of the **A** matrix; it is denoted as $\mathbf{A}^{-1}$. Hence

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{y} \tag{2.6.2}$$

What if **A** has more rows than columns? Suppose that it is an $n\times m$ matrix and that $n$ exceeds $m$; can **x** be calculated from **y** then? This is where things start to get complicated, for the fact that **A** has more rows than columns infers that there is a potential for duplication of information in the **A** matrix and **y** vector. If this is the case, then it is also possible that these two pieces of information conflict with each other. Nevertheless, estimation of **x** from **y** may

be required. In seeking to solve this problem we enter into the realm of parameter estimation. The problem of estimating **x** from **y** will be discussed extensively later in this text.

Returning to square matrices, the strict mathematical definition of the inverse of matrix **A** is

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I} \qquad (2.6.3)$$

Using this definition of the inverse of **A**, pre-multiplication of both sides of (2.6.1) by $\mathbf{A}^{-1}$ leads immediately to (2.6.2).

It is important to note that a matrix must be square to have an inverse. But it is equally important to note that not all square matrices have inverses. A square matrix does not have an inverse if it is rank-deficient. A square matrix which has an inverse is often known as a "regular" matrix. One which does not have an inverse is denoted as "singular".

It is easily shown that if **A** and **B** are regular matrices then

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \qquad (2.6.4)$$

$$(\mathbf{A}^{-1})^{t} = (\mathbf{A}^{t})^{-1} \qquad (2.6.5)$$

$$(\mathbf{A}^{-1})^{-1} = \mathbf{A} \qquad (2.6.6)$$

It is also easy to show that the inverse of a symmetric matrix is itself symmetric.

## 2.7 Determinant of a Matrix

The determinant of a square matrix is a scalar. It is a quantity which is well-suited to characterizing the rank of a matrix. It features in many matrix equations, including that for the multi-dimensional normal distribution. It is only mentioned herein. For a more detailed treatment of matrix determinants see any good book on matrix algebra.

The determinant $|\mathbf{A}|$ of a one-dimensional square matrix **A** is calculated as

$$|\mathbf{A}| = a_{11} \qquad (2.7.1)$$

If **A** is a 2×2 matrix its determinant is calculated as

$$|\mathbf{A}| = a_{11}a_{22} - a_{12}a_{21} \qquad (2.7.2)$$

Formulas for the determinant become rapidly more complex as matrix dimensions rise. Useful properties of the determinant include the following; see, for example, Koch (1999) or Mikhail (1976) for further details.

- The determinant of a triangular matrix (including a diagonal matrix) is the product of its diagonal elements.
- For square matrices **A** and **B**
  $$|\mathbf{AB}| = |\mathbf{A}|\,|\mathbf{B}| \qquad (2.7.3)$$
- The determinant of a matrix is zero if one of its columns is a zero vector.
- The determinant of a matrix with two rows or columns that are identical is zero.
- The determinant of a matrix with one row or column that is a multiple of another row or column is zero.
- $$|\mathbf{A}| = |\mathbf{A}^{t}| \qquad (2.7.4)$$
- If two rows or two columns of a matrix are interchanged then $|\mathbf{A}|$ changes sign.
- If a row or a column of a matrix is multiplied by a constant, the value of the determinant is multiplied by that constant.
- The value of a determinant does not change if a multiple of a row or column is added

to another row or column.

- A matrix is invertible only if its determinant is non-zero.

## 2.8 The Null Space

Let **A** be an arbitrary matrix. It can be square, have more rows than columns, or have more columns than rows. If a non-zero vector **z** can be found such that the following equality holds, then **A** has a null space.

$$\mathbf{0} = \mathbf{Az} \tag{2.8.1}$$

The concept of the null space is important for what lies ahead. Suppose that **y** is calculated from **x** as

$$\mathbf{y} = \mathbf{Ax} \tag{2.8.2}$$

If the above two equations are added, we obtain

$$\mathbf{y} = \mathbf{A}(\mathbf{x}+\mathbf{z}) \tag{2.8.3}$$

Now suppose that we know **y** and wish to back-calculate **x**. It is obvious from (2.8.2) and (2.8.3) that inference of **x** from **y** is nonunique if the matrix **A** has a null space.

Any matrix that has more columns than rows has a null space. This makes sense if back-calculation of **x** from **y** is thought of as an attempt to solve a set of simultaneous equations for the elements of **x**; when a matrix which connects these two vectors has more columns than rows then there are less equations than unknowns.

A square matrix has a null space if it is singular, that is, if it does not have an inverse. As stated above, this arises because of duplication of information in the rows (or columns) of **A**. A matrix with more rows than columns may or may not possess a null space.

## 2.9 The Generalized Inverse

Consider equation (2.8.2). Looking ahead somewhat, let us suppose that **A** in this equation represents the action of a model on its parameters, and that these parameters are represented by the vector **x.** Let the vector **y** represent a set of observations from which we wish to infer values for the parameters **x**. **A** can be of any shape. If there are more observations than parameters **A** will be long in the vertical direction; that is, it will have more rows than columns. If there are more parameters than observations **A** will be long in the horizontal direction; that is, it will have more columns than rows. (Conceptually this is always the case if full account is taken of the inherent heterogeneity of natural systems.)

If **A** has a null space, inference of **x** from **y** is nonunique. This means that many **x**'s are compatible with a single **y**. A matrix from which an **x** which satisfies (2.8.2) can be calculated from **y** is referred to as a generalized inverse of **A**. It is usually denoted using a "-" superscript instead of a "-1" superscript, the latter being reserved for the strict inverse of a square matrix. Thus

$$\underline{\mathbf{x}} = \mathbf{A}^{-}\mathbf{y} \tag{2.9.1}$$

In equation (2.9.1) the underscore under **x** is used to denote the fact that $\underline{\mathbf{x}}$ is an estimate of the **x** of equation (2.8.2) (and a nonunique estimate at that). Where **A** has a null space, $\mathbf{A}^{-}$ is therefore nonunique. Substitution of (2.8.2) into (2.9.1) gives

$$\underline{\mathbf{x}} = \mathbf{A}^{-}\mathbf{Ax} \tag{2.9.2}$$

If both sides of equation (2.9.2) are multiplied by **A**, we obtain

$$\mathbf{A}\underline{\mathbf{x}} = \mathbf{A}\mathbf{A}^{-}\mathbf{A}\mathbf{x} \tag{2.9.3}$$

But, by definition of $\underline{\mathbf{x}}$

$$\mathbf{A}\underline{\mathbf{x}} = \mathbf{A}\mathbf{x} \tag{2.9.4}$$

This leads to the mathematical definition of the generalized inverse $\mathbf{A}^{-}$ of the matrix **A** as

$$\mathbf{A} = \mathbf{A}\mathbf{A}^{-}\mathbf{A} \tag{2.9.5}$$

Contrast this definition with that of the strict inverse of a square, invertible matrix **A** given by equation (2.6.3). As stated above, in contrast to $\mathbf{A}^{-1}$, $\mathbf{A}^{-}$ is nonunique. However where **A** is square and invertible, then $\mathbf{A}^{-}$ and $\mathbf{A}^{-1}$ are the same. Under these conditions $\mathbf{A}^{-}$ is unique.

Consider that **A** has a null space and that $\mathbf{A}^{-}$ is therefore nonunique. There is one special $\mathbf{A}^{-}$, commonly denoted as $\mathbf{A}^{+}$, which has some special properties – including that of uniqueness. $\mathbf{A}^{+}$ is variously known as the pseudoinverse of the matrix **A** or as the Moore-Penrose inverse of **A**. When used to calculate $\underline{\mathbf{x}}$ through equation (2.9.1), it yields the $\underline{\mathbf{x}}$ of minimum norm for which **x** and **y** are related through (2.8.2). In practice $\mathbf{A}^{+}$ is obtainable through singular value decomposition of the matrix **A** (a subject which we will visit shortly). It can be shown that the following properties characterize **A**+ at the same time as they make it unique; see Koch (1999) for more details. Note that the first of the following equations is simply (2.9.5) rewritten for the pseudoinverse.

$$\mathbf{A}\mathbf{A}^{+}\mathbf{A} = \mathbf{A} \tag{2.9.6a}$$

$$\mathbf{A}^{+}\mathbf{A}\mathbf{A}^{+} = \mathbf{A}^{+} \tag{2.9.6b}$$

$$(\mathbf{A}\mathbf{A}^{+})^{t} = \mathbf{A}\mathbf{A}^{+} \tag{2.9.6c}$$

$$(\mathbf{A}^{+}\mathbf{A})^{t} = \mathbf{A}^{+}\mathbf{A} \tag{2.9.6d}$$

It can also be shown that (Albert, 1972)

$$\mathbf{A}^{+} = \lim_{\delta \to 0}\left(\mathbf{A}^{t}\mathbf{A} + \delta^{2}\mathbf{I}\right)^{-1}\mathbf{A}^{t} = \lim_{\delta \to 0}\mathbf{A}^{t}\left(\mathbf{A}\mathbf{A}^{t} + \delta^{2}\mathbf{I}\right)^{-1} \tag{2.9.7}$$

Equation (2.9.7) is important. Looking ahead, it says that the solution of a nonunique inverse problem achieved through Tikhonov regularization is the same as that achieved through singular value decomposition as measurement noise approaches zero. As will be discussed, singular value decomposition and Tikhonov regularization comprise the two great strands of mathematical regularization that are employed to obtain sensible solutions to ill-posed inverse problems of the type that arise in environmental model calibration (and in many other fields of study).

Equation (2.9.2) depicts the relationship between estimated $\underline{\mathbf{x}}$ and true **x**. Recall that $\underline{\mathbf{x}}$ and **x** are indistinguishable after multiplication by **A** because

$$\mathbf{y} = \mathbf{A}\mathbf{x} \tag{2.9.8a}$$

and

$$\mathbf{y} = \mathbf{A}\underline{\mathbf{x}} \tag{2.9.8b}$$

Where **A** has a null space there is no reason why $\underline{\mathbf{x}}$ should equal **x**. Hence $\mathbf{A}^{-}\mathbf{A}$ of (2.9.2) is not the identity matrix. Furthermore, because of the fact that **A** has a null space, $\mathbf{A}^{-}\mathbf{A}$ is rank-deficient. (The identity matrix is definitely not rank-deficient). In fact $\mathbf{A}^{-}\mathbf{A}$ is given a special name, this being the "resolution matrix". Thus

$$\underline{\mathbf{x}} = \mathbf{A}^{-}\mathbf{A}\mathbf{x} = \mathbf{R}\mathbf{x} \qquad (2.9.9)$$

Equation (2.9.6d) shows that the resolution matrix is symmetric when solution of a nonunique inverse problem is achieved using the Moore-Penrose pseudoinverse.

The resolution matrix has much to say about the nature of the vector $\underline{\mathbf{x}}$ that is achieved through solution of a nonunique inverse problem, and about how any such solution should be interpreted. Recalling the definition of vector-by-matrix multiplication, equation (2.9.9) states that each element $\underline{x}_i$ of $\underline{\mathbf{x}}$ is obtained through weighted averaging of all the elements $x_i$ of $\mathbf{x}$; the weights used in this averaging process are the elements of the $i$'th row of the resolution matrix $\mathbf{R}$. (This is why it is called the resolution matrix.) Obviously, the closer that $\mathbf{R}$ resembles the identity matrix $\mathbf{I}$, the better is the resolving power of the inversion process. $\mathbf{R}$ equals $\mathbf{I}$ only when $\mathbf{A}$ is square and regular, for then $\mathbf{A}^{-}$ becomes $\mathbf{A}^{-1}$, and $\mathbf{A}^{-1}\mathbf{A}$ becomes $\mathbf{I}$. If this is not the case, then the resolution matrix is of less than full rank, and hence is non-invertible. There can thus be many different $\underline{\mathbf{x}}$'s for a given $\mathbf{x}$.

## 2.10 Orthogonality and Projections

Two vectors are orthogonal to each other if their scalar product is equal to 0. Thus the vector $\mathbf{x}$ is orthogonal to the vector $\mathbf{y}$ if

$$\mathbf{x}^t\mathbf{y} = 0 \qquad (2.10.1)$$

A matrix $\mathbf{V}$ is orthonormal if each of its columns comprises a unit vector, and if those unit vectors are mutually orthogonal to each other. Let $\mathbf{v}_i$ denote the $i$'th column of $\mathbf{V}$. Then $\mathbf{V}$ can be written as

$$\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_n \end{bmatrix} \qquad (2.10.2)$$

where $m$ is the number of columns in $\mathbf{V}$. If $\mathbf{V}$ has $n$ rows, then each $\mathbf{v}_i$ obviously has $n$ elements. $\mathbf{V}$ is orthonormal if

$$\mathbf{v}_i^t\mathbf{v}_j = 0 \qquad \text{for } i \neq j \qquad (2.10.3a)$$

$$\mathbf{v}_i^t\mathbf{v}_j = 1 \qquad \text{for } i = j \qquad (2.10.3b)$$

If $\mathbf{V}$ is orthonormal, then obviously

$$\mathbf{V}^t\mathbf{V} = \mathbf{I} \qquad (2.10.4)$$

If $\mathbf{V}$ is also square, it follows that $\mathbf{V}^t$ is the inverse of $\mathbf{V}$. Thus the transpose of a square orthonormal matrix is its inverse. From (2.6.3) it then follows that

$$\mathbf{V}\mathbf{V}^t = \mathbf{V}^t\mathbf{V} = \mathbf{I} \qquad (2.10.5)$$

A matrix $\mathbf{A}$ is declared to be idempotent if

$$\mathbf{A}\mathbf{A} = \mathbf{A}^2 = \mathbf{A} \qquad (2.10.6)$$

If the vector $\mathbf{x}$ is multiplied by the idempotent matrix $\mathbf{A}$, then $\mathbf{x}$ is said to have undergone projection onto the range space of $\mathbf{A}$ (i.e. the space of all possible outcomes of multiplication of any vector by $\mathbf{A}$). What defines an operation as a projection is that multiple operations achieve nothing that a single operation has not already achieved. This follows from the idempotency of the operation.

Suppose that the matrix **A** is idempotent; simple matrix multiplication demonstrates that (**I-A**) is also idempotent. Hence **I-A** is also a projection operator. If operating on the vector **x** it can be thought of as projecting **x** in the "other direction" to the projection achieved through multiplication by **A**. If this "other direction" is orthogonal to the original projection direction, that is if

$$(\mathbf{I} - \mathbf{A})^t\mathbf{A} = \mathbf{0} \qquad (2.10.7)$$

then **A** is called an orthogonal projection operator. It can be shown that **A** is an orthogonal projection operator if it is both idempotent and symmetric.

Idempotent matrices have less than full rank. They are not invertible. It can be shown that if a matrix is idempotent and regular (i.e. invertible), then it can only be **I**. See Koch (1999) for further details.

## 2.11 Eigenvectors, Eigenvalues and Positive-Definiteness

Let **A** be an $n \times n$ square matrix. If it is of full rank, then it has $n$ non-zero eigenvalues; more generally it has $m$ non-zero eigenvalues, where $m$ is its rank. By definition, the eigenvalues $\lambda_i$ of a matrix **A** can be obtained through solution of the following equation.

$$(\mathbf{A} - \lambda_i\mathbf{I})\mathbf{x}_i = \mathbf{0} \qquad (2.11.1a)$$

That is

$$\mathbf{A}\mathbf{x}_i = \lambda_i\mathbf{x}_i \qquad (2.11.1b)$$

For each eigenvalue $\lambda_i$ there is a corresponding eigenvector $\mathbf{x}_i$.

The above definition of eigenvectors and eigenvalues seems quite abstract. Furthermore, one could be forgiven for failing to see the purpose of eigenvectors and eigenvalues, if their usefulness is perceived only in terms of their ability to solve the above equation. Let the reader be assured, however, that eigenvectors and eigenvalues are some of the most important concepts in linear algebra.

A symmetric $n \times n$ matrix is positive-definite if

$$\mathbf{x}^t\mathbf{A}\mathbf{x} > 0 \text{ for all } \mathbf{x} \neq \mathbf{0} \qquad (2.11.2a)$$

It is positive semi-definite if

$$\mathbf{x}^t\mathbf{A}\mathbf{x} \geq 0 \text{ for all } \mathbf{x} \neq \mathbf{0} \qquad (2.11.2b)$$

Covariance matrices (see later) are always positive-definite; they have to be thus for probabilities to be non-negative.

It can be shown that a matrix is positive-definite only if all of its eigenvalues are positive. It can also be shown that the eigenvectors of a positive-definite matrix are orthogonal. This is important for covariance matrices as it is the basis for principle component analysis.

## 2.12 Singular Value Decomposition

Let **Z** be an $n \times m$ matrix, where $n < m$. Thus **Z** is long in the horizontal direction. This kind of matrix may be used to simulate the action of a model on its parameters where parameters are many and observations are few. (This is the case in many environmental modelling contexts as soon as the complexity and heterogeneity of the real world is acknowledged). Singular value decomposition of **Z** leads to the calculation of three matrices. These are denoted as **U**, **S** and **V** in the following equation.

$$\mathbf{Z} = \mathbf{U}\mathbf{S}\mathbf{V}^t \qquad (2.12.1)$$

The situation is pictured in figure 2.1.

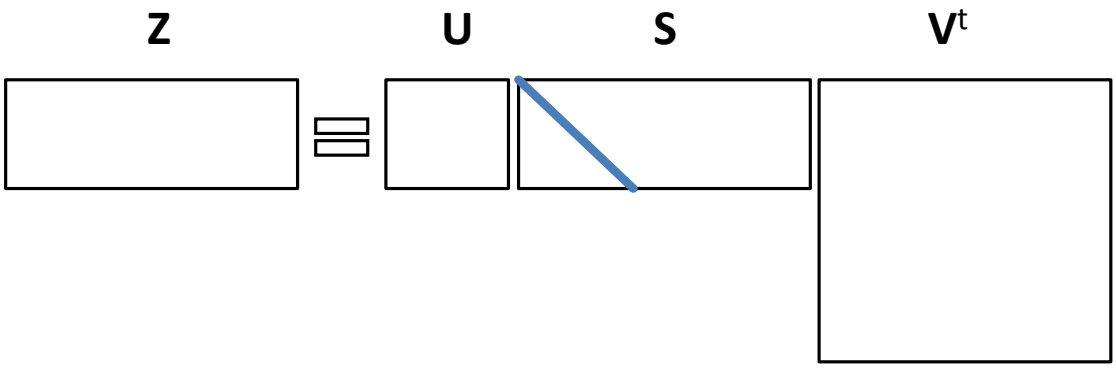


**Figure 2.1. Singular value decomposition of the *n*×*m* matrix Z where *n* < *m*.**

Singular value decomposition would not be so special if the matrices that it produced were not so special. The matrix **U** is an orthonormal matrix. Thus the vectors $\mathbf{u}_i$ which form its columns are each of unit length and are orthogonal to each other. Collectively they encompass the range space of the matrix **Z**. Thus any vector **y** that results from multiplication of any vector **x** by the matrix **Z** through the equation

$$\mathbf{y} = \mathbf{Z}\mathbf{x} \qquad (2.12.2)$$

can be expressed as a linear combination of the $\mathbf{u}_i$ which comprise the columns of **U**. As such, the columns of **U** can be considered to form a new, orthogonal, coordinate system for **Z** output space. (**Z** output space will become model output space later in this text when we use **Z** to represent the action of a model on a set of parameters; the nondescript vector **x** will then be replaced by the parameter vector **k**.) Because **U** is a square orthonormal matrix, it satisfies the following equation.

$$\mathbf{U}\mathbf{U}^t = \mathbf{U}^t\mathbf{U} = \mathbf{I} \qquad (2.12.3)$$

where **I** is the *n*×*n* identity matrix.

**V** is another orthonormal matrix. It is flipped on its side in figure 2.1 which represents its transpose. The columns of **V** span the input space of **Z** which, in the context of the present text, is parameter space. Because it is orthonormal then

$$\mathbf{V}\mathbf{V}^t = \mathbf{V}^t\mathbf{V} = \mathbf{I} \qquad (2.12.4)$$

where **I** is the *m*×*m* identity matrix. Thus any vector **x** on which **Z** can operate can be expressed as a linear combination of the columns of **V**, these comprising the *m* unit vectors $\mathbf{v}_i$ which thereby form the rows of $\mathbf{V}^t$.

All of the elements of the matrix **S** are zero except for those along its diagonal; its diagonal is pictured in figure 2.1. These diagonal elements are all either positive or zero. They are normally arranged from highest to lowest, starting at the top. Singular values either run out at *n* (the number of rows of **Z**) or become zero before that.

Let us now partition **S** at the point where singular values either run out or become zero. Assume that they become zero before they run out. This is illustrated in figure 2.2.

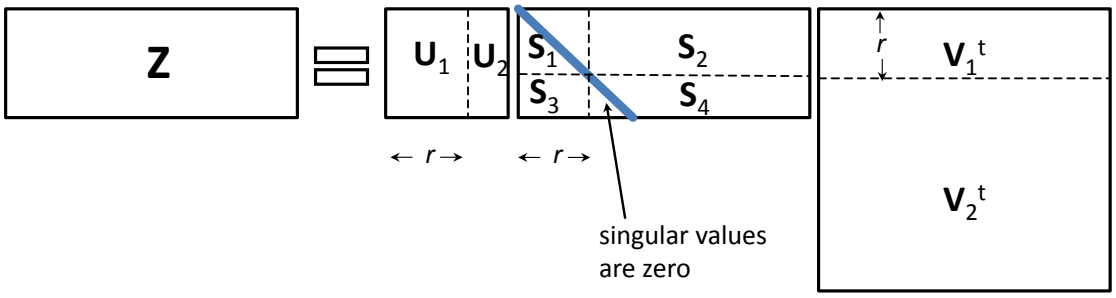


**Figure 2.2. Partitioning of the U, S and V matrices according to whether singular values are zero or non-zero.**

If all singular values are non-zero, then *r* in figure 2.2 is equal to *n*. Otherwise it is less than *n*. With **S** and **V** partitioned accordingly, equation (2.12.1) can be written as

$$\mathbf{Z}=\begin{bmatrix}\mathbf{U}_1 & \mathbf{U}_2\end{bmatrix}\begin{bmatrix}\mathbf{S}_1 & \mathbf{S}_2\\ \mathbf{S}_3 & \mathbf{S}_4\end{bmatrix}\begin{bmatrix}\mathbf{V}_1^t\\ \mathbf{V}_2^t\end{bmatrix} \qquad (2.12.5)$$

$$=\begin{bmatrix}\mathbf{U}_1\mathbf{S}_1+\mathbf{U}_2\mathbf{S}_3 & \mathbf{U}_1\mathbf{S}_2+\mathbf{U}_2\mathbf{S}_4\end{bmatrix}\begin{bmatrix}\mathbf{V}_1^t\\ \mathbf{V}_2^t\end{bmatrix} \qquad (2.12.6)$$

$$= \mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1 + \mathbf{U}_2\mathbf{S}_3\mathbf{V}^t_1 + \mathbf{U}_1\mathbf{S}_2\mathbf{V}^t_2 + \mathbf{U}_2\mathbf{S}_4\mathbf{V}^t_2 \qquad (2.12.7)$$

$$= \mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1 \qquad (2.12.8)$$

The last of the above equations follows from its predecessor because all elements of $\mathbf{S}_2$, $\mathbf{S}_3$ and $\mathbf{S}_4$ are zero. We are now in a position to solve equation (2.12.2) for **x**. Actually we cannot solve this equation for the original **x** but for a vector $\underline{\mathbf{x}}$ which is of minimum norm and which satisfies (2.12.2). (Recall from the discussion of the Moore-Penrose pseudoinverse that singular value decomposition gives us a solution to the inverse problem which is of minimum norm). If both sides of (2.12.2) are pre-multiplied by $\mathbf{U}^t_1$ while the right side of (2.12.8) is substituted for **Z** in (2.12.2) we obtain

$$\mathbf{U}^t_1\mathbf{y} = \mathbf{U}^t_1\mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1\mathbf{x} = \mathbf{S}_1\mathbf{V}^t_1\mathbf{x} \qquad (2.12.9)$$

where equality of $\mathbf{U}^t_1\mathbf{U}_1$ to **I** follows from the orthonormality of $\mathbf{U}_1$. We now multiply each side of the above equation by $\mathbf{S}^{-1}_1$. It is important to note that the inverse of $\mathbf{S}_1$ cannot fail to exist because $\mathbf{S}_1$ is a square diagonal matrix with non-zero elements down the diagonal; partitioning of the **U**, **S** and **V** matrices was designed specifically to achieve this outcome. We obtain (after recalling that the product of a matrix and its inverse is **I**)

$$\mathbf{S}^{-1}_1\mathbf{U}^t_1\mathbf{y} = \mathbf{V}^t_1\mathbf{x} \qquad (2.12.10)$$

Both sides of (2.12.10) are now pre-multiplied by $\mathbf{V}_1$ to obtain

$$\mathbf{V}_1\mathbf{S}^{-1}_1\mathbf{U}^t_1\mathbf{y} = \mathbf{V}_1\mathbf{V}^t_1\mathbf{x} = \underline{\mathbf{x}} \qquad (2.12.11)$$

To verify that $\underline{\mathbf{x}}$ satisfies equation (2.12.2) substitute it into this equation. We obtain

$$\mathbf{Z}\underline{\mathbf{x}} = \mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1\mathbf{V}_1\mathbf{V}^t_1\mathbf{x} = \mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1\mathbf{x} = \mathbf{Z}\mathbf{x} \qquad (2.12.12)$$

where use is made of the fact that $\mathbf{V}^t_1\mathbf{V}_1$ is equal to **I** because of orthonormality of $\mathbf{V}_1$.

Equation (2.12.11) can be re-written as

$$\underline{\mathbf{x}} = \mathbf{V}_1\mathbf{V}^t_1\mathbf{x} \qquad (2.12.13)$$

Obviously $\mathbf{V}_1\mathbf{V}^t_1$ is not equal to $\mathbf{I}$. $\mathbf{V}_1\mathbf{V}^t_1$ is an $m \times m$ matrix, where $m$ is the number of elements in $\mathbf{x}$. (Later in this text this will be equal to the number of parameters used by a model.) In contrast, if we reverse the order of multiplication, $\mathbf{V}^t_1\mathbf{V}_1$ is an $r \times r$ identity matrix where $r$ is, at most, equal to the number of elements in $\mathbf{y}$ (number of observations used in the calibration process later in this text, which is assumed, for the moment, to be less than the number of elements of $\mathbf{x}$). The order of matrix multiplication is very important.

Comparing (2.12.13) with (2.9.9), it is apparent that $\mathbf{V}_1\mathbf{V}^t_1$ is the resolution matrix that specifies the relationship between estimated $\underline{\mathbf{x}}$ and true $\mathbf{x}$ when an ill-posed problem is solved using singular value decomposition. Much more will be said of this later. For now it can be stated that $\mathbf{V}_1\mathbf{V}^t_1$ is an orthogonal projection operator. The fact that it is idempotent and symmetric can be readily verified by direct multiplication. It projects $\mathbf{x}$ from the $m$-dimensional space in which it resides, onto a subspace of $r$ dimensions. This is visualized in figure 2.3, where $m$ is 3 and $r$ is 2.

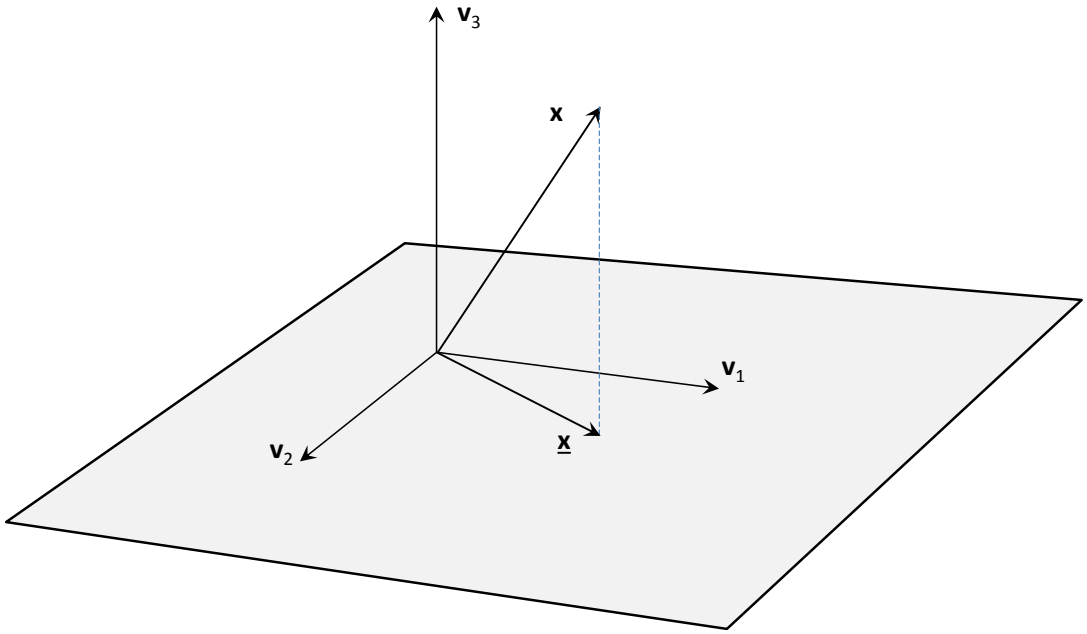


**Figure 2.3. $\underline{\mathbf{x}}$ is related to x through orthogonal projection onto a smaller dimensional subspace.**

The subspace onto which $\mathbf{x}$ is projected to form $\underline{\mathbf{x}}$ is spanned by the column vectors of $\mathbf{V}_1$. Throughout the present text this subspace is referred to as the "calibration solution space", or simply as the "solution space". The orthogonal complement to this subspace is the null space of $\mathbf{Z}$. The null space is spanned by the column vectors of $\mathbf{V}_2$. Hence any vector which lies entirely in the null space of $\mathbf{Z}$ can be formulated as a linear combination of the orthogonal unit vectors which comprise the columns of $\mathbf{V}_2$. Equation (2.12.8), together with mutual orthogonality of the columns of $\mathbf{V}_1$ and $\mathbf{V}_2$, instantly shows that multiplication of such a vector by $\mathbf{Z}$ has an outcome of $\mathbf{0}$.

Because the column vectors of $\mathbf{V}_1$ and $\mathbf{V}_2$ collectively span the entirety of $m$-dimensional space, the following equations holds

$$\mathbf{V}_1\mathbf{V}^t_1 + \mathbf{V}_2\mathbf{V}^t_2 = \mathbf{I} \qquad (2.12.14)$$

where $\mathbf{I}$ is the $m \times m$ identity matrix. An immediate consequence of equation (2.12.14) is that if any vector is simultaneously projected onto the solution space of $\mathbf{Z}$ and onto its null space,

and the two projected vectors are then added together, the result is the original vector. Hence from (2.12.13) $\underline{\mathbf{x}}$ can be considered as the original vector **x** with its null space component removed.

Our discussion of singular value decomposition so far has assumed that the matrix **Z** is elongated in the horizontal direction. The converse case is depicted in figure 2.4.

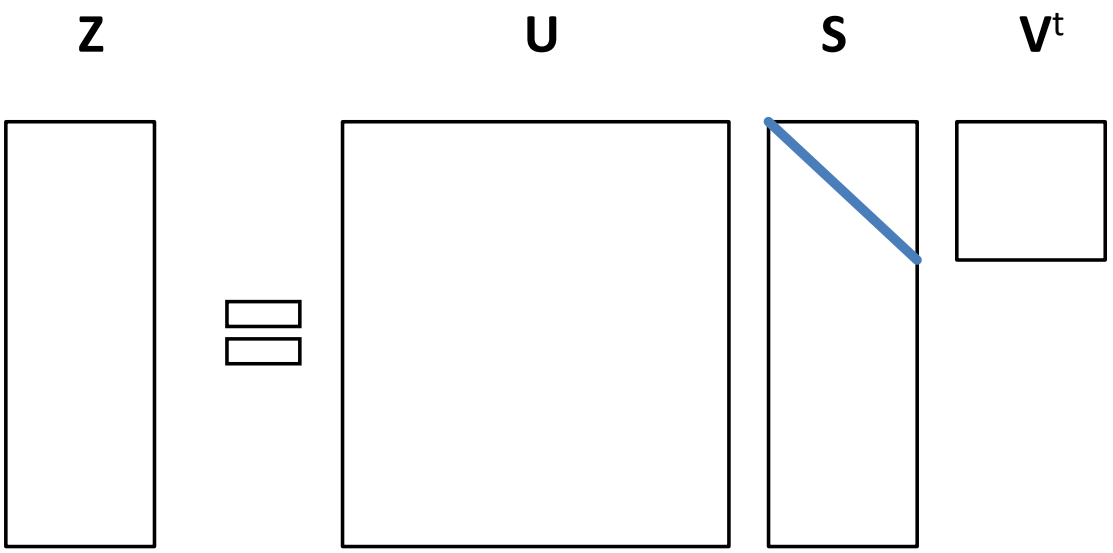


**Figure 2.4. Singular value decomposition of the *n*×*m* matrix Z where *n* > *m*.**

Where **Z** has more rows than columns, singular values are either all positive or become zero before the right side of the **S** matrix is reached. In this case matrix partitioning that is undertaken to isolate non-zero singular values is likely to affect **U** more than **V**. If there are no zero-valued singular values, then **V** is not partitioned at all. In this case the inverse problem is well-posed as there is no null space. See figure 2.5.

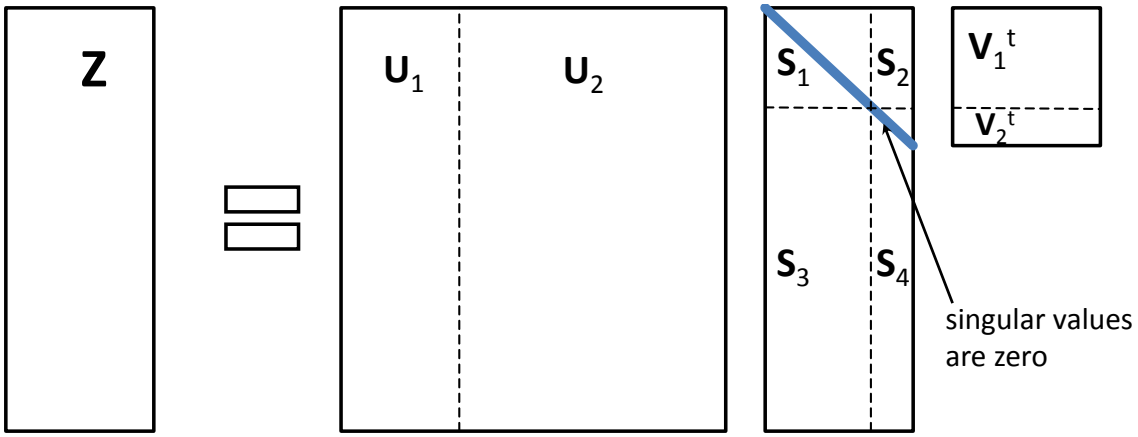


**Figure 2.5. Partitioning of the U, S and V matrices where Z has more rows than columns.**

So what are the implications of partitioning of **U**? Where $m > n$ (i.e. where the number of columns of **Z** is greater than its number of rows) and where **Z** possesses no zero-valued singular values (because there is no room left in the **S** matrix to hold them), then **U** is not partitioned at all. However where $m < n$ (i.e. where the number of columns of **Z** is less than its number of rows), then **U** is indeed partitioned, regardless of whether any singular values are zero or not. Partitioning of **U** restricts the range space of the **Z** matrix. At best, the range

space of **Z** can only be as high as its number of columns. Hence $\mathbf{U}_1$ will possess, at most, only as many columns as there are columns of **Z**.

Say, for example, that the **Z** matrix has 10 columns. (This will happen if a model has 10 parameters). Then any vector that is an outcome of multiplication by **Z** is a linear combination of these 10 columns. Let us further suppose that **Z** has 100 rows (which will occur if the calibration dataset is comprised of 100 observations). There are 100 degrees of freedom in the way that 100 numbers can express themselves. These are expressed by the 100 columns of **U**. However the range space (i.e. output space) of the **Z** matrix can only express 10 degrees of freedom. Hence $\mathbf{U}_1$ has at most 10 columns. The degrees of freedom in the range space of **Z** will actually be less than this if **Z** has a null space; under these circumstances the $\mathbf{U}_1$ matrix will possess fewer than 10 columns.

Suppose that we wish to solve an inverse problem based on the matrix **Z** in which the components of **x** are estimated from the components of an arbitrary vector **y**. Then, to the extent that **y** is not in the range space of **Z** (and of $\mathbf{U}_1$), and is therefore not expressible as a linear combination of the columns of **Z** (and of $\mathbf{U}_1$), any excess variability that it possesses beyond this can only be characterized in terms of the columns of $\mathbf{U}_2$. This excess variability must simply be written off as "noise" and minimized as much as possible, as no **x** can explain it.

## 2.13 More on Positive-Definite Matrices

If **A** is a positive-definite matrix (such as a covariance matrix, as will be discussed shortly) then it is square and symmetric. Furthermore, its eigenvalues are all positive. If it is subjected to singular value decomposition, then the **U** and **V** matrices which emerge from this process are the same. Let us refer to each of these as **E**, and to the square diagonal matrix of singular value as **F**. Subjecting **A** to singular value decomposition, we obtain from (2.12.1)

$$\mathbf{A} = \mathbf{E}\mathbf{F}\mathbf{E}^t \tag{2.13.1}$$

As usual, **E** is an orthonormal matrix; hence its columns are orthogonal unit vectors. Let us denote them as $\mathbf{e}_1$, $\mathbf{e}_2 \ldots \mathbf{e}_n$, where **E** is assumed to be an $n \times n$ matrix. If we now post-multiply both sides of **A** by **E** and invoke orthonormality of **E** to set $\mathbf{E}^t\mathbf{E}$ to **I** we obtain

$$\mathbf{A}\mathbf{E} = \mathbf{E}\mathbf{F} \tag{2.13.2}$$

On partitioning **E** into its individual columns this becomes

$$\mathbf{A}[\mathbf{e}_1 \ \mathbf{e}_2 \ \ldots \ \mathbf{e}_n] = [\mathbf{e}_1 \ \mathbf{e}_2 \ \ldots \ \mathbf{e}_n]\mathbf{F} \tag{2.13.3}$$

Because **F** is a diagonal matrix the above equation can be written as individual equations, each of which features an individual diagonal element of **F**. These diagonal elements are scalars; we denote the $i$'th diagonal element of **F** as $f_i$. We thus obtain

$$\mathbf{A}\mathbf{e}_1 = f_1\mathbf{e}_1 \tag{2.13.4a}$$

$$\mathbf{A}\mathbf{e}_2 = f_2\mathbf{e}_2 \tag{2.13.4b}$$

.

$$\mathbf{A}\mathbf{e}_n = f_n\mathbf{e}_n \tag{2.13.4c}$$

Comparing these equations with equation (2.11.1) we see that $\mathbf{e}_i$ are the eigenvectors of **A** while $f_i$ are its eigenvalues. Because of the orthonormality of **E**, the eigenvectors of **A** are mutually orthogonal.

Singular value decomposition allows us to find the square root of a positive-definite matrix. We define the square root of matrix **A** as a matrix that, if multiplied by itself, equals **A**. Recalling that singular values are always positive, the square root of **A** is readily written as

$$\mathbf{A}^{1/2} = \mathbf{E}\mathbf{F}^{1/2}\mathbf{E}^{t} \qquad (2.13.5)$$

where $\mathbf{F}^{1/2}$ is a diagonal matrix whose elements are the square roots of those of **F**. Simple matrix multiplication shows that

$$\mathbf{F}^{1/2}\mathbf{F}^{1/2}=\mathbf{F} \qquad (2.13.6)$$

Recalling the orthonormality of **E**, from which it follows that $\mathbf{E}^{t}\mathbf{E}$ is equal to **I**, it then follows from (2.13.5) that

$$\mathbf{A}^{1/2}\mathbf{A}^{1/2} = \mathbf{A} \qquad (2.13.7)$$

# 3 Some Basic Probability Theory

## 3.1 A Random Variable

Many books have been written on statistics. Only a light coverage of this broad subject area is provided herein. Only matters that are salient to the following chapters of this text are addressed.

Suppose that $\underset{\sim}{x}$ is a random number. (For the moment we will represent a random variable by underlining it with a squiggle; this notation will be dropped later for the sake of simplicity as nearly all variables that we will employ are probabilistic in nature.) The fact that $\underset{\sim}{x}$ is a random variable means that we do not know its value; it could have a range of values, with some of these values being more likely than others. If we know this range, and if we can differentiate values that $\underset{\sim}{x}$ is likely to take from those which it is not, then we know something about $\underset{\sim}{x}$, if not its exact value. So our ignorance of $\underset{\sim}{x}$ is not complete.

In environmental modelling $\underset{\sim}{x}$ may be the value of a parameter. Suppose that someone calibrated an environmental model and informed an expert that the calibrated value of a certain parameter was a value which the expert considered unlikely. Presumably the expert would complain. He/she would inform the modeller that his/her model needed to be re-calibrated. However other values assigned to this same parameter would not assail the expert's sensibilities in this manner. This tells us something about the nature of expertise, and about the nature of knowledge to which experts lay claim. It tells us that an expert cannot say for certain what the values of environmental system properties are; that is why they need to be informed by the calibration process after all. However it also tells us that an expert can recognize nonsense. In other words, expertise provides certainty about the values that model parameters *cannot* take. However it does not provide certainty about their actual values.

Expert knowledge is thus probabilistic in nature and should therefore be expressed using probabilistic concepts. For a given random variable $\underset{\sim}{x}$, the space of real numbers is occupied by values that $\underset{\sim}{x}$ cannot possibly have, and some that it may have. Within this latter subspace there are some values which $\underset{\sim}{x}$ is more likely to take than others. This notion is expressed mathematically by associating a probability density function with $\underset{\sim}{x}$. This will be denoted as $f(x)$, where $x$ (without a squiggle underline) denotes a value that $\underset{\sim}{x}$ may take. Values of $x$ that $\underset{\sim}{x}$ is more likely to take have higher values of $f(x)$ than those which it is less likely to take.

The notion of "probability" relates to "an event". Different realizations of $\underset{\sim}{x}$ could be generated using a random number generator that expresses $f(x)$. The generation of an individual realization of $\underset{\sim}{x}$ is an event. Conceptually the unknown value of a real world system property that is represented by a model's parameter is the outcome of a random number generation event. Experts do not know the outcome of each event. Ideally, however, their expertise informs them of the probability distribution associated with a parameterization event.

The probability that $\underset{\sim}{x}$ lies between two values $x_1$ and $x_2$ is denoted as $P(x_1 < \underset{\sim}{x} < x_2)$. This probability is always between zero (which means "impossible") to unity (which means "certain"). The probability that $\underset{\sim}{x}$ lies between two values $x_1$ and $x_2$ is calculated from the probability density function of $\underset{\sim}{x}$ as the integral of that function between these two values. That is

$$P(a < \underset{\sim}{x} < b) = \int_a^b f(x)dx \qquad (3.1.1)$$

The area under the total probability density function $f(x)$ integrates to unity. This is because the value of $\underset{\sim}{x}$ forthcoming from any sampling event must lie somewhere in the space of real numbers. Thus

$$\int_{-\infty}^{\infty} f(x)dx=1 \qquad (3.1.2)$$

The probability that $\underset{\sim}{x}$ is less than a value $x$ is itself a function. This is called the cumulative distribution function of $\underset{\sim}{x}$ and is denoted herein as $F(x)$. Formally

$$P(\underset{\sim}{x} < x) = F(x) = \int_{0}^{x} f(u)du \qquad (3.1.3)$$

Equation (3.1.1) can then be expanded as

$$P(a < \underset{\sim}{x} < b) = \int_{a}^{b} f(x)dx = F(b) - F(a) \qquad (3.1.4)$$

Obviously

$$\lim_{x\to-\infty} F(x)=0 \qquad \lim_{x\to\infty} F(x)=1 \qquad (3.1.5)$$

and

$$f(x)=\frac{dF(x)}{dx} \qquad (3.1.6)$$

The "expected value" of any function of $\underset{\sim}{x}$, say $g(\underset{\sim}{x})$, is the weighted average of values of $g(\underset{\sim}{x})$ over all values of $\underset{\sim}{x}$, with the weighting function being the probability density function. If $E[g(\underset{\sim}{x})]$ is used to symbolize the expected value of $g(\underset{\sim}{x})$ then

$$E[g(\underset{\sim}{x})] = \int_{-\infty}^{\infty} g(x)f(x)dx \qquad (3.1.7)$$

In similar fashion, the expected value $E(\underset{\sim}{x})$ of $\underset{\sim}{x}$ is the average of $\underset{\sim}{x}$ over all possibly values that it may take, with these values being weighted according to their respective probability density function values. This is also known as the average value, or mean value $\mu_x$ of $\underset{\sim}{x}$. Thus

$$E(\underset{\sim}{x}) = \mu_x = \int_{-\infty}^{\infty} xf(x)dx$$

The variance of $\underset{\sim}{x}$, denoted as var($\underset{\sim}{x}$) or $\sigma^2_x$, is the expected value of the square of the difference between $\underset{\sim}{x}$ and its mean. That is

$$\sigma^2_x = E[(\underset{\sim}{x} - E(\underset{\sim}{x}))^2] = \int_{-\infty}^{\infty} (x-\mu_x)^2 f(x)dx \qquad (3.1.8)$$

The square root of the variance is known as the standard deviation.

The median of $\underset{\sim}{x}$ is the value of $\underset{\sim}{x}$ that divides the density function in two. If this is denoted as $x_m$ then

$$\int_{-\infty}^{x_m} f(x)dx=\int_{x_m}^{\infty} f(x)dx=\frac{1}{2} \qquad (3.1.9)$$

## 3.2 Some Commonly Used Density Functions

### 3.2.1 Gaussian or Normal Distribution

The Gaussian or normal distribution is given by

$$f(x)=\frac{2}{\sigma_x\sqrt{2\pi}}\exp\left\{-\frac{(x-\mu_x)^2}{2\sigma_x^2}\right\} \qquad (3.2.1)$$

Graphs and tables of the normal distribution function abound. As is commonly known, the probability that a sample of a random normal variable lies within a standard deviation of its mean is 68.27 percent. That is

$$P[-\sigma_x < x - \mu_x < \sigma_x] = .6827 \qquad (3.2.2a)$$

Probabilities related to some other intervals are as follows

$$P[-2\sigma_x < x - \mu_x < 2\sigma_x] = .9545 \qquad (3.2.2b)$$

$$P[-3\sigma_x < x - \mu_x < 3\sigma_x] = .9973 \qquad (3.2.2c)$$

A normal random variable is "standardized" or "normalized" if it is transformed such that its standard deviation is one and its mean is zero. Samples of a standardized normal random variate *z* are calculated from those of a normal random variable *x* using the equation

$$z=\frac{x-\mu_x}{\sigma_x} \qquad (3.2.3)$$

The familiar "bell-shaped curve" which characterizes the normal distribution is illustrated in figure 3.1.

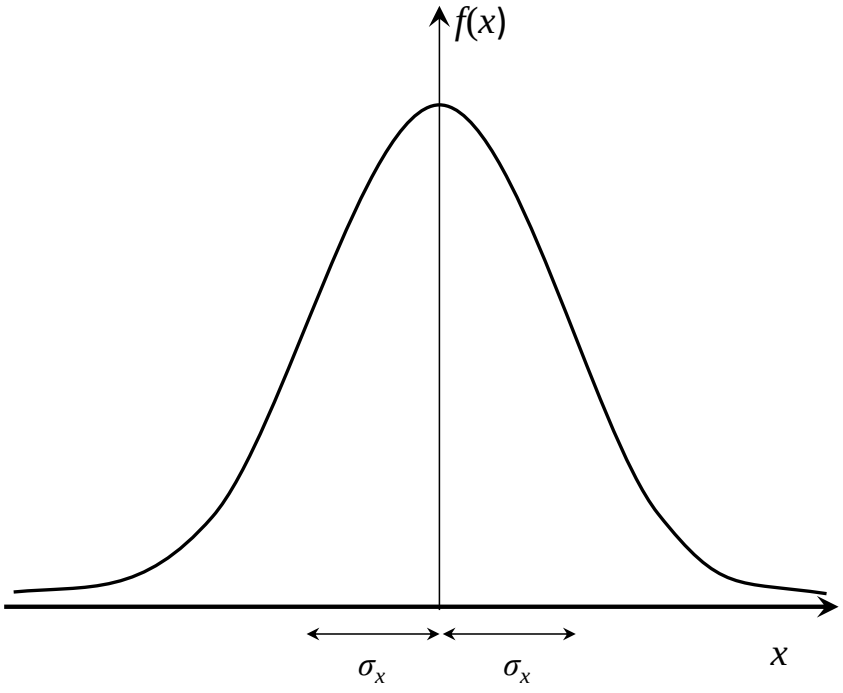


**Figure 3.1. The normal probability distribution.**

A number of other probability density functions feature prominently in testing and sampling.

As for the normal distribution, tables and graphs of these abound. They are only mentioned briefly hereunder.

### 3.2.2 The *t* or Student's *t* Distribution

Let $\underset{\sim}{x}_1, \underset{\sim}{x}_2 \ldots \underset{\sim}{x}_n$ be $n$ independent (see below for a discussion of statistical independence) random variables which each possess a normal distribution with mean $\mu$ and standard deviation $\sigma$. The random variable $\underset{\sim}{t}$ defined by

$$t = \frac{\bar{x} - \mu}{s}\sqrt{n} \qquad (3.2.4a)$$

where

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n} \qquad \text{and} \qquad s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 \qquad (3.2.4b)$$

belongs to a *t* or student's *t* distribution. This distribution describes variability in estimates of the mean of a random normal variable. A *t* distribution defined as above is said to possess $n$-1 degrees of freedom. Where $n$ exceeds about 30 the student *t* distribution is almost identical to the normal distribution with mean of 0 and standard deviation $\frac{\sigma_x}{\sqrt{n}}$.

### 3.2.3 The Chi-Squared Distribution

Let $\underset{\sim}{x}_1, \underset{\sim}{x}_2 \ldots \underset{\sim}{x}_n$ be $n$ independent random variables, each of which is normally distributed with a mean of 0 and a standard deviation of 1. Their sum yields a random variable which belongs to a $\chi^2$ distribution. This distribution depends on $n$ which is referred to as the "degrees of freedom" of the distribution. The expected value of a $\chi^2$ distribution with $n$ degrees of freedom (i.e. the mean of this distribution) is $n$, while its variance is $2n$. As $n$ becomes very large, the $\chi^2$ distribution with $n$ degrees of freedom approaches a normal distribution with this same mean and variance.

### 3.2.4 The F or Fisher Distribution

Let $\underset{\sim}{\chi}_m^2$ designate a random variable belonging to a chi-squared distribution with $m$ degrees of freedom. Thus

$$\underset{\sim}{\chi}_m^2 = \underset{\sim}{x}_1^2 + \underset{\sim}{x}_2^2 + \ldots + \underset{\sim}{x}_m^2 \qquad (3.2.5a)$$

where $\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots, \underset{\sim}{x}_m$ are independent standardized normal variates. Similarly, let $\underset{\sim}{\chi}_n^2$ designate a random variable belonging to a chi-squared distribution with $n$ degrees of freedom. Thus

$$\underset{\sim}{\chi}_n^2 = \underset{\sim}{y}_1^2 + \underset{\sim}{y}_2^2 + \ldots + \underset{\sim}{y}_n^2 \qquad (3.2.5b)$$

where $\underset{\sim}{y}_1, \underset{\sim}{y}_2, \ldots, \underset{\sim}{y}_n$ are also independent standardized normal variates. The random variable $\underset{\sim}{F}_{m,n}$ defined by

$$\underset{\sim}{F}_{m,n} = \frac{\underset{\sim}{\chi}_m^2}{\underset{\sim}{\chi}_n^2} \qquad (3.2.6)$$

possess an $F$ distribution of $m$, $n$ degrees of freedom. The mean and variance of this distribution are as follows

$$\text{mean } (\underset{\sim}{F}_{m,n}) = \frac{n}{n-2} \qquad \text{for } n > 2 \qquad (3.2.7a)$$

$$\text{variance } (\underset{\sim}{F}_{m,n}) = \frac{2n^2(m+n-2)}{m(n-2)^2(n-4)} \qquad \text{for } n > 4 \qquad (3.2.7b)$$

As $n$ approaches infinity, the $F$ distribution with $m,n$ degrees of freedom approaches the chi-squared distribution with $m$ degrees of freedom.

## 3.3 Random Vectors

Most models have more than a single parameter. The calibration dataset against which they are calibrated is comprised of more than one observation; random noise is associated with each of these observations. We must therefore deal with collections of random numbers rather than with individual random numbers. That is, we must deal with random vectors. A random vector is simply a vector whose elements are random numbers.

Where the variability of more than one random number must be characterized then multidimensional probabilities, and multidimensional probability density functions, must be employed.

Consider the $n$-dimensional random vector $\underset{\sim}{\mathbf{x}}$. Its $n$ elements are random variates $\underset{\sim}{x}_i$. (As stated above, the squiggle under a variable that is used to denote its random status will be dropped in later notation.) Thus

$$\underset{\sim}{\mathbf{x}} = [\underset{\sim}{x}_1 \;\; \underset{\sim}{x}_2 \;\; \ldots \;\; \underset{\sim}{x}_n]^t \qquad (3.3.1)$$

An $n$-dimensional probability density function $f(\mathbf{x})$ can be defined that allows event probabilities to be computed for $\underset{\sim}{\mathbf{x}}$ in a similar manner as for a one-dimensional probability distribution. It is defined in following manner.

$$P(a_1 < \underset{\sim}{x}_1 < b_1;\; a_2 < \underset{\sim}{x}_2 < b_2;\; \ldots;\; a_n < \underset{\sim}{x}_n < b_n)$$

$$= \int_{a_1}^{b_1}\int_{a_2}^{b_2}\ldots\int_{a_n}^{b_n} f(x_1, x_2 \ldots x_n)\, dx_1 dx_2 \ldots dx_n \qquad (3.3.2a)$$

or to put it more concisely

$$P(\mathbf{a} < \mathbf{x} < \mathbf{b}) = \int_{\mathbf{a}}^{\mathbf{b}} f(\mathbf{x})\, d\mathbf{x} \qquad (3.3.2b)$$

As for its one-dimensional counterpart

$$\int_{-\infty}^{\infty} f(\mathbf{x})\, d\mathbf{x} = 1 \qquad (3.3.3)$$

The probability that $\underset{\sim}{\mathbf{x}}$ is less than $\mathbf{x}$ is called the joint cumulative distribution function of $\underset{\sim}{\mathbf{x}}$ and is denoted as $F(\mathbf{x})$. Employing vector notation, this can be expressed as

$$P(\underset{\sim}{\boldsymbol{x}} < \boldsymbol{x}) = F(\boldsymbol{x}) = \int_{\mathbf{0}}^{\mathbf{x}} f(\mathbf{u})\, d\mathbf{u} \qquad (3.3.4)$$

so that

$$P(\mathbf{a} < \underset{\sim}{\mathbf{x}} < \mathbf{b}) = \int_{\mathbf{a}}^{\mathbf{b}} f(\mathbf{x})\, d\mathbf{x} = F(\mathbf{b}) - F(\mathbf{a}) \qquad (3.3.5)$$

Similar limits hold for the joint cumulative distribution function as hold for the one-dimensional cumulative distribution function, namely

$$\lim_{\mathbf{x}\to 0} F(\mathbf{x})=0 \qquad \lim_{\mathbf{x}\to\infty} F(\mathbf{x})=1 \tag{3.3.6}$$

Also

$$f(\mathbf{x})=\frac{dF(\mathbf{x})}{d\mathbf{x}} \tag{3.3.7}$$

The expected value of a scalar function of the random vector $\underset{\sim}{\mathbf{x}}$, for example $g(\underset{\sim}{\mathbf{x}})$, is defined as the weighted average of that function over the $n$-dimensional space of $\underset{\sim}{\mathbf{x}}$; the weighting function is the density function of $\underset{\sim}{\mathbf{x}}$. If, as above, the expected value of $g(\underset{\sim}{\mathbf{x}})$ is denoted as $E[g(\underset{\sim}{\mathbf{x}})]$ then

$$E[g(\underset{\sim}{\mathbf{x}})] = \int_{-\infty}^{\infty} g(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} \tag{3.3.8}$$

Notice that the integration takes place over $n$ dimensions. The mean of an element $\underset{\sim}{x}_i$ of $\underset{\sim}{\mathbf{x}}$ is the expected value of that element. It is given by

$$E(\underset{\sim}{x}_i) = \mu_i = \int_{-\infty}^{\infty} x_i f(\mathbf{x}) d\mathbf{x} \tag{3.3.9}$$

The expected values of all of the elements of $\underset{\sim}{\mathbf{x}}$ can be collected into a single vector $\boldsymbol{\mu}_{\mathbf{x}}$ as

$$\boldsymbol{\mu}_{\mathbf{x}} = [\mu_1 \;\; \mu_2 \;\; \ldots \;\; \mu_n]^t \tag{3.3.10}$$

The variance of $\underset{\sim}{x}_i$ is denoted as $\sigma^2_i$ and is given by

$$\sigma^2_i = E[(\underset{\sim}{x}_i - E(\underset{\sim}{x}_i))^2] = \int_{-\infty}^{\infty} (x_i - \mu_i)^2 f(\mathbf{x}) d\mathbf{x} \tag{3.3.11}$$

Once again, the integral is over $n$-dimensional space.

Notice that in the above equations $\sigma^2_{xi}$ has been abbreviated to $\sigma^2_i$ as the "$x$" part of the subscript is redundant when $\underset{\sim}{x}_i$ is part of the greater random vector $\underset{\sim}{\mathbf{x}}$. The same applies to $\mu_{xi}$ which has been abbreviated to $\mu_i$.

The propensity for variability of a single random variable (i.e. a scalar rather than a vector variable) can be characterized by its variance. If the variable is normally distributed this is, in fact, all that is needed to characterize its variability; this is because the mean and the standard deviation alone completely define a normal distribution. (The same does not necessarily apply to other distributions.) Unfortunately, characterization of variability gets a little more complicated in multiple dimensions. This topic will be addressed shortly.

Suppose that we wish to obtain the probability density function of $\underset{\sim}{x}_i$ without regard to the values that other components of the random vector $\underset{\sim}{\mathbf{x}}$ may take. That is, we wish to obtain the probability density function of $\underset{\sim}{x}_i$ while allowing the other components of $\underset{\sim}{\mathbf{x}}$ to have any values that they please. The resulting probability density function is called the marginal probability density function of $\underset{\sim}{x}_i$. It is obtained by integrating out the other components. For illustrative purposes, suppose that $n$ is equal to 3 and that we wish to obtain the marginal probability distribution of $\underset{\sim}{x}_2$. Let us denote this as $f_m(x_2)$. This is obtained as

$$f_m(\underset{\sim}{x}_2) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x_1, x_2, x_3) dx_1 dx_3 \tag{3.3.12}$$

## 3.4 Dependence and Independence

Figure 3.2 shows a probability density function contour pertaining to each of two different two-variable distributions. In each case the peak of the density function lies somewhere

within the contour. Outside the contour the value of the density function diminishes to zero in all directions.

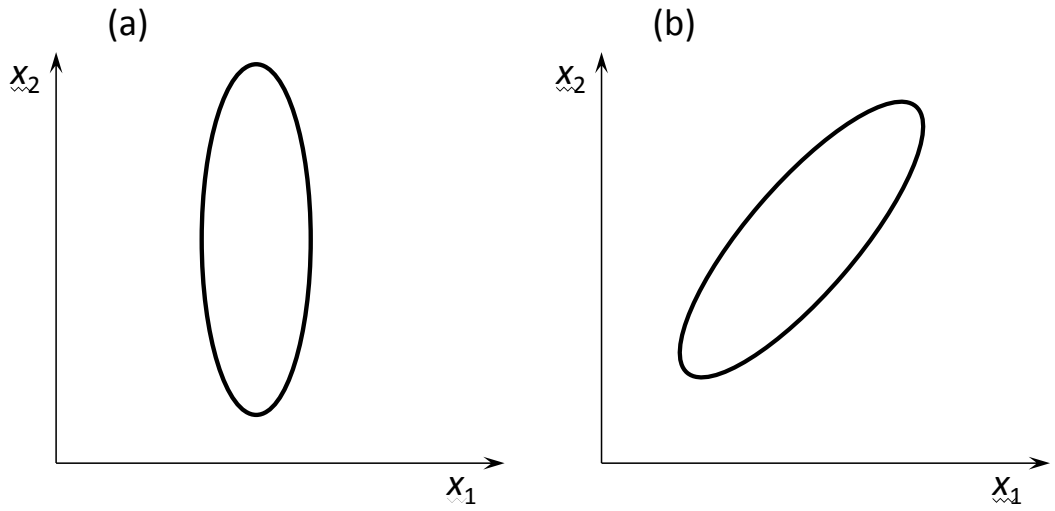


**Figure 3.2. Probability density function contours where (a) random variables are independent and (b) where they are not independent.**

For the distribution function depicted on the left of figure 3.2, the value taken by random variable $x_2$ is independent of that taken by $x_1$. Thus a "statistical event" through which values are generated for both of these variables is effectively comprised of two separate events, namely generation of a value for $x_1$ followed by generation of a value for $x_2$. Formally, this is expressed by the fact that the joint probability density function of $x_1$ and $x_2$ is the product of the separate, marginal probability density functions of each. For a greater number of dimensions than 2, this can be written as

$$f(x_1, x_2 \ldots x_n) = f(x_1)f(x_2)...f(x_n) \qquad (3.4.1)$$

The same multiplicative rule applies for marginal cumulative distributions. Thus

$$F(x_1, x_2 \ldots x_n) = F(x_1)F(x_2)...F(x_n) \qquad (3.4.2)$$

Probabilities associated with events are also multiplicative under these circumstances. Thus, for the two-dimensional case above, if we denote by $P(a)$ the probability that $x_1$ lies between $a_1$ and $a_2$, and by $P(b)$ the probability that $x_2$ lies between $b_1$ and $b_2$, the probability of joint occurrence of these events, denoted by $P(ab)$, is given by

$$P(ab) = P(a)P(b) \qquad (3.4.3)$$

For the joint probability distribution whose contour is depicted on the right of figure 3.2, the values taken by $x_1$ and $x_2$ are not independent of each other. Suppose that a statistical event generates values for these two variables. If this event were to be decomposed into two parts whereby a value for $x_2$ is generated followed by a value for $x_1$, then the probability density function used for generation of $x_1$ would not be its marginal distribution. This is illustrated in figures 3.3 and 3.4. Figure 3.3 shows the marginal probability density functions of the two statistically-dependent random variables. Figure 3.4 shows the so-called conditional probability density function of $x_1$ that must be used for generation of a value for this random variable if a value $\alpha$ has already been drawn for $x_2$. Also shown is the conditional probability density function for $x_1$ if, instead of a value of α, a value of $\beta$ has already been drawn for $x_2$. The differences between each of these two density functions, and between the conditional and

marginal density functions of $x_1$ are obvious.

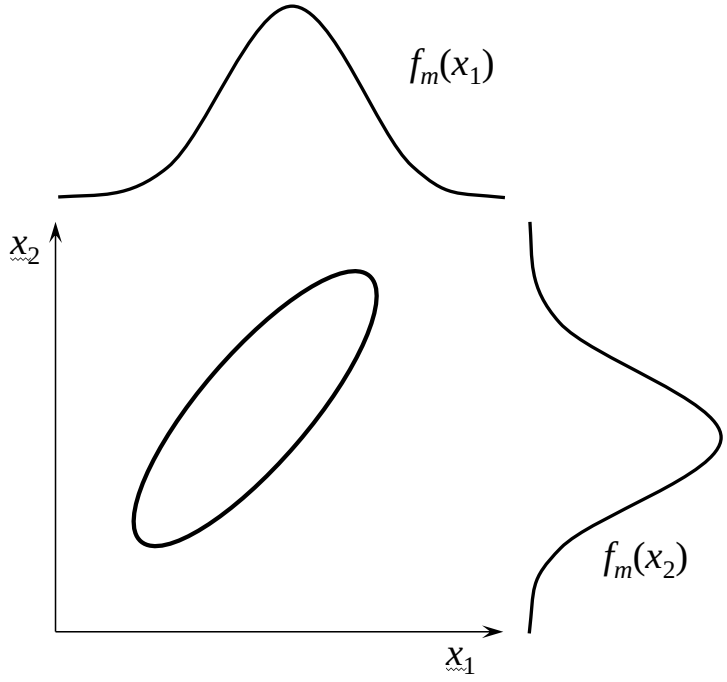


**Figure 3.3. Marginal probability density functions of two random variables which are not statistically independent.**

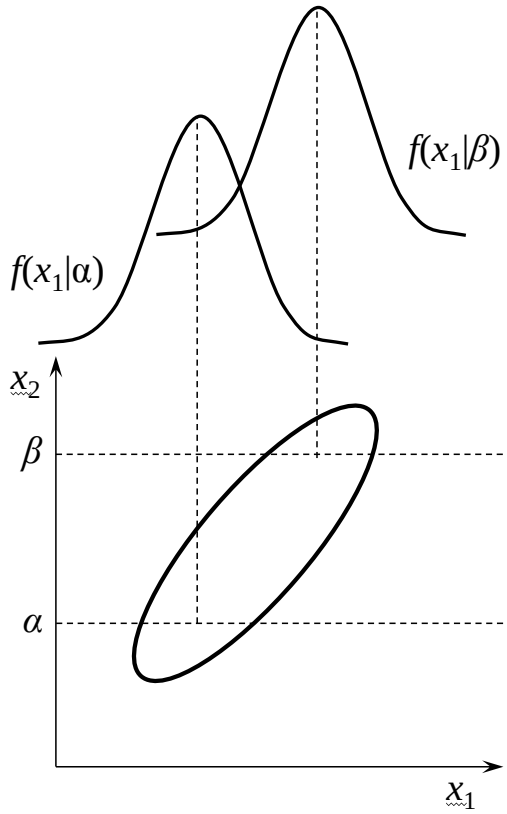


**Figure 3.4. Two conditional probability density functions for random variable $x_1$.**

The simultaneous occurrence of event *a* and event *b* can be denoted as the event *ab*. (An example of such a joint event is that $\underset{\sim}{x}_1$ lies between $\beta_1$ and $\beta_2$ and that $x_2$ lies between $\alpha_1$ and $\alpha_2$). The probably of the joint event *ab* is given by

$$P(ab)=P(b|a)P(a) \tag{3.4.4}$$

where $P(b|a)$ can be read as "the probability of *b* given *a*" or "the probability of *b* conditional on *a*". In similar fashion, the conditional density function for $\underset{\sim}{x}_1$ conditional on $\underset{\sim}{x}_2$ is denoted as $f(x_1|x_2)$. The joint probability density function of $\underset{\sim}{x}_1$ and $\underset{\sim}{x}_2$, i.e. $f(x_1, x_2)$ is given by

$$f(x_1, x_2) = f(x_1|x_2)f_m(x_2) \tag{3.4.5}$$

where $f_m(x_2)$ is the marginal density function of $\underset{\sim}{x}_2$.

The above two formulas are used when decomposing a joint event into its component parts. If a value for $\underset{\sim}{x}_2$ is generated first, no restrictions on the random number generation process are operative while this value is being drawn. Hence a value for $\underset{\sim}{x}_2$ is generated using its marginal density function. However, given the statistical interdependence that exists between $\underset{\sim}{x}_1$ and $\underset{\sim}{x}_2$, this sets a condition on the drawing of a value for $\underset{\sim}{x}_1$. $f(x_1|x_2)$ must therefore be used when drawing a value for $\underset{\sim}{x}_1$.

From (3.4.5) it follows that

$$f(x_1 \mid x_2)=\frac{f(x_1, x_2)}{f_m(x_2)} \tag{3.4.6}$$

If $x_1$ and $x_2$ are statistically independent, their conditional distributions are the same as their marginal distributions. From (3.4.6) and (3.4.1)

$$f(x_1 \mid x_2)=\frac{f(x_1, x_2)}{f_m(x_2)}=\frac{f_m(x_1)f_m(x_2)}{f_m(x_2)}=f_m(x_1) \tag{3.4.7}$$

## 3.5 Covariance and Correlation

The variance of a single random variable was defined above. This characterizes the extent to which random samples of that variable can vary about their mean; see equation (3.1.8). The variance of a random variable which is an element of a random vector is similarly defined; see equation (3.3.11). In the latter case the integration required to calculate the expected value of the squared departure of this random vector element from its mean must be performed over multi-dimensional space, as the random variable is drawn from a multi-dimensional density function that describes both it and other components of the random vector to which it belongs. Alternatively integration can take place over the marginal density function of the individual variable; as (3.3.12) shows, integration over the other random variables has already been performed in defining the marginal probability density function of the individual variable whose variance is sought.

Where a random variable is part of a joint probability distribution, more than just its variance may be needed to characterize its propensity to vary about its mean value, for this conveys nothing about how this propensity is linked to that of other random variables which figure in the joint distribution. Information on statistical interdependence of random variables which share a joint probability distribution can be conveyed through denoting is covariance with those other variables. Like the variance of random variable $\underset{\sim}{x}_1$, the covariance between random variables $\underset{\sim}{x}_1$ and $\underset{\sim}{x}_2$ is expressed as an expected value; it is the expected value of the product of the departures of these two random variables from their respective means. An

expected value of zero for this product indicates independence of these variables. A positive expected value indicates that the random variables tend to vary together in the same direction. A negative expected value indicates that one random variable tends to vary in one direction from its mean as the other varies in the opposite direction.

The covariance between $\underset{\sim}{x}_1$ and $\underset{\sim}{x}_2$ is denoted as $\text{cov}(\underset{\sim}{x}_1, \underset{\sim}{x}_2)$, or more succinctly as $\sigma_{12}$. More generally, the covariance between the $\underset{\sim}{x}_i$ and $\underset{\sim}{x}_j$ components of the random vector $\underset{\sim}{\mathbf{x}}$ is denoted as $\sigma_{ij}$. It is defined as

$$\sigma_{ij} = E[(\underset{\sim}{x}_i - \mu_i)(\underset{\sim}{x}_j - \mu_j)] = \int_{-\infty}^{\infty} (x_i - \mu_i)(x_j - \mu_j) f(\mathbf{x}) d\mathbf{x} \qquad (3.5.1)$$

The variances of individual elements of a random vector, together with inter-element covariances between its elements, can be combined into a single matrix known as the variance-covariance matrix, or simply the covariance matrix for short. If the random vector $\underset{\sim}{\mathbf{x}}$ has $n$ dimensions, then the covariance matrix of $\underset{\sim}{\mathbf{x}}$, designated as $\text{C}(\mathbf{x})$, is a square $n \times n$ matrix defined as

$$\text{C}(\mathbf{x}) = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22}^2 & \cdots & \sigma_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn}^2 \end{bmatrix} \qquad (3.5.2)$$

The covariance matrix is symmetric as $\sigma_{ij} = \sigma_{ji}$ for all $i$ and $j$. It can also be shown that it must be positive-definite if it is to properly characterize the stochasticity of random variables; this ensures that no statistical events have a negative probability of occurrence.

The correlation coefficient $\rho_{ij}$ between random vector elements $\underset{\sim}{x}_i$ and $\underset{\sim}{x}_j$ is calculated as

$$\rho_{ij} = \frac{\sigma_{ij}}{\sigma_i \sigma_j} \qquad (3.5.3)$$

The correlation coefficient varies between -1 and 1. Correlation coefficients of -1 and 1 indicate functional dependence rather than statistical inter-relatedness, so great is the propensity for the random variables to vary in the opposite or same directions respectively from their mean in sympathy. On the other hand, a correlation coefficient of 0 indicates statistical independence of the random variables. Correlation coefficients can be collected into a matrix; naturally enough this is referred to as the correlation coefficient matrix. The diagonal elements of the correlation coefficient matrix are all 1.

## 3.6 The Multinormal Distribution

The multinormal, or multiGaussian, probability distribution is characterized by the following density function

$$f(x_1, x_2 \ldots x_n) = f(\mathbf{x}) = \frac{e^{\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_x)^t C^{-1}(\mathbf{x})(\mathbf{x}-\boldsymbol{\mu}_x)\right]}}{(2\pi)^{n/2}\left|\text{C}(\mathbf{x})\right|^{1/2}} \qquad (3.6.1)$$

As can be seen from this equation, the vector of element means $\boldsymbol{\mu}_x$ and the covariance matrix $\text{C}(\mathbf{x})$ are all that is required for a complete mathematical description of this distribution. For some other distributions more specifications than this are required.

Contours of constant probability in *n*-dimensional parameter space are defined by the equation

$$(\mathbf{x} - \boldsymbol{\mu}_x)^t C^{-1}(\mathbf{x})(\mathbf{x} - \boldsymbol{\mu}_x) = k \qquad (3.6.2)$$

where *k* is a constant associated with the contour. In two dimensions, probability contours form ellipses; in higher dimensions they are hyper-ellipsoids. If there is no correlation between the elements of $\underset{\sim}{\mathbf{x}}$ (i.e. if C(**x**) is a diagonal matrix), then the axes of these hyper-ellipsoids are parallel to the unit vectors $[1\ 0\ 0..]^t$, $[0\ 1\ 0\ ..]^t$, etc. More generally, the axes of hyper-ellipsoids of constant probability point in the directions of the eigenvectors of C(**x**). The lengths of these axes are proportional to the square roots of the corresponding eigenvalues of C(**x**).

## 3.7 Bayes Equation

Equation (3.4.4) states that the probability of simultaneous occurrence of events *a* and *b* is given by the probability that event *a* will occur multiplied by the probability of event *b* conditional on event *a*. This equation is now repeated as (3.7.1).

$$P(ab)=P(b|a)P(a) \qquad (3.7.1)$$

Obviously, the simultaneous occurrence of events *a* and *b* could also be considered as the occurrence of event *b* followed by the occurrence of event *a*. Once *b* has occurred, the probability of event *a* is then conditional on *b* if there is any statistical inter-relatedness between events *a* and *b*. Thus

$$P(ab)=P(a|b)P(b) \qquad (3.7.2)$$

From the above two equations it immediately follows that

$$P(b \mid a)=\frac{P(a \mid b)P(b)}{P(a)} \qquad (3.7.3)$$

This is Bayes equation, a subject on which more will be said later in this text. The same concept can be expressed using density functions. If we drop the "m" subscript from (3.4.5) (the marginal probability density function will become the prior probability density function in later chapters), we obtain

$$f(x_1 \mid x_2)=\frac{f(x_2 \mid x_1)f(x_1)}{f(x_2)} \qquad (3.7.4)$$

Extending the concept from random scalars to random vectors, Bayes equation in multiple dimensions becomes

$$f(\mathbf{x}_1 \mid \mathbf{x}_2)=\frac{f(\mathbf{x}_2 \mid \mathbf{x}_1)f(\mathbf{x}_1)}{f(\mathbf{x}_2)} \qquad (3.7.5)$$

Obviously, if $\underset{\sim}{\mathbf{x}}_1$ and $\underset{\sim}{\mathbf{x}}_2$ are independent, then

$$f(\mathbf{x}_2 \mid \mathbf{x}_1) = f(\mathbf{x}_2) \qquad (3.7.6)$$

which, if substituted into (3.7.5) leads to

$$f(\mathbf{x}_1 \mid \mathbf{x}_2) = f(\mathbf{x}_1) \qquad (3.7.7)$$

However suppose that this is not the case. Suppose also that, following a particular statistical event in which samples of $\underset{\sim}{\mathbf{x}}_1$ and $\underset{\sim}{\mathbf{x}}_2$ are generated, we acquire perfect knowledge of the

values taken by the elements of $\underset{\sim}{\mathbf{x}}_2$. $f(\mathbf{x}_2|\mathbf{x}_1)$ can then be calculated for various values of $\underset{\sim}{\mathbf{x}}_1$ and substituted into the right side of (3.7.5). This modifies the calculated value of $f(\mathbf{x}_1|\mathbf{x}_2)$ on the left side of this equation from $f(\mathbf{x}_1)$, the distribution which it would possess if sampled values of $\underset{\sim}{\mathbf{x}}_2$ are unknown. Presumably $f(\mathbf{x}_1|\mathbf{x}_2)$ will be higher than $f(\mathbf{x}_1)$ for some values of $\underset{\sim}{\mathbf{x}}_1$ and lower than $f(\mathbf{x}_1)$ for other values of $\underset{\sim}{\mathbf{x}}_1$. The probability density function of $\underset{\sim}{x}_1$ is therefore modified by sampling $\underset{\sim}{\mathbf{x}}_2$. It follows that values of $\underset{\sim}{\mathbf{x}}_2$ are informative of values of $\underset{\sim}{\mathbf{x}}_1$. This is also apparent from figures 3.3 and 3.4; in this example, sampling of $\underset{\sim}{\mathbf{x}}_2$ narrows the width of the conditional, or posterior, probability density distribution of $\underset{\sim}{\mathbf{x}}_1$.

## 3.8 Conditional Covariance Matrix

Our notation will now be altered slightly to dispense with the squiggle under a scalar or vector variable to denote its status as a random variable. This was useful up until now in order to distinguish the name of a variable from the value taken by that variable, especially in discussing probability density functions and cumulative probability density functions. As most future discussion of random variables will involve only their covariance matrices, this distinction is no longer needed. The meaning of a symbol will be clear from its context.

The acquisition of knowledge pertaining to some variables through the sampling of other variables with which they are statistically correlated was discussed above. Where the variables are collectively described by a multinormal probability density function this knowledge transfer can be quantified.

Let $\mathbf{x}$ be a random vector. Suppose that we partition $\mathbf{x}$ into the vectors $\mathbf{x}_1$ and $\mathbf{x}_2$ as follows

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} \tag{3.8.1}$$

Suppose that the mean of $\mathbf{x}$ is given by

$$\boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix} \tag{3.8.2}$$

and that the covariance matrix $\mathrm{C}(\mathbf{x})$ of $\mathbf{x}$ can be partitioned according to the partitioning of $\mathbf{x}$ into $\mathbf{x}_1$ and $\mathbf{x}_2$ as

$$\mathrm{C}(\mathbf{x}) = \begin{bmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \mathbf{C}_{21} & \mathbf{C}_{22} \end{bmatrix} \tag{3.8.3}$$

If variability of $\mathbf{x}$ is described by a multinormal distribution, then the marginal distribution of $\mathbf{x}_1$ is completely characterized by $\boldsymbol{\mu}_1$ and $\mathbf{C}_{11}$. Suppose now that we acquire perfect knowledge of values taken by elements of the $\mathbf{x}_2$ vector. As discussed above, this modifies the probability distribution of $\mathbf{x}_1$. Let $\boldsymbol{\mu}_1'$ and $\mathbf{C}'_{11}$ specify the mean and covariance matrix of this modified distribution. It can be shown (see, for example, Koch, 1999) that

$$\boldsymbol{\mu}_1' = \boldsymbol{\mu}_1 + \mathbf{C}_{12}\mathbf{C}^{-1}{}_{22}\,(\mathbf{x}_2 - \boldsymbol{\mu}_2) \tag{3.8.4}$$

and

$$\mathbf{C}'_{11} = \mathbf{C}_{11} - \mathbf{C}_{12}\mathbf{C}^{-1}{}_{22}\mathbf{C}_{21} \tag{3.8.5}$$

## 3.9 Propagation of Covariance

Let $\mathbf{x}$ be a random $n$-dimensional vector. Let $\mathbf{A}$ be an $m \times n$ matrix. Let the $m$-dimensional

vector **y** be calculated from **x** as follows

$$\mathbf{y} = \mathbf{A}\mathbf{x} \tag{3.9.1}$$

If **x** is a random vector, than so too must **y** be a random vector. Hence it possesses an $m \times m$ covariance matrix. It can be shown that

$$C(\mathbf{y}) = \mathbf{A}C(\mathbf{x})\mathbf{A}^t \tag{3.9.2}$$

This relationship will be used extensively in work to follow.

## 3.10 Principal Components

Suppose that the *n*-dimensional random vector **x** has a covariance matrix C(**x**). As has already been discussed, C(**x**) is a positive-definite matrix. Hence, when subjected to singular value decomposition, an orthonormal **E** matrix and a diagonal **F** matrix can be found which satisfy the following equation

$$C(\mathbf{x}) = \mathbf{E}\mathbf{F}\mathbf{E}^t \tag{3.10.1}$$

Let the *n*-dimensional vector **y** be calculated from **x** using the equation

$$\mathbf{y} = \mathbf{F}^{-½}\mathbf{E}^t\mathbf{x} \tag{3.10.2}$$

As was discussed above, the diagonal $\mathbf{F}^{½}$ matrix is calculated from the diagonal **F** matrix by taking the square root of its respective elements. The diagonal $\mathbf{F}^{-½}$ matrix is calculated from the diagonal $\mathbf{F}^{½}$ matrix by individually inverting respective diagonal elements. Through use of equation (3.9.2) the covariance matrix of **y**, that is C(**y**), can be calculated as

$$C(\mathbf{y}) = \mathbf{F}^{-½}\mathbf{E}^t\mathbf{E}\mathbf{F}\mathbf{E}^t\mathbf{E}\mathbf{F}^{-½} = \mathbf{I} \tag{3.10.3}$$

where use is made of the fact that **E** is an orthonormal matrix, so that

$$\mathbf{E}^t\mathbf{E} = \mathbf{I} \tag{3.10.4}$$

The covariance matrix of **y** is thus the identity matrix.

Suppose that **y** possesses a multinormal probability distribution. Then the smaller is the norm of **y**, the higher is its likelihood. This is because the exponent in equation (3.6.1) becomes equal to minus half the square of the norm of a random vector when its covariance matrix is **I**. An inversion methodology such as singular value decomposition which achieves a minimum norm solution to an inverse problem therefore achieves a solution of maximum likelihood to that problem if the prior covariance matrix of parameters is **I**.

Suppose that an inverse problem is posed for **x**, and that the prior covariance matrix of **x** is C(**x**) and not **I**. A solution of maximum likelihood for that problem can be achieved through singular value decomposition if it is first posed in terms of the transformed parameter set **y** where the relationship between **y** and **x** is described by (3.10.2). The solution for **x** can then be back-calculated from that achieved for **y** using the relationship (easily derived from equation 3.10.2)

$$\mathbf{x} = \mathbf{E}\mathbf{F}^{1/2}\mathbf{y} \tag{3.10.5}$$

The transformation depicted in equation (3.10.2) is known as the Kahunen-Loève transformation.

Now define the vector **z** as

$$\mathbf{z} = \mathbf{E}^t\mathbf{x} \tag{3.10.6}$$

**z** and **y** are therefore related through the equation

$$\mathbf{y} = \mathbf{F}^{-½}\mathbf{z} \qquad (3.10.7)$$

Recalling that $\mathbf{F}^{-½}$ is a diagonal matrix, **z** points in the same direction as **y**. The individual elements of **z** are related to those of **y** through an element-specific factor which is the corresponding diagonal element of $\mathbf{F}^{-½}$. From (3.9.2) and (3.10.1) it readily follows that

$$C(\mathbf{z}) = \mathbf{F} \qquad (3.10.8)$$

As **F** is a diagonal matrix, the elements of **z** are not correlated with each other. This is despite the fact that the elements of **x** are indeed correlated with each other if C(**x**) is not a diagonal matrix.

Recall from section 2.13 that the columns of **E** are the eigenvectors of C(**x**) and that the (diagonal) elements of **F** are its eigenvalues. The columns of **E** become the rows of $\mathbf{E}^t$. Each element of the vector **z** which is calculated from **x** using (3.10.6) is thus the scalar product of **x** with an eigenvector of its covariance matrix C(**x**). From (3.10.8) the variance of each of these elements is the corresponding eigenvalue of C(**x**); the standard deviation of each of these elements is therefore the square root of this eigenvalue.

Figure 3.5 depicts the probability density functions of the individual elements of a two-dimensional **z** vector.

