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A study of Ill-conditioning in Linear Techniques with emphasis on some applications in the Earth Sciences.

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November, 1990

A thesis submitted to the University of Adelaide
in fulfillment of the requirements for the
degree of
Doctor of Philosophy.

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Abstract

When linear equations are solved using a computer, factors such as ill-conditioning and numerical stability should be considered. These factors determine the reliability with which a solution to the linear equations may be computed.

This study considers the conditioning of some linear least-squares methods which are applied in the earth sciences. Most attention is directed towards Wiener filtering, emphasis being placed on seismic deconvolution. Two geostatistical techniques, Ordinary Kriging and Co-kriging, are also considered.

The occurrence of ill-conditioned autocorrelation matrices are seen to be related to the fact that deconvolution is a mathematical problem which may have no solution. It is shown that intermediate results of the Wiener-Levinson algorithm provide a measure which can be employed to recognize ill-conditioned normal equations, and that prewhitening always has a beneficial effect on conditioning.

Intermediate results of the Wiener-Levinson algorithm are demonstrated to be useful for determining when that algorithm is over-come by rounding errors. It is seen that the Wiener-Levinson and Conjugate Gradient algorithms, which are employed in geophysical practice to solve the normal equations, introduce more error than classical solution algorithms when solving ill-conditioned problems. It is demonstrated that there is no general guarantee that the Conjugate Gradient algorithm produces solutions to ill-conditioned problems with less error than does the Wiener-Levinson algorithm.

Results obtained for deconvolution are extended to apply to Ordinary Kriging and Co-kriging. It is shown that conditioning of both these methods depends upon properties of covariance and cross-covariance functions, and also that a scaling effect occurs due to the presence of unbiasedness constraints. Via numerical experiments, it is seen that this scaling effect is primarily of importance when covariance and cross-covariance matrices are ill-conditioned.

Statement

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R.J. O'Dowd

September, 1990

Acknowledgements

My supervisor, Dr. Gäbor Korvin, who originally suggested this project, and Dr. Peter Brooker provided encouragement, support in many ways, and friendship throughout the course of this work.

Andy Mitchell provided some of the software which was employed in generating synthetic traces, in addition to the reflection coefficient series and wavelet, which were employed in this study.

John Willoughby provided valuable support and advice with equipment which was employed during this study, and with other work with which the author was involved.

Fellow postgraduate students, including Shanti Rajagopalan, Andrew Lewis, Zhou Shaohua, and Shi Zhi Qun provided companionship and support.

Dr. Sven Treitel corresponded with the author regarding a Research Note and an article written during the course of this work. His words both stimulated and encouraged a young researcher.

My mother and grandparents provided support and encouragement throughout.

The Computing Centre of the University, and the National Centre for Petroleum Geology and Geophysics provided computing facilities. Staff of the University Computing Services provided valuable support. The Department of Geology and Geophysics provided additional facilities.

This thesis was completed under the provisions of a University of Adelaide postgraduate scholarship, typeset using LaTeX, and printed on the University of Adelaide's Apple Laserwriter.

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Introduction

Linear deconvolution has received significant attention in geophysical literature. Processes of Wiener filtering and frequency domain deconvolution have been discussed in a number of texts. The Wiener-Levinson algorithm has been frequently described as a tool for solving the normal equations to obtain deconvolution filters. Despite an extensive discussion of formulation and implementation of deconvolution, there has been little attention towards aspects such as numerical stability of the Wiener-Levinson algorithm, or conditioning of deconvolution. Both of these aspects relate to the reliability of numerically computed solutions to the normal equations. This lack of attention in geophysical literature has been in spite of the fact that there has been substantial discussion in mathematical literature for a number of years. A statement of a similar nature may also be made concerning Fourier series—for example Gibb's phenomenon is rarely mentioned in geophysical literature despite being a fundamental observation in texts on Fourier analysis. Some authors in geophysical literature have noted effects which relate to stability, conditioning, and related limitations of least squares deconvolution or Fourier transforms, and have either made a statement to the effect that "more theoretical development is needed in this area" or called for an explanation.

This thesis addresses a number of issues in the closely connected fields of conditioning and linear stability, focusing on linear least squares methods in the earth sciences. Effects in conditioning relate to the mathematical structure of the methods, and a significant portion of the theory discussed here owes its origins to mathematical literature and texts. The basic aim of discussion is to identify causes of ill-conditioning, methods for recognizing ill-conditioned systems in practice, whether or not this ill-conditioning results in numerical

difficulty or sensitivity to perturbations, and approaches which may be employed when ill-conditioning is encountered. Case studies using simulated data are performed to assess these concepts.

Chapter 1 introduces the basic theory of linear least-squares methods. The basic aims are to establish notation used in later chapters, and to demonstrate the relationships between methods considered in this thesis, and their relationship to standard linear regression techniques. An early and brief discussion of linear and multiple regression is given. Wiener (least-squares) filtering is then introduced. Discrete convolution is defined, the autocorrelation function is introduced, and spiking and predictive deconvolution are discussed. Frequency domain deconvolution is introduced briefly, together with a brief account of FFT's. Basic geostatistical theory is presented, focusing on Ordinary kriging and Co-kriging. The inter-relationship of the simple linear regression techniques and methods being considered in this thesis is discussed.

Chapter 2 introduces various aspects of linear systems, focusing on those with a square coefficient matrix. Various matrix classes (Toeplitz, symmetric, persymmetric, etc) are defined in an early section, and properties of their inverses are given. A number of solution algorithms, both direct and iterative (for general and Toeplitz matrices) are described. Eigenvalues and eigenvectors of matrices are introduced because of their importance in later chapters. Some aspects of algorithms for numerically evaluating eigenvalues and eigenvectors are discussed.

Chapter 3 discusses a number of aspects related to conditioning and numerical stability of the solution of linear equations. The concept of ill-conditioning of numerical problems is described, and aspects such as computational errors (rounding, etc) are introduced. The concept of ill-conditioning of linear equations is discussed. Vector and matrix norms are defined, and used to define condition numbers. A few symptoms of ill-conditioning, other than norms, are described, and limitations of approaches for recognizing ill-conditioned systems are considered. The chapter concludes with a discussion of conditioning of eigenvalue problems.

Chapter 4 begins with a survey of causes of ill-conditioned autocorrelation matrices

from a mathematical point of view. The Wiener-Levinson algorithm is discussed and it is seen that intermediate results of the algorithm may be employed to recognise circumstances in which rounding errors have a significant effect on the computed solution of the normal equations. Finally, an explanation of the effects of prewhitening on conditioning of the normal equations is given.

Chapter 5 is directed towards examples which illustrate some of the concepts of Chapter 4, and determine their usefulness in recognizing and avoiding ill-conditioning. Examples also show the effect of ill-conditioning in the normal equations on deconvolved outputs. Stability of solution algorithms, which was mentioned only as a footnote in Chapter 3, is discussed and used to account for observations that the Wiener-Levinson algorithm produces substantially poorer quality solutions than does the classical Gaussian elimination.

Chapter 6 extends results of previous chapters to apply to conditioning of some geostatistical methods. The topic of robustness, which has received some attention in geostatistical literature, and is closely related to the topic of conditioning, is discussed briefly. The effect of conditioning of the stationary covariance matrix on conditioning of the kriging matrix is described, and conditioning of covariance matrices are considered in light of the discussion of Chapter 4. Results relating to kriging matrices are extended to draw conclusions about conditioning of co-kriging.

Chapter 7 examines, via numerical experiments, some concepts of Chapter 6. It is seen that the unbias constraints of ordinary kriging and co-kriging have a significant effect on the condition number of the respective coefficient matrices. When the equations are solved using a stable algorithm, like Gaussian elimination, this effect does not significantly affect quality of computed solutions unless the stationary covariance matrix is ill-conditioned.

This thesis examines the behaviour of a number of linear methods, when solution is performed on a computer. The basic motivation may be summed up by the following quote from an interview of Milo Backus, which appeared in Geophysics : The Leading Edge of Exploration, 5(9), September 1986 :

> "How much time is invested today in checking the calculations of the computer?
>
> *Not nearly enough. One of the main things I try to teach my students is to never believe what comes out of the computer unless they can independently come up with the same answer within an order of magnitude without the computer. I have more trouble getting them to question the machine than anything else. The fact is that the computer output can be exceedingly misleading, and there's a real danger in thinking that since it's out to five decimal places it must be right. It's not that the computer makes mistakes, but that, not infrequently, a particular program is inappropriately used for a problem, and the machine can't figure out whether the programs it has are applicable to what you're trying to resolve."*
>
> Computers to displace interpreters? Never! says Milo Backus

Chapter 1

Linear Methods

1.1 Introduction and preliminaries

A common problem of statistics is the estimation of a function $Y(X)$ at locations X. This estimation is performed by making use, in some way, of a number of samples y_i which have been obtained at locations $\mathbf{x}_i$. In such a situation, the function Y has a distribution dependent upon the location X at which it is observed. This distribution is generally unknown, and observations y_i are subject to error, so the nature of the function Y can not be described in an entirely deterministic way. In the earth sciences, the determining variable X is often a location (*e.g.* latitude and longitude), and the response variable Y is some quantity such as ore grades at that location. In linear methods, the statistical estimation is performed (either implicitly or explicitly) as a weighted sum of a number of sampled values which occur within a given area A :

$$y^{\star}(\mathbf{x}_u) = w_0 + \sum_{\mathbf{x}_i \in A} w_i y(\mathbf{x}_i) \tag{1.1}$$

Linear least squares methods perform such estimations which minimize the average squared error between the true (unknown) value and the estimated value *i.e.* the techniques perform statistical estimations in an attempt to reduce the spread of error, as measured in a least squares sense, of the estimated values.

This chapter introduces some linear methods which are applied in the Earth Sciences.

Before introducing these methods, simple linear regression will be introduced in some detail to demonstrate the above concepts. The extension of linear regression to multiple determining variables will then be introduced to facilitate the comparison of other linear methods with simple linear regression. Later sections introduce methods which are more usually applied in the Earth Sciences, and are the main focus of this thesis. It will be demonstrated that these methods may be considered as extended versions of the well known linear regression model, and it will be shown how they are interrelated.

1.1.1 Some statistical language

This section introduces some statistical concepts which are exercised, implicitly or explicitly, in discussion in the remainder of this chapter.

Definition 1.1 *A random variable, Y, is a measurable quantity which has a statistical nature. The value of any one measurement may not be predicted in advance. However, if a number of measurements are performed, the measurements will have a distribution which may be characterized.*

Definition 1.2 *A random function $Y(\mathbf{x})$ is a set of random variables $Y(\mathbf{x}_\alpha)$, defined at each point $\mathbf{x}_\alpha$ within an area of interest.*

For example, $Y(\mathbf{x}) = \{Y(\mathbf{x}_\alpha), \forall \mathbf{x}_\alpha \in T\}$, where T may denote a time interval over which seismic amplitudes are measured, or may represent the area of a mineral deposit, over which grades are sampled.