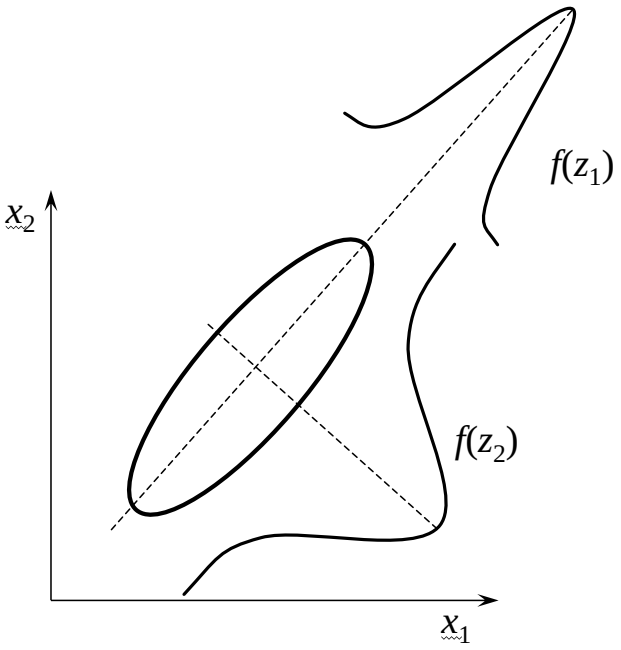


**Figure 3.5. Independent probability density functions for components of z obtained from x using equation (3.10.6).**

## 3.11 Spatial Correlation

In many contexts of PEST usage, expert knowledge of parameters as it exists prior to the calibration process can be expressed through positing spatial correlation between them. This is especially the case in groundwater and subsurface reservoir modelling. Spatial correlation of parameters follows from the likelihood that hydraulic properties at points which are close together are similar. However the likelihood of hydraulic property similarity is likely to decay with increasing separation of the points until, at some separation, there is likely to be no

relationship at all between properties at the two points.

Suppose that a model employs $n$ parameters. Keeping in mind that a covariance matrix is symmetric, the number of values that must be provided for the filling of a $n \times n$ covariance matrix is $n(n+1)/2$. This rises rapidly as $n$ rises.

In contrast to this, only a few numbers are required to fill a spatial covariance matrix if the simplifying assumption of system property stationarity is made. The assumption is that system property correlation is a function only of the distance between points at which the property is specified, and not of the locations of these points. Spatial correlation is thus designated as $\rho(h)$ where $h$ is the distance between any two points for which system property correlation must be calculated. If the variance of the system property in question is similarly uniform, then a covariance function $C(h)$ becomes immediately available. If required, such a function can readily accommodate system property anisotropy whereby spatial correlation can decay at different rates in different orthogonal directions.

As has already been mentioned, a covariance matrix must be positive-definite. The reason for this is clear from an inspection of the exponent of equation (3.6.1). The negative of this exponent cannot become positive, for probabilities must fade as the values of random variables become very large; they cannot grow exponentially. The filling of any covariance matrix must be such as to achieve this fundamental design specification.

Certain functions which relate covariance to distance are guaranteed to achieve positive-definiteness of a spatial covariance matrix. One of these is the exponential decay function through which spatial covariance is expressed as

$$C(h) = C(0)e^{-h/a} \tag{3.11.1}$$

In equation (3.11.1) $C(0)$ is the variance of the system property under consideration. This value occupies the diagonal terms of the covariance matrix which pertains to this property; as such, it specifies the "innate variability" of this property as assessed by expert knowledge. $a$ of equation (3.11.1) determines the rate of decay of spatial correlation with distance; the larger is $a$ the smaller is the rate of this decay.

Spatial covariance matrices are often derived from variograms. The variogram as a means of specifying spatial correlation has its roots in the geostatistical literature. Let us designate the value of a system property at location $\mathbf{r}$ as $k(\mathbf{r})$. Suppose that this property has been measured at two points which are a distance $h$ apart. The value of the variogram for this separation, i.e. $\gamma(h)$, is defined to be half the expected value of the squared difference between property values. That is

$$\gamma(h) = \tfrac{1}{2}E[(k(\mathbf{r}) - k(\mathbf{r}+\mathbf{h}))^2] \tag{3.11.2}$$

where the vector $\mathbf{h}$ is of length $h$. System property anisotropy is taken into account by specifying different dependencies of $\gamma$ on $h$ in different orthogonal directions.

It is easily shown that

$$C(h) = C(0) - \gamma(h) \tag{3.11.3}$$

and that

$$\gamma(\infty) = C(0) \tag{3.11.4}$$

Figure 3.6 depicts a variogram and corresponding spatial covariance function. It also depicts commonly-employed descriptors of variogram characteristics, namely the variogram sill and the variogram range. The sill is the variogram value at large $h$ which, from (3.11.4), is equal

to the variance of the system property. The variogram range is the distance over which spatial correlation of the system property prevails.

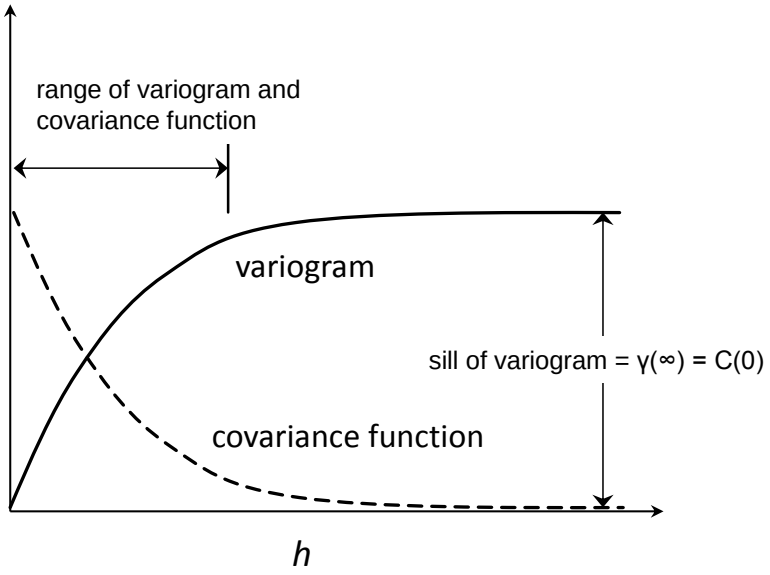


**Figure 3.6. Relationship between a variogram and a spatial covariance function.**

As already stated, mathematical functions that are used to characterize variograms must ensure positive-definiteness of associated covariance matrices. Four commonly-used variogram functions which achieve this purpose are provided below.

*Spherical*

$$\gamma(h)=c\cdot\left[1.5\frac{h}{a}-0.5\left(\frac{h}{a}\right)^3\right] \qquad \text{if } h < a \qquad (3.11.5)$$

$$\gamma(h)=c \qquad \text{if } h \geq a \qquad (3.11.6)$$

*Exponential*

$$\gamma(h)=c\cdot\left[1-\exp\left(-\frac{h}{a}\right)\right] \qquad (3.11.7)$$

*Gaussian*

$$\gamma(h)=c\cdot\left[1-\exp\left(-\frac{h^2}{a^2}\right)\right] \qquad (3.11.8)$$

*Power*

$$\gamma(h)=c\cdot h^a \qquad (3.11.9)$$

## 3.12 Modern Geostatistical Methods

It is well beyond the scope of the present text to provide anything more than brief mention of some features of modern geostatistical methods that are salient to parameter estimation and uncertainty analysis.

Modern geostatistics routinely employs more sophisticated descriptors of lithological and system property variability than the variogram. As implied in the name, spatial correlation expresses the fact that if one acquires knowledge of a system property at one location then some knowledge of that property has thereby been gained at a nearby location; the amount of translated knowledge decreases with increasing separation of the two locations. However such simple, so-called "two-point", statistical descriptors of system property variability do not reflect the true nature of most geological environments, for these environments are the outcomes of complex depositional and structural events that can juxtapose materials of quite different properties. Furthermore, the boundaries that separate one material from another can be complex, elongate and tortuous in shape. A particular concern with two-point statistics is that they fail to express the fact that permeable features within the subsurface tend to be more continuous than impermeable features. This follows from the nature of the processes that produced these features. Features that are outcomes of geological processes are often better simulated using context-dependent geobodies, and/or specialized statistical techniques that attempt to emulate the processes that formed them. Another emerging field in the world of geostatistics is that of "multiple point geostatistics". This technique attempts to capture the salient features of a scanned two- or three-dimensional image as a means of providing multiple realizations of realistic features that are represented in that image.

Modern geostatistical methods recognize the fact that subsurface features which exert a high influence on the movement of fluids through the subsurface tend to be categorical in nature. Consider, for example, a fault, a layer of sand interbedded with less permeable clay layers, or a buried stream channel within more impermeable flood plain deposits. All of these features can exert an important influence on subsurface flow. Each of these features is "either there, or it isn't"; one cannot have half a fault or half a channel. However mathematical adjustment of these features in a complex geological domain in order to promulgate a better fit between model outputs and measurements that comprise a calibration dataset is a difficult procedure, as other features would have to be displaced as well.

Geostatistical software which can generate realizations of complex, flow-determining geological features is freely available. However, as stated, manipulation of features which appear in these realizations in a calibration setting is difficult, if not impossible. Unfortunately, highly parameterized inversion requires that model outputs be continuous with respect to adjustable parameters. A benefit of highly parameterized inversion is that it brings with it the ability to estimate values for large numbers of parameters and, more importantly, to explore the repercussions of the fact that these parameters often cannot be endowed with unique values. In contrast, however, while modern geostatistical methods can generate picturesque representations of the subsurface, and can endow the objects that appear in these pictures with realistically heterogeneous hydraulic properties, the locations and shapes of features which may exert a critical influence on subsurface flow are not continuously adjustable. Hence while categorical geostatistical fields can be used for uncertainty analysis in contexts that do not require the imposition of calibration constraints, they can be used only with difficulty in contexts that do. Future research may overcome these difficulties. Methodologies such as the ensemble Kalman filter, and other developments that are discussed by Mariethoz and Caers (2015), show some potential in this regard. These are not

discussed in this text.

In some modelling contexts it may be possible to overcome the impasse between realistic-but-categorical and abstract-but-continuous parameter fields by improving methodologies for using the latter as surrogates for the former. Improvements may be realized in a number of ways. These may include more flexible methods of interpolation from pilot points to model grids (see Doherty, 2015) together with greater sophistication of Tikhonov regularization. The latter will almost certainly require the use of higher order statistics than the two-point descriptors that are presently employed almost ubiquitously (in the groundwater modelling context at least). This may result in estimated parameter fields that, while being continuous, better represent features of categorical parameter fields that are salient to subsurface flow. This is a field of active research; see, for example, Sarma et al (2008).

In the meantime, limitations of continuous parameter fields that are often assigned to groundwater and subsurface reservoir models must be recognized. Simplified descriptors of geological variability based on two-point statistics may need to over-state geological heterogeneity as partial compensation for their lack of ability to provide superior descriptions of complex geological reality. Of course, all of this must be seen in context. Even the most sophisticated and picturesque geostatistical realization is likely to be a grossly inadequate descriptor of real subsurface variability.

# 4. Situation Statement

## 4.1 Model Parameters

Let the vector **k** denote parameters used by a model. In general, these tend to be properties of the system that the model purports to simulate, for example the permeabilities of porous media, the roughness coefficients of streams, or the coefficients in semi-empirical equations from which water quality is calculated from agricultural practices. However they may also be the values of stresses to which a system is subject, for example recharge or stream inflow.

Conceptually the number of elements comprising the vector **k** will be very large in most instances of real world environmental modelling, especially where the domain of the model is two or three-dimensional. This is because real world environmental processes are infinitely complex, and the properties which govern these processes show considerable spatial heterogeneity. Sometimes spatial heterogeneity is of secondary importance to predictions of management interest, as these predictions are sensitive only to broad scale system behaviour and properties. In other cases a critical model prediction may be sensitive to fine scale spatial heterogeneity. Local spatial property details may not be inferable from direct measurement of these properties because not enough of these measurements may have been made. Nor may they be inferable through model calibration because of inadequacies in the information content of the calibration dataset.

The situation becomes more complex when it is considered that numerical models are grossly imperfect simulators of environmental system behaviour. A model's representation of real world processes and properties may be grossly abstract in nature. Even where a model is loudly proclaimed to be "physically-based", environmental processes and properties can be represented at no finer scale than that of the model's grid or mesh. Hence, as will be discussed in greater detail in later chapters, its parameters may need to adopt roles that compensate for its inadequacies if outputs computed by the model are to replicate real world measurements of the state of the system which the model purports to simulate. For the moment, however, we will assume for convenience that models have no defects; this makes the analysis that follows more simple.

In general, the environmental expert knows the exact values of few if any of the numbers which comprise the elements of **k** at a particular study site. However in most cases, the ignorance of the expert has limits. He/she would complain if confronted with a model whose parameters are wrong or inappropriate. This constitutes knowledge. Direct measurements of system properties may have been made at one or a number of locations within a model domain. This too constitutes knowledge. However these measurements may have been accompanied by error. Furthermore they may pertain to only a point or vertical line (for example a drill hole) in a much more voluminous two- or three-dimensional study area. As such they may only be indicative of the sampled system property at the scale of the model cell or element which houses the measurement point, and may be even less indicative of system properties in neighbouring cells or elements.

Knowledge of the parameter set **k** that is employed by a model is thus probabilistic in nature, reflecting the fact that the exact values of its elements cannot be known, but that limits can be placed on these values. It may be possible to supplement this knowledge with more qualitative, though no less important, descriptions of system property variability. For example

an expert may know scales of spatial correlation that system properties display. In the geological context, he/she may know something of the nature and disposition of structural and/or sedimentary features that are likely to give rise to anomalous system properties.

Conceptually, expert knowledge of **k** can be expressed as a probability density function; we will refer to this probability density function as $f(\mathbf{k})$. Unfortunately, this is unlikely to be a neat and tidy analytical density function such as a multinormal density function. Instead it may be possible to express $f(\mathbf{k})$ only through sampling it. Samples may be obtained, for example, by running a complex geostatistical simulator that generates realizations of geological facies and structural features. These features can then be populated with spatially variable realizations of system properties.

In Bayesian terminology $f(\mathbf{k})$ is the "prior probability density function" of the parameters **k**. As such, it encapsulates expert knowledge as it pertains to a particular study site. Conceptually at least, a covariance matrix can be associated with $f(\mathbf{k})$; let us designate this covariance matrix as $\mathrm{C}(\mathbf{k})$.

## 4.2 History-matching

Suppose that we have at our disposal a set of measurements of historical states of the system which is the subject of our model-based investigations. For a surface water system these may be stream flows. For a groundwater system they may be water levels in wells; these may be "natural", or they may be affected by man-made stresses such as pumping. For an oil reservoir our dataset of historical measurements may be comprised of production rates and water cuts. Being a collection of numbers, these measurements comprise a vector. We will name this vector **h**.

Measurements of system state are accompanied by error – often referred to as "noise". By way of example, samples of river flow during floods may be very noisy because of the high potential for error that accompanies the taking of such measurements. In contrast, other types of measurement can be made with a high level of instrumental accuracy; nevertheless their noise content may still be high because of their questionable representativeness of the system state that they are meant to portray. For example, a borehole measurement on a particular day may not be truly representative of "steady state" or "equilibrium" groundwater conditions. Nor may it be truly representative of the average head within a thick stratigraphic layer that is represented as a single layer in a groundwater model. (The subject of so-called "structural noise" will receive considerable attention in later chapters. For now, discrepancies between measurements of system state and the capacity of a model to represent those states will be classified as a component of overall "measurement error".

Any number which is the outcome of a measurement of system state must therefore be regarded as being "contaminated" to some extent. Therefore it cannot be considered to be a true representation of the state of the system at the time at which the measurement was made. Instead, it is the state of the system plus an unknown error. For measurement $i$ we will designate this as error as $\varepsilon_i$. Collectively all measurement errors comprise the vector $\boldsymbol{\varepsilon}$; the $i$'th component of $\boldsymbol{\varepsilon}$ is the noise associated with the $i$'th component of **h**.

Like **k**, $\boldsymbol{\varepsilon}$ is a stochastic quantity. Therefore, conceptually, it can be ascribed a probability distribution $f(\boldsymbol{\varepsilon})$. This probability distribution can, in turn, be ascribed a covariance matrix $\mathrm{C}(\boldsymbol{\varepsilon})$. The probability distribution associated with measurement noise is often considered to be relatively uncomplicated, unlike that associated with model parameters. In fact, the noise

associated with any one measurement is often considered to be statistically independent of that associated with any other measurement. C(**ε**) thus becomes a diagonal matrix; each diagonal element of this matrix is the variance (square of the standard deviation) of measurement noise associated with the corresponding individual measurement. Furthermore the expected value of **ε** is normally assumed to be **0**. Measurements are thus assumed to be made without bias.

In common history-matching practice, a multiplier is associated with C(**ε**). This is often called the "reference variance" and is designated as $\sigma^2_r$. This recognizes the fact that the level of model-to-measurement fit that can be achieved through the history-matching process may not be known in advance. Hence while a modeller may feel comfortable in specifying the statistics of multi-measurement error in a relative sense through use of an appropriate C(**ε**) matrix, the actual values of the elements of C(**ε**) are determined as part of the history-matching process itself while inter-element relativity is preserved. (This raises the spectre, of course, that it may not be actual measurement noise that is responsible for model-to-measurement misfit. Where higher levels of misfit are encountered than was anticipated on the basis of noise that was thought to be associated with the history-matching dataset, this suggests that model-to-measurement fit may be caused by structural defects of the model. If this is the case, then the pre-specified C(**ε**) may not be correct. This topic will be ignored for the moment, but will receive detailed treatment later in this text.)

Because **h** includes measurement noise, it is a stochastic quantity itself. It can thus be endowed with a probability distribution which we designate as *f*(**h**). Its covariance matrix is the same as that of measurement noise. However, because *E*[***ε***] (i.e. the expected value of measurement noise) is **0**, then *E*[**h**] is **q** where the vector **q** specifies the actual values of system state.

If the model is run using a particular set of parameters **k**, then it produces a set of outputs **o** which are associated with these parameters. The model can be considered to be an operator on these parameters. This operator will be designated as ***Z***[.]. The "***Z***" symbol is italicized to represent the fact that, in general, a model is nonlinear. It is capitalized because it operates on many parameters, these comprising the vector **k**, and because it yields many outputs, these comprising the vector **o**. With this notation, the action of the model over the time span for which historical measurements of system state are available can be written as

$$\mathbf{o} = \boldsymbol{Z}[\mathbf{k}] \qquad (4.2.1)$$

Suppose that we know the correct system properties, and that we run the model using these. (Actually we will also assume that other model inputs such as "known" system stresses and "known" boundary conditions that are not classified as parameters, and hence are not represented in **k**, are also correct). The outputs **o** calculated by the model under these circumstances would not reproduce our measurements **h**, because, as stated above, the latter are contaminated by measurement noise. Hence

$$\mathbf{h} = \boldsymbol{Z}[\mathbf{k}] + \boldsymbol{\varepsilon} \qquad (4.2.2)$$

Equation (4.2.2) states that measurements comprising the history-matching dataset **h** are scattered about the true values of system state **o** that would be calculated by the model using the true set of parameters **k**. This scatter is described by the probability density function *f*(**ε**).

In real world modelling contexts we do not know the true **k**. However, presumably, samples of **k** can be drawn from its prior probability density function *f*(**k**). Suppose that we do this.

For each realization of **k** that we draw, a corresponding set of "phantom measurements" **h** can then be obtained by first calculating **o** using (4.2.1), then sampling $f(\boldsymbol{\varepsilon})$ to obtain a realization of **ε**, and then adding the two together. From this it is apparent that $f(\boldsymbol{\varepsilon})$ can be considered to specify $f(\mathbf{h}|\mathbf{k})$, i.e. the probability density function of **h** given **k**, or the conditional probability of **h**. This can be written formally as

$$f(\boldsymbol{\varepsilon}) = f(\mathbf{h}|\mathbf{k}) \tag{4.2.3}$$

Meanwhile, as just described, the marginal probability density function of **h**, i.e. $f(\mathbf{h})$, can be sampled by repeating the following procedure.

1. Sample **k** (i.e. generate a realization of **k**);
2. Run the model to obtain a corresponding realization of **o**;
3. Sample **ε**;
4. Add it to **o**.

If this were done many times, the marginal probability distribution of **h** could be determined empirically. However empirical estimation of $f(\mathbf{h})$ requires a great many model runs, especially if **k** has many elements. Alternatively, if the density function $f(\mathbf{k})$ can be characterized using a mathematical expression (as can the multinormal distribution), and if the model operator $\boldsymbol{Z}[.]$ can be similarly characterized (for example if $\boldsymbol{Z}[.]$ is linear and can be specified as a matrix), specification of $f(\mathbf{h})$ may become easier; under these circumstances it may be possible to obtain a mathematical expression for $f(\mathbf{h})$. In real world modelling practice, however, models are complex and nonlinear, and no such expressions for $f(\mathbf{h})$ are obtainable. Fortunately, specification of $f(\mathbf{h})$ is unnecessary in most history-matching contexts.

In the real world history-matching context, a modeller has the following items at his/her disposal (or makes the assumptions necessary to place these items at his/her disposal):

- a single sample of **h**, this comprising the measurement dataset;
- knowledge of $C(\boldsymbol{\varepsilon})$ (but not necessarily of the reference variance $\sigma^2_r$);
- knowledge of $f(\mathbf{k})$ (or at least the means to generate samples of **k**).

**h** and **k** are not independent random variables. They are linked by the action of the model. Knowledge of **h** thus has a conditioning effect on $f(\mathbf{k})$. Theoretically (see the previous chapter) it should thus be possible to determine a conditional probability density function for **k**, i.e. $f(\mathbf{k}|\mathbf{h})$, based on knowledge of **h**. Alternatively, it should be possible to at least draw samples from this conditional distribution so that it can be characterized empirically.

From (3.7.5)

$$f(\mathbf{k}\,|\,\mathbf{h}) = \frac{f(\mathbf{h}\,|\,\mathbf{k})\,f(\mathbf{k})}{f(\mathbf{h})} \tag{4.2.4}$$

This is Bayes equation as it pertains to the history-matching context. As stated above $f(\mathbf{k})$, the encapsulation of expert knowledge, is referred to as the prior probability density function of **k**; meanwhile $f(\mathbf{k}|\,\mathbf{h})$ is referred to as the posterior probability density function of **k**. $f(\mathbf{h}|\mathbf{k})$ is often referred to as the likelihood function; the better is the fit between model outputs **o** and field measurements **h**, the higher is the value of the likelihood function. The reduction in uncertainty of **k** achieved through the conditioning process that is history-matching is a measure of the information content of the history-matching dataset **h**. It is important to note that **h** is likely to be more informative of some parameters (and combinations of parameters)

than others. Hence when the history-matched model is used to make predictions of management interest, the uncertainties of some of its predictions are likely to be reduced from those that prevailed prior to conditioning, while those of others may not be reduced much at all by the conditioning process. Moore and Doherty (2006) show an example of a "perfectly calibrated model" for which the uncertainty of one particular model output of potential management interest is hardly reduced at all through the history-matching process, in spite of the conditioning exerted on some combinations of parameter by a noiseless history-matching dataset.

The denominator of (4.2.4) is the marginal probability density function of **h**. If this is written as a conditional (on **k**) density function, and if **k** is then integrated out, (4.2.4) can be re-written as

$$f(\mathbf{k}|\mathbf{h}) = \frac{f(\mathbf{h}|\mathbf{k})f(\mathbf{k})}{\int_{-\infty}^{\infty} f(\mathbf{h}|\mathbf{k})f(\mathbf{k})\mathrm{d}\mathbf{k}} \qquad (4.2.5)$$

By integrating both sides of (4.2.5) with respect to **k**, it is seen that the integral of the posterior density function of **k** over all of **k**-space is unity, as must be the case for any density function.

Let *s*, a scalar, be a prediction of management interest made by a model. Let the model operator under these predictive conditions be designated as ***y***[.]. The bold status of "***y***" indicates that, like ***Z*****[**.], it operates on the vector of model parameters **k**; its italicized status followed by square brackets indicates that it is a nonlinear operator and not a matrix. Use of lower case to symbolize ***y*** indicates that it yields a single number, this being the prediction *s*. Thus

$$s = \boldsymbol{y}[\mathbf{k}] \qquad (4.2.6)$$

Figure 4.1 conceptualizes the prior probability density function of this prediction, which we denote as $f(s)$. This density function could be sampled by first sampling **k** based on its prior probability density function $f(\mathbf{k})$, and then running the model for each sample to obtain a corresponding sample of *s*. A histogram of *s* could then be constructed and its probability density function determined empirically. Also depicted in figure 4.1 is a schematic of the posterior probability density function of this prediction, which we denote as $f(s|\mathbf{h})$. Conceptually, this probability density function could also be constructed empirically by running the model using samples of the posterior density function of **k**, i.e. $f(\mathbf{k}|\mathbf{h})$. The extent to which the posterior predictive uncertainty of *s* is smaller than its prior predictive uncertainty is dependent on the information content of the data, the model parameters to which this information is pertinent, and the parameters to which *s* is most sensitive.

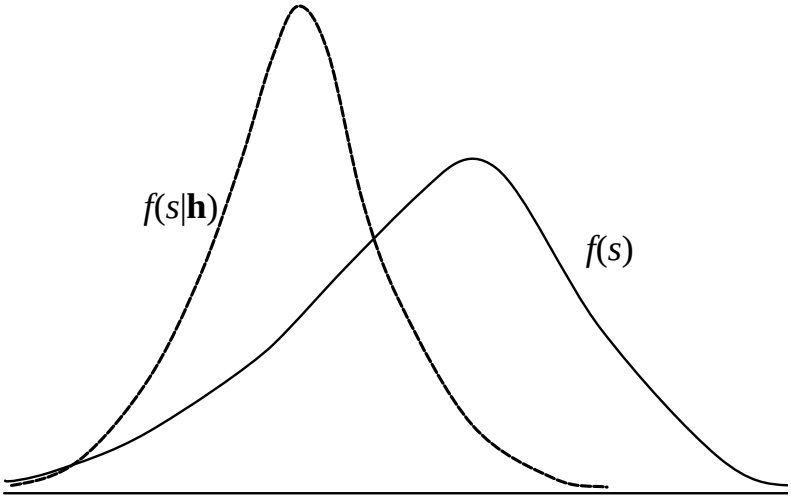


**Figure 4.1. Prior and posterior predictive probability density functions. The integral under both of these is 1.0.**

## 4.3 Sampling the Posterior

### 4.3.1 Rejection Sampling

The concepts expressed by Bayes equation are simple enough. Rudimentary implementation of Bayes equation is also simple enough. Conceptually the prior parameter probability density function could be sampled using an appropriate random process. Where the prior density function is explicit (for example if the potential for variability of parameters **k** can be described by a multinormal probability distribution), the random number generation process by which samples of **k** are obtained is simple enough. However where $f(\mathbf{k})$ is implicit rather than explicit and requires, for example, generation of complex geostatistical parameter fields, then the process of sampling the prior distribution of **k** may be considerably more complex. In either case, prior parameter samples (these are often called prior parameter "fields" where they pertain to a two- or three-dimensional model domain) should be conditioned by direct measurements of these parameters where these are available. A model run is then undertaken based on each such parameter field. The likelihood function is then calculated based on the difference between model outputs and corresponding field data using the probability density function $f(\boldsymbol{\varepsilon})$ of measurement noise. Suppose that the probability forthcoming from this calculation is $p$. This will be a number between 0 and 1. A random number is then generated using a probability density function which is uniform between 0 and 1. If this number is greater than $p$ the sample is rejected. If it is less than $p$ the sample is retained. (Note that, theoretically, the uniform random number should be compared to the computed value of the posterior density function divided by its maximum value; the information required to compute this maximum value is generally unavailable so a value of 1 is used as a safe surrogate.)

This procedure is referred to as "rejection sampling". From the above description it is apparent that it imposes two levels of "filtering" on parameters **k** used by the model. The first is imposed by the prior parameter distribution. In theory, realistic values of **k** are unlikely to be generated if the true $f(\mathbf{k})$ is being sampled. The second filter is comprised of the likelihood function. Parameter fields **k** which give rise to unlikely fits are rejected through this function.

Rejection sampling has the advantage that it is conceptually simple. Furthermore, the

methodology through which it is implemented illustrates some important features of the history-matching process, namely that

a) history-matching can be viewed as a kind of probability density function filtering operation, and that
b) the outcome of this filtering operation is another probability density function.

The last point is important. History-matching does not promise parameter or predictive certainty. This challenges the use of terms such as "calibration" which (quite wrongly) imply a sense of parameter finality and accuracy. This matter will be further discussed below.

Unfortunately, while conceptually simple, rejection sampling is impossible to implement in most practical settings. Even where parameter numbers are very low it is a vastly inefficient procedure, especially where a modeller is entitled to seek a good fit between model outcomes and field data. The "hit to miss ratio" (i.e. the ratio of acceptances to rejections) is too low to be useable, so that many model runs are squandered. Where model run times are high, this is unacceptable.

### 4.3.2 Markov Chain Monte Carlo

Markov chain Monte Carlo (MCMC) and related methods are gaining popularity in environmental model history-matching. Instead of generating parameter samples based on the prior parameter probability density function, a series of parameter samples forming a Markov chain is taken. At any point in parameter space along the chain the next sample is generated using a so-called proposal density function which governs transition from one sample to the next. The model is then run using the new parameter sample; model outputs corresponding to this new sample then become available. Using $f(\boldsymbol{\varepsilon})$, the product $f(\mathbf{h}|\mathbf{k})f(\mathbf{k})$ is then evaluated and its ratio taken with the same product calculated using the previous parameter sample. If this ratio is greater than unity, the new sample of **k** is accepted as the next member of the Markov chain. If it is less than unity the new sample is accepted or rejected after generating a random number from a uniform probability distribution between zero and one. If this random number is less than the ratio of new to old $f(\mathbf{h}|\mathbf{k})f(\mathbf{k})$ the proposed parameter set becomes the next member of the chain. Otherwise the sampled **k** is rejected and another **k** is tested using the proposal density function.

This is the so-called Metropolis-Hastings algorithm. Provided the proposal density function is symmetric, that the Markov chain is irreducible (i.e. all states can be sampled from the current state) and aperiodic (i.e. the number of steps until the chain returns to its current state is not a multiple of an integer greater than 1), it can be shown that samples generated using this methodology are actually samples of $f(\mathbf{k}|\mathbf{h})$, i.e. the posterior probability density function of **k**. See texts such as Gelman et al (2013) for further details.

MCMC constitutes a far more efficient means of sampling the posterior parameter density function than rejection sampling. Furthermore, so-called "structural parameters" such as the reference variance $\sigma^2_r$ can be included in the parameter refinement process; hence the level of noise associated with a measurement dataset **h** can be estimated at the same time as a good fit with that dataset is sought. Nevertheless, despite the fact that powerful, parallel versions of MCMC are available to modellers through packages such as DREAM (see, for example, Laloy and Vrugt, 2012; Vrugt, 2011), model-run efficiency becomes a problem where model run times are long and **k** has many elements (more than about 50 or so); tens of thousands to hundreds of thousands of model runs are then required to ensure adequate sampling of the

posterior parameter probability density function. Furthermore, where parameter numbers are high, the acceptance-to-rejection ratio of the MCMC sampler can become very small, particularly where the parameter null space must be sampled for proper characterization of parameter and predictive uncertainty. This further increases the number of runs required for sampling of the posterior parameter distribution. When it is recalled that the number of parameters employed by geophysical, groundwater and subsurface reservoir models on the one hand, and surface water quality and land use models on the other hand, may number in the thousands, use of MCMC in these contexts is seen to be somewhat problematic.

An obvious way to speed up the MCMC process is to reduce the number of parameters employed by a model. In some situations this may be appropriate. In other situations it may be entirely inappropriate for any of the following reasons.

- Omission of parameters from the MCMC process may artificially reduce the perceived uncertainties of some model predictions of management interest. This will be particularly the case for predictions which are sensitive to parameters which lie in the null space of the model operator ***Z*.** These are the parameters that are typically omitted from MCMC analysis as they have little or no effect on model outcomes that correspond to the history-matching dataset **h**.
- Where parameter simplification is not confined to the null space of ***Z*** it may introduce "structural noise" to model outputs that correspond to **h**, thereby compromising the level of fit that can be attained between these outputs and field measurements of system state. The history-matching process is then further complicated by the fact that the statistics of structural noise are unknown and that its covariance matrix is probably singular; see Doherty and Welter (2010) and chapter 9 of the present text for further details. The likelihood function then becomes more difficult to define and calculate. Its choice may then entail a high degree of subjectivity; see, for example, Beven (2005) and Beven et al (2008).
- Unless parameter simplification is "optimal" (a topic that will be addressed in chapter 9) some parameters will adopt compensatory roles as they are adjusted to ensure goodness of model-to-measurement fit during the history-matching process. Under these circumstances the history-matching process (whether it is undertaken using MCMC or by any other means) can introduce substantial bias to some parameters, and to some predictions. Both linear (White et al, 2014; Watson et al, 2013) and nonlinear analysis (Doherty and Christensen, 2011) demonstrate that the potential for simplification-induced bias in some predictions can be very large indeed. This too, is discussed in chapter 9.

A growing body of literature is exploring the possibility of using surrogate, fast-running, models in MCMC analysis in place of complex, slow-running, but more physically/chemically "realistic" models of environmental processes. Included in these surrogate models are stochastic surrogate-to-real-model correction terms which encapsulate their inadequacies as real-model substitutes. See for example Cui and O'Sullivan (2011). While this strategy has met with some success, to the author's knowledge, parameter numbers involved in surrogate model construction and consequential MCMC analysis remain small.

Another practical difficulty in many modelling environments is that of constructing an appropriate proposal density function. In the groundwater and reservoir modelling contexts, complex geostatistical simulators are often used to express expert geological knowledge.

These simulators can generate "picture perfect" realizations of hydraulically important features such as fracture networks, meandering river channels and lithological layering. All of these features are "categorical" in nature. That is to say, they cannot be varied continuously to generate other realizations (or only with great numerical difficulty, with the level of difficulty rising with the degree of realism with which subsurface features are portrayed). System property contrasts are normally sharp at feature boundaries. Computation times required for generation of such three-dimensional subsurface realisations are often long; run times of models that use these realizations are often much longer. If used in the MCMC context, determination of a suitable proposal density function that allows progression from one categorical realization to another along a Markov chain that can be guaranteed to generate samples that are far enough apart in parameter space to fully define the posterior parameter probability distribution becomes a considerable problem. However progress is being made in this endeavour; see, for example, Mariethoz and Caers (2015).

### 4.3.3 Highly Parameterized Bayesian Methods

Regardless of whether inverse methods (including methods for analysis of posterior uncertainty) have Bayesian roots, subspace roots, or a combination of the two (as do methods documented later in this text), the handling of large numbers of parameters ultimately requires temporary model linearization; this is accomplished by calculating sensitivities of model outputs with respect to these parameters. This provides access to mathematically tractable ways of adjusting these parameters under history-matching constraints. Model nonlinearity is then accommodated by repeating the linearization process as successively better estimates of posterior parameter means are obtained. Where parameter numbers are very large, adjoint methods can be used for calculation of sensitivities; see, for example, Sykes et al (1985). However the programming of an adjoint solver for any particular model may not be a straightforward task.

Fienen et al (2013) developed bgaPEST, which incorporates a Bayesian statistical approach to posterior predictive uncertainty analysis for use in the groundwater modelling context. The algorithms employed by bgaPEST are based on those developed and described by Kitanidis and Vomvoris (1983), Hoeksema and Kitanidis (1984), Kitanidis (1995), Nowak and Cirpka (2004), and others. The notion of conditioning lies at the heart of these methods. A joint probability distribution encompassing both observations **h** and parameters **k** is established. After linearization, equations not unlike (3.8.4) and (3.8.5) are employed to estimate posterior parameter means and covariances. The reference variance $\sigma^2_r$ and/or a similar multiplier on the prior parameter density function can be estimated through the inversion process. A modeller can trade goodness of fit between model outputs and field measurements against heterogeneity introduced to parameter fields to accommodate that fit to achieve what he/she believes to be an optimal compromise between fit and heterogeneity.

This and similar methods (see, for example, Woodbury and Ulrych, 2000) have an advantage over MCMC methods in that they can perform well in parameter spaces of very high dimensions. However they are unable to handle categorical parameter fields which, as stated above, comprise the most realistic expressions of geological expert knowledge. This is because differentiability of model outputs with respect to categorical features is difficult or impossible to attain. The problem is exacerbated by the implicit rather than explicit definition of model parameters that these fields embody. Nevertheless, methodologies such as that encapsulated by bgaPEST are "geostatistical enough" to operate in contexts where

characterization of spatial parameter variability can be based on variograms or some other form of so-called "two-point" statistics. Furthermore their use of continuous parameter fields makes them responsive to "geostatistical surprises" that may emerge from the history-matching process.

This raises an issue that is pertinent to use of all Bayesian methods, namely the faith that a modeller must place in his/her explicit or implicit expression of prior expert knowledge of parameter dispositions and ranges. Calibration of groundwater, subsurface reservoir, surface water quality/quantity and other models often reveals the existence of unforeseen patterns of spatial parameter heterogeneity, and/or unforeseen values that parameters may need to take in order to promulgate good model-to-measurement fit. It is important that the inversion process be capable of revealing such patterns and values, and that their expression not be suppressed because of excessive dedication to a prior parameter probability distribution to the exclusion of all other possible expressions of natural system complexity. As is discussed later in this text, the use of highly parameterized inversion together with Tikhonov regularization does indeed allow expression of unanticipated parameter values and heterogeneity. In contrast, where geostatistically-based categorical parameter fields provide the sole expression of expert knowledge, and where the history-matching process is undertaken in such a way that the posterior parameter distribution must be comprised of such fields, that process is rendered incapable of modifying the expert knowledge of the modeller. Where continuous parameter fields and accompanying expert knowledge are used in their stead, the loss of "picture perfect" realizations of subsurface properties is partially compensated for by the superior ability of continuous parameter fields to internalize unanticipated information contained within the history-matching dataset, even if that information is not necessarily expressed in geostatistically realistic ways in the parameter fields that emerge from the inversion process. This, amongst many other things, is something that must be considered when weighing the use of continuous parameter fields against categorical parameter fields, and indeed Bayesian methods against non-Bayesian methods. Any choice will be accompanied by gains and losses. What is lost through failing to take one alternative may be more than compensated for by taking another.

### 4.3.4 Other Bayesian Methods

The Kalman filter is another Bayesian method that conditions the joint probability distribution of parameters and field observations by values of the latter. It undertakes a series of so-called assimilation steps whereby observed data is progressively integrated into dynamic models to improve estimates of poorly known parameters at the same time as it updates a model's representation of system states. A growing body of literature has demonstrated successful use of this method in conjunction with complex models in a growing suite of environmental modelling contexts. Though its theoretical roots are in linear models and multinormal density functions, algorithms are being progressively enhanced to better accommodate severe departures from both of these assumptions. These include ensemble methods that progressively update parameter and system state fields that collectively represent the uncertainties in both of these. See Aanonsen et al (2009), Emerick and Reynolds (2013), Oliver and Chen (2010) and references cited therein for more details.

## 4.4 Model Calibration

### 4.4.1 What is Calibration?

Bayes equation states that parameter and predictive uncertainty prevail both before and after history-matching, and that the history-matching process may (or may not) reduce the uncertainties of management-critical predictions below their pre-calibration levels.

So what exactly is "model calibration"? Why does the notion of the "calibrated model" carry such an aura of finality – as though the model construction process can be considered to be complete once a model has been calibrated? And why does the environmental industry seem so pre-disposed to place such great faith in predictions made by a model when the model's principle claim to credibility is the fact that it has been calibrated? Sadly these questions can only be answered through recourse to folklore and wishful thinking; mathematics provides little assistance.

The terms "calibration" and "calibrated model" will be used extensively throughout this text; however these terms will be given a specific meaning. It is important to note that this meaning does not imply certainty of parameters, nor of predictions made by a calibrated model. Nor is it meant to diminish the fundamental truth embodied in Bayes equation that history-matching may reduce the uncertainties of some parameters but not others, and may reduce the uncertainties of some model predictions while leaving the uncertainties of other model predictions relatively untouched by the history-matching process.

From a Bayesian perspective, the term "model calibration" has no meaning. Nor can any conclusions regarding the predictive integrity of a model be drawn from the fact that it has been calibrated. If a model has been declared to be "well calibrated", the only conclusion that can be drawn is that the model has been provided with a set of parameters for which model outputs match corresponding measurements of system state reasonably well. However this tells us nothing about whether a very different set of parameters that are equally valid when judged at the bar of expert knowledge also allow the model to match measurements of system state reasonably well.

In everyday usage the term "calibration" carries the implication that defects have been corrected. When applied to modelling this may require that the calibration process force parameters to adopt values which compensate for model simplifications and imperfections. As will be shown in chapter 9, the matter of whether model defects can indeed be "calibrated out" is a complex one that may work for some predictions at the same time as it degrades the capacity of a calibrated model to make other predictions.

The notion of "calibration" implies uniqueness. However Bayes equation informs us that we cannot expect uniqueness, and that parameters and predictions are stochastic quantities. Does it therefore follow that all model-based parameter inference and predictive uncertainty analysis should follow strictly Bayesian principles?

Unfortunately the matter is not that simple. As was discussed above, in the environmental modelling context purely Bayesian analysis is always compromised to at least some extent. Generation of stochastic expressions of expert knowledge, especially as these pertain to subsurface geological details or to the surficial complexities of land use practices and processes, is a difficult undertaking. So too is formulation of a likelihood function that accommodates model imperfections. Added to these conceptual difficulties are the practical

numerical difficulties of enforcing history-matching constraints on model parameters where the latter may need to number in the hundreds, or even thousands, if they are to provide an adequate representation of system heterogeneity. Methods such as Markov chain Monte Carlo, which are completely general and theoretically "pure" in the Bayesian sense, become inadequate where parameter fields are spatially complex, parameter numbers are large and model run times are long.

The need to accommodate large numbers of parameters presents no obstacles, however, to numerical methods which are charged with the task of finding a single set of parameters which fit a historical measurement dataset well. In obtaining this fit, mathematical uniqueness may be achieved by imposing constraints of minimum parameter field curvature, maximum parameter field smoothness, minimum parameter perturbation from a preferred set of expert-knowledge-based values, or some other constraint that is deemed to be appropriate in a particular inverse modelling context. Numerical methods that operate in this manner invariably require problem linearization. However by engaging in an iterative solution process, they do not actually require that the model be linear – only that it be numerically well-behaved.

It thus becomes a matter of numerical expediency that imposition of history-matching constraints on parameters whose numbers are large enough to express the heterogeneity of natural systems requires a processing step in which mathematical uniqueness is sought as an indispensable component of the history-matching process. This is acceptable if two important issues are resolved. The first issue relates to the constraints that are imposed on parameters to achieve uniqueness. Thus the issue of which type of uniqueness is most appropriate to seek in the highly parameterized history-matching process must be addressed. The second issue is that of finding other sets of parameters which also fit the historical dataset well once the first set has been found, while ensuring that these complementary sets collectively span the range of parameter fields that expert knowledge of system properties allows. By making model predictions of management interest with all of these parameter sets, the uncertainties in these predictions can thereby be explored. While this process may not be implemented using an algorithm that is "strictly Bayesian" in the sense that it can be shown theoretically to sample the posterior parameter probability distribution, this is a secondary consideration if it achieves similar outcomes but in a far more efficient manner. The problem of "Bayesian purity" fades further into the background once one acknowledges the approximations and conceptual difficulties that inevitably accompany Bayesian analysis in highly parameterized modelling contexts anyway.

Uniqueness of solution of highly parameterized inverse problems is achieved through so-called "regularization". This is a subject which will receive much attention in this text. Indeed this is a topic that has received a considerable amount of attention in the mathematical literature as it relates to the solution of so-called ill-posed inverse problems. The purpose of regularization is to attain uniqueness where none in fact exists. The nature of the solution to the inverse problem is then highly dependent on the nature of the regularization that is employed in its solution.

Regularization therefore provides the means through which an ill-posed inverse problem can be solved. The benefit of regularization is the attainment of parameter uniqueness. This is also its cost. Of necessity, a unique solution to an inverse problem will almost certainly be in error. Model predictions that are made using parameter fields that are in error may themselves be in error. The best regularization method to use is obviously that which

minimizes the potential for parameter and predictive error. Exploration of the potential for post-calibration parameter and predictive error, if it can be done efficiently, then achieves a similar outcome to quantification of posterior parameter and predictive uncertainty. However exploration of post-calibration parameter and predictive error may be a far easier numerical task to undertake than exploration of posterior parameter and predictive uncertainty. It is for this reason that methodologies described in the present text adopt this strategy.

The situation is schematized in figure 4.2. This is virtually a repeat of figure 4.1. However a prediction $\underline{s}$ made by a calibrated model has been added to the figure. Ideally, the value of that prediction should lie somewhere near the centre of the uncertainty band of the prediction. In this way, the potential for predictive error is minimized. This potential may not be small; in fact it will be large if the posterior uncertainty of the prediction is large. Nevertheless to the extent that a prediction of interest made by a calibrated model lies somewhere near the centre of the posterior uncertainty distribution of that prediction, the potential for error of that prediction is minimized precisely because of the symmetry of that error which is thereby attained. Of course the situation becomes somewhat more complicated when the posterior predictive probability distribution is skewed (which, among other things, can be an outcome of model nonlinearity). However the principle of minimizing the error variance of a prediction made by a calibrated model by ensuring that the prediction lies somewhere near the centre of its posterior probability distribution remains intact. (The reader may notice that this discussion is focussing on a model prediction rather than on model parameters, in insisting on the necessity to minimize error variance through the calibration process. If a model is a perfect simulator of real world behaviour the two are the same; if a model is defective, the two can be very different. This is discussed in chapter 9.)

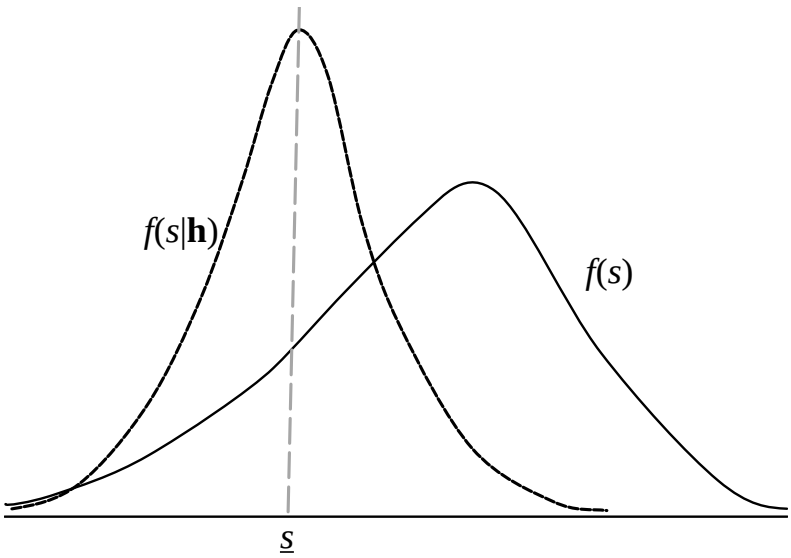


**Figure 4.2. A prediction $\underline{s}$ of minimized error variance made by a calibrated model.**

As used in this text, "model calibration" now takes on a specific meaning. It is not simply the finding of a parameter field that allows the model to fit a historical dataset. It is the attainment of a parameter field that allows the model to achieve an acceptable fit with historical observations of system state, and which also allow it to make one or more predictions of management interest with minimized potential for error (even though this potential may be high because of the innate posterior uncertainty of those predictions). It is

through attainment of this status of minimum predictive error variance that parameter uniqueness is achieved.

If a model is free of imperfections, then achievement of a parameter field of minimum error variance would provide the basis for the making of predictions of minimum error variance, regardless of those predictions. (It is normally the predictions that a model makes, rather than values taken by its parameters, that we care about in the end.). As stated above, however, the link between minimization of parameter error variance and minimization of predictive error variance is broken once model defects are considered. We will put this issue to one side until chapter 9. In the meantime we will pursue inverse problem uniqueness through seeking a parameter field of minimum error variance. For a while at least, it will be assumed that minimization of predictive error variance automatically follows.

Of fundamental importance is the fact that model calibration must be considered as the first step of a two-step process. The second step is that of defining the potential for error in predictions of interest made by a calibrated model subject to two constraints. The first constraint is that the fit between model outputs and the calibration dataset does not deteriorate by any more than a modeller-prescribed amount, this being dictated by the level of measurement noise associated with the calibration dataset and/or by the amount of structural noise that is generated by the model. The second constraint is that in exploring the potential for predictive error, parameters span the range of realistic values which expert knowledge allows them to adopt. Thus can the precepts of Bayes equation be respected.

### 4.4.2 Regularization

As stated above, in its broadest sense, regularization is the word given to the process through which uniqueness of solution to an ill-posed inverse problem is achieved. By definition, an ill-posed inverse problem is one which does not have a unique solution. As was discussed above, and eluded to in our discussion of the resolution matrix (see equation 2.9.9), regularization does not guarantee correctness; it only guarantees uniqueness. The most to which regularized inversion can aspire is calculation of a parameter field which allows a model to make predictions of future system behaviour which possess minimum potential for error. This does not mean that predictive error is eliminated, or even small. As has been discussed, minimization of predictive error variance is attained through trying to ensure that a prediction is roughly at the centre of its posterior probability distribution. Exploration of post-calibration predictive error then becomes roughly (but not exactly) equivalent to exploration of posterior predictive uncertainty. (As will be shown later in this text, post-calibration predictive error is, at best, slightly greater than posterior predictive uncertainty.) At the same time the calibration process should add as little “man-made error” to the post-calibration probability distribution of predictive error as possible.

This text discusses three broad approaches to regularization. These are

- parameter simplification (i.e. manual regularization);
- singular value decomposition;
- Tikhonov regularization.

Parameter simplification is the oldest form or regularization. It can be implemented by fixing some parameters at their prior mean values while estimating the values of other parameters. Alternatively, (or as well) it can be implemented through estimating values for combinations of parameters rather than for individual parameters. Parameter combinations can be formed

by tying parameters together so that they vary as one while maintaining a fixed ratio to each other. Meanwhile, parameters which are fixed rather than estimated should ideally be those to which model outputs used in the calibration process are insensitive. In a spatial model, simplification can be attained by endowing large areas within the model domain with the same set of system properties. The rationale that underpins this regularization strategy is that average or broad scale system properties are estimable through the calibration process while system property details are not; hence system property homogeneity is assumed to prevail within each of a small number of different zones into which the model domain is subdivided for the purpose of attaining inverse problem uniqueness.

The idea of subdividing parameters into one subspace comprised of individual parameters and combinations of parameters that are estimable, and another subspace comprised of individual parameters and combinations of parameters that are not, is formalized through the mathematical device of singular value decomposition. As will be discussed in subsequent chapters, not only can this subdivision of parameter space be achieved with greater efficiency and correctness when undertaken mathematically; the cost of regularization in terms of the potential for parameter and predictive error that it incurs can also be quantified. As is apparent from the above discussion, this provides the wherewithal to deliver estimates of post-calibration parameter and predictive uncertainty.

The third great strand of regularization discussed herein is Tikhonov regularization. Unlike manual regularization and singular value decomposition which seek uniqueness through inverse problem reduction, Tikhonov regularization seeks uniqueness through inverse problem expansion. Given the information content of a calibration dataset, manual regularization and singular value decomposition reduce the number of parameters that are estimated through the calibration process to a number that is commensurate with that information content. Tikhonov regularization does the opposite. It expands the information content of the calibration dataset by supplementing it with other observations. These may be "observations" of the prior mean values of parameters, or "observations" that the preferred spatial relationship of estimated parameters to their neighbours is one of smoothness or homogeneity. These "regularization observations" can be overruled by information that is resident in field measurements which comprise the actual calibration dataset. However the extent to which parameters are allowed to depart from the preferred condition that is encapsulated in these regularization observations in achieving a user-specified level of fit with the measurement dataset is minimized. In this way is inverse problem uniqueness attained.

If model numerical behaviour is good enough, and if model run times are small enough, there can be little doubt that regularization achieved through mathematical means is superior to that achieved through manual means. Some of the reasons for this are as follows.

- Where regularization is undertaken mathematically, complex spatial parameterization schemes involving possibly large numbers of parameters can provide flexibility of response to information contained in the calibration dataset. The modeller does not need to establish in advance whether a particular parameter is estimable or not, as this is irrelevant to its inclusion in the calibration dataset. Meanwhile parameters are free to respond to the information content of the calibration dataset, regardless of where in the spatial model domain this information is directed.
- If properly formulated, mathematical regularization can provide a guarantee of minimum error variance for both estimable parameters (and combinations of

parameters) and inestimable parameters (and combinations of parameters). The metrics defined above for optimal regularization are thus honoured.

- The cost of uniqueness in terms of penchant for parameter error incurred through use of a specific mathematical regularization methodology can be quantified. This allows parameter and predictive error to be quantified, and with it parameter and predictive uncertainty.

So which is the better mathematical regularization device to employ – singular value decomposition or Tikhonov regularization? A combination of the two is normally best.

## 4.5 Model Linearization

### 4.5.1 The Jacobian Matrix

As was mentioned above, history-matching in the highly parameterized context generally requires that a model be temporarily linearized. This allows deployment of a suite of numerical methods that facilitate inversion, Bayesian analysis, definition and exploration of the null space, and attainment of many other benefits that are discussed in detail in subsequent chapters. When undertaking any type of linear analysis, the operation of the model on its parameters is replaced by a matrix equation. At the heart of this equation is the so-called Jacobian matrix.

Equation (4.2.1) represents the action of a model on its parameters under calibration conditions, that is under the environmental conditions that prevailed when the measurements **h** comprising the calibration dataset were acquired. For the *n* individual model outputs $o_i$ comprising the model output vector **o**, equation (4.2.1) can be written as

$$o_1 = \mathbf{z}_1[\mathbf{k}] \tag{4.5.1a}$$

$$o_2 = \mathbf{z}_2[\mathbf{k}] \tag{4.5.1b}$$

…

$$o_n = \mathbf{z}_n[\mathbf{k}] \tag{4.5.1c}$$

Using Taylor's theorem equation (4.2.1) can be expanded as

$$\mathbf{o} = \mathbf{o}_0 + \mathbf{J}\delta\mathbf{k} + \text{other terms} \tag{4.5.2}$$

where

$$\mathbf{o}_0 = \boldsymbol{Z}[\mathbf{k}_0] \tag{4.5.3}$$

$$\delta\mathbf{k} = \mathbf{k} - \mathbf{k}_0 \tag{4.5.4}$$

and **J** is the Jacobian matrix. This is a matrix of partial derivatives of the *n* model outputs which correspond to measurements comprising the calibration dataset with respect to the *m* (adjustable) parameters employed by the model. Specifically, the Jacobian matrix is defined as

$$\mathbf{J} = \begin{bmatrix} \frac{\partial \mathbf{z}_1}{\partial k_1} & \frac{\partial \mathbf{z}_1}{\partial k_2} & \cdot & \frac{\partial \mathbf{z}_1}{\partial k_m} \\ \frac{\partial \mathbf{z}_2}{\partial k_1} & \frac{\partial \mathbf{z}_2}{\partial k_2} & \cdot & \frac{\partial \mathbf{z}_2}{\partial k_m} \\ \cdot & \cdot & \cdot & \cdot \\ \frac{\partial \mathbf{z}_n}{\partial k_1} & \frac{\partial \mathbf{z}_n}{\partial k_2} & \cdot & \frac{\partial \mathbf{z}_n}{\partial k_m} \end{bmatrix} \qquad (4.5.5)$$

The Jacobian matrix is often referred to as the "sensitivity matrix" for obvious reasons. The *m* elements comprising the *i*'th row of the Jacobian matrix are the derivatives of the model operator as it pertains to the *i*'th model output; these derivatives are taken with respect to each of the *m* parameters used by the model. The *j*'th column of the Jacobian matrix contains the derivatives with respect to the *j*'th parameter of all *n* model outputs.

In equations (4.5.2) to (4.5.4) $\mathbf{k}_0$ specifies a set of "base parameters" or "reference parameters" while $\mathbf{o}_0$ specifies model outputs calculated using these reference parameters. Where a model is temporarily linearized as part of an iterative, nonlinear parameter estimation or uncertainty analysis procedure, $\mathbf{k}_0$ changes from iteration to iteration of that procedure. The Jacobian matrix is re-calculated on every occasion that $\mathbf{k}_0$ changes. Because the model is nonlinear, the values of elements of the Jacobian matrix change with $\mathbf{k}_0$. By definition, if a model were truly linear, the Jacobian matrix would not be a function of $\mathbf{k}_0$.

### 4.5.2 Linear Model Analysis

A linear model is a model that can be represented by a matrix; the values taken by elements of this matrix are independent of values taken by model parameters. The operator $\boldsymbol{Z}[.]$ therefore becomes a matrix operator.

Rarely is an environmental model linear. However the assumption of near linear behaviour for small variations of parameters from a set of reference values facilitates many useful analyses. It underpins algorithms that improve parameter values in successive iterations of a nonlinear parameter estimation process. The benefits of linear analysis go well beyond this however. Where reference parameter values $\mathbf{k}_0$ are obtained through model calibration and presumably therefore represent minimum error variance estimates of a real world parameter set $\mathbf{k}$, reasonable estimates of the uncertainties of thus-estimated parameters, and of predictions that are sensitive to them, can be readily obtained if linear behaviour in the vicinity of the estimated $\mathbf{k}_0$ parameter set is assumed. In addition to this, linear analysis can teach a modeller much about the benefits (or lack thereof) that are accrued through model calibration in a particular modelling context, and of the sources of parameter and predictive uncertainty that remain after calibration has taken place. Much will be said on this subject in later chapters of this book.

To facilitate analyses that are described throughout this text, and to make the equations that emerge from these analyses somewhat simpler, equation (4.5.2) is written as

$$\mathbf{o} = \mathbf{Z}\mathbf{k} \qquad (4.5.6)$$

In equation (4.5.6) $\mathbf{Z}$ replaces the Jacobian matrix; the model is thus assumed to be truly linear instead of just locally near-linear. Furthermore $\mathbf{k}$ in equation (4.5.6) replaces $\delta\mathbf{k}$ of (4.5.2). It is thus equal to $\mathbf{k} - \mathbf{k}_0$. $\mathbf{k}_0$ will be taken to represent the pre-calibration expected value of $\mathbf{k}$. That is, $\mathbf{k}_0$ represents the prior mean of $\mathbf{k}$ expressed as

$$\mathbf{k}_0 = E[\mathbf{k}] \qquad (4.5.7)$$

**k** of equation (4.5.6) thus represents departures of parameters from their pre-calibration expected values. As such, if pre-calibration uncertainty of parameters is expressed by the covariance matrix C(**k**), this matrix is just as applicable to the **k** of (4.5.6) as it is to the **k** of (4.2.1).

Because

$$\mathbf{0} = \mathbf{Z0} \qquad (4.5.8)$$

**o** of equation (4.5.6) represents departures of model outputs from $\mathbf{Zk}_0$. If **h** represents the observed values of these departures then (4.2.2) becomes

$$\mathbf{h} = \mathbf{Zk} + \boldsymbol{\varepsilon} \qquad (4.5.9)$$

Measurement noise is presumably independent of **k**. Furthermore its expected value is **0**. That is

$$E[\boldsymbol{\varepsilon}] = \mathbf{0} \qquad (4.5.10)$$

**ε** of equation (4.5.10) has the same statistical properties as **ε** of equation (4.2.2) and is thus characterized by the same covariance matrix C(**ε**).

For the linear model, equation (4.2.6) becomes

$$s = \mathbf{y}^t\mathbf{k} \qquad (4.5.11)$$

where the element $y_i$ of the vector **y** expresses the sensitivity of the prediction *s* to parameter $k_i$, this comprising the *i*'th element of the parameter vector **k**. If, as above, **k** in equation (4.5.11) is considered to represent the departure of parameter values from their prior expected values, then the value of the prediction *s* represented in equation (4.5.11) represents the departure of this prediction from that which the model would make if provided with prior expected parameter values.

As has already been discussed, in most cases of environmental interest **k** will have many elements. It will probably cite more parameters than can be uniquely estimated. The matrix **Z** may thus possess a null space. In some cases **k** will have more elements than **h**; if this is the case the matrix **Z** will be long in the horizontal direction and will certainly possess a null space. Linear model analysis is well equipped to explore the repercussions of this situation.

# 5. Manual Regularization

## 5.1 Formulation of Equations

In this chapter we start by assuming linear model behaviour. Equations for solution of the inverse problem will be formulated and then solved. The means through which nonlinear problems can be solved using the same theory in slightly modified form will then be explored.

We start with equation (4.5.9), which is now repeated.

$$\mathbf{h} = \mathbf{Zk} + \boldsymbol{\varepsilon} \qquad (5.1.1)$$

Manual regularization achieves calibration uniqueness through parameter simplification. Suppose that the outcome of the simplification process is a reduced set of parameters **p**. (The number of elements comprising the vector **p** must be less than that comprising the vector **h** or the inverse problem cannot possibly be well-posed.) Let it further be supposed that the elements of **p** are defined through combining some elements of the larger parameter set **k** into single elements of **p** and through fixing other elements of **k** at "known" values so that they do not need to be estimated at all. As a result, **p** has fewer elements than **k**. Ideally this leads to a well-posed (often referred to as "over-determined") inverse problem through which elements of **p** can be uniquely estimated. The attainment of uniqueness is, of course, the goal of regularization. As we shall see, however, it will often not be possible to judge the success or otherwise of a manual regularization enterprise until solution of the newly-posed inverse problem is attempted. Furthermore, as we shall also see, it will probably not ever be possible to judge the optimality or otherwise of the manual regularization process. (Recall the metric for optimal regularization presented in the previous chapter.)

The relationship between **k** parameters and **p** parameters can be expressed through the following matrix equation

$$\mathbf{k} = \mathbf{Lp} \qquad (5.1.2)$$

In equation (5.1.2) **L** is a matrix that calculates values for elements of the complex parameter set **k** from those of the simple parameter set **p**. For example, if a 3-element vector **p** represents the values of system properties in each of three zones of assumed (for the purpose of parameter estimation) piecewise constancy into which the domain of a spatial model has been subdivided, and if **k** (a 13-element vector) represents a more complex set of model parameters which characterize spatial heterogeneity at a finer scale, then equation (5.1.2) may be written as

$$\begin{bmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \\ k_5 \\ k_6 \\ k_7 \\ k_9 \\ k_{10} \\ k_{11} \\ k_{12} \\ k_{13} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} \qquad (5.1.3)$$

In this example an element of **k** simply takes the value of the **p**-zone in which it lies; **L** is a selection matrix. If (5.1.2) is substituted into (5.1.1) we obtain

$$\mathbf{h} = \mathbf{ZLp} + \boldsymbol{\varepsilon} \qquad (5.1.4)$$

If **X** is now defined as

$$\mathbf{X}=\mathbf{ZL} \qquad (5.1.5)$$

then

$$\mathbf{h} = \mathbf{Xp} + \boldsymbol{\varepsilon} \qquad (5.1.6)$$

We now have a modified equation that represents the action of the model under calibration conditions. However this equation uses a simplified parameter set **p** instead of the more complex parameter set **k**. If **X** does not have a null space then each member $p_i$ of the reduced parameter set **p** is, conceptually at least, uniquely estimable. Let us denote the estimated parameter set as $\underline{\mathbf{p}}$.

Equation (5.1.2) allows us to calculate an estimated **k** (i.e. $\underline{\mathbf{k}}$) from an estimated **p** (i.e. $\underline{\mathbf{p}}$). It is important to note, however, that even if $\underline{\mathbf{p}}$ is uniquely estimable from **h**, the same does not apply to $\underline{\mathbf{k}}$. Hence the $\underline{\mathbf{k}}$ that emerges from solution of the manually-regularized inverse problem may be very different from the correct **k**; it will be unique, but probably incorrect. $\underline{\mathbf{k}}$ will approach **k** only if there is no variability of properties within a zone of assumed piecewise constancy that is used to define **p**.

A modeller undertakes manual regularization when he/she is presented with an inverse problem that he/she perceives to be ill-posed. However parameterization simplification (defined by the matrix **L**) that defines this regularization strategy must be strategic. If possible, manual regularization should not compromise the model's ability to fit the calibration dataset (or should do so as little as possible). If parameter simplification induces too much model-to-measurement misfit, then it can be concluded that more parameters than are offered to the inversion process through the vector **p** are in fact estimable.

Ideally, a parameter simplification strategy **L** is sought for which the following equation holds

$$\mathbf{ZLp} - \mathbf{Xp} = (\mathbf{ZL} - \mathbf{X})\mathbf{p} = \mathbf{0} \qquad (5.1.7)$$

for all **p**. An **L** which achieves (5.1.7) has no impact on model-to-measurement misfit.

However even if an **L** can be found for which (5.1.7) holds true, another important question arises. While (5.1.2) can be used for computation of $\underline{\mathbf{k}}$ from $\underline{\mathbf{p}}$, what exactly is the relationship between the estimated $\underline{\mathbf{k}}$ and the true **k**, and between the estimated $\underline{\mathbf{p}}$ and the true **k**? Can $\underline{\mathbf{p}}$ be construed to be an estimate of the average of **k** within each **p**-zone which encapsulates multiple **k** parameters? The answer to this is "no", unless special measures are taken in an effort to achieve this status for $\underline{\mathbf{p}}$. These measures are described in Cooley (2004) and Cooley and Christensen (2006). They will be discussed later in this chapter; so too will the nature of the relationships between $\underline{\mathbf{k}}$ and **k** and between $\underline{\mathbf{p}}$ and **k**.

In most cases, an **L** cannot be found for which (5.1.7) holds exactly. Hence the outcomes of manual regularization are visible to the inversion process as simplification-induced model-to-measurement misfit. Starting from (5.1.1)

$$\mathbf{h} = \mathbf{Zk} + \boldsymbol{\varepsilon}$$

$$\mathbf{h} = \mathbf{Zk} - \mathbf{Xp} + \mathbf{Xp} + \boldsymbol{\varepsilon}$$

$$\mathbf{h} = \mathbf{Xp} + (\mathbf{ZL} - \mathbf{X})\mathbf{p} + \boldsymbol{\varepsilon}$$

$$\mathbf{h} = \mathbf{Xp} + \boldsymbol{\eta} + \boldsymbol{\varepsilon} \qquad (5.1.8)$$

$$\mathbf{h} = \mathbf{Xp} + \boldsymbol{\tau} \qquad (5.1.9)$$

where

$$\boldsymbol{\eta} = (\mathbf{ZL} - \mathbf{X})\mathbf{p} \qquad (5.1.10)$$

and

$$\boldsymbol{\tau} = \boldsymbol{\eta} + \boldsymbol{\varepsilon} \qquad (5.1.11)$$

Equation (5.1.9) is the same as (5.1.6) except for the fact that it acknowledges the presence of simplification-induced noise $\boldsymbol{\eta}$ in addition to measurement noise $\boldsymbol{\varepsilon}$. Continuing with the above zonal example, this "structural noise" $\boldsymbol{\eta}$ will only be zero if model outputs under calibration conditions are completely insensitive to any heterogeneity which exists within each zone of assumed piecewise constancy which underpins definition of **p**; that is, structural noise will only be zero if equation (5.1.7) holds. Regardless of this, equation (5.1.9) defines the inverse problem that must be solved for **p**.

The logic above is equally applicable to other forms of parameter simplification such as the fixing of some parameters at values that are based on expert knowledge and the estimation of others. In all cases it is possible to formulate an equation which describes an inverse problem which features a simplified parameter set **p** in place of a more complex parameter set **k**. Ideally, solution of this problem provides a unique $\underline{\mathbf{p}}$ from which a unique $\underline{\mathbf{k}}$ can be calculated using an appropriate **L** matrix on which basis simplification is defined. However while $\underline{\mathbf{p}}$ may be unique, its relationship to the real system properties **k** remains unknown; so too does the relationship between estimates of $\underline{\mathbf{k}}$ achieved through the manual regularization process and the real system properties **k**. As will be discussed, this makes analysis of parameter and predictive error difficult, if not impossible, in the manually-regularized context.

As demonstrated above, structural noise can be introduced to the inverse problem through the parameter simplification process. The existence of this noise has a number of repercussions.

Firstly it may limit the fit between model outcomes and field measurements that is achieved through the parameter estimation process. Information contained within the calibration dataset therefore does not get to inform model parameters. What is worse is that while we may know something about the statistics of measurement noise, generally we know nothing about the statistics of structural noise. It thus becomes very difficult to establish the potential for error in $\underline{\mathbf{p}}$ as an estimate of $\mathbf{p}$. This further compounds the problem of assessing post-calibration parameter and predictive uncertainty.

These problems will be ignored for a while as we focus on solution of the inverse problem that manual regularization delivers to us.

## 5.2 Well-posed Inverse Problem

### 5.2.1 Data without Noise

Let us put aside for the moment the fact that, in the environmental modelling context, well-posed inverse problems rarely happen naturally but are the outcomes of regularization. Instead, let us suppose that the parameters of the real world are as simple as those employed by a model. Hence simplification-induced structural noise is zero. At the same time, questions pertaining to the relationship between estimated parameters and real world parameters can be dispensed with. In doing this, critical questions related to parameter and predictive uncertainty can also be put to one side – for the moment at least.

We start with equation (5.1.9) but replace $\boldsymbol{\tau}$ with $\boldsymbol{\varepsilon}$. Thus

$$\mathbf{h} = \mathbf{X}\mathbf{p} + \boldsymbol{\varepsilon} \tag{5.2.1}$$

If there were no noise associated with the measurement dataset, (5.2.1) would become

$$\mathbf{h} = \mathbf{X}\mathbf{p} \tag{5.2.2}$$

While this equation is simpler than (5.2.1) it still cannot be solved for $\mathbf{p}$ as $\mathbf{X}$ is not a square matrix. Instead it is a matrix with more rows than columns (as must be the case for uniqueness of $\mathbf{p}$), and hence is long in the vertical direction; as such, it does not have an inverse.

Let us now multiply both sides of (5.2.2) by $\mathbf{X}^t$. Then

$$\mathbf{X}^t\mathbf{h} = \mathbf{X}^t\mathbf{X}\mathbf{p} \tag{5.2.3}$$

$\mathbf{X}^t\mathbf{X}$ is a square matrix. If $\mathbf{X}$ does not have null space, $\mathbf{X}^t\mathbf{X}$ is invertible. We can thus multiply both sides of (5.2.3) by $(\mathbf{X}^t\mathbf{X})^{-1}$ to obtain $\mathbf{p}$.

$$(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{h} = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{X}\mathbf{p} = \mathbf{p} \tag{5.2.4}$$

If, instead of multiplying both sides of (5.2.2) by $\mathbf{X}^t$ and then $(\mathbf{X}^t\mathbf{X})^{-1}$, we had multiplied by $\mathbf{X}^t\mathbf{Q}$ and then $(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}$ where $\mathbf{Q}$ is a square matrix of full rank so that $(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}$ exists, we would have obtained

$$(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{h} = \mathbf{p} \tag{5.2.5}$$

The assumption of no noise implies a perfect fit between model outputs and the calibration dataset. An underscore is not used to distinguish estimated $\underline{\mathbf{p}}$ from true $\mathbf{p}$ as was done in the preceding section. Values for $\mathbf{p}$ obtained through (5.2.4) and (5.2.5) are identical; both are equal to the true $\mathbf{p}$.

### 5.2.2 Data with Noise

We now acknowledge the presence of noise in the calibration dataset. It will be seen that the equations derived in the previous section can still be used for estimation of **p**, notwithstanding noise contamination of the calibration dataset. However the estimate of **p** obtained through these equations is no longer the true **p**; as such it is denoted as $\underline{\mathbf{p}}$. This estimate has a potential for error. A task that awaits us is to quantify this potential.

Before proceeding further, equation (5.2.1) will be transformed slightly to a form that promulgates estimates of **p** that are of minimum error variance. Recall from the previous chapter that this is the calibration metric that we have set ourselves. Let us suppose that measurement noise can be characterized by the covariance matrix C(**ε**). As such, C(**ε**) this is a positive-definite matrix; hence it possesses an inverse. Let a matrix **Q** be defined as being proportional to this inverse, with the proportionality constant being denoted as $\sigma^2_r$. Then

$$\mathbf{Q} = \sigma^2_r \mathbf{C}^{-1}(\boldsymbol{\varepsilon}) \tag{5.2.6}$$

Note that if C(**ε**) is diagonal, then so too is **Q**; it is also invertible and hence of full rank. **Q** is referred to as the "weight matrix". $\sigma^2_r$ is variously referred to as the "reference variance" and "variance of unit weight".

We now define the vector of residuals **r** as that which lists differences between model outputs and corresponding field measurements. Thus

$$\mathbf{r} = \mathbf{h} - \mathbf{X}\mathbf{p} \tag{5.2.7}$$

A so-called objective function Φ can be formulated as the sum of weighted squared residuals. Thus

$$\Phi = \mathbf{r}^t\mathbf{Q}\mathbf{r} = (\mathbf{h} - \mathbf{X}\mathbf{p})^t\mathbf{Q}(\mathbf{h} - \mathbf{X}\mathbf{p}) \tag{5.2.8}$$

The lower is the objective function, the better is the fit between model outputs and field data. Notice the similarity of this definition of the objective function to the exponent appearing in the equation for the multinormal density function; see equation (3.6.1). If measurement noise is characterized by a multinormal distribution, then minimization of the objective function defined by (5.2.8) is the same as maximization of the likelihood of the residuals which describe model-to-measurement misfit.

In a few lines of calculus it is easily shown that minimization of (5.2.8) leads to the following estimate $\underline{\mathbf{p}}$ of model parameters **p**

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{h} \tag{5.2.9}$$

This is the same equation as (5.2.5); it is comforting that solution of the inverse problem with noise taken into account is the same as that without noise. Use of (5.2.9) to solve the inverse problem constitutes use of the Gauss-Newton method for estimation of parameters.

We now explore the potential for error in the parameter set $\underline{\mathbf{p}}$ that is estimated using (5.2.9). If (5.2.1) is substituted into (5.2.9) we obtain

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{X}\mathbf{p} + (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\boldsymbol{\varepsilon} = \mathbf{p} + (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\boldsymbol{\varepsilon} \tag{5.2.10}$$

So that the error in estimated $\underline{\mathbf{p}}$ becomes

$$\underline{\mathbf{p}} - \mathbf{p} = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\boldsymbol{\varepsilon} \tag{5.2.11}$$

If **ε** is zero, then so too is parameter error. Hence $\underline{\mathbf{p}}$ is estimated without bias. Under any other

circumstances we cannot know parameter error as we do not know **ε**. However we can say something about the propensity for parameter error through calculation of its covariance matrix. Using equation (3.9.2) for propagation of covariance, we obtain for C($\underline{\mathbf{p}}$ - **p**), the covariance matrix of parameter error

$$C(\underline{\mathbf{p}} - \mathbf{p}) = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}C(\boldsymbol{\varepsilon})\mathbf{Q}\mathbf{X}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1} \quad (5.2.12)$$

Here we have used the fact that $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ is a symmetric matrix and that therefore its inverse is symmetric; the transpose of a symmetric matrix is the original matrix. If the weight matrix **Q** is chosen in accordance with (5.2.6), (5.2.12) becomes

$$C(\underline{\mathbf{p}} - \mathbf{p}) = \sigma_r^2(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1} \quad (5.2.13)$$

It can be shown (see for example Koch, 1999) that with this choice of **Q**, $\underline{\mathbf{p}}$ satisfies our calibration metric. It is the so-called best linear unbiased estimator of **p**; as an estimate of **p** it has less error variance than any other estimate. The above choice of **Q** is critical to achieving this status as it minimizes the trace of C($\underline{\mathbf{p}}$ - **p**). This choice of **Q** can also be shown to minimize the error variance of any linear combination of parameters calculated as

$$\underline{s} = \mathbf{w}^t\underline{\mathbf{p}} \quad (5.2.14)$$

If the components of the vector **w** comprise sensitivities of a model prediction to parameters **p**, then equation (5.2.14) is the equation which is used to make that prediction using the calibrated model. The "real" value of the prediction is

$$s = \mathbf{w}^t\mathbf{p} \quad (5.2.15)$$

By subtracting (5.2.15) from (5.2.14), predictive error is calculated as

$$\underline{s} - s = \mathbf{w}^t(\underline{\mathbf{p}} - \mathbf{p}) \quad (5.2.16)$$

From (3.9.2) the covariance matrix of predictive error, which for a scalar such as a single prediction is simply the variance of that error (recall that the variance of a random variable is the square of its standard deviation), is then given by

$$\sigma^2_{\underline{s}-s} = \mathbf{w}^tC(\underline{\mathbf{p}} - \mathbf{p})\mathbf{w} = \sigma_r^2\mathbf{w}^t(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{w} \quad (5.2.17)$$

As stated above, this is minimized through choosing **Q** according to (5.2.6).

Let $\Phi_0$ represent the minimized value of the objective function defined according to equation (5.2.8). An unbiased estimate $\underline{\sigma}^2_r$ of the reference variance $\sigma^2_r$ can be calculated from this minimized objective function as

$$\underline{\sigma}_r^2 = \frac{\Phi_0}{n-m} \quad (5.2.18)$$

where *n* is the number of observations featured in the calibration dataset (i.e. the number of elements of **h**) and *m* is the number of estimated parameters (i.e. number of elements of **p**).

If the reference variance $\sigma^2_r$ does not need to be estimated from the minimized objective function because it is known in advance, then if measurement noise has a multinormal distribution, so too does $\underline{\mathbf{p}} - \mathbf{p}$ (if the model is linear). The same applies to $\underline{s} - s$ for any prediction *s* made by the model. However if $\underline{\sigma}^2_r$ needs to be estimated using (5.2.18), then parameter and predictive error have student *t* distributions with *n-m* degrees of freedom. Meanwhile $\underline{\sigma}^2_r$ itself has a chi-squared distribution with $n - m$ degrees of freedom. See Koch (1999) for details.

Before completing this section, it is worth pointing out that equation (5.2.1) is often transformed in order to make some of the above equations a little less cumbersome. If all terms of (5.2.1) are pre-multiplied by $\mathbf{Q}^{½}$, where $\mathbf{Q}$ is chosen according to (5.2.6), we obtain

$$\mathbf{Q}^{½}\mathbf{h} = \mathbf{Q}^{½}\mathbf{X}\mathbf{p} + \mathbf{Q}^{½}\boldsymbol{\varepsilon} \quad (5.2.19)$$

This can be written as

$$\mathbf{g} = \mathbf{Y}\mathbf{p} + \boldsymbol{\xi} \quad (5.2.20)$$

where

$$\mathbf{g} = \mathbf{Q}^{½}\mathbf{h} \quad (5.2.21)$$

$$\mathbf{Y} = \mathbf{Q}^{½}\mathbf{X} \quad (5.2.22)$$

$$\boldsymbol{\xi} = \mathbf{Q}^{½}\boldsymbol{\varepsilon} \quad (5.2.23)$$

Using (3.9.2) and (5.2.6) the covariance matrix $C(\boldsymbol{\xi})$ of $\boldsymbol{\xi}$ can be written as

$$C(\boldsymbol{\xi}) = \mathbf{Q}^{½}C(\boldsymbol{\varepsilon})\mathbf{Q} = \sigma^2_r\mathbf{I} \quad (5.2.24)$$

$\underline{\mathbf{p}}$ can then be estimated as

$$\underline{\mathbf{p}} = (\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t\mathbf{g} \quad (5.2.25)$$

Meanwhile the covariance matrix of parameter error is

$$C(\underline{\mathbf{p}} - \mathbf{p}) = \sigma^2_r(\mathbf{Y}^t\mathbf{Y})^{-1} \quad (5.2.26)$$

Substitution of (5.2.21) and (5.2.22) into (5.2.25) and (5.2.26) readily confirms that the latter two equations are equivalent to (5.2.9) and (5.2.13).

### 5.2.3 Prior Information

To increase the estimability of model parameters, measurements of system state can be supplemented by "observations" that pertain directly to these parameters. Such observations are often referred to as "prior information". These supplementary observations may be comprised of direct measurements of system properties which the parameters represent. Alternatively, they can express expert knowledge of likely parameter values. Let the vector **b** designate the values of these observations, and let the matrix **B** designate the relationship of these observations to system parameters. For example, if the extent of prior information that is included in the parameter estimation process is a single observation that the difference between $p_i$ and $p_j$ is likely to be 2.0, then **b** will have a single element (this being 2.0), while the matrix **B** will be a $1 \times m$ matrix, where $m$ is the number of elements in the parameter vector **p**. The $i$'th element of the single row of **B** will be 1 and the $j$'th element of its single row will be -1.

Prior information can be included in the inversion process simply by adding elements to the **h** matrix and rows to the **X** matrix as appropriate. However it is sometimes useful to separate terms which pertain to prior information from those which pertain to measurements of system state so that these two aspects of the calibration dataset can be given separate treatment if desired. This will be especially the case when prior information is used to express Tikhonov regularization; see the next chapter.

With specific mention made of prior information, equation (5.2.1) can be written as

$$\begin{bmatrix}\mathbf{h}\\ \mathbf{b}\end{bmatrix}=\begin{bmatrix}\mathbf{X}\\ \mathbf{B}\end{bmatrix}\mathbf{p}+\begin{bmatrix}\boldsymbol{\varepsilon}\\ \boldsymbol{\zeta}\end{bmatrix} \qquad (5.2.27)$$

In equation (5.2.27) $\boldsymbol{\zeta}$ is the "noise" associated with **b**. If the value of **b** is based on expert knowledge then this "noise" arises from prior uncertainty of **p**. If this uncertainty is characterized by the covariance matrix C(**p**), then

$$C(\boldsymbol{\zeta}) = \mathbf{B}C(\mathbf{p})\mathbf{B}^t \qquad (5.2.28)$$

Equation (5.2.9), when applied to (5.2.27), becomes

$$\underline{\mathbf{p}}=\left\{\begin{bmatrix}\mathbf{X}^t & \mathbf{B}^t\end{bmatrix}\begin{bmatrix}\mathbf{Q}_w & \mathbf{0}\\ \mathbf{0} & \mathbf{Q}_p\end{bmatrix}\begin{bmatrix}\mathbf{X}\\ \mathbf{B}\end{bmatrix}\right\}^{-1}\begin{bmatrix}\mathbf{X}^t & \mathbf{B}^t\end{bmatrix}\begin{bmatrix}\mathbf{Q}_w & \mathbf{0}\\ \mathbf{0} & \mathbf{Q}_p\end{bmatrix}\begin{bmatrix}\mathbf{h}\\ \mathbf{b}\end{bmatrix} \qquad (5.2.29)$$

where $\mathbf{Q}_w$ is the weight matrix assigned to the measurement dataset, and $\mathbf{Q}_p$ is the weight matrix assigned to prior information. Ideally, following (5.2.6), $\mathbf{Q}_p$ should be formulated as

$$\mathbf{Q}_p = \sigma^2_r C^{-1}(\boldsymbol{\zeta}) \qquad (5.2.30)$$

Note that, for consistency, the same reference variance must be used in formulation of $\mathbf{Q}_p$ as is used in formulation of $\mathbf{Q}_w$. Using (5.2.6) for $\mathbf{Q}_w$, the latter is formulated as

$$\mathbf{Q}_w = \sigma^2_r C^{-1}(\boldsymbol{\varepsilon}) \qquad (5.2.31)$$

After due processing, equation (5.2.29) becomes

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{Q}_w\mathbf{X} + \mathbf{B}^t\mathbf{Q}_p\mathbf{B})^{-1}(\mathbf{X}^t\mathbf{Q}_w\mathbf{h} + \mathbf{B}^t\mathbf{Q}_p\mathbf{b}) \qquad (5.2.32)$$

If the prior information component of the observation dataset consists simply of a series of "observations" that each parameter is ideally equal to its prior expected value, then **B** becomes the identity matrix **I**. Furthermore, by cancelling out the reference variance as it is featured in the $\mathbf{Q}_w$ and $\mathbf{Q}_p$ matrices appearing in inverted and non-inverted components of the matrix product on the right of (5.2.32), this equation becomes

$$\underline{\mathbf{p}} = [\mathbf{X}^t\mathbf{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{X} + \mathbf{C}^{-1}(\mathbf{p})]^{-1}\mathbf{X}^t\mathbf{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{h} \qquad (5.2.33a)$$

Equivalently, if the reference variance is not cancelled, the equation is

$$\underline{\mathbf{p}} = [\mathbf{X}^t\mathbf{Q}_w\mathbf{X} + \mathbf{Q}_p]^{-1}\mathbf{X}^t\mathbf{Q}_w\mathbf{h} \qquad (5.2.33b)$$

The absence of **b** in equations (5.2.33a) and (5.2.33b) is an outcome of the linearization procedure discussed in section 4.5.2 whereby the pre-calibration (i.e. prior) expected values of all parameters are zero.