Definition 1.3 *Particular measured, or measurable, values $y(\mathbf{x})$ of the random function $Y(\mathbf{x})$ are realizations.*

Under this definition, the true value at any location (which is generally unknown, but may be measured) may be interpreted as a realization. Similarly, any sample value may be interpreted as a realization.

A set of k realizations, from different locations $\mathbf{x}_i$, of the random function Y may be denoted by :

$$\{Y(\mathbf{x}_1), Y(\mathbf{x}_2), \ldots, Y(\mathbf{x}_k)\}$$

and characterized by a k-variable distribution function :

$$F_{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_k}(y_1, y_2, \ldots, y_k) = Prob\{Y(\mathbf{x}_1) < y_1, Y(\mathbf{x}_2) < y_2, \ldots, Y(\mathbf{x}_k) < y_k\}$$

Definition 1.4 *A random function is said to be stationary if the distribution function is invariant under translation :*

$$F_{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_k}(y_1, y_2, \ldots, y_k) = F_{\mathbf{x}_1+\mathbf{h},\mathbf{x}_2+\mathbf{h},\ldots,\mathbf{x}_k+\mathbf{h}}(y_1, y_2, \ldots, y_k)$$

Stationarity is essentially the assumption, commonly made in statistical theory, that the set of realizations (*e.g.* measurements) $y(\mathbf{x}_i)$ are drawn from the same population, and may be grouped, so statistical inferences about that population may be drawn from them.

1.2 Simple Linear Regression

Suppose that the values y_i are values which are measured corresponding to levels x_i of the determining variable. In this case, the vectors $\mathbf{x}_i$ have only one element and are therefore scalars. The aim of linear regression is to fit a straight line :

$$y = a + bx \tag{1.2}$$

where a and b are constants (the intercept and slope of the line respectively). The constants a and b are chosen so that the positive quantity

$$d = \sum_{i=1}^{n} (y_i - a - bx_i)^2$$

is minimized. The quantity d is referred to as the *Residual Sum of Squares*.

The quantities a and b may be obtained by the following approach :

1. From the raw data five quantities may be calculated :

(a) totals

$$x_T = \sum_{i=1}^{n} x_i \qquad y_T = \sum_{i=1}^{n} y_i$$

(b) raw sums of squares and products

$$S_{xx} = \sum_{i=1}^{n} x_i^2 \quad S_{xy} = \sum_{i=1}^{n} x_i y_i \quad S_{yy} = \sum_{i=1}^{n} y_i^2$$

2. From these five quantities, three more may be calculated :

$$P = S_{xy} - \frac{x_T y_T}{n} \quad Q = S_{yy} - \frac{y_T^2}{n} \quad R = S_{xx} - \frac{x_T^2}{n}$$

3. The estimates may then be obtained :

(a) Slope : $b = \frac{P}{R}$

(b) Intercept : $a = \frac{(y_T - b x_T)}{n}$

(c) Residual Sum of Squares : $d = Q - \frac{P^2}{R}$

An estimate of y corresponding to any value of x may be calculated by applying Equation 1.2.

Linear regression may be expressed as a linear weighting scheme, as described in Section 1.1, by manipulating the above formulae to obtain the following values for the weights of Equation 1.1 :

$$\begin{aligned} w_0 &= 0 \\ w_i &= \left(x_i - \frac{x_T}{n}\right)\left(1 - \frac{x_T \times x_u}{n}\right) + \frac{x_u}{n} \end{aligned}$$

It should be noted that the weights obtained are dependent upon the location of the point where a value is being estimated, and on the location of the data points *i.e.* the weights applied are dependent upon the data configuration.

1.3 Multiple regression analysis

Linear regression is a method whereby a least-squares "best" fit of a set of observations of a dependent variable y and an independent variable x may be obtained of the form :

$$y = a + bx$$

Similarly, multiple regression is a method used to obtain a least-squares "best" fit of a set of observations of a dependent variable y and of a number of independent variables $x_j, j = 1 \ldots m$ of the form :

$$y = a + \sum_{j=1}^{m} b_j x_j \tag{1.3}$$

To obtain the values of a and $b_j, j = 1 \ldots m$ on the basis of n samples :

$$(y_i, x_{1,i}, x_{2,i}, \ldots x_{m,i}), \; i = 1 \ldots n$$

the following procedure, which is analogous to that followed in Section 1.2, may be used :

1. Calculate average values :

$$\begin{aligned} \overline{y} &= \frac{1}{n} \sum_{i=1}^{n} y_i \\ \overline{x_j} &= \frac{1}{n} \sum_{i=1}^{n} x_{j,i} \quad j = 1 \ldots m \end{aligned}$$

2. The coefficients b_j can be obtained by solving the following set of simultaneous equations, which are referred to as the *normal equations* :

$$\sum_{i=1}^{m} \left\{ \sum_{t=1}^{n} (x_{j,t} - \overline{x_j})(x_{i,t} - \overline{x_i}) \right\} b_i = \sum_{t=1}^{n} (x_{j,t} - \overline{x_j})(y_t - \overline{y}) \quad j = 1 \ldots m \tag{1.4}$$

3. The value a can be obtained as :

$$a = \overline{y} - \sum_{j} b_j \overline{x_j}$$

The values of a and b_j $j = 1 \ldots n$ thus obtained are those which minimize the quantity :

$$E = \sum_{t=1}^{n} \left(y_t - a - \sum_{j=1}^{m} b_j x_{j,t} \right)^2$$

which is the total deviation between the (multi-dimensional) plane surface described in Equation 1.3 and the various sample points.

1.4 Seismic Deconvolution

The aim of an exploration geophysicist in the petroleum industry is to determine, on the basis of a number of methods, whether or not it is viable to drill for oil and/or gas at a given location. There are a number of methods used for such a reconnaissance, for example gravity and magnetic methods are employed to determine depth to basement, and hence the possible thickness of the sedimentary sequences in which hydrocarbons will be found. A frequently used method, after such initial reconnaissance has been performed, is the reflection seismic method. Although this method introduces the greatest cost into the exploration effort, the resolution of the method and the information it provides more than justifies this cost.

In the reflection seismic method a source is used to generate an acoustic wave which is filtered by the earth (dispersion, reflection, and transmission through various stratigraphic layers). The returned waveform is then measured by geophones at the surface. The aim of the method is to gain information about the structure of the earth. This structure is then used to determine where (and if) it is viable to drill.

In order to obtain this structure, it is necessary to have a model relating the input waveform, the earth filter, and the output waveform. Because the seismic method more commonly makes use of digital as opposed to analog data, the following discussion will refer to the digital filtering process.

The digital filtering process may be described by the discrete convolution formula :

$$y_\tau = x_t * e_t = \Delta t \sum_t x_t e_{\tau - t} \tag{1.5}$$

where x_t is the input, e_t is the filter, y_τ is the output, and Δt is the sampling increment. No loss of generality occurs if we assign $\Delta t = 1$, and this will be assumed in all that follows, unless otherwise stated. The output y_τ of Equation 1.5 is a weighted sum of values of the input, x_t, in the same fashion described in Equation 1.1. In terms of seismic theory, the input x_t represents the seismic source wavelet, the filter e_t is the "earth filter", which is intimately related to geological structure, and y_t represents the measured seismic trace.

In the field there is often a boundary with a sharp velocity and/or density contrast at or near the surface. On land this boundary can result from the presence of a "low velocity layer", which results in a significant reflection coefficient at the boundary between this layer and the higher velocity layers below. The surface of the earth also has a high reflection coefficient. At sea, high reflection coefficients occur both at the sea surface and at the sea bed. Because of these highly reflecting boundaries, the acoustic wave is continually reflected between them, the amplitude only gradually decreasing with time, and the seismic section thus obtained takes on a reverberatory nature. These reverberations, or multiples, of the initial reflection event, conceal later primary reflection events which may be of much smaller amplitude. In order to detect these reflection events, it is necessary to remove the effects of the reverberations.

The predictive deconvolution technique aims to remove contaminating effects of multiples. It amounts essentially to determining a filter w_t which, when convolved with the seismic trace, removes the effects of multiples. Deconvolution techniques are also employed to remove contaminating effects of the seismic wavelet to improve temporal resolution and aid seismic interpretation.

This section is primarily concerned with least squares deconvolution, which is also referred to as Wiener filtering. The section concludes with a brief discussion of frequency domain filtering. Most of the following theory is described by Peacock and Treitel (1969), Rice (1962), Robinson (1967b), Robinson (1983), and Yilmaz (1987). Notation has been altered from that in the above texts to enable comparison of deconvolution with other methods discussed in this chapter. The primary purpose here is the introduction of Wiener filtering as the solution of a linear system. The theory described here is implicitly based on a number of assumptions :

- source and receivers are coincident,
- geological boundaries are horizontal, and wave paths are strictly vertical (perpendicular to the boundaries),
- the seismic disturbance is stationary (*i.e.* it does not change form with time),

- data is free of noise.

In practice, these assumptions are not strictly true :

- geophones are generally spread in an array, or along a line, separate from the source of the seismic disturbance.
- geological boundaries are not, in general, horizontal,
- a loss of amplitude occurs due to spherical divergence and inelastic absorption,
- random noise occurs in experimental data *e.g.* instrument error, back scattering

These aspects are discussed more extensively in geophysical literature, *e.g.* Yilmaz (1987). In practice, deviations from the assumptions being made are minor, unless the geology is quite complex. A number of additional approaches in processing (*e.g.* common depth point (CDP) stacking, correction for spherical divergence, migration) are employed, either before or after deconvolution, to correct field data to conform, in at least an approximate fashion, to assumptions being made in theory.

1.4.1 Wiener Filtering

The Wiener filter, w_t, is a particular filter which minimizes the mean-square error :

$$I = E\left\{(z_\tau - y_\tau)^2\right\} \tag{1.6}$$

where :

- z_τ is some arbitrary desired output,
- y_τ is the actual output, obtained by convolving the input sequence, x_t, with the Wiener filter :

$$y_\tau = x_t * w_t$$

The n-length Wiener filter results from the solution of the *normal equations* :

$$\sum_{t=0}^{n-1} w_\tau r_{\tau-t} = g_\tau \ \forall \tau = 0, 1, \ldots, n-1 \tag{1.7}$$

where :

- r_τ is the autocorrelation of the input :

$$r_\tau = E\{x_t x_{t+\tau}\} \tag{1.8}$$

  It may also be shown, by a change of variables, that $r_{-\tau} = r_\tau$.