In similar fashion to (5.2.13), the post-calibration covariance matrix of parameter error under these circumstances is easily calculated as

$$C(\underline{\mathbf{p}} - \mathbf{p}) = \sigma^2_r[\mathbf{X}^t\mathbf{Q}_w\mathbf{X} + \mathbf{Q}_b]^{-1} \qquad (5.2.34)$$

which is equivalent to

$$C(\underline{\mathbf{p}} - \mathbf{p}) = [\mathbf{X}^t\mathbf{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{X} + \mathbf{C}^{-1}(\mathbf{p})]^{-1} \qquad (5.2.35)$$

Where $\sigma^2_r$ is known to be unity, and where prior parameter uncertainties and measurement noise are normally distributed, equation (5.2.35) is derivable from Bayes equation as expressing the posterior uncertainties of parameters; see chapter 7. For this over-determined (i.e. well-posed) case, the post-calibration potential for parameter error and the posterior

parameter uncertainty are the same.

### 5.2.4 Objective Function Contours

If a model is linear, and if the inverse problem is well-posed, contours of the objective function form hyper-ellipsoids if plotted in parameter space. At their centre is the unique minimum of the objective function. This is schematized for a two-dimensional inverse problem in figure 5.1.

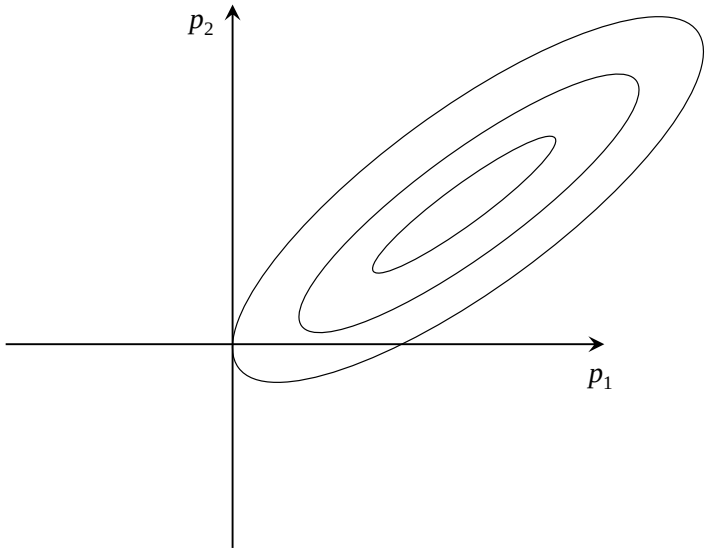


**Figure 5.1. Objective function contours for a two-parameter, linear inverse problem.**

If an inverse problem is nonlinear, then objective function contours do not form hyper-ellipsoids. Nevertheless, if the inverse problem is well-posed, the objective function contours close around a discrete minimum. This is illustrated for a two-parameter problem in figure 5.2.

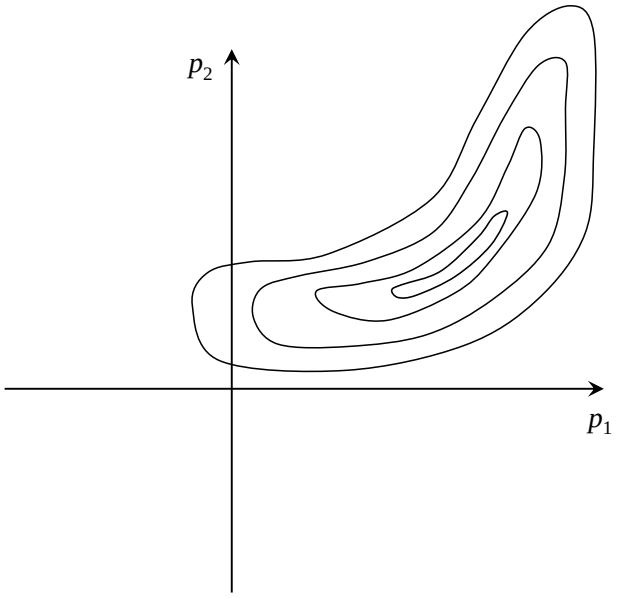


**Figure 5.2. Objective function contours for a two-parameter, nonlinear, inverse problem.**

Where a problem is ill-posed the objective contours do not close. Objective function contours for an ill-posed, nonlinear, two-parameter, inverse problem are schematized in figure 5.3.

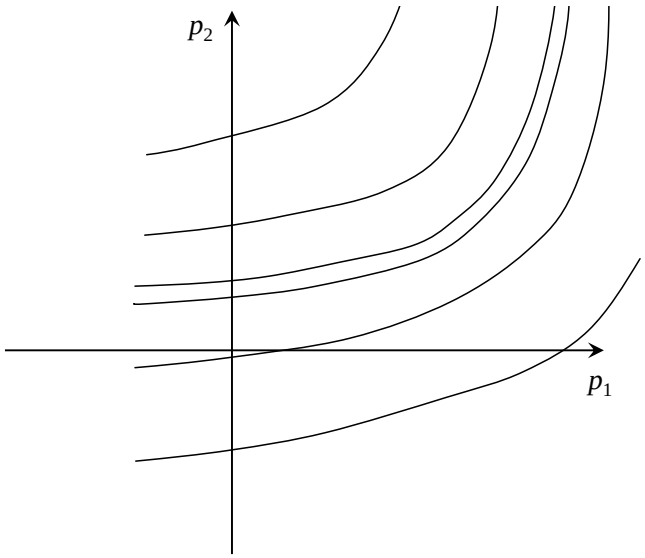


**Figure 5.3. Objective function contours for a nonlinear, two-parameter, ill-posed inverse problem.**

Where a problem is highly nonlinear, the objective function may contain local optima. Where it is nonlinear and ill-posed, objective function contours may not close about these local objective function minima.

### 5.2.5 Probability Density Contours of Posterior Parameter Error

As discussed in section 3.6, probability density function contours for a normal distribution are elliptical in two dimensions, ellipsoidal in three dimensions and hyper-ellipsoidal in greater than three dimensions. The same applies for the student *t* distribution.

If a model is linear, and if measurement noise is normally-distributed, the post-calibration probability distribution of parameter error is multinormal if the reference variance is not estimated through the calibration process, and student *t* if it is. In both cases the distribution is centred on estimated parameter values as inferred through the calibration process. Under these circumstances objective function contours and contours of equal posterior parameter error probability (also known as parameter error confidence ellipsoids) coincide. The association of an objective function value with a parameter error probability value depends on the dimensionality of parameter space, and on whether a multinormal or student *t* distribution is used to characterize parameter error; see chapter 8. Where a model is mildly nonlinear the relationship between objective function value and post-calibration parameter error probability value is still maintained. However the relationship fades as a model becomes very nonlinear.

As was stated in section 3.6, the eigenvectors of the covariance matrix of a multinormally distributed set of variables point along the axes of hyper-ellipsoids of constant probability. As was also stated, the ratios of the lengths of these axes for a hyper-ellipsoid associated with any probability value are the ratios of the square roots of respective covariance matrix eigenvalues. Because of the coincidence of hyper-ellipsoids of constant probability with objective function contours, eigenvector and eigenvalue associations of the former are valid

for the latter.

### 5.2.6 Residuals

The discussion so far has focused on the fate of parameters as a model is calibrated. Some features of calibrated model outputs and corresponding residuals are also of interest. These features are easier to examine if we formulate the inverse problem using equation (5.2.20) so that the covariance matrix of measurement noise is proportional to the identity matrix **I**. Thus **Y** replaces **X** as the model matrix, **g** replaces **h** as the observation dataset, and $\xi$ replaces $\varepsilon$ as the vector of measurement noise. Transformed residuals **f** are calculated as

$$\mathbf{f} = \mathbf{g} - \mathbf{Y}\mathbf{p} \tag{5.2.36}$$

We denote residuals for a calibrated model as $\underline{\mathbf{f}}$ to complement the fact that they are calculated using parameters $\underline{\mathbf{p}}$. Thus

$$\underline{\mathbf{f}} = \mathbf{g} - \mathbf{Y}\underline{\mathbf{p}} \tag{5.2.37}$$

From (5.2.25) this becomes

$$\underline{\mathbf{f}} = \mathbf{g} - \mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t\mathbf{g} = (\mathbf{I} - \mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t)\mathbf{g} \tag{5.2.38}$$

Let **e** designate outputs calculated by the model **Y**. Thus

$$\mathbf{e} = \mathbf{Y}\mathbf{p} \tag{5.2.39}$$

For the calibrated model these become

$$\underline{\mathbf{e}} = \mathbf{Y}\underline{\mathbf{p}} = \mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t\mathbf{g} \tag{5.2.40}$$

From (5.2.40) and (5.2.38)

$$\underline{\mathbf{e}}^t\underline{\mathbf{f}} = \mathbf{g}^t\mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t(\mathbf{I} - \mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t)\mathbf{g} = 0 \tag{5.2.41}$$

Equation (5.2.41) states that, for a calibrated model, residuals are normal to model outputs. The calibration process can thus be conceived of as having extracted as much information from the measurement dataset as it can by fitting it as well as it can. That part of the calibration dataset that has not been fit is simply out of reach of the columns of **Y** because there is nothing left in the observation dataset **g** that can project onto the columns of **Y**. Hopefully, this is because all that remains in the data is measurement noise – noise that cannot be expressed as a linear combination of the columns of **Y** because of the random nature of noise. In practice, however, it will normally be the incapacity of the model to simulate all details of an environmental system's behaviour that is responsible for the greater part of a model's incapacity to fit a calibration dataset exactly. Part of that behaviour is inexpressible as a linear combination of the columns of **Y** because of the inadequacy of **Y** as a descriptor of real world behaviour.

The fact that, in most real world modelling circumstances, model-to-measurement misfit is dominated by so-called structural (rather than measurement) noise has many repercussions. Some of these will be discussed in chapter 9. In the meantime it is worth pointing out that if such noise is to be treated as if it were measurement noise so that the theory presented in this chapter can be applied with rigour, then its covariance matrix must be known. This is required so that a measurement weighting strategy, embodied in a weight matrix **Q**, can be determined from its inverse. Regrettably the covariance matrix of structural noise can rarely, if ever, be known. Even more sadly, it is likely to be singular, and hence noninvertible, for reasons that are discussed in chapter 9.

Let us continue with our analysis nevertheless. The matrix $\mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t$ is idempotent, as can be readily verified by multiplying it by itself. It is also symmetric, as can be readily verified by taking its transpose and recalling the fact that the inverse of a symmetric matrix is itself symmetric. Hence it is an orthogonal projection operator. Equation (5.2.40) states that outputs calculated by the calibrated model are the orthogonal projection of measurements comprising the calibration dataset onto the range space of the model (i.e. the space spanned by the columns of the model matrix **Y**). As can also be readily verified, $\mathbf{I} - \mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t$ is an idempotent symmetric matrix too. It projects onto the orthogonal complement of the range space of **Y**. Equation (5.2.38) states that residuals pertaining to the calibrated model are the orthogonal projection of measurements onto this space.

## 5.3 Post-Calibration Analysis

### 5.3.1 Problem Well-Posedness

*5.3.1.1 Nonuniqueness*

All of the equations presented in the previous section which involve estimation of parameters require that a matrix be inverted. Where no prior information is included in the parameter estimation process, this matrix is $\mathbf{X}^t\mathbf{Q}\mathbf{X}$.

If **X** has a null space then $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ is not invertible. If PEST is asked to solve an ill-posed inverse problem using no mathematical regularization device (which occurs if it runs in "estimation" mode), it may not work. The objective function may not fall. Problems may also be encountered if the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix is near-singular. It can be shown that attempted inversion of a near-singular matrix (or attempted solution of a set of linear equations in which near-singular matrix inversion is implied) leads to gross amplification of tiny numerical errors that are incurred when matrix and vector elements are stored in a computer. This amplification of numerical noise can easily dominate the "solution" to the inverse problem; the solution may therefore be meaningless.

In spite of this, PEST may nevertheless obtain a solution to an ill-posed inverse problem. The resulting parameter set may indeed fit the calibration dataset well. This occurs because addition of the Marquardt lambda (see later) to the diagonal of the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix may facilitate a "false inversion" of this matrix, and the achievement of a set of parameters which minimize the objective function. The set of parameters thus obtained will not be unique however. Under a slightly different weighting scheme, or through use of a different Marquardt lambda selection strategy, an entirely different set of parameters may be obtained which also minimize the objective function. It is unlikely that either of these parameter sets will approach that of minimized post-calibration error variance; recall that this was the goal that we set ourselves in Section 4.4.

Where inversion is undertaken using so-called "global" methods, the attainment of different parameter sets that fit the calibration dataset equally well is often offered as proof of the existence of local minima in the objective function – a phenomenon that can indeed accompany attempts to calibrate some types of highly nonlinear models. It is the author's experience, however, that the discovery of multiple sets of parameters that fit a calibration dataset equally well may illustrate nothing more than the inadvertent formulation of an ill-posed inverse problem. Chance plays a large role in "solution" of an ill-posed inverse problem where regularisation is eschewed. Of the many solutions that can be obtained to that

problem, only one can be of minimum error variance.

*5.3.1.2 Parameter Variance-Covariance Analysis*

Invertibility of the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix is a necessary, but not a sufficient, condition for success of the manually-regularized parameter estimation process. Another requirement is that post-calibration error variances that are computed for estimated parameters be reduced below their pre-calibration levels. The latter are their prior uncertainties. ("Pre-calibration error variance" characterizes the extent to which parameters may depart from their prior expected values. This, of course, is nothing other than a characterization of parameter uncertainty. Recall that variances constitute the diagonal elements of a covariance matrix and that the variance of a random variable is the square of its standard deviation.)

If an inversion dataset includes prior information on all parameters which specifies that each parameter is "observed" to have a value equal to its prior mean then, provided that this prior information is weighted appropriately, the error variance of no parameter should be assessed to rise through the inversion process. In this case parameter estimation is based on equation (5.2.33). In practice, prior information is often omitted from formulation of a manually-regularized inverse problem. There are a number of reasons for this. One reason is that modellers often do not want to commit themselves to prior expected parameter values, especially if the inverse problem is "well-posed enough" for the information content of the calibration dataset to dominate that of prior expert knowledge. Another reason is that it is often difficult to derive a weighting scheme which adequately balances the uncertainties of prior information against those of measurement error. This is especially the case where "measurement error" is actually dominated by model structural error (as it often is); this is a topic to which we will return later.

Manually-regularized parameter estimation is thus often accomplished using equation (5.2.9) without prior information. Post-calibration parameter error variance is then assessed using equation (5.2.13). If the post-calibration error variances of some parameters are unacceptably high, the modeller then generally repeats the parameter estimation process with manual regularization strengthened. This can involve the fixing of some parameters at their prior expected values and/or the combining of others into composite parameters. The number of estimated parameters is thereby reduced. Presumably parameters which are eliminated from the revised inversion process are those whose error variances rose, rather than fell, during the previous inversion process. These will have been revealed by studying the post-calibration parameter error covariance matrix that emerged from that process.

While the covariance matrix of post-calibration parameter error may indeed reveal that post-calibration error variances for some parameters are unacceptably high, the reasons for inflated post-calibration error variance may not be readily apparent from an inspection of this matrix. There are, in fact, two reasons why the post-calibration error variance of a parameter may be high. One is that the calibration dataset contains little or no information on this parameter. The second is that the information that the calibration dataset contains for this parameter is actually shared with one or a number of other parameters; therefore each parameter cannot be resolved individually. These two situations are illustrated for a simple two-parameter problem in figure 5.4.

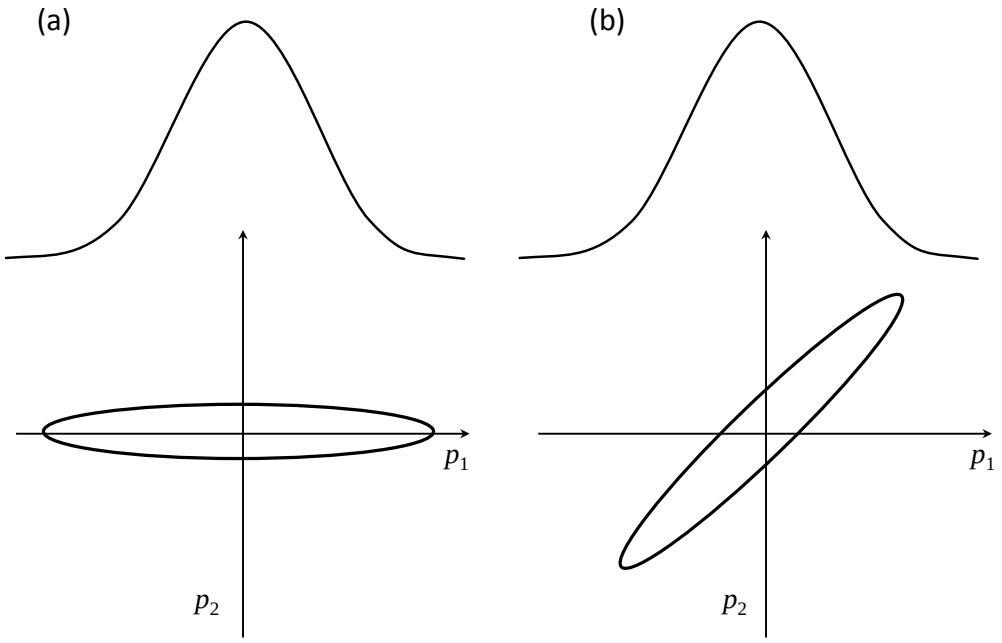


**Figure 5.4. A contour of post-calibration parameter error variance, and the post-calibration marginal probability distribution of error for parameter $p_1$. In part (a) of this figure parameter $p_1$ has a high post-calibration error variance because the calibration dataset has little information that pertains to this parameter. In part (b) of this figure the calibration dataset does contain information which pertains to parameter $p_1$. However that information is shared with parameter $p_2$.**

A modeller can readily distinguish between the two cases depicted in figure 5.4 by inspecting the post-calibration parameter error correlation coefficient matrix. Correlation coefficients are calculated from covariances using equation (3.5.3). Recall that the diagonal elements of a correlation coefficient matrix are all 1. Meanwhile off-diagonal elements of this matrix lie between 1 and -1; the matrix is symmetric. The closer that an off-diagonal element approaches 1 or -1, the greater is the degree to which parameters associated with the row and column pertaining to that element are correlated; hence the greater the degree to which a contour of the post-calibration parameter error probability density function looks like part (b) of figure 5.4 rather than part (a) of this figure. Actually as correlation coefficients approach 1 or -1, error variance contours become narrower than illustrated in the figure. In the limit that they are actually 1 or -1, the contours are so narrow that they become straight lines. In the limit they do not close. At this stage the matrix **X** has a null space.

The contour that is depicted in part (b) of figure 5.4 illustrates positive parameter correlation, and hence a correlation coefficient that is greater than zero. An ellipse which slopes upwards to the left indicates negative correlation between parameters. A circle, or an ellipse which is oriented along a parameter axis, indicates zero correlation between respective parameters.

The correlation coefficient matrix thus informs a modeller whether excessive correlation with other parameters may be the reason for high post-calibration error variance of a particular parameter. Unfortunately, however, there is a practical problem associated with use of this matrix. The closer a covariance matrix approaches singularity (a matrix is singular when it cannot be inverted) the greater is the amount of numerical error that is associated with calculation of correlation coefficients. This applies especially to correlation coefficients that

should be calculated as approaching 1 and -1. High levels of post-calibration parameter correlation may therefore go unnoticed.

Fortunately, the same does not apply to calculation of eigenvectors and eigenvalues of a post-calibration parameter error covariance matrix. Hence these are probably the best source of information on well- or ill-posedness of a parameter estimation problem and, if ill-posed, the reason for this. If the ratio of highest to lowest eigenvalue of a post-calibration parameter error covariance matrix is large, this indicates that post-calibration parameter error probability ellipses are unduly long in at least one direction of parameter space; this direction is that of the eigenvector corresponding to the highest eigenvalue. If a number of eigenvalues are unduly large in comparison to others, then there are a number of directions of probability ellipse elongation; once again, elongation is in the direction of the corresponding eigenvectors. (Recall that eigenvalues and eigenvectors are matched to each other.) If the eigenvector corresponding to an unduly large eigenvalue is dominated by a single parameter, then the situation is as depicted in figure 5.4a. However if a number of parameter components are equally large, then the situation is as depicted in figure 5.4b. Eigenvectors listed on PEST printouts are normalized so that their magnitude is 1.0. Hence a modeller can see at a glance whether an eigenvector is dominated by a single parameter, or whether a number of parameters feature strongly in this vector.

It is apparent that the information content of the eigenvectors and eigenvalues of the post-calibration parameter error covariance matrix is large. Furthermore, this information is presented in a form that is readily digestible by the modeller. In addition to this, numerical calculation of these quantities is relatively robust. If there is a single number that can characterize the health (or otherwise) of the inversion process as undertaken using manual regularization, it is the ratio of highest to lowest eigenvalue of the post-calibration parameter error covariance matrix. This is equal to the so-called "condition number" of this covariance matrix. It is apparent from (5.2.9) that it is also the condition number of the matrix that must be inverted to estimate parameter values (it is easy to show that the condition number of the inverse of a matrix is the same as that of the original matrix). Matrices that have a high condition number are difficult to invert, as numerical errors are amplified in their inversion. In PEST usage, the predominant source of numerical error in the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix is the calculation of finite-difference derivatives required to fill the $\mathbf{X}$ matrix.

Experience in using PEST suggests that if the ratio of highest to lowest eigenvalue of the post-calibration parameter error covariance matrix is greater than about $5\times10^7$, the numerical integrity of the inversion process is highly questionable. (Parameterization integrity of the inversion process generally loses its integrity at much lower eigenvalue ratios than this.) Refinement of the manual regularization strategy then becomes essential. If the eigenvector associated with the highest eigenvalue is dominated by a single parameter, then that parameter should not be estimated in the reformulated inverse problem. Instead it should be held at a value equal to its prior expected value. If, on the other hand, a number of parameters feature strongly in this vector, then one of them should probably be fixed at its prior expected value in the reformulated inverse problem. The parameter, or parameters, with which it is correlated will then have lower post-calibration error variances. This is illustrated in figure 3.4. However this same figure illustrates that the values estimated for parameters that are correlated with the newly fixed parameter may be highly dependent on the value at which this parameter is fixed. Hence their apparent post-calibration certainty may be illusory. Obviously, when choosing the parameter to fix from a group of correlated parameters, the

parameter with least prior uncertainty should be chosen, as this is the one that a modeller is least likely to fix at the wrong value.

Unfortunately, a fundamental problem with analysis of the post-calibration parameter error covariance matrix is that this matrix cannot be computed if the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix of equation (5.2.9) cannot be inverted. Hence just when the information that the post-calibration parameter error covariance matrix can provide is needed most in order to shed light on the origins of inverse problem ill-posedness, it cannot be calculated. Later in this text singular value decomposition is used to solve ill-posed inverse problems. It provides the same information that the post-calibration parameter error covariance matrix would have provided if it was not incapable of being inverted. However the information is available prior to solving the inverse problem instead of afterwards. Furthermore, at the same time as it identifies the causes of inverse problem ill-posedness, singular value decomposition removes those causes prior to estimating parameters.

*5.3.1.3 Composite Parameter Sensitivities*

One means through which parameters which give rise to the situation depicted in figure 5.4a can be identified is through calculation of the so-called "composite" sensitivities of all parameters that feature in the manually-regularized inverse problem and then comparing these sensitivities with each other. Those parameters whose composite sensitivities are low relative to those of other parameters are candidates for removal from the inversion process if that process seems to be feeling the deleterious effects of incipient inverse problem ill-posedness. A disadvantage of this statistic however is that it does not identify the problem that is depicted in figure 5.4b, for a parameter may have a high composite sensitivity but still be highly correlated with other parameters. However an advantage of the composite sensitivity statistic over eigen-analysis of the post-calibration parameter error covariance matrix is that it does not require calculation of that covariance matrix. Hence it can still be used even if the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix cannot be inverted.

The composite sensitivity of a parameter is the magnitude of the column of the $\mathbf{X}$ matrix pertaining to that parameter, with weighting taken into account. This is generally then divided by the number of observations featured in the parameter estimation process; that is, it is divided by the number of rows of $\mathbf{X}$. If the weighting matrix (i.e. the $\mathbf{Q}$ matrix) is diagonal, the composite sensitivity of parameter $i$ (i.e. $csp_i$) can therefore be calculated as

$$csp_i = \frac{\left[\sum_j^n q_{jj} x_{ji}^2\right]^{\frac{1}{2}}}{n} \qquad (5.3.1a)$$

Where $\mathbf{Q}$ is non-diagonal the composite sensitivity of parameter $i$ can be calculated as

$$csp_i = \frac{\left[\mathbf{X}^t\mathbf{Q}\mathbf{X}\right]_{ii}^{\frac{1}{2}}}{n} \qquad (5.3.1b)$$

In both of these equations $n$ is, as usual, the number of observations comprising the calibration dataset.

Hill and Tiedeman (2007) suggest normalization of the composite parameter sensitivity by dividing it by the value of the pertinent parameter. If a parameter is log transformed for the

purpose of parameter estimation (see below), this happens automatically. If parameters are subjected to Kahunen-Loève transformation prior to estimation then, once again, scaling occurs automatically.

Experience in using PEST suggests that if the ratio of highest to lowest composite parameter sensitivity is of the order of 200 or greater, then those parameters with lowest composite sensitivities should be removed from the manually-regularized inversion process as the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix is probably approaching singularity and is therefore invertible only with difficulty.

### 5.3.2 Analysis of Residuals

*5.3.2.1 Goodness of Fit*

Ideally, the goodness of fit attained through solution of an inverse problem should be commensurate with the level of measurement noise associated with the calibration dataset. If this level of fit cannot be attained, this suggests that the model may be somewhat defective in simulating environmental processes. To most environmental modellers this should come as no surprise. On the other hand, attainment of a higher level of fit than that expected on the basis of measurement noise is to be treated with extreme caution. Such "over-fitting" is often an indication of under-regularization and consequential inflation of post-calibration parameter error variance.

Where regularization is manual, it may not be model defects that are responsible for a less-than-pleasing fit between model outcomes and field measurements. An unsatisfactory model-to-measurement fit may result from excessively heavy-handed manual regularization whereby too few parameters are estimated in order to avoid problem ill-posedness. The details of the consequential parameter-simplification-induced misfit may suggest to the modeller how best to revise parameter definition in order to reduce this misfit on the next inversion run, without at the same time inducing inverse problem ill-posedness.

An often-used measure of fit between model outcomes and field measurements is referred to as the correlation coefficient (which should not be confused with the correlation coefficient defined in equation 3.5.3). It is calculated as

$$R = \frac{\left(\mathbf{Q}^{1/2}\mathbf{h} - \boldsymbol{\mu}_h\right)^t \left(\mathbf{Q}^{1/2}\mathbf{o} - \boldsymbol{\mu}_o\right)}{\left[\left(\mathbf{Q}^{1/2}\mathbf{h} - \boldsymbol{\mu}_h\right)^t \left(\mathbf{Q}^{1/2}\mathbf{h} - \boldsymbol{\mu}_h\right)\left(\mathbf{Q}^{1/2}\mathbf{o} - \boldsymbol{\mu}_o\right)^t \left(\mathbf{Q}^{1/2}\mathbf{o} - \boldsymbol{\mu}_o\right)\right]^{1/2}} \qquad (5.3.2)$$

where

$$\boldsymbol{\mu}_{hi} = \frac{\sum_{j=1}^{n}\left(\mathbf{Q}^{1/2}\mathbf{h}\right)_j}{n} \qquad \text{for all } i \qquad (5.3.3a)$$

and

$$\boldsymbol{\mu}_{oi} = \frac{\sum_{j=1}^{n}\left(\mathbf{Q}^{1/2}\mathbf{o}\right)_j}{n} \qquad \text{for all } i \qquad (5.3.3b)$$

*R* defined through (5.3.2) provides a measure of the extent to which variability of field measurements is explained by the calibrated model compared to that which can be construed

as purely random. Some modellers recommend that success of a calibration exercise should be judged on whether or not a certain correlation coefficient is attained (for example 0.9). It is the author's opinion however, that this statistic provides little assistance to the necessarily subjective process of judging the success or otherwise of the parameter estimation process. Its usefulness is further degraded where observations are of different types, and where observation weighting includes a subjective component which, in the author's opinion, is important to the success of the parameter estimation process in the presence of structural noise; see chapter 9.

*5.3.2.2 Statistical Analysis of Residuals*

Many texts on parameter estimation discuss methods through which post-calibration residuals can be analysed. Much of this analysis is undertaken in order to verify that assumptions regarding the statistical characterization of measurement noise are correct. When working with well-posed inverse problems (which, in the environmental context, are normally the outcomes of manual regularization) much may depend on this characterization. An appropriate weight matrix **Q** is formulated in a way that complements this characterization; see equation (5.2.6). Parameters are then estimated using formulas that include this weight matrix. The uncertainties associated with these estimates, and ultimately the uncertainties of model predictions, are also evaluated using formulas which include this weight matrix. Ultimately parameter and predictive uncertainty are attributed in large part, if not entirely, to measurement noise. Proper statistical characterization of measurement noise is thus essential.

As has been alluded to already, and as will be discussed later in this text, in most environmental modelling contexts the bulk of model-to-measurement misfit cannot be attributed to noise associated with the making of measurements. In fact, it is attributable to shortcomings of a model as a simulator of complex environmental behaviour. If calibration is based on manual regularization, parameter simplification can also introduce substantial amounts of structural noise. The covariance matrix of structural noise is unknown, and is probably singular. Statistical characterization of what is mostly a deterministic quantity is generally impossible. Much of the theory on which manually-regularized parameter estimation and uncertainty quantification is based is therefore invalidated.

For complex models that simulate system state, and changes to system state, at many different locations in a three-dimensional model domain, it is unlikely that quantitative post-calibration analysis of residuals will do anything other than invalidate statistical characterizations of measurement noise upon which construction of a weight matrix is based. Hence methodologies for residuals analysis are not discussed herein. This is not meant to suggest that a modeller should not inspect residuals carefully in space and in time, and draw whatever conclusions that he/she can about model or parameterization inadequacy from differences between model outputs and true system behaviour. This, in fact, is an essential component of good calibration practice. It is suggested however that a serious statistical analysis of residuals is unlikely to yield results that are useful to the history-matching process.

While this may seem at first to be a rather depressing conclusion, the situation should be seen in context. An important feature of this context is that for many predictions of management interest, predictive uncertainty is not so much a function of measurement noise as it is of information deficits in the calibration dataset. Integrity of characterization of predictive uncertainty therefore depends more on proper characterization of prior parameter uncertainty

than it does on the stochastic character of measurement noise. A second redeeming feature is that formulation of an objective function in most real world modelling contexts will often be a matter that requires considerable subjectivity and more than a little creativity. The objective function will often be at least partly formulated in such a way as to compare observations which are processed in some way with respective model outputs which are processed in the same manner. As will be discussed in chapter 9, such a strategy can mitigate some of the more deleterious impacts of structural noise by partially filtering out those aspects of it which have too much structure and too little stochasticity. Weighting of different components of an objective function formulated in this way is a necessarily subjective matter. Some of this subjectivity is unavoidably inherited by values ascribed to estimated parameters, and by assessments of the uncertainties associated with these estimates. With acknowledgement of the necessarily high subjective input into history-matching in particular, and environmental modelling in general, comes the freedom to dispense with certain aspects of quantitative analysis that are unlikely to add much value to the overall process.

### 5.3.3 Influence Statistics

*5.3.3.1 Background*

A number of statistics have been developed for comparing the relative information content of different observations comprising the calibration dataset. These have been designed for use in the over-determined parameter estimation context that is the subject of the present chapter. As such, they inherit limitations which pertain to manual regularization as a device for solution of inverse problems in the environmental modelling context. These limitations will be discussed later in this chapter. It is worth noting, however, that the need for excessive manual regularization may be mitigated if a large number of parameters is retained in the parameter estimation process while, at the same time, supplementing the calibration dataset with correctly weighted prior information; see equation (5.2.33). This, of course, introduces the problem of ensuring correct relativity of weighting between prior information and measurements of system state when formulating the overall objective function. This too will be discussed later.

It is of interest to note that some of the statistics that are discussed in the present and previous sections of this chapter (and many statistics that will be discussed in future chapters of this text) require only sensitivities of model outputs with respect to adjustable model parameters as encapsulated in the **X** matrix; they do not require that actual parameter values be supplied or that measurement values be provided. These statistics can thus be employed even if a model has not been calibrated, and even if data that will comprise an hypothesized calibration dataset has not been gathered. In this context they can be used to examine the benefits of a future calibration process, and inquire into the source of these benefits. Where required, estimates of the objective function that will be achieved in the future calibration process can be guessed; this guess can be supported by an assessment of the amount of measurement noise that the real or posited calibration dataset is likely to carry.

In real world modelling practice, where earth system behaviour and the models which simulate this behaviour are nonlinear, the **X** matrix on which calibration-pertinent statistics are based must be replaced by a Jacobian matrix. Ideally this matrix should be calculated using a parameter set that is the outcome of a model calibration process. If a model is truly linear the Jacobian matrix does not, of course, vary with parameter values. If a model is

nonlinear this is not the case. Nevertheless, if a model has not yet been calibrated, an **X** matrix that is calculated using non-calibrated parameters can suffice for formulation of some of the statistics discussed in the present section and many of those discussed in later chapters of this book. Prior parameter expected values constitute a sound basis for calculation of the **X** matrix under these circumstances.

The following discussion is brief. Those interested in this topic should refer to Hadi (1982), Yager (1998), Cook and Weisberg (1982), and Belsley et al (1980) for further details.

*5.3.3.2 The Statistics*

The composite observation sensitivity constitutes a crude influence statistic. This complements the composite parameter sensitivity discussed above. It is the magnitude of the row of the **X** matrix corresponding to the observation of interest, divided by the number of parameters. Where the weight matrix is diagonal the composite sensitivity of observation *i* can be written as follows.

$$cso_i = \frac{q_i\left[\sum_j^m x_{ij}^2\right]^{\frac{1}{2}}}{m} \qquad (5.3.4a)$$

Here *m* is the number of parameters featured in the manually-regularized calibration process. More generally

$$cso_i = \frac{\left[\mathbf{Q}^{1/2}\mathbf{X}\mathbf{X}^t\mathbf{Q}^{1/2}\right]_{ii}^{1/2}}{m} \qquad (5.3.4b)$$

If the composite sensitivity of an observation is low, then the model output which corresponds to that observation is sensitive to no parameter. As a consequence the observation carries little information with respect to any parameter.

For the remainder of this section we will employ the mathematical characterization of the inversion process introduced above that endows (transformed) measurement noise with a covariance matrix that is proportional to **I**; see equation (5.2.20) and subsequent equations. This simplifies the equations to follow.

Let the matrix **H** be defined as follows

$$\mathbf{H} = \mathbf{Y}(\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y} \qquad (5.3.5)$$

Recall from section 5.2.6 that **H** is an orthogonal projection operator onto model output space. Equation (5.2.40) can now be re-written as

$$\underline{\mathbf{e}} = \mathbf{H}\mathbf{g} \qquad (5.3.6)$$

Recall also that $\underline{\mathbf{e}}$ is the vector of outputs calculated by the calibrated model that correspond to members of the calibration dataset, while **g** comprises the calibration dataset itself. The covariance matrix of $\underline{\mathbf{e}}$ can be calculated as

$$C(\underline{\mathbf{e}}) = \mathbf{H}C(\mathbf{g})\mathbf{H}^t \qquad (5.3.7)$$

The covariance matrix of **g** is simply the covariance matrix of $\xi$, that is the covariance matrix of weight-transformed measurement noise. This is $\sigma^2_r\mathbf{I}$. Hence

$$C(\underline{\mathbf{e}}) = \sigma^2_r \mathbf{H}\mathbf{H}^t = \sigma^2_r \mathbf{H} \tag{5.3.8}$$

Similarly, for residuals $\underline{\mathbf{f}}$ pertaining to the calibrated model (see equation 5.2.38)

$$C(\underline{\mathbf{f}}) = \sigma^2_r(\mathbf{I} - \mathbf{H}) \tag{5.3.9}$$

The variance of the *i*'th element of $\underline{\mathbf{e}}$ divided by the variance of the *i*'th element of $\underline{\mathbf{f}}$ is denoted as the "leverage" of observation *i*. From (5.3.8) and (5.3.9) it is readily calculated as

$$L_i = \frac{h_{ii}}{1-h_{ii}} \tag{5.3.10}$$

where, of course, $h_{ii}$ is the *i*'th diagonal element of **H**.

The Cook's D statistic takes the value of a weighted residual specifically into account when computing the influence of the corresponding observation. The Cook's D statistic for observation *i* can be thought of as the relative distance between the centre of confidence ellipsoids for $\underline{\mathbf{p}}$ based on the full calibration dataset on the one hand, and the centre of the confidence ellipsoids for $\underline{\mathbf{p}}$ based on a calibration dataset with observation *i* omitted on the other hand. (This concept is easily extended to the omission of more than one observation from the calibration dataset.) It is calculated as

$$D_i = \frac{1}{m} v_i^2 \frac{h_{ii}}{1-h_{ii}} \tag{5.3.11}$$

Where *m* is the number of parameters, and $v_i$ is the weighted "studentized" residual corresponding to observation *i*. The latter is computed as

$$v_i = \frac{\underline{f}_i}{\underline{\sigma}_r \sqrt{1-h_{ii}}} \tag{5.3.12}$$

$\underline{\sigma}_r$ is the square root of the reference variance $\underline{\sigma}^2_r$ estimated from the minimized objective function using equation (5.2.18).

Focusing on outliers, Hadi (1982) suggests the following statistic for characterizing the influence of the *i*'th observation on estimated parameters as a whole

$$H_i^2 = \frac{m}{1-h_{ii}} \frac{\underline{f}_i^2}{\left(\underline{f}^t \underline{f} - \underline{f}_i^2\right)} + \frac{h_{ii}}{1-h_{ii}} \tag{5.3.13}$$

$DFBETAS_{ij}$ is a measure of the influence of observation *i* on estimated parameter *j*. It is calculated as

$$\beta_{ij} = \frac{c_{ji}}{\sqrt{\sum_{k=1}^{n} c_{jk}^2}} \frac{\underline{f}_i}{s(i)(1-h_{ii})} \tag{5.3.14}$$

where $c_{jk}$ is an element of the matrix product $\mathbf{C} = (\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t$. $s(i)$ is calculated as follows (Belsley et al, 1980)

$$s^2(i) = \frac{1}{(n-m-1)} \left[ (n-m)\underline{\sigma}_r^2 - \frac{\underline{f}_i^2}{1-h_{ii}} \right] \tag{5.3.15}$$

Much more will be said on the subject of data worth in chapter 7 of this document. There the discussion will focus on assessment of data worth in highly parameterized contexts wherein the null space may contribute substantially to parameter and predictive uncertainty.

## 5.4 Nonlinear Models

### 5.4.1 The Jacobian Matrix

The theory presented so far in this chapter assumes that the relationship between parameters **p** of a model and model outputs **o** to which there are corresponding field measurements **h** is linear, and hence can be represented by a matrix operation. In the over-determined context made possible by manual regularization, that matrix has been designated as **X**. Theory presented above has demonstrated how a parameter set $\underline{\mathbf{p}}$ that supposedly satisfies the calibration metric stated in section 4.4 of this text can be estimated from **h**. (We will review whether this metric can really be met in the manually-regularized context later in this chapter.) Formulas were derived for calculation of the post-calibration parameter error covariance matrix C($\underline{\mathbf{p}}$ - **p**). Strategies were presented for discerning the well-posedness or otherwise of the manually-regularized inverse problem. Means through which the influence of different observations on the parameter estimation process could be assessed were provided. Equations which underpin all of these calculations use the matrix **X**.

A nonlinear model must be linearized before any of the theory presented above can be implemented. This is achieved through replacing the **X** matrix featured in the above equations with the Jacobian matrix. See section 4.5.1 for specifications of the Jacobian matrix. For a nonlinear model this matrix is a function of parameter values. The parameter values on which its computation should be based depend on what it is being computed for. If it is being computed during one iteration of an objective function minimization procedure, then parameter values pertaining to the current iteration of that procedure should be used in its calculation. If it is being computed in order to calculate the post-calibration parameter error covariance matrix, then parameter values estimated through the calibration process should be used in its calculation. The same applies to calculation of observation influence statistics. In some cases formulas for the latter require values of minimized residuals as well; obviously their calculation should be preceded by a calibration exercise in which both optimized parameters and optimized residuals are calculated.

There may be occasions, however, where some of the equations presented above are deployed in contexts that are not preceded by estimation of parameters. This may occur, for example, where a modeller would like to obtain estimates of calibration-constrained parameter error variance, and/or establish the well-posedness or otherwise of a manually-regularized inverse problem, before actually attempting the inversion. In this case Jacobian matrix calculation may be based on prior expected parameter values.

Statistics such as post-calibration parameter error variance calculated for a nonlinear model using a linearized substitute for that model are, of course, likely to be approximate. Nevertheless they may be useful. If, for example, the ratio of highest to lowest eigenvalue of a post-calibration parameter error covariance matrix indicates ill-posedness of the inverse problem, then the problem is indeed ill-posed as charged. Parameters identified as being responsible for its ill-posedness through being either individually insensitive, or through

being part of a group of parameters identified as making major contributions to an eigenvector whose corresponding eigenvalue is very large, are indeed problematic. Attention must therefore be given to these parameters when formulating a revised manual regularization strategy. Linear estimates of post-calibration parameter error variance may indeed be approximately correct; as will be discussed in later chapters however, the linearized post-calibration parameter error covariance matrix can provide a useful starting point for more robust nonlinear analysis. Meanwhile comparative parameter error variances provided by this matrix are likely to be valid.

It is in the inversion process itself where the need for modification of linear theory is most urgent. It is to this topic that we now turn.

### 5.4.2 Nonlinear Parameter Estimation

The means by which the linear theory presented so far can be adapted to estimation of parameters of a nonlinear model is now addressed.

#### *5.4.2.1 Formulation of Equations*

As has already been discussed, where a model is nonlinear the parameter estimation process becomes an iterative procedure. This is schematized for a two-parameter model in figure 5.5.

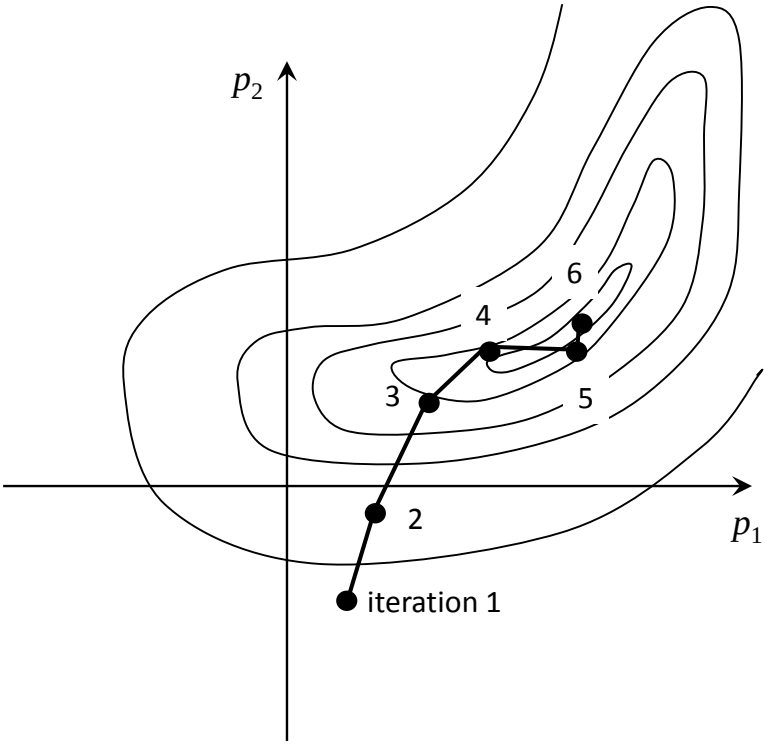


**Figure 5.5. Iterative adjustment of parameters toward the objective function minimum during a nonlinear parameter estimation process.**

During each iteration of the objective function minimization process, equation (5.2.9) is used to improve the values assigned to parameters from those which they inherit from the previous iteration. Parameter improvements are obtained using the following formula

$$\mathbf{p} - \mathbf{p}_0 = (\mathbf{J}^t\mathbf{Q}\mathbf{J})^{-1}\mathbf{J}^t\mathbf{Q}\mathbf{r} \qquad (5.4.1)$$

In equation (5.4.1) $\mathbf{p}_0$ designates parameter values at the start of the iteration while **r** designates model-to-measurement residuals calculated using the $\mathbf{p}_0$ parameter set. **J** is the Jacobian matrix calculated using the $\mathbf{p}_0$ parameter set.

*5.4.2.2 The Marquardt Lambda*

Use of equation (5.4.1) directly to estimate parameters for a nonlinear model is numerically inefficient. In practice, the diagonal terms of the $\mathbf{J}^t\mathbf{Q}\mathbf{J}$ matrix are enhanced through use of the following equation to calculate parameter improvements

$$\mathbf{p} - \mathbf{p}_0 = (\mathbf{J}^t\mathbf{Q}\mathbf{J} + \lambda\mathbf{I})^{-1}\mathbf{J}^t\mathbf{Q}\mathbf{r} \qquad (5.4.2)$$

$\lambda$ is the so-called "Marquardt parameter", or simply "Marquardt lambda", named after Marquardt (1963) who employed this strategy. However use of this parameter was, in fact, pioneered by Levenberg (1944).

Suppose that $\lambda$ is very high. Then (5.4.2) becomes

$$\mathbf{p} - \mathbf{p}_0 = \lambda^{-1}\mathbf{J}^t\mathbf{Q}\mathbf{r} \qquad (5.4.3)$$

It is not difficult to show that the gradient of the objective function in parameter space is given by

$$\nabla\Phi = \begin{bmatrix} \frac{\partial\Phi}{\partial p_1} \\ \frac{\partial\Phi}{\partial p_2} \\ \dot{} \\ \frac{\partial\Phi}{\partial p_m} \end{bmatrix} = -2\mathbf{J}^t\mathbf{Q}\mathbf{r} \qquad (5.4.4)$$

Equation (5.4.3) states that if the Marquardt lambda is very high, then the parameter estimation process simply moves parameters down the objective function gradient. Also, the higher is the Marquardt lambda, the less movement takes place.

Moving down-gradient makes sense early in the parameter estimation process. This accommodates non-ellipticity of the objective function contours arising from model nonlinearity. However as the objective function minimum is approached, efficiency of the objective function minimization process requires that the Marquardt lambda be decreased. This avoids the phenomenon of "hemstitching", which is shown schematically in figure 5.6. The threat posed by hemstitching is especially high where objective function contours are long and narrow. A strength of equation (5.4.2) is that parameter estimation is able to proceed with great efficiency even where the objective function surface is characterized by this type of topography.

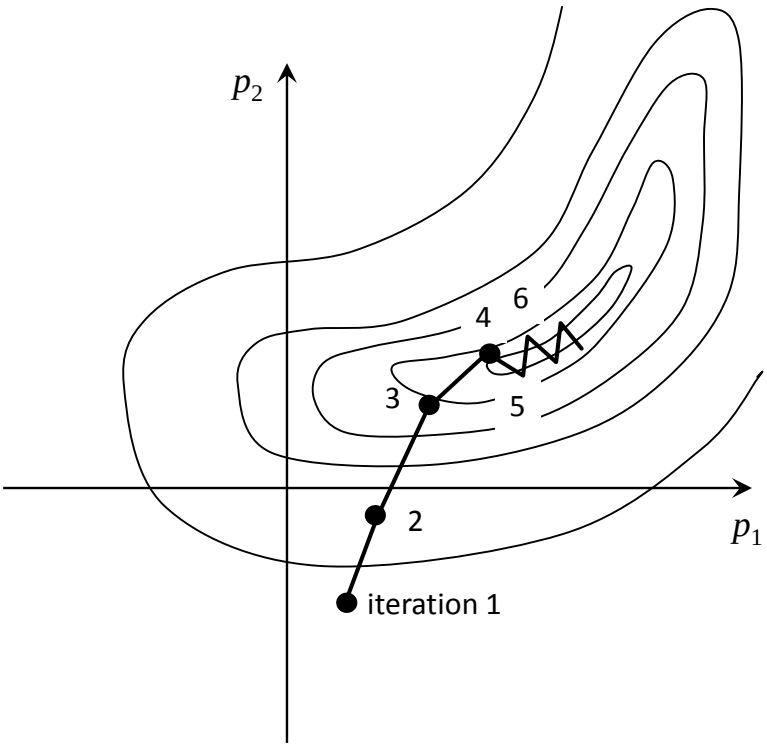


**Figure 5.6. "Hemstitching" in search of the objective function minimum.**

It follows from the above discussion that a nonlinear parameter estimation process should commence with the Marquardt lambda set to a value which is large enough to promulgate a reasonable component of direct down-gradient movement of parameters. However as the parameter estimation process progresses, the Marquardt lambda should ideally decrease in value; this allows the parameter estimation process to squeeze into narrow objective function valleys if this is required.

Parameter estimation based on equation (5.4.2) is variously referred to as the "Gauss-Marquardt-Levenberg", "Levenberg-Marquardt", or "damped least squares" method. Alternative implementations of this method differ in the way that the Marquardt lambda is calculated at different stages of the parameter estimation process. PEST implements a trial and error procedure that makes maximum use of spare computing capacity in a parallel environment.

Some numerical advantages can be gained by modifying equation (5.4.2) to prevent corruption of the parameter estimation process by numerical round-off errors. Let **S** be a square $m \times m$ matrix (where $m$ is the number of parameters featured in the parameter estimation process) with diagonal elements only. Let the $i$'th diagonal element of **S** be given by

$$s_{ii} = (\mathbf{J}^t\mathbf{Q}\mathbf{J})_{ii}^{-1/2} \qquad (5.4.5)$$

If **S** is introduced into equation (5.4.2) the following equation is obtained for $\mathbf{S}^{-1}(\mathbf{p} - \mathbf{p}_0)$

$$\mathbf{S}^{-1}(\mathbf{p} - \mathbf{p_0}) = ((\mathbf{JS})^t\mathbf{QJS} + \lambda\mathbf{S}^t\mathbf{S})^{-1}(\mathbf{JS})^t\mathbf{Qr} \qquad (5.4.6)$$

It can be shown that although equation (5.4.6) is mathematically equivalent to equation (5.4.2) it is numerically superior. If $\lambda$ is zero, all of the diagonal elements of $(\mathbf{JS})^t\mathbf{QJS} + \lambda\mathbf{S}^t\mathbf{S}$ are equal to unity. For a non-zero $\lambda$ the diagonal elements of $(\mathbf{JS})^t\mathbf{QJS} + \lambda\mathbf{S}^t\mathbf{S}$ are greater than

unity, though in general they will not be equal. Let the largest element of $\lambda\mathbf{S}^t\mathbf{S}$ be denoted as $\lambda_p$. This is the value that PEST reports as its Marquardt lambda. Then the largest diagonal element of $(\mathbf{JS})^t\mathbf{QJS} + \lambda\mathbf{S}^t\mathbf{S}$ is equal to $1 + \lambda_p$.

As well as being useful in adjusting the direction of parameter improvement during the early stages of the parameter estimation process where that process is not able to "see" the closed contours of the objective minimum at the bottom of the objective function valley, the Marquardt lambda has a secondary role. This is a role that it probably should not have, but can be extremely valuable nevertheless.

If the $\mathbf{J}^t\mathbf{QJ}$ matrix of equation (5.4.2) cannot be inverted, then the addition of positive terms to its diagonal renders it invertible. The Marquardt lambda thus becomes a primitive regularization device. If the Marquardt lambda is assigned values on a trial and error basis (as PEST does), the amount of applied regularization can be adjusted to suit the need for regularization at any particular point during the iterative parameter estimation process. Ideally, regularization should not be applied in such an ad hoc fashion. Nevertheless, where model nonlinear behaviour is such that sensitivities encapsulated in the **J** matrix can vary greatly from iteration to iteration, then singularity of $\mathbf{J}^t\mathbf{QJ}$ can occur unexpectedly. Temporary non-invertibility of this matrix may then bring the parameter estimation process to a halt. However with the Marquardt lambda restoring the invertibility status of $\mathbf{J}^t\mathbf{QJ}$, another set of parameters can be calculated for use in the next iteration of the parameter estimation process; in many contexts this allows the overall parameter estimation process to then proceed without further problems.

In some modelling contexts the Marquardt lambda can play yet another useful role. If an environmental model has problematic numerical behaviour (for example if its solver experiences convergence difficulties), the integrity of finite-difference derivatives that are used to fill the Jacobian matrix may be compromised. Through trial-and-error variation of the Marquardt lambda, a direction of parameter improvement may nevertheless be found in spite of the fact that no parameter improvement at all may be forthcoming from direct application of equation (5.4.1).

### *5.4.2.3 Optimum Length of the Parameter Upgrade Vector*

A parameter upgrade vector is calculated during every iteration. Actually, PEST calculates a number of different parameter upgrade vectors, each based on a different value of the Marquardt lambda; that which provides the largest reduction in the objective function is used for calculation of parameters to take into the next iteration.

Let the (Marquardt-lambda dependent) parameter upgrade vector be designated as **u**. Thus

$$\mathbf{u} = \mathbf{p} - \mathbf{p}_0 \qquad (5.4.7)$$

The optimal length of this vector can be calculated using information that is available through local model linearization. Let the new set of parameters be actually calculated as

$$\mathbf{p} - \mathbf{p}_0 = \alpha\mathbf{u} \qquad (5.4.8)$$

By varying α, the magnitude of parameter movement in the direction of the parameter upgrade vector can also be varied. As has already been discussed, the objective function Φ, whose task it is for the parameter estimation process to minimize, is calculated as

$$\Phi = \mathbf{r}^t\mathbf{Qr} \qquad (5.4.9)$$

Suppose that model outputs are $\mathbf{o}_0$ when model parameters are $\mathbf{p}_0$. When parameters are updated to $\mathbf{p}$ using (5.4.8) a linear approximation to updated residuals can be computed as

$$\mathbf{r} = \mathbf{h} - [\mathbf{o}_0 + \alpha\mathbf{J}(\mathbf{p} - \mathbf{p}_0)] = \mathbf{r}_0 - \alpha\mathbf{J}\mathbf{u} \qquad (5.4.10)$$

where the $\mathbf{r}_0$ vector denotes current residuals (i.e. residuals corresponding to parameters $\mathbf{p}_0$). The objective function then becomes

$$\Phi = (\mathbf{r}_0 - \alpha\mathbf{J}\mathbf{u})^t\mathbf{Q}(\mathbf{r}_0 - \alpha\mathbf{J}\mathbf{u}) \qquad (5.4.11)$$

After multiplication and collecting terms this becomes

$$\Phi = \mathbf{r}^t_0\mathbf{Q}\mathbf{r}_0 - 2\alpha\mathbf{r}^t_0\mathbf{Q}\mathbf{J}\mathbf{u} + \alpha^2\mathbf{u}^t\mathbf{J}\mathbf{Q}\mathbf{J}\mathbf{u} \qquad (5.4.12)$$

If this equation is now differentiated with respect to α, and the differential set to zero (as this minimizes Φ), we obtain the optimal factor by which to multiply the length of the parameter upgrade vector. This is

$$\alpha = \frac{\mathbf{r}_0^t\mathbf{Q}\mathbf{J}\mathbf{u}}{\mathbf{u}^t\mathbf{J}^t\mathbf{Q}\mathbf{J}\mathbf{u}} \qquad (5.4.13)$$

*5.4.2.4 Broyden's Jacobian Update*

Each iteration of the nonlinear parameter estimation process is effectively divided into two parts. During the first part of each iteration the Jacobian matrix is calculated. During the second part of each iteration the optimal direction and length of the parameter upgrade vector are determined. As implemented in PEST, this second segment of each iteration requires that a number of model runs be undertaken as different values assigned to the Marquardt lambda are tested in order to establish that which is most effective in lowering the objective function. The best set of upgraded parameters, as well as the lambda that achieved it, are then inherited by the next iteration of the nonlinear parameter estimation process.

When a model is run in order to test a parameter upgrade, this provides an opportunity to compare changes to model outputs computed using the Jacobian matrix to those which actually occur. The difference between predicted and actual changes can then be used to partially correct the Jacobian matrix so that it is more effective in upgrading parameters in directions that are similar to that of the parameter upgrade that was just attempted. If the directions of parameter upgrades computed on the basis of different Marquardt lambdas are not too different from each other, improvements made to the Jacobian matrix based on lessons learned in testing one Marquardt lambda may make calculation of the next upgrade vector based on the next Marquardt lambda more effective.

Let $(\mathbf{p}_n - \mathbf{p}_0)$ denote the upgrade vector calculated using one particular value of the Marquardt lambda. The subscript "n" stands for "new" while the "0" subscript indicates current parameter values. If the model were linear then the altered model outputs could be calculated from the existing Jacobian matrix as

$$\mathbf{o}_n = \mathbf{o}_0 + \mathbf{J}(\mathbf{p}_n - \mathbf{p}_0) \qquad (5.4.14)$$

Let model outputs as calculated by the actual model be designated as $\mathbf{o}_m$. The difference between actual and linear-predicted model outputs, divided by the norm of the difference in parameter values that was responsible for the change in outputs, is calculated as

$$\mathbf{w} = \frac{\mathbf{o}_m - \mathbf{o}_0 - \mathbf{J}(\mathbf{p}_n - \mathbf{p}_0)}{(\mathbf{p}_n - \mathbf{p}_0)^t(\mathbf{p}_n - \mathbf{p}_0)} \quad (5.4.15)$$

An updated Jacobian matrix $\mathbf{J}_n$ can then be calculated as

$$\mathbf{J}_n = \mathbf{J} + \mathbf{w}(\mathbf{p}_n - \mathbf{p}_0)^t \quad (5.4.16)$$

For the *i*'th model output $o_i$ of **o**, equation (5.4.16) distributes the correction to the Jacobian matrix among parameters in proportion to the relative amount that each parameter is featured in the upgrade direction.

### *5.4.2.5 Restricting Parameter Movement*

Notwithstanding use of the Marquardt lambda to accommodate nonlinear model behaviour, calculation of parameter upgrades still relies heavily on the assumption of model linearity. This assumption is workable if parameters don't need to change too much during any iteration of the nonlinear parameter estimation process. However if a parameter change vector is calculated whose length grossly exceeds the region of applicability of the linearity assumption on which its calculation rests, then the objective function may rise instead of fall as the upgrade vector crosses the objective function valley and proceeds up the other side of the objective function hill. On the next iteration of the nonlinear parameter estimation process, a new parameter upgrade vector will be calculated which tries to correct the previous overshoot. The result may be over-correction and another overshoot of the objective function valley.

This problem can be prevented by placing limits on the length of the parameter upgrade vector. Different parameter estimation packages differ in how they do this. PEST offers a number of options. The length of the upgrade vector may be limited such that

- the value of no parameter alters by more than a certain factor;
- the value of no parameter alters by more than a certain fraction of its current value;
- no parameter changes by more than a certain parameter-specific amount.

In all cases the direction of the parameter upgrade vector as calculated by the procedures described above is not altered. Only the length of the upgrade vector is changed.

Another methodology for preventing parameter overshoot on successive iterations is through detecting parameters whose changes on successive iterations are of opposite sign, and then subjecting such parameters to especially strong damping. PEST implements this kind of damping using a method described by Cooley (1983) and implemented in Hill (1992).

### *5.4.2.6 Parameter and Observation Transformations*

The more linear is a model's behaviour, the more efficient is the Gauss-Marquardt-Levenberg method in minimizing the objective function on which the calibration process is based. There are many modelling contexts in which linearity can be more closely approached if parameters and/or observations are appropriately transformed prior to being used in the parameter estimation process. Logarithmic transformation of parameters is often highly effective in this regard, particular for parameters such as permeability and electrical resistivity whose values can span many orders of magnitudes.

Sometimes particular care also needs to be taken in definition of observations. For example, rate of spring flow may comprise part of the observation dataset used to calibrate a

groundwater model. However if model-calculated heads are below the level of the spring, then model-calculated spring flow will be zero; at the same time the sensitivity of model-calculated spring flow to changes in parameter values will be zero if no spring flow actually occurs. Problems associated with such "asymmetric observations", and means by which they can be ameliorated, are discussed in chapter 10 of this book. For the spring example, the actual spring flow observation may need to be supplemented with an observation that groundwater head is at the elevation of the spring. The residual for this supplementary observation will be positive if the model-calculated head is below the level of the spring, and the spring is therefore not flowing; this observation will indeed be sensitive to at least some model parameters when the spring flow observation is not. See chapter 10 for more details.

### *5.4.2.7 Parameter Bounds*

Bounds are normally placed on values taken by parameters during the inversion process for one of two reasons. One reason is to prevent them from adopting values that will cause a model to crash. For example, a groundwater or subsurface reservoir model is unlikely to tolerate a negative value supplied for porosity; similarly, a surface water model is unlikely to tolerate a negative value supplied for soil moisture zone store volume. The other reason for which a modeller may wish to place bounds on values taken by parameters is to prevent the parameter estimation process from endowing parameters with values which a modeller believes to be unrealistic.

Numerically, the imposition of bounds on parameters requires more than simply replacing the value of a parameter that has transgressed its bound with the value of the bound that it has transgressed. The bounds imposition algorithm implemented by PEST is more sophisticated than this. If a parameter upgrade vector **u** is calculated which would cause a parameter to move beyond its upper or lower bound, PEST reduces the length of the upgrade vector **u** such that this does not occur. The offending parameter is thereby placed at its bound. On later iterations, special treatment is then provided for this, and any other parameters, which are at their allowed limits. If the components of both the upgrade vector and the negative of the gradient vector pertaining to a parameter which is at its upper or lower limit are such as to take the parameter further out of bounds, then the parameter is temporarily frozen at its bound and the parameter estimation problem is reformulated accordingly with that parameter omitted from the reformulated inverse problem; hence the new upgrade vector will not result in any adjustment of that parameter. If, after reformulation of the problem in this manner, there are other parameters at their limits for which the parameter upgrade vector still points outward, but for which the negative of the gradient vector points inward, then these parameters, too, are temporarily frozen at their respective bounds. This process continues until a parameter upgrade vector is calculated which either moves parameters from their bounds back into the allowed parameter domain, or leaves them fixed.

The strength of this strategy is that it allows PEST to search along the boundaries of the user-limited parameter domain for the smallest objective function to which it has access, in spite of the fact that the global minimum of the objective function may lie outside that part of parameter space to which PEST is granted access.

At the beginning of each new iteration of the nonlinear parameter estimation process all temporarily-frozen parameters are freed. This allows them to move back inside the permitted part of parameter space if solution of equation (5.4.2) deems this necessary. The stepwise, temporary freezing of parameters is then repeated as described above.

Figure 5.7 schematizes parameter trajectories where the objective function minimum lies outside that part of parameter space wherein parameters are allows to roam.

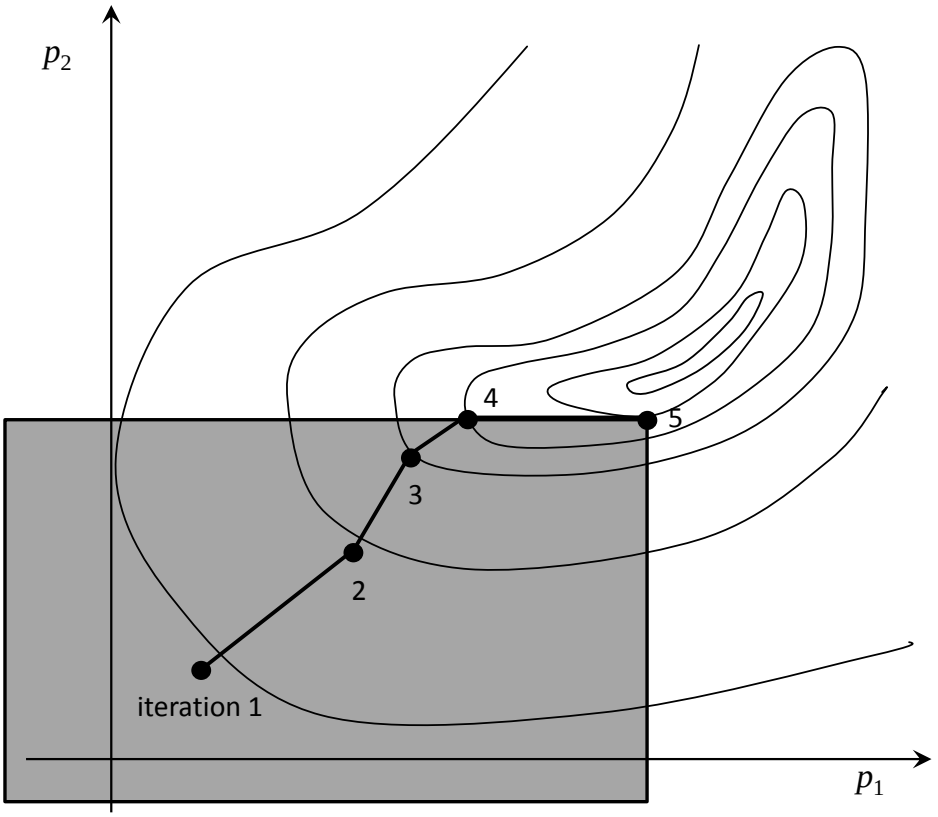


**Figure 5.7. The shaded region shows that part of parameter space that is bounded by user-supplied upper and lower parameter limits. Also shown is the trajectory taken by parameters during the parameter estimation process.**

Care should be taken when imposing bounds on parameters. In many instances of manually-regularized parameter estimation, bounds act as a de-facto regularization device. It is often the problematic parameters (i.e. parameters whose composite sensitivities are small or that share occupancy of an eigenvector whose eigenvalue is unduly large) that equation (5.4.2) deems to require the largest alterations. This, of course, follows from the fact that large alterations to individually or collectively insensitive parameters are required if the objective function is to improve. More often than not, these parameters are virtually inestimable, and should have been fixed at their prior expected values prior to embarking on the parameter estimation process. However if a wayward parameter encounters its bound, and is effectively removed from the parameter estimation process, this has the same regularising effect as that which a modeller would introduce to the parameter estimation process if he/she had fixed the parameter him/herself. However fixing the parameter at its limiting value constitutes a far inferior form of regularization than fixing the parameter at its prior expected value. "Regularization by bounds" is thus not a recommended procedure, as estimated parameter values can hardly claim a status of minimum error variance.

## 5.5 Critique of Manual Regularization

In the next chapter of this book the focus shifts to mathematical regularization. Meanwhile,

the present chapter has assumed that parameter uniqueness is achieved through manual regularization. In the author's opinion, mathematical regularization provides a far better means of achieving parameter uniqueness. A solution to an inverse problem achieved through mathematical regularization normally has a greater right to claim a status of minimum error variance than that achieved through manual regularization. Furthermore, when regularized mathematically, model calibration can take place in a highly-parameterized context wherein the process complexity of environmental simulators is partnered with parameterization complexity that respects the natural heterogeneity of the real world.

Prior to introducing mathematical regularization, the shortcomings of manual regularization are first discussed in detail.

### 5.5.1 Man-Made Structural Noise

This chapter has discussed how inverse problem well-posedness can be achieved manually. It has also discussed how some of the vectors and matrices that are an outcome of the manually-regularized inversion process can be analysed to check whether the problem is in fact well-posed. The analysis presented in this chapter is based on the concept that the following equation describes the action of the model under calibration conditions

$$\mathbf{h} = \mathbf{X}\mathbf{p} + \boldsymbol{\varepsilon} \qquad (5.5.1)$$

It is also assumed that a statistical description of measurement noise is available, and that this is encapsulated in a covariance matrix $C(\boldsymbol{\varepsilon})$. As has been discussed, knowledge of $C(\boldsymbol{\varepsilon})$ is important. It provides the basis for choice of a weighting matrix $\mathbf{Q}$ that supports the search for a minimum error variance solution $\underline{\mathbf{p}}$ to the inverse problem. It also underpins quantification of that error variance. The latter is expressed through the post-calibration parameter error covariance matrix $C(\underline{\mathbf{p}} - \mathbf{p})$.

The present chapter has shown how the Gauss-Marquardt-Levenberg method can be used to solve the inverse problem posed by equation (5.5.1). Other methods can also be used, including so-called global methods that do not rely on calculation of a Jacobian matrix. Generally these are not nearly as numerically efficient as the Gauss-Marquardt-Levenberg method; however they can accommodate high degrees of model nonlinearity and poor model numerical behaviour. Alternatively, a modeller may dispense with the quest for uniqueness and employ a Bayesian methodology such as Markov chain Monte Carlo to sample the posterior probability distribution of $\mathbf{p}$; the mean of this posterior distribution can be considered as the $\underline{\mathbf{p}}$ that is sought in the present chapter.

Regardless of the method that is employed to solve the problem posed by (5.5.1), and regardless of the methodology that is adopted to quantify the uncertainty or potential for error in that solution, the imperative to weight individual members of the calibration dataset in a way that reflects their credibility remains. Thus a modeller cannot avoid the task of adopting either a $C(\boldsymbol{\varepsilon})$ matrix, or a matrix that is proportional to it; in the latter case the constant of proportionality $\sigma^2_r$ can be estimated as part of the inverse problem solution procedure. Normally $C(\boldsymbol{\varepsilon})$ is specified as a diagonal matrix; this choice rests on the assumption that errors afflicting different measurements of system state that comprise a calibration dataset are independent of each other.

Calibration of just about any environmental model inevitably leads to the discovery that the level of model-to-measurement misfit achieved through the calibration process is far greater than can be explained by measurement noise alone. In fact misfit is often dominated by a so-

called structural component. This reflects the fact that a numerical model is a less-than-perfect simulator of complex environmental processes that are operative at a particular study site. It also reflects the fact that the parameterization scheme employed by an environmental model does not encapsulate the complex spatial variability of physical/chemical properties that characterize that system.

Equation (5.1.10) shows the component of this structural noise term that arises from parameter simplification. A challenge that faces manual regularization is how to make this term as small as possible while still achieving a matrix **X** to use in place of the "real" model matrix **Z** for which the matrix $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ is invertible. However this is not the only condition that **X** must satisfy. Not only must $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ be invertible; post-calibration parameter error variances must be smaller than pre-calibration parameter variances.

Manual attainment of an appropriate **X** matrix is normally hard work, requiring much laborious trial and error. On the one hand a modeller wants to reduce structural noise to a minimum. On the other hand, all attempts to do so by increasing the number of parameters that are estimated through the inversion process increase the chances that the resulting **X** matrix will either be rank-deficient (i.e. it will possess a null space), or that the error variance of some parameters will be amplified rather than diminished through the inversion process.

The question must be asked "why manufacture structural noise through manual parameter simplification when mathematical regularization can promise far lower levels of regularization-induced structural noise?" Of course parameter simplification is not the only model structural defect whose presence can engender structural noise; the model itself is a simplification of reality - a matter that will receive more attention in chapter 9. To mitigate structural noise arising from model defects, modellers often deploy complex simulators that are sometimes characterized by high run times and problematic numerical behaviour. The above question then becomes even more salient. Why drape a simplistic parameterization scheme over the domain of a complex model, thereby eroding the capacity of that model to replicate the historical behaviour of the environmental system that it purports to represent?

It will be shown in the next chapter that even under the best of circumstances it is not possible to completely eliminate regularization-induced structural noise as long as the measurement dataset is contaminated by even a little measurement noise. (Recall that all attempts to seek parameter uniqueness involve regularization; the only way to eliminate the need to regularise is to eschew the quest for uniqueness altogether and employ Bayesian methods to directly explore posterior parameter and predictive uncertainty. However, with present technology, this can be achieved only with great difficulty, if at all, for highly parameterized systems; so the need for regularization remains.) In fact, as will be shown, the best that can be done in a regularization setting is to reduce regularization-induced structural error to a level that is commensurate with measurement error; the $\eta$ term of equation (5.1.8) therefore becomes commensurate with the $\varepsilon$ term. However because it is commensurate with this term and not zero, it cannot be ignored (as is effectively done if a weight matrix **Q** is chosen strictly on the basis of equation 5.2.6).

In all of the theoretical developments presented in the current chapter, with the exception of the brief introduction to manual regularization provided in section 5.1, we have used $\boldsymbol{\varepsilon}$ instead of $\boldsymbol{\tau}$ to characterize noise associated with the calibration dataset; regularization-induced structural noise has been ignored. For characterization of measurement noise, a modeller must address the mechanics of the measurement process; through this means a suitable

covariance matrix of measurement noise C(**ε**) (normally diagonal) can be established. It is now apparent that, if an appropriate weighting matrix **Q** must be developed to achieve parameter estimates of minimum error variance, it is C(**τ**) that must be characterized and not just C(**ε**). From (5.1.8) this requires that C(**η**) be specified.

Sadly, calculation of C(**η**) is rarely possible. From (5.1.10) C(**η**) can be conceptually calculated as

$$C(\boldsymbol{\eta}) = (\mathbf{ZL} - \mathbf{X})C(\mathbf{p})(\mathbf{ZL} - \mathbf{X})^t \qquad (5.5.2)$$

If C(**η**) is calculated using equation (5.5.2) pertinent Jacobian matrices must replace **Z** and **X**. **X** is easily calculated; in fact it must be calculated routinely in estimating parameters **p** through the Gauss-Marquardt-Levenberg method. The same is not the case for **Z** as **Z** includes all model parameters – not just those which are adjusted through the calibration process; it includes those that are fixed and tied through manual regularization. Its calculation is therefore much more laborious than that of **X**. And even if it were to be calculated, another question immediately arises. Why not use the mathematical regularization methods discussed in the following chapter to estimate **k** of equation (5.1.1) instead of a parsimonious set of parameters **p** based on a regularization strategy that may be far from optimal?

The C(**p**) term in equation (5.5.2) is even more problematic. As was discussed in section 5.1, the relationship of **p** to the real world parameter set **k** is unknown. However it is **k** to which expert knowledge can be applied, and not **p**. Hence while it is conceptually possible for an expert to arrive at a suitable C(**k**) matrix, the same cannot be said for C(**p**). We will return to this subject shortly.

There is yet another problem. Doherty and Welter (2010) show that C(**η**) is generally singular. This is not really surprising as it is not noise at all, but (as Doherty and Welter point out), "information with nowhere to go". The singular status of C(**η**) can also be gleaned intuitively from equation (5.5.2). Presumably the small-dimensional covariance matrix C(**p**) is non-singular, for otherwise it cannot be a covariance matrix. It is conceptually impossible to create a vector **η** with a greater number of elements than that of **p** (as must occur for observations to outnumber parameters – a fundamental condition of over-determined parameter estimation), and for the degrees of freedom of **η** to be greater than that of **p**. This restriction in the degrees of freedom of **η** to that of **p** is expressed as singularity of the C(**η**) covariance matrix.

Hence in situations where model-to-measurement misfit is dominated by parameter-simplification-induced structural noise (or actually any kind of structural noise) C(**τ**) will approach singularity. Its inverse $C^{-1}(\boldsymbol{\tau})$ from which the weight matrix **Q** used in the inversion process should be calculated therefore does not exist, or can be obtained only with a high amount of numerical error. Achievement of a minimum error variance solution to the inverse problem, and quantification of this variance, therefore becomes difficult or impossible. Certainly a good fit can be achieved with field measurements using the Gauss-Marquardt-Levenberg method (or some other method). But assessment of how wrong estimated parameters may be becomes subjective at best, and impossible at worst.

It is worthy of note that these problems are not limited to calibration; they apply equally to direct posterior uncertainty analysis. If a Markov chain Monte Carlo methodology is employed to directly sample the posterior probability distribution of **p** following a parameter simplification strategy which supports the use of this methodology by reducing the number of

parameters that it must accommodate, then the integrity of this sampling becomes questionable because of failure to properly characterize the likelihood term of Bayes equation that characterizes model-to-measurement misfit.

### 5.5.2 Parameter and Predictive Error Variance at the Scale that Matters

Instead of achieving model simplification by defining **p** in terms of **k**, equation (5.1.2) achieves parameter simplification by defining **k** in terms of **p**. This is a matter of practicality, and cannot be avoided. A complex model requires **k** parameters; these can number in the hundreds or even thousands (or even greater if they pertain to the scale of a model grid). As was discussed in section 5.1, a simplistic **p** parameterization scheme may comprise, for example, zones of piecewise constancy (in which case groups of **k**-parameters are assumed to be equal to each other), or parameters combined according to fixed ratios (in which case groups of **k**-parameters are assumed to vary in harmony), or parameters which are fixed (in which case some **k**-parameters are not estimated at all while a handful or other **k**-parameters, or grouped **k**-parameters, are estimated). In all cases the modeller defines the groups, supplies the ratios, and fixes non-adjustable **k** parameters at appropriate values. Each adjustable parameter or parameter group that emerges from this process defines an element $p_i$ of **p**. The modeller (or the inversion process) then assigns values to elements of $\underline{\mathbf{p}}$. Corresponding values for $\underline{\mathbf{k}}$ are calculated for use by the model on the basis of the user-specified **L** matrix.

Suppose then that $\underline{\mathbf{p}}$ has been estimated using equation (5.2.9) or one of its nonlinear counterparts. The modeller will have chosen a suitable weight matrix **Q**, notwithstanding the conceptual difficulties implied in such a choice discussed above, and will have proceeded with the parameter estimation process using this **Q**. Once $\underline{\mathbf{p}}$ has been estimated, the **k**-scale estimated parameter set $\underline{\mathbf{k}}$ that is actually provided to the model is calculated as

$$\underline{\mathbf{k}} = \mathbf{L}\underline{\mathbf{p}} = \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{h} = \mathbf{G}\mathbf{h} \qquad (5.5.3)$$

The matrix **G** through which $\underline{\mathbf{k}}$ is estimated from **h** is defined through the above equation. If (5.1.1) is substituted for **h** in (5.5.3) we obtain

$$\underline{\mathbf{k}} = \mathbf{L}\underline{\mathbf{p}} = \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{Z}\mathbf{k} + \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\boldsymbol{\varepsilon} \qquad (5.5.4)$$

Suppose that measurement noise ("real" measurement noise this time, and not the mixture of measurement and parameter-simplification-induced structural noise that dominates model-to-measurement misfit under a regime of manual regularization that forces us to work with **p**-scale parameters) is zero. Equation (5.5.4) then becomes

$$\underline{\mathbf{k}} = \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{Z}\mathbf{k} \qquad (5.5.5)$$

This equation shows the relationship between estimated parameters $\underline{\mathbf{k}}$ and true system parameters **k**. These, and not the parsimonized parameters **p**, are the parameters that matter, for these are the parameters that the model uses when it makes a prediction of future system behaviour.

Equation (5.5.5) defines the resolution matrix that arises from manual regularization. Specifically

$$\mathbf{R} = \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{Z} \qquad (5.5.6)$$

Recall from section 2.9 that the resolution matrix defines the relationship between estimated and real parameters. Recall also that each row of the resolution matrix defines the conceptual parameter averaging process that is implied in estimating each element $\underline{k}_i$ of $\underline{\mathbf{k}}$ through an ill-

posed inverse problem. It demonstrates that the value of each such estimated element is, in fact, an average over many real parameter elements. A modeller cannot know **k**; all that he/she obtains through the calibration processes is a "blurred", "averaged" version of parameter reality, and not reality itself.

From (5.5.4) the error in estimated **k**-scale parameters can be calculated as

$$\underline{\mathbf{k}} - \mathbf{k} = -(\mathbf{I} - \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{Z})\mathbf{k} + \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\boldsymbol{\varepsilon} \qquad (5.5.7)$$

That is

$$\underline{\mathbf{k}} - \mathbf{k} = -(\mathbf{I} - \mathbf{R})\mathbf{k} + \mathbf{G}\boldsymbol{\varepsilon} \qquad (5.5.8)$$

where **R** is defined above and

$$\mathbf{G} = \mathbf{L}(\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q} \qquad (5.5.9)$$

If **k** is statistically independent of **ε** (which is a reasonable assumption), then the covariance matrix of post-calibration parameter error can be calculated as

$$\mathrm{C}(\underline{\mathbf{k}} - \mathbf{k}) = (\mathbf{I} - \mathbf{R})\mathrm{C}(\mathbf{k})(\mathbf{I} - \mathbf{R})^t + \mathbf{G}\mathrm{C}(\boldsymbol{\varepsilon})\mathbf{G} \qquad (5.5.10)$$

Equation (5.5.10) is completely general. It does not depend on the type of regularization employed to achieve parameter uniqueness. The **R** and **G** matrices are regularization-specific; however the equation is not. A choice for **R** and **G** can be said to be optimal when the trace of $\mathrm{C}(\underline{\mathbf{k}} - \mathbf{k})$ is minimized. (Actually when model defects are considered, perhaps a more practical definition of optimality of regularization is that the error variance of predictions of interest be minimized. As will be shown in chapter 9 of this text, where model defects are considered, minimization of parameter error variance and minimization of predictive error variance become two different things. For the moment however, we consider the **Z** model to have no defects.)

What is immediately apparent from equation (5.5.10) is that computation of parameter error variance at the scale that matters - the scale of **k** rather than the scale of **p** - requires two terms instead of the single term embodied in equation (5.2.13). If **Q** is chosen as $\mathrm{C}^{-1}(\boldsymbol{\varepsilon})$ (so that the reference variance is unity), the single term of equation (5.2.13) is indeed present as the second term on the right side of equation (5.5.10). However equation (5.5.10) has another term on its right side. This is the "cost of uniqueness" term. This term emerges from the necessity to simplify parameters prior to calibration in order to achieve calibration uniqueness. This term is zero only if **R** is equal to **I** (i.e. the identity matrix). This can happen only if **k** is the same as **p** (and **Z** is the same as **X** because **L** is equal to **I**), and hence the world is as simple as the model. Under any other circumstances the cost of uniqueness must be taken into account in assessing the potential for parameter error at the scale that matters, i.e. the **k**-scale. If it is not taken into account, then the error variances of at least some **k**-scale parameters are likely to be grossly under-estimated as the first term of (5.5.10) is thereby ignored. For example, where a spatial model domain is endowed with zones of piecewise constancy as a manual regularization device, **k**-scale error arises from the erroneous assumption that real world system properties are actually piecewise constant. To the extent that they are not, enforced piecewise homogeneity of **k**-scale parameters creates a potential for **k**-scale error. This is in addition to errors that arise in estimation of **p**-scale parameters from the presence of noise in the calibration dataset.

Let *s* be a prediction of interest. Let the vector **y** express the sensitivity of this prediction to parameters **k**. Then the prediction is made as

$$s = \mathbf{y}^t\mathbf{k} \qquad (5.5.11a)$$

In contrast, predictions made by the calibrated model are actually made using the estimated parameter set $\underline{\mathbf{k}}$. Let this prediction be characterized as $\underline{s}$. Hence

$$\underline{s} = \mathbf{y}^t\underline{\mathbf{k}} \qquad (5.5.11b)$$

Predictive error is thus

$$\underline{s} - s = \mathbf{y}^t(\underline{\mathbf{k}} - \mathbf{k}) \qquad (5.5.12)$$

From (5.5.10), the variance of predictive error can be written as

$$\sigma^2_{\underline{s}-s} = \mathbf{y}^t\mathrm{C}(\underline{\mathbf{k}} - \mathbf{k})\mathbf{y} = \mathbf{y}^t(\mathbf{I} - \mathbf{R})\mathrm{C}(\mathbf{k})(\mathbf{I} - \mathbf{R})^t\mathbf{y} + \mathbf{y}^t\mathbf{G}\mathrm{C}(\boldsymbol{\varepsilon})\mathbf{G}\mathbf{y} \qquad (5.5.13)$$

Hence the cost of parameter simplification flows through to predictive error. The extent to which it affects any prediction is dependent on the prediction itself; that is, it is dependent on the sensitivity **y** of that prediction to the different parameters **k** used by the model. If we continue to use zonal regularization as an example, then to the extent that any prediction *s* is sensitive to within-zone heterogeneity, that prediction will incur an error through suppression of that heterogeneity in the calibrated model. To be sure, within-zone heterogeneity may not be estimable regardless of the regularization device deployed for attainment of parameter uniqueness; the information content of the calibration dataset **h** may simply not support such estimation. What is important, however, is that the parameters that express the potential for within-zone heterogeneity (i.e. the **k** parameters) be retained in the model so that their inestimability can be taken into account when computing predictive error variance. This is done in equation (5.5.13). It is not done in equation (5.2.17) which is typically used to compute predictive error variance in the manual regularization context; equation (5.2.17) includes only the second term on the right of (5.5.13) and not the first, important, cost-of-uniqueness term.