- g_τ is the cross-correlation between the desired output and the input :

$$g_\tau = E\{z_t x_{t+\tau}\} \tag{1.9}$$

- w_t is the Wiener filter.

The expressions given here for the autocorrelation and cross-correlation functions may be seen to be identical in form to convolution given in Equation 1.5, except for a sign change in one term. and the use of $E\{\ldots\}$ (the mathematical expectation) instead of summation terms. In fact, one may write :

$$g'(\tau) = z(t) * x(-t) = \sum_t z_t x_{t+\tau}$$

where $g'(\tau)$ differs from $g(\tau)$ by only a scale factor. The first form is commonly expressed in seismic literature (*e.g.* Rice (1962), Robinson (1967a), Kulhanek (1976)) whilst the second is consistent with the definition of convolution and correlation between functions (*e.g.* Bracewell (1978)). This difference of definition will be ignored in all that follows—the autocorrelation and cross-correlation functions will be expressed as either expectations or convolutions as is more convenient to the discussion in hand. In particular, autocorrelations which occur in examples of Chapter 5 are computed as summations :

$$\sum_t x_t x_{t+\tau}$$

rather than as expectations

$$\frac{1}{n(\tau)} \sum_t x_t x_{t+\tau}$$

where $n(\tau)$ is the number of pairs contributing to the summation. Claerbout (1976) has noted that dividing by $n(\tau)$ to obtain an expectation may introduce difficulties in practice when $n(\tau)$ is not constant (*e.g.* due to end effects).

Equation 1.7 may be expressed in matrix form :

$$\begin{pmatrix} r_0 & r_1 & \cdots & r_{n-1} \\ r_1 & r_0 & \cdots & r_{n-2} \\ & & \vdots & \\ r_{n-1} & r_{n-2} & \cdots & r_0 \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_{n-1} \end{pmatrix} = \begin{pmatrix} g_0 \\ g_1 \\ \vdots \\ g_{n-1} \end{pmatrix} \tag{1.10}$$

or more compactly as :

$$\mathbf{Rw} = \mathbf{g} \tag{1.11}$$

The resulting minimum mean-square-error is :

$$I_0 = r_0 - \left(w_0 r_\alpha - \sum_{j=1}^{n-1} w_j r_{\alpha+j} \right) \tag{1.12}$$

Robinson (1967a, p. 43) has stated that the coefficient matrix, $\mathbf{R}$, referred to as the autocorrelation matrix, is Toeplitz, symmetric, and positive indefinite[1]. Throughout this thesis, except where stated otherwise, the autocorrelation matrix is considered to be positive definite. More properties of this matrix will be discussed in Section 4.4.1.

1.4.1.1 The prediction operator

If a_t is the prediction operator, with prediction distance α, then the output y_τ will be an estimate of the input x_t at a future time $t + \alpha$:

$$y_\tau = \sum_t x_t a_{\tau - t} = x^\star_{t+\alpha} \tag{1.13}$$

An error series may then be defined as the difference between the true value $x_{t+\alpha}$ and the estimated value $x^\star_{t+\alpha}$:

$$\epsilon_{t+\alpha} = x_{t+\alpha} - x^\star_{t+\alpha} \tag{1.14}$$

[1]The terms Toeplitz, symmetric, positive definite, and positive indefinite, are defined in Chapter 2.

This prediction error series is the non-predictable part of the series x_t. It is of interest to the geophysicist because it represents information contained within the seismic trace which is not contaminated due to reverberations—the non-predictable component of the trace may be attributed to primary reflections, which are due to geological boundaries, while the predictable component represents multiple reflections.

The cross-correlation between the input and desired output is :

$$g_\tau = E\left\{x_t x_{t+\alpha+\tau}\right\} = r_{\tau+\alpha}$$

therefore the Wiener prediction filter, a_t is obtained by solving the linear system :

$$\begin{pmatrix} r_0 & r_1 & \cdots & r_{n-1} \\ r_1 & r_0 & \cdots & r_{n-2} \\ & & \vdots & \\ r_{n-1} & r_{n-2} & \cdots & r_0 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} = \begin{pmatrix} r_\alpha \\ r_{\alpha+1} \\ \vdots \\ r_{\alpha+n-1} \end{pmatrix} \tag{1.15}$$

1.4.1.2 The spiking operator

The spiking operator, s_τ, produces, as output, a unit spike :

$$y_\tau = \sum_t x_t s_{\tau-t} = \begin{cases} 1 & \text{if } \tau = 0. \\ 0 & \text{otherwise.} \end{cases} \tag{1.16}$$

This operator is also known as the *inverse operator*, and may be employed to compress the seismic wavelet.

As for the prediction operator, the Wiener spiking operator may be obtained by solving a linear system :

$$\begin{pmatrix} r_0 & r_1 & \cdots & r_{n-1} \\ r_1 & r_0 & \cdots & r_{n-2} \\ & & \vdots & \\ r_{n-1} & r_{n-2} & \cdots & r_0 \end{pmatrix} \begin{pmatrix} s_0 \\ s_1 \\ \vdots \\ s_{n-1} \end{pmatrix} = \begin{pmatrix} x_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

This means that there is little mathematical difference between Wiener prediction filtering and Wiener spiking filtering.

1.4.2 Frequency domain deconvolution

Previous sections have been primarily concerned with time domain deconvolution, with an emphasis placed on Wiener filters. In this section, deconvolution in the frequency domain is considered.

The Fourier transform of a continuous function $x(t)$ is defined as :

$$X(\omega) = \int_{-\infty}^{\infty} x(t)e^{-i\omega t}dt \qquad (i = \sqrt{-1}).$$

provided that certain conditions are met, for example :

- The integral

$$\int_{-\infty}^{\infty} |x(t)|dt$$

  exists,

- Any discontinuities in $x(t)$ are finite.

In cases where no Fourier transform in the ordinary sense exists, the transform may be expressed in a limiting sense by means of generalized functions. More details on conditions for existence are provided by texts on Fourier analysis, *e.g.* Arsac (1966) and Bracewell (1978). For example if the function $x(t)$ is such that

$$\int_{-\infty}^{\infty} |x(t)|^2 dt$$

exists (in which case $x(t)$ is referred to as "square integrable" in this thesis) the Fourier transform is defined as above.

The Fourier transform is a reversible process *i.e.* given the function $X(\omega)$, $x(t)$ may be reconstructed :

$$x(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} X(\omega)e^{i\omega t}d\omega$$

If $x(t)$ is represented by discrete samples (with sampling interval $\Delta t = 1$) :

$$x_0, x_1, \ldots x_{n-1}$$

then the discrete Fourier transform may be written :

$$X(\omega) = \sum_{t=0}^{n-1} x_t e^{-i\omega t}$$

Frequency domain deconvolution is based on the fact that convolution in the time domain corresponds to multiplication in the frequency domain :

$$x(t) * e(t) \leftrightarrow X(\omega)E(\omega)$$

which means that Equation 1.5 may be expressed in the frequency domain as :

$$Y(\omega) = X(\omega)E(\omega)$$

and spiking deconvolution may be expressed as a division in the frequency domain :

$$E(\omega) = \frac{Y(\omega)}{X(\omega)}$$

1.4.2.1 Fast Fourier Transforms

In practice, the Fourier transform of the discrete series :

$$x_0, x_1, \ldots x_{n-1}$$

may be represented by n values in the frequency domain corresponding to :

$$\omega = \frac{2\pi j}{n}, \quad j = 0 \ldots n-1$$

This is possible without loss of information because the discrete Fourier transform is periodic :

$$H(\omega) = H(\omega + 2\pi)$$

and the discrete time series may be reproduced from these discrete Fourier values. This does *not* mean that the function $x(t)$ may be reproduced from either the discrete time series or discrete Fourier series—if the function $x(t)$ contained frequencies higher than $\pi/\Delta t$ (the aliasing frequency), then these higher frequencies will be mapped to other parts of the spectrum. This effect is known as aliasing.

The discrete Fourier transform may be performed quite readily on a computer. The process is, however, relatively inefficient, requiring approximately n^2 multiplications. For certain values of n, the algorithm may be rearranged to calculate the Fourier transform much more rapidly, using the order of $n \log n$ multiplications. Such algorithms were originally introduced by Cooley and Tukey (1965) and have been discussed further by Tukey (1967) and Nussbaumer (1982). These efficient methods are referred to as "Fast Fourier Transforms" or more briefly as FFT's. The most common FFT routine employed in seismic processing is the radix 2 form, in which the length of the series, n, is a power of 2.

1.4.2.2 Truncation of the series

One consideration which often arises in practice is the computation of a spectrum from a small part of a computed autocorrelation. Truncating the series causes the computed spectrum to be an erratic function of frequency. For this reason a weighting operation which results in a smoother computed spectrum is often applied to the computed autocorrelation. This consideration is covered quite extensively in literature *e.g.* Jenkins (1961), Parzen (1961). A number of different weighting schemes are applied in practice, and there are different advantages to be offered by each scheme. Examples of weighting, or windowing, schemes include :

- the Triangular weighting function :

$$w_t = \begin{cases} 1 - |t/M| & t \leq M \\ 0 & |t| > M \end{cases}$$

- the Hamming weighting function :

$$w_t = \begin{cases} 0.54 + 0.46 \cos(\pi t/M) & t \leq M \\ 0 & |t| > M \end{cases}$$

1.5 Geostatistical techniques

Geostatistical techniques aim to estimate values of some measurable attribute of a phenomenon (*e.g.* grades of ore or concentrations of pollutants), either at unsampled

points, or averaged over a region R (*e.g.* a mining block), on the basis of a number of samples which occur in the neighbourhood of the point or region being estimated. This section introduces two geostatistical techniques, Ordinary Kriging and Co-kriging. Most of the theory is discussed by Journel and Huijbregts (1978), David (1977), and Rendu (1981). To facilitate comparison with other methods described in this thesis, notation and symbols have been changed from those given in these texts.

1.5.1 Stationarity of order 2

Stationarity, defined in Section 1.1.1, requires that the spatial law, F, is invariant under translation. However in linear geostatistics, which is being considered here, *stationarity of order 2* is sufficient and this constraint may be reduced to :

1. the mathematical expectation $E\{Y(\mathbf{x})\}$ exists and is independent of factors such as size of samples (*e.g.* length of the drill core) or methods employed to obtain samples (*e.g.* type of drilling). Thus :

$$E\{Y(\mathbf{x})\} = m \tag{1.17}$$

2. for any pair of random variables $\{Y(\mathbf{x}), Y(\mathbf{x}+\mathbf{h})\}$ the covariance function exists and depends exclusively on the separation $\mathbf{h}$:

$$C(\mathbf{h}) = E\{Y(\mathbf{x}+\mathbf{h})Y(\mathbf{x})\} - m^2 \quad \forall \mathbf{x} \tag{1.18}$$

1.5.2 Linear Kriging

All linear kriging techniques use a linear estimator to give estimates of the form :

$$\overline{Y}^{\star}_{R}(\mathbf{x}) = w_0 + \sum_{\alpha=1}^{n} w_\alpha \times y(\mathbf{x}_\alpha) \tag{1.19}$$

(*c.f.* Equation 1.1) where :

- $\overline{Y}^{\star}_{R}(\mathbf{x})$ is the estimate of the mean value of the random variable $Y(\mathbf{x})$ over a region R. The random variable $Y(\mathbf{x})$ is either the variable of interest (*e.g.* ore grade) or some appropriately transformed version of it.