Omission of **k** parameters, and their replacement with **p** parameters, carries a further disadvantage. In general, it cannot be known in advance whether the calibration dataset does indeed carry at least some information that can inform this level of parameterization detail. Optimality of the calibration process cannot be assured if such information is refused entry into that process.

While the above discussion focuses on contexts wherein a model is first calibrated and parameter and predictive error variance are then quantified as surrogates for parameter and predictive uncertainty, arguments pertaining to parameter simplification are no less salient where simplification is undertaken as a precursor to using methods such as Markov chain Monte Carlo for direct exploration of posterior parameter and predictive uncertainty. The temptation to simplify parameterization in this context is overwhelming, as methods such as Markov chain Monte Carlo cannot accommodate large number of parameters, especially where model run times are long. The cost of using a parameter set **p** instead of a more complex parameter set **k** which embodies all aspects of parameterization detail to which a prediction of interest may be sensitive, is expressed by the first term of equation (5.5.10). As equation (5.5.13) demonstrates, this term contributes to predictive error. Its omission results in underestimation of predictive uncertainty. (In many environmental modelling contexts it is, in fact, the dominant contributor to predictive error/uncertainty.) If model predictive uncertainty analysis must be preceded by a set of parameter simplification assumptions in order for it to become numerically feasible, then sadly, its feasibility may have been purchased at the cost of its validity.

### 5.5.3 What is being Estimated?

In the previous section the relationship between estimated $\underline{\mathbf{k}}$ and real $\mathbf{k}$ was quantified. This section addresses the issue of just what is the simplified parameter set $\mathbf{p}$ and what is its estimated counterpart $\underline{\mathbf{p}}$.

In a similar manner to what was done in the last section we can substitute (5.1.1) into (5.2.9) to obtain

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{Z}\mathbf{k} + (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\boldsymbol{\varepsilon} \qquad (5.5.14)$$

Where measurement noise is zero, this becomes

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{Z}\mathbf{k} = \mathbf{R}'\mathbf{k} \qquad (5.5.15)$$

$\mathbf{R}'$ is a kind of resolution matrix for $\underline{\mathbf{p}}$. However, unlike a real resolution matrix $\mathbf{R}$ which links $\underline{\mathbf{k}}$ to $\mathbf{k}$, it is not square. Nevertheless each row of the $\mathbf{R}'$ matrix provides the averaging coefficients through which an element of $\underline{\mathbf{p}}$ is formed from the elements of $\mathbf{k}$.

The matrix $\mathbf{L}$ appears implicitly in equation (5.5.15) through equation (5.1.5) which is repeated here for convenience

$$\mathbf{X} = \mathbf{Z}\mathbf{L} \qquad (5.5.16)$$

It is important to note that the relationship between $\underline{\mathbf{p}}$ and $\mathbf{k}$ is "discovered" through the calibration process; it is not pre-assigned (unless the methodology discussed in the following section is followed). Hence if, for example, $\mathbf{L}$ is a matrix such as that depicted in equation (5.1.3) which forms the basis for subdivision of a model domain into zones of piecewise constancy, it does not follow that the averaging of elements of $\mathbf{k}$ specified by the rows of $\mathbf{R}'$ endows elements of $\underline{\mathbf{p}}$ with a status of average system property within their respective zones. In fact there is no reason whatsoever why the averaging process specified by any row of $\mathbf{R}'$ should preclude contributions to the value of an element $p_i$ of $\underline{\mathbf{p}}$ from elements $k_i$ of $\mathbf{k}$ that lie outside of its zone. See Moore and Doherty (2006), Gallagher and Doherty (2007) and Watson et al (2013) for a further discussion of this issue and examples. It is wrong, therefore, to inspect the outcomes of a calibration process which features zones of piecewise constancy and infer that the calibration process has provided estimates of the average system property within each zone. Similar considerations apply to regularization devices other than zones of piecewise constancy.

These considerations have consequences for parsimonization in general, whether this is being undertaken as a form of manual regularization, or whether it is being undertaken as a means of bestowing numerical feasibility on other types of analysis such as Markov chain Monte Carlo. The problem of defining a likelihood function when implementing Markov chain Monte Carlo following parameter simplification was discussed above. Another problem is that of defining the prior probability density function of $\mathbf{p}$. From the above discussion it is obvious that a pre-calibration relationship between $\mathbf{p}$ and $\mathbf{k}$ cannot be assumed. The prior probability distribution of $\mathbf{p}$ cannot therefore be calculated from that of $\mathbf{k}$. With the two terms on the right of Bayes equations (see equation 4.2.4) therefore compromised, claims that are sometimes heard that Bayesian analysis, and only Bayesian analysis, must form the basis for model parameter and predictive uncertainty analysis, are somewhat misleading. Like all other model-based data-processing, Bayesian analysis cannot be pure, but can nevertheless be useful.

Where calibration-constrained parameter error analysis is undertaken by first manually

regularizing a model's parameter set, by then calibrating the model, and by finally analysing the post-calibration propensity for parameter error through calculation of C($\underline{\mathbf{p}} - \mathbf{p}$) (see equation 5.2.13), similar considerations apply. The question of "just what is this **p** whose propensity for error we are quantifying" does not go away. In many contexts it matters little, as most environmental models are built to make predictions; they are not necessarily built for estimation of system properties. However if this is the case, then to the extent that a prediction of interest is sensitive to parameterization detail that is represented in **k** but not in **p**, **k** must feature in any strategy that is employed to quantify the uncertainty of that prediction.

While equation (5.5.13) provides such a strategy, its use raises some obvious questions. These include the following.

- If the parsimonious parameter set **p** devised for implementation of manual regularization must be dispensed with when undertaking predictive uncertainty analysis, then why not dispense with **p** during calibration as well? Why not employ a mathematical regularization strategy that can readily accommodate a high dimensional **k**?
- Is the post-calibration potential for error in a prediction made by a model that has been calibrated using a manual regularization strategy higher than it needs to be because the **R** and **G** matrices that emerge from that strategy are sub-optimal?

As will be discussed in the following chapter, the answer to the first of these questions is that mathematical regularization methods are indeed available that are capable of handling **k** vectors of arbitrary size. The answer to the second question is that these methods provide a mathematical guarantee of regularization optimality.

### 5.5.4 Cooley's Strategy

While focusing on calibration of a groundwater model with a heterogeneous parameter field, Cooley (2004) and Cooley and Christensen (2006) proposed a calibration strategy which can avoid some of the problems outlined above, while still employing manual regularization to achieve inverse problem well-posedness. At the same time their theory accommodates nonlinear model behaviour when applied to calculation of post-calibration parameter and predictive error variance.

As usual, let **k** designate the "true parameterization" of a model domain, and let **p** designate a parsimonious set of parameters that are used in its place. Suppose that it is desired that **p** have a pre-defined relationship to **k**. Thus this relationship is designated before calibration is undertaken rather than being "discovered" after the event. Suppose that this relationship is specified as follows

$$\mathbf{p} = \mathbf{N}\mathbf{k} \qquad (5.5.17)$$

For the case where **p** designates values taken by system properties over zones of piecewise constancy, **p** may be pre-defined as the average **k** within each such zone; the **N** matrix then performs the desired averaging.

More generally, **N** may be related to **L** of equation (5.1.2) through

$$\mathbf{N} = (\mathbf{L}^t\mathbf{L})^{-1}\mathbf{L} \qquad (5.5.18a)$$

or

$$\mathbf{N} = (\mathbf{L}^t\mathbf{Q}\mathbf{L})^{-1}\mathbf{L}^t\mathbf{Q} \qquad (5.5.18b)$$

Note from equation (2.9.5) that **N** thus constitutes a generalized inverse of **L**. At the same time, from equation (5.2.9), **p** can be considered to be a simplified parameter set for which the complementary model parameter field calculated from it using (5.1.2) is the best approximation (in the weighted least squares sense) to the original complex parameter field from which **p** was derived using **N**. That is to say, after **p** is calculated from **k** using (5.5.17) a simplified model-scale parameter field **j** can be calculated from **p** using (5.1.2) as

$$\mathbf{j} = \mathbf{L}\mathbf{p} \qquad (5.5.19)$$

Through (5.5.18) **j** becomes the closest approximation to **k** in the weighted least squares sense. Where **p** represents zones of piecewise constancy, the elements of **p** can thus represent the spatial average of those elements of **k** that lie within the zone defined by each element of **p**. At the same time, **j** parameters are uniform within each **p**-zone.

A workflow similar to the following is then implemented.

1. Generate a stochastic realization of **k** using the C(**k**) prior covariance matrix of **k**.
2. Run the model using **k**. Record model outputs **o** corresponding to the measurement dataset **h** that will be used to calibrate the model. Add a realization of measurement noise to **o** to generate a "pseudo **h**".
3. Calculate **j** from **k** using (5.5.17) followed by (5.5.19). Where zones of piecewise constancy are employed as a manual regularization device, this amounts to assigning all **j** elements within a particular zone a value equal to the average of all **k** elements within that same zone. Run the model using the **j** parameter set and obtain values for model outputs that correspond to **h**.
4. Repeat steps 1 to 3 many times. Then calculate an empirical C($\boldsymbol{\tau}$) matrix based on differences between outputs of the **k**-model and corresponding outputs of the **j**-model.
5. Estimate $\underline{\mathbf{p}}$ from the real world **h** using (5.2.9), with **Q** calculated as $C^{-1}(\boldsymbol{\tau})$.
6. Calculate parameter and predictive error variance using theory described in this chapter, optionally with appropriate enhancements to accommodate model nonlinearity.

Cooley (2004) and Cooley and Christensen (2006) show that an estimate of $\underline{\mathbf{p}}$ obtained in this way constitutes the minimum error variance estimate of **Nk**. Where regularization is based on replacing geological heterogeneity with zones of piecewise constancy, they thus specify before undertaking the calibration process that they would like to estimate the average value of system properties within each zone. They then obtain the minimum error variance estimate of those average properties.

An advantage of this approach to manual regularization is that it recognizes the existence of system property complexity behind the parsimonious parameterization scheme that is used to calibrate the model. It attempts to make a formal, pre-defined connection between these two levels of parameterization. However it is doubtful, in the author's opinion, that the methodology will find much use in everyday modelling practice for the following reasons.

- Modellers must decide on the number of **p** parameters to estimate before the parameter estimation process begins rather than have mathematical regularization determine the optimal dimensionality of the calibration solution space itself. The modeller therefore cannot know until post-calibration statistics are available whether he/she is attempting to estimate too many or too few parameters.

- If measurement noise is small in comparison to structural noise induced through parameter simplification, many model runs are required before a stable empirical estimate of the $C(\boldsymbol{\tau})$ matrix is obtained because of near singularity of this matrix.
- While minimum error variance estimates of the elements of **p**, defined according to a modeller's specifications, may be obtained through this process, this is often of secondary or tertiary importance to obtaining minimum error variance estimates of predictions of management interest. The above methodology does not try to minimize structural noise. Instead it embraces it. Error variances of important predictions may be larger than they need to be, given the information content of the calibration dataset and the information content of expert knowledge.
- While the methodology presented by Cooley (2004) and Cooley and Christensen (2006) quantifies structural noise induced by parameter simplification, other sources of structural noise are ignored. In real world modelling contexts, these may be considerably greater in magnitude than those induced by parameter simplification. A weight matrix that is specified as $C^{-1}(\boldsymbol{\tau})$, where $\boldsymbol{\tau}$ includes only parameter-simplification-induced structural noise may therefore fail as a guarantor of minimum error variance of **p** as an estimate of **Nk**.

### 5.5.5 The Role of Prior Information

As has been discussed, a calibration dataset can be expanded to include expert knowledge of parameter values that existed prior to the calibration process. Conceptually such knowledge always exists; the uncertainties that are associated with it will, of course, vary from case to case. Ideally there is no reason why expert knowledge should not be included in the parameter estimation process as a matter of course, especially where the information content of the calibration dataset is limited and parameter nonuniqueness therefore prevails. Practically, however, there are difficulties in doing this where regularization is undertaken manually.

The first (and probably most significant) problem with the use of prior information in the manual regularization process is that of weighting it. As has been discussed extensively in this chapter, weights should ideally be inversely proportional to the "noise" associated with measurements comprising the calibration dataset. In the case of prior information this "noise" is the uncertainty of that information. This is where the first problem arises; how does an expert quantify the uncertainty associated with his/her expert knowledge?

The second problem is that of maintaining correct relativity between prior information weights and weights assigned to measurements of system state. The problem here is that model-to-measurement misfit is not an outcome of measurement noise; so measurement instrument specifications cannot be used to estimate it. In fact, the amount of "measurement noise" that is associated with the calibration dataset is usually estimated through the calibration process itself; see equation (5.2.18). Furthermore, that estimate pertains to the calibration dataset as a whole, and not to separate parts of it. Hence even if a modeller can quantify the uncertainty of his/her expert knowledge, it is not possible for him/her to maintain correct relativity between weights assigned to prior information on the one hand, and to members of the measurement dataset on the other hand when the noise associated with the latter is not known until the calibration process is complete.

This is an unfortunate situation as correct relativity of weighting between measurements of system state on the one hand, and prior information on the other hand, that collectively

comprise a calibration dataset is important. If prior information is weighted too strongly, the inversion process will ignore measurements of system state in favour of prior information. If prior information is not weighted strongly enough, it may not exert a sufficiently strong regularizing influence on the inversion process. The latter may remain ill-posed; nonuniqueness will then prevail, as will the numerical difficulties that attend inversion of near-singular matrices.

Yet another problematic aspect of using prior information in the manual regularization context is that of defining the meaning of individual members of the parsimonized parameter set that is being estimated. Equation (5.5.15) shows that individual members of the parsimonized parameter set bear complex relationships to the real world parameters to which expert knowledge actually pertains. Furthermore, this relationship is rarely quantifiable as equation (5.5.15) includes a sensitivity matrix (the **Z** matrix) that is generally not available. In addition to this, the averaging process that is implied by rows of the pseudo-resolution matrix $\mathbf{R}'$ of equation (5.5.15) may include parameters of multiple types in the characterization of one particular parsimonized parameter. Hence just because a simplified parameter used in the manually-regularized inversion process is named after a particular system property, this does not mean that it is being estimated as such. The difficulties of associating expert knowledge with such a parameter, and of weighting such an association, are thus compounded.

The following chapters of this text abandon **p**-scale parameters in favour of **k**-scale parameters to which, hopefully, expert knowledge is more directly applicable. This creates the context wherein expert knowledge can indeed play an important role in the inversion process.

### 5.5.6 Information Criteria Statistics

The following post-calibration statistics are sometimes employed to assist a modeller in deciding how many parameters to include in a parsimonious parametrization scheme on which manual regularization is based. They are also sometimes used to assist a modeller in ranking parsimoniously calibrated models. This ranking allows weights to be assigned to predictions made by these models so that they can be used collectively in a predictive uncertainty analysis exercise in which different system conceptualizations are taken into account. See Poeter and Hill (2007) for more details.

AIC: Akaike Information Criterion

$$\mathrm{AIC} = n\ln\left(\sigma^2\right) + 2k \tag{5.5.20}$$

AICc: second order bias-corrected AIC

$$\mathrm{AICc} = n\ln\left(\sigma^2\right) + 2k + \left(\frac{2k(k+1)}{n-k-1}\right) \tag{5.5.21}$$

BIC: Bayesian Information Criterion

$$\mathrm{BIC} = n\ln\left(\sigma^2\right) + k\ln(n) \tag{5.5.22}$$

KIC: Kashyap Information Criterion

$$\mathrm{KIC} = (n-(k-1))\ln\left(\sigma^2\right) - (k-1)\ln(2\pi) + \ln\left|\mathbf{J}^t\mathbf{Q}\mathbf{X}\right| \tag{5.5.23}$$

In all of these formulas

- $n$ is the number of observations and prior information equations employed in the parameter estimation process;
- $k$ is equal to $m+1$ where $m$ is the number of adjustable parameters involved in the parameter estimation process;
- $\sigma^2$ is $\Phi_{min}/n$, where $\Phi_{min}$ is the minimized objective function;
- $\mathbf{X}$ is the Jacobian matrix computed on the basis of optimised (or almost optimised) parameters;
- $\mathbf{Q}$ is the weight matrix.

The formula for each of these statistics has two terms. The first decreases as the objective function falls, and the level of model-to-measurement fit thereby improves. The second rises as the number of parameters rises. Supposedly, the optimal number of parameters to employ in the calibration process is that which fits the data well enough to have extracted its information, but not so well that over-fitting has occurred and parameters are thereby "informed" by measurement noise rather than measurement information. This "sweet spot" is supposed to occur where the various information criteria listed above are minimized with respect to the number of parsimonized parameters.

In the author's opinion, these formulas have little meaning in the environmental modelling context. The balance between under-fitting and over-fitting can be formalized using theory based on singular value decomposition that is presented in the next chapter. That theory employs **k**-level parameters rather than **p**-level parameters; hence it avoids problems associated with discerning the exact meaning of the latter. It is also directly applicable to the calibration context.

Use of the above statistics in ranking alternative model conceptualizations is also questionable. As is addressed in chapter 9 of this text, many model defects are invisible to the calibration process. Yet their effect on some model predictions may be profound; the deleterious effects of model defects on these predictions may be amplified through the calibration process. At the same time, as far as other model predictions are concerned, model defects can be happily "calibrated out". Model parameterization and calibration strategies must therefore be prediction-specific rather than model-specific. The matter is much more complicated than the above statistics imply.

# 6. Mathematical Regularization

## 6.1 General

### 6.1.1 Formulation of Equations

As in the previous chapter, we start by assuming linear model behaviour. This allows us to develop theory and explore concepts. Adaptation of the theory to nonlinear models is then discussed.

Once again, we start with the equation that describes a linear model **Z** running under calibration conditions acting on *m* parameters encapsulated in the vector **k**. Measurements of system state **h** (*n* of these are available so that **h** has *n* elements) are accompanied by noise **ε** so that

$$\mathbf{h} = \mathbf{Zk} + \boldsymbol{\varepsilon} \tag{6.1.1}$$

In this chapter we assume that **k** represents model parameters on the same scale as that to which expert knowledge applies. Hence we assume that the prior probability distribution of **k**, together with its covariance matrix C(**k**), are a direct outcome of expert knowledge as it pertains to the system being simulated. We also assume that **k** encapsulates system property heterogeneity at a scale that is pertinent to predictions that the model must make. For now, we further assume that the model has no defects; hence any misfit between model outcomes and field measurements is a product purely of measurement noise. Of course, in real world modelling, none of this is true. Some upscaling will be required in definition of **k**; the model will have defects incurred through space and time discretization, improper representation of initial and boundary conditions, and of course through imperfections in its simulation algorithm. Model defects are discussed in a later chapter.

### 6.1.2 Measurement Noise

For convenience in developing the equations that follow, we assume that an appropriate weight matrix **Q** has been built into equation (6.1.1). Ideally this matrix is chosen in such a way as to render measurement noise, as seen by the inversion process, homoscedastic and independent so that its covariance matrix is proportional to the identity matrix **I**. An appropriate **Q** matrix is

$$\mathbf{Q} = \sigma^2_{\varepsilon}\mathbf{C}^{-1}(\boldsymbol{\varepsilon}) \tag{6.1.2}$$

Note that we specify the scalar multiplier in the above equation as $\sigma^2_{\varepsilon}$ rather than $\sigma^2_{r}$ because of the slightly different treatment which this multiplier receives in equations which follow from that which it received in the previous chapter. If all terms of (6.1.1) are multiplied by $\mathbf{Q}^{1/2}$, equation (6.1.2) becomes

$$\mathbf{Q}^{½}\mathbf{h} = \mathbf{Q}^{½}\mathbf{Zk} + \mathbf{Q}^{½}\boldsymbol{\varepsilon} \tag{6.1.3}$$

If, as in section 5.2.2, we define

$$\mathbf{g} = \mathbf{Q}^{½}\mathbf{h} \tag{6.1.4}$$

$$\mathbf{Y} = \mathbf{Q}^{½}\mathbf{Z} \tag{6.1.5}$$

$$\boldsymbol{\xi} = \mathbf{Q}^{½}\boldsymbol{\varepsilon} \tag{6.1.6}$$

equation (6.1.3) becomes

$$\mathbf{g} = \mathbf{Yk} + \boldsymbol{\xi} \tag{6.1.7}$$

From (3.9.2) and (6.1.2) the covariance matrix of measurement noise $\boldsymbol{\xi}$ as represented in this equation is

$$C(\boldsymbol{\xi}) = \sigma^2_{\varepsilon} C^{-½}(\boldsymbol{\varepsilon}) C(\boldsymbol{\varepsilon})\, C^{-½}(\boldsymbol{\varepsilon}) = \sigma^2_{\varepsilon}\mathbf{I} \tag{6.1.8}$$

The benefits of choosing a weight matrix **Q** defined by (6.1.2) were discussed in the context of well-posed inverse problems in the previous chapter. If (6.1.7) constitutes a well-posed inverse problem, an objective function could be formulated whose minimization constitutes solution of that problem. The objective function introduced in the previous chapter is

$$\Phi = (\mathbf{g} - \mathbf{Yk})^t(\mathbf{g} - \mathbf{Yk}) \tag{6.1.9}$$

This is a sum of squared residuals. With substitution of (6.1.4) and (6.1.5) into (6.1.9) this becomes

$$\Phi = (\mathbf{h} - \mathbf{Zk})^t\mathbf{Q}(\mathbf{h} - \mathbf{Zk}) \tag{6.1.10a}$$

That is

$$\Phi = \mathbf{r}^t\mathbf{Q}\mathbf{r} = \sigma^2_{\varepsilon}\mathbf{r}^t C^{-1}(\boldsymbol{\varepsilon})\mathbf{r} \tag{6.1.10b}$$

where residuals **r** are defined as

$$\mathbf{r} = \mathbf{h} - \mathbf{Zk} \tag{6.1.11}$$

If measurement noise is characterized by a multinormal probability distribution, then minimization of the above-defined objective function maximizes residual likelihood. See the exponent of equation (3.6.1). However, as will be discussed later in this chapter, where a problem is ill-posed, this function is not actually minimized. Where enough parameters are featured in the inverse problem, it may actually be possible to reduce the objective function to nearly zero, in spite of the presence of measurement noise in **h**. For reasons which will become obvious shortly, a parameter set which achieves such "ultimate minimization" of the objective function cannot be construed as being an optimal solution to the inverse problem of model calibration. Instead, parameters are adjusted until $\Phi$ is reduced to a value that is commensurate with measurement noise. If $\boldsymbol{\varepsilon}$ is multinormal and $\sigma^2_{\varepsilon}$ is unity, $\Phi$ possesses a chi-squared distribution with *n* degrees of freedom, where *n* is the number of observations comprising the calibration dataset **h**, and hence the number of residuals featured in equation (6.1.10). The expected value of $\Phi$ is therefore *n*; see section 3.2.3.

Because we will assume in the discussion that follows that equation (6.1.1) has already been transformed through pre-multiplication of all terms by a user-specified **Q** matrix, this matrix will not appear in the equations to follow; nevertheless its presence will be implied in definition of **Z**, so that we will use **Z** (and not **Y**) to characterize the action of the model. If the **Z** model is defect-free, then **Q** should have been calculated using (6.1.2). If **Z** is not defect free (as no models are), then greater sophistication needs to be applied in formulation of the objective function and in choice of **Q**. This will be discussed later.

### 6.1.3 Parameter and Predictive Error Variance

The discussion in this section is similar to that of section 5.5.2. However it is repeated here for the sake of completeness of the present chapter. The discussion is also slightly more general than in section 5.5.2; this makes it more relevant to all regularization methodologies,

including mathematical regularization.

Suppose that a vector $\underline{\mathbf{k}}$ has been found that can be said to "calibrate" the model **Z**. Suppose further that the manner of its calculation from **h** can be encapsulated in a matrix **G**. Different means of solving an ill-posed inverse problem will result in calculation of different **G** matrices, this depending on the adopted regularization method; as has been previously discussed, there can be no unique solution to an ill-posed inverse problem without regularization of one kind or another. Thus

$$\underline{\mathbf{k}} = \mathbf{Gh} \tag{6.1.12}$$

Substitution of (6.1.1) into (6.1.12) gives

$$\underline{\mathbf{k}} = \mathbf{GZk} + \mathbf{G}\boldsymbol{\varepsilon} \tag{6.1.13a}$$

or

$$\underline{\mathbf{k}} = \mathbf{Rk} + \mathbf{G}\boldsymbol{\varepsilon} \tag{6.1.13b}$$

where

$$\mathbf{R} = \mathbf{GZ} \tag{6.1.14}$$

As has already been discussed, **R** is the resolution matrix. If there is no noise associated with the calibration dataset it describes the relationship between estimated parameters $\underline{\mathbf{k}}$ and real world parameters **k**. Obviously **R** is a square matrix. If the inverse problem is well-posed, then **R** is equal to the identity matrix **I**. If the inverse problem is ill-posed then it can be shown that **R** is rank-deficient and hence non-invertible. As has also been discussed, each row of the resolution matrix provides weights through which an individual element of $\underline{\mathbf{k}}$ can be calculated from all elements of **k**. If **R** is not **I** (as it cannot be if an inverse problem is ill-posed) then some averaging of the elements of **k** thus takes place in calculation of the elements of $\underline{\mathbf{k}}$. $\underline{\mathbf{k}}$ cannot possibly be **k** under these circumstances. The best that can be hoped for is that **R** somehow approaches **I** so that this "blurring" of estimated parameters in the ill-posed context is minimized. However the more ill-posed is the inverse problem, the less is this possible. It follows that even where measurement noise is zero, $\underline{\mathbf{k}}$ is always in error, with the magnitude of this error increasing with ill-posedness of the inverse problem. This is the cost of seeking parameter uniqueness (and hence the cost of calibrating a model).

Other interesting properties of **G** and **R** emerge if $\boldsymbol{\varepsilon}$ is zero. These define asymptotic properties of these matrices in more realistic cases where $\boldsymbol{\varepsilon}$ is non-zero. Where $\boldsymbol{\varepsilon}$ is zero a modeller is entitled to seek a perfect fit between model outputs and the calibration dataset **h**. Thus

$$\mathbf{h} = \mathbf{Z}\underline{\mathbf{k}} \tag{6.1.15}$$

From (6.1.1) with no noise, (6.1.12) and (6.1.15) we obtain

$$\mathbf{h} = \mathbf{Zk} = \mathbf{Z}\underline{\mathbf{k}} = \mathbf{ZGh} = \mathbf{ZGZk} \tag{6.1.16}$$

and hence

$$\mathbf{Z} = \mathbf{ZGZ} \tag{6.1.17}$$

which, through comparison with (2.9.5), establishes that **G** is a generalized inverse of **Z**. Pre-multiplication of both sides of (6.1.17) by **G** establishes that the resolution matrix **R** is idempotent and hence is a projection operator. If it is symmetric it becomes an orthogonal projection operator. As will be discussed, such is the case where parameter uniqueness is

achieved through use of singular value decomposition as a regularization device.

From (6.1.13), the error in the estimated parameter set $\underline{\mathbf{k}}$ in the presence of measurement noise can be calculated as

$$\underline{\mathbf{k}} - \mathbf{k} = -(\mathbf{I} - \mathbf{R})\mathbf{k} + \mathbf{G}\boldsymbol{\varepsilon} \qquad (6.1.18)$$

Characterization of parameter error thus requires two terms. One of these terms (the second term on the right of equation 6.1.18) arises from the presence of noise in the measurement dataset. The other term would arise even if there were no noise in the calibration dataset. As stated above, this contribution to estimated parameter error arises to the extent that **R** is different from **I**. It is thus an unavoidable outcome of seeking a unique solution to an ill-posed inverse problem.

Whenever a unique solution is sought to an ill-posed inverse problem, a resolution matrix is implied or, in cases where regularization is mathematical, can be explicitly calculated. This resolution matrix **R** cannot be **I**. The resolution matrix that emerges from manual regularization was discussed in the previous chapter. Rarely, if ever, is the resolution matrix explicitly calculated in the manual regularization context.

An advantage of formalized mathematical regularization over manual regularization is that the **G** matrix as it pertains to model parameters **k**, and hence the **R** matrix, becomes available as the inverse problem is solved. Hence the cost-of-uniqueness term of equation (6.1.18) can be explored. Despite this, however, the error in estimated parameters $\underline{\mathbf{k}}$ cannot be known. This is because **k**, the vector of real world parameters whose values are being estimated, is not known. **k** is featured on the right side of equation (6.1.18); so too is the unknown vector $\boldsymbol{\varepsilon}$ of measurement noise. Hence (6.1.18) cannot be used to calculate $\underline{\mathbf{k}} - \mathbf{k}$. However while parameter error itself cannot be determined, much can be said about the *propensity* for parameter error. This can be expressed by the covariance matrix of post-calibration parameter error $C(\underline{\mathbf{k}} - \mathbf{k})$. Using (3.9.2) $C(\underline{\mathbf{k}} - \mathbf{k})$ can be calculated from (6.1.18) as

$$C(\underline{\mathbf{k}} - \mathbf{k}) = (\mathbf{I} - \mathbf{R})C(\mathbf{k})(\mathbf{I} - \mathbf{R})^t + \mathbf{G}C(\boldsymbol{\varepsilon})\mathbf{G}^t \qquad (6.1.19)$$

Two covariance matrices are featured on the right side of (6.1.19); these are $C(\mathbf{k})$ and $C(\boldsymbol{\varepsilon})$. It follows that if we seek to quantify the post-calibration potential for parameter error (or the post-calibration potential for predictive error for which an equation will be derived shortly), then we need to know more than just the statistics of measurement noise; recall that this is all that we need for quantification of parameter error variance in the well-posed context. In the ill-posed context we also need to encapsulate expert knowledge in a $C(\mathbf{k})$ matrix which quantifies the innate variability of parameters **k**. Conceptually this is available from the prior parameter probability distribution, the same probability distribution that is required by Bayes equation. As well as denoting innate parameter variability, off diagonal terms of $C(\mathbf{k})$ must denote any correlation (spatial or otherwise) that system properties are likely to possess.

Let *s* be a prediction of management interest. Let the sensitivity of this prediction to parameters **k** be expressed by the vector **y**. The true value of this prediction is calculated as

$$s = \mathbf{y}^t\mathbf{k} \qquad (6.1.20)$$

Through propagation of covariance (i.e. equation 3.9.2), the variance of this prediction is then given by

$$\sigma^2_s = \mathbf{y}^t C(\mathbf{k})\mathbf{y} \qquad (6.1.21)$$

$\sigma^2_s$ can be viewed in a number of different ways. It describes the prior uncertainty of the prediction *s*. (Recall that variance is the square of standard deviation.) That is, it describes the uncertainty of this prediction if made on the basis of expert knowledge alone. $\sigma^2_s$ can also be viewed as the pre-calibration error variance of the prediction. If a single value were to be sought for this prediction based on expert knowledge alone, then this value would be calculated using prior expected values (i.e. prior means) of all of the parameters encapsulated in **k**. According to the concepts used to linearize the model, these are all zero; see section 4.5. Hence the prior mean of the prediction *s* is also zero. $\sigma^2_s$ quantifies the potential for error in making such a zero-valued prediction.

The prediction made by the calibrated model is calculated as

$$\underline{s} = \mathbf{y}^t\underline{\mathbf{k}} \qquad (6.1.22)$$

Hence predictive error is

$$\underline{s} - s = \mathbf{y}^t(\underline{\mathbf{k}} - \mathbf{k}) \qquad (6.1.23)$$

Using the propagation of variance formula once again, the variance of post-calibration predictive error becomes

$$\sigma^2_{\underline{s}-s} = \mathbf{y}^t\mathrm{C}(\underline{\mathbf{k}} - \mathbf{k})\mathbf{y} \qquad (6.1.24)$$

which, from (6.1.19), is

$$\sigma^2_{\underline{s}-s} = \mathbf{y}^t(\mathbf{I} - \mathbf{R})\mathrm{C}(\mathbf{k})(\mathbf{I} - \mathbf{R})^t\mathbf{y} + \mathbf{y}^t\mathbf{G}\mathrm{C}(\boldsymbol{\varepsilon})\mathbf{G}^t\mathbf{y} \qquad (6.1.25)$$

Equation (6.1.25) quantifies the potential for error in a prediction $\underline{s}$ when made using a calibrated model.

For a nonlinear model predictive error variance as calculated using equation (6.1.25) is only approximately correct. However in chapter 8 this equation will be adapted for use in the nonlinear context.

### 6.1.4 Overview of Mathematical Regularization

Regularization in its broadest sense refers to the process through which a unique solution is sought to an ill-posed inverse problem. By definition, many solutions exist to an ill-posed inverse problem. A metric through which one of these can be selected as optimal was suggested in section 4.4. There it was suggested that the optimal solution to the inverse problem of model calibration is that which endows the model with the ability to make predictions of future system behaviour which are of minimized error variance. It may be argued that the minimum error variance metric should actually be applied to parameters rather than to predictions, for if estimated parameters are of minimum error variance then minimization of predictive error variance follows automatically. Unfortunately this is not the case when model imperfections are taken into account, for under these circumstances the link between parameter and predictive error variance is broken. This is a subject for a later chapter. In the present chapter, however, it will be assumed that models have no defects.

As has already been shown, uniqueness comes at a cost; that cost is the potential for error in estimated parameters. Pivotal to the evaluation of this cost is the resolution matrix. Where regularization is implemented under mathematical control this can be calculated. So too then can the propensity for parameter and predictive error. Post-calibration predictive error analysis as a substitute for posterior uncertainty analysis thus becomes possible. This

provides mathematical regularization with a huge advantage over manual regularization.

This is not the only advantage that mathematical regularization holds over manual regularization. Where a model has spatially distributed parameters, all of these parameters can be retained in the calibration process as elements of the vector **k**. This endows the inversion process with maximum flexibility in introducing system property heterogeneity to locations within the model domain at which the calibration dataset suggests that such heterogeneity should exist. Of course the process of heterogeneity emplacement must take place under the control of a regularization strategy which precludes the introduction of spurious heterogeneity. In principle it is not difficult to find such a strategy; see the discussion of Tikhonov regularization below. Contrast this with manual regularization wherein heterogeneity must express itself in pre-defined spatial patterns, such as a small number of zones of piecewise constancy whose geometries may or may not be appropriate, and whose number may or may not be adequate to reflect the information content of the calibration dataset.

Whether or not parameterization is spatial, the practicalities of implementing mathematical regularization make it a far easier option than manual regularization. In principal, decisions of which parameters to estimate, which parameters to lump together, and which parameters to fix, never need to be made under a mathematical regularization regime. Instead an approach of "if in doubt, declare it as adjustable" can prevail. If it transpires that the information content of a calibration dataset is insufficient to allow estimation of a particular parameter or group of parameters, then the post-calibration value of the parameter, or group of parameters taken as a whole, will be unchanged from their pre-calibration values. At the same time, numerical instability incurred through attempts to invert non-invertible matrices is avoided as mathematical regularization alters these matrices to enhance their invertibility.

This chapter introduces the two broad approaches to mathematical regularization. These are broadly known as "subspace methods" (of which singular value decomposition is the flagship) and "Tikhonov". Each has advantages and disadvantages. In practice, it is best to use both of them together.

Subspace methods work through reducing the inverse problem to that of estimating only as many parameters as are actually estimable on the basis of the calibration dataset. In this they resemble manual regularization. However a significant point of difference with manual regularization is that the inversion process itself determines the number of parameters that are actually estimable. These estimable parameters are often optimally-defined linear combinations of the original model parameters. If model parameters are subjected to an appropriate transformation prior to undergoing inversion (see below), not only can a minimum error variance status be guaranteed for estimated parameters, but the process is also guaranteed to be numerically stable as no matrices must be inverted that cannot, in fact, be easily inverted.

In contrast to subspace methods, Tikhonov regularization addresses information deficits in the calibration dataset relative to parameters that require estimation by supplementing the calibration dataset with expert knowledge pertaining to the parameters themselves. A challenge in formulating the inverse problem, particularly in contexts where parameters have spatial connotations and may need to express complex patterns of spatial heterogeneity, is to find the best way to express such expert knowledge in a mathematical way that the inversion process understands. However while challenging, formulation of an appropriate Tikhonov

regularization scheme can also be very flexible. Expressions of expert knowledge do not need to be linear. Hence complex, nonlinear inter-parameter relationships can promulgate the appearance of desirable features within an estimated parameter field such as sharp edges, anisotropy, proximity of heterogeneity to certain points or lines within the model domain, and much else besides. While doing this, Tikhonov regularization is able to ensure correct relativity of weighting between the expert knowledge and measurement components of the overall calibration dataset. This forestalls numerical difficulties at the same time as it ensures that the two sources of information act in concert rather than in opposition to each other.

## 6.2 Singular Value Decomposition

### 6.2.1 Estimation of Parameters

Singular value decomposition (SVD) was discussed in section 2.12. The reader is referred to that section for details of the orthonormal matrices that emerge from the singular value decomposition process. It is now applied to estimation of parameters in an inversion context described by equation (6.1.1).

Under singular value decomposition, the **Z** matrix of equation (6.1.1) can be decomposed as

$$\mathbf{Z} = \mathbf{U}\mathbf{S}\mathbf{V}^t \qquad (6.2.1)$$

Recall from section 2.12 that the orthogonal unit vectors which form the columns of **U** span *n*-dimensional space, where *n* is the number of rows of **Z**. This space includes the output space of **Z** (i.e. the output space of the model). The unit vectors which comprise the columns of **V** span parameter space. The **S** matrix has elements only on its diagonal. These are all non-negative. Their values become smaller as the diagonal is descended. Eventually they either become zero, or the diagonal runs out of elements. The latter occurs if the number of parameters *m* used by the model exceeds the number of observations *n* comprising the calibration dataset.

With appropriate partitioning of **U**, **S** and **V** as described in section 2.12, equation (6.2.1) can be written as

$$\mathbf{Z} = \mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1 + \mathbf{U}_2\mathbf{S}_2\mathbf{V}^t_2 \qquad (6.2.2)$$

In defining the partition embodied in equation (6.2.2) the $\mathbf{S}_2$ matrix is designed to be either completely zero-valued, or to contain only small singular values along its diagonal. Meanwhile the unit vectors which comprise the columns of $\mathbf{V}_1$ and $\mathbf{V}_2$ span two orthogonal subspaces which collectively comprise the whole of parameter space. If (6.2.2) is substituted into (6.1.1) we obtain

$$\mathbf{h} = (\mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1 + \mathbf{U}_2\mathbf{S}_2\mathbf{V}^t_2)\mathbf{k} + \boldsymbol{\varepsilon} \qquad (6.2.3)$$

The solution $\underline{\mathbf{k}}$ of the inverse problem is calculated as (see section 2.12)

$$\underline{\mathbf{k}} = \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\mathbf{h} \qquad (6.2.4)$$

Calculation of $\underline{\mathbf{k}}$ can proceed without any conceptual or numerical difficulties if partitioning of the **S** matrix (and with it the implied partitioning of the **U** and **V** matrices) is such that $\mathbf{S}_1$ is square and contains only non-zero diagonal elements. If $\mathbf{S}_2$ is entirely zero-valued and $\mathbf{S}_1$ contains no zero-valued singular values, the columns of $\mathbf{V}_2$ span the null space of the matrix **Z**. We will refer to its orthogonal complement (which is spanned by the columns of $\mathbf{V}_1$) as the "solution space" of **Z**. Because $\mathbf{V}_1$ is the first-occurring matrix on the right side of (6.2.4), the

solution $\underline{\mathbf{k}}$ to the inverse problem is a linear combination of the vectors which define its columns.

Any vector **j** which is a linear combination of the columns of $\mathbf{V}_2$ can be written as

$$\mathbf{j} = \mathbf{V}_2\mathbf{p} \tag{6.2.5}$$

where **p** is an arbitrary vector with as many elements as there are columns in $\mathbf{V}_2$. In this equation the multiplier of column *i* of $\mathbf{V}_2$ is $p_i$, the *i*'th element of **p**. From (6.2.2)

$$\mathbf{Zj} = \mathbf{U}_1\mathbf{S}_1\mathbf{V}^t{}_1\mathbf{V}_2\mathbf{p} + \mathbf{U}_2\mathbf{S}_2\mathbf{V}^t{}_2\mathbf{V}_2\mathbf{p} \tag{6.2.6}$$

The first term on the right of equation (6.2.6) is zero because of the orthogonality of $\mathbf{V}_1$ and $\mathbf{V}_2$. The second term is zero if all elements of $\mathbf{S}_2$ are zero. Hence **Zj** is zero, so that **j** is in the null space of **Z**.

Normally the partitioning of **S** into $\mathbf{S}_1$ and $\mathbf{S}_2$, and with it the partitioning of **V** into $\mathbf{V}_1$ and $\mathbf{V}_2$, for the purpose of estimating $\underline{\mathbf{k}}$ using equation (6.2.4) is not strictly according to the onset of zero diagonal elements of $\mathbf{S}_2$. Normally the leading diagonal elements of $\mathbf{S}_2$ are small but nonzero; the reasons for this will become apparent shortly. Hence **j** defined according to (6.2.5) when substituted into (6.2.6) will produce a non-zero outcome. Nevertheless the outcome will be small as the first term on the right of (6.2.6) will continue to be zero while the second term of (6.2.6) will be small because of the small diagonal elements of $\mathbf{S}_2$.

In the discussion that follows we will continue to refer to the subdivision of parameter space into $\mathbf{V}_1$ and $\mathbf{V}_2$ along the lines described above as subdivision of this space into the "solution space" and the "null space". This is in spite of the fact that it is not completely correct to equate the null space with the $\mathbf{V}_2$ space unless all diagonal elements of $\mathbf{S}_2$ are strictly zero. Nevertheless, adoption of this protocol makes the following discussion easier.

### 6.2.2 An Example

Figure 6.1 shows a simple, one-dimensional groundwater model. Steady-state flow from right to left is *q*; for convenience in the equations that follow we assume that *q* is equal to 1. The head at the left boundary is fixed at zero. The calibration dataset is comprised of the head measured in a single well at the extreme right end of the model domain. Let this head be *h*. Two model parameters determine the head in this well. These are the resistances within each of the two zones through which groundwater flows. Hence

$$h = (r_1 + r_2) \tag{6.2.7a}$$

or, to write this in matrix form,

$$\begin{bmatrix} h \end{bmatrix} = \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} \tag{6.2.7b}$$

In equation (6.2.7) the **Z** matrix of equation (6.1.1) is [1 1], the **k** vector is $\begin{bmatrix} r_1 \\ r_2 \end{bmatrix}$, while the **h** vector is $\begin{bmatrix} h \end{bmatrix}$.

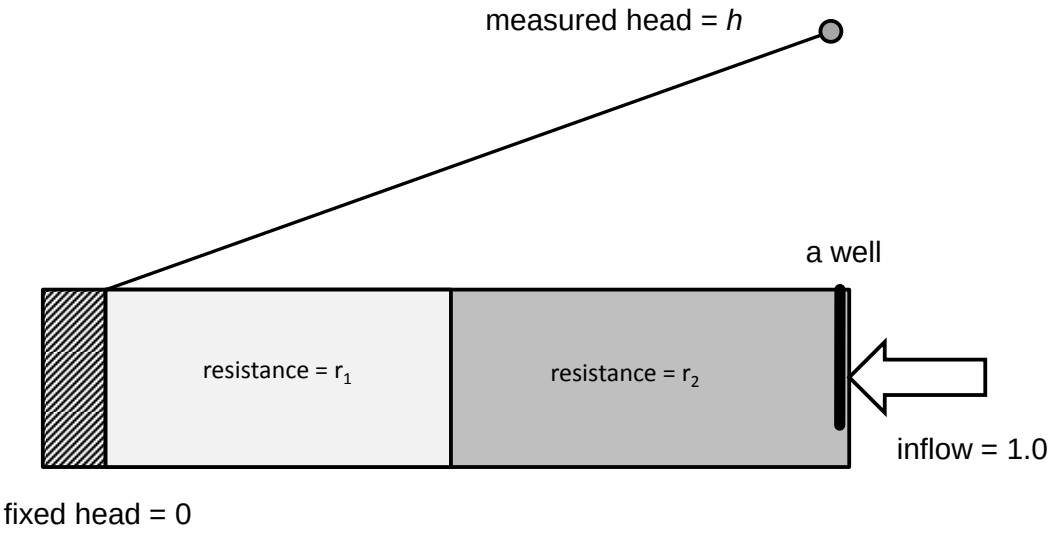


**Figure 6.1. A one-dimensional groundwater model domain in which water flows toward a boundary in which the head is fixed at zero.**

It can be verified with ease that the vector $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$ is a unit vector. It can also be verified that

$$\mathbf{Z}\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} = \mathbf{0} \qquad (6.2.8)$$

Hence this vector is in the null space of **Z**. It thus comprises the $\mathbf{V}_2$ matrix of equation (6.2.2); obviously, in the present example, this matrix has just one column. Meanwhile the vector $\begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ comprises the $\mathbf{V}_1$ matrix; it can also be readily verified that this is orthogonal to the vector comprising the single column of $\mathbf{V}_2$. The $\mathbf{V}_1$ matrix too has just one column, this comprising the one-dimensional solution space of the **Z** matrix. Hence any solution to the ill-posed inverse problem of estimating $r_1$ and $r_2$ must be a multiple of this vector. Hence $r_1$ and $r_2$ must be estimated as equal.

Intuition readily informs us that the single head which comprises the observation dataset **h** allows estimation of only the sum of the resistances $r_1$ and $r_2$ that occupy the model domain. Because the inverse problem is ill-posed, there are an infinite number of possible values which $r_1$ and $r_2$ can take which, when added together, form this single estimable sum. Uniqueness is achieved by assuming that $r_1$ and $r_2$ are equal, for unless there is information to the contrary, this constitutes the "safest" solution to the inverse problem, and hence the solution of minimum error variance.

Differences between $r_1$ and $r_2$ are irresolvable because they lie in the null space; see equation

(6.2.8). For safety, this difference is assigned a value of zero in achieving the minimum error variance solution to the inverse problem of figure 6.1; as discussed in section (2.12) this minimum error variance solution must have a null space projection of zero. This does not mean, of course, that $r_1$ and $r_2$ are necessarily equal. It only means that the probability of $r_1$ being greater than $r_2$ is the same as the probability of $r_2$ being greater than $r_1$. The middle path is chosen in seeking a minimum error variance solution to the inverse problem. Meanwhile the predictive repercussions of $r_1$ and $r_2$ being different from each other can be explored later when post-calibration error analysis is undertaken. When undertaking this analysis, $r_1$ and $r_2$ can indeed be endowed with different values; however their sum must always be unity so that calibration constraints are respected.

### 6.2.3 Relationship between Estimated and Real Parameters

With substitution of (6.2.3) into (6.2.4) we obtain

$$\underline{\mathbf{k}} = \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\mathbf{U}_1\mathbf{S}_1\mathbf{V}^t{}_1\mathbf{k} + \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\mathbf{U}_2\mathbf{S}_2\mathbf{V}^t{}_2\mathbf{k} + \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\boldsymbol{\varepsilon} \qquad (6.2.9a)$$

Because $\mathbf{U}^t{}_1\mathbf{U}_1$ is $\mathbf{I}$ and $\mathbf{U}^t{}_1\mathbf{U}_2$ is $\mathbf{0}$ this becomes

$$\underline{\mathbf{k}} = \mathbf{V}_1\mathbf{V}^t{}_1\mathbf{k} + \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\boldsymbol{\varepsilon} \qquad (6.2.9b)$$

Equation (6.2.9b) is in the form of equation (6.1.13b). Hence, for singular value decomposition as a regularization device

$$\mathbf{R} = \mathbf{V}_1\mathbf{V}^t{}_1 \qquad (6.2.10)$$

$$\mathbf{G} = \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1 \qquad (6.2.11)$$

As can be readily verified from its symmetry and idempotency, $\mathbf{R}$ is an orthogonal projection operator. The relationship between the estimated parameter set $\underline{\mathbf{k}}$ and the true parameter set $\mathbf{k}$ is thus that $\underline{\mathbf{k}}$ is the projection of $\mathbf{k}$ into the solution space of the model matrix $\mathbf{Z}$. This is the subspace of parameter space spanned by the unit vectors comprising the columns of $\mathbf{V}_1$. The relationship is illustrated in figure 6.2. This is a repeat of figure 2.3 with $\mathbf{k}$ substituted for $\mathbf{x}$ which features in the previous figure. For the three-dimensional parameter space schematized in figure 6.2, $\mathbf{V}$ is given by

$$\mathbf{V} = [\mathbf{v}_1\ \mathbf{v}_2\ \mathbf{v}_3] \qquad (6.2.12)$$

The solution space of $\mathbf{Z}$ is spanned by $\mathbf{v}_1$ and $\mathbf{v}_2$ while the null space of $\mathbf{Z}$ is spanned by $\mathbf{v}_3$.

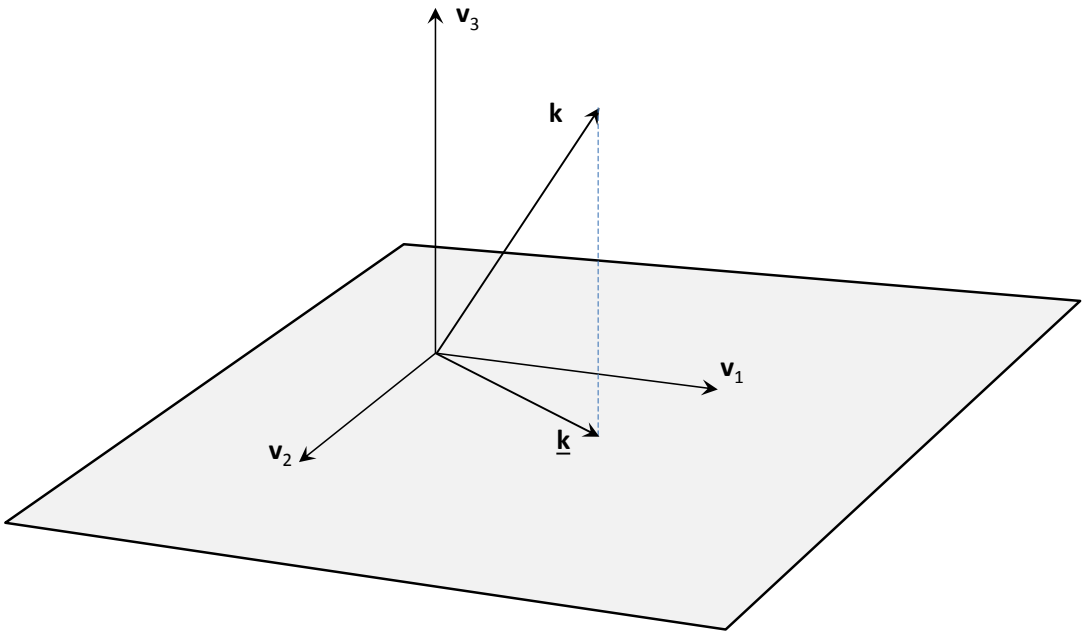


**Figure 6.2. The relationship between estimated and true parameters is that of orthogonal projection onto a limited dimensional solution space.**

From (6.2.9b) and (2.12.14) parameter error is calculated as

$$\underline{\mathbf{k}} - \mathbf{k} = -(\mathbf{I} - \mathbf{V}_1\mathbf{V}^t_1)\mathbf{k} + \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\boldsymbol{\varepsilon} = -\mathbf{V}_2\mathbf{V}^t{}_2\mathbf{k} + \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\boldsymbol{\varepsilon} \qquad (6.2.13)$$

It follows that the error in the estimated parameter set $\underline{\mathbf{k}}$ is comprised of two orthogonal terms. The first is the projection of the true parameter set onto the null space of **Z**; this is the first term on the right of equation (6.2.13). The second contribution to parameter error lies in the solution space of **Z**. This is the error that is incurred in estimating the projection of the true parameter vector **k** onto this space through the presence of noise **ε** in the calibration dataset **h**. The situation is depicted in figure 6.3.

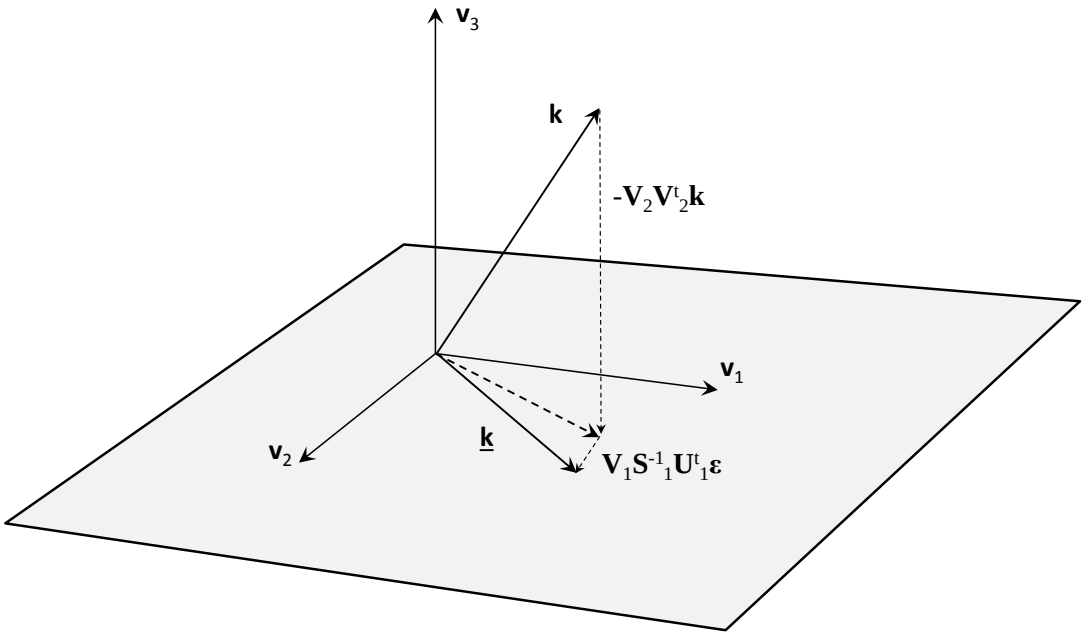


**Figure 6.3. The two components of error in the estimated parameter set $\underline{\mathbf{k}}$.**

The decision to exclude any null space component of **k** from $\underline{\mathbf{k}}$ is fundamental to seeking a solution to the inverse problem which has minimum potential for error, and hence is of minimum error variance. We do not know **k**. We cannot know its null space component because **h** does not provide this information; this is because model outputs can fit the calibration dataset **h** without parameters venturing into the null space at all. Meanwhile our estimate of the solution space component of **k** from **h** is somewhat in error because of the presence of measurement noise **ε** in the calibration dataset. We refer to the estimated solution space component of **k** as $\underline{\mathbf{k}}$; we deem our model to be calibrated once we have calculated this. At the same time we exclude anything that has a non-zero projection onto the calibration null space from $\underline{\mathbf{k}}$, for it is just as likely that any null space component that we may include in $\underline{\mathbf{k}}$ would take us further from **k** rather than closer to it. So we stay on the solution space hyperplane depicted in figure 6.3. This is the safest option – the minimum error variance option. It does not give us "the truth" as far as estimation of **k** is concerned. However it gives us maximum protection from inadvertent falsehood.

### 6.2.4 Kahunen-Loève Transformation

*6.2.4.1 The need for Kahunen-Loève Transformation*

Where there is no noise in the calibration dataset and hence **ε** of equation (6.1.1) is **0**, partitioning of **S** into $\mathbf{S}_1$ and $\mathbf{S}_2$ can take place exactly at the point where $\mathbf{S}_2$ is zero. (The reason why this should not happen if **ε** is non-zero will be provided shortly.) In that case, as discussed in section 2.12, equation (6.2.4) provides the minimum norm (i.e. minimum magnitude) solution for $\underline{\mathbf{k}}$; calculation of $\underline{\mathbf{k}}$ from **h** takes place using the Moore-Penrose pseudoinverse of **Z**.

If the prior probability distribution of **k** is multinormal with mean **0** (recall that a mean of **0** is a design specification that we have adopted for model linearization, and have formulated the definition of **k** accordingly), and if the elements of **k** are statistically independent and have the same standard deviation, this solution is also that of highest probability density function

value according to the prior distribution of **k**. Under these conditions the exponent of equation (3.6.1) coincides with the equation for the $L_2$ norm of vector **k**; hence the estimated parameter set $\underline{\mathbf{k}}$ deviates from the prior mean parameter set of **0** to the smallest extent required to satisfy the condition that model outputs fit field measurements. This is obviously a good outcome, for it guarantees a high level of credibility for the estimated parameter set. It does not guarantee that this parameter set is right; it does guarantee however that it is minimally wrong.

In most cases of real world modelling interest the prior probability distribution of **k** is not such that

$$C(\mathbf{k}) = \sigma^2_k \mathbf{I} \qquad (6.2.14)$$

as is required for minimum norm to coincide with maximum pre-calibration probability. However a parameter set **m** can be calculated from a model's parameter set **k** that has these properties; see section 3.10. As usual, let C(**k**) denote the prior covariance matrix of **k**. Let the eigenvector matrix **E** and the diagonal eigenvalue matrix **F** be obtained from C(**k**) through singular value decomposition as follows

$$C(\mathbf{k}) = \mathbf{E}\mathbf{F}\mathbf{E}^t \qquad (6.2.15)$$

Then the parameter set **m** defined as

$$\mathbf{m} = \mathbf{F}^{-½}\mathbf{E}^t\mathbf{k} \qquad (6.2.16)$$

has the desired property that its covariance matrix is **I**.

Minimization of the $L_2$ norm of **m** requires minimization of $\mathbf{m}^t\mathbf{m}$. From (6.2.16)

$$\mathbf{m}^t\mathbf{m} = \mathbf{k}^t\mathbf{E}\mathbf{F}^{-½}\mathbf{F}^{-½}\mathbf{E}^t\mathbf{k} = \mathbf{k}^tC^{-1}(\mathbf{k})\mathbf{k} \qquad (6.2.17)$$

As seen from equation (3.6.1), a parameter set **k** of maximum prior probability density function value is thus attained. From (6.2.16), **k** is calculated from **m** as

$$\mathbf{k} = \mathbf{E}\mathbf{F}^{½}\mathbf{m} \qquad (6.2.18)$$

It is thus apparent that use of singular value decomposition to solve the inverse problem of model calibration requires that the prior probability distribution of model parameters be taken into account if the solution to that inverse problem is to be of minimum error variance; this is done by subjecting model parameters to Kahunen-Loève transformation before actually estimating them. Accommodation of the prior parameter probability distribution of parameters thus becomes an indispensable feature of an appropriately-formulated inverse problem. (In later sections of this chapter prior knowledge of parameters will be introduced to the parameter estimation process through Tikhonov regularization, as this provides more flexible ways to express expert knowledge; however singular value decomposition will still play a strategic role in solving the inverse problem because of its ability to calculate, and then invert, a matrix that is guaranteed to be invertible.)

### *6.2.4.2 Repercussions of not Transforming*

Suppose that we solve an ill-posed inverse problem for $\underline{\mathbf{k}}$ and that we do not pre-transform **k** to obtain an **m** to which equation (6.2.14) applies. From (6.2.9b) without measurement noise, the estimated $\underline{\mathbf{k}}$ is related to the true **k** through the equation

$$\underline{\mathbf{k}} = \mathbf{V}_1\mathbf{V}^t_1\mathbf{k} \qquad (6.2.19)$$

Transformation and back-transformation between **m**-space and **k**-space is available through equations (6.2.16) and (6.2.18). Through use of these two equations the relationship between estimated **m** (i.e. $\underline{\mathbf{m}}$) and real **m** parameters when singular value decomposition is undertaken in **k**-space is

$$\underline{\mathbf{m}} = \mathbf{F}^{-½}\mathbf{E}^{t}\,\mathbf{V}_1\mathbf{V}^{t}_1\,\mathbf{E}\mathbf{F}^{½}\mathbf{m} = \mathbf{R}'\mathbf{m} \qquad (6.2.20)$$

As can be readily verified, the resolution matrix $\mathbf{R}'$ of (6.2.20) is idempotent. Hence it is a projection operator. However, in general, it is not symmetric. Therefore it is not an orthogonal projection operator. What this means is that $\underline{\mathbf{m}}$ may include some **m**-space null space components. The presence of these null space components invalidates any claims to minimum error variance status that $\underline{\mathbf{m}}$ may make; the same then applies to predictions made by the model. This is because, for a given (unknown) **m**, $\underline{\mathbf{m}}$ achieved through **k**-space singular value decomposition provides a biased estimate of its value. Watson et al (2013) discuss this matter further, and show an example of calibration bias incurred in this way for a simple model.

The fact that singular value decomposition conducted in the wrong space can lead to inverse problem solution bias through unwitting entrainment of null space components in the calibrated parameter field can be further demonstrated as follows. Using (6.2.18), equation (6.1.1), which poses the inverse problem which is the subject of this chapter, can be expressed in **m**-space as

$$\mathbf{h} = \mathbf{Z}\mathbf{E}\mathbf{F}^{½}\mathbf{m} + \boldsymbol{\varepsilon} = \mathbf{Y}\mathbf{m} + \boldsymbol{\varepsilon} \qquad (6.2.21)$$

where **Y**, the model matrix in **m**-space, is defined through the above equation as

$$\mathbf{Y} = \mathbf{Z}\mathbf{E}\mathbf{F}^{½} \qquad (6.2.22)$$

If (6.2.22) is post-multiplied by $\mathbf{F}^{-½}$ and then by $\mathbf{E}^{t}$ if follows that

$$\mathbf{Z} = \mathbf{Y}\mathbf{F}^{-½}\mathbf{E}^{t} \qquad (6.2.23)$$

Suppose that a vector **m** is in the null space of **Y**. Then

$$\mathbf{Y}\mathbf{m} = \mathbf{0} \qquad (6.2.24)$$

If, in this equation, (6.2.22) is substituted for **Y** and (6.2.16) is substituted for **m**, it immediately follows that

$$\mathbf{Z}\mathbf{E}\mathbf{F}^{½}\mathbf{F}^{-½}\mathbf{E}^{t}\mathbf{k} = \mathbf{Z}\mathbf{k} = \mathbf{0} \qquad (6.2.25)$$

Hence a vector in **m**-space which is in the null space of **Y** transforms to a vector in **k**-space which is in the null space of **Z**. The reverse is also true. Suppose that **k** is in the null space of **Z** so that (6.2.25) holds. If (6.2.23) is substituted for **Z** and (6.2.18) is substituted for **k** in (6.2.25) then

$$\mathbf{Y}\mathbf{F}^{-½}\mathbf{E}^{t}\,\mathbf{E}\mathbf{F}^{½}\mathbf{m} = \mathbf{Y}\mathbf{m} = \mathbf{0} \qquad (6.2.26)$$

It follows that the null spaces of **Z** and **Y** are directly transferrable between **k**-space and **m**-space. However it was demonstrated above that the orthogonal complement to the **Z** matrix null space in **k**-space does not transform to the orthogonal complement of the **Y** matrix null space in **m**-space. Conversely, if a vector in **m**-space is orthogonal to the null space of **Y**, it does not follow that the **k**-space equivalent of this vector will not contain a null space component of **Z**.

### 6.2.5 Predictive Error Variance

*6.2.5.1 Expressing Predictive Error Variance*

From equation (6.2.13) the covariance matrix of parameter error can be obtained using the propagation of variance relationship (3.9.2) as

$$C(\underline{\mathbf{k}} - \mathbf{k}) = \mathbf{V}_2\mathbf{V}^t_2C(\mathbf{k})\mathbf{V}_2\mathbf{V}^t_2 + \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t_1C(\boldsymbol{\varepsilon})\mathbf{U}_1\mathbf{S}^{-1}{}_1\mathbf{V}^t_1 \qquad (6.2.27)$$

Suppose that

$$C(\mathbf{k}) = \sigma^2_k\mathbf{I} \qquad (6.2.28)$$

$$C(\boldsymbol{\varepsilon}) = \sigma^2_\varepsilon\mathbf{I} \qquad (6.2.29)$$

Ideally (6.2.28) should have been achieved through pre-inversion Kahunen-Loève parameter transformation while (6.2.29) should have been achieved through pre-inversion weight matrix observation transformation, both of which have been discussed above. Equation (6.2.27) then becomes

$$C(\underline{\mathbf{k}} - \mathbf{k}) = \sigma^2_k\mathbf{V}_2\mathbf{V}^t_2 + \sigma^2_\varepsilon\mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t_1 \qquad (6.2.30)$$

Let $s$ be a prediction of interest whose sensitivity to parameters $\mathbf{k}$ is expressed by the vector $\mathbf{y}$. The error in this prediction, as made by the calibrated model, is given by

$$\underline{s} - s = \mathbf{y}^t(\underline{\mathbf{k}} - \mathbf{k}) \qquad (6.2.31)$$

so that, through propagation of variance,

$$\sigma^2_{\underline{s}-s} = \sigma^2_k\mathbf{y}^t\mathbf{V}_2\mathbf{V}^t_2\mathbf{y} + \sigma^2_\varepsilon\mathbf{y}^t\mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t_1\mathbf{y} \qquad (6.2.32)$$

This, of course, is equation (6.1.25) formulated for the specific conditions wherein regularization is undertaken using singular value decomposition and the covariance matrices of prior parameter uncertainty and measurement error are expressed by (6.2.28) and (6.2.29).

*6.2.5.2 Optimum Truncation Point*

Equation (6.2.32) can be used to design optimal partitioning of the **U**, **S** and **V** matrices to define $\mathbf{V}_1$, $\mathbf{S}_1$ and $\mathbf{U}_1$ for use in equation (6.2.4). Such partitioning is often referred to as "truncation"; singular value decomposition is often referred to as "truncated singular value decomposition".

It will be recalled that singular values are arranged in the **S** matrix from highest to lowest down its diagonal. Obviously, truncation should occur before singular values become zero, for if this does not occur then equation (6.2.4) is asked to invert a non-invertible matrix. However, as will now be shown, the optimum truncation point should occur before this, where singular values become small rather than zero. This prevents so-called "over-fitting" to the calibration dataset, and the consequential potential for parameter and predictive error that over-fitting can incur.

Suppose that we truncate **S** after $w$ singular values. Recalling that the number of parameters featured in the inverse problem is $m$, equation (6.2.32) can be written as

$$\sigma^2_{\underline{s}-s} = \sigma^2_k\sum_{i=w+1}^{m}\left(\mathbf{y}^t\mathbf{v}_i\right)^2 + \sigma^2_\varepsilon\sum_{i=1}^{w}s_i^{-2}\left(\mathbf{y}^t\mathbf{v}_i\right)^2 \qquad (6.2.33)$$

where $\mathbf{v}_i$ are the unit vectors comprising the columns of **V**. All terms in both of the

summations featured on the right side of equation (6.2.33) are positive. Therefore the first summation decreases as *w* increases and the second summation increases as *w* increases. Where there is no truncation at all and *w* is equal to 0, then

$$\sigma^2_{\underline{s}\text{-}s} = \sigma^2_k \mathbf{y}^t \mathbf{V}\mathbf{V}^t \mathbf{y} = \sigma^2_k \mathbf{y}^t \mathbf{y} = \mathbf{y}^t C(\mathbf{k}) \mathbf{y} \qquad (6.2.34)$$

When *w* is zero the null space is equivalent to the entirety of parameter space as there is no calibration. Equation (6.2.34) states that the predictive error variance is then equal to the prior uncertainty of the prediction which, of course, depends only on C(**k**).

As *w* increases from 0, the first term of equations (6.2.32) and (6.2.33) falls monotonically as the number of terms in the summation falls. Eventually it becomes zero when *w* is equal to *m*, the number of parameters featured in the inverse problem; at this point the dimensions of the null space have shrunk to zero. This first term of equations (6.2.32) and (6.2.33) will be referred to as the "null space term". It quantifies the cost of uniqueness that is paid in seeking a solution to an ill-posed inverse problem. For singular value decomposition this cost is paid by seeking a value only for the projection of the real world parameter set **k** onto the solution space of **Z** and thereby foregoing entry into the null space of **Z**.

The behaviour of the second term of equations (6.2.32) and (6.2.33) is opposite to that of the first; it rises monotonically as *w* increases from zero. It is zero when *w* is zero because the summation has no terms; then it rises with *w* as the number of terms in the summation increases. The rate of increase of the summation becomes very rapid as singular values become small because of the presence of $s_i^{-2}$ in this term. When singular values become zero, this term becomes infinite. It is referred to herein as the "solution space term". It quantifies the effect of measurement noise on the error variance of a prediction. Note that a prediction can also be the value of a single parameter; this occurs when all elements in **y** are zero except for the element corresponding to the pertinent parameter which is set to one.

The solution and null space terms of equations (6.2.32) and (6.2.33) sum to the total predictive error variance.

The situation is depicted in figure 6.4. As the truncation point increases from zero, predictive error variance initially falls. As the truncation point is increased further to include more singular values, the dimensions of the null space decrease while the dimensions of the solution space increase. This provides more receptacles for information contained within the calibration dataset; these receptacles are the coefficients by which individual $\mathbf{v}_i$ are multiplied before vector addition to form the overall $\underline{\mathbf{k}}$ vector calculated through equation (6.2.4). However as the null space term of equations (6.2.32) and (6.2.33) falls, the solution space term rises. Eventually the cost of achieving a better fit with the calibration dataset outweighs the benefit of reducing the dimensionality of the null space. The total predictive error variance curve, which has hitherto fallen with increasing number of singular values, now starts to rise as measurement noise is more greatly amplified because of the presence of $s_i^{-2}$ in the solution space term. "Over-fitting" to the calibration dataset is now occurring. The optimal singular value truncation point corresponds to the minimum of the predictive error variance curve.

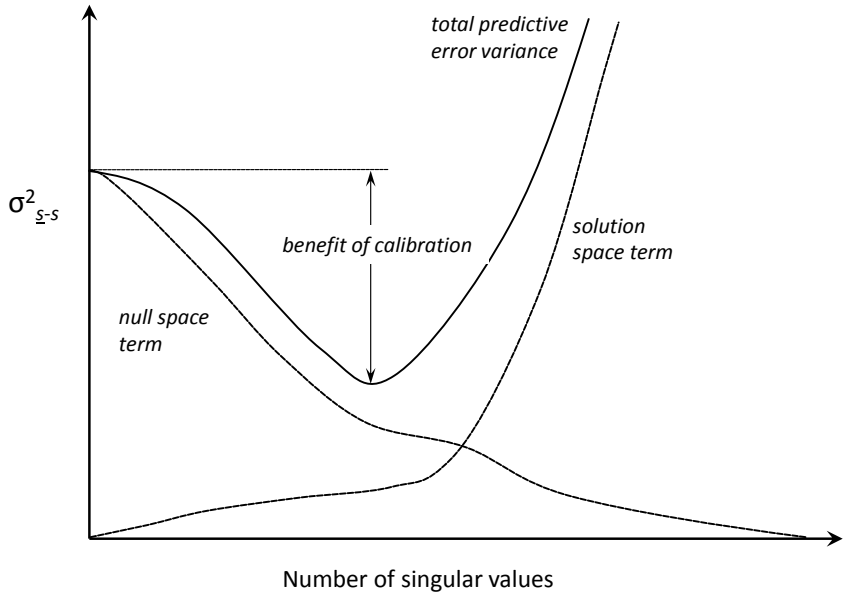


**Figure 6.4. Predictive error variance as a function of number of singular values used in the inversion process. Note that as the number of singular values increases, the fit between model outputs and the calibration dataset improves. The horizontal axis of the above figure could therefore be alternatively labelled as "goodness of fit".**

Equations (6.2.32) and (6.2.33) can be used to calculate the benefits of model calibration as these pertain to a specific prediction. This benefit is the reduction in the error variance of that prediction below its pre-calibration level that is accrued through the calibration process. Recall that the pre-calibration error variance of a prediction is equal to the variance of its pre-calibration uncertainty. Maximum predictive benefit is gained where singular value truncation accords with the minimum of the predictive error variance curve. See figure 6.4.

It will be shown below that the minimized error variance of a prediction cannot fall below the posterior uncertainty of that prediction as calculated through direct application of Bayes equation; in fact it will probably be a little higher. The difference between post-calibration predictive error variance and the variance of posterior predictive uncertainty is the cost of firstly calibrating a model and then exploring post-calibration error as a substitute for direct calculation of posterior uncertainty. However, as stated in an earlier chapter, strict Bayesian analysis is generally numerically intractable, and always approximate, where parameter numbers are high and model run times are long. So the benefit of taking the calibration route is generally worth the cost, for the benefit is being able to calculate a quantity that approaches predictive uncertainty where direct evaluation of predictive uncertainty may otherwise be impossible.

Plots such as that depicted in figure 6.4 reveal the components of predictive error variance at any number of singular values, including the optimum number of singular values. A modeller is thus able to ascertain the relative contributions made to predictive error variance by the solution and null space terms of (6.2.32) and (6.2.33). If minimized predictive error variance (and hence posterior predictive uncertainty for which it is a surrogate) is dominated by the null space term, then it is the deficit of information in the calibration dataset that is responsible for this error variance. On the other hand, if minimized predictive error variance is dominated by the solution space term then, to the extent that parameters to which a

prediction is sensitive are informed by the calibration process, estimates of their values are contaminated by noise associated with the calibration dataset.

The nature of the curve that is obtained by plotting predictive error variance against singular value truncation point is prediction-specific. However the location of the minimum is unlikely to vary greatly from prediction to prediction. Equation (6.2.32) indicates that if a prediction is sensitive to predominantly null space components of **Z** then its error variance (and hence uncertainty) will be reduced very little from its pre-calibration level through the calibration process; in this case the calibration dataset contains little information pertaining to parameters to which the prediction is most sensitive. Predictions which depend on system property detail, predictions of system state which are very different from those for which measurements are available in the calibration dataset, and predictions of system response to a stress regime which is very different from that which prevailed when the calibration dataset was acquired, are all likely to fall into this category. This is something that those who are unfamiliar with highly parameterized inversion may not always appreciate. Just because a model has been "calibrated", it does not follow that its predictive abilities have thereby been enhanced, for this depends entirely on the prediction.

It should be especially noted that failure to represent null space parameterization in a model (as is often done as a manual regularization device to achieve inverse problem well-posedness) may prevent a modeller from ever realizing the inadequacies of the calibration process in lowering the uncertainties of critical model predictions. If null space parameterization is eradicated from a model, the first term of equation (6.2.32) is eliminated; predictive error variance may therefore be grossly underestimated.

It is of interest to note that calculation of predictive error variance using equation (6.2.32) requires only sensitivities of model outputs to model parameters. These sensitivities comprise the elements of the vector **y** and the elements of the matrix **Z**. The latter is subjected to singular value decomposition to yield the **S** and **V** matrices featured in this equation. Values of parameters **k**, values of measurements **h**, and the value of the prediction *s* do not feature in this equation. This provides some interesting possibilities. For example if the error variance of a prediction can be calculated using the current calibration dataset through equation (6.2.32), then its error variance can also be calculated using an expanded dataset. The values of measurements comprising that expanded dataset are not required. All that is required is that the model calculate the sensitivities of model outputs that correspond to these measurements and supplement the **Z** matrix accordingly. The ability of different data acquisition strategies to lower the error variances of predictions of interest can thereby be explored. For a nonlinear model, sensitivities will depend on parameter values, so data worth analysis using equation (6.2.32) can only be approximate. Nevertheless it may be informative. This is further discussed in the following chapter where a Bayesian alternative to linear data worth analysis is proposed.

Equations (6.2.32) and (6.2.33) were derived under the assumption that C(**k**) and C(**ε**) are specified by (6.2.28) and (6.2.29). In the more general case where C(**k**) and C(**ε**) are not described by these equations, it follows from (6.2.27) that

$$\sigma^2_{\underline{s}\text{-}s} = \mathbf{y}^t\mathbf{V}_2\mathbf{V}^t{}_2C(\mathbf{k})\mathbf{V}_2\mathbf{V}^t{}_2\mathbf{y} + \mathbf{y}^t\mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1C(\boldsymbol{\varepsilon})\mathbf{U}_1\mathbf{S}^{-1}{}_1\mathbf{V}^t{}_1\mathbf{y} \qquad (6.2.35)$$

If $\sigma^2_{\underline{s}\text{-}s}$ is plotted against number of pre-truncation singular values, monotonicity of the first and second terms of equation (6.2.35) cannot be guaranteed where (6.2.28) and (6.2.29) do not apply. Furthermore the minimized predictive error variance will be greater than it would

have been if Kahunen-Loève and weight matrix transformation had first been undertaken in order to achieve the conditions expressed by (6.2.28) and (6.2.29).

*6.2.5.3 Optimizing Truncation without a Prediction*

The assistance that equation (6.2.32) can provide in identifying the point of optimal singular value truncation was discussed above. It was shown that the best truncation point is that at which the benefits of further extraction of information from the calibration dataset are balanced by the propensity for parameter and predictive error to increase as a better fit is sought with the calibration dataset. This occurs because the values estimated for some combinations of parameters (these combinations being the vectors $\mathbf{v}_i$ of the matrix **V**) become more reflective of measurement noise that accompanies **h** than of information that is resident in **h** itself, as singular values $s_i$ associated with respective $\mathbf{v}_i$ decrease in value.

The exact shape of the curve that emerges from application of (6.2.32) will vary from prediction to prediction. Some predictions will have their error variances reduced very little through the calibration process. The opposite is the case for others. Also, the exact location of the minimum of the total error variance curve may vary slightly from prediction to prediction, this depending on alignment of the vector **y** with the vectors $\mathbf{v}_i$ comprising the columns of **V**.

So which prediction should a modeller use when establishing the optimum singular value truncation point for calibration of a model? The answer is "probably none". Generally, predictive sensitivities are unavailable when a model is being calibrated.

A more practical means of securing truncation point optimality is to examine each term of the two summations that are made explicit when equation (6.2.32) is re-written as (6.2.33). Furthermore, in each term of these summations, the vector **y** should be replaced by the respective $\mathbf{v}_i$ vector. The prediction is thus different for each $i$ in the overall summation. For each term the prediction thus becomes $\sigma^2_k \mathbf{v}^t_i \mathbf{v}_i$, which is $\sigma^2_k$ times the magnitude of $\mathbf{v}_i$; this is, of course, equal to $\sigma^2_k$. Starting at the first singular value, the solution and null space estimates for the error variance of the estimated value of $\sigma^2_k \mathbf{v}^t_i \mathbf{v}_i$ should be compared. The solution space error variance is $\sigma^2_\varepsilon s_i^{-2} (\mathbf{v}^t_i \mathbf{v}_i)^2$ (which is, of course, equal to $\sigma^2_\varepsilon s_i^{-2}$), while the null space error variance is $\sigma^2_k (\mathbf{v}^t_i \mathbf{v}_i)^2$ (which is, of course, equal to $\sigma^2_k$). For low values of $i$, where $s_i$ is likely to be large, the null space error variance will normally be higher than the solution space error variance. The term should therefore be relegated to the solution space. However eventually an $i$ will be encountered where the opposite occurs. This marks the $i$ at which singular value truncation should occur. If $\sigma^2_\varepsilon$ is equal to $\sigma^2_k$ this occurs where $s_i$ becomes less than 1.0.

## 6.2.6 Well-posedness and Flow of Information

*6.2.6.1 Already Well-Posed*

Suppose that the inverse problem described by equation (6.1.1) is well-posed. Let us also assume that weight matrix transformation of the problem has taken place so that equation (6.2.29) is satisfied. Then, based on theory presented in the previous chapter, $\underline{\mathbf{k}}$ can be estimated as

$$\underline{\mathbf{k}} = (\mathbf{Z}^t\mathbf{Z})^{-1}\mathbf{Z}^t\mathbf{h} \qquad (6.2.36)$$

If (6.2.1) is substituted for **Z** in this equation, (6.2.4) results. It is therefore apparent that singular value decomposition and the Gauss-Newton method described in the previous

chapter are equivalent when an inverse problem is well-posed.

From (6.2.1)

$$\mathbf{Z}^t\mathbf{Z} = \mathbf{V}\mathbf{S}^2\mathbf{V}^t \qquad (6.2.37)$$

The singular values of $\mathbf{Z}^t\mathbf{Z}$ are thus the squares of the singular values of **Z**. If (6.2.37) is post-multiplied by **V** we obtain

$$\mathbf{Z}^t\mathbf{Z}\mathbf{V} = \mathbf{V}\mathbf{S}^2 \qquad (6.2.38)$$

From (2.11.1) it is apparent that the vectors $\mathbf{v}_i$ are the eigenvectors of $\mathbf{Z}^t\mathbf{Z}$ while the scalars $s^2_i$ comprising the diagonals of $\mathbf{S}^2$ are its eigenvalues. That is, the eigenvalues of $\mathbf{Z}^t\mathbf{Z}$ are the squares of the singular values of **Z**.

It is easily verified that

$$(\mathbf{Z}^t\mathbf{Z})^{-1} = \mathbf{V}\mathbf{S}^{-2}\mathbf{V}^t \qquad (6.2.39)$$

and that

$$(\mathbf{Z}^t\mathbf{Z})^{-1}\mathbf{V} = \mathbf{V}\mathbf{S}^{-2} \qquad (6.2.40)$$

Recall from the previous chapter that, after multiplication by the reference variance, $(\mathbf{Z}^t\mathbf{Z})^{-1}$is the post-calibration covariance matrix of parameter error. As was discussed in section 5.3, much can be learned about the well-posedness or otherwise of an inverse problem through examining the eigenvectors and eigenvalues of this matrix. If the ratio of largest to smallest eigenvalue of this matrix is very large, then the inverse problem is verging on ill-posedness and should be reformulated with stronger manual regularization. Unfortunately, however, if the inverse problem is entirely ill-posed, then the $\mathbf{Z}^t\mathbf{Z}$ matrix cannot be inverted at all to obtain the post-calibration parameter error covariance matrix. The parameter combinations that feature in the eigenvector corresponding to the highest eigenvalue of this matrix are not therefore available for inspection in order for one or a number of salient parameters to be eliminated in improved manual regularization. This illustrates an important flaw in manually-regularized inversion that was discussed in the previous chapter; the ill-posedness, or incipient ill-posedness, of an inverse problem is not apparent until after one has tried (and possibly failed) to solve it.

Singular value decomposition allows a modeller to inspect the would-be eigenvalues of a post-calibration parameter error covariance matrix before, rather than after, this matrix is obtained. These are simply the inverse of the squares of the singular values of **Z**. If some singular values are zero, or are very low relative to the highest singular value, then ill-posedness, or incipient ill-posedness, of the inverse problem is thereby identified. The eigenvectors corresponding to would-be troublesome eigenvalues are also available in the columns of **V**.

*6.2.6.2 Well-Posed through SVD*

From (6.1.1) and (6.2.2)

$$\mathbf{h} = \mathbf{Z}\mathbf{k} + \boldsymbol{\varepsilon} = \mathbf{U}_1\mathbf{S}_1\mathbf{V}^t_1\mathbf{k} + \mathbf{U}_2\mathbf{S}_2\mathbf{V}^t_2\mathbf{k} + \boldsymbol{\varepsilon} \qquad (6.2.41)$$

Adopting the same symbolism as in section 5.1, equation (6.2.41) can be written as

$$\mathbf{h} = \mathbf{X}\mathbf{p} + \boldsymbol{\eta} + \boldsymbol{\varepsilon} \qquad (6.2.42)$$

where

$$\mathbf{X} = \mathbf{U}_1\mathbf{S}_1 \tag{6.2.43}$$

$$\mathbf{p} = \mathbf{V}^t{}_1\mathbf{k} \tag{6.2.44}$$

$$\boldsymbol{\eta} = \mathbf{U}_2\mathbf{S}_2\mathbf{V}^t{}_2\mathbf{k} \tag{6.2.45}$$

With appropriate singular value truncation, equation (6.2.42) constitutes a well-posed inverse problem. Meanwhile $\boldsymbol{\eta}$ is the structural noise incurred through the simplification that was required to achieve well-posedness of the inverse problem. The fewer non-zero singular values that feature in $\mathbf{S}_2$, the smaller will $\boldsymbol{\eta}$ be. The elements of $\mathbf{p}$ are the scalar projections of the unknown parameter vector $\mathbf{k}$ onto each of the unit vectors that comprise the columns of $\mathbf{V}_1$; recall that the columns of $\mathbf{V}_1$ span the solution space of $\mathbf{Z}$. Once $\underline{\mathbf{p}}$ has been estimated, the solution vector in $\mathbf{k}$-space can be recovered from the solution vector in $\mathbf{p}$-space by multiplying each of these scalar projections by the corresponding unit vector onto which it is projected. Thus

$$\underline{\mathbf{k}} = \mathbf{V}_1\underline{\mathbf{p}} \tag{6.2.46}$$

A solution to this well-posed inverse problem can be obtained, according to methods discussed in the last chapter, as

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{h} = (\mathbf{S}_1\mathbf{U}^t{}_1\mathbf{U}_1\mathbf{S}_1)^{-1}\mathbf{S}_1\mathbf{U}^t{}_1\mathbf{h} = \mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\mathbf{h} \tag{6.2.47}$$

which, combined with (6.2.46), leads to (6.2.4).

So singular value decomposition has in common with manual regularization the fact that it achieves inverse problem solution uniqueness through parameter simplification. The simplification strategy adopted by singular value decomposition is the estimation of strategic combinations of parameters in place of individual parameters of the original inverse problem. While estimation of parameter combinations sometimes constitutes a simplification strategy sought through manual regularization (where, for example, a modeller may link parameters in constant ratios or combine them to form homogenous zones), parameter combinations defined by singular value decomposition are optimal. Provided it is preceded by Kahunen-Loève transformation of parameters, the outcome of regularization achieved through singular value decomposition is a solution of minimum error variance to the inverse problem. This occurs because simplification is carried by the parameter estimation process itself which, through its ability to separate combinations of parameters which are estimable (columns of the $\mathbf{V}_1$ matrix) from combinations of parameters which are inestimable (columns of the $\mathbf{V}_2$ matrix), is able to isolate the latter so that only the former are estimated.

*6.2.6.3 Flow of Information*

If both sides of equation (6.2.4) are multiplied by $\mathbf{V}^t{}_1$ the following equation is obtained

$$\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\mathbf{h} = \mathbf{V}^t{}_1\underline{\mathbf{k}} \tag{6.2.48}$$

If there is no noise in the calibration dataset $\mathbf{V}^t{}_1\underline{\mathbf{k}}$ can be replaced by $\mathbf{V}^t{}_1\mathbf{k}$ in the above equation. Because $\mathbf{S}^{-1}{}_1$ is a diagonal matrix (6.2.48) can be re-written as a series of equations as follows

$$s_i{}^{-1}\mathbf{u}^t{}_i\mathbf{h} = \mathbf{v}^t{}_i\mathbf{k} \tag{6.2.49}$$

$\mathbf{u}^t{}_i\mathbf{h}$ is the scalar projection of the calibration dataset onto a single column of the $\mathbf{U}_1$ matrix. (The columns of $\mathbf{U}_1$ span part or all of the range space of $\mathbf{Z}$.) $\mathbf{v}^t{}_i\mathbf{k}$ is the scalar projection of the parameter set $\mathbf{k}$ into the $i$'th column of the $\mathbf{V}_1$ matrix. (The columns of $\mathbf{V}_1$ span the

solution space of **Z**.) Each of these scalar projections is, of course, a scalar. There is one scalar that links the scalar projection on the left side of (6.2.49) to that on its right side. This scalar is $s_i^{-1}$. This, together with the orthonormality of **U** and **V**, implies that $\mathbf{u}^t_i\mathbf{h}$ is uniquely and entirely informative of $\mathbf{v}^t_i\mathbf{k}$. $\mathbf{u}_i$ is thus the "characteristic" or "signal" in the dataset **h** that speaks solely and uniquely about the "characteristic" or "signal" that is $\mathbf{v}_i$ in the model's parameter set. To put it another way, (6.2.49) identifies orthogonal combinations of observations (i.e. "signals" in the calibration dataset) that are uniquely and entirely informative of orthogonal combinations of parameters (i.e. "characteristics" of the model's parameter field).

The $\mathbf{u}_i$ defined through singular value decomposition of **Z** thus constitute individual and separate sources of information in the observation dataset. Regardless of the size of this dataset (i.e. regardless of the number of elements of **h**), there are only as many of these sources of information available to the parameter estimation process as there are pre-truncation singular values employed in that process. $\mathbf{v}_i$ constitutes the receptacle for the information that is $\mathbf{u}_i$.

Where observations and parameters have spatial or temporal associations, it is sometimes interesting to plot the elements of high index $\mathbf{u}_i$ and $\mathbf{v}_i$ vectors in space and time. The spatial/temporal distribution of measurement data that constitutes a single piece of information on the one hand, and the spatial/temporal distribution of properties of an environmental system that constitutes the receptacle for that information on the other hand, then become apparent.

After model parameters have been estimated, residuals can be calculated as

$$\mathbf{r} = \mathbf{h} - \mathbf{Z}\underline{\mathbf{k}} = \mathbf{h} - \mathbf{Z}\mathbf{V}^1\mathbf{S}_1^{-1}\mathbf{U}^t{}_1\mathbf{h} \qquad (6.2.50)$$

which, after substitution of $\mathbf{USV}^t$ for **Z**, becomes

$$\mathbf{r} = (\mathbf{I} - \mathbf{U}_1\mathbf{U}^t{}_1)\mathbf{h} \qquad (6.2.51)$$

Direct multiplication shows that

$$\mathbf{r}^t\mathbf{Z}\underline{\mathbf{k}} = \mathbf{0} \qquad (6.2.52)$$

Residuals are thus orthogonal to outputs generated by the calibrated model. It does not necessarily follow, however, that the measurement dataset **h** has thereby been emptied of all of its information. To the extent that singular value truncation takes place prior to singular values becoming zero, the residuals vector **r** may have a non-zero projection onto some of the $\mathbf{u}_i$ vectors which comprise the columns of $\mathbf{U}_2$. However if singular value truncation is optimal, the information that is associated with these $\mathbf{u}_i$ vectors cannot be assimilated into the model's parameter set because noise within the measurement dataset that is also projected on to these $\mathbf{u}_i$ has the potential to worsen, rather than improve, estimates of parameter combinations to which that information is directed.

### 6.2.7 Strengths and Weaknesses of Singular Value Decomposition

As a method for solving an ill-posed inverse problem, singular value decomposition has many attractive features. Its numerical stability in the face of problem ill-posedness is an obvious advantage. Another nice feature of singular value decomposition is the conceptual insights that it offers into what can be achieved, and what cannot be achieved, in solving an ill-posed inverse problem. These have been discussed above.

A further numerical benefit that singular value decomposition offers is illustrated by equations (6.2.42) to (6.2.45). Once a singular value truncation point has been selected, a set of parameters **p** can be defined through (6.2.44). In PEST parlance, these are so-called "super parameters". In many modelling contexts the number of parameters featured in the **p** vector will be much smaller than those featured in the **k** vector. For a given **p**, a corresponding **k** can be calculated as

$$\mathbf{k} = \mathbf{V}_1\mathbf{p} \qquad (6.2.53)$$

In a parameter estimation setting where the Jacobian matrix must be computed using finite parameter differences, a **Z** matrix can first be computed by undertaking *m* model runs, where *m* is the number of elements in **k**. A smaller set of parameters **p** can then be defined using (6.2.44). This smaller set of parameters can then form the basis for further iterations of the nonlinear parameter estimation process. Finite differences of **p**-parameters and corresponding model outputs can be used to compute a Jacobian matrix to represent **X**; for every **p** vector used in finite differencing to fill the Jacobian matrix, or in testing updated parameters calculated using different Marquardt lambdas, a corresponding **k** vector is calculated using (6.2.53) prior to running the model. Actually, there is no need for the singular value truncation process on which basis **p** is calculated to be such as to guarantee a well-posed inverse problem; singular value decomposition of **X** can be used to estimate **p** so that numerical stability is ensured. Once the inverse problem has been solved, and $\underline{\mathbf{p}}$ has been estimated, a corresponding $\underline{\mathbf{k}}$ is then calculated using (6.2.53). This is the basis of the "SVD-assist" methodology implemented in PEST; see Tonkin and Doherty (2005) for further details. (Note that it is recommended practice for Tikhonov regularization to be included in "SVD-assisted" solution of an ill-posed inverse problem.)

One weakness of singular value decomposition as a parameter estimation device in the environmental modelling context is the rigidity of the receptacles that it provides for expert knowledge. As has already been discussed, use of singular value decomposition to attain a minimum error variance solution to an ill-posed inverse problem requires that model parameters be subjected to Kahunen-Loève transformation prior to commencement of the inversion process. In many environmental contexts it may be difficult or impossible to provide such a transformation. In the discussion above, Kahunen-Loève transformation was based on the prior covariance matrix C(**k**). However the complexity and heterogeneity of natural systems (for example geological media) is such that a C(**k**) matrix may be very difficult to formulate at best, and may provide an inappropriately simple descriptor of prediction-relevant heterogeneity at worst.

Suppose that a C(**k**) matrix that encapsulates expert knowledge of system property variability and correlation is indeed formulated. Singular value decomposition can then be used to estimate coefficients of its eigencomponents; see section 6.2.4. While this may provide the benefit that the prior covariance matrix of estimated, transformed parameters is **I**, the inversion process is then locked into the use of these eigencomponents as the sole expression of system property variability and heterogeneity. This suppresses the ability of the inversion process to reveal the presence of system property heterogeneity of which the modeller may have been previously unaware. This annuls one of the benefits of adopting a highly parameterized approach to inversion in the first place, this being an ability to formulate the inverse problem in such a way as to provide the inversion process with as much freedom as it needs to respond to information contained in the calibration dataset in ways that are flexible and informative to the modeller.

Another practical problem with the use of singular value decomposition in real world model calibration is the prevention of over-fitting. While the theory of singular value decomposition provides elegant concepts through which over-fitting can be defined and avoided (see figure 6.4), in many environmental contexts neither C(**k**) nor C(**ε**) is known. Furthermore model-to-measurement misfit is likely to be dominated by structural noise born of model defects rather than noise associated with the measurement dataset. Because of this, a modeller often learns through the calibration process itself the extent of parameter variability and the magnitude of model-to-measurement misfit that he/she will tolerate. In fact these are often subjectively traded off against each other until a modeller finds a level of parametric heterogeneity and a corresponding level of model-to-measurement misfit with which he/she feels comfortable. Where singular value decomposition is a modeller's only means of regularization, the only control that he/she can exert on the level of model-to-measurement fit attained through the inversion process is the number of singular values at which truncation takes place; either this, or the ratio of highest to lowest pre-truncation singular value can be used to define the truncation point. One or the other of these must be provided by the modeller prior to the commencement of the inversion process. Unfortunately, the relationship between either of these and the final objective function attained through the inversion process is often unclear, and must be ascertained through trial and error. This can be a computer-intensive and time-consuming business.

Fortunately, as will now be discussed, Tikhonov regularization as implemented by PEST, offers the modeller more direct control over the level of model-to-measurement fit that is sought through the inversion process.

## 6.3 Tikhonov Regularization

### 6.3.1 Concepts

Tikhonov regularization achieves well-posedness of an inverse problem by supplementing the information content of a calibration dataset with expert knowledge that makes up for the deficit of information in that dataset. Conceptually the idea is very simple, and has already been expressed through equation (5.2.33) wherein prior information pertaining to all parameters is added to the calibration dataset. In this equation prior information is weighted in inverse proportion to the prior parameter covariance matrix. Hence its influence on the outcome of the inversion process is proportional to the strength of expert knowledge in comparison to the credibility of the measurement dataset as expressed through weights assigned to various components of that dataset; ideally weights should vary in inverse proportion to measurement noise. As was stated earlier, where the prior probability distributions of parameters on the one hand and measurement noise on the other hand are both multinormal, the outcome of the inversion process formulated as (5.2.33) is a set of parameters that correspond to the mean of the posterior parameter probability distribution, which is itself multinormal if the model is linear.

In practice, it is rarely possible to balance prior knowledge against measurement noise in this way. As has been stated, the level of "measurement noise" (which in most real world environmental modelling contexts is predominantly structural noise) is rarely known before inversion is attempted; in fact knowledge of its magnitude and characteristics is often forthcoming from the inversion process itself. The same applies to expert knowledge; furthermore, the uncertainties and characteristics of spatial variability of system properties

are often very difficult to characterize. Flexible methods of mathematically encapsulating expert knowledge that extend beyond a simple prior covariance matrix are often required by an inversion process for the parameter field which emerges from that process to reflect the complex dispositions of environmental property heterogeneity that characterize the real world. At the same time, flexibility is required in balancing expert knowledge, regardless of how it is mathematically expressed, against field measurements so that over-fitting is prevented while, at the same time, freedom is granted to the inversion process in transferring information from the calibration dataset to the parameters employed by the model.

Let the calibration dataset **h** be supplemented by expert knowledge **w**. Equation (6.1.1) then becomes

$$\begin{bmatrix}\mathbf{h}\\ \mathbf{w}\end{bmatrix}=\begin{bmatrix}\mathbf{Z}\\ \mathbf{Z}_w\end{bmatrix}\mathbf{k}+\begin{bmatrix}\boldsymbol{\varepsilon}\\ \boldsymbol{\omega}\end{bmatrix} \qquad (6.3.1a)$$

In equation (6.3.1) $\mathbf{Z}_w$ is a "regularization model" which operates on **k** to produce a set of regularization outcomes. **w** is the "observed value" of these outcomes. **ω** is the "noise" associated with **w**. It is thus a measure of the strength of expert belief in **w**. As such it expresses the extent to which failure of the inversion process to produce a set of parameters **k** which respects **w** will be tolerated.

Equation (6.3.1a) can be written as two separate matrix equations. The first of these is the same as (6.1.1). The second of these expresses regularization constraints on parameter values. The equations are

$$\mathbf{h} = \mathbf{Z}\mathbf{k} + \boldsymbol{\varepsilon} \qquad (6.3.1b)$$

$$\mathbf{w} = \mathbf{Z}_w\mathbf{k} + \boldsymbol{\omega} \qquad (6.3.1c)$$

The nature of expert knowledge that is expressed by $\mathbf{Z}_w$ varies with context. It can be as simple as the observation that each parameter **k** is equal to its prior mean value, as was done for equation (5.2.33). Alternatively, it can be considerably more complex than this. In spatial parameterization contexts to which Tikhonov regularization is commonly applied, $\mathbf{Z}_w$ may express a homogeneity condition through which it is "observed" that the value of each parameter is equal to that of its neighbour, or possibly to those of many of its neighbours. Weights assigned to these observations may decrease with increasing parameter separation; see, for example, Doherty (2003). In other cases a parameter smoothness condition may be expressed whereby differences of differences (i.e. second spatial derivatives) of parameter values are observed to be zero; this type of regularization is sometimes employed in geophysical data processing contexts where a parameter is associated with every grid cell of a spatial model domain. If spatial heterogeneity arises in solving the inverse problem, it will therefore arise in a smooth "spread out" way. In other spatial parameterization contexts, however, this may be an inappropriate way for parameter heterogeneity to arise. In such cases it may be desired that spatial heterogeneity, should it need to arise, be confined to as small an area as possible, and perhaps have reasonably sharp boundaries with neighbouring areas where homogeneity prevails. Alternatively, or at the same time, it may be desired that heterogeneity be aligned in a certain direction, or that it arise in as close proximity to a certain geological feature as possible. All of these conditions can be formulated through appropriate Tikhonov constraints on parameter values estimated through the inversion process. These constraints may not be linear as implied by the $\mathbf{Z}_w$ matrix of equation (6.3.1). But then neither is the model generally linear. These types of complex nonlinear constraints

are then accommodated in the same way as the nonlinear behaviour of the model, that is through computing an appropriate Jacobian matrix and updating it during every iteration of the nonlinear parameter estimation process.

A fundamental difference between "regularization observations" encapsulated in **w** and observations of system state encapsulated in **h** is that the former are expected to be violated while the latter are not. In a spatial model where Tikhonov regularization embodies a parameterization smoothness constraint, it is not expected that the solution to the inverse problem will express no system property heterogeneity whatsoever. Tikhonov constraints are formulated in full knowledge of the fact that heterogeneity will arise, and hence that these constraints will be violated; however the importance of their formulation is that they give the modeller control over *how* heterogeneity will arise, and hence *how* the constraints are optimally violated. At the same time, a modeller does not want heterogeneity to arise unless its existence is supported by the measurement dataset; nor does he/she want over-fitting of model outputs to field measurements to precipitate the emergence of spurious heterogeneity. For both of these reasons it is important that the parameter estimation process be given control over the relative commitment of that process to respecting measurements represented by **h** on the one hand, and regularization constraints encapsulated in **w** on the other hand.

Of course it is not necessary that Tikhonov regularization be confined to spatial parameterization schemes such as are employed by groundwater and subsurface reservoir models and models used in geophysical data interpretation. Tikhonov regularization can also play an important role in calibration of surface water and land use models. In doing so they may form the basis for parameter regionalization. Thus parameters which pertain to complex physical or chemical processes in neighbouring watersheds may be "observed" to have similar values if land use and soil conditions are the same in those watersheds; however they may be allowed to differ if a good fit with stream flows measured in respective watershed gauging stations deems this necessary.

Because regularized inversion places no limits on the number of parameters that can be accommodated in an inversion process, calibration of multiple submodels associated with multiple watersheds feeding multiple stream gauges can all be done at once. This allows the modeller to "suggest", through Tikhonov constraints, that certain ordering relationships prevail among parameters, these reflecting the physical/chemical characteristics of the watersheds that feature in the inversion process. Alternatively, certain relationships may be posited between watershed parameters and independently measurable characteristics of these watersheds; perhaps these relationships may be encapsulated in a regression equation. The parameters governing the regression equation can then be estimated at the same time as parameters for the individual watershed models. Regression and watershed model parameters can then be linked through Tikhonov constraints which suggest maximum respect by the watershed parameters for the regional regression relationships, while tolerating departures from these relationships where these are necessary to fit local stream flow data.

In short, there is no limit to the flexibility that a modeller can exercise in formulating a set of Tikhonov constraints that constitute expressions of expert knowledge that are most pertinent to a particular study site.

The Tikhonov regularization process may be viewed in a number of ways. One of these has just been described. Another is to view Tikhonov constraints as encapsulating a default parameter condition. This is the condition that will prevail unless there is information to the

contrary contained in the calibration dataset. They thus express a condition which is deemed to be of minimum parameter error variance where the only available information is expert knowledge. The status of minimum prior parameter error variance does not make this condition right; it only minimizes its potential for wrongness. The formulation of Tikhonov constraints which instruct the inversion process to respect this prior parameter condition is then "safe" or "conservative". This is because it instructs the inversion process to express no departures from this preferred condition that cannot be supported by data. What is of equal importance is that the manner in which these (possibly nonlinear) Tikhonov constraints are formulated and weighted must also specify *how* departures from this prior parameter condition should arise if indeed they need to arise.

### 6.3.2 Formulation of Equations

Ideally, with **h** supplemented by **w**, the inverse problem of equation (6.3.1) is well-posed and can thus be solved using the Gauss-Newton method.

Let the weight matrix used for measurements be designated as **Q**; normally this matrix is diagonal. As usual, measurement weighting should reflect the relative noise contents of different components of the observation dataset. Where the overall objective function has a number of components, an adopted weighting strategy may also ensure that these different components have roughly the same visibility in the initial objective function. More will be said on this topic later.

In the case of regularization weights, relative weighting between different constraints should reflect the comparative tolerance of a modeller to their violation. For some or all of these constraints the weight matrix may be non-diagonal. It may, for example, comprise the inverse of a C(**k**) matrix which expresses correlation between parameters arising from spatial proximity or physical/chemical property co-dependence on a more fundamental attribute of the medium to which they pertain. We will denote this matrix as $\mu^2\mathbf{Q}_r$. The factor $\mu^2$ is made explicit to denote the fact that the regularized inversion process is allowed to adjust this factor. This factor is referred to as the "regularization weight multiplier" in the discussion that follows.

The solution to the presumably well-posed inverse problem described by equation (6.3.1) is

$$\underline{\mathbf{k}} = \left\{ \begin{bmatrix} \mathbf{Z}^t & \mathbf{Z}_w^t \end{bmatrix} \begin{bmatrix} \mathbf{Q} & \mathbf{0} \\ \mathbf{0} & \mu^2\mathbf{Q}_r \end{bmatrix} \begin{bmatrix} \mathbf{Z} \\ \mathbf{Z}_w \end{bmatrix} \right\}^{-1} \begin{bmatrix} \mathbf{Z}^t & \mathbf{Z}_w^t \end{bmatrix} \begin{bmatrix} \mathbf{Q}^t & \mathbf{0} \\ \mathbf{0} & \mu^2\mathbf{Q}_r \end{bmatrix} \begin{bmatrix} \mathbf{h} \\ \mathbf{w} \end{bmatrix} \qquad (6.3.2a)$$

which, when all the matrix multiplications are carried out, becomes

$$\underline{\mathbf{k}} = [\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mu^2\mathbf{Z}^t_w\mathbf{Q}_r\mathbf{Z}_w]^{-1}[\mathbf{Z}^t\mathbf{Q}\mathbf{h} + \mu^2\mathbf{Z}^t_w\mathbf{Q}_r\mathbf{w}] \qquad (6.3.2b)$$

Let us assume that **w** is equal to **0**. This does not have to be the case, but is often so in practice. This follows from its role of expressing a preferred parameter condition and the fact that, for a linearized model, prior parameter expected values are zero; see section 4.5. In this case equation (6.3.2b) becomes

$$\underline{\mathbf{k}} = [\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mu^2\mathbf{Z}^t_w\mathbf{Q}_r\mathbf{Z}_w]^{-1}\mathbf{Z}^t\mathbf{Q}\mathbf{h} \qquad (6.3.3)$$

It will be recalled from the previous chapter that equations (6.3.2) and (6.3.3) constitute solutions to a problem in which an objective function is minimized. In the present case the objective function has two components, one pertaining to model-to-measurement misfit and

the other pertaining to respect for Tikhonov constraints. These will be called the measurement and regularization objective functions respectively; they will be designated as $\Phi_m$ and $\Phi_r$. They are defined as follows

$$\Phi_m = (\mathbf{h} - \mathbf{Zk})^t\mathbf{Q}(\mathbf{h} - \mathbf{Zk}) \quad (6.3.4)$$

$$\Phi_r = (\mathbf{w} - \mathbf{Z}_w\mathbf{k})^t\mathbf{Q}_r(\mathbf{w} - \mathbf{Z}_w\mathbf{k}) \quad (6.3.5)$$

If **w** is **0**, (6.3.5) becomes

$$\Phi_r = \mathbf{k}^t\mathbf{Z}^t{}_w\mathbf{Q}_r\mathbf{Z}_w\mathbf{k} \quad (6.3.6)$$

The total objective function $\Phi_t$ which is minimized through solution of (6.3.2) or (6.3.3) is

$$\Phi_t = \Phi_m + \mu^2\Phi_r \quad (6.3.7)$$

### 6.3.3 Optimization of Regularization Weight Factor

Equations that have just been presented in the present chapter are similar to those that were presented in the previous chapter for solution of a well-posed inverse problem where well-posedness was attempted by supplementing the calibration dataset with expert knowledge. Fundamental to robust implementation of Tikhonov regularization, however, is that $\mu^2$ be adjusted as part of the inversion process together with model parameters whose estimates are sought through that process. There are a number of different ways in which this can be done. A numerically costly, but very instructive, option is to solve for $\underline{\mathbf{k}}$ using (6.3.2) or (6.3.3) for many different values of $\mu^2$, starting with very high values of $\mu^2$. For (6.3.3) the solution to the inverse problem with $\mu^2$ very high is obviously that **k** is equal to **0**; for this value of **k** the regularization objective function defined by (6.3.5) is zero. Meanwhile the measurement objective function is probably seriously non-zero as model outputs under these conditions are unlikely to provide a good match with the calibration dataset.

As $\mu^2$ is lowered, the measurement dataset **h** starts to have some impact on estimated values of $\underline{\mathbf{k}}$. The regularization objective function starts to rise as **k** departs from its preferred condition and the measurement objective function starts to fall. Normally this process continues until a point is reached where the regularization objective function rises very quickly for only a small decrease in the measurement objective function. Figure 6.5 shows a real world example. (The numbers on this graph are case-specific.)

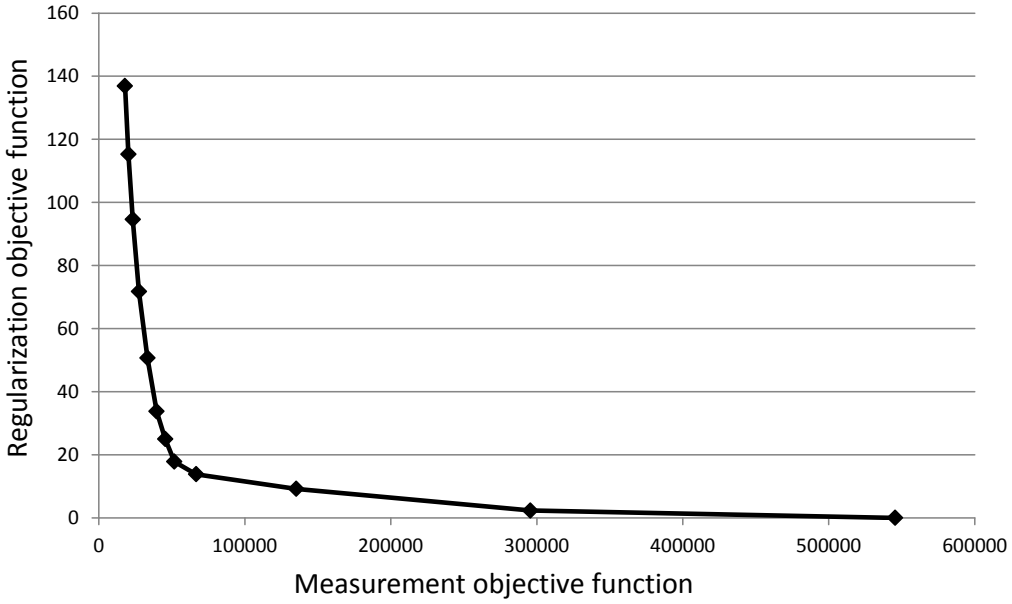


**Figure 6.5. Trade-off between measurement and regularization objective functions.**

The curve shown in figure 6.5 is often referred to as an "L-curve". Intuitively, the optimum value of $\mu^2$ is that at which the curve deflects sharply upwards. The requirement that parameters deviate markedly and pervasively from their preferred condition at this point for very little improvement in model-to-measurement fit suggests that they are responding to measurement or structural noise that is associated with the measurement dataset rather than to real information that is contained within that dataset. (In some modelling contexts it may not be possible to track the curve too far to the left of its sharp upward bend because the inverse problem becomes too ill-posed for numerical solvers to accommodate the near-singular matrix which must be inverted when regularization constraints are given so little weight.)

PEST is able to compute an L-curve when it is run in Pareto mode. The term "Pareto" is often used to describe a numerical process wherein two or more competing objective functions are traded off against each other.

Another option in seeking an optimal value of $\mu^2$ is that suggested by de Groot-Hedlin and Constable (1990) and Doherty (2003); this is also implemented in PEST. Instead of directly seeking a value for $\mu^2$, the modeller sets a desired value for $\Phi_m$, the measurement objective function. This value is referred to herein as the "target measurement objective function" and is designated as $\Phi^t_m$. The Tikhonov inversion process then becomes a constrained minimization process formulated thus:

> *Minimize the regularization objective function* $\Phi_r$ *subject to the constraint that* $\Phi_m$ *is equal to a user-specified target measurement objective function* $\Phi^t_m$.

The inversion software then determines $\mu^2$ itself. If a modeller supplies a value for $\Phi^t_m$ that is too low to achieve, then $\mu^2$ should not be reduced any lower than a value that maintains numerical stability of the inversion process while $\Phi_m$ is lowered as much as possible.

The Tikhonov-regularized inversion process, formulated as above, is thus asked to seek a certain level of fit with the measurement dataset. At the same time it is informed that it must not seek a level of fit which is any better than this. The measurement objective function is not therefore minimized. In the previous chapter, it was minimization of the objective function

that established uniqueness of the inverse problem. Things are different in the present chapter. Presumably many sets of parameters are compatible with a target measurement objective function that is elevated above its minimum. The Tikhonov-regularized inversion process maintains uniqueness by insisting that the set of parameters that it deems to have solved the inverse problem are those that require least deviation from the default parameter condition for which the regularization objective function $\Phi_r$ is zero. If the default parameter condition is one of minimized parameter error variance from an expert knowledge point of view, then the solution to the inverse problem can lay partial claim to a status of minimized post-calibration parameter error variance due to the fact that in fitting the calibration dataset it pays maximum respect to expert knowledge. It is important to note, however, that this can constitute only part of the basis for such a claim. The other important factor that complements proximity to the default parameter condition is the manner in which deviations from that condition have arisen in order to attain the desired level of fit. It is the design details of $\Phi_r$, and the $\mathbf{Q}_r$ matrix used in formulation of $\Phi_r$, that achieves this.

So at what value should a modeller set $\Phi^t_m$? If measurement noise associated with the calibration dataset is the only determinant of model-to-measurement misfit, and if this noise is normally distributed, and if $\Phi^t_m$ is calculated from residuals $\mathbf{r}$ as $\mathbf{r}^t\mathbf{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{r}$, then setting $\Phi^t_m$ equal to $n$, the number of observations comprising the calibration dataset, seems appropriate. This is the expected value of a chi-squared distribution with $n$ degrees of freedom. In practice however (as has been stated many times herein), it is not measurement noise that determines model-to-measurement misfit. In most cases, model-to-measurement misfit is dominated by so-called structural noise which reflects the fact that an environmental model is not a perfect simulator of complex, real world, environmental processes. It is unlikely in the extreme that structural noise will be homoscedastic, independent, or multinormally distributed. Furthermore its magnitude must generally be discovered during the calibration process itself. Selection of an appropriate $\Phi^t_m$ thus becomes subjective.

One option for the setting of $\Phi^t_m$ is to first estimate parameters with $\Phi^t_m$ set unachievably low. This will inform the modeller just how good a fit with the calibration dataset it is possible to obtain. Signs of over-fitting will probably be plainly visible in the calibrated parameter field which achieves this level of fit. In the ensuing inversion process $\Phi^t_m$ can then be set 5% to 10% higher than this minimum. It is normally found that with only a slight diminution of model-to-measurement fit, a parameter field can be obtained that deviates from its Tikhonov-defined default condition by a readily-acceptable amount. This is suggested by L-curves such as that plotted in figure 6.5.

### 6.3.4 Relationship between Estimated and Real Parameters

With substitution of (6.1.1) into (6.3.3) we obtain

$$\underline{\mathbf{k}} = [\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mu^2\mathbf{Z}^t_w\mathbf{Q}_r\mathbf{Z}_w]^{-1}\mathbf{Z}^t\mathbf{Q}\mathbf{Z}\mathbf{k} + [\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mu^2\mathbf{Z}^t_w\mathbf{Q}_r\mathbf{Z}_w]^{-1}\mathbf{Z}^t\mathbf{Q}\boldsymbol{\varepsilon} \qquad (6.3.8)$$

From this equation the **G** and **R** matrices that are associated with Tikhonov regularization can be inferred as follows

$$\mathbf{G} = [\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mu^2\mathbf{Z}^t_w\mathbf{Q}_r\mathbf{Z}_w]^{-1}\mathbf{Z}^t\mathbf{Q} \qquad (6.3.9)$$

$$\mathbf{R} = [\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mu^2\mathbf{Z}^t_w\mathbf{Q}_r\mathbf{Z}_w]^{-1}\mathbf{Z}^t\mathbf{Q}\mathbf{Z} \qquad (6.3.10)$$

With these matrices defined, the covariance matrix of parameter error can be calculated using equation (6.1.19). Predictive error variance can be calculated using equation (6.1.25).

If, for a given prediction made by a calibrated, Tikhonov-regularized model, the first, second and summed terms of equation (6.1.25) are plotted against $1/\mu^2$, curves similar to those depicted in figure 6.4 result. A low value for $1/\mu^2$ (i.e. a high value for $\mu^2$) signifies no calibration at all. A high value for $1/\mu^2$ (i.e. a low value for $\mu^2$) signifies over-fitting. An optimum value for $\mu^2$ lies between the two. For this value of $\mu^2$ predictive error variance is minimized. See Moore and Doherty (2005) for further details.

Suppose that C(**ε**) is the identity matrix **I**. (If necessary, this can be achieved through the transformations listed in equations 6.1.2 to 6.1.6). The weight matrix **Q** can then be chosen as **I**, so that equation (6.3.3) becomes

$$\underline{\mathbf{k}} = [\mathbf{Z}^t\mathbf{Z} + \mu^2\mathbf{Z}^t{}_w\mathbf{Q}_r\mathbf{Z}_w]^{-1}\mathbf{Z}^t\mathbf{h} \qquad (6.3.11)$$

Now let us further suppose that Tikhonov regularization is formulated to constrain all parameters to be individually equal to their prior expected values, and that the weighting matrix that is associated with these constraints is $C^{-1}(\mathbf{k})$, the inverse of the prior parameter covariance matrix. The above equation then becomes

$$\underline{\mathbf{k}} = [\mathbf{Z}^t\mathbf{Z} + \mu^2C^{-1}(\mathbf{k})]^{-1}\mathbf{Z}^t\mathbf{h} \qquad (6.3.12)$$

Now, instead of solving for $\underline{\mathbf{k}}$, let us assume that we are solving for $\underline{\mathbf{m}}$, a Kahunen-Loève transformed parameter set for which C(**m**) = **I**. $\underline{\mathbf{k}}$ can then be calculated from $\underline{\mathbf{m}}$ using (6.2.18). **Z** in (6.3.12) must therefore be replaced by **Y** defined by equation (6.2.22). Because C(**m**) is **I**, then so too is its inverse $C^{-1}(\mathbf{m})$. Equation (6.3.12) then becomes

$$\underline{\mathbf{m}} = [\mathbf{Y}^t\mathbf{Y} + \mu^2]^{-1}\mathbf{Y}^t\mathbf{h} \qquad (6.3.13)$$

Let $\mathbf{Y}^+$ denote the Moore-Penrose pseudoinverse of **Y**. As was discussed in section 2.9, this is the unique generalized inverse of **Y** that leads to a minimum norm solution to the noise-free inverse problem; this minimum norm solution is the solution of minimum error variance if C(**m**) is **I** and **m** is multinormally distributed. It is also the solution to the noise-free inverse problem achieved through singular value decomposition. As previously discussed in section 2.9, Albert (1972) shows that

$$\mathbf{Y}^+ = \lim_{\mu^2\to 0}\left(\mathbf{Y}^t\mathbf{Y} + \mu^2\mathbf{I}\right)^{-1}\mathbf{Y}^t = \lim_{\mu^2\to 0}\mathbf{Y}^t\left(\mathbf{Y}\mathbf{Y}^t + \mu^2\mathbf{I}\right)^{-1} \qquad (6.3.14)$$

If the first of these equalities is compared to (6.3.13) it is apparent that, like singular value decomposition acting on a Kahunen-Loève transformed parameter set, a Tikhonov regularized solution to the inverse problem approaches the Moore-Penrose pseudoinverse as measurement noise approaches zero.

So is one of these forms of regularization just as good as the other? This has already been discussed to some extent. In fact they complement each other. The attraction of Tikhonov regularization is the flexibility that it offers in expressing expert knowledge. A $\mathbf{Z}_r$ matrix, or a more elegant nonlinear expression of features which are desirable in a calibrated parameter field, constitutes a much more flexible expression of expert knowledge, and the uncertainties associated therewith, than pre-inversion Kahunen-Loève transformation. Flexibility of Tikhonov regularization is further enhanced by the ability of the Tikhonov-regularized inversion process to adjust weights associated with Tikhonov constraints as part of the inversion process itself. On the other hand, singular value decomposition guarantees unequivocal numerical stability of the inversion process. The same applies to more sophisticated iterative solvers which are related to singular value decomposition but are much

faster and can handle very large numbers of parameters; see the next section.

The best regularization method to use is a combination of the two. The inverse problem can be formulated using Tikhonov regularization; the equations that emerge from this formulation can then be solved using singular value decomposition, or a fast iterative solver which operates along similar orthogonalization lines.

## 6.4 Practical Implementation

### 6.4.1 Nonlinear Model Behaviour

Most models are, of course, nonlinear. Hence they can only be temporarily represented by a matrix during each iteration of step-wise progression toward the ultimate solution to the inverse problem. During each of these iterations, the equations presented above are employed to calculate improvements to parameters, rather than the parameters themselves. These improvements are calculated from current residuals rather than directly from the calibration dataset **h**. During each iteration, the Jacobian matrix replaces the **Z** matrix. Each column of this matrix is a vector of length *n* (the number of observations comprising the calibration dataset) whose elements represent the partial derivatives of model outputs used in the calibration process with respect to a particular parameter; see section 5.4. The regularization function represented by $\mathbf{Z}_w$ in equations presented in the preceding section may be linear or nonlinear. If it is nonlinear then $\mathbf{Z}_w$ will also need to be updated during each iteration of the inversion process with an equivalent matrix of partial derivatives.

Means through which nonlinear model behaviour can be best accommodated during each linearized iteration of the inversion process are similar for the highly parameterized context to those described for the parsimonious parameterization context in chapter 5. They include logarithmic transformation of some parameters, limiting the length of the parameter upgrade vector, employment of Broyden's Jacobian upgrade procedure, and use of the Marquardt lambda. Where a model is highly nonlinear, the possibility of convergence to a local objective function minimum can never be completely removed. However the probability of this happening can often be greatly reduced through creative formulation of a multi-component measurement objective function in which some components are more immune to model nonlinearities than are other components. If these objective function components are supplemented with others that encapsulate regularization constraints that guide the inversion process towards a sensible parameter set that achieves a good fit with the measurement dataset, then the purpose of the calibration process will have been served. As will be recalled from earlier chapters, this is to obtain a parameter set whose status approaches that of minimum error variance, which can then provide a foundation for subsequent exploration of parameter and predictive error variance as a surrogate for parameter and predictive uncertainty. As has been discussed, calibration should not be an end in itself.

The Marquardt lambda can be just as useful in nonlinear highly parameterized inversion as it is in nonlinear parsimonious inversion that is the outcome of manual regularization. At early stages of the nonlinear inversion process, parameters can be guided directly down the objective function gradient through use of a moderate to high value of the Marquardt lambda. As has been discussed, PEST implements a trial and error procedure for selection of an appropriate Marquardt lambda during each iteration of the inversion process; linearized equations for parameter upgrades are solved using different values of the Marquardt lambda and the upgraded parameters are then tested for their efficacy in lowering the overall

objective function. The Marquardt lambda which results in greatest objective function improvement is retained. It then forms the starting value for a similar Marquardt lambda selection process that is implemented in the following iteration. While this procedure requires that a higher number of model runs be undertaken per iteration than that required for Jacobian matrix calculation, it can be implemented efficiently in a parallel computing environment where it is just as cost-effective to attempt many parameter upgrades as it is to attempt just one. Ideally the value of the Marquardt lambda should fall with iteration count. If it does not, this may indicate that formulation of Tikhonov constraints needs revision as the Marquardt lambda may be adopting a de facto regularization role itself.

With the Jacobian matrix used in place of the **Z** matrix, with the inverse problem formulated in terms of parameter upgrades, and with use made of the Marquardt lambda, equation (6.3.2b) becomes

$$\underline{\mathbf{k}} - \underline{\mathbf{k}}_0 = [\mathbf{J}^t\mathbf{Q}\mathbf{J} + \mu^2\mathbf{J}^t_w\mathbf{Q}_r\mathbf{J}_w + \lambda\mathbf{I}]^{-1}[\mathbf{J}^t\mathbf{Q}\mathbf{h} + \mu^2\mathbf{J}^t_w\mathbf{Q}_r\mathbf{w}] \qquad (6.4.1)$$

while equation (6.3.3) becomes

$$\underline{\mathbf{k}} - \underline{\mathbf{k}}_0 = [\mathbf{J}^t\mathbf{Q}\mathbf{J} + \mu^2\mathbf{J}^t_w\mathbf{Q}_r\mathbf{J}_w + \lambda\mathbf{I}]^{-1}\mathbf{J}^t\mathbf{Q}\mathbf{r} \qquad (6.4.2)$$

As will be discussed shortly, it is often easier to solve equation (6.3.1a) directly using singular value decomposition, or a related algorithm, than it is to solve equation (6.3.2) or (6.3.3). With inclusion of the Marquardt lambda and the $\mu^2$ multiplier for the regularization term, (6.3.1a) becomes

$$\begin{bmatrix}\mathbf{h}\\ \mathbf{w}\\ \mathbf{0}\end{bmatrix} = \begin{bmatrix}\mathbf{Z}\\ \mu^2\mathbf{Z}_w\\ \lambda\mathbf{I}\end{bmatrix}\mathbf{k} + \begin{bmatrix}\boldsymbol{\varepsilon}\\ \boldsymbol{\omega}\\ \zeta\end{bmatrix} \qquad (6.4.3)$$

Alternatively, in applying singular value decomposition to solution of (6.3.1a), direct use of the Marquardt lambda can be foregone. Instead, singular values emerging from that decomposition can be adjusted upwards to achieve a similar outcome to the Marquardt lambda.

### 6.4.2 Solution of Equations

Suppose that highly parameterized model calibration takes place in the absence of Tikhonov regularization, and that singular value decomposition constitutes the only regularization device. Solution of the inverse problem could take place in one of two ways. One option is to proceed directly from equation (6.1.1) by subjecting **Z** to singular value decomposition and then computing $\underline{\mathbf{k}}$ through (6.2.4). A second option is to proceed as if the inverse problem is well-posed, and then formulate the Gauss-Newton equations as in (6.2.36). The $\mathbf{Z}^t\mathbf{Z}$ matrix could then be subjected to singular value decomposition as per equation (6.2.37). With removal of zero and very low singular values, a generalized inverse of the $\mathbf{Z}^t\mathbf{Z}$ matrix can then be found as $\mathbf{V}_1\mathbf{S}_1^{-2}\mathbf{V}^t_1$ where truncation of singular values to form $\mathbf{S}_1$ follows similar considerations to those already discussed. The solution $\underline{\mathbf{k}}$ to the inverse problem would then be calculated as

$$\underline{\mathbf{k}} = \mathbf{V}_1\mathbf{S}_1^{-2}\mathbf{V}^t_1\mathbf{Z}\mathbf{h} \qquad (6.4.4)$$

With substitution of (6.2.2) for **Z**, (6.2.4) follows immediately. The two approaches are thus mathematically identical. Numerically, however, direct use of equation (6.2.4) is often

numerically more practical as formulation of the $\mathbf{Z}^t\mathbf{Z}$ matrix can require a great deal of numerical work where parameter and/or observation numbers are high. Numerical round-off errors may also corrupt formulation of $\mathbf{Z}^t\mathbf{Z}$ to some extent.

Where Tikhonov regularization is included in the inversion process there may be no need to use singular value decomposition at all in obtaining the matrix inverse required for solution of the inverse problem through use of equations (6.3.2) and (6.3.3). Unfortunately, however, it is not a foregone conclusion that Tikhonov regularization will achieve unconditional invertibility of this matrix even where multiple regularization weight multipliers are employed instead of the single $\mu^2$ multiplier featured in these equations; the use of multiple regularization weight multipliers is further discussed below. Hence implementation of Tikhonov-based regularized inversion should accommodate the fact that further regularization may be required. The Marquardt lambda can help; however as far as regularization is concerned it is a "blunt instrument" that should only be used as the regularization device of last resort so that it can be left to fill its primary role of accommodating model nonlinearity.

As mentioned above, singular value decomposition can be used for regularization reinforcement. However when used in this reinforcement role, singular value truncation should take place only on the basis of numerical considerations, and not on the basis of minimization of parameter and predictive error variance. Where Tikhonov regularization is being implemented, sensibility of inverse problem solution and prevention of over-fitting are best handled using the regularization weight multiplier.

As stated above, however, it is better to apply singular value decomposition directly to equation (6.3.1a) than to equation (6.3.2) or (6.3.3). It is thus applied to the $\begin{bmatrix} \mathbf{Z} \\ \mathbf{Z}_w \end{bmatrix}$ matrix featured in the former equation. This avoids the numerical burden and round-off errors incurred in assembling the matrices that are featured in equations (6.3.2) and (6.3.3).

In practice, better solution methods than singular value decomposition are available for solving large matrix equations of this type. Numerically, singular value decomposition of a matrix becomes very slow once parameters start to number more than about two thousand. Iterative solution algorithms such as LSQR (Paige and Saunders, 1982a; 1982b) and PROPACK (Larsen, 1998) are much faster. Solutions provided by these algorithms are very similar to those provided by singular value decomposition (especially for PROPACK that preserves the full orthogonalization properties of singular value decomposition), but are achieved very much more quickly. Furthermore they can be employed even where parameters number in the hundreds of thousands.

In many practical contexts, packages like LSQR and PROPACK have a further numerical advantage. The discussion above assumes that first a Jacobian matrix is calculated and then a large equation is solved to calculate an upgraded set of parameters. In the environmental modelling context the Jacobian is often calculated using finite parameter differences. This is the case where a model-independent package such as PEST is used to calibrate a complex environmental model that may simulate many physical and chemical processes at a particular study site. It may not be the case, however, where specialist packages such as geophysical models and imaging software comprise the model. These packages can calculate their own derivatives, often using fast procedures such as adjoint methods. Furthermore, they can calculate, often with great efficiency, a single column or row of the Jacobian matrix without

having to calculate other columns and rows of this matrix. Iterative solvers such as LSQR and PROPACK can make use of this. On any call to the model to obtain derivatives they may require only that $\mathbf{J}^t\mathbf{x}$ or $\mathbf{Jy}$ be calculated, where $\mathbf{x}$ and $\mathbf{y}$ are vectors that the solver provides. Each such call requires that only one model run or adjoint model run be undertaken. Parameters employed by the model can be progressively updated as these calls are made. Furthermore, during any iteration of the nonlinear inversion process, such model calls may be limited to a number that is much smaller than the number of parameters requiring estimation.

### 6.4.3 Multiple Regularization Weight Factors

As was mentioned above, while Tikhonov regularization provides mechanisms for sophisticated and flexible expressions of expert knowledge, numerical stability of the Tikhonov-regularized inversion process cannot always be guaranteed. To understand why this is so, let us suppose that we are estimating parameters for a spatial model whose domain is two-dimensional and covers a large area. Suppose also that measurements comprising the calibration dataset are concentrated in some parts of the model domain but are virtually absent from other parts. In those parts of the model domain where measurement density is high, the calibration dataset may support unique estimation of system properties. However in other parts of the model domain the local information content of the calibration dataset may be too low to warrant alteration of parameter values from their defaults. It follows that in parts of the model domain where information density is high there is no need for the regularization weight factor to be high, as the local information content of the calibration dataset may not need expert knowledge enhancement. At the same time, the weight factor may need to be relatively high in those other parts of the model domain where information density is low or non-existent in order to ensure that parameters which occupy these areas do not deviate from their preferred values. Unfortunately a single weight factor cannot accomplish both of these tasks. The assignment of a low value to a single weight factor in order to achieve the level of fit with the calibration dataset that is requested through the user-specified target measurement objective function may undermine numerical stability in those parts of the model domain where the calibration dataset is under-represented and solution of the inverse problem is nonunique.

Similar problems can occur where model parameters represent different system properties. Information density within the calibration dataset as it pertains to one of these system property may be high, while system properties of other types may be relatively uninformed by the calibration dataset. In this context, differential weighting of expert knowledge as it pertains to different parameter types is warranted to ensure stability of an inverse problem that is relatively well-posed with respect to some parameters and relatively ill-posed with respect to others. Such differential relative weighting of Tikhonov constraints can be provided by the modeller in his/her filling of the $\mathbf{Q}_r$ matrix of equations (6.3.2) and (6.3.3). However it is unlikely that the relativities that are thus provided will complement relativities in measurement dataset information content in such a way as to guarantee stability of the inversion process while at the same time allowing maximum transfer of information from the measurement dataset to those parameters which are estimable. Of course, numerical stability can be guaranteed through use of singular value decomposition to undertake the necessary matrix inversions. But without pre-inversion Kahunen-Loève transformation of parameters, the cost of numerical stability may be loss of minimum error variance status of some components of the estimated parameter field.

Conceptually, the best way to handle this problem is to allow the inversion process itself to assign differential regularization weight factors to different subsets of Tikhonov regularization. Equation (6.3.3) thus becomes

$$\underline{\mathbf{k}} = [\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mu_1^2\mathbf{Z}^t_{w1}\mathbf{Q}_{r1}\mathbf{Z}_{w1} + \mu_2^2\mathbf{Z}^t_{w2}\mathbf{Q}_{r2}\mathbf{Z}_{w2} + \mu_3^2\mathbf{Z}^t_{w3}\mathbf{Q}_{r3}\mathbf{Z}_{w3} + \ldots]^{-1}\mathbf{Z}^t\mathbf{Q}\mathbf{h} \qquad (6.4.5)$$

The problem of estimating a suitable value for one regularization weight multiplier $\mu^2$ then becomes that of estimating suitable values for multiple weight multipliers $\mu_i^2$. There are a number of ways to go about this. A method employed by PEST that has proven effective in many calibration contexts is to estimate the ratios of the $\mu_i^2$ first and then apply a global weight multiplier to all Tikhonov regularization in the manner described in previous sections. As usual, this global weight multiplier is chosen in order to achieve a user-specified target measurement objective function. One easy option for choosing relative regularization weight multipliers is to assign them values such that composite observation sensitivities pertaining to all rows of each $\mathbf{Z}_{wi}$ sum to the same value after each of these matrices is multiplied by its respective $\mu_i^2$; see equation (5.3.4) for definition of composite observation sensitivity. Thus expressions of expert knowledge embodied in the different $\mathbf{Z}_{wi}$ all make an impact on the total regularization objective function, regardless of the number of rows in each of the $\mathbf{Z}_{wi}$ matrices.

Another option is to assign higher $\mu_i^2$ values to groupings of expert knowledge that pertain to parameters that are ill-informed by the calibration dataset **h**. One measure of the information content of the calibration dataset with respect to a particular parameter is the composite sensitivity of that parameter as calculated from the **Z** matrix; see equation (5.3.1). Meanwhile the parameters that feature in the expert knowledge to which a particular regularization weight factor $\mu_i^2$ pertains can be gleaned from the $\mathbf{Z}_{wi}$ matrix with which it is associated. Those $\mathbf{Z}_{wi}$ which feature parameters whose average or maximum composite sensitivity is low receive a higher $\mu_i^2$ than those which feature parameters that are well informed by the calibration dataset.

An even more sophisticated attempt to weight regularization that pertains to inestimable parameters more highly than that which pertains to estimable parameters is to examine the projection of each row of each $\mathbf{Z}_{wi}$ matrix onto the null space of the **Z** matrix. Those which have a higher null space projection receive a greater relative regularization weight.

For all of these options new values for $\mu_i^2$ are calculated during every iteration of the inversion process. See PEST documentation for details.

### 6.4.4 Working with "Super Parameters"

The greatest practical challenge that must be overcome in implementing highly parameterized inversion in the environmental modelling context is that of calculating a new Jacobian matrix during every iteration of the nonlinear inversion process. Where sensitivities are computed using finite parameter differences, this requires that at least one model run be undertaken for each parameter featured in **k**; extra accuracy in computation of these derivatives may require that two, or even four, model runs be undertaken for each parameter. Where model runs can be parallelized so that they are undertaken on different processors, this task can become numerically feasible even where model run times are long. The running of simplified surrogate or proxy models for filling of the Jacobian matrix may also ease the computational burden of filling it; see chapter 10 of this text and Burrows and Doherty (2015) for details.

Another means through which the computational burden of highly parameterized inversion

can be eased was discussed in section 6.2.6. So-called "super parameters" **p** can be estimated in lieu of actual model parameters **k**. Super parameters are the coefficients by which orthogonal combinations of parameters are multiplied to form the overall estimated parameter set $\underline{\mathbf{k}}$. These combinations of parameters are the columns of the $\mathbf{V}_1$ matrix calculated through singular value decomposition undertaken on **Z**. These combinations can be evaluated just once, at the start of the inversion process; hence the full Jacobian matrix associated with the **Z** matrix needs to be evaluated just this once. Alternatively, super parameters can be reformulated at strategic intervals throughout the nonlinear parameter estimation process. In the latter case the Jacobian matrix associated with **Z** must be re-calculated a small number of times. In either case the numeral burden of highly parameterized inversion is greatly reduced. This is because a Jacobian matrix is required only for super parameters during intervening iterations; super parameters **p** are normally far fewer in number than base model parameters **k**.

Estimation of super parameters does not need to be a well-posed inverse problem; hence the number of super parameters employed in the inversion process can (and should) increase with availability of computing resources. Ideally, Tikhonov regularization should support their estimation. The expert knowledge that is embedded in Tikhonov constraints should pertain to the original **k** parameter set in spite of the fact that super parameters **p** are being estimated. Sensitivities of Tikhonov constraints to super parameters **p** can be calculated through finite differencing (with respect to **p** parameters) during each iteration of the inversion process. Regardless of the use or otherwise of Tikhonov regularization, solution for $\underline{\mathbf{p}}$ can be sought through singular value decomposition in order to guarantee of numerical stability of the inverse problem solution process.

### 6.4.5 Optimizing the Level of Fit

When undertaking highly parameterized inversion, the attainment of a good fit between model outputs and field measurements may not be too difficult. However just because a high level of fit with a measurement dataset *can* be attained, this does not mean that it necessarily *should* be attained. The adverse consequences of over-fitting are dramatically illustrated by figure 6.4 and by the equations which support it.

If using only singular value decomposition as a regularization device, over-fitting can be prevented through suitable singular value truncation. If using Tikhonov regularization, the target measurement objective function becomes the mechanism through which a modeller can prevent over-fitting. Presumably, the level of fit which is sought through either of these mechanisms should be no greater than that which is expected on the basis of measurement noise.

As has been mentioned many times in this text (and as will be discussed from a theoretical perspective in chapter 9), the level of model-to-measurement fit achieved through the calibration process is not usually determined by measurement noise. It normally reflects, more than anything else, the adequacy, or otherwise, of the model as a simulator of real world behaviour. Normally the best level of fit to attain in any particular modelling context is not known in advance. Instead it must be "discovered" through the inversion process itself. In over-determined parameter estimation contexts this is formalized through calculation of a value for the reference variance $\sigma^2_r$ using equation (5.2.18) from the best objective function achieved through an adopted manual regularization strategy. However when regularization is mathematical rather than manual, the objective function is not minimized. The desired level

of model-to-measurement fit must actually be specified by the user. While its selection may be supported by the availability of an L-curve, more often than not its specification is a matter of some subjectivity.

If C(**k**) and C(**ε**) are known, then selection of an optimal level of fit could be made using figures such as 6.4 and supporting equations. Alternatively a well-posed inverse problem could be formulated, and its parameters estimated, using equation (5.2.33). Solution of this equation minimizes an objective function that is composed of both measurements and prior information in which weights are correctly balanced based on knowledge of C(**k**) and C(**ε**).

Balancing of the constraints imposed by both C(**k**) and C(**ε**) underpins both of these approaches. Respect for C(**k**) requires that estimated parameters be realistic; respect for C(**ε**) requires that a good level of fit with the measurement dataset be obtained unless that data is untrustworthy. If such balancing cannot be done mathematically because C(**ε**) is not known and C(**k**) can only be approximately known, then it must be done manually. One way of achieving this is to implement several Tikhonov-regularized inversion processes with different target measurement objective functions. If computer resources permit, a more continuous description of the interplay between measurement and regularization objective functions can be obtained by generating an L-curve using PEST's Pareto functionality. In either case, a modeller will decree a level of model-to-measurement fit to be "too good" when unacceptable values must be assigned to model parameters in order to achieve this fit. Such a judgement of low **k** likelihood implies violation of an explicit or implicit C(**k**). A looser fit with the calibration dataset must then be sought, as this will reduce the requirement that **k** adopt unlikely values. On the other hand, if the cost for respect for C(**k**) is a poor level of fit with the measurement dataset, then this suggests that too much information contained within that dataset has been rejected. It follows that either the parameters **k** have a greater penchant for variability than was originally anticipated (and that C(**k**) therefore needs revision), that the model is not a good simulator of environmental behaviour, or that its parameterization scheme is not up to the task of providing receptacles for all of the information contained within the measurement dataset.

The subjective balancing of level of fit against acceptability of parameters can provide a modeller with the opportunity to learn much about the properties of the system which he/she is modelling at the same time as it provides him/her with the opportunity to learn much about his/her model. The decision to accept a certain level of misfit constitutes conditional acceptance of the calibrated model for the making of predictions of future system behaviour. These predictions will often form the basis for management of that system. Uncertainty will accompany these predictions. Part of this uncertainty will be inherited from "measurement noise" in the calibration dataset which, of course, is heavily loaded with structural noise whose covariance matrix is unknown. Nevertheless, at least some attempt to estimate the magnitude and characteristics of the collective "noise" that is responsible for model-to-measurement misfit must be made, for its characterization (as much as this is possible) is required for analysis of the post-calibration uncertainties associated with decision-critical model predictions. The calibration process provides the only opportunity for such characterization.

Similarly, a modeller may learn that system properties are more variable, and perhaps more heterogeneous, than he/she expected. In a groundwater or reservoir modelling context, it is far from uncommon that the calibration process may suggest, or even definitively expose, the existence of subsurface heterogeneity whose existence was previously unsuspected. If such

heterogeneity can exist in places where its presence was exposed by the calibration dataset, then perhaps it can exist in other places as well. Expert knowledge, and with it the explicit or implicit formulation of C(**k**), can thus be enhanced by the calibration process. Given the important role played by expert knowledge in calculating predictive uncertainty, its probabilistic characterization may therefore need revision based on lessons learned through model calibration before embarking on post-calibration predictive uncertainty analysis.

Uncertainty analysis is the subject of the next chapter.

# 7. Linear Uncertainty and Error Analysis

## 7.1 General

The present chapter discusses a variety of easily-completed analyses that provide useful information on the estimability of parameters, the uncertainties of predictions, the information content of data, and other matters related to model usage in calibration and in calibration-constrained predictive settings. All of these analyses require a Jacobian matrix; such a matrix will normally have been computed as part of the parameter estimation process, or can easily be computed after the calibration process has been completed. Some analyses require predictive sensitivities as well.

Normally the analyses described herein will be undertaken after calibration has taken place and a Jacobian matrix based on the calibrated parameter set is available. A Jacobian matrix based on estimated parameters is likely to promote greater integrity of these analyses than a Jacobian matrix based on an alternative set of parameter values. Conceptually at least, calibrated parameter values are expected to lie roughly at the centres of their posterior uncertainty distributions. The intent of many of the analyses discussed herein is to explore the estimability and potential for error of these estimated parameters, and of calibration-constrained predictions which are sensitive to them.

Nevertheless, many of the statistics that are discussed in this section are useful enough for their calculation to be worth the effort even before calibration has taken place. For example, they may be used to ascertain whether calibration is a worthwhile undertaking, or whether, for some predictions of interest, posterior uncertainty is little less than prior uncertainty, and can perhaps therefore be better explored using the latter. This will be particularly the case where prior predictive uncertainty can be explored using complex geostatistical realizations of system properties which may be considered, at a particular study, to constitute better expressions of expert knowledge than the continuous parameterization devices that may be employed for the purpose of model calibration.

Some of the concepts that are discussed in the present chapter have already been discussed in previous chapters. However some repetition is justified in the interests of keeping similar topics in the one place. An additional linear analysis option will be presented in chapter 9 where the effects of model defects are explored.

As usual, the inverse problem that forms the basis of present discussions is embodied in the following equation

$$\mathbf{h} = \mathbf{Z}\mathbf{k} + \boldsymbol{\varepsilon} \qquad (7.1.1)$$

The prior covariance matrix of $\mathbf{k}$ is denoted as $C(\mathbf{k})$ and the covariance matrix of measurement noise is denoted as $C(\boldsymbol{\varepsilon})$.

Where a model prediction $s$ is being considered, the sensitivity of this prediction to model parameters is denoted as $\mathbf{y}$. Hence

$$s = \mathbf{y}^t\mathbf{k} \qquad (7.1.2)$$

## 7.2 Post-Calibration Subspace-Based Analyses

### 7.2.1 Parameter Identifiability

Doherty and Hunt (2009) define the identifiability of a parameter as the square of the cosine between a vector pointing in the direction of the parameter and the projection of that vector onto the calibration solution space. This projection is zero where a parameter lies entirely within the null space; it is one when a parameter lies entirely within the solution space. If the identifiability of a parameter is zero, then its uncertainty is not reduced through the calibration process. However if its identifiability is unity, this does not mean that its estimation takes place without any potential for error. What it does indicate is that all of its potential for error is inherited from noise in the measurement dataset.

A parameter's identifiability is readily calculated from the outcomes of singular value decomposition undertaken on the Jacobian matrix that is used in place of **Z** featured in equation (7.1.1). In fact, singular value decomposition should be undertaken on the weighted Jacobian matrix which represents $\mathbf{Q}^{1/2}\mathbf{Z}$, where **Q** is chosen such that

$$\mathbf{Q} \propto \mathrm{C}^{-1}(\boldsymbol{\varepsilon}) \qquad (7.2.1)$$

As was discussed in previous chapters, while the magnitude of C(**ε**) may become apparent through the calibration process, the influence of structural noise on model-to-measurement misfit ensures that the values of off-diagonal elements of C(**ε**) cannot be known. C(**ε**) is normally assumed to be diagonal. However, as will be discussed in chapter 9, to some extent at least, the presence of structural noise can be accommodated by assembling a measurement dataset that includes observations that are processed in multiple ways in order to shield parameter estimates, to some extent at least, from the worst effects of its presence.

Ideally, a parameter set **k** should have been Kahunen-Loève transformed prior to calculation of identifiability for reasons discussed in the previous chapter. However this may not always be convenient or useful, as Kahunen-Loève transformed parameters may be difficult for a modeller to recognize because they pertain to the eigencomponents of the C(**k**) prior parameter covariance matrix. A modeller may therefore find that identifiability estimates for these parameters are not too informative. Hence identifiabilities are normally calculated for **k** parameters rather than for transformed parameters. These should be viewed with caution, however, where the prior parameter covariance matrix C(**k**) is non-diagonal.

The repercussions of failure to acknowledge the non-diagonal nature of C(**k**) in calculation of identifiabilities of individual elements of **k** can be illustrated as follows. Suppose that two elements of **k**, say $k_i$ and $k_j$, exhibit prior correlation. Suppose also that the information content of the calibration dataset **h** is directly informative of $k_i$ but not of $k_j$. The posterior uncertainty of $k_j$ is therefore smaller than its prior uncertainty because of the conditioning effect of $k_i$ (whose uncertainty is directly reduced through the calibration process). However this will not be reflected in a reduced identifiability for $k_j$ if identifiability is calculated using $\mathbf{Q}^{1/2}\mathbf{Z}$ based on the **Z** matrix of equation (7.1.1). (Note that other statistics will be presented later in this chapter which better accommodate a non-diagonal C(**k**).)

The projection operator onto the calibration solution space is $\mathbf{V}_1\mathbf{V}^{\mathrm{t}}_1$. As was discussed in section 6.2, partitioning of the **V** matrix arising from singular value decomposition of $\mathbf{Q}^{1/2}\mathbf{Z}$ into $\mathbf{V}_1$ and $\mathbf{V}_2$ submatrices is not generally such that the singular values associated with $\mathbf{V}_2$ are all zero. Instead singular value truncation takes place prior to singular values becoming

zero in order to prevent amplification of measurement noise when estimating values for parameters. Selection of the optimum truncation point is often inexact; this can affect the identifiabilities that are calculated for some parameters. This adds to the somewhat arbitrary nature of this statistic.

Let **x** be an arbitrary vector, and let **y** be its projection into the calibration solution space spanned by the columns of $\mathbf{V}_1$. Then

$$\mathbf{y} = \mathbf{V}_1\mathbf{V}^t_1\mathbf{x} \tag{7.2.2}$$

The cosine of the angle between **x** and **y** is their scalar product divided by the magnitude of each. Let us refer to this angle as θ. Then

$$\cos\theta = \frac{\mathbf{x}^t\mathbf{V}_1\mathbf{V}_1^t\mathbf{x}}{\sqrt{\mathbf{x}^t\mathbf{V}_1\mathbf{V}_1^t\mathbf{x}}\sqrt{\mathbf{x}^t\mathbf{x}}} \tag{7.2.3}$$

So that

$$\cos^2\theta = \frac{\mathbf{x}^t\mathbf{V}_1\mathbf{V}_1^t\mathbf{x}}{\mathbf{x}^t\mathbf{x}} \tag{7.2.4}$$

If **x** is a unit vector that points in the direction of one of the elements of **k**, let us say $k_i$, then all of its elements are zero except for its *i*'th element, which is one. For this vector

$$\cos^2\theta = (\mathbf{V}_1\mathbf{V}^t_1)_{ii} \tag{7.2.5}$$

From equation (6.2.10) it follows that the identifiability of parameter *i* is the *i*'th diagonal element of the resolution matrix that emerges from the use of singular value decomposition as a regularization device. Recall that the "ideal" resolution matrix is the identity matrix. However such an ideal resolution matrix can only emerge from a parameter estimation process wherein there is no null space. Where there is no null space all parameters possess an identifiability of unity.

As has been extensively discussed, the columns of matrix $\mathbf{V}_1$ are comprised of unit orthogonal vectors which we have denoted as $\mathbf{v}_i$. Thus

$$\mathbf{V}_1 = [\mathbf{v}_1 \;\; \mathbf{v}_2 \; \ldots \; \mathbf{v}_i \; \ldots \; \mathbf{v}_w] \tag{7.2.6}$$

where *w* is the number of singular values before truncation. If this is substituted into (7.2.5) and expanded we obtain

$$\cos^2\theta = \sum_{j=1}^{w}\left(\mathbf{v}_j\mathbf{v}^t_j\right)_{ii} \tag{7.2.7}$$

$(\mathbf{v}_j\mathbf{v}^t_j)_{ii}$ is the square of the cosine of the angle between a unit vector in the direction of parameter $k_i$ and its projection onto the unit $\mathbf{v}_j$ vector. If this angle is denoted as $\theta_j$, then

$$\cos^2\theta = \sum_{j=1}^{w}\cos^2\theta_j \tag{7.2.8}$$

The above equations can form the basis for some interesting and informative post-calibration plots. Where parameters have a spatial setting, identifiability maps can be drawn. Simple bar charts of identifiability are also readily plotted. These bar charts can be stacked so that contributions to total parameter identifiability by each of the $\mathbf{v}_j$ vectors are visible in each bar.

If these contributions are colour-coded according *j*, with warmer colours (i.e. shades of red) assigned to *j*'s for which corresponding singular values are higher, the effect is not only stunning but informative. If the identifiability bars pertaining to two different parameters are the same height, but one bar has warmer colours than the other, this signifies that a value can be estimated for the former parameter with less potential for error than for the latter parameter as its estimate is less likely to be contaminated by measurement noise. See section 6.2.5.

As stated, a parameter's identifiability is 1.0 or less. Perhaps the complement to this should be named "non-identifiability". It is easy to show that the number obtained by subtracting a parameter's identifiability from 1.0 is the squared cosine of the angle between a vector pointing in the direction of that parameter and its projection onto the null space of $\mathbf{Q}^{1/2}\mathbf{Z}$. The latter is spanned by unit vectors comprising the columns of $\mathbf{V}_2$. If a parameter has a high "non-identifiability" then the calibration dataset carries little or no information pertaining to this parameter. Note however that, as discussed above, if the parameter exhibits prior correlation with an identifiable parameter, then its uncertainty will nevertheless be reduced through the calibration process as an outcome of that correlation.

While parameter identifiability and non-identifiability statistics are informative, they must be used with caution. Indeed, as stated above, there is some degree of arbitrariness associated with these statistics, for their values depend on where singular value truncation takes place. Where singular value truncation aims to minimize parameter and predictive error variance, the truncation point may be based on a curve such as that depicted in figure 6.4. In practice the minimum of this curve may be broad, perhaps spanning tens of singular values. The identifiabilities of parameters whose projections onto corresponding $\mathbf{v}_i$ vectors is high will be very sensitive to the truncation point.

### 7.2.2 Other Subspace-Based Statistics

#### *7.2.2.1 Transformed Equations*

In addition to parameter identifiability, a number of other post-calibration statistics can easily be computed based on subspace concepts. These can reveal much about the status of the just-completed inversion process. They are often worth including in a report on the calibration process because of the insights that they provide not just into that process, but into the information content of the calibration dataset, and into the flow of that information from data to parameters. Ideally, calculation of these statistics should take place in a Kahunen-Loève transformed parameter environment, regardless of whether Kahunen-Loève transformation was undertaken prior to the actual calibration process. Where the inversion process took place under Tikhonov regularization constraints, then pre-calibration Kahunen-Loève transformation will probably not have been undertaken as Tikhonov constraints will have been the primary mechanism for expression of expert knowledge. However as it can be difficult to include Tikhonov constraints, and weight them appropriately, when calculating subspace-based post-calibration statistics, Kahunen-Loève transformation constitutes the most practical expression of prior knowledge when calculating these statistics.

As usual we take (7.1.1) as our starting point and assume that a weight matrix has been chosen according to (7.2.1). As has been done previously we will suppose that C(**k**) can be decomposed through singular value decomposition as

$$C(\mathbf{k}) = \mathbf{EFE}^t \qquad (7.2.9)$$

If the nature of system property heterogeneity at a particular study site is such that a C(**k**) matrix does not constitute a satisfying expression of expert knowledge, then it may nevertheless be possible to construct an approximate C(**k**) matrix for the purpose of calculating the following statistics anyway. For example, an assumption of multinormality accompanied by a variogram may be invoked for statistical characterization of layer-specific parameters within the domain of a groundwater or reservoir model in spite of the fact that higher order statistics may be required to properly characterize geological heterogeneity within the model domain. Statistics such as the following that provide a useable position statement on the inversion process do not need to be exact for them to be informative.

From (7.2.9) a Kahunen-Loève transformed parameter set **m** can be calculated as

$$\mathbf{m} = \mathbf{F}^{-½}\mathbf{E}^{t}\mathbf{k} \tag{7.2.10}$$

so that

$$C(\mathbf{m}) = \mathbf{I} \tag{7.2.11}$$

Back-transformation from **m**-space to **k**-space is achieved through the equation

$$\mathbf{k} = \mathbf{E}\mathbf{F}^{½}\mathbf{m} \tag{7.2.12}$$

With appropriate weight transformation, equation (7.1.1) can now be written as

$$\mathbf{g} = \mathbf{Y}\mathbf{m} + \boldsymbol{\xi} \tag{7.2.13}$$

where

$$\mathbf{g} = \mathbf{Q}^{½}\mathbf{h} \tag{7.2.14}$$

$$\mathbf{Y} = \mathbf{Q}^{½}\mathbf{Z}\mathbf{E}\mathbf{F}^{½} \tag{7.2.15}$$

$$\boldsymbol{\xi} = \mathbf{Q}^{1/2}\boldsymbol{\varepsilon} \tag{7.2.16}$$

Obviously, if **Q** is chosen such that

$$\mathbf{Q} = C^{-1}(\boldsymbol{\varepsilon}) \tag{7.2.17}$$

then

$$C(\boldsymbol{\xi}) = \mathbf{I} \tag{7.2.18}$$

Let us now undertake singular value decomposition on **Y**, so that

$$\mathbf{Y} = \mathbf{U}\mathbf{S}\mathbf{V}^{t} \tag{7.2.19}$$

*7.2.2.2 Model Matrix Products*

From (7.2.19) it immediately follows that

$$\mathbf{Y}\mathbf{Y}^{t} = \mathbf{U}\mathbf{S}^{2}\mathbf{U}^{t} \tag{7.2.20}$$

and that

$$\mathbf{Y}^{t}\mathbf{Y} = \mathbf{V}\mathbf{S}^{2}\mathbf{V}^{t} \tag{7.2.21}$$

If measurement noise is ignored, then from (7.2.13)

$$C(\mathbf{g}) = \mathbf{Y}C(\mathbf{m})\mathbf{Y}^t = \mathbf{Y}\mathbf{Y}^t \qquad (7.2.22)$$

Hence $\mathbf{Y}\mathbf{Y}^t$ is the covariance matrix that denotes the variability of model outputs **g** as this arises from the natural variability of parameters **m**. (This can be compared with the variability that **g** possesses by virtue of its noise content; with transformations as above, this is described by the covariance matrix **I**.) The variability of individual model outputs arising from natural parameter variability is therefore described by the diagonal elements of $\mathbf{Y}\mathbf{Y}^t$. This variability is a measure of their information content with respect to parameters. High parameter-induced variability compared to a noise variance of unity indicates high information content with respect to the parameters that induce that variability. The diagonal elements of $\mathbf{Y}\mathbf{Y}^t$ are closely related to the composite observation sensitivities defined in equation (5.3.4).

$\mathbf{Y}^t\mathbf{Y}$ can be viewed in a number of ways. As is apparent from equation (5.3.1), each diagonal element of this matrix is closely related to the composite sensitivity of the corresponding Kahunen-Loève-transformed parameter. Because Kahunen-Loève transformation effectively scales parameters by their innate variabilities, the diagonal elements of $\mathbf{Y}^t\mathbf{Y}$ are somewhat reminiscent of the composite scaled sensitivity statistic of Hill and Tiedeman (2007); however scaling is a little more theoretically based. If the inverse problem is well-posed $(\mathbf{Y}^t\mathbf{Y})^{-1}$ is the post-calibration parameter covariance matrix. However if it is not well-posed this matrix cannot be formed. Because the diagonal elements of $(\mathbf{Y}^t\mathbf{Y})^{-1}$ denote individual post-calibration parameter uncertainties, the diagonal elements of $\mathbf{Y}^t\mathbf{Y}$ can be loosely viewed as denoting post-calibration "parameter certainties". A low value of post-calibration "parameter certainty" denotes a low ability to be inferred through the calibration process. The post-calibration uncertainties of such parameters must therefore be constrained by expert knowledge, as information that is resident in the calibration dataset is insufficient to constrain them.

There is another, slightly more abstract way, to view the diagonal elements of $\mathbf{Y}^t\mathbf{Y}$. From (7.2.21) $\mathbf{Y}^t\mathbf{Y}$ can be written as

$$\mathbf{Y}^t\mathbf{Y} = \sum_{j=1}^{m} s_j^2 \mathbf{v}_j \mathbf{v}_j^t \qquad (7.2.22)$$

where $s^2_j$ are singular values and $m$ is the number of parameters featured in the inverse problem. From considerations presented in the preceding section, each diagonal element of $\mathbf{Y}^t\mathbf{Y}$ can thus be seen as being equal to the sum of weighted squared cosines between each transformed parameter $m_i$ and each unit vector $\mathbf{v}_j$ emerging from the singular value decomposition process; weights used in the summation are corresponding squared singular values. If parameter $m_i$ projects strongly onto $\mathbf{v}_j$ unit vectors that span the null space, or onto $\mathbf{v}_j$ unit vectors for which corresponding singular values are very low, then the $i$'th diagonal element of $\mathbf{Y}^t\mathbf{Y}$ will be small.

### *7.2.2.3 Singular Values*

As has been much discussed in the preceding chapter, the **S** matrix has only diagonal elements, these being singular values. Singular values are listed from highest to lowest down the diagonal; all are positive. Where an inverse problem is ill-posed their values diminish to

zero or near zero. An inspection of these singular values can be most informative. If they decay rapidly to zero, this informs the modeller that the information content of the calibration dataset is directed to only a small number of receptacles. These receptacles comprise the few $\mathbf{v}_i$ vectors for which corresponding singular values are high. Alternatively, if singular value decay is slow, then the information content of the calibration dataset is informative of many combinations of parameters (i.e. many $\mathbf{v}_i$ vectors). Where singular values decay to about $10^{-3}$ to $10^{-4}$ of the highest singular value, this marks the point where, from numerical considerations alone, the workable solution space ends in parameter estimation settings where the Jacobian matrix is calculated using finite parameter differences. In such settings this marks the point where numerical noise incurred through finite-difference derivatives calculation may be too grossly amplified to allow parameter combinations defined by corresponding $\mathbf{v}_i$ vectors to be estimated with integrity; see equations (6.2.27) and (6.2.30).

In practice, as has already been discussed, singular value truncation should take place before this point is reached because of the presence of measurement noise in the calibration dataset. A method for determining the optimal truncation point was suggested in section 6.2.5.3. In the present context this consists of determining the singular value at which $s^{-2}{}_i(\mathbf{v}^t{}_i\mathbf{v}_i)^2$ is greater than $(\mathbf{v}^t{}_i\mathbf{v}_i)^2$, that is where $s^{-2}{}_i$ is greater than 1 (as $\mathbf{v}^t{}_i\mathbf{v}_i$ is always equal to 1). This, of course, occurs where $s_i$ falls below 1.This is the point where the calibration process has the potential to incur more error in estimation of the $\mathbf{v}_i$ parameter combination than the uncertainty that this combination of parameters already possesses based on expert knowledge alone. This defines the optimal dimensionality of the solution space (and hence the optimal dimensionality of the orthogonal complementary null space). This, of course, is highly informative; it is worth reporting along with other statistics discussed herein that are easily calculated following calibration of a model.

*7.2.2.4 Transformed Parameter Status*

Once a singular value truncation point has been determined, and parameter space has thereby been subdivided into mutually orthogonal solution and null subspaces, the identifiabilities and non-identifiabilities of **m**-space parameters are easily computed as the diagonal elements of $\mathbf{V}_1\mathbf{V}^t{}_1$ and $\mathbf{V}_2\mathbf{V}^t{}_2$ respectively.

The diagonal elements of $\mathbf{V}_1\mathbf{S}^2{}_1\mathbf{V}^t{}_1$ and $\mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t{}_1$ are also worth recording in a state-of-calibration report. If the calibration solution space comprises the whole of parameter space the diagonal elements of $\mathbf{V}_1\mathbf{S}^2{}_1\mathbf{V}^t{}_1$ are equal to the diagonal elements of $\mathbf{Y}^t\mathbf{Y}$. If not, they are equal to or less than these. If the solution space comprises the entirety of parameter space, $\mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t{}_1$ is equal to $(\mathbf{Y}^t\mathbf{Y})^{-1}$; this is the post-calibration covariance matrix of Kahunen-Loève transformed parameter error. If not, each diagonal element of $\mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t{}_1$ is equal to the solution space component of post-calibration Kahunen-Loève transformed parameter error. In both cases the *i*'th diagonal element pertains to the *i*'th element of **m**. For each such parameter the sum of this diagonal element and the respective diagonal element of $\mathbf{V}_2\mathbf{V}^t{}_2$ is the total post-calibration error variance. That is

$$C(\underline{\mathbf{m}} - \mathbf{m}) = \mathbf{V}_2\mathbf{V}^t{}_2 + \mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t{}_1 \qquad (7.2.23)$$

From (7.2.12) the post-calibration covariance matrix of native model parameter error is

$$C(\underline{\mathbf{k}} - \mathbf{k}) = \mathbf{E}\mathbf{F}^{1/2}\mathbf{V}_2\mathbf{V}^t{}_2\mathbf{F}^{1/2}\mathbf{E}^t + \mathbf{E}\mathbf{F}^{1/2}\mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t{}_1\,\mathbf{F}^{1/2}\mathbf{E}^t \qquad (7.2.24)$$

(Note that this formulation differs from equation (6.2.30) because, in the present subsection,

singular value decomposition is undertaken on **Y** of equation (7.2.15) rather than on **Z**. Back-transformation to **k**-space is therefore necessary. Either equation can be used.)

*7.2.2.5 Relative parameter error variance reduction*

The *i*'th diagonal element of C($\underline{\mathbf{k}}$ – **k**) is the post-calibration error variance of parameter *i*. This can be denoted as $\sigma^2_{ei}$. Let $\sigma^2_i$ denote the prior error variance of this same parameter; this is the same as the error variance of its prior uncertainty. We denote the relative error variance reduction of parameter *i* as $rev_i$. This can be written as

$$rev_i = 1 - \frac{\sigma^2_{ei}}{\sigma^2_i} \qquad (7.2.25)$$

Ideally, the relative error variance reduction of a parameter should, like the identifiability of a parameter, range between zero and one. However there is no guarantee that $rev_i$ will always be non-negative. Negativity of $rev_i$ will occur if singular value truncation takes place at a point where the parameter's post-calibration error variance, as depicted in a plot such as that shown in figure 6.4, is greater than its pre-calibration error variance. The potential for this to occur will, of course, be exacerbated for those parameters for which the minimum of the error variance curve is only shallow.

*7.2.2.6 Model Output Statistics*

The diagonal elements of $\mathbf{U}_1\mathbf{S}^2{}_1\mathbf{U}^t{}_1$ can sometimes be informative. Where **U** is not truncated through inversion (as will occur if the number of estimable parameters is greater than the number of observations), or if the inversion problem is well-posed, then the $\mathbf{U}_1\mathbf{S}^2{}_1\mathbf{U}^t{}_1$ matrix is equal to the $\mathbf{YY}^t$ matrix. If not, the diagonal elements of $\mathbf{U}_1\mathbf{S}^2{}_1\mathbf{U}^t{}_1$ will be slightly less than those of $\mathbf{YY}^t$. These provide a measure of variability of weight-matrix-scaled model outputs arising from variability of solution space components of Kahunen-Loève transformed parameters. As such, the diagonal elements of $\mathbf{U}_1\mathbf{S}^2{}_1\mathbf{U}^t{}_1$ are the variances of respective model outputs arising from natural parameter variability as described by expert knowledge.

*7.2.2.7 Flow of Information*

The solution to the inverse problem of estimating Kahunen-Loève transformed parameters **m** is

$$\underline{\mathbf{m}} = \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t\mathbf{g} \qquad (7.2.26)$$

which can also be written as

$$\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\mathbf{g} = \mathbf{V}^t{}_1\underline{\mathbf{m}} \qquad (7.2.27)$$

As was discussed in section 6.2.6.3, the orthogonal unit vectors $\mathbf{u}_i$ comprising the columns of **U** constitute the "signals" or "characteristics" of the measurement dataset that contain its information. For the *i*'th such signal, the information itself is the *i*'th singular value $s_i$. This information flows uniquely and entirely to the *i*'th parameter receptacle; the latter is the vector $\mathbf{v}_i$ comprising the *i*'th column of **V**.

Identification of these signals and receptacles can sometimes be very useful. Where observations and/or parameters have spatial and/or temporal connotations, then it can sometimes be very instructive to plot the individual elements that comprise the elements of $\mathbf{u}_i$ and $\mathbf{v}_i$ in space and/or time. For example, if the calibration dataset is comprised of a stream

flow time series, decomposition of the time series in this manner may allow a modeller to see the features of this time series which are most information-rich, at the same time as he/she sees the parameter combinations that these various stream flow characteristics inform. However before making such a plot, Kahunen-Loève parameters must be back-transformed to native parameters, and weight-transformed measurements must be back-transformed to native measurements. From (7.2.10) and (7.2.14), (7.2.27) becomes

$$\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1\mathbf{Q}^{1/2}\mathbf{h} = \mathbf{V}^t{}_1\mathbf{F}^{-1/2}\mathbf{E}^t\underline{\mathbf{k}} \qquad (7.2.28)$$

The vectors comprising the columns of $\mathbf{Q}^{1/2}\mathbf{U}_1$ and $\mathbf{E}\mathbf{F}^{-1/2}\mathbf{V}_1$, even though they are no longer orthogonal unit vectors, define "information signals" in native observation space on the one hand, and the receptacles for that information in native parameter space on the other hand. The elements of these vectors thus have space and/or time connotations and can be plotted as such.