- $y(\mathbf{x}_\alpha), \alpha = 1, .., n$ are the sample values being used to make this estimate ($\mathbf{x}_\alpha \in N$).
- w_α is the weight being applied to the sample, $y(\mathbf{x}_\alpha)$, at location $\mathbf{x}_\alpha$.

The estimator chosen is the particular one which minimizes the expected squared error (also called the estimation variance) between the true (unknown) values and the estimated values, which is denoted by $E\{[\overline{Y}_R(\mathbf{x}) - \overline{Y}^\star_R(\mathbf{x})]^2\}$. Note the similarity between Equations 1.19 and 1.1—the estimates provided by these equations are both weighted sums of sample values.

1.5.3 Non-bias conditions

An estimator is said to be globally unbiased if the expected value of all the estimates is the same as the expected value of the true results. Mathematically this is :

$$E\{\overline{Y}^\star_R(\mathbf{x})\} = E\{\overline{Y}_R(x)\} \tag{1.20}$$

This condition can be enforced in a number of ways. One way is to satisfy the following conditions :

$$\begin{aligned} \sum_{\alpha}^{N} w_\alpha &= 1 \\ w_0 &= 0 \end{aligned} \tag{1.21}$$

Journel and Huijbregts (1978, pp. 560-561) describe other non-bias constraints, which apply to non-stationary systems. The constraint given above is the only one considered in this study, as attention is being directed towards Ordinary Kriging.

1.5.4 Ordinary Kriging

The Ordinary Kriging procedure is one of finding a linear estimator, as given in Equation 1.19 which minimizes the expected squared error of the estimated results, subject to the nonbias constraints given in Equation 1.21. It may be shown using Calculus of

Variations that the weights $w_\alpha, \alpha = 1, \ldots, n$ satisfy the following system of simultaneous equations :

$$\begin{aligned} \sum_{\beta=1}^{n} w_\beta \times C(\mathbf{x}_\alpha, \mathbf{x}_\beta) - \mu &= \overline{C}(\mathbf{x}_\alpha, R) \quad \forall \alpha = 1..n \\ \sum_{\alpha=1}^{n} w_\alpha &= 1 \end{aligned} \tag{1.22}$$

where :

- μ is a Lagrange multiplier applied to the system
- the function $C(\mathbf{x}_\alpha, \mathbf{x}_\beta)$ is the covariance between points $\mathbf{x}_\alpha$ and $\mathbf{x}_\beta$ which are separated by a vector $\mathbf{h} = \mathbf{x}_\alpha - \mathbf{x}_\beta$. This is defined as :

$$C(\mathbf{x}_\alpha, \mathbf{x}_\beta) = E\{[Y(\mathbf{x}_\alpha) - m(\mathbf{x}_\alpha)][Y(\mathbf{x}_\beta) - m(\mathbf{x}_\beta)]\} \tag{1.23}$$

  where :

  - $m(\mathbf{x}_\alpha)$ and $m(\mathbf{x}_\beta)$ are the expectations of the random variable $Y(\mathbf{x})$ at locations $\mathbf{x}_\alpha$ and $\mathbf{x}_\beta$ respectively
  - if the covariance is available for any possible combination of $\mathbf{x}_\alpha$ and $\mathbf{x}_\beta$ the bivariate distribution of $Y(\mathbf{x}_\alpha)$ and $Y(\mathbf{x}_\beta)$ is totally described.

- $\overline{C}(\mathbf{x}_\alpha, R)$ denotes the mean value of the covariance function, evaluated between the location $\mathbf{x}_\alpha$ and all locations within the region R.

Equation 1.22 may be expressed in matrix form as :

$$\begin{pmatrix} & & & 1 \\ & \mathbf{C} & & \vdots \\ & & & 1 \\ 1 & \ldots & 1 & 0 \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_n \\ -\mu \end{pmatrix} = \begin{pmatrix} \mathbf{c} \\ \\ 1 \end{pmatrix} \tag{1.24}$$

where :

- **C** is the covariance matrix with elements $C_{\alpha\beta} = C(\mathbf{x}_\alpha, \mathbf{x}_\beta)$ $\alpha, \beta = 1 \ldots n$. This matrix is symmetric and positive indefinite in general, meaning that all its eigenvalues are non-negative. Throughout this thesis, except where stated otherwise, the covariance matrix is implicitly assumed positive definite, and therefore non-singular.

- **c** is a vector of mean covariance values with elements $c_\alpha = \overline{C}(\mathbf{x}_\alpha, R)$

It is apparent from Equation 1.23 that in order to make statistical inferences it is necessary, in general, to have a large number of realizations of random variable pairs $\{Y(\mathbf{x}_\alpha), Y(\mathbf{x}_\beta)\}$ as the covariance is dependent upon both the location of the aggregate of two data points $\mathbf{x}_\alpha$ and $\mathbf{x}_\beta$, as well as on their separation. In practice, this difficulty is relieved by assuming stationarity of order 2, which means that the covariance function of Equation 1.23 depends only upon the separation $\mathbf{h} = \mathbf{x}_\alpha - \mathbf{x}_\beta$.

1.5.5 Ordinary Kriging with the semivariogram

The semivariogram function, which is one characteristic of the bivariate distribution of $Y(\mathbf{x})$ and $Y(\mathbf{x} + \mathbf{h})$, may be defined as :

$$\gamma(\mathbf{h}) = \frac{1}{2} E\{[Y(\mathbf{x} + \mathbf{h}) - Y(\mathbf{x})]^2\} \tag{1.25}$$

The semivariogram may be rewritten in terms of the covariance function :

$$\gamma(\mathbf{h}) = C(\mathbf{0}) - C(\mathbf{h}) \tag{1.26}$$

Under an assumption of stationarity, this may be substituted into Equation 1.22 to obtain an equivalent set of simultaneous equations :

$$\begin{aligned} \sum_{\beta=1}^{n} w_\beta \times \gamma(\mathbf{x}_\alpha, \mathbf{x}_\beta) + \mu &= \overline{\gamma}(\mathbf{x}_\alpha, R) \quad \forall \alpha = 1 \ldots n \\ \sum_{\alpha=1}^{n} w_\alpha &= 1 \end{aligned} \tag{1.27}$$

which may be expressed in a matrix form similar to Equation 1.24 :

$$\begin{pmatrix} & & & 1 \\ & \boldsymbol{\Gamma} & & \vdots \\ & & & 1 \\ 1 & \dots & 1 & 0 \end{pmatrix} \begin{pmatrix} w_1 \\ \vdots \\ w_n \\ \mu \end{pmatrix} = \begin{pmatrix} \mathbf{g} \\ \\ 1 \end{pmatrix} \tag{1.28}$$

where :

- $\boldsymbol{\Gamma}$ is the semivariogram matrix ($\Gamma_{\alpha\beta} = \gamma(\mathbf{x}_\alpha, \mathbf{x}_\beta)$ $\alpha, \beta = 1 \dots n$).
- $\mathbf{g}$ is a vector of mean semivariogram values with elements $g_\alpha = \overline{\gamma}(\mathbf{x}_\alpha, R)$

The estimation variance associated with the weights produced may be expressed in terms of semivariograms as :

$$\sigma_E^2 = 2\overline{\gamma}(R, v) - \overline{\gamma}(R, R) - \overline{\gamma}(v, v) \tag{1.29}$$

where :

- R is the region for which the estimate is being calculated
- v denotes the set of sample points used to perform the estimation
- $\overline{\gamma}(A, B)$ represents the mean value of the semivariogram as measured/evaluated between the two sets of points (or regions) A and B.

In practice, the experimental semivariogram (or covariance) is fitted with some form of analytical function. This modelling is of vital interest, and is discussed further in Section 1.6. Modelled semivariograms which depart significantly from the underlying (unknown) semivariogram can be expected, intuitively, to give lower quality results (*e.g.* a larger spread of error in kriged estimates) than would a model which does not depart significantly from the underlying semivariogram. However, it will be seen in Chapters 6 and 7, that models which fit the experimental data relatively well may still result in poor quality results, because certain models may result in a non-robust[2] kriging system and/or

[2]The topic of robustness is discussed in Section 6.1.

numerical difficulty obtaining kriging weights. This means that it is possible to obtain a model which does not depart significantly from the underlying situation, but numerical errors introduced when solving the kriging equations may still mean kriged estimates are of little value.

1.5.6 Positive-definite conditions

Equation 1.29 provides the estimation variance in terms of the semivariogram function $\gamma(\mathbf{h})$, if stationarity is assumed. However this form will not necessarily ensure a non-negative predicted estimation variance. However, an estimation variance must always be non-negative. This means that semivariogram functions must be chosen in such a way that a negative result in Equation 1.29 is impossible. This is a far from trivial problem. Armstrong and Diamond (1984b) give an account of the problems involved, and present a method which may be used to test if a given model provides a non-negative estimation variance. This constraint may be related to the positive indefiniteness of the covariance matrix, $\mathbf{C}$. Functions which ensure non-negative estimation variances are said to be conditionally positive definite.

In geostatistical practice, the covariance is usually modelled as a monotonic (decreasing) function of lag, $|h|$ (or, conversely, the semivariogram is modelled as a monotonic (increasing) function). This consideration is not necessary to satisfy the positive definite constraint. It relates back to the observation that the correlation between data values can often be expected to decrease as the distance between them increases. However, this assumption is not generally true, *e.g.* Journel and Huijbregts (1978) describe the "hole effect" in which the covariance model does not monotonically decay. Frequently, in practice, natural variability observed within an ore body causes hole effects to be associated with other structures, which result in a dampening of the hole effect. Therefore, hole effects are often ignored in geostatistical practice, and experimental covariances are modelled as monotonically decaying functions. All discussion of geostatistical methods in this thesis assumes that covariances are positive valued functions which monotonically decay towards

zero, and corresponding covariance matrices are positive definite, as is often assumed in geostatistical practice. However, it must be noted that, in practice, the assumption of a monotonically decaying function may only be an approximation to a more general situation.