*7.2.2.8 Influence Statistics*

Observation influence statistics were discussed in section 5.3.3. Though formulated for well-posed inverse problems, they can still be used in the highly parameterized context if an ill-posed problem is re-formulated as a well-posed problem. This can be done by supplementing the calibration dataset with appropriately weighted prior information. Alternatively it may be accomplished by restricting the search for the solution to the ill-posed inverse problem to the subspace of parameter space that is spanned by the vectors comprising the columns of the $\mathbf{V}_1$ matrix obtained through singular value decomposition of $\mathbf{Y}$. However the information gained from such an analysis may not be very helpful.

To the extent that a prediction of interest is sensitive to parameters, or combinations of parameters, that occupy the null space, its uncertainty will not have been diminished through calibration. If such a prediction is of management interest, the need for reduction of its uncertainty is strong. Investments may need to be made in data acquisition that is targeted at achieving such a reduction. The most effective means by which to achieve this reduction is to reduce the dimensionality of the null space in a manner that is specific to this prediction. In particular, parameters and parameter combinations to which the prediction is sensitive should be shifted from the null space to the solution space. Influence statistics must accommodate the existence of the null space if they are to identify observations, or potential observations, which can achieve the most in this regard. Influence methodologies which achieve this purpose are presented shortly.

# 7.3 Post-Calibration Uncertainty Analysis

## 7.3.1 Posterior Parameter Uncertainty

*7.3.1.1 Formulation of Equations*

The previous section explored the propensity for error in calibrated model parameters. It also introduced a number of statistical quantities that provide an understanding of the workings of the calibration process, and can track the flow of information that takes place through the calibration process. In formulating the equations presented in the previous section, model calibration was presumed to take place through the theoretically optimal mechanism of truncated singular value decomposition applied to a Kahunen-Loève-transformed parameter set. Such calibration is, of course "conceptual"; it takes place only in the equations that are

used to calculate the statistical quantities of interest. Furthermore, all equations are matrix equations based on the assumption of a linear model in which expert knowledge presumes preferred parameter values of zero. In spite of these shortcomings and approximations, the equations that were derived in the previous section can provide a modeller with important insights into what a real world nonlinear history-matching process can and cannot achieve.

The same theme is continued in the present section. However the matrix equations which form the basis of the analysis presented in this section do not imitate the estimation of model parameters through a calibration process. Instead, they describe the conditioning of model parameters by field measurements of system state. The same measurement dataset is employed as in the previous section. However a Bayesian approach is adopted wherein the role of that dataset is to reduce the uncertainties of model parameters below their pre-calibration levels.

As usual, equation (7.1.1) is our starting point. To this we add a rather obvious equation.

$$\mathbf{k} = \mathbf{I}\mathbf{k} \tag{7.3.1}$$

This equation says nothing other than that parameters are related to themselves through the identity matrix. If this is combined with (7.1.1) in a single matrix equation we obtain

$$\begin{bmatrix}\mathbf{k}\\ \mathbf{h}\end{bmatrix}=\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{Z} & \mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{k}\\ \boldsymbol{\varepsilon}\end{bmatrix} \tag{7.3.2}$$

From the standard matrix relationship for propagation of covariance (i.e. equation 3.9.2) the joint covariance matrix of parameters and observations of system state can be written as

$$\begin{aligned}\mathrm{C}\left(\begin{bmatrix}\mathbf{k}\\ \mathbf{h}\end{bmatrix}\right)&=\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{Z} & \mathbf{I}\end{bmatrix}\begin{bmatrix}\mathrm{C}(\mathbf{k}) & \mathbf{0}\\ \mathbf{0} & \mathrm{C}(\boldsymbol{\varepsilon})\end{bmatrix}\begin{bmatrix}\mathbf{I} & \mathbf{Z}^{\mathrm{t}}\\ \mathbf{0} & \mathbf{I}\end{bmatrix}\\ &=\begin{bmatrix}\mathrm{C}(\mathbf{k}) & \mathrm{C}(\mathbf{k})\mathbf{Z}^{\mathrm{t}}\\ \mathbf{Z}\mathrm{C}(\mathbf{k}) & \mathbf{Z}\mathrm{C}(\mathbf{k})\mathbf{Z}^{\mathrm{t}}+\mathrm{C}(\boldsymbol{\varepsilon})\end{bmatrix}\end{aligned} \tag{7.3.3}$$

Using equation (3.8.5) we can now formulate the conditional covariance matrix of **k**, the condition being that we have gained perfect knowledge of **h** through having acquired a calibration dataset. We denote this matrix as C′(**k**). It must be remembered, however, that use of equation (3.8.5) rests on the assumption that the probability distributions with which the C(**k**) and C(**ε**) covariance matrices are associated are multinormal. We obtain

$$\mathrm{C}'(\mathbf{k}) = \mathrm{C}(\mathbf{k}) - \mathrm{C}(\mathbf{k})\mathbf{Z}^{\mathrm{t}}[\mathbf{Z}\mathrm{C}(\mathbf{k})\mathbf{Z}^{\mathrm{t}} + \mathrm{C}(\boldsymbol{\varepsilon})]^{-1}\mathbf{Z}\mathrm{C}(\mathbf{k}) \tag{7.3.4}$$

The first term on the right of equation (7.3.4) is the prior covariance matrix. The second term on the right shows how acquisition of the calibration dataset **h** alters this matrix. In general one or more of the diagonal elements of C(**k**) will be reduced through subtraction of this second term from the first. The extent to which it is reduced for a particular parameter depends on the information content of the calibration dataset with respect to that parameter.

C′(**k**) is the covariance matrix associated with the posterior probability distribution of parameters. Equation (7.3.4) expresses Bayes equation under the assumptions of parameter and measurement noise multinormality together with the assumption of model linearity.

Calculation of C′(**k**) through equation (7.3.4) requires that a $n \times n$ matrix be inverted, where $n$

is the number of observations comprising the calibration dataset. An equivalent formula will now be derived in which a matrix of size $m \times m$ must be inverted, where $m$ is the number of parameters in the parameter vector $\mathbf{k}$.

To derive this equation we start with an obvious matrix identity

$$\mathbf{B}^t\mathbf{D}^{-1}\mathbf{B}\mathbf{A}\mathbf{B}^t + \mathbf{B}^t = \mathbf{B}^t\mathbf{D}^{-1}\mathbf{B}\mathbf{A}\mathbf{B}^t + \mathbf{B}^t \qquad (7.3.5)$$

Then, noting that

$$\mathbf{D}^{-1}\mathbf{D} = \mathbf{I} \qquad (7.3.6)$$

and that

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{I} \qquad (7.3.7)$$

we re-write (7.3.5) as

$$\mathbf{B}^t\mathbf{D}^{-1}\mathbf{B}\mathbf{A}\mathbf{B}^t + \mathbf{B}^t\mathbf{D}^{-1}\mathbf{D} = \mathbf{B}^t\mathbf{D}^{-1}\mathbf{B}\mathbf{A}\mathbf{B}^t + \mathbf{A}^{-1}\mathbf{A}\mathbf{B}^t \qquad (7.3.8)$$

Thus

$$\mathbf{B}^t\mathbf{D}^{-1}(\mathbf{B}\mathbf{A}\mathbf{B}^t + \mathbf{D}) = (\mathbf{B}^t\mathbf{D}^{-1}\mathbf{B} + \mathbf{A}^{-1})\mathbf{A}\mathbf{B}^t \qquad (7.3.9)$$

By premultipyling both sides of (7.3.9) by $(\mathbf{B}^t\mathbf{D}^{-1}\mathbf{B} + \mathbf{A}^{-1})^{-1}$ and post-multiply both sides by $(\mathbf{B}\mathbf{A}\mathbf{B}^t + \mathbf{D})^{-1}$ we then obtain

$$(\mathbf{B}^t\mathbf{D}^{-1}\mathbf{B} + \mathbf{A}^{-1})^{-1}\mathbf{B}^t\mathbf{D}^{-1} = \mathbf{A}\mathbf{B}^t(\mathbf{B}\mathbf{A}\mathbf{B}^t + \mathbf{D})^{-1} \qquad (7.3.10)$$

Applying this identity to (7.3.4) we obtain

$$\mathrm{C}'(\mathbf{k}) = \mathrm{C}(\mathbf{k}) - [\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + \mathrm{C}^{-1}(\mathbf{k})]^{-1}\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z}\mathrm{C}(\mathbf{k}) \qquad (7.3.11)$$

That is

$$\mathrm{C}'(\mathbf{k}) = \{\mathbf{I} - [\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + \mathrm{C}^{-1}(\mathbf{k})]^{-1}\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z}\}\mathrm{C}(\mathbf{k}) \qquad (7.3.12)$$

From the obvious identity

$$\mathbf{I} = [\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + \mathrm{C}^{-1}(\mathbf{k})]^{-1}[\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + \mathrm{C}^{-1}(\mathbf{k})] \qquad (7.3.13)$$

it follows from (7.3.12) that

$$\mathrm{C}'(\mathbf{k}) = \{[\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + \mathrm{C}^{-1}(\mathbf{k})]^{-1}\,[\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + \mathrm{C}^{-1}(\mathbf{k}) - \mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z}]\}\mathrm{C}(\mathbf{k}) \qquad (7.3.14)$$

from which it follows that

$$\mathrm{C}'(\mathbf{k}) = [\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + \mathrm{C}^{-1}(\mathbf{k})]^{-1} \qquad (7.3.15)$$

Equation (7.3.15) is equivalent to equation (5.2.34) if $\sigma^2_r$ is unity. Thus where $\mathrm{C}(\mathbf{k})$ and $\mathrm{C}(\boldsymbol{\varepsilon})$ are known and pertain to multinormal distributions, and where the observation dataset is supplemented by prior information which is weighted according to prior parameter uncertainty (while members of the calibration dataset are weighted according to measurement noise), the post-calibration distribution of parameter error following Gauss-Newton parameter estimation is the same as the posterior parameter uncertainty distribution obtained through Bayes equation.

It is also easy to show that under the same circumstances parameter values estimated using the Gauss-Newton method are equal to their posterior expected values when conditioned by members of the calibration dataset. Recalling that prior expected values of $\mathbf{k}$ and $\mathbf{h}$ are $\mathbf{0}$, equation (3.8.4) becomes

$$\underline{\mathbf{k}} = C(\mathbf{k})\mathbf{Z}^t[\mathbf{Z}C(\mathbf{k})\mathbf{Z}^t + C(\boldsymbol{\varepsilon})]^{-1}\mathbf{h} \quad (7.3.16)$$

Notice the similarity of this equation to the second equation on the right of (6.3.14). With appropriate weight matrix and Kahunen-Loève transformation they are the same.

With application of the identity expressed by (7.3.10) equation (7.3.16) becomes

$$\underline{\mathbf{k}} = [\mathbf{Z}^tC^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + C^{-1}(\mathbf{k})]^{-1}\mathbf{Z}^tC^{-1}(\boldsymbol{\varepsilon})\mathbf{h} \quad (7.3.17)$$

This equation is identical to (5.2.33).

*7.3.1.2 Relative Parameter Uncertainty Variance Reduction*

The diagonal elements of $C'(\mathbf{k})$ express the posterior variances of parameter uncertainty. A similar statistic to the relative parameter error variance reduction can be formulated for parameter uncertainty. This denotes the ability (or otherwise) of the calibration dataset to reduce the uncertainty of a particular parameter.

Let the $i$'th diagonal element of $C'(\mathbf{k})$ be denoted by $\sigma^2_{ui}$. Let $\sigma^2_i$ denote its prior uncertainty variance, this being the corresponding diagonal element of $C(\mathbf{k})$. We denote the relative uncertainty variance reduction of parameter $i$ as $ruv_i$. This can be written as

$$ruv_i = 1 - \frac{\sigma^2_{ui}}{\sigma^2_i} \quad (7.3.18)$$

Like parameter identifiability, $ruv_i$ ranges between zero and one. Unlike relative parameter error variance reduction it cannot be negative. It is a more robust statistic than either identifiability or relative parameter error variance reduction as it does not depend on selection of a singular value at which the subdivision of parameter space into solution and null subspaces is deemed to occur.

## 7.4 Predictions

### 7.4.1 Predictive Uncertainty and Error Variance

*7.4.1.1 Formulation of Equations*

The focus of this chapter so far has been on the parameter estimation process (or the parameter conditioning process, depending on whether one adopts a subspace or Bayesian perspective). Using linear analysis it has been relatively easy to derive a suite of statistics which reflect the capacity or otherwise of a measurement dataset to inform model parameters.

Most models are not built simply for the sake of estimating system properties. Most models are built to make predictions of future environmental behaviour under similar or altered stress regimes to those which prevailed at the time of model calibration. It is to the making of model predictions that we now turn our attention.

From (7.1.2) and (7.3.4) the posterior uncertainty of a prediction $s$ can be calculated as

$$\sigma^2_s = \mathbf{y}^tC(\mathbf{k})\mathbf{y} - \mathbf{y}^tC(\mathbf{k})\mathbf{Z}^t[\mathbf{Z}C(\mathbf{k})\mathbf{Z}^t + C(\boldsymbol{\varepsilon})]^{-1}\mathbf{Z}C(\mathbf{k})\mathbf{y}^t \quad (7.4.1)$$

From (7.3.15) this can also be written as

$$\sigma^2_s = \mathbf{y}^t[\mathbf{Z}^tC^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + C^{-1}(\mathbf{k})]^{-1}\mathbf{y} \quad (7.4.2)$$

From (7.2.24) the post-calibration error variance of this same prediction can be written as

$$\sigma^2_{\underline{s}\text{-}s} = \mathbf{y}^t\mathbf{E}\mathbf{F}^{1/2}\mathbf{V}_2\mathbf{V}^t_2\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{y} + \mathbf{y}^t\mathbf{E}\mathbf{F}^{1/2}\mathbf{V}_1\mathbf{S}^{-2}{}_1\mathbf{V}^t{}_1\,\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{y} \qquad (7.4.3)$$

It must not be forgotten that in equation (7.4.3) the **U**, **S** and **V** matrices are calculated through singular value decomposition undertaken on the **Y** matrix of equation (7.2.15). This matrix accounts for weight transformation of observations and Kahunen-Loève transformation of parameters.

*7.4.1.2 Effect of Transformation*

The importance of weight-transformation of measurements and Kahunen-Loève transformation of parameters in minimizing the error variances of estimated parameters and predictions made by a calibrated model has been discussed extensively in this text. It is because of pre-calibration Kahunen-Loève transformation of parameters that the **E** and **F** matrices that emerge from singular value decomposition of the C(**k**) prior covariance matrix appear in equation (7.4.3). It was shown in section 6.2.4.2 that orthogonal projection in the space of Kahunen-Loève transformed parameters (i.e. **m**-space) does not constitute orthogonal projection in native parameter space (i.e. **k**-space). If solution to the inverse problem is therefore undertaken in **k**-space using singular value decomposition, the estimated $\underline{\mathbf{k}}$ vector, once transformed to **m**-space, may have a non-zero projection onto the null space of the model as it operates in that space. The minimum error variance status of the solution to the inverse problem is thereby lost. The potential for parameter and predictive error is thereby increased.

The same does not apply to parameter and predictive uncertainty (as distinct from error). To demonstrate this we first estimate parameters in **m**-space using the Bayesian approach. We then transform to **k**-space. We obtain the same equations that we would have obtained if we had worked directly in **k**-space.

From (7.3.17) applied in **m**-space, together with (7.2.11) and (7.2.18), the posterior mean of Kahunen-Loève transformed parameters can be calculated as

$$\underline{\mathbf{m}} = [\mathbf{Y}^t\mathbf{Y} + \mathbf{I}]^{-1}\mathbf{Y}^t\mathbf{g} \qquad (7.4.4)$$

With pertinent substitutions for $\underline{\mathbf{m}}$, **Y** and **g**, this becomes

$$\underline{\mathbf{k}} = \mathbf{E}\mathbf{F}^{1/2}[\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{Z}^t\mathbf{Q}\mathbf{Z}\mathbf{E}\mathbf{F}^{1/2} + \mathbf{I}]^{-1}\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{Z}^t\mathbf{Q}^{1/2}\mathbf{Q}^{1/2}\mathbf{h} \qquad (7.4.5)$$

From (7.2.9)

$$\mathbf{I} = \mathbf{F}^{1/2}\mathbf{E}^t\mathrm{C}^{-1}(\mathbf{k})\mathbf{E}\mathbf{F}^{1/2} \qquad (7.4.6)$$

If this and (7.2.17) are substituted into (7.4.5) we obtain

$$\underline{\mathbf{k}} = \mathbf{E}\mathbf{F}^{1/2}\{\mathbf{F}^{1/2}\mathbf{E}^t[\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mathbf{C}^{-1}(\mathbf{k})]\mathbf{E}\mathbf{F}^{1/2}\}^{-1}\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{h} \qquad (7.4.7)$$

Applying (2.6.4) and recalling that **E** is an orthonormal matrix, this becomes

$$\underline{\mathbf{k}} = \mathbf{E}\mathbf{F}^{1/2}\mathbf{F}^{-1/2}\mathbf{E}^t[\mathbf{Z}^t\mathbf{Q}\mathbf{Z} + \mathbf{C}^{-1}(\mathbf{k})]^{-1}\mathbf{E}\mathbf{F}^{-1/2}\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{Z}^t\mathrm{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{h} \qquad (7.4.8)$$

from which (7.3.17) follows.

A similar procedure can be followed to show that the computed uncertainty of a prediction is also immune to Kahunen-Loève and weight transformation. We start with (7.4.2). If measurement dataset conditioning is done in **m**-space we obtain

$$\sigma^2_s = \mathbf{w}^t[\mathbf{Y}^t\mathbf{Y} + \mathbf{I}]^{-1}\mathbf{w} \qquad (7.4.9)$$

where **w** expresses the sensitivity of a prediction *s* to parameters **m**. From (7.1.2) and (7.2.12)

$$\mathbf{w} = \mathbf{F}^{1/2}\mathbf{E}^t\mathbf{y} \tag{7.4.10}$$

Through expansion of **w** and **Y**, equation (7.4.9) becomes

$$\sigma^2_s = \mathbf{y}^t\mathbf{E}\mathbf{F}^{1/2}[\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{Z}^t\mathbf{Q}^{1/2}\mathbf{Q}^{1/2}\mathbf{Z}\mathbf{E}\mathbf{F}^{1/2} + \mathbf{I}]^{-1}\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{y} \tag{7.4.11}$$

From (7.4.6) and (7.2.17) this becomes

$$\sigma^2_s = \mathbf{y}^t\mathbf{E}\mathbf{F}^{1/2}\{\mathbf{F}^{1/2}\mathbf{E}^t[\mathbf{Z}^t\mathbf{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + C^{-1}(\mathbf{k})]\mathbf{E}\mathbf{F}^{1/2}\}^{-1}\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{y} \tag{7.4.12}$$

From (2.6.4) we then obtain

$$\sigma^2_s = \mathbf{y}^t\mathbf{E}\mathbf{F}^{1/2}\mathbf{F}^{-1/2}\mathbf{E}^t[\mathbf{Z}^t\mathbf{C}^{-1}(\boldsymbol{\varepsilon})\mathbf{Z} + C^{-1}(\mathbf{k})]^{-1}\mathbf{E}\mathbf{F}^{-1/2}\mathbf{F}^{1/2}\mathbf{E}^t\mathbf{y} \tag{7.4.13}$$

from which (7.4.2) follows.

*7.4.1.3 Comparing Predictive Error and Predictive Uncertainty*

Equation (7.4.3) can be written as

$$\sigma^2_{\underline{s}\text{-}s} = \mathbf{w}^t\mathbf{V}_2\mathbf{V}^t_2\mathbf{w} + \mathbf{w}^t\mathbf{V}_1\mathbf{S}^{-2}_1\mathbf{V}^t_1\mathbf{w} \tag{7.4.14}$$

Equation (7.4.9) is the equation for the variance of predictive uncertainty under equivalent conditions. It was shown above that parameter and predictive uncertainty are the same, regardless of whether the measurement dataset conditions native or transformed parameters. Hence parameter and predictive uncertainty are functions solely of expert knowledge and the information content of the calibration dataset.

In contrast, parameter and predictive error variance depend on the way in which calibration is implemented. They depend on the regularization methodology through which parameter and predictive uniqueness is attained, and on parameter transforms that are undertaken (or not) prior to calibration. Parameter and predictive error variance are minimized when regularization is undertaken using singular value decomposition applied to estimation of Kahunen-Loève transformed parameters. At the same time, the model matrix to which singular value decomposition is applied must be weight-matrix-transformed, with the weight matrix being proportional to the inverse of the covariance matrix of measurement noise. Equation (7.4.14) shows the error variance of a prediction calculated under such conditions.

Equation (7.4.14) can be written as

$$\sigma^2_{\underline{s}-s} = \sum_{i=1}^{w} s_i^{-2}\left(\mathbf{w}^t\mathbf{v}_i\right)^2 + \sum_{i=w+1}^{m}\left(\mathbf{w}^t\mathbf{v}_i\right)^2 \tag{7.4.15}$$

where *m* is the number of parameters, *w* is the number of pre-truncation singular values and $\mathbf{v}_i$ is the *i*'th column of the **V** matrix. Note that the first and second terms on the right of the equality sign have been interchanged between equations (7.4.14) and (7.4.15) in order to preserve the order of summation.

Now let us examine equation (7.4.9). From (7.2.21) and the fact that

$$\mathbf{V}\mathbf{V}^t = \mathbf{I} \tag{7.4.16}$$

(7.4.9) can be written as

$$\sigma^2_s = \mathbf{w}^t[\mathbf{V}\mathbf{S}^2\mathbf{V}^t + \mathbf{V}\mathbf{V}^t]^{-1}\mathbf{w} \tag{7.4.17}$$

Hence

$$\sigma^2_s = \mathbf{w}^t[\mathbf{V}(\mathbf{S}^2 + \mathbf{I})\mathbf{V}^t]^{-1}\mathbf{w} \quad (7.4.18)$$

$(\mathbf{S}^2 + \mathbf{I})$ is a diagonal matrix. The *i*'th term along its diagonal is $s_i^2 + 1$. Its inverse is thus also a diagonal matrix. The *i*'th term along the diagonal of its inverse is $1/(s_i^2 + 1)$. Equation (7.4.18) therefore becomes

$$\sigma^2_s = \mathbf{w}^t[\mathbf{V}(\mathbf{S}^2 + \mathbf{I})^{-1}\mathbf{V}^t]\mathbf{w} \quad (7.4.19)$$

This can be written in the same form as (7.4.15) as

$$\sigma_s^2 = \sum_{i=1}^{m} \frac{\left(\mathbf{w}^t\mathbf{v}_i\right)^2}{\left(s_i^2 + 1\right)} \quad (7.4.20)$$

The scalar multiplier of each term of (7.4.20) is always less than or equal to 1 (it is equal to 1 where the singular value is equal to 0 for a particular *i*), and always less than $s_i^{-2}$. Hence every term in (7.4.20) is less than or equal to the corresponding term in (7.4.15). Predictive error variance is therefore greater than predictive uncertainty variance. This means that the decision to calibrate first and then quantify the potential for predictive error, though normally far more numerically convenient than direct use of Bayes equation, comes at a cost. That cost is the introduction of "man-made error". Fortunately this cost is not hidden. If predictive error variance is quantified, the cost is included. Hence predictive error (and predictive uncertainty for which it is used as a surrogate) is not under-estimated.

In section 7.2.2.3 it was shown that where Kahunen-Loève and weight transformation take place, singular value truncation should occur where singular values fall below 1. Where singular values are more than slightly greater than 1, the terms of equation (7.4.20) are almost equal to those of (7.4.15). The first summation of the latter equation is relevant in this case. Where singular values are below a value that is slightly less than 1, then the terms of equation (7.4.20) are again almost equal to those of (7.4.15), and when singular values are zero exact equality prevails. The second summation of the latter equation is relevant in this case. Significant differences between the two equations exist only over that range of singular values that are close to unity. Thus "man-made error" is not likely to be high, and predictive error variance will often not exceed predictive uncertainty by much.

The matter can be viewed in another way by continuing the above analysis slightly. Consider the estimate of the conditional mean for **m** obtained through (7.4.4). Though undertaking singular value decomposition of **Y** this becomes.

$$\underline{\mathbf{m}} = [\mathbf{V}\mathbf{S}^2\mathbf{V}^t + \mathbf{I}]^{-1}\mathbf{V}\mathbf{S}\mathbf{U}^t\mathbf{g} \quad (7.4.21)$$

If we ignore measurement noise and set **g** equal to **Ym**, where **m** is the true but unknown parameter set, the following equation is obtained. We also expand the matrix expression inside the inverse term as above

$$\underline{\mathbf{m}} = [\mathbf{V}(\mathbf{S}^2 + \mathbf{I})\mathbf{V}^t]^{-1}\mathbf{V}\mathbf{S}\mathbf{U}^t\mathbf{U}\mathbf{S}\mathbf{V}^t\mathbf{m} \quad (7.4.22)$$

This becomes

$$\underline{\mathbf{m}} = \mathbf{V}(\mathbf{S}^2 + \mathbf{I})^{-1}\mathbf{S}^2\mathbf{V}^t\mathbf{m} \quad (7.4.23)$$

which can be written as

$$\underline{\mathbf{m}} = \sum_{i=1}^{m} \frac{s_i^2}{\left(1 + s_i^2\right)}\mathbf{v}_i\mathbf{v}_i^t\mathbf{m} \quad (7.4.24)$$

When singular values are high, $\frac{s_i^2}{\left(1+s_i^2\right)}$ approaches unity. **m** projects onto a vector $\mathbf{v}_i$ within the solution space of **Y** to obtain a component of **m** in the same way as if **m** had been estimated using singular value decomposition. When singular values are small or zero, the scalar term of (7.4.24) becomes small or zero. For these singular values **m** contains very little, if any, of **m**. It is the same for estimation of **m** using singular value decomposition as these singular values are below the singular value truncation threshold. For singular values just above unity however, less of **m** is projected onto the solution space of **Y** as would be the case if **m** were estimated using singular value decomposition. For singular values just below unity, **m** is partly informed by **m**, even though it would not be informed by **m** at all if **m** were estimated using singular value decomposition, as this is below the singular value truncation threshold of 1.

*7.4.1.4 Data Worth*

The uncertainty of a model prediction can be calculated using either of equations (7.4.1) or (7.4.2). These equations require that a Jacobian matrix be calculated to replace the matrix **Z** that is featured in these equations. It also requires that a predictive sensitivity vector **y** be calculated. A covariance matrix expressing expert knowledge, namely C(**k**), and a covariance matrix expressing measurement noise, namely C(**ε**), must also be supplied.

There is no reason, of course, why a "prediction" cannot be a parameter. All that is required of **y** for this to occur is that its only non-zero element be that which corresponds to the parameter in question; this element should be 1.

Neither equation (7.4.1) nor equation (7.4.2) requires the values of parameters. Nor do they require the values of observations, nor of the prediction whose uncertainty is being evaluated. Hence for a linear model it is only sensitivities and covariances that matter. This has the important repercussion that it is not necessary for the history-matching process that is expressed through the matrix **Z** to have actually been accomplished for the posterior uncertainty of a prediction to be evaluated. Nor, in fact, do the measurements comprising the history-matching dataset need to have even been made. All that is required is that the pertinent sensitivities comprising the matrix **Z** be computed.

If the worth of data is judged by its ability to reduce the uncertainties of predictions of management interest, then data worth assessment based on linear analysis becomes a comparatively simple task. The worth of data with respect to a particular prediction can be assessed before it is gathered. The comparative worth of different data acquisition strategies can be assessed before those strategies are actually implemented. The uncertainties of one or a number of predictions of interest can be calculated using the above equations with and without the addition of the extra data to the existing history-matching dataset. The extent to which uncertainties of predictions of interest are reduced through acquisition of that data can thereby be assessed.

Similar strategies can be used for evaluating the worth of data that already exists. One option for evaluating the worth of an individual data element, or of all data of a certain type, is to employ equation (7.4.1) or (7.4.2) to evaluate the uncertainty of a prediction of interest under the assumption that this data comprises the entirety of the measurement dataset. The amount by which the uncertainty of that prediction is reduced below its pre-calibration uncertainty (the latter is calculated using the first term on the right of equation 7.4.1) is a measure of the

worth of that data to that prediction.

A slightly different way to assess the worth of existing data is to calculate the uncertainty of a prediction of interest with and without inclusion of that data in the existing measurement dataset. The extent to which the uncertainty of the prediction rises with omission of the data from the existing history-matching dataset is a measure of the uniqueness of its information to that prediction. See Dausman et al (2010) for further discussion and some practical applications.

Data whose worth is being assessed need not be restricted to measurements of system state. Direct measurements of system properties can also be included in the analysis. A row of the **Z** matrix for data of this type is comprised of zeros except for the element pertaining to the parameter whose value is measured. This element has a value of 1.

*7.4.1.5 Parameter Contributions to Predictive Uncertainty*

Let us define "the contribution that an individual parameter makes to the uncertainty of a prediction" as the fall in the uncertainty of the prediction that would be accrued through the acquisition of perfect knowledge of the value of that parameter. A similar definition can be made for the contribution that a group of parameters makes to the uncertainty of a prediction. These contributions are readily evaluated using equation (7.4.1) or (7.4.2) in one of two ways. One way is to add rows to the **Z** matrix simulating direct measurements of system properties in the manner described in the previous section; zero measurement noise would be associated with such measurements. An alternative procedure is to re-calculate the uncertainty of the prediction with the number of elements of **k** reduced to account for the reduced number of unknown parameters; C(**k**) would require conditioning if there is prior correlation between parameters whose values are now notionally known and those whose values are still unknown.

If desired, the contributions that individual or grouped parameters make to the uncertainty of a prediction can be graphed or plotted in space. Inspection of such plots can be highly informative.

Parameter contribution analysis may help to resolve arguments about such issues as correctness or proximity of boundary conditions. "Parameters" which may not necessarily have been included in the actual model calibration process can be included in parameter contribution analysis. These parameters may include boundary value properties. If the contributions that these properties make to the uncertainties of predictions of interest are small, then possible errors in boundary conditions will have been shown to contribute little to the potential for error in these predictions. Approximations in designing these boundary conditions will therefore have been shown to be acceptable. If these approximations have enabled the area of the model domain to be reduced, or have enhanced the numerical stability of the model, then this may have allowed calibration and uncertainty analysis to proceed where it would have otherwise been difficult or impossible. The losses incurred by making the approximations will have been shown to be less than the gains that they have enabled.

Parameter contributions to predictive uncertainty can be computed under both pre- and post-calibration conditions. In the former case only the first term of equation (7.4.1) is employed in calculation of uncertainty. In many cases it is found that the post-calibration contribution of a parameter or parameter group to the uncertainty of a prediction is less than its pre-calibration contribution. The size of the parameter contribution reduction may illustrate why

the calibration process was successful in reducing the uncertainty of the prediction.

In some cases the contribution that a parameter makes to the uncertainty of a prediction is actually seen to increase, rather than decrease, through the history-matching process. In explaining this, the definition given above for "contribution to uncertainty" must be remembered. Sometimes a parameter makes little contribution to the uncertainty of a prediction prior to the history-matching process because the prediction is not sensitive to that parameter. At the same time the information contained within the measurement dataset may be shared between this parameter and another parameter; hence the post-calibration correlation between the two parameters may be high. In a case such as this, acquisition of knowledge of the first parameter will reduce the post-calibration uncertainty of the second parameter. If the model prediction of interest is sensitive to the second parameter, then its uncertainty will be reduced through acquisition of knowledge of the first parameter, notwithstanding the lack of direct sensitivity of the prediction to the first parameter.

## 7.5 Minimizing the Cost of Parameter Reduction

### 7.5.1 Background

Suppose that a modeller has built a complex model with many parameters and wishes to reduce the number of parameters that are adjusted in calibrating that model. An obvious way to accomplish this would be through the use of so-called "super parameters" defined through singular value decomposition of the weighted Jacobian matrix calculated using prior expected parameter values. See section 6.4.4. In principle, as will be discussed in chapter 9, singular value decomposition constitutes an "ideal" form of parameter simplification which, if properly implemented, reduces the risk of predictive bias incurred through subsequent calibration of the simplified model.

Suppose, however, that a modeller wishes to avoid the use of "abstract" super parameters, preferring instead to reduce the number of adjustable parameters by fixing some at values which are deemed to be of minimum error variance from an expert knowledge point of view, and linking other parameters together so that their values maintain equality, or fixed ratios, during the parameter adjustment process.

As usual, let the original model be denoted by **Z** and let its parameters be denoted by **k**. Let the simplified model be denoted by **X** and its parameters by **p**. Simplification is implicitly defined by the relationship

$$\mathbf{k}_s = \mathbf{L}\mathbf{p} \tag{7.5.1}$$

Here $\mathbf{k}_s$ denotes a set of **k**-parameters for use of the model **Z** which are in fact simplified from the normal set of parameters **k** employed by **Z** due to the fact that they have their roots in **p**. Thus, for example, if one parameter is used in the simplified model to represent two parameters in the complex model, then the elements of $\mathbf{k}_s$ which correspond to this single **p** parameter are both equal in value to this simple parameter. In this case the **L** matrix acts as a kind of "selection matrix" through which values are assigned to elements of $\mathbf{k}_s$ according to the element of **p** with which each element of $\mathbf{k}_s$ is associated. A particular row of **L** will then be all zeroes except for the element that corresponds to the selected element of **p**. Fixed ratios between elements of $\mathbf{k}_s$ which are assigned to the same element of **p** are easily accommodated through using values other than 1 in selecting an element of **p** for value assignment to an element of $\mathbf{k}_s$.

Alternatively if elements of $\mathbf{k}_s$ are fixed during the parameter simplification process, they are assigned values of zero for the purpose of linear analysis, for these are their prior expected values; see section 4.5.2. Rows of the **L** matrix that correspond to these $\mathbf{k}_s$ parameters are thus all zero.

Running of the model on the basis of a set of parameters $\mathbf{k}_s$ calculated from a simplified parameter set **p** through (7.5.1) to produce a set of outputs **o** can be symbolized as

$$\mathbf{o}_s = \mathbf{Z}\mathbf{k}_s = \mathbf{ZLp} \qquad (7.5.2)$$

from which it is apparent that

$$\mathbf{X} = \mathbf{ZL} \qquad (7.5.3)$$

where, as stated above, **X** represents the action of the simplified model on the simplified parameter set **p**.

Parameter simplification may reduce the level of fit that it is possible to achieve between model outputs and the calibration dataset, as use of a smaller number of parameters reduces the dimensionality of the range space of the model. Let us define "simplification residuals" $\mathbf{r}_x$ as

$$\mathbf{r}_x = \mathbf{Zk} - \mathbf{X}\underline{\mathbf{p}} = \mathbf{Zk} - \mathbf{ZL}\underline{\mathbf{p}} \qquad (7.5.4)$$

where $\underline{\mathbf{p}}$ is a set of parameters that are estimated through calibration of **X** to achieve as good a fit as possible with outputs of **Z** calculated on the basis of arbitrary values for **k**.

A number of simplification options are normally open to a modeller. Each of these results in an **L** matrix which embodies the simplification strategy, together with a corresponding **X** matrix calculated using (7.5.3). One way to discover the best simplification strategy of the various options available (where "best" is defined, for the moment, as that which incurs least rise in the calibration objective function) is to calibrate the model on the basis of each such simplification strategy to see which incurs least cost in terms of objective function increase. However time and/or the numerical burden of this procedure may prohibit this approach. Another option is to use linear analysis to establish the least costly simplification strategy prior to actually implementing it; the model can then be calibrated on the basis of this strategy.

### 7.5.2 Estimating Simplification Residuals

We will assume that the calibration process through which $\underline{\mathbf{p}}$ of equation (7.5.4) is estimated is achieved through singular value decomposition. As has been discussed previously, this is equivalent to use of the Gauss-Newton method if the problem of estimating $\underline{\mathbf{p}}$ is well-posed. $\underline{\mathbf{p}}$ is thus calculated as

$$\underline{\mathbf{p}} = \mathbf{V}_{x1}\mathbf{S}_{x1}^{-1}\mathbf{U}^t_{x1}\mathbf{Zk} \qquad (7.5.5)$$

The subscript "x" following **V**, **S** and **U** denotes singular value decomposition undertaken on **X** (i.e. **ZL**). From (7.5.4) $\mathbf{r}_x$ becomes

$$\mathbf{r}_x = \mathbf{Zk} - \mathbf{XV}_{x1}\mathbf{S}_{x1}^{-1}\mathbf{U}^t_{x1}\mathbf{Zk} \qquad (7.5.6)$$

Writing **X** as

$$\mathbf{X} = \mathbf{U}_x\mathbf{S}_x\mathbf{V}^t_x \qquad (7.5.7)$$

and substituting this into (7.5.6) we obtain

$$\mathbf{r}_x = (\mathbf{I} - \mathbf{U}_{x1}\mathbf{U}^t_{x1})\mathbf{Z}\mathbf{k} = \mathbf{U}_{x2}\mathbf{U}^t_{x2}\mathbf{Z}\mathbf{k} \qquad (7.5.8)$$

Suppose that, in testing one particular simplification strategy, we conceptually generate many realizations of **k** and that, for each such realization, we estimate a corresponding simplified parameter set **p** through calibration of the simplified **X** model against outputs of the **Z** model. From (7.5.8) the covariance matrix of residuals emerging from repeated calibration of the simplified **X** model in this way can be calculated as

$$C_x(\mathbf{r}) = \mathbf{U}_{x2}\mathbf{U}^t_{x2}\mathbf{Z}C(\mathbf{k})\mathbf{Z}^t\mathbf{U}_{x2}\mathbf{U}^t_{x2} \qquad (7.5.9)$$

If $C(\mathbf{k})$ is equal to **I**, this becomes

$$C_x(\mathbf{r}) = \mathbf{U}_{x2}\mathbf{U}^t_{x2}\mathbf{Z}\mathbf{Z}^t\mathbf{U}_{x2}\mathbf{U}^t_{x2} \qquad (7.5.10)$$

The diagonal elements of $C_x(\mathbf{r})$ represent the variances of individual elements of $\mathbf{r}_x$; the square roots of these represent their standard deviations.

Using equation (7.5.9) different simplification strategies embodied in different **L** matrices can be rapidly compared. A simple summary statistic is the sum of elements along the diagonal of $C_x(\mathbf{r})$. We denote this as $\Phi_x$ (because of its resemblance to an objective function). It is calculated as

$$\Phi_x = \mathrm{tr}(C_x(\mathbf{r})) \qquad (7.5.11)$$

where tr() is the matrix trace operator. $\Phi_x$ can be thought of as the contribution made to the overall calibration objective function by parameter simplification. If this number is low (or even zero), it indicates that the simplified model retains enough adjustable parameters to guarantee a fit with field data that is little worse than that which would prevail through calibration of the original **Z** model. This does not mean that simplification is therefore "ideal", for it is possible that the parameters of the simplified model may play roles that compensate for parameter simplification in achieving this level of fit, and that this may bias some model predictions; see chapter 9. Nevertheless it does indicate that enough parameters exist in the simplified model, and that these parameters are defined in such a way, for a good fit between model outputs and the measurement dataset to be attained. These parameters therefore span the solution space of the **Z** model.

In the subsurface reservoir or groundwater modelling contexts, different simplification strategies (embodied in different **L** matrices) may result from alternative representations of the presence, locations and geometries of zones of piecewise constancy reflecting rock types of contrasting, but relatively homogeneous, hydraulic properties. Lower values of $\Phi_x$ arising from some of these tested dispositions may indicate better representation of subsurface heterogeneity. It must be remembered, however, that all simplified **X** models are children of the original **Z** model and that all simplified **p** parameter fields are derived from the original **k** field. The greater is the number of elements that **k** possesses, the greater is the number of simplification options that are open to the modeller.

# 8. Nonlinear Uncertainty and Error Analysis

## 8.1 Some General Comments

### 8.1.1 Model Parameterization

The focus of the present chapter is on exploration of posterior predictive uncertainty, for which exploration of post-calibration predictive error is a computationally feasible surrogate. It is assumed that in exploring posterior predictive variability, parameter variability must be constrained by the fact that model outputs under calibration conditions must respect measurements of system state to within limits that are considered appropriate. Much of the discussion of this chapter pertains to models that are highly parameterized and that simulate environmental processes in model domains wherein system properties are heterogeneous. Exploration of parameter and predictive uncertainty in this context is a demanding task, and one that can be implemented only approximately.

Section 4.3 discussed some Bayesian options for sampling the posterior probability distribution of model parameters. Some of the difficulties that can be encountered in implementing these methods in highly parameterized contexts were mentioned. Where parameter numbers are large, sampling of the posterior parameter probability distribution using Bayesian methods can require an inordinately large number of model runs. Numerical challenges are exacerbated if the parameter null space has many dimensions and if model run times are long. Under these circumstances, derivative-based methods such as those discussed herein become the preferred option for exploration of post-calibration parameter and predictive error/uncertainty.

Posterior parameter and predictive uncertainty analysis requires adequate representation of the prior probability distribution of model parameters. This is especially the case where the uncertainties associated with predictions of management interest are not greatly diminished through the history-matching process. This can be quite challenging in some modelling contexts. One such context is subsurface reservoir modelling, and some instances of groundwater modelling where expressions of expert knowledge may take the form of complex geostatistical realizations of subsurface heterogeneity which endeavour to represent geological units and their complex spatial interrelationships with picture-perfect integrity. Geological units are often categorical rather than continuous in nature. For example a fault or fracture is either present or it is not at a certain location; it is either intersected or not by another fault. At any one location within a sedimentary unit, lithology may be any of $n$ different types where $n$ is a small integer. The generation and adjustment of random realizations of discrete depositional and structural features in a way that allows a model to replicate historical observations of system state while maintaining their geological integrity is a problem which has yet to be fully solved.

If using methodologies discussed in the present chapter for exploration of posterior parameter and predictive uncertainty, these categorical, geostatistically-based parameter fields must be replaced with alternative spatial parameterization schemes that are more easily manipulated to respect calibration constraints. A primary design specification of these alternative parameter fields is that model outputs be differentiable with respect to the parameters which define them so that the model can be replaced by a Jacobian matrix. This may compromise

their geological integrity. It may also compromise the integrity of model outputs that are sensitive to the types of details which these categorical parameter fields can uniquely portray. This cost must be played against the principal benefit of employing a non-categorical parameter field to which model outputs bear a continuously differential relationship. This benefit is that the parameters which comprise such parameter fields can be efficiently adjusted so that model outputs respect calibration constraints. This benefit can be realized even where parameters number in the hundreds of thousands.

Having stated the above, it must also be stated that there are some highly-parameterized posterior uncertainty analysis contexts where the requirements for parameter differentiability can be somewhat relaxed. In previous sections it was explained that the quest for uniqueness that underpins the concept of model calibration can only be justified if a minimum error variance parameter field is the outcome of the calibration process. Where the calibration dataset is information-poor, the minimum error variance parameter field may be relatively simple, this being an outcome of its minimum error variance status. Differences between such a calibrated parameter field and complex geostatistically-based realizations of the subsurface can be profound. However if these differences are irresolvable by the calibration process because they lie within the calibration null space, then calibration-constrained representation of them may not be too difficult. It may simply require that realizations of categorical parameter fields remain "centred" on the minimum error variance calibrated parameter field. If necessary, the latter can be adjusted on a realization-by-realization basis to accommodate elements of solution space variability that different categorical realizations introduce.

In the more usual case where system parameterization complexity does not lie completely within the calibration null space, probabilistic representation of this complexity in a calibration-constrained setting becomes more difficult. Suppose that continuous, calibration-constrained parameter fields, centred on the calibrated parameter field, are randomly generated as surrogates for more complex geostatistically-based parameter fields. Even in this case it may be possible to relax the necessity for model outputs to be differentiable with respect to all aspects of these parameter fields. The solution space component of each of these parameter fields must indeed be continuously adjustable; this allows constraints imposed by the necessity for model outputs to match the calibration dataset to be met. However the null space components of these parameter fields do not need to be adjusted to meet calibration constraints because, by definition, the calibration dataset is uninformative of these components. Complex statistical realizations of null space parameter components which represent non-inferable spatial parameterization detail can then, conceptually at least, "ride on the back" of continuous solution space components of these stochastic parameter fields that are adjusted in order to maintain the model in a calibrated state.

While this concept may provide some latitude in developing parameterization schemes for use in calibration-constrained exploration of parameter and predictive uncertainty in complex environmental settings, in practice many difficulties remain, especially in groundwater and reservoir modelling contexts. The principle difficulty is that a discrete separation of an environmentally realistic parameterization scheme into solution and null space components that can be independently manipulated may not always be possible.

The above considerations suggest that in modelling complex environmental systems, post-calibration uncertainty analysis will always be approximate. The categorical nature of environmental heterogeneity in many modelling contexts is just one of the many factors which will contribute to its difficulties. Another important factor is that models themselves

constitute simplified representations of environmental processes. What is important, however, is that regardless of the parameterization and simulation approximations that must necessarily precede exploration of the range of predictive possibilities that exist after calibration constraints are met, this range of possibilities must be over-stated rather than under-stated. Such a strategy prevents the occurrence of a type II statistical error wherein the occurrence of an unwanted future environmental event is deemed to be unlikely when this is not in fact the case; such an error constitutes failure as far as attempts to explore predictive uncertainty in the decision-making context are concerned.

It follows that where model and parameter simplifications are adopted in order to expedite the numerically difficult task of exploring post-calibration predictive uncertainty, the compromises must be worth it. They will, indeed, be worth the costs if the reduction in predictive uncertainty that is accrued through respecting calibration constraints is greater than the "man-made" uncertainty that is required to impose these constraints. This "man-made" uncertainty is born of the model and parameterization simplifications that must be made in order to implement numerical algorithms such as those outlined in this chapter. It is incumbent on a modeller to ensure that this man-made uncertainty is included in assessments of the ultimate uncertainty of model predictions of management interest in order to forestall the occurrence of a type II statistical error. By its very nature, this "margin of safety" term will only be approximately calculable in most modelling contexts. However it must be over-stated rather than under-stated.

Because of the compromised and approximate nature of post-calibration predictive uncertainty analysis in the environmental modelling context, an alternative strategy may be to not enforce calibration constraints at all. Hence a more complex model, parameterized with categorical representations of system properties, may be deployed in unconstrained Monte Carlo analysis of predictive uncertainty. The "man-made" uncertainty that accompanies this strategy is, of course, that incurred by failing to enforce history-matching constraints on model parameter fields. If, however, the cost of failing to exert history-matching constraints is thought to be small (this can be explored by undertaking linear analysis using methods discussed in the previous chapter based on a continuous surrogate parameter field), then such a strategy may constitute a realistic means of exploring the post-calibration uncertainties of those predictions whose posterior uncertainties are likely to be diminished only marginally from their prior uncertainties. It may also be the preferred option for exploration of posterior predictive uncertainty where enforcement of calibration constraints on parameter fields that populate a defective model has the potential to incur bias in some of its management-critical predictions; see the next chapter.

In some modelling contexts another alternative for posterior predictive uncertainty analysis may be to enforce calibration constraints only very loosely. Hence high levels of misfit between model outputs and the calibration dataset are deemed to be tolerable. This strategy may allow deployment of complex categorical parameter fields together with, for example, a Markov chain Monte Carlo sampler.

Whatever strategy is chosen for exploration of post-calibration predictive uncertainty analysis, it must not be forgotten that a compromise that works well for one prediction may not work well for another prediction. If a prediction is well-informed by the calibration dataset, then the methodologies presented in the present chapter for exploration of posterior uncertainty may indeed be appropriate; however their implementation may require that some parameter field simplification be undertaken. Alternatively, if a prediction is not informed by

the calibration dataset, then uncertainty analysis methodologies that provide the most effective expression of expert knowledge may need to be employed instead of those which expedite history-matching and therefore provide most effective expression of information contained in the calibration dataset.

We finish this section on a philosophical note. The prediction-specific nature of model-based data analysis and decision support alluded to above calls into question the use of a single model, supported by a single calibration process, to make a suite of different predictions within a study area. It is a paradox of our times, however, that this is often the way that environmental models are built and then deployed to support the making of important environmental decisions. See Doherty and Simmons (2013) and Doherty and Vogill (2015) for a discussion of this issue.

### 8.1.2 Looking Ahead

The methodologies discussed in the present chapter for exploration of post-calibration predictive uncertainty follow two broad approaches. The first is Monte Carlo. This approach dedicates itself to the production of many parameter fields, all of which reflect expert knowledge as best they can, and all of which respect calibration constraints as best they can. The uncertainty associated with any prediction required of a model can then be assessed by making that prediction with all of these parameter fields; a histogram of the prediction can thereby be constructed.

An advantage of Monte Carlo methods is that a modeller is not committing him/herself to any specific prediction when assembling a set of post-calibration parameter fields. Once such a set of parameter fields has been generated, they can be used at any time in the future for the making of one or many predictions of the behaviour of the system under any proposed management strategy. A disadvantage of Monte Carlo methods however is that the number of parameter fields that are used in the making of these predictions may not be sufficient to define the extremities of predictive probability distributions. This may result in under-estimation of the potential for unwanted consequences to follow the adoption of a proposed management strategy. Another potential drawback follows from inadequacies in defining parameter fields that properly express expert knowledge, especially where these parameter fields must also respect calibration constraints; see above. This may suppress the range of predictive possibilities that emerge from uncertainty analysis such that this range does not encompass the range of predictions that may actually occur.

A problem with Monte Carlo methods in general, whether these employ simplified or complex parameter fields, is that they leave little room for "surprises". It may not require too much of a departure from hardwired expressions of expert knowledge embodied in these parameter fields for some unwanted environmental event to occur.

The above problems can be partially overcome by using a predictive analysis methodology that is prediction-specific. This is the focus of the second class of strategies examined in this chapter. A disadvantage of prediction-specific methods is that the algorithms which implement them normally require that the model compute the value of a prediction many times in the course of analysing its uncertainty. In this regard they resemble linear predictive uncertainty analysis methods discussed in the previous chapter in which calculation of a predictive sensitivity vector (i.e. a **y** vector) is required. However, in the nonlinear context, the numerical burden of prediction-specific uncertainty analysis is exacerbated by the fact

that this vector may need to be re-computed during each of many successive linear iterations of a nonlinear optimization process. Where predictions of management interest occur well into the future, these calculations may consume considerable computing resources.

## 8.2 Calibration-Constrained Monte-Carlo

### 8.2.1 Linear-Assisted Monte Carlo

Calibration-constrained Monte Carlo analysis aims to generate many parameter realizations for the use of a model. Collectively these realizations should reflect the range of possibilities that expert knowledge allows for model parameters. Individually, each parameter field should respect the information content of the calibration dataset by ensuring that model outputs fit that dataset. The collection of parameter sets that emerge from Markov chain Monte Carlo sampling of the posterior parameter probability distribution (see section 4.3.2) satisfies these criteria. Unfortunately, as has been discussed, the numerical cost of obtaining a set of calibration-constrained parameter fields in this way may be prohibitive where model parameters are many and model run times are long. Hence more efficient methods must be employed in this context. However the cost of greater efficiency is that sampling of the posterior parameter probability distribution is likely to be approximate.

Approximations in sampling the posterior parameter probability distribution must be put into perspective. This matter has already been addressed in chapter 5. Claims that users of Markov chain Monte Carlo methods sometimes make of Bayesian purity can only be supported by demonstrable purity of the prior parameter probability distribution as a true expression of expert knowledge, and by demonstrable purity of the likelihood function as being reflective of "noise" in the calibration dataset. Neither of these conditions are met in most real world modelling contexts. As has been discussed, most model-to-measurement misfit in most environmental modelling contexts is more of a reflection of model imperfections than it is of measurement noise. While some posterior sampling methodologies allow a modeller to employ a "subjective likelihood function" as a means of accommodating this situation (see for example Beven et al, 2008), this approach has not secured the unanimous approval of the Bayesian community (see, for example, Mantovan and Todini, 2006).

Once a model has been calibrated, then hopefully a parameter set has been obtained that approximates the posterior mean parameter set. The associated covariance matrix of posterior uncertainty $C'(\mathbf{k})$ can be approximated using equation (7.3.4) or, equivalently, equation (7.3.15). The "accuracy" of this approximation may be enhanced if the Jacobian matrix used in place of the $\mathbf{Z}$ matrix in these equations is calculated using calibrated parameter values. If necessary, a multiplier greater than unity can be applied to this matrix as partial compensation for the assumptions required in its calculation. Recall that these assumptions are linear model behaviour and multi-normality of the probability distributions of prior parameter uncertainty and measurement noise.

Samples of an approximation to the posterior parameter distribution can then be obtained by sampling a multinormal distribution whose mean is the parameter set obtained through the calibration process, and whose covariance matrix is the linear approximation to the posterior covariance matrix obtained as above. If desired, a sampling methodology such as Latin Hypercube could be employed to achieve maximum coverage of posterior parameter space with only a limited number of samples. (Note however that this strategy will be difficult to implement if parameter numbers are high.)

Unfortunately, if the model is run using any sample of the above approximation to the posterior parameter distribution, it will probably be found that the parameter set which comprises this sample does not satisfy calibration constraints; in other words, the calibration objective function calculated on the basis of model outputs computed using this parameter set is too high. This can be rectified by adjusting these parameters using inversion methodologies discussed in previous chapters in order to reduce the objective function to a suitably low level. The numerical burden of parameter adjustment should not be too great as the parameter set constitutes a sample of a linear approximation to the posterior parameter distribution. Furthermore, the first iteration of the nonlinear parameter adjustment process can employ the Jacobian matrix that has already been used to compute the linear approximation to the posterior covariance matrix. In many modelling contexts this may be the only iteration that is required for the adjusted parameters to meet calibration constraints; if so, this makes the parameter adjustment process numerically very cheap indeed. This sampling and re-calibration process can then be repeated many times to obtain a suite of parameter fields which all satisfy calibration constraints, at the same time as they are all realistic from an expert knowledge point of view. The latter is guaranteed by the prominent place that C(**k**) takes in equations (7.3.4) and (7.3.15).

Theoretically, as well as generating random parameter sets based on a linear approximation to the posterior covariance matrix, samples of measurement noise based on C(**ε**) should also be generated. These should be added to the measurement dataset - a different sample for each random parameter sample. Alternatively, a series of new "measurement datasets" could be generated by adding measurement noise to the model-generated counterpart of the measurement dataset that is calculated by the calibrated model. However while these strategies can accommodate the presence of random noise in the calibration dataset, and account for its presence in samples of the posterior parameter distribution, a major problem is that of knowing the probability distribution of the combination of measurement and structural noise that is actually responsible for model-to-measurement misfit.

In generating and constraining random parameter fields in the way just described, a user must decide on an objective function for which the model is deemed to be "calibrated". Theory is presented below on which this decision can be based. In the author's opinion, however, the assumptions on which this theory rests will be violated on every occasion on which it is applied in real world modelling contexts. Measurement noise may not possess a multinormal distribution (as is required by the theory). What is more problematic, however, is that model-to-measurement misfit will probably have a large non-random component that expresses the inability of the model to replicate all nuances of system behaviour. This component of "measurement noise" does not cancel; nor do more measurements that are accompanied by this type of "measurement noise" (which is in fact structural noise) decrease the uncertainties of estimated parameters. (If measurement noise were purely random and independent, the uncertainties of estimable parameters would decrease as roughly the square root of $n$, where $n$ is the number of measurements comprising the calibration dataset.) In fact where "noise" is actually an expression of model structural defects, then beyond a certain number of measurements, parameter uncertainty is not reduced at all with the taking of further measurements. Instead, the inability of the model to fit certain aspects of the measurement dataset is simply made more obvious. In this case a modeller is justified in employing his/her own "subjective likelihood function", and deem the objective function to be low enough for the model to be considered as calibrated when model-to-measurement misfit is visibly "good enough".

### 8.2.2 Null Space Monte Carlo

The null space Monte Carlo (NSMC) methodology is similar to the linear-assisted Monte Carlo methodology outlined in the previous section. However its implementation is much more numerically efficient where parameter numbers are high and where the null space has many dimensions.

The starting point of null space Monte Carlo analysis is equation (6.2.27). It is again assumed that the model has just been calibrated, and that a parameter field $\underline{\mathbf{k}}$ has thereby been obtained that approaches the posterior mean parameter field. It is also assumed that the error in the estimated parameter field is null-space-dominated so that the first term in equation (6.2.27) dominates the second.

As for the linear-assisted Monte Carlo methodology described above, null space Monte Carlo random parameter generation is implemented in two steps. The first step is the generation of random parameter fields that "almost" calibrate the model. The second step is the adjustment of these parameter fields until they do, in fact, calibrate the model. However each of these steps is slightly different from the methodology described in the previous section.

Random parameter fields are first generated using the C(**k**) prior covariance matrix centred on the calibrated parameter field $\underline{\mathbf{k}}$. Let one such parameter field be designated as **k**. The calibrated parameter field $\underline{\mathbf{k}}$ is then subtracted from this field to yield $\mathbf{k} - \underline{\mathbf{k}}$. This parameter difference is then projected onto the null space of **Z** to yield $(\mathbf{k} - \underline{\mathbf{k}})_n$. The latter is thus calculated as

$$(\mathbf{k} - \underline{\mathbf{k}})_n = \mathbf{V}_2\mathbf{V}^t{}_2(\mathbf{k} - \underline{\mathbf{k}}) \qquad (8.2.1)$$

This null-space-projected parameter difference is then added back to $\underline{\mathbf{k}}$. The outcome is $\underline{\mathbf{k}}+(\mathbf{k}-\underline{\mathbf{k}})_n$. If the model were linear, then model outputs computed on the basis of this parameter set would fit the calibration dataset just as well as the calibrated parameter field. This is because differences between it and the calibrated parameter field are strictly in the null space. However because the model is nonlinear, some parameter adjustment is required.

The second difference between the null space Monte Carlo method described in the present section and the linear-assisted Monte Carlo methodology described in the previous section is in the way that parameter adjustment occurs in order to enforce calibration constraints. Conceptually, if the $\underline{\mathbf{k}}+(\mathbf{k}-\underline{\mathbf{k}})_n$ parameter set fails to calibrate the model, it is because its solution space projection is in error. This projection is comprised of individual projections onto the $\mathbf{v}_i$ vectors which comprise the columns of the $\mathbf{V}_1$ matrix which emerges from singular value decomposition of $\mathbf{Q}^{1/2}\mathbf{Z}$. Hence it is only these solution space parameter components that require adjustment. This can be achieved using the "SVD-assist" methodology implemented in PEST and described in section 6.4.4 of the present document. So-called "super parameters" **p** are adjusted until model outputs fit the calibration dataset **h**. There only need to be as many elements of **p** as there are dimensions in the solution space (though there can be more than this if desired). They can be defined through equation (6.2.44) using a Jacobian matrix calculated on the basis of the calibrated parameter set $\underline{\mathbf{k}}$. The same set of super parameters can be reused for all random parameter realizations and hence all incidences of $\underline{\mathbf{k}}+(\mathbf{k}-\underline{\mathbf{k}})_n$. Furthermore, the first iteration of the parameter adjustment process for all parameter realizations can reuse the same set of super parameter sensitivities; these are calculated from the calibrated model Jacobian matrix using (6.2.43). In many circumstances the objective function after this first iteration of parameter adjustment will be low enough for

the model to be deemed to be "calibrated". If a second iteration is required, then sensitivities of model outputs with respect to super parameters can be calculated using finite super parameter differences. However the numerical burden of doing this is light because of the usually small number of super parameters (i.e. elements of **p**) whose values are adjusted compared to the possibly large number of parameters that are actually used by the model (i.e. elements of **k**).

Optionally, a new realization of measurement noise can be added to the calibration dataset **h** before each incidence of random parameter generation, null space projection, and adjustment to satisfy calibration constraints; problems with this strategy are discussed in the previous section.

As for the linear-assisted Monte-Carlo methodology described in the previous section, a modeller must decide on an objective function which is low enough for the model to be considered as "calibrated". Theory will now be presented that addresses this issue. However further theory will be presented in chapter 9 which takes model defects into account. The latter theory suggests that this objective function is best chosen on the basis of visual appeal of model-to-measurement fit.

## 8.3 Objective Function Thresholds

### 8.3.1 Some Theory

Suppose that the *n* elements of the vector **j** belong to a multinormal distribution. Let the mean of this distribution be **0** and let its covariance matrix be C(**j**). If C(**j**) is subjected to singular value decomposition then

$$C(\mathbf{j}) = \mathbf{E}\mathbf{F}\mathbf{E}^t \tag{8.3.1}$$

Define **m** such that

$$\mathbf{m} = \mathbf{F}^{-1/2}\mathbf{E}^t\mathbf{j} \tag{8.3.2}$$

Hence

$$\mathbf{j} = \mathbf{E}\mathbf{F}^{1/2}\mathbf{m} \tag{8.3.3}$$

Obviously

$$C(\mathbf{m}) = \mathbf{I} \tag{8.3.4}$$

It follows that $\mathbf{m}^t\mathbf{m}$ has a chi-squared distribution with *n* degrees of freedom. From (8.3.2)

$$\mathbf{m}^t\mathbf{m} = \mathbf{j}^t\mathbf{E}\mathbf{F}^{-1}\mathbf{E}^t\mathbf{j} = \mathbf{j}^tC^{-1}(\mathbf{j})\mathbf{j} \tag{8.3.5}$$

from which it follows that $\mathbf{j}^tC^{-1}(\mathbf{j})\mathbf{j}$ also has a chi-squared distribution with *n* degrees of freedom.

Let **q** be a vector with *n* elements. Suppose that we wish to inquire whether **q** could have been generated using a multinormal distribution with a mean of **0** and a covariance matrix C(**j**). We could compute $\mathbf{q}^tC^{-1}(\mathbf{j})\mathbf{q}$ and then refer to a chi-squared distribution table to see where this computed value lies with respect to the range of values that a chi-squared distribution with *n* degrees of freedom should possess. Suppose, for example, that *n* is 10. After referring to a chi-squared distribution table we find that $\chi^2_{.975}$ is 3.247 while $\chi^2_{.025}$ is 20.483. This means that there is a 97.5% chance that a chi-squared variate with *n* degrees of freedom is above 3.247 but only a 2.5% chance that it is above 20.483. In other words, there

is a 95% chance that it is between 3.247 and 20.483. Hence if the value that we compute for $\mathbf{q}^t C^{-1}(\mathbf{j})\mathbf{q}$ is outside of this interval then the hypotheses that **q** is multinormal with mean **0** and covariance matrix C(**j**) can be rejected with a 95% level of confidence.

This is actually not a very strong test. This can be demonstrated by example. Suppose that C(**j**) is **I**. Suppose further that all of the elements of our test vector **q** are zero except for one of them, and that this element is 4. $\mathbf{q}^t C^{-1}(\mathbf{j})\mathbf{q}$ is therefore 16. Based on the above chi-squared test, we cannot reject the hypothesis at the 95% confidence level that **q** belongs to a normal distribution with a mean of **0** and a covariance matrix of **I**; that is, we cannot reject the hypothesis that $\mathbf{q} \sim N(\mathbf{0},\mathbf{I})$. However reference to a normal distribution table quickly informs us that the chances of an individual standard normal variate being 4 or above are about 0.003%.

A stronger test is required.

Let us form the scalar product between a known vector **m** and a random vector **q** which has a mean of **0** and for which we wish to test whether it has a covariance matrix of C(**j**). Let us refer to this scalar product as *s*. Then

$$s = \mathbf{m}^t\mathbf{q} \tag{8.3.6}$$

If C(**q**) is the same as C(**j**) then, applying the usual formula for propagation of covariance, we obtain

$$\sigma^2_s = \mathbf{m}^t C(\mathbf{j})\mathbf{m} \tag{8.3.7}$$

Because we know **m** and because we know **q** we can compute the scalar product (8.3.6) of **m** with the variable **q** whose statistical adherence to C(**j**) we wish to test. The outcome of this calculation can be evaluated using $\sigma^2_s$ of (8.3.7). If *s* lies outside its expected confidence region then C(**j**) must be rejected as representing C(**q**) of which **q** is supposedly a realization.

This test can be made more convenient if the vector **m** is normalized through division by $[\mathbf{m}^t C(\mathbf{j})\mathbf{m}]^{1/2}$. The scalar *s* that we use as the basis for our test then becomes

$$s = \frac{\mathbf{m}^t\mathbf{q}}{\left(\mathbf{m}^t C(\mathbf{j})\mathbf{m}\right)^{1/2}} \tag{8.3.8}$$

for which the variance, if C(**q**) is the same as C(**j**), is

$$\sigma_s^2 = \frac{\mathbf{m}^t}{\left(\mathbf{m}^t C(\mathbf{j})\mathbf{m}\right)^{1/2}} C(\mathbf{j}) \frac{\mathbf{m}}{\left(\mathbf{m}^t C(\mathbf{j})\mathbf{m}\right)^{1/2}} = \frac{\mathbf{m}^t C(\mathbf{j})\mathbf{m}}{\mathbf{m}^t C(\mathbf{j})\mathbf{m}} = 1 \tag{8.3.9}$$

Hence if **q** is multinormally distributed with a covariance matrix of C(**j**), then the scalar $\frac{\mathbf{m}^t\mathbf{q}}{\left(\mathbf{m}^t C(\mathbf{j})\mathbf{m}\right)^{1/2}}$ has a normal distribution with a mean of zero and standard deviation of 1. This forms the basis for a stricter test of **q**.

The basis for this stricter test is easily appreciated when contours of a two-dimensional $N(\mathbf{0},\mathbf{I})$ distribution are considered. These are circles. The projection of the distribution along any line that passes through its centre in any direction (including the axes which pertain to individual variables) is a normal distribution with unit variance.

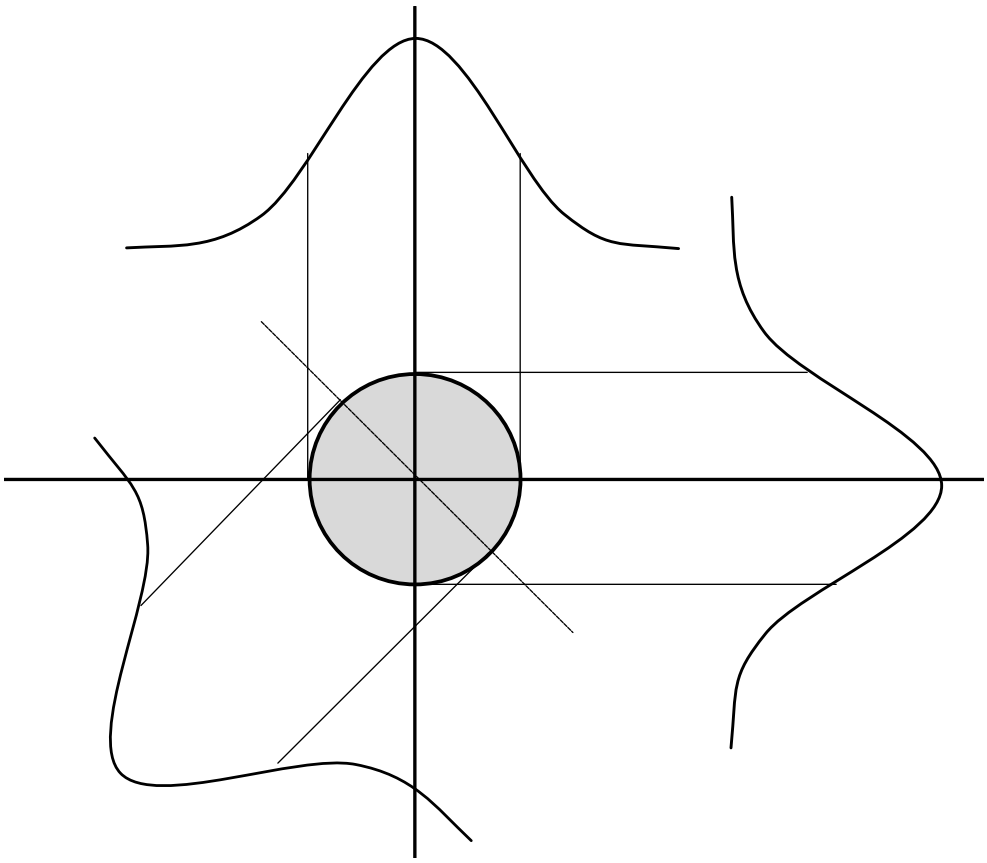

**Figure 8.1. A contour corresponding to one individual standard deviation of a two-dimensional *N*(0,1) distribution. This standard deviation can apply to the two individual variates, or to a one-dimensional variate formed through projection of the two-dimensional normal variate onto any line through its centre.**

The non-random vector **m** that is best used to test stochastic credibility of a particular random vector **q** depends on the context. If all elements of **m** are 0 except for one element, then the test can be applied to an individual element of a random vector, for example to an individual parameter; this is what was done for the **q** vector in the above example when demonstrating the looseness of the chi-squared test. Alternatively, **m** may be derived from a predictive sensitivity vector; this will be done below. Direct tests of predictive credibility can thereby be implemented.

### 8.3.2 Repercussions for Objective Functions

We will assume that measurement noise has a multinormal distribution. To begin with, we will also assume that C(**ε**) is known. Hence, if we are solving a well-posed inverse problem, the reference variance is not estimated as part of the inversion process using equation (5.2.18). If the inverse problem includes prior-knowledge-based estimates of parameter values, then we will also assume that C(**k**) is known and that the prior distribution of parameters is multinormal. We will further assume that the weight matrix **Q** is chosen as $C^{-1}(\boldsymbol{\varepsilon})$ for the case with no prior information, or expanded appropriately to include $C^{-1}(\mathbf{k})$ in cases where prior information features in the inversion process. However to simplify the following equations we will not explicitly represent the presence of prior information in the inversion process.

The objective function Φ is formulated from residuals **r** as

$$\Phi = \mathbf{r}^t\mathbf{Q}\mathbf{r} = \mathbf{r}^t C^{-1}(\boldsymbol{\varepsilon})\mathbf{r} \qquad (8.3.10)$$

Because residuals supposedly represent a realization of **ε**, then Φ of equation (8.3.10) should have a chi-squared distribution. Furthermore the two statistics discussed in the preceding section can be used to establish an objective function threshold above which it is very unlikely that discrepancies between model outputs and field measurements can be explained by measurement noise and/or (if prior information figures in the objective function) innate parameter variability.

Based on the first of the two tests presented in the previous section, let us designate as $\Phi_0$ the upper limit of the range of values which Φ is likely to take. Let the confidence level associated with this upper limit be (1-α). Then

$$\Phi_0 = \chi^2_\alpha \qquad (8.3.11)$$

where $\chi^2_\alpha$ denotes the value of a variate which belongs to a chi-squared distribution with *n* degrees of freedom (*n* is the number of elements in the measurement dataset) for which the integral over greater values is α.

A tighter confidence level for Φ, based on the second of the two tests presented in the previous section, is

$$\Phi_0 = N^2_{\alpha/2} \qquad (8.3.12a)$$

That is

$$\Phi_0^{1/2} = N_{\alpha/2} \qquad (8.3.12b)$$

where $N_{\alpha/2}$ denotes the value of a standard normal variate for which the integral of the normal distribution for values greater than this is α/2. The use of α/2 rather than α in these last equations arises from the fact that the objective function can only be positive. Residuals, however, can be positive or negative; for a two-dimensional case, a given set of residuals **r** can be in any quadrant of the circle depicted in figure 8.1.

In most calibration contexts C(**ε**) is not known. However it is often assumed to be known to within a factor. As was described in chapter 5 of this text, in over-determined parameter estimation contexts, this factor is evaluated from the minimized objective function; see equation (5.2.18). Because the statistical properties of measurement noise are not completely known in advance, the above equations must be modified. Suppose that the objective function associated with the (possibly prior-information-enhanced) inversion problem has been minimized, and that this minimum is unique; let it be designated as $\Phi_{min}$. The *F* distribution must be used in place of the chi-squared distribution, and the student *t* distribution must be used in place of the normal distribution in assessing objective function credibility using the two statistical tests discussed above. Equations (8.3.11) and (8.3.12) become

$$\Phi_0 = \Phi_{\min}\left[\frac{m}{n-m}F_\alpha(m, n-m)+1\right] \qquad (8.3.13)$$

and

$$\Phi_0 = \Phi_{\min}\left[\frac{t^2_{\alpha/2}(n-m)}{(n-m)}+1\right] \qquad (8.3.14)$$

where, as usual, *n* is the number of observations (plus prior information equations) comprising the calibration dataset and *m* is the number of parameters that are featured in the inverse problem. The parameter confidence interval that is implicitly defined by the first of these equations is often referred to as the "simultaneous" or "Scheffé" confidence interval, while that defined by the second is referred to as the "individual" confidence interval. Christensen and Cooley (1999) and Cooley (2004) point out that a correction factor should be applied to the right side of equation (8.3.14) to accommodate nonlinear model behaviour. However they also point out that this factor is mostly close to 1.0. See the above authors and Vechhia and Cooley (1987) for more details.

## 8.4 Constrained Predictive Maximization/Minimization

### 8.4.1 Concepts

Figure 8.2 schematizes two-dimensional parameter space. Objective function contours are depicted as full lines. The minimum of the objective function is marked by a cross. Problem well-posedness is assumed as this minimum is unique; the calibration dataset may have been supplemented with appropriately-weighted prior estimates of parameter values to achieve this. As above, it is assumed that the weight matrix is proportional to $\mathbf{C}^{-1}(\boldsymbol{\varepsilon})$. If prior information is included in the objective function, then the subset of the weight matrix associated with this prior information is assumed to be proportional to $\mathbf{C}^{-1}(\mathbf{k})$; the same constant of proportionality is applied to $\mathbf{C}^{-1}(\mathbf{k})$ as that which is applied to $\mathbf{C}^{-1}(\boldsymbol{\varepsilon})$. In figure 8.2 the innermost contour is associated with an objective function value of $\Phi_0$. This is assumed to indicate a certain level of objective function confidence as calculated using equation (8.3.13) or equation (8.3.14).

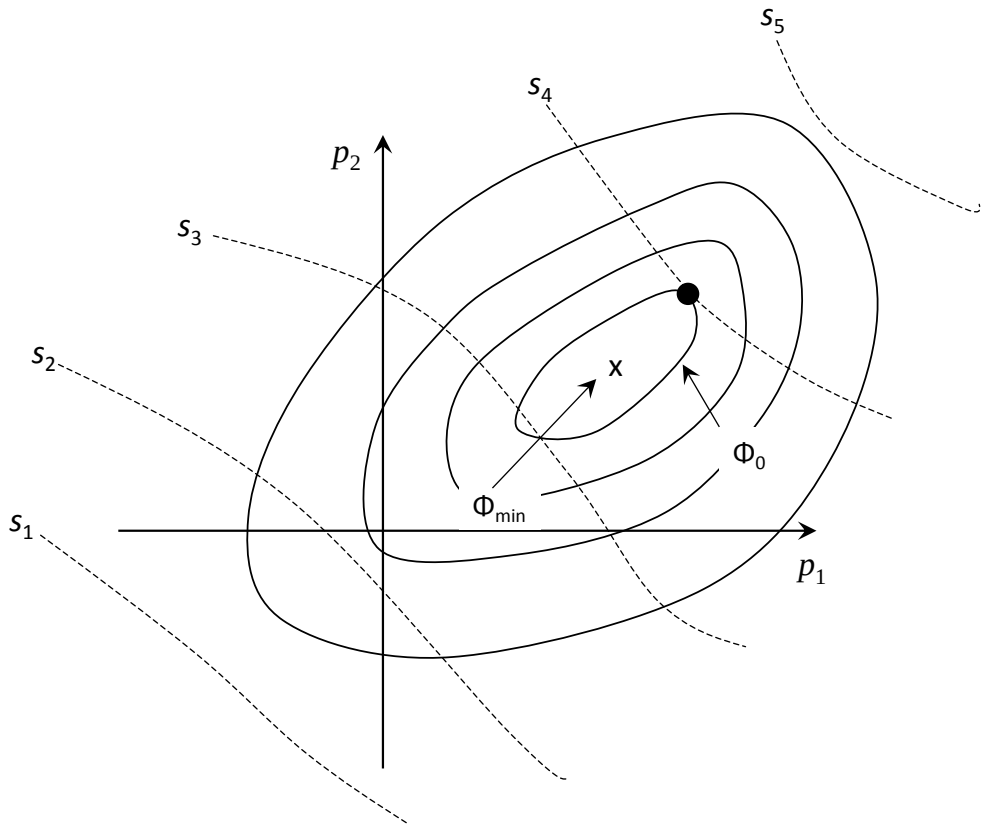


**Figure 8.2. The dashed contours depict the dependence of a prediction on a set of parameters. The full contours depict the calibration objective function. The contour labelled $\Phi_0$ is that at which model-to-measurement misfit is deemed to be too great for the model to be considered as calibrated. The dark spot marks the parameter set for which the prediction is maximized subject to the model remaining calibrated.**

Figure 8.2 also shows contoured values of a prediction *s* of interest. Let it be assumed that the value of the prediction increases with increasing contour index, so that $s_2$ is greater than $s_1$, $s_3$ is greater than $s_2$, etc.

Suppose that we wish to establish the 1-α posterior confidence interval of the prediction *s*. This can be done by solving a constrained maximization problem followed by a constrained minimization problem. In the first of these, the prediction is maximized subject to the constraint that the objective function rises no higher than $\Phi_0$ where $\Phi_0$ corresponds to this level of objective function confidence. In the second of these, the prediction is minimized subject to this same constraint. The difference between these two prediction values defines the 1-α confidence interval of the prediction.

In some contexts a modeller may wish to calculate a wider interval than this, referred to as the "prediction interval". In contrast to the predictive confidence interval, the predictive prediction interval takes account of noise that may be associated with the prediction – the same kind of noise as that which contaminates members of the calibration dataset. The prediction interval therefore pertains to the range of values that the prediction may take if it were in fact an observation. If "noise" associated with a prediction actually includes model-generated structural noise, then the inclusion of such noise in predictive uncertainty assessment includes the effects of model imperfections on the prediction. The stochastic

properties of this "predictive noise" must of course be known if the prediction interval is to be calculated. If a prediction is similar in character to members of the calibration dataset, this has been inferred through the calibration process through equation (5.2.18).

If the prediction interval is sought, the objective function $\Phi_0$ that is used to enforce constraints on predictive variability must be expanded to accommodate the predictive noise term. This is accomplished by adding the term $(w_e e)^2$ to the normal objective function given by equation (8.3.10) so that

$$\Phi = \mathbf{r}^t\mathbf{Q}\mathbf{r} + (w_e e)^2 = (\mathbf{h} - \mathbf{X}\mathbf{p})^t\mathbf{Q}(\mathbf{h} - \mathbf{X}\mathbf{p}) + (w_e e)^2 \qquad (8.4.1)$$

In the above equation $e$ is the (unknown) value of noise associated with the prediction and $w_e$ is its weight. This weight must be consistent with weights defined in the **Q** matrix.

With expansion of the definition of $\Phi$ in this manner, equations (8.3.13) and (8.3.14) for the limiting objective function associated with the 1-α prediction interval become

$$\Phi_0 = \Phi_{\min}\left[\frac{m+1}{n-m}F_\alpha(m+1, n-m)+1\right] \qquad (8.4.2)$$

and

$$\Phi_0 = \Phi_{\min}\left[\frac{t^2_{\alpha/2}(n-m)}{(n-m)}+1\right] \qquad (8.4.3)$$

Equation (8.4.3) is identical to equation (8.3.14) despite the fact that the predictive error term $(ew_e)^2$ is included in the objective function $\Phi$. As for equation (8.3.14), Christensen and Cooley (1999) and Cooley (2004) point out that a correction factor (which is not too different from unity) should be applied to the right side of equation (8.4.3) to accommodate nonlinear model behaviour.

### 8.4.2 Implementation

As usual, let the scalar $s$ denote a model prediction of interest, and let the vector **y** denote the sensitivity of this prediction to model parameters **p**. (We use **p** rather than **k** in this section to remind the reader that the focus of the present discussion is on well-posed inverse problems.) Hence for a linear model

$$s = \mathbf{y}^t\mathbf{p} \qquad (8.4.4)$$

For a model whose action under calibration conditions is given by the matrix **X** (see equation 5.2.1), Vecchia and Cooley (1987) show that the constrained predictive maximization or minimization problem depicted in figure 8.2 can be solved for **p** using the following formula

$$\mathbf{p} = \left(\mathbf{X}^t\mathbf{Q}\mathbf{X}\right)^{-1}\left\{\mathbf{X}^t\mathbf{Q}\mathbf{h} - \frac{\mathbf{y}}{2\lambda}\right\} \qquad (8.4.5)$$

where

$$\left(\frac{1}{2\lambda}\right)^2 = \pm\frac{\Phi_0 - \mathbf{h}^t\mathbf{Q}\mathbf{h} + \mathbf{h}^t\mathbf{Q}\mathbf{X}\left(\mathbf{X}^t\mathbf{Q}\mathbf{X}\right)^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{h}}{\mathbf{y}^t\left(\mathbf{X}^t\mathbf{Q}\mathbf{X}\right)^{-1}\mathbf{y}} \qquad (8.4.6)$$

As usual, the **h** vector is comprised of observations (possibly including prior information observations) employed in the calibration process. The positive or negative square root of

$\left(\frac{1}{2\lambda}\right)^2$ is chosen according to whether prediction maximization or prediction minimization is being performed.

Where $\Phi_0$ includes the effect of predictive error (and therefore includes the term $(w_e e)^2$ where $w_e$ is the weight assigned to predictive noise and $e$ is the predictive error itself) equation (8.4.5) is still employed to calculate **p**. However (8.4.6) becomes

$$\left(\frac{1}{2\lambda}\right)^2 = \pm\frac{\Phi_0 - \mathbf{h}^t\mathbf{Q}\mathbf{h} + \mathbf{h}^t\mathbf{Q}\mathbf{X}\left(\mathbf{X}^t\mathbf{Q}\mathbf{X}\right)^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{h}}{\mathbf{y}^t\left(\mathbf{X}^t\mathbf{Q}\mathbf{X}\right)^{-1}\mathbf{y} + w_e^{-2}} \qquad (8.4.7)$$

while the actual predictive error $e$ is calculated as

$$e = -w_e^{-2}/2\lambda \qquad (8.4.8)$$

For nonlinear models, equations (8.4.5) to (8.4.7) are solved for **p** using an iterative procedure in which **X**, **y** and **h** (which is actually replaced by the residuals vector **r**) are updated during every optimization iteration in accordance with current values of **p**. Theoretically, this iterative procedure can commence from any desired starting values of the elements of **p**. Practically, a choice of **p** equal to $\mathbf{p}_{min}$ which minimizes the objective function $\Phi$ (i.e. for which the objective function is equal to $\Phi_{min}$) can reduce the number of model runs required for solution of the maximization/minimization problem.

Note that the above procedure can be employed to analyse parameter as well as predictive uncertainty. Where the uncertainty of a parameter is the subject of inquiry, the predictive sensitivity vector **y** is replaced by a vector whose elements are all zero except for that which pertains to the parameter in question; this element has a value of one.

### 8.4.3 Some Practicalities

*8.4.3.1 General*

While the constrained, nonlinear predictive maximization/minimization problem through which the posterior confidence or predictive interval of a prediction can be obtained is theoretically solvable using the equations provided above, use of these equations in a real world modelling context is often plagued by difficulties. Some of these difficulties are now briefly discussed.

*8.4.3.2 Numerical Considerations*

Practical experience in solving the constrained maximization/minimization problem discussed above indicates that its numerical solution may require many model runs. As for the nonlinear parameter estimation problem which must precede it (in order to evaluate $\Phi_{min}$), an iterative procedure is required. Each iteration of this procedure is comprised of two steps. The first step involves calculation of the Jacobian matrix that replaces **X** in the above equations and the predictive sensitivities that replace **y**. If these sensitivities cannot be computed by the model itself, then they must be computed using finite parameter differences. The second step requires calculation of parameter upgrade vectors using different trial values of the Marquardt lambda. As in equation (5.4.2) the Marquardt lambda term is added to the $\mathbf{X}^t\mathbf{Q}\mathbf{X}$ matrix of equation (8.4.5). Conceptually the Marquardt lambda should approach zero as the iterative solution process nears completion; furthermore it should start at a low value if

this process commences with **p** equal to $\mathbf{p}_{min}$. The iterative solution process is terminated when parameters change no further between iterations and $\Phi$ is suitably close to the user-specified $\Phi_0$.