1.5.7 Co-kriging

Co-kriging is a method which was developed for situations where samples of two or more correlated variables exist (*e.g.* uranium and gold). The method uses values of a number of variables to estimate one of them, making use of correlation between variables. For example, a better estimate of gold content may be made by using both gold and uranium data to make the estimate, rather than using only the gold values. The method was primarily directed towards the case in which one variable has been undersampled relative to the other variables, and estimation of this undersampled variable is desired.

Mathematically, Co-kriging may be considered as an extension of Ordinary Kriging—it is a procedure which produces a linear estimator consisting of a weighted sum of sample values of a number of variables or attributes :

$$\overline{Y}^{\star}_{k_0,R}(\mathbf{x}) = \sum_{k=1}^{K} \sum_{\alpha_k=1}^{n_k} w_{\alpha_k} \times y_k(\mathbf{x}_{\alpha_k}). \tag{1.30}$$

where :

- K is the number of sampled variables being used to perform the estimate *e.g.* if a Co-kriging approach is employing samples of gold and uranium to estimate gold grades, then $K = 2$
- n_k is the number of samples available of the variable y_k
- $y_k(\mathbf{x}_{\alpha_k})$ denotes sample values at locations $\mathbf{x}_{\alpha_k}$ of y_k which are being used to perform the estimation
- k_0 denotes the variable whose average value is being estimated over the region R
- w_{α_k} is the weight applied to the sample $y(\mathbf{x}_{\alpha_k})$

The weights are chosen to minimize the expected squared error between true (unknown) values and estimated values of the particular variable, k_0, of interest. As in Section 1.5.2 a set of equations may be obtained :

$$\begin{aligned}
\sum_{k'=1}^{K}\sum_{\beta_{k'}=1}^{n_{k'}} w_{\beta_{k'}}\overline{C}_{k'k}(x_{\beta_{k'}}, x_{\alpha_k}) - \mu_k &= \overline{C}_{k_0k}(R, x_{\alpha_k}) \quad \forall\alpha_k = 1,..n_k, \quad \forall k = 1,\ldots,K \\
\sum_{\beta_{k_0}=1}^{n_{k_0}} w_{\beta_{k_0}} &= 1 \\
\sum_{\beta_k=1}^{n_k} w_{\beta_k} &= 0 \quad \forall k \neq k_0
\end{aligned} \tag{1.31}$$

where $C_{k'k}$ is the cross-covariance between variables k' and k, defined (*c.f.* Equation 1.23) as :

$$C_{k'k}(\mathbf{x}_\alpha, \mathbf{x}_\beta) = E\{[Y_{k'}(\mathbf{x}_\alpha) - m_{k'}(\mathbf{x}_\alpha)][Y_k(\mathbf{x}_\beta) - m_k(\mathbf{x}_\beta)]\} \tag{1.32}$$

where $m_k(\mathbf{x})$ denotes the expectation of the random variable Y_k at the location $\mathbf{x}$.

Note the presence of non-bias conditions in the system of Equations 1.31—in order to satisfy the global non-bias conditions of Equation 1.20, the weights applied to the variable being estimated must add to unity and the weights applied to all other variables must add to zero for each variable.

If stationarity may be assumed, this system may be expressed in terms of cross-variograms as follows :

$$\begin{aligned}
\sum_{k'=1}^{K}\sum_{\beta_{k'}=1}^{n_{k'}} w_{\beta_{k'}}\overline{\gamma}_{k'k}(\mathbf{x}_{\beta_{k'}}, \mathbf{x}_{\alpha_k}) + \mu_k &= \overline{\gamma}_{k_0k}(R, \mathbf{x}_{\alpha_k}) \quad \forall\alpha_k = 1,..n_k, \quad \forall k = 1,..K \\
\sum_{\beta_{k_0}=1}^{n_{k_0}} w_{\beta_{k_0}} &= 1 \\
\sum_{\beta_k=1}^{n_k} w_{\beta_k} &= 0 \quad \forall k \neq k_0
\end{aligned} \tag{1.33}$$

where the cross-variogram function is defined, in a similar fashion to the semivariogram function of Equation 1.25 :

$$\gamma_{k'k}(\mathbf{h}) = \frac{1}{2}E\left\{[Y_{k'}(\mathbf{x}+\mathbf{h}) - Y_{k'}(\mathbf{x})]\,[Y_k(\mathbf{x}+\mathbf{h}) - Y_k(\mathbf{x})]\right\} \tag{1.34}$$

Equations 1.31 and 1.33 may be expressed in matrix forms similar to those given in Equations 1.24 and 1.28 for Ordinary Kriging. The estimation variance associated with the Co-kriging weights thus produced may be expressed in terms of variogram functions as :

$$\sigma_E^2 = \sum_{k=1}^{K} \sum_{\alpha_k=1}^{n_k} \{w_{\alpha_k} \overline{\gamma}_{k_0 k}(R, \mathbf{x}_{\alpha_k})\} - \overline{\gamma}_{k_0 k_0}(R, R) + \mu_{k_0} \tag{1.35}$$

But, what happens if all available data sets are sampled at every sample location, so that one is not undersampled relative to the others? Journel and Huijbregts (1978) state that if all variables coexist at all sample locations and coregionalization is intrinsic (*i.e.* all semivariograms and cross variograms are proportional to one basic model), Co-kriging provides no advantage over Ordinary Kriging, as the estimation variance obtained using Ordinary Kriging will be identical to that obtained using Co-kriging. However it has been shown by Journel (1984) that if coregionalization is not intrinsic then Co-kriging will always provide a smaller estimation variance. This in turn implies a smaller spread of error in the results.

1.5.8 Properties of the cross-variogram and cross-covariance

In the foregoing discussion, the Co-kriging system was expressed in terms of cross-covariance functions, and then converted into an expression involving cross-variogram functions in an analogous way to that presented in Section 1.5.2 for expressing the kriging system in terms of semivariograms. In the case of Co-kriging, however, the cross-variogram is symmetric in (k', k) and $(h, -h)$, whilst this is not necessarily true for the cross-covariance :

$$\gamma_{k'k}(h) = \gamma_{kk'}(h) \quad \text{and} \quad \gamma_{k'k}(h) = \gamma_{k'k}(-h) \tag{1.36}$$

$$C_{k'k}(h) = C_{kk'}(h) \quad \text{and} \quad C_{k'k}(h) \neq C_{k'k}(-h) \tag{1.37}$$

The cross-covariance may be asymmetric if one variable lags behind another (*e.g.* rich lead grades may lag behind rich zinc grades in a given direction due to replacement phenomena). This lag effect will not appear on the cross-variogram, but it will on the cross-covariance. However, in many cases, it is sufficient to assume that the cross-covariance is symmetric, and to use the co-kriging system expressed in terms of cross-variogram functions. This is

assumed throughout this thesis in discussion of Co-kriging. As this effect does not occur in the covariance, no such consideration is required for Ordinary Kriging.

1.5.9 The linear model for a coregionalization

The linear model for a coregionalization is a mathematical model which enables the establishment of a matrix of cross-variograms, $[\gamma_{kk'}(\mathbf{h})]$ (or more generally cross-covariances, $[C_{kk'}(\mathbf{x},\mathbf{h})]$) which is positive definite to ensure that the variances of all finite linear combinations of the random functions $Y_k(\mathbf{x})$ are non-negative. The model consists of defining all direct and cross-variograms for all variables $k, k' = 1,..,K$ as linear combinations of m basic variogram models :

$$\gamma_{kk'}(\mathbf{h}) = \sum_{i=1}^{m} a_{kk',i} \times \gamma_i(\mathbf{h}) \tag{1.38}$$

For combinations of the i^{th} basic model, $\gamma_i(\mathbf{h})$, this may be expressed in the form :

$$\begin{pmatrix} \gamma_{11,i}(\mathbf{h}) & \dots & \gamma_{1K,i}(\mathbf{h}) \\ \vdots & \ddots & \vdots \\ \gamma_{K1,i}(\mathbf{h}) & \dots & \gamma_{KK,i}(\mathbf{h}) \end{pmatrix} = \underbrace{\begin{pmatrix} a_{11,i} & \dots & a_{1K,i} \\ \vdots & \ddots & \vdots \\ a_{K1,i} & \dots & a_{KK,i} \end{pmatrix}}_{\mathbf{A}} \begin{pmatrix} \gamma_i(\mathbf{h}) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \gamma_i(\mathbf{h}) \end{pmatrix} \tag{1.39}$$

For each component i, the coefficient matrix $\mathbf{A}$ must be positive definite—all its eigenvalues must be real and positive. The following K conditions may also be applied (refer to Bellman (1960, Chapter 4)) :

$$a_{11,i} > 0, \begin{vmatrix} a_{11,i} & a_{12,i} \\ a_{21,i} & a_{22,i} \end{vmatrix} > 0 \dots, \begin{vmatrix} a_{11,i} & \dots & a_{1K,i} \\ \vdots & \ddots & \vdots \\ a_{K1,i} & \dots & a_{KK,i} \end{vmatrix} > 0. \tag{1.40}$$

It may be seen that the matrix $\mathbf{A}$ is symmetric because $\gamma_{kk'}(\mathbf{h}) = \gamma_{kk'}(-\mathbf{h}) = \gamma_{k'k}(\mathbf{h})$.

When samples of two different regionalized variables, say $Y_1(\mathbf{x})$ and $Y_2(\mathbf{x})$, are available (*i.e.* $K = 2$) and both will be used to produce estimates of one of them (say Y_1), the positive definite constraints reduce to the following :

$$\left.\begin{aligned} a_{Y_1Y_1,i} &> 0 \\ a_{Y_2Y_2,i} &> 0 \\ a_{Y_1Y_1,i} \times a_{Y_2Y_2,i} - a_{Y_1Y_2,i} \times a_{Y_2Y_1,i} &> 0 \end{aligned}\right\} \forall i = 1, m \tag{1.41}$$

1.6 The inter-relationship of methods

There is fundamentally little difference between multiple regression, Wiener filtering, and Ordinary Kriging. Information provided by the autocorrelation function for Wiener filtering, in Equation 1.7, is given by the covariance or semivariogram functions for Ordinary Kriging, in Equations 1.22 and 1.27. Terms on the left hand side of Equation 1.4 provide the same information for multiple regression.

Multiple regression fits a planar surface based on all data locations. Wiener filtering and Ordinary kriging use information provided by the autocorrelation or covariance in performing estimation *i.e.* the surface fitted to perform an estimate is dependent upon the data. Geostatistical practice often involves imposing a functional model, examples of which are employed in Chapter 7, to the covariance or semivariogram. This modelling is performed because geostatistical estimates are often desired for arbitrary locations and/or averaged over a region, R. Referring to Equation 1.22, this means that it is necessary to have some form of knowledge of the covariance or semivariogram function at lags, h, for which there is no experimental estimate, and a model of some type is required to provide these values. Predictive deconvolution, as applied in seismic processing, involves estimation using regularly spaced data along a seismic trace to predict values at locations which also occur on the trace. This means that experimental autocorrelation values provide all the information needed in Equation 1.15, and no model of the autocorrelation function need be invoked. The nature of the selected covariance or semivariogram function affects the behaviour of Ordinary Kriging estimates. For example, the geostatistical practice of assuming that a covariance function is a monotonically decaying function obviously has some bearing on results of Ordinary Kriging. Ordinary Kriging also imposes the nonbias constraint to ensure that the mean value of estimates is the same as the mean of the data.

It must be noted that all the linear techniques discussed in this chapter implicitly assume a linear model with the aim of making useful inferences. No claim may be made, in general, that the linear model describes reality. For example, no claim is made in geostatistical theory that grades in any given deposit are randomly distributed—the theory of random

variables is utilized because any deposit with a given set of properties (*e.g.* mean grade, or covariance structure, etc.) may be considered as one possibility (*i.e.* a realization) of all possible deposits which could give rise to those properties.

1.6.1 Relating the correlation and covariance functions

It may be seen that Equations 1.7 and 1.22, are of similar form, except for the presence of nonbias conditions in Equation 1.22. Both methods being described attempt to minimize an average squared difference, but Equation 1.10 is described in terms of correlation functions while Equation 1.22 is described in terms of the covariance function.

Stationarity is assumed so the covariance function is described by :

$$C(h) = C(\mathbf{h}) = C_{xx}(h) = r_h - (E\{x\})^2 \tag{1.42}$$

where r_h denotes the autocorrelation function, defined in Section 1.4.1. This equation is simply a re-expression of Equation 1.18, establishing the relationship between the covariance and autocorrelation functions. Similarly, the cross-covariance may be written as :

$$C_{xz}(h) = g_h - E\{x\} \times E\{y\} \tag{1.43}$$

The relationship between these various functions allows the conclusion that Ordinary Kriging and Co-kriging are extended (*e.g.* multi-dimensional) deconvolution processes. Alternatively, the weighting process used by kriging may be described as an extended convolution process. This concept has been mentioned by Dietrich (1989), who focused on conditioning of one-dimensional kriging matrices. The mathematical relationship between autocorrelation and covariance functions is described by Robinson and Treitel (1980) and Robinson (1981). It should also be noted that if data is regularly spaced along a line (as is the case in seismic deconvolution), then the kriging operator is applied via a discrete convolution process, in the fashion of Equation 1.5.

Chapter 2

Linear Equations

The solution of a set of equations of the form :

$$\mathbf{Ax} = \mathbf{b}$$

where $\mathbf{A}$ is a known n by n coefficient matrix, and $\mathbf{b}$ a known right hand side vector, is central to linear least squares methods described in Chapter 1. This chapter presents a number of aspects appropriate to linear systems with square coefficient matrices. A description of some important matrix classes, and their inverses, is presented, and a number of computational methods for solving linear equations are introduced. The chapter concludes with a brief description of numerical techniques for calculations of eigenvalues of a matrix, because of the importance of eigenvalues to error analysis. The aim is to identify concepts and techniques, rather than to discuss them in exhaustive detail. Appropriate references are given. Chapter 3 introduces concepts related to conditioning of linear equations.

2.1 Different matrix classes

The linear methods considered in this project result in linear systems, in which the coefficient matrices exhibit various properties. These properties often have important consequences because they may be exploited by various methods to solve a given linear equation more efficiently. This section introduces a number of these properties, their relationships,

and consequences. More details, including proofs of results, are provided by Cornyn (1974).

Table 2.1 defines a number of matrix classes of interest, and states which class the corresponding inverse matrices belong to. Knowledge of the matrix class to which the inverse of a given matrix belongs is useful because this information can often be used to significantly reduce the number of operations and memory locations required to invert a matrix, or, equivalently, solve a linear equation. For example, the inverse of a symmetric matrix may be stored in $\frac{n(n+1)}{2}$ elements, where n is the order of the matrix. It may also

Class	Property ($\mathbf{A} = [a_{ij}]$)	4x4 matrix example	Inverse class
Symmetric	$a_{ij} = a_{ji}$ or $\mathbf{A} = \mathbf{A}^T$	$\begin{pmatrix} a & b & c & d \\ b & e & f & g \\ c & f & h & p \\ d & g & p & q \end{pmatrix}$	Symmetric
Persymmetric	$a_{ij} = a_{n-1-j,n-1-i}$	$\begin{pmatrix} a & b & c & d \\ e & f & g & c \\ h & p & f & b \\ q & h & e & a \end{pmatrix}$	Persymmetric
Centrosymmetric	$a_{ij} = a_{n-1-i,n-1-j}$	$\begin{pmatrix} a & b & c & d \\ e & f & g & h \\ h & g & f & e \\ d & c & b & a \end{pmatrix}$	Centrosymmetric
Toeplitz	$a_{ij} = r_{i-j}$	$\begin{pmatrix} a & b & c & d \\ e & a & b & c \\ f & e & a & b \\ g & f & e & a \end{pmatrix}$	Persymmetric
Hankel	$a_{ij} = r_{i+j}$	$\begin{pmatrix} a & b & c & d \\ b & c & d & e \\ c & d & e & f \\ d & e & f & g \end{pmatrix}$	Symmetric

Table 2.1: Square Matrix Classes and Inverses

be seen that the classes are not exclusive—a matrix may appear in two or more classes. In particular, it should be observed that :

- all Toeplitz matrices are persymmetric and all Hankel matrices are symmetric.
- the class of centrosymmetric matrices includes (but not exclusively) all matrices which

are both persymmetric and symmetric *i.e.* symmetric Toeplitz matrices, persymmetric Hankel matrices, and their inverses are centrosymmetric.

Although Hankel matrices are not examined in this thesis, they are mentioned here because of their close relationship with Toeplitz matrices.

2.2 Solution of linear systems

There are a number of numerical methods for solving linear systems, both for general coefficient matrices and for coefficient matrices which exhibit forms of symmetry. These methods fall into two distinct classes—direct and iterative. This section introduces methods in each of these classes. Some available methods for solution or inversion of Toeplitz equations (both symmetric and asymmetric) are then introduced.

2.2.1 Direct methods

Direct methods for solving a linear system (or equivalently inverting a matrix) evaluate the exact solution (or inverse) in a finite number of steps if no errors are incurred in the process. If errors, such as rounding errors are incurred in the process, the resultant solution can not be expected to be exact. Gaussian and Gauss-Jordan elimination may be applied to general linear systems, whilst the Cholesky Decomposition is applicable to symmetric positive definite[1] matrices. Other methods are available, but are not considered further in this thesis.Examples are : Crout elimination, which is described by Robinson (1981); rank annihilation, a method of matrix inversion described by Wilf (1960).

2.2.1.1 Gaussian Elimination and Gauss-Jordan elimination

Gaussian elimination is by far the most commonly used direct method for solving a general linear system. The procedure involves reduction of the coefficient matrix to an upper triangular form by means of row operations—exchanging rows and pivoting. Identical

[1] Positive definiteness and indefiniteness of a matrix are defined in Section 2.3.2.

operations are performed on the right hand side matrix, $\mathbf{b}$. The solution is then obtained by back substitution. This method, and its variations (*e.g.* different pivoting schemes) is described by most elementary texts *e.g.* Kreyszig (1988), Gerald and Wheatley (1984). Solutions computed using Gaussian elimination are presented for most examples of this thesis. Except where stated otherwise, the variation employed is (partial) pivoting on the maximum non-zero element, for both single and double precision results.

Gauss-Jordan elimination is a method which is closely related to Gaussian elimination, the only real difference being that the coefficient matrix is reduced to the identity matrix instead of to an upper triangular form. Back substitution is unnecessary because, in reducing the coefficient matrix to the identity matrix, the right hand side vector is reduced to the solution of the linear equation. This method has the added property that the operations performed on the coefficient matrix may be performed simultaneously on a matrix which is initially the identity matrix. This matrix then yields the inverse matrix. Computationally, this method is not as commonly used as is Gaussian elimination because it involves more arithmetic operations and therefore requires more computation time and is, in addition, more sensitive to error.

2.2.1.2 Cholesky Decomposition

This method is based on the observation that a real, symmetric, positive definite matrix, $\mathbf{A}$ may be written as the product :

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T \tag{2.1}$$

where $\mathbf{L}$ is a lower triangular matrix. The system $\mathbf{Ax} = \mathbf{b}$ may then be solved by first solving the system :

$$\mathbf{Lz} = \mathbf{b} \tag{2.2}$$

and then solving the system :

$$\mathbf{L}^T\mathbf{x} = \mathbf{z} \tag{2.3}$$

Both Equations 2.2 and 2.3 are rapidly solvable using the back-substitution procedure which is employed by Gaussian elimination. More details on this method are provided by

Martin et al. (1971b).

2.2.2 Iterative methods

Iterative methods choose an initial solution, either arbitrarily or by some other solution method, and it is altered in such a way that it approaches the true solution. The choice of change at each step is one which causes an optimal (measured in some sense) change in the estimated solution. Iterative methods are of use for improving the solution obtained using a direct method whose result has been affected by rounding errors. Another important use is in the solution of sparse matrix systems (*i.e.* the coefficient matrix contains many zero elements). Unlike direct methods, iterative methods can be infinite—they may continually converge on a solution but never quite reach it. For this reason iterative methods are performed by fixing the maximum number of iterations allowed and/or allowing a tolerance—when an error criterion, usually an expression in terms of vector norms[2] which will be zero at the true solution, is nearly enough satisfied, the method completes. Iterative solution of linear equations is discussed in more detail by Varga (1963).

2.2.2.1 The Conjugate Gradient method

The Conjugate Gradient method is an n-step iterative one. When it is applied to a linear equation $\mathbf{Ax} = \mathbf{b}$, where $\mathbf{A}$ is a n by n matrix, then a solution, if it exists, is obtained in n or less steps of the algorithm if computations are done with complete accuracy.

The method aims to obtain an estimate, $\mathbf{x}_n$ such that the length of the residual vector $\mathbf{r}_n = \mathbf{b} - A\mathbf{x}_n$ is minimized. Various aspects of this method are given by Beckman (1960), Hestenes and Stiefel (1952), Ginsberg (1971), and Strikwerda (1981).

The basic algorithm assumes a symmetric, positive definite coefficient matrix. Extensions for real, asymmetric coefficient matrices are described by Beckman (1960) and Strikwerda (1981). Wang and Treitel (1973) have reported that, for applications in seismic deconvolution (involving a symmetric positive definite Toeplitz coefficient matrix), the

[2]Vector norms are defined in Section 3.3.

conjugate gradient method can be programmed to work more efficiently on an array processor, with subsequent reductions in processing time (this will be true only for large order systems because of overhead in communicating with the array processor).