In practice it is found that many iterations can be required to solve the nonlinear constrained maximization/minimization problem, even where the nonlinear solution procedure commences with **p** equal to $\mathbf{p}_{min}$. Experience also shows that its solution may require a line search along directions of parameter upgrade calculated using different values of the Marquardt lambda. In contrast to filling the Jacobian matrix using model runs based on finite parameter differences, a line search procedure is not inherently parallelizable. This further adds to the numerical inefficiency of the solution process.

Numerical problems are exacerbated where model outputs are contaminated by model numerical noise. This can lead to degradation of the quality of the Jacobian matrix, and of the predictive sensitivity vector **y**. The $\Phi$ and *s* contours of figure 8.2 can then become serrated. If the two sets of contours intersect at shallow angles, the location of the black dot depicted in this figure may then become difficult to find; in fact contour serrations may introduce multiple black dots.

*8.4.3.3 Predictive Model Runs*

In many practical modelling contexts, the model run time required for the making of a prediction can far exceed that required for calculation of outputs corresponding to members of the calibration dataset **h**. This is because the time period over which measurements comprising a calibration dataset were taken is often relatively small in comparison to that for which a prediction must be computed.

As already stated, each iteration of the nonlinear predictive maximization/minimization procedure described above requires two separate steps. The first of these steps is calculation of the Jacobian matrix which replaces **X**, and of predictive sensitivities that replace **y**. The "model" as seen by software such as PEST which implements this procedure may thus be comprised of a batch or script file in which two separate model runs are undertaken – one in which the model is supplied with stresses that prevailed during the calibration period and the other in which it is supplied with stresses that will prevail under predictive conditions. If the prediction of interest is far into the future, considerable computing resources may be required for the second of these runs. It follows that, based on model run times alone, the predictive maximization/minimization procedure may be computer-intensive. (Nevertheless, there are some modelling contexts where this is not the case. If the "prediction" of interest is the value of a parameter, or the value of a model output that is different from that used in the calibration process but that pertains to the calibration period, then the calibration and predictive model runs become the same.)

If a modeller is interested in defining the two-sided predictive confidence or prediction interval, the problem of long model run times is exacerbated, for two complementary constrained optimization problems must then be solved – one in which the prediction is maximized and one in which it is minimized. If, in addition to this, predictive intervals corresponding to a number of different confidence levels are required, the constrained optimization problem must be solved for a number of different values of $\Phi_0$. If confidence intervals for more than one prediction are needed then the entire process must be repeated for the other predictions.

*8.4.3.4 Limiting Objective Function*

Equations (8.3.13), (8.3.14), (8.4.2) and (8.4.3) can be used to define the objective function constraint $\Phi_0$. Where the number of observations comprising the calibration dataset **h** is large, it will often be found that $\Phi_0$ is very close to $\Phi_{min}$, this leaving very little "wriggle room" in parameters **p** in defining a predictive confidence or prediction interval. If employed, the predictive noise term then becomes the dominant contributor to predictive variability. Where a prediction is similar in character to members of the calibration dataset **h**, assistance in estimating the magnitude of this term will have been provided by the calibration process. Where it is different in character from members of the calibration dataset, the modeller must estimate it him/herself.

The reduction in constrained parameter variability that follows from increasing the size of the calibration dataset **h** follows from the fact that "noise cancels". Conceptually, regardless of the magnitude of random error that accompanies each measurement of system state, if enough of these measurements have been made, a good estimate of parameters can be obtained (if the inverse problem is well-posed). In contexts such as that of surface water model calibration where a daily or hourly stream flow time series may comprise the calibration dataset, use of equations (8.3.13), (8.3.14), (8.4.2) and (8.4.3) may suggest that posterior parameter uncertainty is very small indeed, so that predictive confidence is therefore very high. Intuition suggests, however that this cannot be the case.

As has been stated often in this text, in practical environmental modelling contexts most model-to-measurement misfit is an outcome of so-called structural noise rather than measurement noise. As will be discussed in the following chapter, structural noise does not cancel. Hence increasing the number of measurements comprising a calibration dataset does not result in better estimates of parameters if use of those parameters leads to computation of model outcomes which are persistently wrong. The problem is exacerbated by the probable non-invertibility of the covariance matrix of structural noise (see the next chapter); this makes calculation of a **Q** matrix for use in the predictive maximization/minimization process difficult. Association of a value of $\Phi_0$ with a certain level of parameter and predictive confidence becomes virtually impossible.

Selection of a suitable value for $\Phi_0$ is therefore generally a subjective matter. In practice, a modeller may select a value that corresponds to visible deterioration of model-to-measurement misfit from that attained through minimization of $\Phi$ – enough deterioration for the modeller to deem that the model is "no longer calibrated". While mathematical purity is thereby foregone in exploring parameter and predictive confidence, solution of the predictive maximization/minimization problem posed with a somewhat arbitrary value assigned to $\Phi_0$ may still provide an effective means of establishing the amount of parameter and predictive variability that is consistent with expert knowledge on the one hand and respect for the information content of the calibration dataset on the other hand.

The presence of structural noise can introduce further problems to the predictive uncertainty analysis process. Equations presented above assume that predictive noise is independent of noise associated with the calibration dataset. In fact it is the same model imperfections that degrade calibration fit that can also impair the integrity of a model's predictions. Statistical correlation of predictive noise with measurement "noise" follows immediately. Thus, for example, a model's error in predicting future peak river flows will be correlated with its inability to fit flow peaks within the calibration dataset.

### 8.4.4 Handling Large Numbers of Parameters

*8.4.4.1 Some Problems*

Where parameter numbers are high, numerical difficulties described above that are encountered in undertaking direct predictive maximization/minimization tend to be exacerbated. The inclusion of a large number of parameters in the predictive maximization/minimization process contributes to the number of calibration and predictive model runs that are required for calculation of the **X** matrix and **y** vector. Experience also demonstrates that numerical solution to the maximization/minimization problem is impaired as the dimensionality of parameter space increases.

Where parameter numbers are high, the likelihood of inverse problem ill-posedness increases. Uniqueness of solution of the inverse problem which precedes solution of the constrained predictive maximization/minimization problem becomes dependent on the inclusion of appropriately weighted linear or nonlinear prior information in the calibration dataset. Problems associated with the relative weighting of prior information and measurements of system state have been discussed in preceding sections. These can be overcome through use of Tikhonov regularization in which the inversion process itself adjusts weights applied to prior information. The modeller may then be tempted to employ the prior information weight multiplier calculated through a preceding Tikhonov-constrained inversion exercise in an ensuing constrained predictive maximization/minimization process.

This is not an advisable procedure. Weights assigned to prior information during a Tikhonov-constrained inversion process are such as to suppress any parameter variability that arises through the calibration process except for that which must be present if the user-specified target measurement objective function is to be achieved. Where a prediction is of a different type from that comprising the calibration dataset, this prediction may be sensitive to parameter combinations that comprise the calibration null space. Pertinent parameter heterogeneity must be allowed to arise in exploring the uncertainty of this prediction, with the limits on this heterogeneity being set by expert knowledge – not by the demands of a previous calibration process. In practice these limits must be expressed by pertinent weights (or preferably a covariance matrix) associated with linear or nonlinear prior information that, along with the measurement component of the calibration dataset, comprises the constraints on parameters that are imposed during predictive maximization/minimization. As these prior information weights will almost certainly be different from those that emerged as a by-product of solution of a Tikhonov-constrained inverse problem, the objective function minimum $\Phi_{min}$ appearing in equations (8.3.13), (8.3.14), (8.4.2) and (8.4.3) cannot be inherited from the previous Tikhonov-regularized inversion process.

Other problems can arise when undertaking predictive maximization/minimization in the highly-parameterized context. Suppose that a modeller defines an appropriate C(**k**) matrix that encapsulates parameter variability with the intention of applying this C(**k**) matrix to prior information that is featured in the constrained predictive maximization/minimization process. The purpose of a prior information constraint such as this is to subdue the occurrence of predictions that require unrealistic parameter variability. However it may be found that the parameter field that emerged from the previous calibration exercise would be considered unlikely when judged in terms of this same C(**k**). There may be a number of reasons why heterogeneity in excess of that which is compatible with C(**k**) was introduced to the calibrated parameter field. Perhaps the C(**k**) matrix (or other descriptor of parameter

variability applied to linear or nonlinear prior information) provides inappropriate characterization of geological variability. (If so, this is hardly surprising in the groundwater or reservoir modelling contexts, given the simple nature of C(**k**) and the complex nature of real world geological heterogeneity.) Perhaps some parameters needed to adopt roles which compensate for model imperfections; this may have required that they be awarded out-of-range values in order to enable reduction of model-to-measurement misfit to a user-specified level. For reasons described in the next chapter, a modeller may or may not be uncomfortable with this. On the other hand, perhaps too good a fit was sought with field data during the previous calibration exercise; the calibration point may thus be situated to the right of the error variance minimum depicted in figure 6.4. The previous calibration process may therefore need to be repeated.

Suppose, however, that a modeller considers the calibrated parameter field to be acceptable, despite being somewhat unlikely when considered in terms of an adopted C(**k**) matrix. Suppose further that he/she would nevertheless like to enforce this same C(**k**) constraint on introduction of further heterogeneity to the calibrated parameter field during the constrained predictive maximization/minimization process to follow. This can be achieved through working with parameter differences rather than with the actual values of parameters. Expert knowledge constraints embodied in the C(**k**) matrix can then be applied to $\mathbf{k}-\underline{\mathbf{k}}$, where $\underline{\mathbf{k}}$ denotes the calibrated parameter field and **k** denotes parameter fields that emerge during the predictive maximization/minimization process. This will be further discussed shortly.

In summary, problems that must be overcome in undertaking predictive maximization/minimization following Tikhonov-constrained calibration are thus potentially two-fold. First, equations (8.3.13), (8.3.14), (8.4.2) and (8.4.3) cannot be used to set the objective function limit $\Phi_0$, as the objective function which must be employed in predictive maximization/minimization is not necessarily the same as that which was minimized through the preceding calibration process. This arises from the modeller's need to set C(**k**) him/herself in the predictive maximization/minimization process rather than have it altered, as was done through the regularized inversion process. Second, it is far from impossible that the parameter field with which the model was endowed during the previous calibration process may be judged as unlikely, or verging on unlikely, through use of this simple characterization of parameter variability, despite the fact that the existence of such variability seems to be supported by the measurement dataset. Direct application of what a modeller may still consider to be an appropriate C(**k**) matrix to the parameter field that emerges from predictive maximization/minimization may thus artificially limit assessments of predictive uncertainty, as constraints on new parameter variability are suppressed by the low likelihood calculated for parameter variability that already exists in the calibrated parameter field.

*8.4.4.2 Overcoming these Problems*

The above problems can be largely overcome by formulating the predictive maximization/minimization problem in terms of parameter and model output differences. Let $\underline{\mathbf{k}}$ be the set of parameters that was obtained through the previous parameter estimation process. Let $\underline{\mathbf{o}}$ be the corresponding set of model outputs. As usual, let **Z** be the linearized model operator (we use **Z** rather than **X** at this point in recognition of the highly parameterized context in which we are now operating). From (6.1.18) the relationship between estimated parameters $\underline{\mathbf{k}}$ achieved through the previous inversion process and real world parameters **k** is given by

$$\underline{\mathbf{k}} - \mathbf{k} = -(\mathbf{I} - \mathbf{R})\mathbf{k} + \mathbf{G}\boldsymbol{\varepsilon} \qquad (8.4.9)$$

As was discussed in chapter 6, **R** and **G** depend on the regularization methodology that was employed to solve the previous inverse problem. Where solution of that problem was achieved through singular value decomposition, (**I** - **R**) is an orthogonal projection operation onto the calibration null space. That is

$$(\mathbf{I} - \mathbf{R}) = \mathbf{V}_2\mathbf{V}^t_2 \qquad (8.4.10)$$

$\mathbf{V}_2$ emerges from singular value decomposition undertaken on $\mathbf{Q}^{1/2}\mathbf{Z}$ where **Z** represents the action of the model. As was discussed in section 6.3.4, where inversion is based on Tikhonov regularization that constrains parameters to deviate as little as possible from their prior means, (**I** – **R**) approaches this.

The purpose of calibration-constrained predictive maximization/minimization can be considered to be that of introducing variability to **k** - $\underline{\mathbf{k}}$ in search of a high or low prediction, subject to two constraints. These are that parameter integrity is maintained, and that model-to-measurement fit that was achieved through the previous calibration process is maintained. Credibility of **k** – $\underline{\mathbf{k}}$ is maintained through respect for its covariance matrix. This is readily calculated from (8.4.9) as

$$C(\mathbf{k} - \underline{\mathbf{k}}) = (\mathbf{I} - \mathbf{R})C(\mathbf{k})(\mathbf{I} - \mathbf{R})^t + \mathbf{G}C(\boldsymbol{\varepsilon})\mathbf{G}^t \qquad (8.4.11)$$

which, for inversion based on singular value decomposition, becomes

$$C(\mathbf{k} - \underline{\mathbf{k}}) = \mathbf{V}_2\mathbf{V}^t_2C(\mathbf{k})\,\mathbf{V}_2\mathbf{V}^t_2 + \mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1C(\boldsymbol{\varepsilon})\mathbf{U}_1\mathbf{S}^{-1}{}_1\mathbf{V}^t{}_1 \qquad (8.4.12)$$

Variability of the first term on the right of equations (8.4.11) and (8.4.12) is subject only to the constraints imposed by expert knowledge. Meanwhile variability of the second term on the right of these equations is subject only to the constraints imposed by the necessity for model outputs to fit the calibration dataset. This fit is expressed by the measurement component of the objective function. If the latter is employed to constrain model-to-measurement misfit during prediction maximization/minimization, then only the first term on the right of equations (8.4.11) and (8.4.12) need be employed to exert expert knowledge constraints on parameter variability.

In practice, it is generally easier to use equation (8.4.12) than (8.4.11), even if the previous inversion exercise was implemented under Tikhonov constraints, as the first term of (8.4.12) is relatively easy to compute. Suppose that the effective dimensionality of the solution space as discovered during the previous calibration exercise is *w*. Regardless of the regularization method that was employed in solving the previous inverse problem, *w* can be readily estimated using the methodology provided in section 6.2.5.3; calculations required to implement this methodology can employ a Jacobian matrix based on optimized parameters $\underline{\mathbf{k}}$.

Let **o** describe model outputs corresponding to a general **k**. The difference between **o** and model outputs $\underline{\mathbf{o}}$ calculated from the calibrated parameter set $\underline{\mathbf{k}}$ is **o** – $\underline{\mathbf{o}}$. Obviously, when **k** is equal to $\underline{\mathbf{k}}$, then **o** is equal to $\underline{\mathbf{o}}$.

A new objective function is now defined for use in the post-calibration constrained predictive maximization/minimization process. It is

$$\Phi_p = (\mathbf{o} - \underline{\mathbf{o}})^t\mathbf{C}^{-1}(\boldsymbol{\tau})(\mathbf{o} - \underline{\mathbf{o}}) + (\mathbf{k} - \underline{\mathbf{k}})^tC_n^{-1}(\mathbf{k} - \underline{\mathbf{k}}) \qquad (8.4.13)$$

where $\mathbf{C}^{-1}(\boldsymbol{\tau})$ is discussed below, and $C_n(\mathbf{k} - \underline{\mathbf{k}})$ is the first term on the right of (8.4.12). ("n" stands for "null space".) Obviously, for **k** equal to $\underline{\mathbf{k}}$, (8.4.13) is zero. The first term of

(8.4.13) exerts constraints on model-to-measurement misfit so that it does not rise too much higher than that attained during the previous inversion exercise. The second term constrains parameters to adopt values that are realistic from an expert knowledge point of view.

Let us suppose that a weight matrix $\mathbf{Q}_h$ was applied to the measurement dataset **h** during the previous inversion process. As has been much discussed, "noise" associated with this dataset is comprised of both measurement and structural noise. Let us denote this total noise as $\boldsymbol{\tau}$. Ideally (though never practically) $\mathbf{Q}_h$ is related to $\boldsymbol{\tau}$ through the equation

$$\mathbf{Q}_h = \sigma^2_r C^{-1}(\boldsymbol{\tau}) \qquad (8.4.14)$$

In practice, $\mathbf{Q}_h$ will probably be supplied as a diagonal matrix, this implying (wrongly) that $C(\boldsymbol{\tau})$ is also diagonal. However the presence of structural noise may have been partially accommodated through formulation of a multi-component objective function in ways described in the following chapter. In either case the implied $C(\boldsymbol{\tau})$ can be calculated from the user supplied $\mathbf{Q}_h$ using (8.4.14) once a value has been estimated for $\sigma^2_r$.

The previous inversion process will not have actually minimized the measurement component of the objective function; instead a target measurement objective function $\Phi^t_m$ will have been attained. Hence (5.2.18) cannot be used to calculate an estimate $\underline{\sigma}^2_r$ of $\sigma^2_r$. Nevertheless the level of model-to-measurement misfit that is represented by $\Phi^t_m$ should be commensurate with the level of measurement/structural noise that is associated with the calibration dataset **h**. Hence $\underline{\sigma}^2_r$ can be approximated as

$$\underline{\sigma}^2_r = \frac{\Phi^t_m}{n} \qquad (8.4.15)$$

where *n* is the number of measurements comprising **h**. (Note that this does not include prior information employed in Tikhonov regularization.) Once an estimate for $\underline{\sigma}^2_r$ has been obtained in this way it can be substituted into (8.4.14) to obtain an estimate of $C^{-1}(\boldsymbol{\tau})$ for use in equation (8.4.13).

With this new formulation of the objective function, the predictive maximization/minimization process can then be implemented using equations (8.4.5) to (8.4.7) with **k** awarded a starting value of $\underline{\mathbf{k}}$. Meanwhile $\Phi_0$ can be set using equation (8.3.11) or (8.3.12) as deemed appropriate. At the beginning of the predictive maximization/minimization process both the measurement and prior information components of the objective function (i.e. the first and second terms respectively of equation 8.4.13) are zero. They are summed to compute the total objective function which $\Phi_0$ then constrains. See Tonkin et al (2007) for details.

The constrained maximization/minimization process just described is mathematically equivalent to the null space Monte Carlo process described in section 8.2.2. However its implementation is normally far more costly than that of null space Monte Carlo for reasons already outlined, particularly where parameter numbers are high and the predictive model run is long.

## 8.5 Model-Based Hypothesis-Testing

### 8.5.1 Calibration as Hypothesis-Testing

Hypothesis-testing, as a concept, lies at the heart of the so-called "scientific method". A

hypothesis is proposed, and evidence is collected to test it. If the evidence allows rejection of the hypothesis then something has been learned; the range of possible explanations for a scientific phenomenon has thereby been reduced.

A hypothesis that explains the behaviour of a system can never be *accepted* as truth, for there may be more than one explanation for its behaviour. However it may be possible to *reject* certain hypotheses that purport to explain the cause-and-effect relationships that govern system behaviour. Hypothesis rejection can occur if a hypothesis is demonstrably incompatible with observations of system state, and/or with other knowledge of a system that has been previously acquired and has been demonstrated to have integrity.

A numerical model of environmental processes constitutes a hypothetical explanation for the behaviour of an environmental system. The hypothesis that is embodied in the numerical model can be partially tested through attempting to calibrate the model. If the model is able to replicate historical system behaviour "reasonably well", using parameters that are "reasonable" from an expert knowledge point of view, then the hypothesis that the model is a useable descriptor of environmental behaviour cannot be rejected. Note that reasonableness of fit may need to be traded off against reasonableness of parameter values using L-curve concepts such as are discussed in section 6.3.3.

Of course, a lot hangs on the definition of "reasonable". If a certain level of model-to-measurement misfit is deemed by a modeller to be tolerable, then knowledge of the noise associated with the calibration dataset is implied. Of course, this "noise" is partly measurement noise, and partly "structural noise" that is attributable to model defects. Whatever its source, the fact that the model is retained as a possibly valid descriptor of system behaviour implies at least an approximate definition of C($\boldsymbol{\varepsilon}$), the covariance matrix of measurement/structural noise. (We retain the use of $\boldsymbol{\varepsilon}$ rather than $\boldsymbol{\tau}$ to denote combined measurement/structural noise to preserve notational consistency, even though $\boldsymbol{\tau}$ has been used on several occasions in this text to acknowledge the contribution that structural noise makes to model-to-measurement misfit.) Exploration of parameter and predictive uncertainty requires knowledge of this matrix. Normally C($\boldsymbol{\varepsilon}$) is denoted as diagonal in spite of the fact that this is demonstrably incorrect where model-to-measurement misfit includes structural noise. However diagonal matrices are easy to store and manipulate. Furthermore, knowledge of its off-diagonal elements is scanty or absent.

"Reasonableness" of values estimated for model parameters is also required if the hypothesis that a model is an adequate descriptor of environmental processes at a particular site is not to be rejected. Obviously, the values that must be assigned to a model's parameters in order for model outputs to fit the calibration dataset must be judged according to metrics set by expert knowledge. If, in order for the model to replicate historical system behaviour, its parameters must adopt values that contravene the range of values that are considered reasonable for the system properties that they represent, the validity of the model is called into question. If the calibration process has been enabled by a suitable regularization scheme, then unreasonableness of estimated parameter values indicates that parameters are adopting roles for which they were not designed in order for the model to provide an acceptable fit with field measurements. Nevertheless, for reasons that are outlined in the next chapter, some degree of parameter unreasonableness may be considered acceptable if it is judged by the modeller that the surrogate roles that some parameters must play if model outputs are to fit the calibration dataset do not introduce errors to predictions of interest required of the model. Alternatively, a modeller may judge that estimated system properties do in fact constitute a

true reflection of actual system properties, even if he/she has been surprised by some of the properties that have been estimated. In either case, the decision not to reject the hypothesis that the model is a reasonable simulator of environmental behaviour at a particular study site, may oblige a modeller to accept a C(**k**) matrix of prior parameter covariance that expresses greater parameter variability than that which would have been expected on the basis of expert knowledge alone. The modeller has thus expanded the horizons of his/her expert knowledge through the calibration process. As for the C(**ε**) matrix, knowledge of the C(**k**) matrix is fundamental to exploring the uncertainties associated with model predictions of future system behaviour.

With these considerations in mind, the role of the model calibration process can be seen as multi-faceted. On the one hand it constitutes a hypothesis-testing device through which the reasonableness of the model as a simulator of local system behaviour is assessed. At the same time as this assessment is being made, the metrics for this assessment are simultaneously reviewed as knowledge is also being acquired about them. This constitutes a significant point of departure from the nature of scientific inquiry as it takes place in many other disciplines where the metrics for hypothesis rejection do not necessarily alter as hypotheses are being tested. However this departure is unavoidable if a modeller does not have access to a superior simulator of environmental behaviour at his/her study site. The modeller's task in assessing the integrity of his/her model therefore becomes one of assessing its limitations as well. If the latter are not too great, the calibrated model may serve as a suitable device for testing hypotheses pertaining to future system behaviour. However its capacity to reject those hypotheses may be degraded by its own limitations as exposed through the process of calibration it.

The outcomes of a "successful" model calibration process are thus fourfold. First, the model retains its status as a provisional descriptor of environmental processes at a particular study site, this following from the fact that the hypothesis that the model constitutes an inadequate description of environmental behaviour at that site cannot not rejected. Second, values that are hopefully of minimum error variance (though probably far from correct as explained in previous sections of this document) have been awarded to model parameters. Third and fourth, the modeller has acquired important knowledge of C(**ε**) and C(**k**) that take into account not only measurement noise on the one hand and expert knowledge on the other hand, but also the imperfections of the model as a simulator of local environmental processes. Future usage of the model must take account of all four of these outcomes of the calibration process. Future usage will normally require that the model simulate the behaviour of the system under conditions which are altered from those which prevailed at calibration.

The fact that knowledge of C(**ε**) and C(**k**) has been acquired through the calibration process is significant, for these outcomes of the calibration process are just as important as the minimum error variance estimates of model parameters that are traditional outcomes of the calibration process. This is because these matrices are an integral part of the hypothesis that the calibration process has failed to reject. In particular, the hypothesis that has not been rejected through calibrating the model is that the model constitutes a simulator of system behaviour to within a misfit tolerance set by C(**ε**) (for model outputs of the type that are used in the calibration process), and to within a parameter variability tolerance set by C(**k**).

It is worth nothing that in most practical modelling circumstances C(**k**) is a simplistic descriptor of far more complex system property variability that exists in reality. The values assigned to elements of C(**k**) should accommodate limitations in its ability to characterize

true parameter variability, at the same time as they may reflect the need for some parameters to adopt roles that compensate for model structural defects. Hence some elements of C(**k**) may overstate the true variability of those system properties that the corresponding elements of **k** purport to represent.

### 8.5.2 The Decision-Making Context

In most decision-making contexts, models are built to make predictions of future environmental system behaviour under management regimes which are different from those which prevailed when the calibration dataset was gathered. Looming large in most decision-making contexts is the thought that something may go wrong following implementation of the new management regime. The new management regime must be such as to preclude the occurrence of such unwanted eventualities. These unwanted eventualities are normally well defined and acknowledged by all stakeholders.

The uncertainties that are associated with predictions of the environmental future (especially where that future involves stresses to which a system has not been subjected in the past) are such that it may not be possible to say that an unwanted event, or a "bad thing", definitely will not happen. Hence environmental management is accompanied by risk. Risk is often defined as the probability of an unwanted occurrence times the cost of its occurrence. Where the cost of something going wrong is low, then decision-makers can accept the fact that considerable uncertainty may be associated with predictions that it will not eventuate. In contrast, where the cost of something going wrong is high, good environmental management demands that the certainty of its non-occurrence be correspondingly high.

The decision-making process is thus one of risk-management. Ideally, environmental modelling assists this process by assigning probabilities to one or a number of unwanted events. See Freeze et al (1990) for an illuminating discussion of this issue.

An unwanted event can take many forms. An important concept is that, in the decision-making context, an unwanted event constitutes a hypothesis that we would like to reject - at a certain level of confidence. The unwanted event may be a "bad thing" from a financial point of view; for example it may be that a proposed mine dewatering system allows more inflow to a mine than can be removed by installed pumps. Alternatively, an unwanted event may be a "bad thing" from an environmental point of view; for example, it may be that a proposed development plan results in depletion of stream flow and the creation of conditions that are thereby harmful to stream biota. In another management context the "bad thing" may be that system managers have made the wrong decision by adopting management plan B over management plan A when in fact management plan A would have provided a better outcome according to prevailing decision criteria.

Unwanted events can be defined in arbitrarily complex ways that reflect the specific demands of environmental decision-making, and the uncertainties that are associated with environmental management at any particular study site. For example it may not be possible to reject the hypothesis that a certain development plan will have an unwanted environmental consequence. However it may be possible to reject the hypothesis that if development is accompanied by a suitable monitoring network to which developers will immediately respond by curtailing their activities if monitoring thresholds are crossed, then the bad thing will not happen. Rejection of this hypothesis may then allow development to proceed with the monitoring network in place. Meanwhile modelling provides the assurance that the

monitoring network is adequate, through specifically testing and rejecting the hypothesis that it is inadequate.

With the decision-making context viewed in this way, the contribution that environmental modelling can make to the decision-making process is aligned with implementation of the scientific method. The task of modelling is to test the hypothesis that if a certain course of management action is followed, then the eventuality of a bad thing can be rejected at a certain level of confidence. The higher is the cost associated with the eventuality of the bad thing, the higher does the level of confidence need to be.

In the environmental management context (and in many other contexts) a hypothesis can be rejected if it is demonstrated to be incompatible with either or both of expert knowledge, and/or with the historical behaviour of the system whose management is being considered. The environmental model constitutes a unique scientific instrument for the testing of environmental hypotheses because of its ability to provide receptacles for these two types of information. Expert knowledge resides in the C(**k**) matrix (or more complex statistical descriptor of system property variability that is employed in the modelling process). Information pertaining to the historical behaviour of the system is embodied in the parameter set $\underline{\mathbf{k}}$ achieved through the calibration process. The basis for rejection of a hypothesis pertaining to the occurrence of a future unwanted event lies in demonstrating that this occurrence requires that the model be endowed with a parameter field that is not in accordance with C(**k**), and/or that it removes from the model its ability to replicate, to within a level set by C(**ε**), historical system behaviour. The latter will occur if the occurrence of a hypothesized bad thing demands that the model adopt parameter values **k** for which $\mathbf{k} - \underline{\mathbf{k}}$ has too great a projection onto the calibration solution space, and is therefore not confined almost completely to the calibration null space.

As C(**k**) and C(**ε**) are both stochastic quantities it should be possible, in theory at least, to associated a level of confidence with rejection of the hypothesis that an unwanted event will occur.

### 8.5.3 Configuring a Model for Hypothesis-Testing

If a model is to test the hypothesis that a future unwanted event will not occur under a proposed management plan, then it must be provided with stresses that allow it to simulate the outcomes of that plan. In other words it must be configured to predict values associated with the unwanted event. Presumably, for a particular prediction of management interest, a certain range of these values are "unwanted" and therefore constitute a "bad thing", while values outside this range are considered as benign.

As stated above, the hypothesis that a bad thing will occur can be rejected if its occurrence is demonstrated to be incompatible with past behaviour of the system, or requires that the model be endowed with unrealistic system properties. C(**ε**) constitutes the metric for the first comparison while C(**k**) constitutes the metric for the second comparison.

If the model prediction as made using the calibrated parameter set $\underline{\mathbf{k}}$ is bad, then naturally the hypothesis that the bad thing will happen cannot be rejected. In contrast, if the prediction made using the calibrated parameter set $\underline{\mathbf{k}}$ is benign, this does not constitute grounds for rejection of the hypothesis that the bad thing will occur. As has been extensively discussed, there is no reason to presume that a prediction made using the parameter set $\underline{\mathbf{k}}$ is correct; all that the calibration process can promise is that this prediction is minimally wrong. This does

not mean, however, that the margin of potential wrongness is not high.

Rejection of the hypothesis that a bad thing will happen requires demonstration that the particular model prediction that corresponds to the bad thing is benign for any set of parameters that calibrate the model to within a level set by C(**ε**) and that are reasonable from an expert knowledge point of view to a level set by C(**k**).

Hypothesis-testing of this kind can be undertaken using calibration-constrained Monte Carlo methods discussed earlier in this chapter. The pertinent model prediction is made using many realizations of **k** drawn from the posterior parameter distribution (or an approximation to it). If all of these predictions are benign, the hypothesis that a bad thing will happen can be rejected. If only a handful of predictions are bad, the hypothesis that the bad thing will happen can be rejected with a high level of confidence.

While this constitutes a conceptually correct strategy for testing the hypothesis that a bad thing will happen, it has a number of drawbacks. The first drawback is one that accompanies all Monte Carlo methods. Rejection of a hypothesis at a high level of confidence requires that many model run be undertaken, each based on different samples of the posterior parameter distribution. The higher the level of confidence for which hypothesis rejection is required, the greater is the number of model runs required. This number increases dramatically as parameter numbers increase.

The second problem is that parameter fields used by a calibrated model often embody simplified representations of real world parameter variability. This applies especially to groundwater and subsurface reservoir models. As was discussed earlier in this chapter, this is an outcome of the fact that efficient imposition of calibration constraints in a highly parameterized context requires that model outputs vary continuously with parameters. This forestalls the use of some of the more picturesque and geologically realistic expressions of parameter variability afforded by modern geostatistical software. It is quite possible then that calibration-constrained random parameter fields generated using techniques such as null space Monte Carlo will fail to include parameter structures that may promulgate the occurrence of an unwanted event, even though such structures are geologically realistic.

These problems can be partially overcome by formalizing model-based hypothesis-testing through adoption of a strategy that resembles, to some extent, the calibration-constrained predictive maximization/minimization process described above. In implementing this strategy a package such as PEST which is capable of highly-parameterized inversion is asked to run the model under both calibration and predictive conditions. The normal calibration dataset is expanded to include just one extra "observation". This is the observation that a bad thing happens at some time in the future. The inversion engine is then asked to fit the calibration dataset (as it did when the model was calibrated) at the same time as it also fits the new "observation". If the inversion engine is able to derive a parameter set that maintains a reasonable fit with the calibration dataset (as judged according to the C(**ε**) metric), while maintaining parameter reasonableness (as judged by the C(**k**) metric), then the hypothesis that the bad thing will happen cannot be rejected.

The expanded parameter estimation process will normally use previously estimated parameter values $\underline{\mathbf{k}}$ as starting parameters. Tikhonov constraints may be used (in conjunction with a suitable C(**k**) matrix) to minimize parameter deviations from these values as the expanded calibration dataset is fitted. The use of a large number of parameters, particularly in strategic parts of the model domain that are most salient to the prediction of interest, allows

heterogeneity to arise if it needs to arise for the bad thing to happen. Thus the occurrence of the bad thing is not precluded by inappropriate parameter parsimony in critical parts of the model domain.

If the model is indeed able to replicate the bad thing at the same time as it simultaneously respects the historical calibration dataset, then assessment of the likelihood of occurrence of the bad thing may be made either subjectively or in a statistically formal manner; this is the modeller's choice. In many cases subjectivity is mandatory, this arising from the inadequate nature of C(**ε**) as a descriptor of model-to-measurement misfit, and of C(**k**) as a descriptor of complex system property reality.

In a particular groundwater or reservoir modelling context, the occurrence of a bad thing may require that a spatially continuous feature be introduced to the model domain as the geological agent for its eventuality. The spatial continuity of this feature may violate the statistical demands of a particular C(**k**) covariance matrix. If this is the case, then such a feature would never emerge if null space Monte Carlo analysis were employed to explore predictive uncertainty. Nevertheless, on inspection of the parameter field that emerges from the direct hypothesis-testing procedure just described, a modeller may, upon reflection, deem such a feature to be a geological possibility. He/she may therefore decide not to reject the hypothesis that the unwanted event will occur. This is a great strength of direct hypothesis-testing. In making the system fail, the inversion process must introduce a failure mechanism. Inspection of this mechanism provides the grounds for the most failsafe rejection of its eventuality, at the same time as it suggests appropriate locations for monitoring points to provide early warning of failure, should the worst occur.

If a more formal, statistically-based, criterion is required for rejection of the hypothesis that an unwanted event will occur, and for assigning a level of confidence to such rejection, this can be accomplished using theory presented in sections 8.3 and 8.4. See, for example, Moore et al (2010). Alternatively, the theory can be partially applied. Suppose, for example, that the inversion process is able to derive a parameter field that allows an unwanted event to happen, and that the fit between model outputs and the calibration dataset is deemed to be "visibly good". A modeller may then decide that testing of the "bad thing hypothesis" will take place on the basis of parameter field credibility alone. Theory described in section 8.3 of this text can then be applied. This may be applied to differences between parameter values obtained through the hypothesis-testing process and either prior mean parameter values or posterior mean parameter values as obtained through model calibration. In the latter case the parameter covariance matrix through which statistical credibility is assessed can be calculated using the first term of equations (8.4.11) or (8.4.12); alternatively it can be calculated using equation (7.3.4) or (7.3.15), both of which are derivable from Bayes equation. It is the author's opinion, however, that whichever option is chosen, the inadequacies of C(**ε**) and C(**k**) as statistical descriptors of model-to-measurement misfit on the one hand, and expert knowledge on the other hand, makes subjective assessment inescapable.

Implementation of the direct hypothesis-testing methodology described in this section requires that a weight be assigned to the observation that the bad thing happens. Some trial and error may be required in assigning this weight. So too may some trial and error be required in assigning an "observed bad value" to the "observed prediction" which is added to the calibration dataset. Ideally the weight assigned to this prediction should provide a strong incentive to the inversion process to actually make the bad thing happen. However if this weight is too large then parts of the remainder of calibration dataset may be ignored; at the

same time numerical errors may compromise the inversion process as some parameters become very sensitive because of the high weight that is assigned to the predictive model outcome that is sensitive to them.

These problems can be circumvented if PEST is run in "Pareto" mode. The weight ascribed to the observed bad thing is then gradually applied. At first this weight can be zero (it is the modeller's choice). If the initial parameter set is equal to the parameter set **k** achieved through the previous calibration process, then the hypothesis-testing process will commence with the model calibrated. The weight assigned to the observed bad thing is then gradually increased. As this happens, model parameters will start to depart from **k**; however departures will be minimized, particular if prior information which limits perturbations of **k** from **k** is included in the hypothesis-testing process. As the weight ascribed to the prediction is increased even further, the calibration component of the objective function will start to rise; at the same time parameters will depart even further from their preferred **k** values. At some stage the modeller may judge that parameter or calibration credibility has been strained to breaking point. The process can then be halted. The hypothesis that the bad thing will happen can then be rejected.

As it traverses the so-called "Pareto front" in this manner, PEST records parameter values and corresponding model outputs. The modeller can associate credibility with each parameter set on the basis of a supplied or implied C(**k**), and with each set of model outputs on the basis of a supplied or implied C(**ε**) as he/she sees fit. On this basis he/she can then establish the value of the prediction at which its occurrence becomes unlikely.

# 9. Model Defects

## 9.1 Introduction

No model is a perfect simulator of environmental processes at any study site. While this does not invalidate the use of models in environmental decision-making, it does mean that they should be used with caution. It also means that modellers should be aware of the repercussions of model defects so that, when called upon to make the many subjective decisions that modelling entails, these decisions can be as informed as possible.

Model defects arise from many sources. They may arise from approximations used in the model algorithm, in failure to provide enough parameters to represent system property heterogeneity, in erroneous definition of temporal and spatial boundary conditions, in the need for spatial and temporal discretization that supports numerical representation of partial differential equations, from improper definition of system stresses and source terms, and from many other sources. Defects may become visible as a model is calibrated through failure of the calibration process to provide a good fit between model outputs and measurements of system state. Alternatively they may remain invisible to the calibration process, especially in highly parameterized contexts where parameters may adopt roles which compensate for model defects, so that a good fit between model outputs and the calibration dataset is attained for the wrong reason. As will be shown below, for some predictions this may be a good thing as model defects are thereby "calibrated out". For other predictions made by the same model it will be a bad thing as the calibration process introduces a potential for error to those predictions that would not have been present if the model had not been calibrated.

Once model defects are taken into account, assessment of the potential for error in calibrated model parameters and in predictions made by a calibrated or uncalibrated model becomes complicated. It also becomes subjective, because the nature and extent of model defects is normally unknown and cannot be quantified. As will be discussed, steps can be taken to reduce the deleterious effects of model defects on calibrated model parameters and on predictions made by a calibrated model. However the nature and efficacy of these strategies will also be a matter of subjectivity.

This chapter summarizes work presented in three papers in which a detailed analysis of model defects is presented, together with suggested methodologies through which, in some cases, it may be possible to analyse and correct for these defects. Not all of the material that appears in these papers is presented in this chapter. The interested reader is therefore referred to Doherty and Welter (2010), Doherty and Christensen (2011) and White et al (2014) if he/she wishes to pursue the matter further.

## 9.2 An Example

Figure 9.1 shows a simple one-dimensional groundwater model. Water flows into the model domain at a known rate through its right boundary. The groundwater head is fixed at the left side of the model domain. Transmissivity within the model domain is uniform. Four observation wells are situated within the domain of this simple model. Heads are measured in these wells; these head measurements are accompanied by measurement noise.

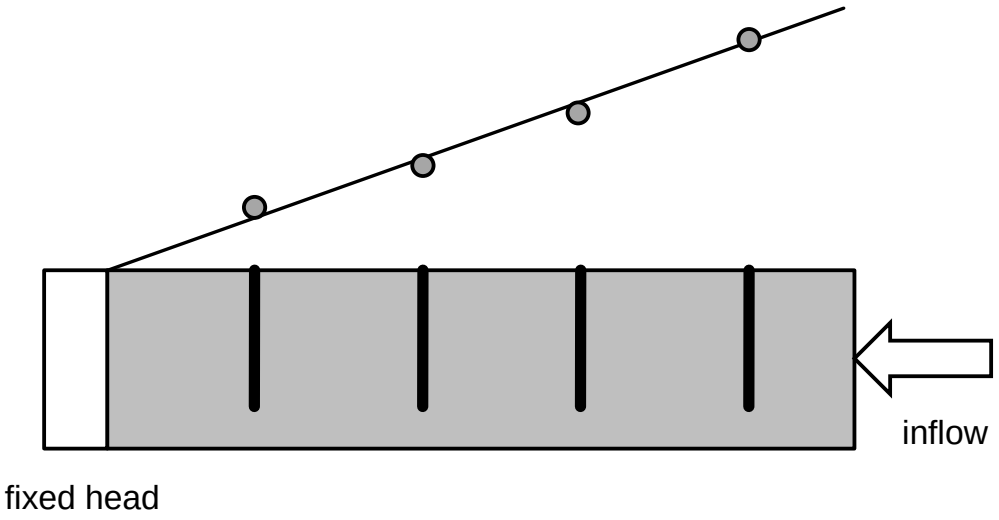


**Figure 9.1. A simple groundwater model. The four circles show water levels recorded in four wells. The solid line shows heads throughout the model domain calculated using a uniform, calibrated transmissivity value. This and subsequent figures are modified from those presented in Doherty and Welter (2010).**

Suppose that the model is calibrated against the four borehole water level measurements depicted in figure 9.1 in order to estimate the single parameter that characterizes its transmissivity. The solid line in figure 9.1 shows heads calculated by the model throughout its domain using the single estimated transmissivity value. The fit between model-calculated and measured heads is good. Measured heads are scattered randomly about this line of best fit; the amount of this scatter is commensurate with measurement noise.

A defect is introduced to the model in figure 9.2. The head at the left side of the model domain is assigned an incorrect value. The model is then re-calibrated to estimate the uniform domain transmissivity by fitting the measured heads. The straight line of model-calculated heads depicted in figure 9.2 provides the best fit between model-calculated and measured heads in the least squares sense. However in this case the scatter of measured heads about the line of model-calculated heads appears to show some “structure”; uphill heads are over-estimated and downhill heads are underestimated by the calibrated model.

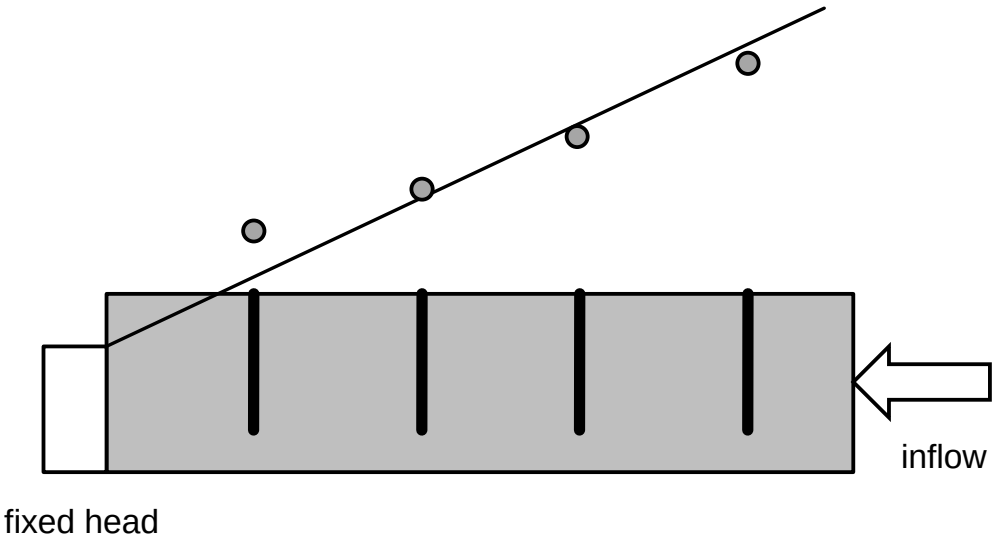


**Figure 9.2. The same model domain as that depicted in figure 9.1, but with an incorrect boundary condition. The solid line shows heads throughout the one-dimensional model domain generated by the calibrated model.**

The modeller who built the model that appears in figures 9.1 and 9.2 may recognize that his/her attempt to estimate model domain transmissivity has been corrupted by the presence of a model defect. In the present example that defect is easy to recognize. In other cases it may not be so easy to spot model defects which may be damaging the calibration process. Nevertheless a modeller may recognize that measurements of one type, or at one location, can only be fit well by sacrificing goodness of model fit with data of other types, or at other locations. Indeed, recognition that a model's inadequacies often prevent it from fitting all data at all locations equally well has given rise to the support that global optimization software provides for Pareto methods. These allow the estimation of many sets of parameters along a so-called Pareto front in which two or more components of the overall calibration objective function are traded off against each other. The rationale behind this approach to calibration is as follows.

1. It explicitly recognizes the existence of structural defects, and incorporates such recognition into the calibration process.
2. By deriving a suite of parameter sets which respect each data type individually, and all combinations of data types in between, the effect of model defects on estimated parameter error has been implicitly quantified. When predictions of management interest are then made by the calibrated model, the contributions to predictive error that originate from these defects will also be implicitly quantified if these predictions are made with many of these parameter sets. See, for example, Vrugt et al (2003) and Wöhling and Vrugt (2008).

Figure 9.3 implements this strategy for the simple model. Two lines are shown in this figure. These lines pass through the extremes of the observation dataset. One of these lines has the maximum slope that it is possible for a line to possess and still respect any of the borehole head measurements. The other line is its minimum slope complement. It is apparent that estimation of the true transmissivity value requires a smaller slope than either of these lines. The true value of parameter uncertainty has therefore eluded this Pareto strategy.

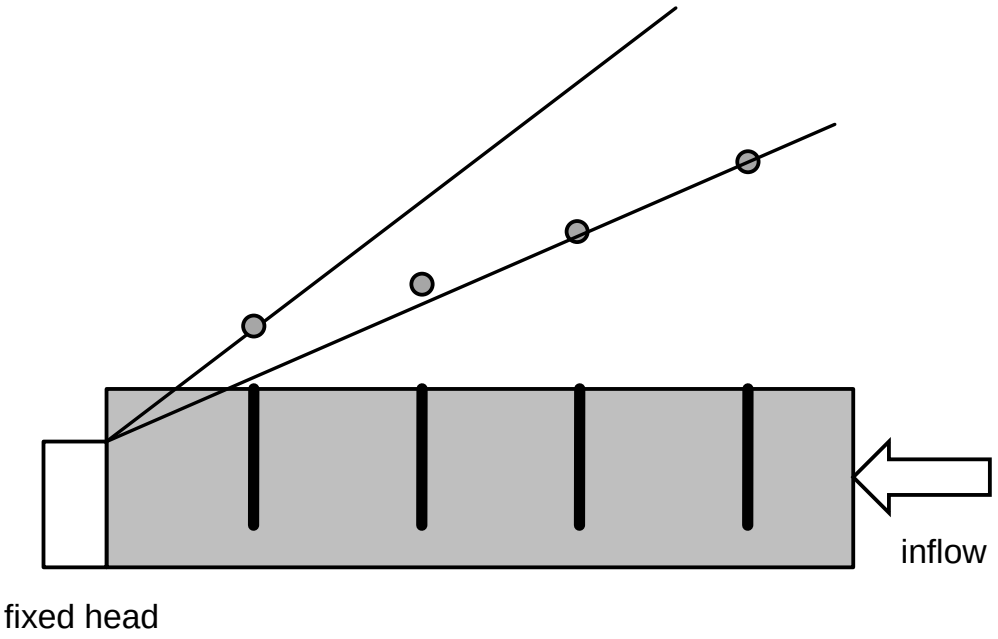


**Figure 9.3. An attempt is made to bracket the true transmissivity by fitting data extremes.**

The "best fit" though the four head measurements comprising the calibration dataset is that depicted in figure 9.4. The line of model-generated heads passes through none of the measured heads. However the slope of this line is correct; hence estimated transmissivity is correct.

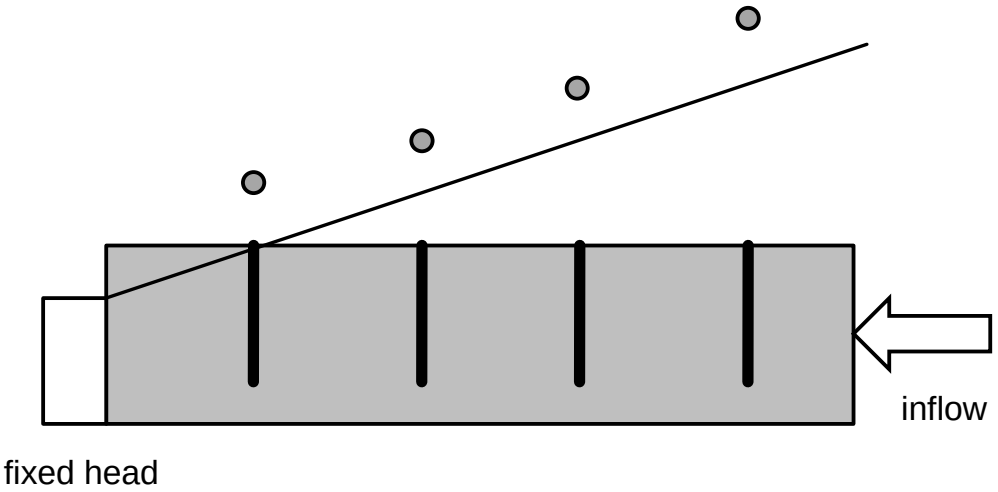


**Figure 9.4. Line of "best fit" through the calibration dataset.**

So would a modeller pursue a fit like that depicted in figure 9.4 when calibrating his/her model? Perhaps so. If the calibration process is reformulated so that the model is asked to fit three observed lateral head differences rather than four observed heads, then exactly this fit is obtained and the value estimated for model domain transmissivity will be correct. That is because, for this particular model, its defect does not affect computed lateral head differences; it only affects computed heads. Calibration using lateral head differences is

schematized in figure 9.5

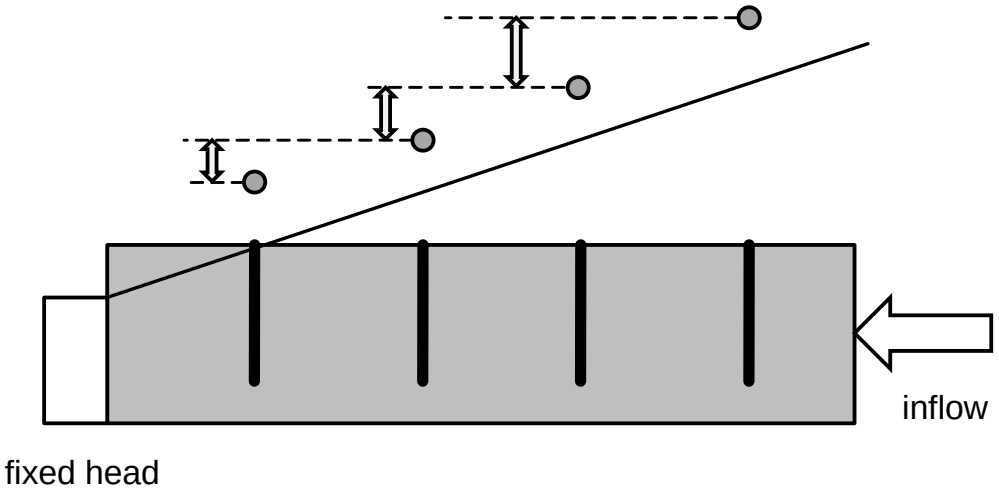


**Figure 9.5. Calibration is achieved through matching lateral differences in measured heads rather than heads directly.**

Rather than sensing a model defect, a modeller may attribute failure to connect all borehole heads to the left model boundary with a single straight line as evidence of the presence of transmissivity heterogeneity within the model domain. He/she may then introduce parameters that can represent that heterogeneity. Figure 9.6 shows the outcome of a calibration exercise that employs two transmissivity parameters. A good fit is obtained between model outputs and field measurements. This calibration strategy results in correct estimation of the $T_1$ parameter; at the same time the $T_2$ parameter "absorbs" structural noise by adopting a transmissivity value that, while being erroneous, provides the opportunity for the calibration process to achieve a good fit with the field data despite the defective nature of the model which was calibrated.

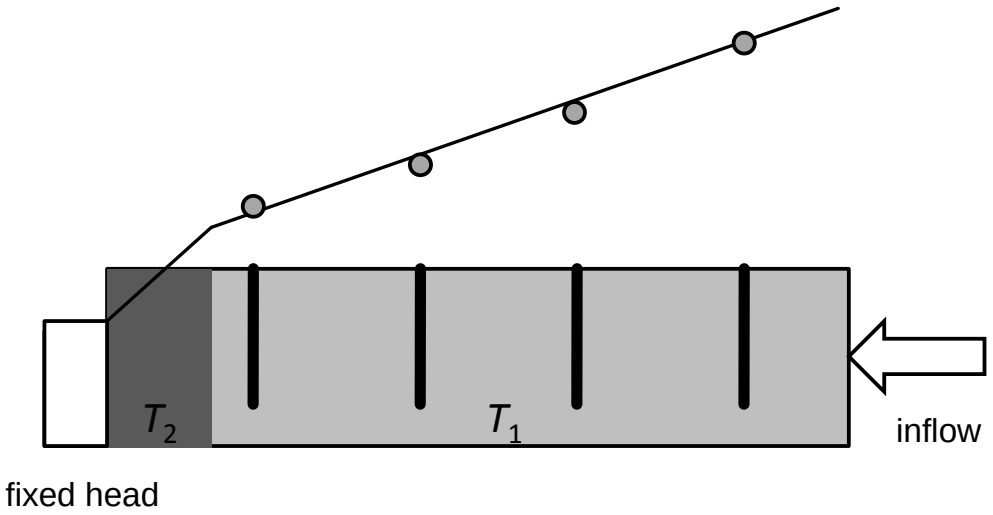


**Figure 9.6. Estimation of an extra transmissivity parameter allows attainment of a good fit with borehole head data.**

How "valid" is the calibration exercise of figure 9.6? It obviously has some validity as the correct transmissivity has been awarded to the greater part of the model domain. If the model

is asked to predict drawdowns in and near a pumping well installed to the right of the $T_2$ boundary, its predictions will be correct. However if the model is asked to predict heads throughout the model domain following an increase in inflow from the right, then its predictions will be wrong; see figure 9.7. In fact its predictions will be more wrong than those made by the calibrated model of figure 9.2 over a substantial part of the model domain.

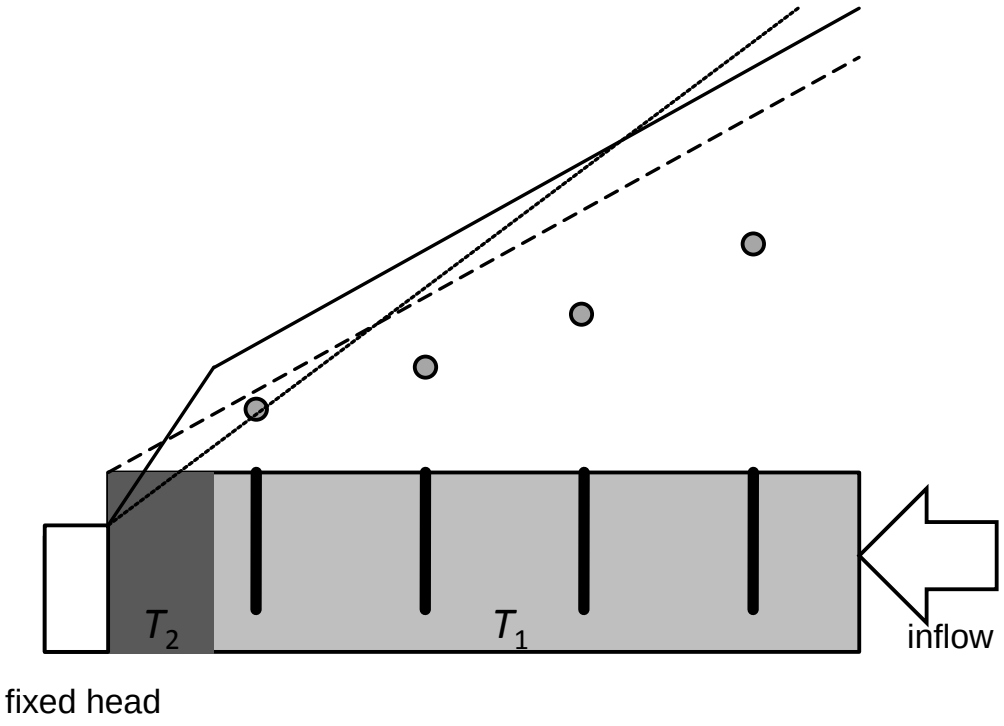


**Figure 9.7. The full line shows heads predicted by the calibrated defective model of figure 9.6 following increased uphill inflow. The dashed line shows the correct heads under these conditions. The dotted line shows predictions calculated by the calibrated model depicted in figure 9.2 which employs no compensatory parameters.**

During the calibration process of the defective model the $T_2$ parameter plays a role which compensates for its defect. Its playing of this same compensatory role provides integrity to some model predictions (namely predictions of drawdown following pumping introduced to the right of the model domain) that they would not otherwise possess. For another prediction however (namely the response of the system to increased lateral inflow) this compensatory role incurs error, as this role is not appropriate for that prediction.

## 9.3 Mathematical Formulation of the Problem

### 9.3.1 A Defective Model

Up until this point, the action of a model under calibration conditions has been described using the equation

$$\mathbf{h} = \mathbf{Zk} + \boldsymbol{\varepsilon} \qquad (9.3.1)$$

All derivations that have proceeded from this equation have not questioned the fact that the linearized model **Z** is a perfect simulator of the system that it purports to represent. Hence no error terms have been introduced to estimated parameters to account for the fact that this may

not be so.

To facilitate the analyses presented in the present chapter, let the following be assumed

$$C(\boldsymbol{\varepsilon}) = \sigma^2_{\varepsilon}\mathbf{I} \qquad (9.3.2)$$

$$C(\mathbf{k}) = \sigma^2_{k}\mathbf{I} \qquad (9.3.3)$$

In practice the former is achieved through use of an appropriate weight matrix while the latter is achieved either explicitly through Kahunen-Loève transformation of parameters, or implicitly through use of appropriate Tikhonov constraints in the model calibration process.

Defects will now be introduced to the model. Equation (9.3.1) becomes

$$\mathbf{h} = \mathbf{Z}_m\mathbf{k}_m + \mathbf{Z}_d\mathbf{k}_d + \boldsymbol{\varepsilon} \qquad (9.3.4)$$

$\mathbf{Z}_m$ and $\mathbf{k}_m$ of equation (9.3.4) correspond to $\mathbf{Z}$ and $\mathbf{k}$ of equation (9.3.1); these pertain to the model as it is "seen" by the modeller. Equation (9.3.3) is then re-written as

$$C(\mathbf{k}_m) = \sigma^2_{km}\mathbf{I} \qquad (9.3.5)$$

The $\mathbf{k}_d$ vector of equation (9.3.5) is comprised of "correction parameters", while the $\mathbf{Z}_d$ matrix is comprised of "correction processes" that act on these parameters. Of course representation of model defects in this way is linear; however, as in previous sections of this document, the linearity assumption allows us to draw some useful conclusions. These conclusions can be extrapolated to nonlinear models.

The $\mathbf{Z}_d\mathbf{k}_d$ term of equation (9.3.4) embodies a (normally unknown) "correction term" for model outputs. The (normally unknown) $\mathbf{k}_d$ parameters can be conceived of as expressing the reasons for which corrections are necessary. Take, for example, the model of figure 9.2. While not explicitly represented in the model's parameter set, the single parameter comprising the $\mathbf{k}_d$ vector for that model is the difference between the elevation of the left fixed-head boundary as represented in the model and its true elevation. Whether the modeller is aware of it or not, this parameter is present in the model's parameter set (conceptually at least) as long as a modeller has the capacity to misassign this elevation. The fact that the modeller is unaware of the possibility of this error, or does not wish to consider the boundary elevation as an adjustable parameter, relegates this parameter to the $\mathbf{k}_d$ vector rather than to the $\mathbf{k}_m$ vector. Inasmuch as model outputs used in the calibration process are sensitive to this parameter, a corresponding $\mathbf{Z}_d$ matrix exists.

As for all linear analysis undertaken in this document, parameters express perturbations from prior expected values of the system properties that they represent. If a parameter's value is zero, this indicates that the parameter has been awarded its prior preferred value. The same applies to correction parameters. If a particular element of $\mathbf{k}_d$ has a value of zero, then the defect which it represents does not exist. This is the case in figure 9.1 where the elevation of the left fixed-head boundary is correct.

For many other types of model defects, appropriate "defect parameters" can also be conceptualized. For example, if a steady-state groundwater model is calibrated under conditions that are partly transient, $\mathbf{k}_d$ parameters comprise recharge rate perturbations from their assumed steady-state values, as well as storage properties that do not feature in steady state simulations; meanwhile the pertinent $\mathbf{Z}_d$ matrix represents the time-varying action of the model over the time interval through which steady-state conditions are assumed to prevail. Where a groundwater or reservoir model is assumed to possess a single layer instead of the

many layers which may actually characterize the subsurface, $\mathbf{k}_d$ parameters are comprised of the differences between individual layer properties and the properties of the single layer which replaces them in the model; meanwhile the $\mathbf{Z}_d$ matrix computes model output correction terms that emerge from these layer property differences and from vertical head gradients. In other cases, for example those arising from simplified representation of complex chemical process, or from overly-coarse spatial and temporal discretization in the vicinity of major system stressors, conceptual identification of $\mathbf{k}_d$ and $\mathbf{Z}_d$ may be a little more subtle. This does not matter; it is their presence rather than their exact definition that is of primary importance.

Through comparison of equations (9.3.4) and (9.3.1) it is obvious that it is to $\mathbf{Z}_d\mathbf{k}_d$ that the term "structural noise" should be applied. In practice, it is often ascribed to its visible expression, these being residuals that are incurred by its presence as the model is calibrated. As will be discussed below, however, it is its invisible expression that inflicts damage on the parameter estimation process.

### 9.3.2 Parameters and Residuals

Through calibration, a model's "adjustable" parameters are estimated. These are the $\mathbf{k}_m$ parameters of equation (9.3.4). Suppose that, when subjected to singular value decomposition, $\mathbf{Z}_m$ can be written as

$$\mathbf{Z}_m = \mathbf{U}_m\mathbf{S}_m\mathbf{V}^t_m \tag{9.3.6}$$

Following determination of a suitable singular value truncation point based on considerations presented in section (6.2.5), $\mathbf{k}_m$ can be estimated as

$$\underline{\mathbf{k}}_m = \mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\mathbf{h} \tag{9.3.7}$$

The assumption implied in using equation (9.3.7) to estimate $\underline{\mathbf{k}}_m$ is, of course, that the model $\mathbf{Z}_m$ has no defects. However in recognition of the fact that the model is indeed defective, we now substitute (9.3.4) into (9.3.7) to obtain (after a little simplification)

$$\underline{\mathbf{k}}_m = \mathbf{V}_{m1}\mathbf{V}^t_{m1}\mathbf{k}_m + \mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d\mathbf{k}_d + \mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} \tag{9.3.8}$$

Suppose that $\mathbf{Z}_d$ can be decomposed as

$$\mathbf{Z}_d = \mathbf{U}_d\mathbf{S}_d\mathbf{V}^t_d \tag{9.3.9}$$

Then (9.3.8) can also be written as

$$\underline{\mathbf{k}}_m = \mathbf{V}_{m1}\mathbf{V}^t_{m1}\mathbf{k}_m + \mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\mathbf{U}_d\mathbf{S}_d\mathbf{V}^t_d\,\mathbf{k}_d + \mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} \tag{9.3.10}$$

Residuals associated with the calibrated model are

$$\mathbf{r} = \mathbf{h} - \mathbf{Z}_m\underline{\mathbf{k}}_m \tag{9.3.11}$$

With substitution of (9.3.8) into (9.3.11) this becomes

$$\mathbf{r} = \mathbf{h} - \mathbf{Z}_m\mathbf{V}_{m1}\mathbf{V}^t_{m1}\mathbf{k}_m - \mathbf{Z}_m\mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d\mathbf{k}_d - \mathbf{Z}_m\mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} \tag{9.3.12}$$

Substituting (9.3.6) for $\mathbf{Z}_m$, this becomes

$$\mathbf{r} = \mathbf{h} - \mathbf{U}_{m1}\mathbf{S}_{m1}\mathbf{V}^t_{m1}\mathbf{k}_m - \mathbf{U}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d\mathbf{k}_d - \mathbf{U}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} \tag{9.3.13}$$

If (9.3.4) is substituted for $\mathbf{h}$ and use is made of the relationship

$$\mathbf{U}_{m1}\mathbf{U}^t_{m1} + \mathbf{U}_{m2}\mathbf{U}^t_{m2} = \mathbf{I} \tag{9.3.14}$$

and the relationship

$$\mathbf{U}_m\mathbf{S}_m\mathbf{V}^t_m = \mathbf{U}_{m1}\mathbf{S}_{m1}\mathbf{V}^t_{m1} + \mathbf{U}_{m2}\mathbf{S}_{m2}\mathbf{V}^t_{m2} \quad (9.3.15)$$

we finally obtain for residuals

$$\mathbf{r} = \mathbf{U}_{m2}\mathbf{S}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m + \mathbf{U}_{m2}\mathbf{U}^t_{m2}\mathbf{Z}_d\mathbf{k}_d + \mathbf{U}_{m2}\mathbf{U}^t_{m2}\boldsymbol{\varepsilon} \quad (9.3.16a)$$

which, using (9.3.9) can also be written as

$$\mathbf{r} = \mathbf{U}_{m2}\mathbf{S}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m + \mathbf{U}_{m2}\mathbf{U}^t_{m2}\mathbf{U}_d\mathbf{S}_d\mathbf{V}^t_d\mathbf{k}_d + \mathbf{U}_{m2}\mathbf{U}^t_{m2}\boldsymbol{\varepsilon} \quad (9.3.16b)$$

The first term on the right of equations (9.3.16) is nonzero if singular values are truncated before they become zero. There is a good reason for doing this, as section 6.2.5 explains. However if a problem is well-posed (whereby, as explained in previous sections, singular value decomposition becomes equivalent to the Gauss-Newton method), this term disappears. The second and third terms on the right of (9.3.16) constitute vector projections of structural noise ($\mathbf{Z}_d\mathbf{k}_d$) and measurement noise $\boldsymbol{\varepsilon}$ respectively onto the orthogonal complement of the range space of $\mathbf{Z}_m$ (i.e. onto the subspace that is spanned by $\mathbf{U}_{m2}$). Any vector that occupies this subspace cannot be expressed as a linear combination of the columns of $\mathbf{Z}_m$; hence no parameters can be given to the model which will allow it to fit data that is described by this vector. All terms on the right of (9.3.16) lie in this subspace; being therefore "unfitable", they comprise residuals. (Actually, this is not quite true if the calibration-utilized range of $\mathbf{Z}_m$ is slightly reduced from its actual range through singular value truncation; columns of $\mathbf{U}_{m2}$ that are associated with small, but non-zero, singular values of $\mathbf{Z}_m$ span that part of the range space of $\mathbf{Z}_m$ that is not used in the calibration process; see below.)

Equations (9.3.8) and (9.3.10) make it obvious that values estimated for $\mathbf{k}_m$ parameters are likely to be influenced by the fact that a model is defective. Quantification of how much they are thus influenced, the extent to which predictions of future system behaviour will inherit error because of this, and whether any defences can be mounted against contamination of estimated parameters by model defects, are issues which will be addressed shortly.

Equations (9.3.8) and (9.3.10) state that if a model has no defects and hence $\mathbf{k}_d$ is zero, and if no measurement noise is associated with the calibration dataset, then estimated values for all $\mathbf{k}_m$ parameters are "correct" in the sense that $\underline{\mathbf{k}}_m$ is the projection of $\mathbf{k}_m$ onto the solution space of $\mathbf{Z}_m$. With the introduction of model defects, however, the situation becomes more complicated. To the extent that the range space of the $\mathbf{Z}_d$ matrix is aligned with that of the $\mathbf{U}_{m1}$ matrix, expressions of model defects are "captured" by the calibration process and thereby affect values estimated for the solution space projection of $\mathbf{k}_m$ parameters. This happens where $\mathbf{u}_{1mi}$ vectors comprising the columns of $\mathbf{U}_{1m}$ have non-zero projections onto $\mathbf{u}_{dj}$ vectors comprising the columns of $\mathbf{U}_d$ for which corresponding elements of the diagonal $\mathbf{S}_d$ matrix are non-zero. (Diagonal elements of the $\mathbf{S}_{1m}$ matrix are all non-zero by definition). In contrast, equation (9.3.16b) shows that, to the extent that any $\mathbf{u}_{dj}$ vector whose corresponding $\mathbf{S}_d$ singular value is seriously non-zero is orthogonal to all $\mathbf{u}_{1mi}$ vectors (and hence has a non-zero scalar product with one or more $\mathbf{u}_{2mi}$ vectors), the real world system which the model attempts to emulate produces "signals" which the model simply cannot capture, for there is no place within the simplified model to store this information. This contributes to the values of residuals, and hence to model-to-measurement misfit. It becomes the "visible" component of structural noise. However, the component of structural noise that can be (erroneously) absorbed by model parameters (i.e. the part that projects onto $\mathbf{U}_{m1}$) is the invisible (and far more insidious) component of structural noise.

The above can be restated as follows. The model provides a limited number of receptacles for the information content of the calibration dataset. These receptacles are the elements of $\mathbf{k}_m$. Meanwhile, the elements of $\mathbf{k}_d$ are fixed in the defective model that is being used to simulate processes that are operative in an environmental system of interest. Because they are fixed, they do not provide receptacles for information contained within the calibration dataset. Furthermore they may be fixed at values which are different from those of the system under study. Information to this effect may be available through the calibration dataset. Two things can happen to this information, neither of which constitutes its correct fate, namely to provide the means to correct $\mathbf{k}_d$. Some of this information may flow wrongly into $\mathbf{k}_m$ receptacles, as the defective model's $\mathbf{k}_d$ receptacles are closed to the entry of that information. Elements of $\mathbf{k}_m$ are thus awarded erroneous values which compensate for model defects; in doing so they reduce the visible expression of structural noise through "absorbing" some of it. Other aspects of this information simply have nowhere to go. The latter "orphaned" information thus express itself through the only option available to it, namely as residuals that constitute model-to-measurement misfit, or so-called "structural noise".

There is a fundamental difference, however, between "structural noise" and measurement noise. This difference calls into question the everyday practice of lumping the two together and treating them as one from the parameter estimation point of view.

Suppose that an inverse problem is well-posed. Suppose also that, in accordance with recommended practice, weights are chosen such that equation (9.3.2) is obeyed after weight-transformation of the $\mathbf{Z}_m$ matrix. Then the visible component of measurement noise that manifests itself as residuals after minimization of the calibration objective function can be used to estimate the invisible component of this same noise; see equation (5.2.18). It is the invisible component of measurement noise which introduces errors to estimated parameters, as this noise is "absorbed" by the parameter estimation process. In contrast, the visible component of measurement noise appears as the last term in equations (9.3.16). As the same $\boldsymbol{\varepsilon}$ that appears in (9.3.16) also appears in equations (9.3.8) and (9.3.10) (and in simular equations derived in previous chapters which omit model defects), noise-induced parameter error can therefore be estimated. Unfortunately, however, there is no such relationship between the visible and invisible components of structural noise. Without explicit knowledge of $\mathbf{Z}_d$, its visible component says nothing about its invisible component. In fact its visible component may be zero while its invisible component (the component that inflicts errors on parameters) may be substantial; see figure 9.6.

Despite this, some attempts have been made to assign a covariance matrix to structural noise so that it can be treated in a similar way to measurement noise; see for example Cooley (2004) and Cooley and Christensen (2006). These authors show that where the nature of model defects can be characterized stochastically, an empirically-determined covariance matrix of structural noise may sometimes be used to support minimum error variance estimation of averaged parameters over a heterogeneous model domain. If the measurement noise contribution to model-to-measurement misfit is small, however, problems can arise in implementing this procedure. These arise from the fact that the covariance matrix of structural noise may be singular or near-singular. Hence it cannot be inverted and then used as a weighting (i.e. $\mathbf{Q}$) matrix.

Let structural noise be denoted using the vector $\boldsymbol{\eta}$. Hence from (9.3.4)

$$\boldsymbol{\eta} = \mathbf{Z}_d\mathbf{k}_d \tag{9.3.17}$$

Its covariance matrix can then be written as

$$\mathrm{C}(\boldsymbol{\eta}) = \mathbf{Z}_d \mathrm{C}(\mathbf{k}_d) \mathbf{Z}^t_d \qquad (9.3.18)$$

$\mathrm{C}(\boldsymbol{\eta})$ is an $n \times n$ matrix, where $n$ is the number of observations comprising the calibration dataset. The rank of this matrix cannot be greater than the rank of $\mathrm{C}(\mathbf{k}_d)$ from which it is derived. If $\mathrm{C}(\boldsymbol{\eta})$ is not of full rank (i.e. $n$), then it cannot be inverted. It can only be of full rank if the number of elements of $\mathbf{k}_d$ equals or exceeds $n$. This does not occur for the model depicted in figure 9.2. $\mathbf{k}_d$ has a dimension of 1 in this example. It is the single erroneous fixed-head boundary elevation parameter that induces head misfit in all 4 observation wells. Hence the 4×4 covariance matrix of structural noise that is associated with these head observations is singular, and therefore noninvertible. That is why the line of best fit does not pass through any of the measured heads. It is also why, as in this example, structural noise does not "cancel out"; hence more measurements do not reduce the uncertainties of estimated parameters.

In many environmental modelling contexts the calibration dataset is large. Nevertheless structural noise may be dominated by only a few model defects, far fewer defects than there are members of the calibration dataset. (This, after all, can be construed as the mark of a "good model" – a model that can replicate historical system behaviour well.) $\mathrm{C}(\boldsymbol{\eta})$ is therefore likely to approach singularity in most real world modelling contexts. Treating it as if it were measurement noise then becomes impossible. Furthermore, even if it does not approach singularly, neither $\mathbf{Z}_d$ nor $\mathbf{k}_d$ is generally known. Hence inference of the invisible component of structural noise (the component that does the damage) from its visible component (the component that contributes to residuals) is impossible. Its effect on parameter (and predictive) error is therefore impossible to calculate.

### 9.3.3 Unavoidable "Structural Noise"

Suppose that a model has no defects. Equation (9.3.16a) and (9.3.16b) then become

$$\mathbf{r} = \mathbf{U}_{m2}\mathbf{S}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m + \mathbf{U}_{m2}\mathbf{U}^t_{m2}\boldsymbol{\varepsilon} \qquad (9.3.19)$$

Let us suppose that the inverse problem of model calibration is ill-posed. Hence the first term of equation (9.3.19) cannot be eliminated through minimization of an objective function because the objective function does not possess a unique minimum. Instead, when solving a highly-parameterized inverse problem, a less-than-perfect fit is sought with the calibration dataset in order to minimize parameter and predictive error variance in ways that have already been described. Singular value truncation therefore occurs before singular values become zero.

From (9.3.10), parameter error is calculated as

$$\underline{\mathbf{k}}_m - \mathbf{k}_m = -\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m + \mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} \qquad (9.3.20)$$

Let $w$ mark the singular value truncation point above which the null space is deemed to begin. The scalar projection of parameter error onto the $i$'th unit vector of the $\mathbf{V}_m$ matrix is then

$$e_i = \mathbf{v}^t_{mi}(\underline{\mathbf{k}}_m - \mathbf{k}_m) = s^{-1}_{mi}\mathbf{u}^t_{mi}\boldsymbol{\varepsilon} \qquad \text{for } i \le w \qquad (9.3.21a)$$

$$e_i = \mathbf{v}^t_{mi}(\underline{\mathbf{k}}_m - \mathbf{k}_m) = -\mathbf{v}^t_{mi}\mathbf{k} \qquad \text{for } i > w \qquad (9.3.21b)$$

From (3.9.1), (9.3.2) and (9.3.3), and recalling that $\mathbf{v}_i$ and $\mathbf{u}_i$ are unit vectors, the variance of

each of these error terms is

$$\sigma^2_{ei} = s^{-2}_{\mathrm{m}i}\sigma^2_{\varepsilon} \qquad \text{for } i \le w \qquad (9.3.22a)$$

$$\sigma^2_{ei} = \sigma^2_{\mathrm{k}} \qquad \text{for } i > w \qquad (9.3.22b)$$

Following from the discussion of section (6.2.5) truncation should occur where these terms are about equal. Beyond this truncation point the benefits of estimating the value of a parameter's projection onto a particular $\mathbf{v}_{\mathrm{m}i}$ vector are outweighed by the potential for error that is associated with this estimation. From the above equations, this occurs where

$$s^2_{\mathrm{m}i} = \frac{\sigma^2_{\varepsilon}}{\sigma^2_{\mathrm{k}}} \qquad (9.3.23)$$

From (9.3.19) the residuals vector **r** can be expressed as

$$\mathbf{r} = \sum_{i=w+1}^{n} \mathbf{u}_{\mathrm{m}i}\left(s_{\mathrm{m}i}\mathbf{v}^{\mathrm{t}}_{\mathrm{m}i}\mathbf{k}_{\mathrm{m}} + \mathbf{u}^{\mathrm{t}}_{\mathrm{m}i}\boldsymbol{\varepsilon}\right) = \sum_{i=w+1}^{n} \eta_i \mathbf{u}_{\mathrm{m}i} \qquad (9.3.24)$$

where $\eta_i$ is defined by the above equation. From (3.9.2) the variance of each of the $\eta_i$ variables featured in equation (9.3.24) is

$$\sigma^2_{\eta i} = s^2_{\mathrm{m}i}\sigma^2_{\mathrm{k}} + \sigma^2_{\varepsilon} \qquad (9.3.25)$$

At truncation, where (9.3.23) prevails, this becomes

$$\sigma^2_{\eta i} = 2\sigma^2_{\varepsilon} \qquad (9.3.26)$$

As $i$ increases, and $s^2_{\mathrm{m}i}$ falls below the value given in (9.3.23), the contribution that $\sigma^2_{\varepsilon}$ makes to $\sigma^2_{\eta i}$ dominates that made by $s^2_{\mathrm{m}i}\sigma^2_{\mathrm{k}}$. Eventually it becomes the sole contributor to residual components as singular values fall to zero.

From the above discussion it follows that even where a model has no defects, there is an unavoidable component of model-to-measurement misfit which does not have its origins in measurement noise. Nor does it have its origins in model defects. It has "structure", in that it projects onto each of the $\mathbf{u}_{\mathrm{m}i}$ differently. However it does not project onto those $\mathbf{u}_{\mathrm{m}i}$ for which $i$ is at or below the singular value truncation point. Hence it induces no error in estimated parameters. Nevertheless it is visible. Furthermore, in circumstances where singular values do not decay rapidly to zero, its size may be commensurate with model-to-measurement misfit induced by random measurement noise.

## 9.4 Defence against Structural Noise

### 9.4.1 Theory

Equations (9.3.8) and (9.3.10) show that calibration of a defective model may induce errors in the estimation of some parameters. We now investigate whether it is possible to calibrate a defective model in a way that affords parameters some protection from these errors.

Let us suppose that we can find an orthonormal matrix **W** which has the following important property

$$\mathbf{W}\mathbf{W}^{\mathrm{t}}\mathbf{Z}_{\mathrm{d}} \approx \mathbf{0} \qquad (9.4.1)$$

$\mathbf{W}\mathbf{W}^{\mathrm{t}}$ is thus an orthogonal projection operator. Decomposing $\mathbf{Z}_{\mathrm{d}}$ through (9.3.9) we obtain

$$\mathbf{W}\mathbf{W}^t\mathbf{U}_d\mathbf{S}_d\mathbf{V}^t_d \approx \mathbf{0} \qquad (9.4.2)$$

From (9.4.1), **W** is chosen such that all of its columns are orthogonal to all of the columns of $\mathbf{Z}_d$ (or at least approximately so). If the $\mathbf{Z}_d$ matrix does not have many columns (because the number of $\mathbf{k}_d$ parameters is small), then it should not be too hard to find such a matrix. For reasons which will become obvious in a moment, the larger is the range space of **W** (that is, the larger the number of linearly independent columns that **W** contains) the more useful will this matrix be. A small dimensionality of $\mathbf{k}_d$ assists in this pursuit.

As any environmental model is likely to be replete with defects, the number of elements comprising $\mathbf{k}_d$ is likely to be large. However, as stated above, in many circumstances a few obstinate defects are likely to dominate the others, for if a model is defective in too many ways it cannot be used. The number of seriously non-zero singular values featured in the diagonal $\mathbf{S}_d$ matrix is thus likely to be small. The columns of **W** need only be orthogonal to those columns of $\mathbf{U}_d$ for which corresponding $\mathbf{S}_d$ singular values are significantly non-zero.

If (9.3.4) is pre-multiplied by $\mathbf{W}^t$, we obtain

$$\mathbf{W}\mathbf{W}^t\mathbf{h} = \mathbf{W}\mathbf{W}^t\mathbf{Z}_m\mathbf{k}_m + \mathbf{W}\mathbf{W}^t\mathbf{Z}_d\mathbf{k}_d + \mathbf{W}\mathbf{W}^t\boldsymbol{\varepsilon} \approx \mathbf{W}\mathbf{W}^t\mathbf{Z}_m\mathbf{k}_m + \mathbf{W}\mathbf{W}^t\boldsymbol{\varepsilon} \qquad (9.4.3)$$

Equation (9.4.3) defines an inverse problem through which solution for $\mathbf{k}_m$ can be sought. Because of (9.4.1) and (9.4.2), **W** must have fewer columns than rows if all of these columns are linearly independent, for if it is of full rank then $\mathbf{W}^t$ cannot possess a null space. The more linearly independent columns does **W** possess, the more of the information content of **h** does $\mathbf{W}\mathbf{W}^t$ preserve.

Equation (9.4.3) transforms an inverse problem in which there are *n* observations into one in which there are effectively fewer than *n* observations. Under favourable conditions this may not reduce the dimensionality of the calibration solution space; the fewer the number of parameters that are being estimated (i.e. the fewer is the number of elements in $\mathbf{k}_m$) the more likely is this to be the case. Note however, that with fewer observations effectively comprising the calibration dataset, errors in estimated parameters induced by measurement noise may be higher because (supposedly random) measurement noise has less opportunity to cancel out. Under less favourable conditions, however, it may not be possible to estimate as many parameters as is possible without pre-multiplication of (9.3.4) by $\mathbf{W}\mathbf{W}^t$. However parameter combinations that thereby become inestimable are those whose estimates would have been contaminated by structural noise anyway.

### 9.4.2 Practice

In everyday modelling practice, it is generally not too difficult to find ways of processing field measurements and corresponding model outputs in ways that "orthogonalize out" (i.e. filter out) at least the worst manifestations of model-generated structural noise.

For example, when calibrating a groundwater model, vertical differences in heads between model layers can be used explicitly in the calibration process rather than (or in addition to) heads in individual layers. Intuitively this makes sense. Vertical head differences may be small; however they are likely to be rich in information on the vertical conductance of an aquitard which separates model layers representing aquifers. For many models the integrity of calculated head differences is likely to be maintained even if the integrity of individual heads from which these differences are calculated is likely to be degraded by errors in representation of recharge and boundary conditions. If using PEST, these head differences

can be placed into an observation group that is separate from that containing head measurements. They can then be weighted to guarantee visibility of the pertinent objective function component in the overall objective function.

The benefits of matching lateral head differences calculated by a model to observed lateral head differences was discussed above; see figure 9.5.

A similar logic applies to temporal head differences calculated by a groundwater model, especially where this model is being used to support water use sustainability. The information content of temporal head differences with respect to storage and recharge-related parameters employed by a model is likely to be high, notwithstanding the fact that these differences may be small in relation to the heads themselves, and that the integrity of model-calculated heads from which these differences are calculated may be degraded by defective boundary conditions or erroneous representation of permeability heterogeneity. By extracting these temporal differences from head observations and corresponding model outputs before matching them, and by then assigning weights to temporal head differences that guarantee their visibility in the overall objective function, the calibration process is empowered to endow the model with parameters that allow it to replicate these temporal head differences, even if it cannot replicate the individual heads themselves. Integrity of estimation of parameters to which these differences are sensitive is thereby enhanced.

In surface water model calibration a modeller may, in similar fashion, formulate a multi-component objective function in which a stream flow time series is processed in a number of different ways in order to expose to the calibration process different aspects of that time series that are rich in information pertaining to different sets of watershed properties. For example, peak flows are informative of surface parameters such as roughness; post-peak recessions are informative of soil moisture store parameters; base flows are informative of groundwater store parameters; monthly-averaged flows are informative of parameters controlling seasonality of evapotranspiration, etc. For each type of processing to which the flow time series is subjected, a different objective function component can be calculated by comparing processed outcomes of the observed flow time series with similarly processed outcomes of the modelled flow time series. The overall calibration dataset then includes all of these outcomes of time series processing. Weights applied to individual processing outcomes should be such as to guarantee visibility of each in the overall objective function.

Procedures such as these use the same calibration dataset in different ways. Hence they do not explicitly implement equation (9.4.3). Moreover, they actually increase the number of elements in the calibration dataset beyond that of the original **h**, thus creating a model matrix that has far more rows than previously. At the same time, the weighting scheme is unashamedly pragmatic. In theory, use of equation (9.4.3) would require adoption of a transformed measurement noise vector $\boldsymbol{\tau}$ calculated as

$$\boldsymbol{\tau} = \mathbf{W}\mathbf{W}^t\boldsymbol{\varepsilon} \qquad (9.4.4)$$

From (9.3.2), the covariance matrix associated with this transformed noise becomes

$$C(\boldsymbol{\tau}) = \sigma^2_{\varepsilon}\mathbf{W}\mathbf{W}^t \qquad (9.4.5)$$

$C(\boldsymbol{\tau})$ is rank-deficient and hence non-invertible. Hence an "ideal" **Q** matrix for use in the calibration process cannot be obtained through inversion of $C(\boldsymbol{\tau})$.

In spite of this, the above heuristic strategy for defending the inversion process against model-defect-incurred error has distinct benefits. The nature and extent of model structural

defects will never be exactly known. Hence determination of a suitable **W** for use in equation (9.4.3) can only ever be approximate. In fact, a modeller may not even be sure whether, in a particular modelling context, it is required at all. Meanwhile he/she may feel uncomfortable about reducing the effective size of the calibration dataset through undertaking the filtering operation implied by $\mathbf{WW}^t$, and possibly thereby decreasing the dimensions of the calibration solution space. This will especially be the case if he/she is unsure of whether, and how much, the calibration process is actually affected by model defects. He/she may decide that the best strategy for handling potential model defects is to "place a bet each way". The modeller can do this by using the calibration dataset in its original form, as well as in a processed form, or in multiply-processed forms. Weight-balancing of the different objective function components then becomes a subjective matter. It is probably best for the modeller to adopt a pragmatic weighting strategy based on the practical philosophy that if an objective function component is worth formulating, then it should be visible in the overall calibration objective function. It is thereby protected against dominance of another objective function component, at the same time as it is not allowed to dominate the objective function itself.

The above pragmatic approach to formulation of a multi-component objective function acknowledges the fact that environmental models are defective. However it also acknowledges the fact that the exact nature of their defects cannot generally be known. It requires that the modeller employ his/her understanding of the environmental system which is being modelled to formulate objective function components that effectively "distil" from the calibration dataset the various types of information that are present within that dataset in ways that provide the model calibration process with some immunity from the worst effects of structural noise. To be sure, some information may be repeated in the expanded calibration dataset. However if the modeller cannot be sure which repetition gives the calibration process greater immunity from the effects of model defects of which he/she has little knowledge, then there is little choice other than to present this information in more than one way. Parameter estimation errors will be ameliorated to some extent if one of these ways delivers the desired protection from model defects.

Because the nature of model defects can often only be guessed, and because the defects that have the most insidious effects on model parameters are actually invisible to the modeller, the strategy which a modeller adopts as his/her means of accommodating them during calibration of a model will necessarily be subjective. In some contexts it may involve formulation of a multi-component objective function in the manner described above. In other contexts a modeller may purposefully limit the information that a calibration dataset is allowed to convey to model parameters for fear of that information doing more harm than good. In this case the **W** matrix of equation (9.4.1) may possess far fewer columns than rows, and the information content of the calibration dataset will be limited rather than duplicated. Whatever measure is taken, the purpose is the same, namely to provide the model with a calibration dataset that it can partially or wholly fit "with safety". That is, it can be fit without inducing bias in $\mathbf{k}_m$ parameters born of the necessity for them to compensate for erroneous values awarded to $\mathbf{k}_d$ parameters in the model construction process. This strategy may not necessarily result in a good fit with the calibration dataset; however it may result in a "safe fit".

It is important to note however that, as will be discussed in detail later in this chapter, prevention of bias in estimates of $\mathbf{k}_m$ parameter values may or may not be a good thing. This depends on the predictions that are required of the model. For some predictions, the ability of

$\mathbf{k}_m$ parameters to adopt biased values that compensate for model defects may allow these defects to be effectively "calibrated out" as far as the making of those predictions is concerned. For other predictions the bias introduced to $\mathbf{k}_m$ parameters through the model calibration process may be transferred directly to the predictions themselves; for these predictions model calibration may do more harm than good. We will return to this point shortly.

## 9.5 Defect-Inducing Model Simplification: a Pictorial Representation

Figure 9.8 depicts three-dimensional parameter space with orthogonal axes which coincide with the three parameters that define this space. Two of the parameters specified by these axes are "m" parameters; that is, they are adjustable parameters in a defective model of an environmental system. The third parameter is a "d" parameter. Hence its value is hardwired into the defective model's construction. Let us assume that, collectively, the three parameters span the entirety of parameter space. Hence replication of past and future system behaviour is possible using these three parameters.

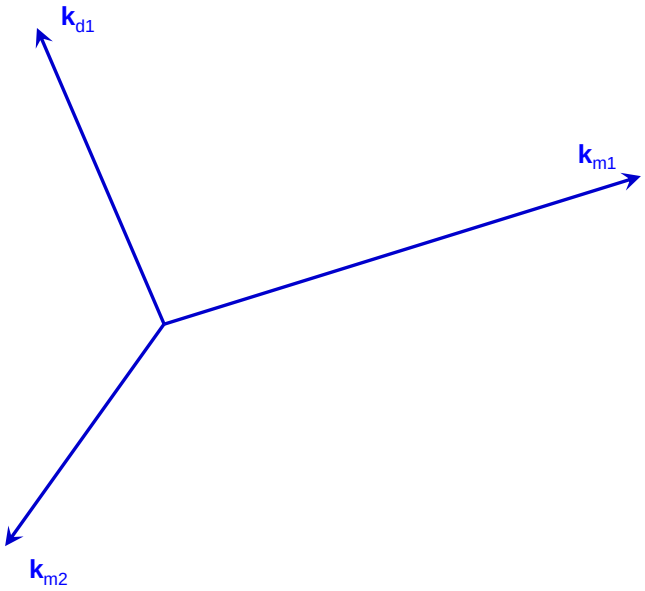


**Figure 9.8. Two "m" parameters and one "d" parameter; collectively they span the entirety of parameter space. This and figures to follow are modified from Doherty and Christensen (2011).**

Let the matrix $\mathbf{Z}$ denote the "reality" model of the system. (The modeller does not have access to this model; he/she has access only to the $\mathbf{Z}_m$ model). Thus

$$\mathbf{h} = \mathbf{Z}\begin{bmatrix}\mathbf{k}_m \\ \mathbf{k}_d\end{bmatrix} + \boldsymbol{\varepsilon} = \begin{bmatrix}\mathbf{Z}_m & \mathbf{Z}_d\end{bmatrix}\begin{bmatrix}\mathbf{k}_m \\ \mathbf{k}_d\end{bmatrix} + \boldsymbol{\varepsilon} = \mathbf{Z}_m\mathbf{k}_m + \mathbf{Z}_d\mathbf{k}_d + \boldsymbol{\varepsilon} \qquad (9.5.1)$$

Let the real world model matrix $\mathbf{Z}$ is subjected to singular value decomposition, so that

$$\mathbf{Z} = \mathbf{USV}^t \qquad (9.5.2)$$

The three $\mathbf{v}_i$ vectors that comprise the columns of $\mathbf{V}$ are added to the three native model parameter vectors in figure 9.9. $\mathbf{v}_1$ and $\mathbf{v}_2$ span the solution space of $\mathbf{Z}$ while $\mathbf{v}_3$ spans its null space.

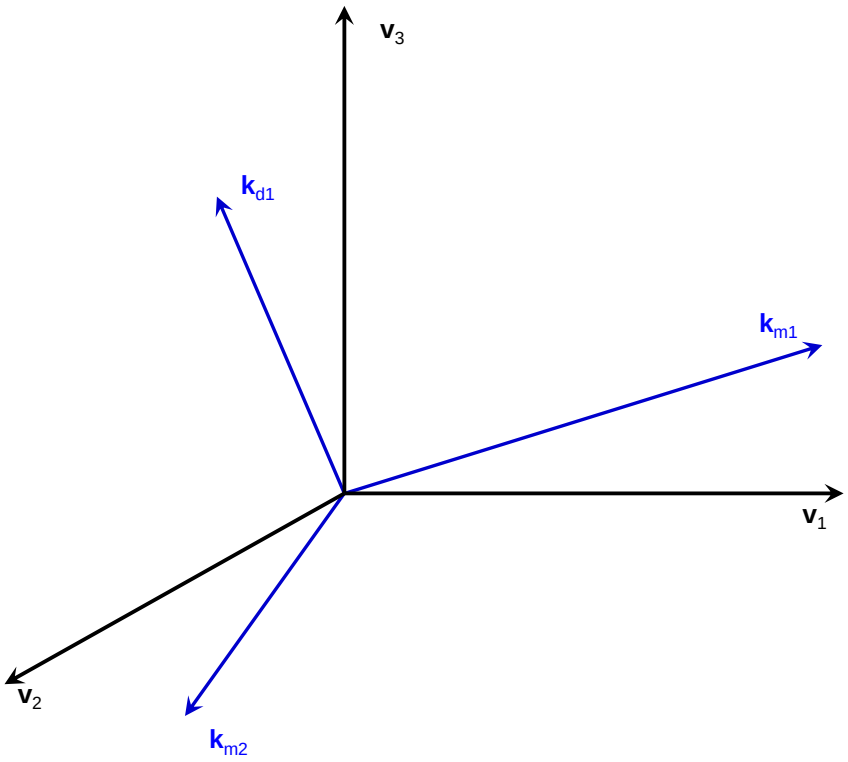


**Figure 9.9. Model parameters together with the eigencomponents (shown in black) of the real world model matrix Z.**

Let the vector **k** represent the three parameters of the real world model **Z**. Suppose that it is possible to actually build and then calibrate this model. The calibration process of the **Z** model would yield the vector $\underline{\mathbf{k}}$ shown in figure 9.10. This is the projection of **k** onto the solution space of the real world model matrix **Z**. This estimate of parameters is not, of course, correct. But it is of minimum error variance (and hence without bias) because the parameter set $\underline{\mathbf{k}}$ allows model outputs to fit the calibration dataset to a level that is commensurate with measurement noise while possessing no null space components; the latter are, by definition, unsupported by the calibration dataset.

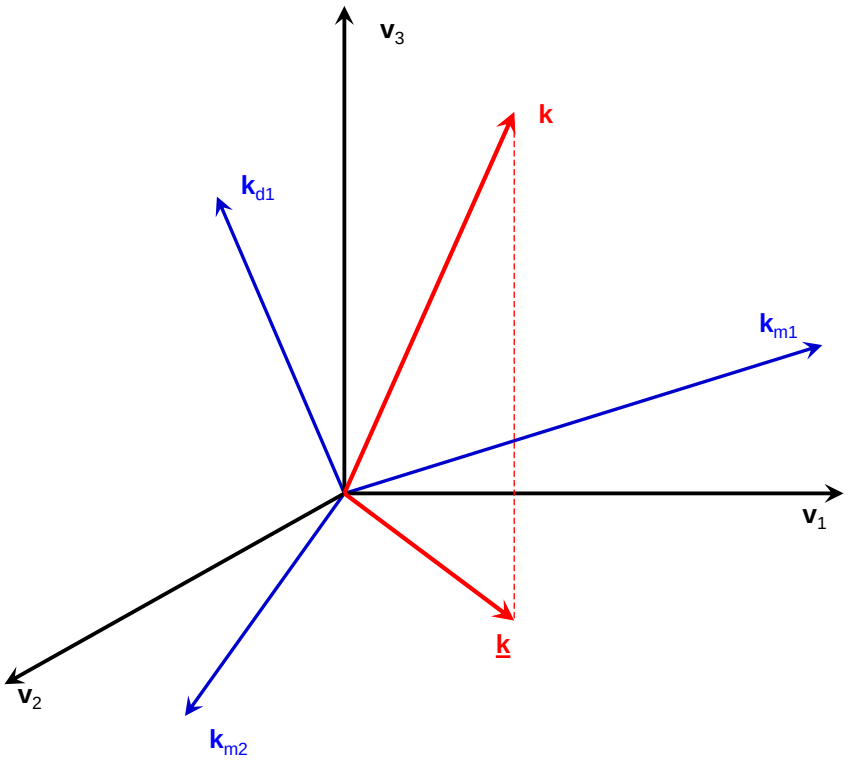


**Figure 9.10. True model parameter set k and parameter set $\underline{\mathbf{k}}$ (shown in red) that would be estimated through an "ideal" calibration process undertaken using the real world model Z.**

Unfortunately, the real world model **Z** cannot be calibrated because a modeller does not have access to it. He/she can only calibrate the simplified model $\mathbf{Z}_m$. It is through estimation of "m" parameters that a good fit is thereby sought with the calibration dataset. In the present example there are just two of these, namely $k_{m1}$ and $k_{m2}$, these comprising the $\mathbf{k}_m$ parameter set. Meanwhile the third parameter $k_d$ of the real world model is fixed at a certain value, this value being implied in construction of the simplified, defective model.

As the dimensionality of the solution space of **Z** is two, the two parameters of the simplified $\mathbf{Z}_m$ model are enough to support a good fit between its outputs and the calibration dataset (provided that neither of its parameters lies entirely within the null space of **Z**). Let $\underline{\mathbf{k}}_m$ denote the parameter set achieved through calibration of the $\mathbf{Z}_m$ model. The vector corresponding to this parameter set must lie in the $k_{m1}/k_{m2}$ plane. At the same time, its projection onto the solution space of the real world model (i.e. the space spanned by $\mathbf{v}_1$ and $\mathbf{v}_2$) must be $\underline{\mathbf{k}}$; if this is not the case then $\underline{\mathbf{k}}_m$ would not allow the model to fit the calibration dataset. This is depicted in figure 9.11.

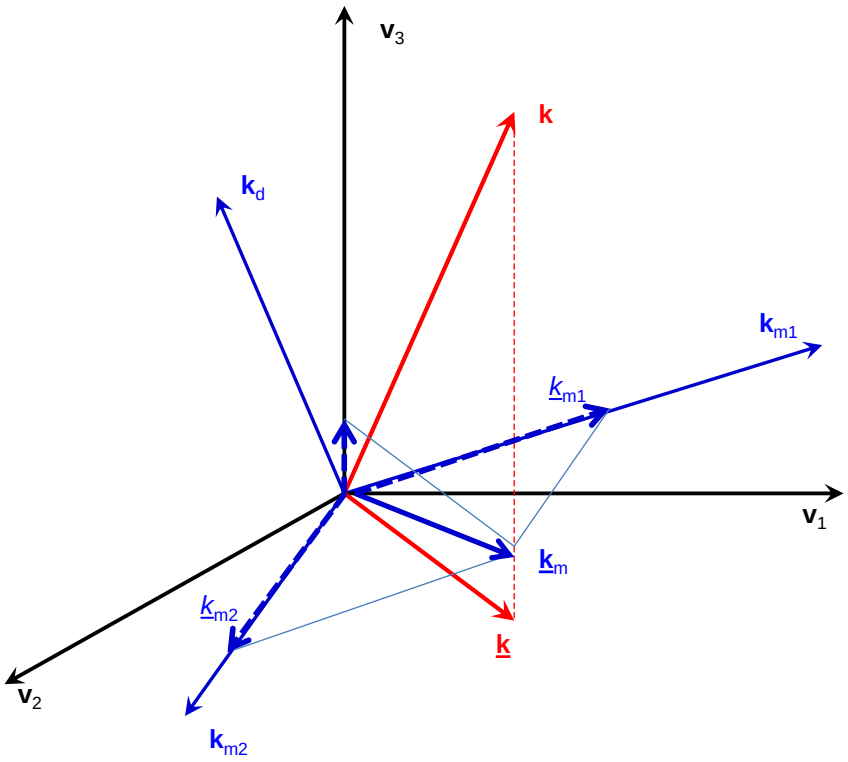


**Figure 9.11. Calibration of the $\mathbf{Z}_m$ model through adjustment of only $k_{m1}$ and $k_{m2}$ with $k_d$ fixed (at zero in this figure) leads to the vector $\underline{\mathbf{k}}_m$ (shown in blue) which projects onto the solution space of the real world model $\mathbf{Z}$ as $\underline{\mathbf{k}}$.**

Immediately apparent from figure 9.11 is the fact that the projection of $\underline{\mathbf{k}}_m$ onto the $\mathbf{v}_3$ axis is non-zero. Hence the solution of what is in reality a three-parameter, ill-posed inverse problem is non-optimal. This occurs because solution of that problem was obtained in a two-dimensional subspace that is not aligned with that which is obtained through singular value decomposition of the real world model $\mathbf{Z}$. Because this subspace is non-orthogonal to the solution space of $\mathbf{Z}$ it is possible to find a $\underline{\mathbf{k}}_m$ vector which fits the calibration dataset. However because it has a nonzero projection onto the null space of $\mathbf{Z}$, this vector has a non-zero projection onto that space. Optimality of solution to the inverse problem is therefore lost.

A paradox here is that $k_d$ is fixed at zero in figure 9.11; according to the concepts that underpin all linear analysis that has been undertaken so far in this text, this is its minimum error variance estimate from an expert knowledge point of view. In reality, of course, $k_d$ is probably not zero, for it has variability that is described by its variance. If the acknowledged variability of all three of the real world model parameters is taken into account, together with the information content of the calibration dataset, which is somewhat informative of all three model parameters but not completely informative of any of them (because none of them has zero projection onto the null space of $\mathbf{Z}$), the best "calibrated" value for $\underline{k}_d$ to take is given by the projection of $\mathbf{k}$ (and not $\mathbf{k}_m$) onto the $k_d$ parameter axis. Collectively $\underline{k}_{m1}$, $\underline{k}_{m2}$ and $\underline{k}_d$ will then have minimum error variance status from a post-calibration point of view; at the same time, the resulting vector $\underline{\mathbf{k}}$ will have zero projection onto the null space of $\mathbf{Z}$.

Suppose that $k_d$ differs from zero. Then a vector of length $k_d$ in the direction of the $k_d$ axis (we call this vector $\mathbf{k}_d$) has a non-zero projection onto the $\mathbf{v}_1/\mathbf{v}_2$ solution space of the real world

model **Z**. In calibrating the $\mathbf{Z}_m$ model, the projection of $\mathbf{k}_d$ onto the $\mathbf{v}_1/\mathbf{v}_2$ subspace must be added to the projections of the $\underline{k}_{m1}$ and $\underline{k}_{m2}$ components of $\underline{\mathbf{k}}_m$ onto that subspace such that the total projection of $\underline{\mathbf{k}}_m$ plus $\mathbf{k}_d$ has the correct projection onto the $\mathbf{v}_1/\mathbf{v}_2$ subspace. The correct projection of $\underline{\mathbf{k}}_m+\mathbf{k}_d$ onto the $\mathbf{v}_1/\mathbf{v}_2$ subspace is, once again, $\underline{\mathbf{k}}$. Given that the $\mathbf{v}_1/\mathbf{v}_2$ subspace is two dimensional, and that unit vectors in the $k_{m1}$ and $k_{m2}$ directions are orthogonal to each other and to $\mathbf{k}_d$, it will always be possible to achieve the correct projection onto $\underline{\mathbf{k}}$ regardless of the value of $k_d$. However the values that the individual $k_{m1}$ and $k_{m2}$ parameters must take to achieve this correct projection will depend on the value of $k_d$. Hence the values that $k_{m1}$ and $k_{m2}$ take through the calibration process (namely $\underline{k}_{m1}$ and $\underline{k}_{m2}$) are dependent on the nature and magnitude of the model's defects. At the same time, the total $\mathbf{k}_d+\underline{\mathbf{k}}_m$ vector is likely to have a non-zero projection onto the null space of the real world model **Z**.

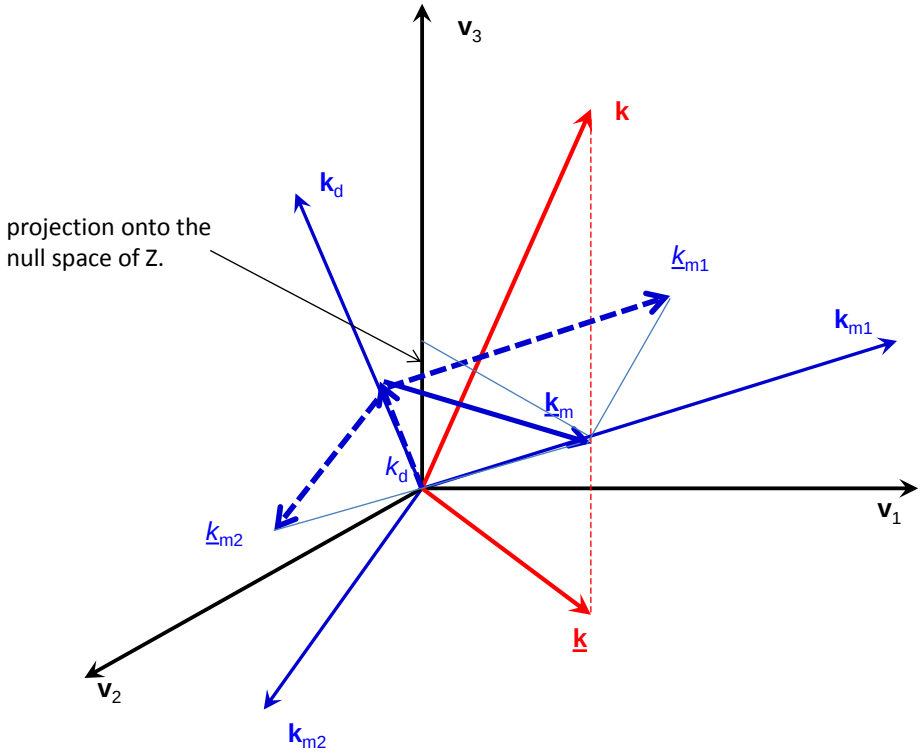


**Figure 9.12. Same as figure 9.11, but with $k_d$ having a non-zero value.**

It is the calibration dataset **h**, together with its information content, that define **Z**, the singular value decomposition of **Z**, and the **V** matrix that emerges from singular value decomposition of **Z**. For the model illustrated in the above figures, the calibration dataset has information which can resolve two *combinations* of parameters, but cannot resolve any *individual* parameter. Each of the three model parameters $k_{m1}$, $k_{m2}$ and $k_d$ project partly onto the solution space of **Z** and partly onto its null space. Because the information content of the calibration dataset is shared between them, and because none of them can be resolved individually, the fixing of a value for any one of these parameters creates a well-posed inverse problem through which values can be estimated for the other two. However these values are dependent on the value ascribed to the fixed parameter. Hence any error in the value ascribed to the fixed parameter will be immediately transferred to the adjustable parameters. Unfortunately the value at which the fixed parameter is actually fixed, is unlikely to be optimal from the point of view of a calibration process that takes into account the true unknown status of all

three parameters. That value is determined through projection of $\underline{\mathbf{k}}$ (the ideal solution to the inverse problem based on the real world model matrix **Z**) onto each of the individual parameter axes. $\underline{\mathbf{k}}$, of course, has a projection of zero onto the null space of **Z**.

Construction of a model which is a necessarily simplified representation of reality thus constitutes an imperfect regularization device. Just as optimal regularization can be defined, so too can optimal simplification. In fact the two definitions are aligned. If construction of a model $\mathbf{Z}_m$ is such that simplifications of the real world **Z** model that are implied in its construction coincide with those which would have been obtained through singular value decomposition of **Z**, then $\mathbf{Z}_m$ model construction is optimal. (Of course Kahunen-Loève pre-transformation of real world model parameters is also required for attainment of model simplification optimality; in the present example we assume that $k_d$, $k_{m1}$ and $k_{m2}$ are statistically independent.)

If $\mathbf{Z}_m$ model construction is such that $\mathbf{k}_d$ parameters which define the $\mathbf{Z}_m$ model's defects lie entirely within the null space of **Z**, this is a reasonable construction outcome, for these parameters then have no effect on **Z** model outputs under calibration conditions; hence they have no opportunity to induce errors in $\mathbf{k}_m$ parameters which are adjusted as the $\mathbf{Z}_m$ model is calibrated. They do have the capacity, of course, to introduce errors to $\mathbf{Z}_m$ model predictions that are sensitive to these $\mathbf{k}_d$ defect parameters. However if the $\mathbf{Z}_m$ model's specifications have been tuned to the predictions that it is required to make, then predictions which are unduly sensitive to $\mathbf{k}_d$ parameters will not be required of the model.

If $\mathbf{Z}_m$ model construction is such that $\mathbf{k}_d$ does not lie in the null space of **Z**, yet the real world simplification process through which $\mathbf{Z}_m$ is built from **Z** is nevertheless aligned with subspaces defined by singular value decomposition of **Z**, then simplification will indeed affect **Z** model outputs that are used in the $\mathbf{Z}_m$ calibration process. However $\mathbf{Z}_m$ model specifications have still achieved the useful outcome that no parameter of the $\mathbf{Z}_m$ model is given the opportunity to compensate for $\mathbf{Z}_m$ model inadequacies as it is calibrated. Calibration of the $\mathbf{Z}_m$ model cannot, therefore, introduce bias to any of its parameters while attempting to estimate them.

Strategies for filtering out structural noise which were described in the preceding section can be seen as attempts to re-align **Z**-matrix-decomposition implied by simplifications required for $\mathbf{Z}_m$ model construction with singular value decomposition of the **Z** model matrix. For the three parameter example described in the previous illustrations, such a process would attempt to remove all information from the calibration dataset that is sensitive to the $k_d$ parameter. $k_d$ is therefore relegated to the null space of the revised (as far as the calibration process is concerned) **Z** model This precludes the possibility of $k_{m1}$ and $k_{m2}$ parameters compensating for an erroneous $k_d$ value.

Yet another important lesson about defective model calibration can be learned from the above three parameter example. Suppose that no steps are taken to mitigate the repercussions of assigning an erroneous value to $k_d$. As has been shown, this does not mean that the simplified, defective $\mathbf{Z}_m$ model cannot be calibrated to achieve a good fit with the calibration dataset. Regardless of the value taken by $k_d$, values for $k_{m1}$ and $k_{m2}$ can be found such that $\underline{\mathbf{k}}_m + \mathbf{k}_d$ projects exactly onto $\underline{\mathbf{k}}$. The latter vector is the optimal solution to the ill-posed inverse problem; it is that which would have been obtained (if this were possible) through singular value decomposition of the real world **Z**, while acknowledging the mutual adjustability of both $\mathbf{k}_d$ and $\mathbf{k}_m$. A direct consequence of this is that any prediction that is sensitive solely to

solution space components of the **Z** matrix (as distinct from solution space components of the $\mathbf{Z}_m$ matrix), will be unaffected by the compensatory roles that $k_{m1}$ and $k_{m2}$ may need to play in calibrating the defective model. In general, predictions which tend to be sensitive solely to solution space parameter components of the real world model tend to be those that are similar in nature and location to measurements comprising the calibration dataset.

## 9.6 Defect-Induced Predictive Error

### 9.6.1 Linear Analysis

*9.6.1.1 Formulation of Equations*

From equation (9.3.8) the error in estimated $\mathbf{k}_m$ parameters is given by

$$\underline{\mathbf{k}}_m - \mathbf{k}_m = -\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m + \mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d\mathbf{k}_d + \mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} \qquad (9.6.1)$$

As usual, let $s$ be a prediction of management interest. Its true value is given by

$$s = \mathbf{y}^t_m\mathbf{k}_m + \mathbf{y}^t_d\mathbf{k}_d \qquad (9.6.2)$$

where the vector $\mathbf{y}_m$ expresses sensitivities of $s$ to $\mathbf{k}_m$ model parameters while the vector $\mathbf{y}_d$ expresses sensitivities of $s$ to $\mathbf{k}_d$ parameters. However the value of the prediction made by the defective, calibrated model is given by

$$\underline{s} = \mathbf{y}^t_m\underline{\mathbf{k}}_m \qquad (9.6.3)$$

Equation (9.6.3) assumes that $\mathbf{k}_d$ is fixed at zero in the defective model. This is its prior expected value. It is reasonable to assume that any simplification strategy would attempt to achieve this conceptual outcome.

The error in the prediction is calculated by subtracting (9.6.2) from (9.6.3) to obtain

$$\underline{s} - s = \mathbf{y}^t_m(\underline{\mathbf{k}}_m - \mathbf{k}_m) - \mathbf{y}^t_d\mathbf{k}_d \qquad (9.6.4)$$

After substitution of (9.6.1) into (9.6.4) followed by some simplification, we obtain

$$\underline{s} - s = -\mathbf{y}^t_m\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m + \mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} + (\mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d - \mathbf{y}^t_d)\mathbf{k}_d \qquad (9.6.5)$$

Under the assumption that $\mathbf{k}_m$ and $\mathbf{k}_d$ are statistically independent, predictive error variance can then be calculated as follows

$$\begin{aligned}\sigma^2_{\underline{s}-s} = {} & \mathbf{y}^t_m\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathrm{C}(\mathbf{k}_m)\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathbf{y}_m + \mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\mathrm{C}(\boldsymbol{\varepsilon})\mathbf{U}_{m1}\,\mathbf{S}^{-1}{}_{m1}\mathbf{V}^t_{m1}\mathbf{y}_m + \\ & (\mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d - \mathbf{y}^t_d)\mathrm{C}(\mathbf{k}_d)(\mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d - \mathbf{y}^t_d)^t \end{aligned} \qquad (9.6.6)$$

This equation can be simplified by making use of the assumptions embodied in equations (9.3.2) and (9.3.5). Let the following additional assumption also be made

$$\mathrm{C}(\mathbf{k}_d) = \sigma^2_{kd}\mathbf{I} \qquad (9.6.7)$$

Equation (9.6.6) then becomes

$$\begin{aligned}\sigma^2_{\underline{s}-s} = {} & \sigma^2_{km}\mathbf{y}^t_m\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathbf{y}_m + \sigma^2_{\varepsilon}\mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-2}{}_{m1}\mathbf{V}^t_{m1}\mathbf{y}_m + \\ & \sigma^2_{kd}\,(\mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d - \mathbf{y}^t_d)\,(\mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d - \mathbf{y}^t_d)^t \end{aligned} \qquad (9.6.8)$$

The first two terms on the right side of equation (9.6.8) are identical to those on the right of equation (6.2.32). As was discussed in section (6.2.5) and illustrated in figure 6.4, they can be used to compute the point at which singular values are best truncated. If truncation takes

place at too few singular values, the calibration process has effectively denied passage of information from the calibration dataset to model parameters that could have reduced the error variances of those parameters, and of predictions that are sensitive to them. However if truncation takes place too late, then the information content of the calibration dataset becomes excessively contaminated by noise associated with that dataset as it passes from observations to parameters. Estimates of parameters therefore lose their credibility.

The contribution that simplifications required for model construction make to predictive error variance is described by the third term on the right side of (9.6.8). Unfortunately a modeller cannot calculate this term as he/she does not have access to the $\mathbf{Z}_d$ matrix that simulates differences between his/her model and the real world, nor to the parameters $\mathbf{k}_d$ on which $\mathbf{Z}_d$ operates. Nevertheless this term can have a significant impact on predictive error variance, and on optimization of predictive error variance.

Lack of direct access to $\mathbf{Z}_d$ and $\mathbf{k}_d$ does not necessarily mean that equation (9.6.8) is unusable. In everyday modelling practice, calculations based on equation (9.6.8) can proceed if a modeller introduces extra parameters to his/her model to represent at least some of the environmental system complexity that his/her model ignores. These will often be parameters that a modeller would not actually adjust through the calibration process, but for which calibration and predictive sensitivities can nevertheless be calculated for inclusion in the $\mathbf{Z}_d$ matrix and the $\mathbf{y}_d$ vector used in equation (9.6.8). In some cases these parameters may be viewed as surrogates for other types of complexity that separate the model from the real world system that it is meant to portray.

By way of example, for the purposes of linear analysis using (9.6.8) a groundwater modeller may parameterize boundary conditions of his/her model. Values associated with boundary conditions are therefore "adjustable" for the purpose of sensitivity calculation instead of being fixed at values that are deemed to be most likely as they may be when the model is calibrated. He/she may also parameterize historical pumping rates that would otherwise be endowed with assumed values that are not actually well known. A geothermal or oil reservoir modeller may add dual porosity parameters to a single porosity model in order to use equation (9.6.8) to determine whether failure to represent dual porosity subsurface flow in his/her model is really detrimental to the model's capacity to predict reservoir behaviour. Of particular interest is the issue of whether calibration of a single porosity model of a dual porosity system introduces bias to calibrated single porosity parameters that compromises the model's ability to make predictions which are important for future reservoir management. A surface water modeller may add time- and space-varying historical rainfall factors to the parameter set employed by his/her model in order to explore the repercussions of calibrating that model against rainfall events of which he/she is somewhat unsure of the temporal and spatial distribution. In all of these examples, implementation of equation (9.6.8) requires only that sensitivities with respect to the added parameters be calculated. It does not require that the more complex model be actually calibrated. Nor does it require that it be subjected to calibration-constrained uncertainty analysis.

Equation (9.6.8) indicates that computation of predictive error variance where the existence of model defects is acknowledged, requires the summation of three terms, rather than the two that would be required if a model was a perfect simulator of real world processes. These terms sum to the total predictive error variance. Figure 9.13 modifies figure 6.4 to illustrate this.

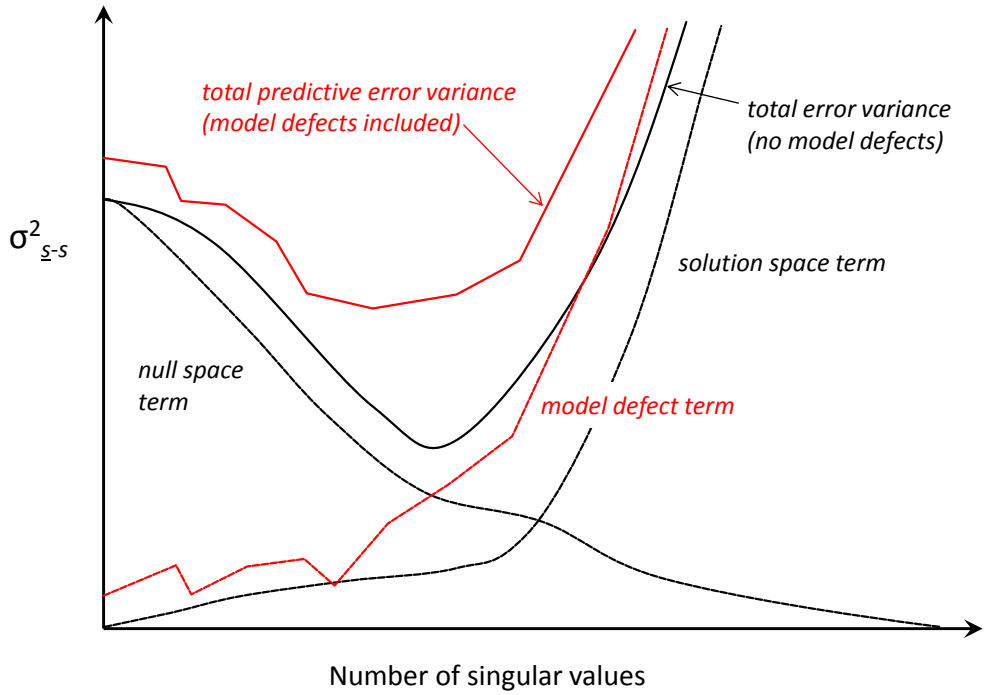


**Figure 9.13. The three terms of equation (9.6.8).**

*9.6.1.2 Insights Gained from Linear Analysis*

Equation (9.6.8) provides many useful insights into the effects that model defects have on parameters that are estimated through model calibration, and on predictions that are made by a calibrated defective model. These insights can have a profound effect on the way that environmental modelling is used to support environmental management.

The last term of equation (9.6.8) can only be zero or positive. However, unlike the first and second terms of this equation, there can be no guarantee that it increases monotonically with increasing number of pre-truncation singular values. Eventually, however, it must rise because it features two incidences of the $\mathbf{S}^{-1}_{m1}$ matrix. When singular values of $\mathbf{Z}_m$ become zero, it rises to infinity. (Recall that singular values decrease with increasing singular value index.)

Where singular value index is low, the general increase that this term exhibits with inclusion of an increasing number of singular values in the inversion process can be slow or rapid, this depending on the prediction. For some predictions this term will be non-zero at the very left of the graph where the number of pre-truncation singular values is zero, and therefore the model does not undergo calibration at all. This occurs where the model defects that are encapsulated in $\mathbf{Z}_d$ have the potential to contribute to the error of the prediction purely because of sensitivity of the prediction to defect parameters $\mathbf{k}_d$. For inclusion of zero singular values in the inversion process (and hence no calibration at all), equation (9.6.8) becomes

$$\sigma^2_{\underline{s}-s} = \sigma^2_{km}\mathbf{y}^t_m\mathbf{y}_m + \sigma^2_{kd}\,\mathbf{y}^t_d\mathbf{y}_d \qquad (9.6.9)$$

Whether the total predictive error variance falls below its initial value as the number of singular values employed in the inversion process increases above zero also depends on the prediction. Experience in using equation (9.6.8) in real world modelling contexts

demonstrates that it is far from impossible for the total error variance to rise and never fall as the number of singular values increases. This type of behaviour is normally associated with predictions that do not benefit much from the calibration process because they are not sensitive to parameters that are well-informed by the calibration dataset. When model defects are taken into account, it is quite possible that, for these particular predictions, any calibration is therefore "bad calibration". This has profound consequences for the way in which a model is constructed and deployed if the purpose of a modelling exercise is to make these particular predictions. For these predictions, a modeller may eschew the "benefits" of calibration in recognition of the fact that calibration may actually do more harm than good. Instead, he/she may build a model that is designed specifically to express expert knowledge with some degree of sophistication, taking into account the fundamentally stochastic nature of expert knowledge. This may involve the use of random, categorical parameter field realizations that make highly parameterized inversion impossible. Meanwhile, justification for this strategy may have relied on the prior use of simpler parameter fields that make computation of the sensitivity matrices and vectors appearing in (9.6.8) possible.

For other predictions the overall predictive error variance may fall with increasing number of singular values. At some number of singular values the predictive error variance is minimized. However because the defect term of equation (9.6.8) is not necessarily monotonic, the total error variance curve may have multiple minima. At some point however the total error variance curve will rise significantly. Meanwhile its minimum will have been shifted to the left (possibly by a large number of singular values) when compared to that which would have been calculated if only the first two terms of (9.6.8) are used. (These are the only terms that are available to a modeller unless he/she is specifically accounting for model defects).

This shift to the left of the total predictive error variance minimum is important to note; it indicates that in calibrating a defective model, a modeller should seek a reduced level of fit from that which he/she is entitled to seek when calibrating a perfect model. This, of course, makes sense as it recognizes the existence of structural noise in addition to measurement noise. Unfortunately, however, in most real world modelling circumstances, a modeller cannot know the extent to which his/her goodness-of-fit ambitions should be reduced in calibrating the defective model.

A significant outcome of the existence of model defects is that the minimum of the predictive error variance curve may be significantly different for some predictions than it is for others. This is in contrast to the case of no model defects where, though error variance curves may differ from prediction to prediction, the number of singular values corresponding to the minimum of these curves is unlikely to differ by too much from prediction to prediction. This allows prediction-independent methods such as that discussed in section 6.2.5.3 to be used in locating the optimum singular value truncation point. Sadly, however, where the existence of model defects is taken into account, the minimum of the predictive error variance curve may be indistinct, possibly serrated, and highly prediction-specific. Hence while, for some predictions, the model calibration process can enable a considerable reduction in the uncertainty of that prediction, for others, as already stated, even a little calibration can do more harm than good. The philosophy that underpins so much current environmental modelling practice that a model can be calibrated once, without regard for the predictions that it will be required to make, and then be employed to make predictions of many and varied types, is thus demonstrably erroneous.

In the previous section it was suggested that some predictions may carry virtual immunity from the deleterious effects of model defects. This will now be demonstrated using equation (9.6.5). For these predictions "any calibration is good calibration" regardless of the surrogate roles that $\mathbf{k}_m$ parameters may adopt through the calibration process, and regardless of the fact that the values estimated for some parameters may transgress the limits of system property credibility. It was suggested above that these predictions are those that are sensitive only to parameters which comprise the solution space of the real world model **Z** (as distinct from the solution space of the defective model $\mathbf{Z}_m$). These tend to be predictions which bear similarities to observations used in the calibration dataset.

The third term on the right side of (9.6.5) is zero if

$$\mathbf{y}^t{}_d\mathbf{k}_d = \mathbf{y}^t{}_m\mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t{}_{m1}\mathbf{Z}_d\mathbf{k}_d \qquad (9.6.10a)$$

This can also be written as

$$\begin{bmatrix}\mathbf{y}_m & \mathbf{y}_d\end{bmatrix}^t\begin{bmatrix}\mathbf{V}_{m1}\mathbf{S}_{m1}^{-1}\mathbf{U}^t_{m1}\mathbf{Z}_d \\ -\mathbf{I}\end{bmatrix}\mathbf{k}_d = \mathbf{0} \qquad (9.6.10b)$$

Suppose that measurement noise is zero. Suppose also that model imperfections can be "calibrated out" because $\mathbf{k}_m$ parameters can be endowed with values that compensate for non-zero $\mathbf{k}_d$ parameter values. It follows that for any defect parameter set $\mathbf{k}_d$ for which a corresponding **h** can be calculated as

$$\mathbf{h} = \mathbf{Z}_d\mathbf{k}_d \qquad (9.6.11)$$

a $\mathbf{k}_m$ parameter set can be found such that

$$\mathbf{h} = \mathbf{Z}_d\mathbf{k}_d = \mathbf{Z}_m\mathbf{k}_m = \mathbf{U}_m\mathbf{S}_m\mathbf{V}^t{}_m\mathbf{k}_m = \mathbf{U}_{m1}\mathbf{S}_{m1}\mathbf{V}^t{}_{m1}\mathbf{k}_m \qquad (9.6.12)$$

The last two equalities in equation (9.6.12) follow from (9.3.6) and (9.3.7). From (9.6.12)

$$\mathbf{k}_m = \mathbf{V}_{m1}\mathbf{S}^{-1}{}_{m1}\mathbf{U}^t{}_{m1}\mathbf{Z}_d\mathbf{k}_d \qquad (9.6.13)$$

From (9.6.13) and (9.6.12) it then follows that

$$\begin{bmatrix}\mathbf{Z}_m & \mathbf{Z}_d\end{bmatrix}\begin{bmatrix}\mathbf{V}_{m1}\mathbf{S}_{m1}^{-1}\mathbf{U}^t_{m1}\mathbf{Z}_d \\ -\mathbf{I}\end{bmatrix}\mathbf{k}_d = \mathbf{Z}\begin{bmatrix}\mathbf{V}_{m1}\mathbf{S}_{m1}^{-1}\mathbf{U}^t_{m1}\mathbf{Z}_d \\ -\mathbf{I}\end{bmatrix}\mathbf{k}_d = \mathbf{0} \qquad (9.6.14)$$

where **Z** is the real world (or total) model matrix. From this it can be concluded that the vector $\begin{bmatrix}\mathbf{V}_{m1}\mathbf{S}_{m1}^{-1}\mathbf{U}^t_{m1}\mathbf{Z}_d \\ -\mathbf{I}\end{bmatrix}\mathbf{k}_d$ is in the null space of the real world model **Z**. Equation (9.6.10.b) therefore states that a prediction will be immune from model structural defects if that prediction is sensitive only to solution space components of **Z**, as was stated above. For the making of such a prediction, the model can be virtually a "black box", as long as it is a well-calibrated black box. (This, of course, is an essential component of black box deployment, as expert knowledge is unlikely to assist in the parameterization of such a device).

This conclusion makes the author wonder how many environmental models have been decreed as "good" simply because they have demonstrated alacrity in making one particular type of prediction. The above theory shows that when a model has defects, calibration-induced aptitude in the making of some types of predictions may guarantee suboptimal performance in the making of other types of predictions.

White et al (2014) demonstrate use of equation (9.6.8) in exploring errors associated with predictions made by a defective groundwater model. They also demonstrate how this equation can be used to explore the efficacy of different objective function formulations in reducing calibration-induced predictive error.

### 9.6.2 Nonlinear Analysis

With the slightest of re-arrangements, equation (9.6.5) can be re-written as

$$s = \underline{s} + \mathbf{y}^t_m\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m - \mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon} - \mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\mathbf{Z}_d\mathbf{k}_d + \mathbf{y}^t_d\mathbf{k}_d \qquad (9.6.15)$$

This formula was used by Doherty and Christensen (2011) who developed a methodology for joint use of two models - a complex model and a complementary simple model – at the same study site. The simple model is calibrated against a measurement dataset, and then used to make predictions of interest. However before it is deployed in this manner, corrections for calibration-induced predictive bias (to which a simple model is prone for reasons outlined in previous sections of this chapter) are established through repeatedly calibrating the simple model against synthetic calibration datasets computed by the complex model as the latter is endowed with a suite of stochastic parameter fields that express expert knowledge of conditions at the study site. This methodology can be used where complex model run times are long, and/or complex model numerical stability is questionable. Furthermore the complex model (if it is a groundwater or reservoir model) can be endowed with complex, geostatistically-based, categorical parameter fields that are difficult or impossible to adjust through inversion. This frees the complex model to express expert knowledge, and the simple model (which is supposedly endowed with a parameter field which can be readily adjusted through inversion) to respond to information that is available in the calibration dataset.

As usual, let **h** denote a measurement dataset that is available at the study site. The complex model is used to simulate conditions at the study site over the calibration period. This is, in fact, done many times; on each occasion it is provided with a different stochastic parameter field. Let us denote each set of complex model outputs that correspond to the calibration dataset **h** as $\mathbf{h}_{ci}$; in this notation the "c" subscript symbolizes "complex-model-generated" while the "*i*" subscript symbolizes the *i*'th parameter field realization. Suppose that this is done *N* times. Suppose also that, for each of these *N* parameter fields, predictions of management interest are also made by the complex model. We will focus on one of these predictions which we denote as *s*; the prediction made using the *i*'th parameter field is denoted as $s_i$. If *N* is large enough, the prior probability distribution of *s* is thereby explored.

Now let the simple counterpart to the complex model be calibrated against each of the *N* realizations of $\mathbf{h}_{ci}$. Let it be supposed that the simple model is complex enough so that it can reproduce these $\mathbf{h}_{ci}$ reasonably well. Thus, for each $\mathbf{h}_{ci}$, a simple model parameter field is calculated corresponding to the complex model parameter field; each of these calibrated parameter fields endows the simple model with the capacity to reproduce the respective $\mathbf{h}_{ci}$. Suppose also that, once the *i*'th simple model has been calibrated against the *i*'th complex model to obtain the *i*'th simple model parameter field, the simple model is then run to make the prediction *s*. We will denote the *i*'th prediction made by a thus-calibrated simple model as $\underline{s}_i$.

After *N* such complex model runs and ensuing simple model calibration exercises have been undertaken, $s_i$ can be plotted against $\underline{s}_i$ for all *i*. Figure 9.14 schematizes such a plot. The prior uncertainty of the prediction is shown in the plot; it comprises the total span of complex

model predictions.

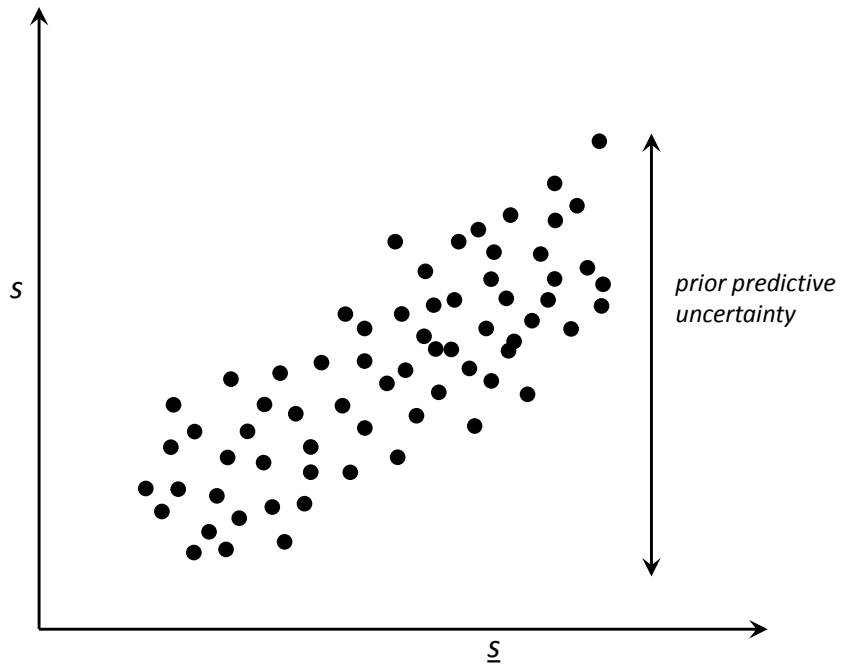


**Figure 9.14. Plot of the value of a prediction *s* made using different parameter field realizations of a complex model against predictions $\underline{s}$ made by partnered simple models. Each simple model is calibrated against a complex-model-generated calibration dataset whose contents are identical to that of a real world calibration dataset.**

The simple model is now calibrated just one more time, this being for the $N$+1'th time. However this time it is calibrated against the real calibration dataset **h**. The thus-calibrated simple model is then used to make the prediction of interest. Suppose that the value that it calculates for this prediction is $\underline{s}_r$; the subscript "r" stands for "real". The post-calibration potential for error in this prediction (which we use as a surrogate for post-calibration predictive uncertainty) can then be obtained in the manner suggested by figure 9.15. The predictive interval depicted in that figure records the range of complex model predictions that is compatible with the prediction made by the simple model calibrated against the real-world measurement dataset **h**.

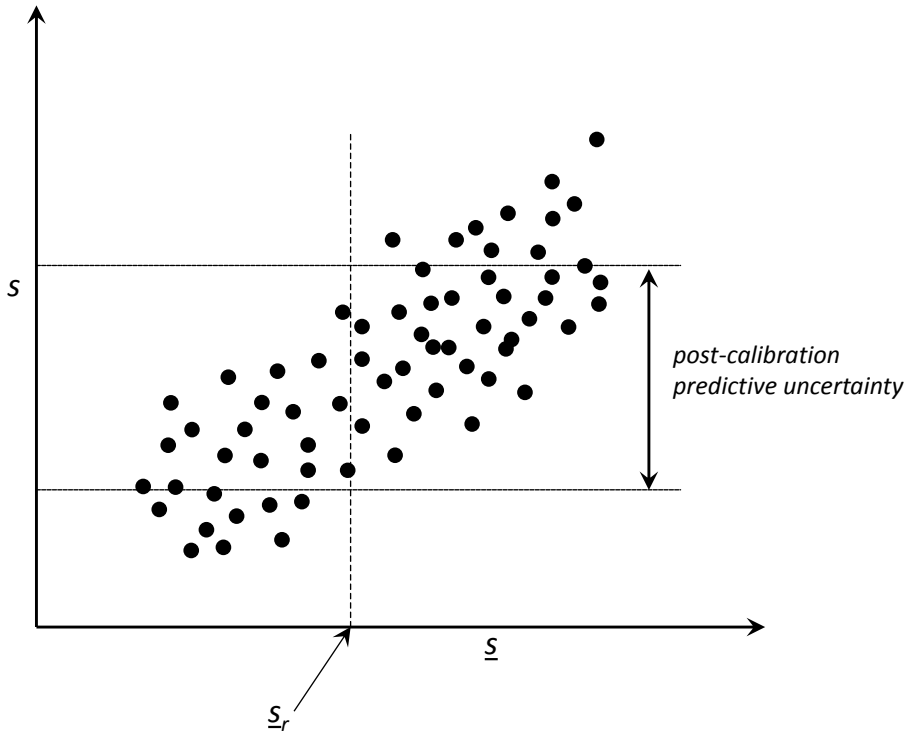


**Figure 9.15. A simple model calibrated against the real world calibration dataset makes the prediction $\underline{s}_r$. The post-calibration uncertainty of that prediction is established as the range of complex model predictions through which a vertical line through $\underline{s}_r$ passes.**

Various aspects of figures 9.14 and 9.15 can be explained by equation (9.6.15).

The second term on the right of (9.6.15) is $\mathbf{y}^t_m\mathbf{V}_{m2}\mathbf{V}^t_{m2}\mathbf{k}_m$. This represents predictive error that prevails if there is no noise in the calibration dataset and no defects in the model. It is simply the null space contribution to post-calibration predictive error. Because this affects *s* rather than $\underline{s}$ in equation (9.6.15), it promotes vertical scatter of the points depicted in figures 9.14 and 9.15. If this is the only contribution to model predictive error (because measurement noise is zero and simple model defects are either non-existent or do not affect the prediction *s*) then the line of best fit through the *s* vs. $\underline{s}$ scatterplot has a slope of 1.

The third term on the right of equation (9.6.15) (i.e. $\mathbf{y}^t_m\mathbf{V}_{m1}\mathbf{S}^{-1}_{m1}\mathbf{U}^t_{m1}\boldsymbol{\varepsilon}$) describes the effect of measurement noise on predictive error. As this affects $\underline{s}$ and not *s*, it promotes horizontal scatter of the points plotted in figures 9.14 and 9.15. In many modelling contexts this contribution to scatter is much smaller than the vertical, null space contribution to scatter; this occurs where, for a prediction of interest, lack of information in the calibration dataset, rather than measurement noise associated with this dataset, is responsible for the greater part of predictive uncertainty.

The contribution made to predictive error by calibration-induced parameter compensation is described by the fourth term on the right of equation (9.6.15). As this affects $\underline{s}$ but not *s*, it promulgates horizontal scatter of an *s* vs. $\underline{s}$ scatterplot. Experience shows that horizontal scatter of this type can be considerable for some predictions. Where this occurs the line of best fit through the *s* vs. $\underline{s}$ scatterplot may have a slope that is considerably less than unity. For some predictions the horizontal width of an *s* vs. $\underline{s}$ scatterplot can be much greater than its vertical width, this providing a clear indication that, for these predictions, the simple model

calibration process has the potential to contribute substantially to the potential for predictive error. In fact, this may result in a potential for post-calibration predictive error which is greater than that which these predictions would possess on the basis of expert knowledge alone. For predictions of these types, simple model calibration can do more harm than good, for calibration actually increases the range of predictive error variance that it attempts to reduce.

The last term on the right of equation (9.6.15) expresses the direct effect of model defects on predictive error. It arises purely from sensitivity of the prediction to these defects. It promotes vertical scatter within the $s$ vs. $\underline{s}$ scatterplot as it affects $s$ and not $\underline{s}$.

Equation (9.6.15) assumes linear model behaviour. However implementation of the paired model methodology described by Doherty and Christensen (2011) does not require that either the complex or simple model be linear. Correction and expansion of a prediction made by a simple calibrated model so that it embraces the range of predictions which a corresponding stochastic, complex model would make if it were to be subjected to calibration-constrained predictive uncertainty analysis is a concept that requires no linearity assumption. For nonlinear models the $s$ vs. $\underline{s}$ scatterplot may show curvature; furthermore, scatter may be wider in some parts of the scatterplot than in others. If a scatterplot possesses nonlinear features such as these, then inference of scatter along a vertical line projected upwards from the $\underline{s}$ axis as in figure 9.15 may be a little more difficult than for linear models wherein scatter is more uniform. This is because scatter assessment involves implicit projection of scatter about other parts of the line of best fit along the direction of this line to the vertical $\underline{s}$ line. Where scatter about this line of best fit is variable, such projection may incur errors. These errors can be accommodated if a modeller is conservative in his/her assessment of scatter about parts of the $s$ vs. $\underline{s}$ best fit line that are used in this projection.

Despite first appearances, construction of an $s$ vs. $\underline{s}$ scatterplot is not necessarily a particularly numerically intensive exercise. Recall that the complex model must be run a total of $N$ times, where $N$ is the number of points comprising the scatterplot. The simple model must, of course, be run many more times than this, for it must be calibrated $N$ times. However if it runs reasonably quickly then the numerical burden of conducting $N$ calibration exercises may not be great.

# 10 Other Issues

## 10.1 Introduction

The purpose of this final chapter is to address a number of issues which do not fall under the direct embrace of subjects to which previous chapters were devoted. Its purpose is also to conclude this book.

## 10.2 Objective Function Formulation

### 10.2.1 General

The previous chapter devoted some discussion to formulation of an objective function expressing model-to-measurement misfit for use in solution of an inverse problem. Minimization of this objective function is explicit if the inverse problem is solved using the Gauss-Marquardt-Levenberg method. Its reduction is implicit in solution of the inverse problem using singular value decomposition. Its reduction is also implicit in formulation of equations which feature Tikhonov regularization.

The lower is the objective function, the better is the fit between model outputs and corresponding field measurements. When undertaking model predictive uncertainty analysis in pursuit of a level of confidence to assign to a parameter or a prediction of interest, the constraint that parameter values must be such as to maintain the model in a calibrated state is often expressed through this objective function. Parameter sets are construed as maintaining respect for information contained in the calibration dataset (at a certain level of confidence) if the objective function is at or below a certain threshold.

In the previous chapter it was recommended that consideration be given to processing field data and corresponding model outputs in one or a number of different ways before differencing them to form residuals; weighted residuals are then summed to form the overall objective function. Processed field measurements and complementary model outputs may comprise the entirety of the calibration dataset. Alternatively, unprocessed measurements and model outputs may be retained to form one component of the total objective function. As has been described, if measurement and model output processing can be designed in such a way as to "orthogonalize out" expressions of structural noise in model outputs, this strategy can inoculate the inversion process, to some extent at least, against the effects of model defects on estimated parameters

The present section discusses some other contexts in which creativity should be exercised in formulating the objective function. The discussion is limited, however, to the measurement component of the objective function. As was discussed in section 6.3, considerable creativity can (and should) be exercised in formulating the regularization component of an objective function in ways that best express expert knowledge of parameter values and the likely nature of parameter heterogeneity as it pertains to a particular calibration setting. That topic will not be addressed further in the present chapter however.

There can be no formula for a universally best approach to formulation of an objective function. However an underlying principle is universal – that is to ensure that as much information as possible is transferred, in as "safe" a way as possible, to the parameters of an environmental model. A number of issues that may challenge that principle are now

discussed. Ways in which these challenges may be met are proposed.

### 10.2.2 Some Issues

*10.2.2.1 Large Observation Range*

Measurements comprising some calibration datasets may span many orders of magnitude. Flows within ephemeral streams are an example. Groundwater contaminant concentrations in the vicinity of a contaminated site comprise another example. In both of these cases the calibration dataset may include measured values of zero.

Where measurements span a large range of values, it may be inappropriate to assign an equal weight to all of them. A strategy of equal weighting ensures that observations whose values are large dominate the objective function while observations whose values are small are correspondingly "lost". In the case of stream flow, this strategy may ensure that the inversion process is able to match flood peaks well, but may not be able to match flood recessions, nor stream flows over periods of drought. In the case of groundwater contaminant concentrations, a strategy of equal weighting may ensure that the inversion process is able to match concentrations close to a contaminant source, but is unable to reproduce concentrations near the periphery of a contaminant plume. In both of these cases important information may be lost unless these low-valued measurements are rendered more "visible" in the objective function. Furthermore, predictions of management interest required of a model may pertain to times and/or locations within the model domain which are similar to those at which low-valued calibration measurements were recorded; the information that is implied in a low value of stream flow or contaminant concentration may be very relevant to these predictions.

This situation is easily rectified. Measurements and model outputs can be transformed (for example log-transformed) before being matched to each other so that small observed values are visible to the inversion process. Alternatively, weights may be calculated from observation values in such a way as to ensure that higher weights are assigned to lower-valued observations.

In the author's opinion, the best guide to formulation of an appropriate weighting strategy is common sense. If high measurement values are rich in information pertaining to one aspect of a system, and low measurement values are rich in information pertaining to another aspect of a system, a modeller may decide to formulate two components of a multi-component objective function. Each component uses the same measurement dataset. In the first of these components weights may be uniform. In the second of these components, measurements whose values are low or intermediate in value may be rendered more visible in the overall objective function through logarithmic (or other) transformation. A group-specific weight multiplier can then be applied to each of these two groups of observations so that the contribution made to the overall objective function by each of them is roughly equal at the commencement of the inversion process. Neither group then dominates the inversion process, nor is dominated by the other group.

*10.2.2.2 Non-Detects*

Suppose that a model is being calibrated for which part of the observation dataset is comprised of measurements of contaminant concentration. Suppose also that values below a certain concentration are recorded as "non-detect". The non-detect threshold will normally have varied over time – a fact that needs to be taken into account where calibration datasets

span many years.

As was mentioned in the preceding section, measurements of low or non-detectable concentration are often an important component of a calibration dataset. In a groundwater remediation context these define the periphery of a contaminant plume. Hence high weights may need to be assigned to these observations.

A numerical value must be assigned to "non-detect" for use in the calibration process. If "non-detect" is associated with a value of zero, then the inversion process may alter model parameters so that model-calculated concentrations which are below the detection threshold, but are not exactly zero, are moved downwards towards zero. Declaring non-detects as zero thus provides misinformation to the inversion process.

A better option is to declare observed non-detects as equal to the detection limit. Meanwhile a model post-processor (or the model itself) should raise model-calculated concentrations up to the detection limit if they are below it. A zero-valued residual is thus achieved if both modelled and observed concentrations are at or below the detection limit. A non-zero residual is recorded if either is at or below this limit and the other is above it. Meanwhile continuity of model outputs with respect to parameters is preserved as modelled concentrations cross the detection limit.

#### *10.2.2.3 Asymmetric Observations*

Another problem that is often associated with concentration observations in the groundwater modelling context is their nonlinearity. Suppose that the calibration dataset includes observations of contaminant concentrations at a certain well. When endowed with a certain set of parameters, the model may calculate a contaminant concentration of zero at that well. If this is the case, then the derivative of the model-calculated well concentration with respect to every model parameter will also be zero, especially if the tip of the model-calculated plume is far from the well. The inversion process therefore has no opportunity to adjust parameters such that the plume reaches the well.

There are a number of ways in which this problem can be addressed. One option is to introduce to the calibration dataset another observation, this being the distance from the well to a certain iso-concentration line as calculated by the model. If the observed concentration in the well is below the concentration associated with this iso-concentration line, then the "observed value" for this distance is zero. Meanwhile, as long as the model places the iso-concentration line at some distance from the well, the model-calculated value for this distance is non-zero. At the same time, this distance is likely to be sensitive to at least some model parameters. This provides the inversion process with an incentive to adjust these parameters in order to move the plume towards the well.

The above strategy accommodates the existence of a naturally asymmetric (and hence nonlinear) observation by introducing another asymmetric observation to the calibration dataset which complements the original observation.

A similar strategy may be necessary where spring flow comprises part of the calibration dataset of a groundwater model. If the head calculated by the groundwater model is above the level of the spring, then model-calculated spring flow is non-zero; presumably model-calculated spring flow is then sensitive to at least some model parameters. Alternatively, if the model-calculated groundwater head is below the level of the spring, then the spring does not flow. Because model-calculated spring flow is then zero it is insensitive to all model

parameters; the inversion process is therefore unable to adjust these parameters in order for the model to calculate a non-zero spring flow. For this particular type of asymmetric observation, a complementary asymmetric observation of groundwater head at the spring may be introduced to the calibration dataset. The observed value of this quantity is the elevation of the spring. As long as the model-calculated head is below the elevation of the spring, a non-zero residual will be associated with this observation; furthermore the value of this residual should be sensitive to at least some model parameters. However when the model-calculated head rises to the level of the spring, the residual for this observation becomes zero; it then becomes insensitive to all model parameters. However just as this happens, model-calculated spring flow becomes non-zero, and is therefore sensitive to at least some model parameters.

More elaborate strategies than this will often be required. Returning to the concentration example presented above, calculation of the distance between a well and an iso-concentration line is a difficult numerical undertaking which a modeller may wish to avoid. An alternative strategy is to introduce particles to the model domain at the same location as the contaminant source; a suitable asymmetric observation may then be the distance between the observation well and the closest particle. This will be positive if the plume has not reached the well, and very small otherwise.

Another possibility may be to introduce a series of asymmetric observations that pertain to collections of model cells centred on the observation well. These collections may represent expanding areas comprised of increasing numbers of model cells. The "measured value" associated with each of these introduced observations is assigned a value of zero. Meanwhile the model-calculated value with which each of these measurements is compared is the observed well concentration minus the maximum concentration computed for any cell within each of these cell groups; however an upper limit equal to the concentration observed in the well is imposed on all of these model-calculated concentrations. Hopefully, at least one of these model-calculated concentrations would be non-zero for any reasonable parameter set. Furthermore the residual associated with at least one of these observations would presumably be reduced as the plume moves toward the well. Eventually the plume would reach the well and all residuals associated with these "asymmetry balancing" observations would be zero.

Similar considerations apply to the location of a salt water wedge in sea water intrusion modelling, and to the location of a separate fluid phase in reservoir modelling.

#### *10.2.2.4 Differencing*

Environmental models are generally better at calculating differences than absolutes – for example horizontal, vertical and temporal differences of system state. These differences therefore tend to be more immune from model defects than absolute quantities calculated by models. As was discussed in the previous chapter, the inclusion of system state differences instead of (or as well as) system state absolutes as components of the calibration dataset to be matched by the model, therefore provides some defence against estimation of erroneous parameter values.

## 10.3 Derivatives

Methodologies for highly parameterized inversion and calibration-constrained uncertainty analysis that are discussed in this text depend on an ability to successively linearize the action of a model on its parameters. The Jacobian matrix that is thereby calculated replaces the **Z** or

**X** matrices in equations that have been used throughout this book.

Sometimes a model itself can calculate derivatives of its outputs with respect to its parameters through an extension of its normal numerical solution procedure. Rarely is this the case for environmental models however. Furthermore, even if it were the case, the need for flexibility in formulation of a multi-component objective function may make such model-calculated derivatives difficult to use. Hence derivatives of model-generated counterparts to members of the calibration dataset are generally calculated using finite parameter differences.

PEST provides many options for calculation of finite-difference derivatives. It also provides some mechanisms for detecting problematic derivatives (often a consequence of poor model algorithmic design or difficulties experienced by model numerical solvers), and for taking remedial action during the inversion process. See PEST documentation for details. However there is a limit to the measures which PEST can take to ameliorate the effects that bad finite-difference derivatives can have on an inversion process. Hence a modeller must take whatever steps that he/she can to enhance the integrity of finite-difference derivatives.

Calculation of finite-difference derivatives requires that the value of a parameter be varied incrementally, and that differences in model outputs be computed on that basis. Because a parameter's value is varied only incrementally, alterations to model outputs will also be small. The first few significant figures of many of these outputs will therefore be the same for both the original and incremented parameter; hence numerical precision of the last few significant figures is important. (Unfortunately, opportunities for these last few significant figures to suffer degradation can be increased if, following the advice provided above, horizontal, vertical and/or temporal differences of system state are included in the calibration dataset; such quantities must be differenced twice in formulation of finite-difference derivatives.)

The following is a short checklist of measures that a modeller should consider taking to maintain or enhance the integrity of finite-difference derivatives calculation. All of these suggestions attempt to ensure that model outputs reflect as accurately as possible the parameters that the model uses to calculate them.

- When using a model-independent parameter estimator such as PEST which reads numbers from a model's output files, these numbers should be recorded by the model with maximum numerical precision, using scientific notation. Note that between 6 and 7 significant figures are required for representation of a single precision real number that is stored using 4 bytes. Around 16 significant figures are required for representation of a double precision real number that is stored using 8 bytes.
- If, as is often the case, the model with which PEST is interacting is a batch or script file comprised of multiple executable programs (for example a model and a number of pre- and post-processors), these executable programs should transfer numbers between each other without loss of numerical precision.
- Convergence settings for model numerical solvers should be set tight.
- If possible, strategies such as adaptive time-stepping that can hasten model execution speed, but which may result in differences in numerical solution paths for different sets of parameters, should be avoided. (It is recognized, however, that for many models the cost of eschewing powerful solution stabilizers like adaptive time-stepping may result in unduly long execution times and/or model solver non-convergence. Under these circumstances, PEST will just have to cope with errors that adaptive time

stepping may introduce to finite-difference derivatives. Its tolerance for adaptive time-stepping is normally high; however this is model-specific.)

Despite the dangers that sometimes accompany finite-difference derivatives calculation, experience has shown that highly parameterised inversion and highly parameterized, calibration-constrained uncertainty analysis, when undertaken using software such as PEST that implements methodologies that are documented herein, is remarkably robust. However, experience has also shown that where the numerical performance of these methodologies does not live up to expectations, problematic calculation of finite-difference derivatives is nearly always the reason.

## 10.4 Proxy and Surrogate Models

Calculation of finite-difference derivatives is the most time-consuming (and the most error-prone), part of highly parameterized inversion and uncertainty analysis. Fortunately, the computational burden of derivatives calculation can be lightened considerably by parallelizing the model runs required for this process. However, where parameters are many, and where model numerical performance is questionable, problems may still remain. In cases such as these it may be possible to use a simpler version of the model for the calculation of derivatives. The simpler model may employ coarser temporal and/or spatial discretization than the model that is actually being calibrated. Other simplification strategies may also be employed. For example the PEST suite provides the means to construct a proxy model in which a relationship based on an enhanced second degree polynomial is developed between each model output used in the calibration process and all model parameters. This suite of enhanced polynomials (each member of which is calibrated by PEST itself against outputs of the real model calculated using strategically sampled parameter values) can then be used for derivatives calculation when calibrating the complex model against a real calibration dataset.

Naturally, the use of a simplified or proxy version of the real model for derivatives calculation compromises the integrity of finite difference derivatives to some extent. Nevertheless, experience has demonstrated that the method can be successful; see Burrows and Doherty (2015). Success of the methodology rests partly on the fact that, while absolute values computed by a simple model are indeed afflicted by model simplification errors, differences between these outputs calculated using marginally different parameter values are less afflicted. Use of the complex model to test parameter upgrades calculated using different values of the Marquardt lambda also contributes to the success of the methodology.

## 10.5 Conclusions

This present text was written for two purposes. Firstly, it records in one place the theory on which PEST, PEST++ and utility software which supports these two programs, relies. It thus constitutes a useful reference for those who use this software.

The other purpose of this text is to provide a comprehensive theoretical basis for the use of highly parameterised methods in calibration and uncertainty analysis of environmental and reservoir models Unfortunately, at the time of writing, despite the extensive use in many other scientific disciplines of methods that are based on theory that is the same or similar to that presented herein, use of these methods in the environmental and reservoir modelling contexts is still limited. Part of the reason for this is the absence of high-end workflow software that expedites their use in these contexts. However another reason is the lack of

acquaintance with these methods by environmental modellers. It is hoped that the present text goes some of the way towards rectifying this situation.

Many insights can be gained into the possibilities and shortcomings of environmental modelling through understanding the roles that parameterization and history-matching play in the modelling process. Important issues which have been addressed using the theory presented herein include uniqueness, uncertainty, data worth, appropriate complexity, the effect that a model's defects has on its capacity to predict the environmental future, and whether these defects can be "calibrated out". A theoretical examination of these issues has called into question some aspects of everyday modelling practice. The author considers this to be an important justification for the writing of this text. It is the author's fervent hope, that this same theory can thereby provide the grounds for improving current modelling practice.

The science of environmental modelling is still young. The science of model-based environmental decision-making is even younger. There is a long way to go in both. The ideas and theory presented herein demonstrate unequivocally that a model cannot exist in isolation from other, equally sophisticated, numerical software if it is to provide a scientific basis for environmental decision-making. A model can play its defining role in the decision-making process when it is partnered by an inversion engine such as PEST, together with appropriate statistical and geostatistical packages that can express the stochastic nature of expert knowledge. The dance that these, and other software packages, must perform is still being choreographed.

# 11. References

Aanonsen, S.L., Naevdal, G., Oliver, D.S., Reynolds, A.C. and Vallès, B., 2009. The ensemble Kalman filter in reservoir engineering – a review. *Soc Petrol Eng J,* 14(3), 393-412, doi:10.2118/117274-PA.

Albert, A., 1972. Regression and the Moore-Penrose pseudoinverse. Academic Press, New York.

Belsley, D.A, Kuh, E. and Welsch, R.E., 1980. Regression Diagnostics: Identifying Influential Data and Source of Collinearity. John Wiley, New York.

Beven, K., 2005. On the concept of model structural error. *Water Sci.Technol,* 52(6), 167–175.

Beven, K.J., Smith, P.J. and Freer, J., 2008. So just why would a modeller choose to be incoherent? *J Hydrol,* 345 (1), 15-32.

Burrows, W. and Doherty, J., 2015. Effficient calibration/uncertainty analysis using paired complex/simple models. *Ground Water,* doi: 10.1111/gwat.12257

Christensen, S. and Cooley, R.L., 1999. Evaluation of prediction intervals for expressing uncertainties in groundwater flow model predictions. *Water Resour Res,* 35 (9), 2627-2639.

Cook, R.D. and Weisberg, S., 1982. Residuals and Influence in Regression. *Monogr. Stat. Appl. Probability,* vol 18, Chapman and Hall, New York, 1982.

Cooley, R.L., 1983. Some new procedures for numerical solution of variably saturated flow problems. *Water Resour. Res,* 19 (5), 1271-1285.

Cooley, R.L. and Christensen, S., 2006. Bias and uncertainty in regression-calibrated models of groundwater flow in heterogeneous media. *Adv Water Resour,* 29, 639-656.

Cooley R.L., 2004. A theory for modeling ground-water flow in heterogeneous media. *U.S. Geological Survey Professional Paper 1679,* 2004. 220 pp.

Cui, T., Fox, C. and O'Sullivan, M.J., 2011. Bayesian calibration of a large-scale geothermal reservoir model by a new adaptive delayed acceptance Metropolis Hastings algorithm. *Water Resour. Res,* 47, W10521, doi:10.1029/2010WR010352.

Dausman, A.M., Doherty, J., Langevin, C.D., and Sukop, M.C., 2010. Quantifying data worth toward reducing predictive uncertainty. *Ground Water,* 48 (5), 729-740.

De Groot-Hedlin, C. and Constable, S., 1990. Occam's inversion to generate smooth, two-dimensional models from magnetotelluric data. *Geophysics,* 55 (12), 1613-1624.

Doherty, J., 2003. Groundwater model calibration using Pilot Points and Regularization. *Ground Water,* 41 (2), 170-177.

Doherty, J. and Christensen, S., 2011. Use of paired simple and complex models in reducing predictive bias and quantifying uncertainty. *Water Resour Res,* doi:10.1029/2011WR010763.

Doherty, J. and Hunt, R.J., 2009. Two statistics for evaluating parameter identifiability and error reduction. *J Hydrol,* 366, 119-127.

Doherty, J. and Simmons, C.T., 2013. Groundwater modelling in decision support: reflections on a unified conceptual framework. *Hydrogeol J,* 21, 1531–1537.

Doherty, J. and Welter, D., 2010, A short exploration of structural noise, *Water Resour. Res*, 46, W05525, doi:10.1029/2009WR008377.

Doherty, J., 2015. PLPROC: A Parameter List Processor. Watermark Numerical Computing, Queensland, Australia.

Emerick, A., and Reynolds, A., 2013. Investigation of the sampling performance of ensemble-based methods with a simple reservoir model. *Computat Geosci*, 17, 1-26.

Fienen, M.N. D'Oria, M., Doherty, J. and Hunt, R., 2013. Approaches in Highly Parameterized Inversion: bgaPEST, a Bayesian Geostatistical Approach Implementation with PEST – Documentation and Instructions. *Techniques and Methods, Book 7, Section C9*. U. S. Geological Survey.

Freeze R.A., Massmann J., Smith L., Sperling T., James B., 1990. Hydrogeological decision analysis: 1 A framework. *Ground Water* 28 (5),738–766.

Gallagher, M. R., and Doherty, J., 2007. Parameter interdependence and uncertainty induced by lumping in a hydrologic model, *Water Resour Res*, 43, W05421, doi:10.1029/2006WR005347.

Gelman, A., Carlin, J.B. and Stern, H.S., 2013. Bayesian Data Analysis. *Chapman and Hall/CRC Texts in Statistical Science*. Third Edition.

Hadi, A.S., 1992. A new measure of overall potential influence in linear regression. *Comput Stat Data An*, 14, 1-27.

Hill, M. C., 1992. A Computer Program (MODFLOWP) for Estimating Parameters of a Transient, Three-Dimensional, Ground-Water Flow Model using Nonlinear Regression. *U. S. Geological Survey Open-File Report 91-484*.

Hill, M.C. and Tiedeman, C.R., 2007. Effective groundwater model calibration: With analysis of data, sensitivities, predictions, and uncertainty. Wiley and Sons, New York, New York, 455 p

Kitanidis, P.K., 1995, Quasi-linear geostatistical theory for inversing: *Water Resour. Res*, 31 (10), 2411–2419, doi:10.1029/95WR01945.

Kitanidis, P.K., and Vomvoris, E.G., 1983. A geostatistical approach to the inverse problem in groundwater modeling (steady state) and one-dimensional simulations: *Water Resour. Res*, 19 (3), 677–690, doi:10.1029/WR019i003p00677.

Koch, K-R. 1999. Parameter Estimation and Hypothesis-Testing in Linear Models. Springer, Berlin, Heidelberg.

Hoeksema, R.J., and Kitanidis, P.K., 1984, An application of the geostatistical approach to the inverse problem in two-dimensional groundwater modeling: *Water Resour. Res*, 20 (7), 1003–1020, doi:10.1029/WR020i007p01003.

Laloy,E., and Vrugt, J.A., 2012. High-dimensional posterior exploration of hydrologic models using multiple-try DREAM(ZS) and high-performance computing. *Water Resour. Res*, 48, W0156. DOI 10.1029/2011WR010608.

Larsen, R.M., 1998, Lanczos bidiagonalization with partial reorthogonalization: Aarhus, Denmark, Aarhus University, Computer Science Department, 90 p. *PROPACK is downloadable from http://sun.stanford.edu/~rmunk/PROPACK/*

Levenberg, K., 1944. A method for the solution of certain non-linear problems in least

squares. *Q Appl Math*, 2, 164-168.

Mantovan, P. and Todini, E., 2006. Hydrological forecasting uncertainty assessment: incoherence of the GLUE methodology. *J Hydrol*, 330, 368–381.

Mariethoz, G. and Caers, J., 2015. Multiple-Point Geostatistics. Stochastic Modeling with Training Images. John Wiley and Sons, UK.

Marquardt, D. W., 1963. An algorithm for least-squares estimation of nonlinear parameters. *Journal of the Society of Industrial and Applied Mathematics*, 11 (2), p431-441.

Mikhail, E.M., 1976. Observations and Least Squares. IEP Series in Civil Engineering. Dun-Donnelley, New York.

Moore, C. and Doherty, J., 2005. The role of the calibration process in reducing model predictive error. *Water Resour Res*, 41, W05020, doi:10/1029/2004WR003501.

Moore, C. and Doherty, J., 2006. The cost of uniqueness in groundwater model calibration. *Adv in Water Resour*, 29, (4), 605 – 623.

Moore, C., Wöhling, T., and Doherty, J., 2010. Efficient regularization and uncertainty analysis using a global optimization methodology. *Water Resour Res*, 46, W08527, doi:10.1029/2009WR008627.

Nowak, W., and Cirpka, O.A., 2004. A modified Levenberg-Marquardt algorithm for quasi-linear geostatistical inversing: *Adv. in Water Resour*, 27, (7), 737–750, doi:10.1016/j.advwatres.2004.03.004.

Oliver, D.S. and Chen, Y., 2010. Recent progress on reservoir history matching: a review. *Computat Geosci*, 15 (1), 185-221.

Paige, C.C., and Saunders, M.A., 1982a. LSQR: An algorithm for sparse linear equations and sparse least squares. *ACM T Math Software*, 8 (1), 43–71.

Paige, C.C., and Saunders, M.A., 1982b. Algorithm 583 LSQR: Sparse linear equations and least squares problems. *ACM T Math Software*, 8 (2), 195–209.

Poeter, E.P. and Hill, M.C., 2007. MMA, A Computer Code for Multi-Model Analysis. *U.S. Geological Survey Techniques and Methods*, 6-E3, 113p.

Sarma, P., Durlofsky, L.J., and Azis, K., 2008. Kernel principal component analysis for efficient, differentiable, parameterization of multipoint geostatistics. *Math Geosci*, 40, 3-32.

Sykes, J.F., Wilson, J.L and Andrews, R.W., 1985. Sensitivity analysis for steady state groundwater flow using adjoint operators. *Water Resour Res*, 21 (3), 359-371. doi:10.1029/WR021i003p00359.

Tonkin, M. and Doherty, J., 2005. A hybrid regularised inversion methodology for highly parameterised models. *Water Resour Res*, 41, W10412, doi:10.1029/2005WR003995, 2005.

Tonkin, M., Doherty, J. and Moore, C., 2007. Efficient nonlinear predictive error variance for highly parameterized models. *Water Resour Res*, 43, W07429, doi:10.1029/2006WR005348.

Vecchia, A.V. and Cooley, R.L., 1987. Simultaneous confidence and prediction intervals for nonlinear regression models with application to a groundwater flow model. *Water Resour Res*, 23 (7), 1237-1250.

Vrugt, J.A., Gupta, H.V., Bastidas, L.A., Bouten, W and Sorooshian W., 2003. Effective and efficient algorithm for multiobjective optimization of hydrologic models. *Water Resour Res*,

39(8), 1214, doi:10,1029/2002WR001746.

Vrugt, J. A., 2011. DREAM: an adaptive markov chain Monte Carlo simulation algorithm to solve discrete, noncontinuous, posterior parameter estimation problems. *Hydrol. Earth Syst. Sc*, 8, 4025-4052, doi:10.5194/hessd-8-4025-2011.

Watson, T.A., Doherty, J.E. and Christensen, S., 2013. Parameter and predictive outcomes of model simplification. *Water Resour Res*, 49 (7), 3952-3977. DOI: 10.1002/wrcr.20145.

Welter, D.E., White, J.T., Doherty, J.E., and Hunt, R.J. 2015. PEST++ Version 3. A Parameter ESTimation and Uncertainty Analysis Software Suite Optimized for Large Environmental Models. *U.S. Geological Survey Techniques and Methods Report.* In review.

White, J.T., Doherty, J.E. and Hughes, J.D., 2014. Quantifying the predictive consequences of model error with linear subspace analysis. *Water Resour Res*, 50(2), 1152-1173. doi: 10.1002/2013WR014767.

White, J.T., Fienen, M.N., and Doherty, J.E., 2015. pyEMU: A Python Framework for Linear-Based Environmental Model Uncertainty Analysis. *Environ Modell Softw*, in review.

Wöhling, T. and Vrugt, J.A., 2008. Combining multiobjective optimization and Bayesian model averaging to calibrate forecast ensembles of soil hydraulic properties. *Water Resour Res*, 44, W12432, doi:10.1029/2008WR007154.

Woodbury, A. and Ulrych, T., 2000. A full-Bayesian approach to the groundwater inverse problem for steady state flow. *Water Resour Res*, 36 (8), 2081-2093, doi:10.1029/2000WR900086.

Yager, R.M., 1998. Detecting influential observations in nonlinear regression modelling. *Water Resourc Res*, 34 (7), 1623-1633.