In practice, computational errors often prevent the exact solution of the linear equation being obtained in n or less steps, particularly when the system is poorly conditioned (refer Chapter 3). This problem may be remedied by simply allowing the algorithm to proceed for a greater number of steps, and terminating when some error criterion is satisfied. This approach suggests that better results could be obtained by a judicious selection of the initial estimate of the solution. The simplest way of obtaining a better initial estimate is to solve the equation using a direct method to obtain an initial solution and iterate to improve it. In another approach, which is applicable if a large number of systems with similar coefficients are being solved, the solution of one system is used as the initial estimate of the solution to the next. It has been reported by Wang and Treitel (1973) that such an approach gives convergence in a very small number of iterations.

2.2.2.2 Other iterative methods

The Gauss-Seidel method is an iterative method which is described, amongst others, by Norton (1960), Kreyszig (1988, pp. 810-813). It produces, after m iterations, an estimated solution $\mathbf{x}_m$ from which a residual $\mathbf{r} = \mathbf{A}\mathbf{x}_m - \mathbf{b}$ may be calculated. It is referred to as a relaxation technique because, at each stage, the estimated solution is modified (relaxed) to reduce one component of the residual to zero. Although not considered further in this thesis, this method is of interest because, as stated by Norton (1960), it will converge for any initially estimated vector, if the coefficient matrix is symmetric and positive definite.

Two other methods, which are very closely related to the Gauss-Seidel iteration, are the Jacobi iteration, discussed briefly by Kreyszig (1988), and over- or under-relaxation techniques, which are based on the Gauss-Seidel technique, but instead multiply the change in the solution so that, respectively, the appropriate element of the residual vector passes zero, or does not reach it.

There are a number of other iterative methods *e.g.* Monte-Carlo methods, described

by Oswald (1960). The major differences between iterative methods is in the criterion used to determine a "good" solution, and how they change the estimated solution. For example, the Conjugate Gradient method alters all components of the estimated solution in each step, whilst the Gauss-Seidel method alters only one component in each step. It may be expected that such characteristics will affect the numerical properties of the methods. Some methods also require that the coefficient matrix satisfy special conditions, which may be difficult to satisfy in general. For example, the Monte-Carlo method given by Oswald (1960), and the Jacobi iteration mentioned in the last paragraph, require that all eigenvalues of the matrix $I - A$, where I is the identity matrix, have a magnitude less than unity.

2.2.3 Methods for Toeplitz matrices

There are a number of direct methods available for solving linear systems involving Toeplitz matrices, or equivalently inverting a Toeplitz matrix. Related methods also exist which are applicable to Hankel matrices, and these methods can, in some cases, be extended to apply to Toeplitz matrices. Details on some of these approaches are provided by Cornyn (1974).

The two main approaches which will be considered in this thesis, are the Wiener-Levinson algorithm, and Trench's algorithm. Some related methods are discussed in literature *e.g.* Bareiss (1969) describes a method of inversion of Toeplitz matrices. "Superfast" algorithms (*e.g.* Ammar and Bragg (1988), Bitmead and Anderson (1980), Hoog (1987)), based on the use of Fast Fourier Transform (FFT) techniques, provide a more rapid solution than the "standard" techniques, when the matrix system is of large order.

2.2.3.1 The Wiener-Levinson Algorithm

The Wiener-Levinson Algorithm is a very simple one which was, in fact, trivialized by it's author (refer, for example, to Levinson (1946)). It is an algorithm for solving a system involving a symmetric Toeplitz coefficient matrix. Computationally, it requires

storage proportional to n (n being the order of the system being solved) and computer time proportional to n^2. This is a marked advantage over general methods which require storage proportional to n^2 and computer time proportional to n^3. This algorithm has found wide use in seismic deconvolution. The major constraint required for the system to be solved is that all principal sub-matrices of the system are non-singular (this constraint is a function of the algorithm—it is not true that a Toeplitz matrix is singular if one of its principal submatrices is). The discussion here is essentially that given by Claerbout (1976).

The Wiener-Levinson Algorithm is based on the recursive property by which, given the values $a_1, a_2, \ldots, a_i$ and ν_i, for the system of order i, such that :

$$\begin{pmatrix} r_0 & \ldots & \ldots & r_i \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ r_i & \ldots & \ldots & r_0 \end{pmatrix} \begin{pmatrix} 1 \\ a_1 \\ \vdots \\ a_i \end{pmatrix} = \begin{pmatrix} \nu_i \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

the corresponding values $a_1', a_2', \ldots, a_i'$ and ν_{i+1} for the system of order $i+1$ may be obtained by calculating :

$$e = r_{i+1} + \sum_{j=1}^{i} a_j r_{i+1-j}$$

Defining $c = \frac{-e}{\nu_i}$ the desired values may then be calculated :

$$\begin{aligned} \nu_{i+1} &= \nu_i + ce \\ a_j' &= a_j + c a_{j+1-i} \; j = 1 \ldots n \\ a_{i+1} &= c \end{aligned}$$

The algorithm thus has a recursive property in the sense that results for a system of order i are used to calculate results for a system of order $i+1$. This approach may be readily extended to obtain a solution vector for any given right hand side vector. The quantities ν_i are discussed further in Section 4.4.1 where they are referred to as prediction error variances.

2.2.3.2 Trench's Algorithm

Trench's Algorithm, presented by Trench (1964) and improved by Zohar (1969), is a method for inverting a general Toeplitz matrix, rather than for solving a linear system directly. The approach also has a similar advantage in computer time and storage to that of the Wiener-Levinson Algorithm—namely, it requires storage proportional to n and computer time proportional to n^2. However, the basic algorithm does not produce the inverse directly. It produces two vectors of length n from which the inverse may be obtained by simple recursion relations (similarly to the Wiener-Levinson Algorithm these vectors are also produced by recursive relations). The method may be simplified if the coefficient matrix is symmetric. As for the Wiener-Levinson Algorithm, this algorithm also requires that all principal sub-matrices be non-singular. The computer algorithm used in this study is based on that given by Cornyn (1974).

2.3 Eigenvalues and Eigenvectors

As will be seen later in Sections 3.3 and 3.4, eigenvalues of a matrix are important to discussions about conditioning of linear systems. Eigenvalues will also be important for some developments in later chapters. This section summarises some properties of eigenvalues and eigenvectors, which may be obtained from most basic texts, *e.g.* Kreyszig (1988). Conditioning of the eigenvalue problem is discussed in Section 3.6.

Consider a system of linear equations :

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \tag{2.4}$$

where $\mathbf{A}$ is a known n by n matrix, λ is a scalar, and $\mathbf{x}$ is a non-null vector. There are n vectors $\mathbf{x}_i$ for which Equation 2.4 is true, referred to as *eigenvectors* or *characteristic vectors* or *invariant directions*. The corresponding values $\lambda_i$are referred to as the *eigenvalues* or *characteristic values*.

It may be shown that the eigenvalues λ_i are the roots of the characteristic (polynomial)

equation :

$$det(\mathbf{A} - \lambda I) = 0 \tag{2.5}$$

where $\mathbf{I}$ is the identity matrix and *"det"* represents the determinant.

Eigenvalues of a real, symmetric matrix are real (Parlett (1980)). In this case, the eigenvalues may be considered, without loss of generality, to be ordered :

$$\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$$

2.3.1 Eigenvalues of the inverse matrix

Each eigenvalue of the matrix $\mathbf{A}^{-1}$ is the reciprocal of an eigenvalue of the matrix A :

$$\lambda_i(\mathbf{A}^{-1}) = \frac{1}{\lambda_{n-i}(\mathbf{A})} \tag{2.6}$$

The matrices $\mathbf{A}^{-1}$ and $\mathbf{A}$ also have the same set of eigenvectors :

$$\mathbf{x}_i(\mathbf{A}^{-1}) = \mathbf{x}_{n-i}(\mathbf{A}) \tag{2.7}$$

2.3.2 Positive definite and indefinite matrices

A real positive definite matrix, $\mathbf{A}$, is defined as one for which the scalar quantity $\mathbf{x}^T\mathbf{A}\mathbf{x}$ is positive for all non-zero vectors, $\mathbf{x}$:

$$\mathbf{x}^T\mathbf{A}\mathbf{x} > 0 \ \forall \mathbf{x} \neq \mathbf{0} \tag{2.8}$$

An equivalent condition, discussed by Bellman (1960), is that the real component of all eigenvalues of the matrix $\mathbf{A}$ are positive *i.e.* all eigenvalues appear in the right half-plane of the complex number coordinate system. The eigenvalues of a real, symmetric, positive definite matrix are real and positive.

In a similar fashion, a positive indefinite matrix is one for which :

$$\mathbf{x}^T\mathbf{A}\mathbf{x} \geq 0 \ \forall \mathbf{x} \neq \mathbf{0}$$

The eigenvalues of a real, symmetric, positive indefinite matrix are non-negative. A positive indefinite matrix may also be referred to as a positive semidefinite matrix.

Analogous definitions hold for definitions of negative definite and negative indefinite matrices. The term "indefinite matrix" without qualification is used to describe a matrix which does not belong in any of the above classes *e.g.* the eigenvalues of a real, symmetric, indefinite matrix may be either positive or negative.

2.3.3 Further properties of eigenvalues

Further properties of eigenvalues of a real matrix are as follows :

- the sum of all eigenvalues of the matrix $\mathbf{A}$ is equivalent to the trace of $\mathbf{A}$, the sum of its diagonal elements :
$$\sum_{i}^{n} \lambda_i = tr(\mathbf{A}) = \sum_{i}^{n} a_{ii}$$
- the product of all the eigenvalues of $\mathbf{A}$ is equivalent to the determinant of $\mathbf{A}$:
$$\prod_{i} \lambda_i = det(\mathbf{A})$$

2.4 Numerical evaluation of eigenvalues

The standard eigenvalue problem may be posed very simply as the determination of non-trivial solutions of Equation 2.4. Unfortunately, the numerical determination of these solutions is a far from trivial task, usually requiring significantly more effort than does the solution of the corresponding linear equation. Many algorithms are required to deal efficiently with the wide range of problems which are encountered in practice, for example :

- Eigenvalues and/or eigenvectors may be required,
- The complete set of eigenvalues and/or eigenvectors may be required, or a comparatively small number, *e.g.* the k largest or smallest eigenvalues,
- The coefficient matrix $\mathbf{A}$ may be symmetric or asymmetric.

The purpose of this section is to identify some of the more commonly used methods of evaluation of the eigenvalues of a matrix, with little emphasis being placed on evaluation

of the eigenvectors. It is not the intention to present a comprehensive description of such methods. More details may be found in literature, for example Greenstadt (1960), Wilkinson (1965), Martin et al. (1971a), Rutishauser (1971), and Parlett (1980).

2.4.1 Jacobi methods

Jacobi methods are amongst the most elegant devised for solving the complete eigenproblem. The basic algorithm produces all eigenvalues and (optionally) eigenvectors of a symmetric matrix. The algorithm is essentially a repetition of the process :

$$\mathbf{A}_{new} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P} \tag{2.9}$$

where $\mathbf{P}$ is non-singular and referred to as a permutation matrix. This process has the feature that the matrix $\mathbf{A}_{new}$ has the same eigenvalues as the matrix $\mathbf{A}$. The most common permutation matrix employed is one representing a plane rotation in the form :

$$\begin{pmatrix}
1 & 0 & & & \cdots & & & 0 \\
0 & \ddots & & & & & & \\
 & & 1 & & & & & \\
 & & & cos(\theta) & & sin(\theta) & & \\
 & & & & 1 & & & \\
\vdots & & & & & \ddots & & \vdots \\
 & & & & & & 1 & \\
 & & & -sin(\theta) & & cos(\theta) & & \\
 & & & & & & & 1 \\
 & & & & & & \ddots & 0 \\
0 & & & & \cdots & & 0 & 1
\end{pmatrix}$$

Jacobi algorithms make a judicious choice of plane rotations so that each step annihilates an off-diagonal element (*i.e.* that element in $\mathbf{A}_{new}$ will be zero), the aim being to annihilate all off-diagonal elements as far as possible. When all off-diagonal elements have been annihilated, the eigenvalues are found on the main diagonal. The algorithm is essentially iterative because, when annihilating one off-diagonal element, a previously annihilated

element may be made non-zero. For this reason, the process is either repeated for a fixed number of iterations, or until the off-diagonal elements are acceptably small.

Eigenvectors may be found by applying the same sequence of plane rotations to the identity matrix as are applied to the original coefficient matrix $\mathbf{A}$. The algorithm has the advantage that it is simply formulated, and all eigenvalues and eigenvectors may be obtained to working accuracy reasonably efficiently, regardless of the existence of any multiple or pathologically close eigenvalues. Extensions for asymmetric matrices also exist, described by, for example, Eberlein and Boothroyd (1971).

2.4.2 Power methods

Power methods are based on the observation that the sequence :

$$\mathbf{x}_{i+1} = \mathbf{A}\mathbf{x}_i$$

repeated indefinitely with an appropriate non-zero starting vector $\mathbf{x}_0$ will produce a sequence of vectors in which the situation :

$$\mathbf{x}_{j+1} = c\mathbf{x}_j$$

will be approached for large j. That is, the situation will eventually be reached where consecutive vectors in the sequence will eventually be a scalar multiple of each other. The value c thus produced will approach the eigenvalue of largest magnitude and the corresponding $\mathbf{x}_j$ will approximate the corresponding eigenvector. When the matrix $\mathbf{A}$ is real and complex eigenvalues may occur, it is necessary to choose the starting vector $\mathbf{x}_0$ to have some complex component so that the largest magnitude eigenvalue can be obtained, even if it is complex. This approach requires some modification if a number of eigenvalues all have maximum magnitude.

From this simple formulation more powerful methods, such as the LR and QR algorithms, have been developed. The basic algorithms apply to general square matrices, although various forms are available for different special cases, and approaches which result in more rapid and/or reliable evaluation of the eigenvalues. Algorithms exist for evaluating

all eigenvalues of a matrix (*e.g.* Martin et al. (1971a), Bowdler et al. (1971)), or a number of the eigenvalues of smallest magnitude (*e.g.* Martin et al. (1971c)).

2.4.3 Eigenvalues of Toeplitz matrices

There are a number of efficient algorithms for the solution of linear systems with Toeplitz coefficient matrices, which exploit the Toeplitz structure. However, this is not true for the problem of determining eigenvalues. Algebraic properties of eigenvalues of Toeplitz forms have been discussed by, for example, Grenander and Szego (1958), Nevai (1980), Grunbaum (1981a, b), Bini and Capovani (1983), and Trench (1985). However, to the authors knowledge, no efficient computational methods for calculation of eigenvalues of Toeplitz forms, which exploit their structure, currently exist. For this reason general methods, such as the QR-algorithm or Jacobi plane rotations, must be applied.

Chapter 3

Errors in Linear Systems

A number of classes of linear equations of the form :

$$\mathbf{Ax} = \mathbf{b} \tag{3.1}$$

were introduced in Chapter 2. A number of numerical methods for solving linear equations were also discussed.

The concern of this chapter is the effect of the difference $\mathbf{x}_d = \mathbf{x} - \mathbf{y}$ where $\mathbf{y}$ is the solution of the disturbed system :

$$(\mathbf{A} + \mathbf{A}_d)\mathbf{y} = \mathbf{b} + \mathbf{b}_d \tag{3.2}$$

where $\mathbf{A}_d$ and $\mathbf{b}_d$ are matrices of perturbations in the matrix $\mathbf{A}$ and vector $\mathbf{b}$ respectively. Some causes of these perturbations are discussed in Section 3.1. The errors in the solution of such a perturbed system will affect any later results or interpretations made using this solution.

Any perturbations $\mathbf{A}_d$ or $\mathbf{b}_d$ will cause an error in the solution. What is important, however, is not that the error in the solution will occur, but rather how significant that error will be *i.e.* does a small perturbation result in a small or large error in the solution, or in later results calculated using it? This problem may be considered in two ways :

1. do small perturbations, $\mathbf{A}_d$ and $\mathbf{b}_d$ result in a solution vector $\mathbf{y}$ which is significantly (in some sense) in error relative to the true (desired, but generally unknown) solution

vector $\mathbf{x}$? If the vector $\mathbf{y}$ is significantly in error, any results calculated using it may be expected to have significant error.

2. Do small errors in the solution vector $\mathbf{y}$ cause significant errors in any quantities calculated later using it ?

These two problems are closely related—both refer to how any errors produced at any stage in a series of calculations propagate through into the final results. The remainder of this chapter is directed towards the first of these problems—namely, the definition of ill-conditioning in linear systems—and any use of terminology will be considered as it applies to linear systems. However, the term "ill-conditioning" can apply to any stage in any series of computations. Any computational problem may be described as ill-conditioned if a small error at any stage manifests as a more significant error at a later stage. The theory which follows is provided by a number of texts, *e.g.* Barnett (1979), Ralston and Rabinowitz (1978), Deif (1982), Householder (1964), and Press et al. (1986) but is mainly due to Wilkinson (1961, 63, 65).

3.1 Errors and computer arithmetic

The perturbations described in Equation 3.2 may arise in a number of ways :

1. The elements of $\mathbf{A}$ or $\mathbf{b}$ may be measured quantities subject to observation error :
   (a) noise
   (b) the blunder — a gross human error
2. elements of $\mathbf{A}$ and/or $\mathbf{b}$ may be estimated. Examples are :
   (a) in predictive deconvolution, the autocorrelation is estimated from the data, affecting both the coefficient matrix and right hand side vector,
   (b) in kriging, the covariance or semivariogram is estimated from the data. A model is also imposed. This affects both $\mathbf{A}$ and $\mathbf{b}$ when kriging estimates are

point locations. When kriging a mean value over an area, $\mathbf{b}$ may, in addition, be poorly known because the fitted function may not be mathematically integrated. The gaussian function, which occurs in examples of Chapter 7, is a function which can not be analytically integrated, and which is employed in geostatistical practice.

3. The elements may be known exactly, but when stored in a computer they can only be stored to a fixed number of decimal places. For example, $\frac{1}{3}$ may be stored (to 5 decimal places) as 0.33333 which is not exact. The difference between the true and actual values is referred to as rounding error. More details are given in Section 3.1.1.

4. The elements may be a result of prior computations, hence subject to rounding errors, which will be described in Section 3.1.1. That is, previous errors will have an effect on the results of the current calculation, which may also introduce a component of error.

3.1.1 Floating point arithmetic

Errors may arise in a number of ways in floating point arithmetic. The first of these is adding two numbers of different orders of magnitude. For example, consider a hypothetical computer which carries seven significant figures in it's calculations, and assume there are two numbers $a = 234.5372$ and $b = 0.0002848905$ from which it is desired to calculate $a + b$. The computer will return the result $a + b = 234.5375$ instead of the true result $a + b = 234.5374848905$, which represents a loss of significant figures in the result.

Errors may be magnified by dividing by small numbers. Consider a number a' which is the current value in storage representing a number a, so $a' = a + \Delta a$ where Δa is the error introduced by storing the value in finite computer storage. If, at some time, the operation $c = a/b$ is performed where b is small in magnitude, the result c obtained will have a much larger absolute error than did the value a'. When the calculated value of c is used in later calculations, large errors may result—an initial error can propagate through the solution.

Because small numbers are often produced during a series of calculations (*e.g.* subtracting two very close values), this type of error occurs frequently.

In a series of calculations, the errors introduced may be positive or negative, therefore an error in one calculation may cancel out, or significantly reduce, the effect of an error produced by an earlier calculation. For this reason, final results will not necessarily be as inaccurate as may be expected from the above discussion. However, in general, it may be expected that an error at any stage in a series of calculations will manifest itself in the final results. More details of the effects of this type of error, together with considerations applicable to this study, may be found in Appendix A.

3.2 Ill-conditioned Linear Systems

Definition 3.1 *A matrix equation is said to be ill-conditioned when a small relative error, in the coefficient matrix, the right hand side, or the solving process, produces a much larger relative error in the solution.*

A matrix equation which is not ill-conditioned is said to be "well-conditioned".

Ill-conditioning may be considered in a number of related ways :

1. An approach towards singularity. Conventionally, matrices are divided into two groups—non-singular and singular (meaning respectively those having an inverse and those which do not). However, this classification does not fully describe the situation when the system is solved on a computer. Ill-conditioned systems fall into a class which are, by definition, analytically solvable. However, their solutions often can not be numerically obtained because the ill-conditioning manifests itself by a loss of significant figures during computation, making it difficult to obtain an accurate solution. Conversely, singularity may be considered as a very severe form of ill-conditioning.

2. One definition of singularity is that at least one of the rows (columns) of the coefficient matrix is a linear combination of the others. An ill-conditioned system may be

regarded as an approach to this situation : at least one of the rows (columns) of the coefficient matrix is "very nearly" a linear combination of the others.

Figure 3.1 illustrates the contrast between an ill-conditioned and a well-conditioned system of two linear equations in two unknowns. The pairs of lines in each case are the lines which may be defined by the respective system, with the point of intersection being the desired solution. If the system is ill-conditioned, the lines are "almost parallel", whilst this is not true for a well conditioned system. Analogous results hold for systems with more unknowns/equations.

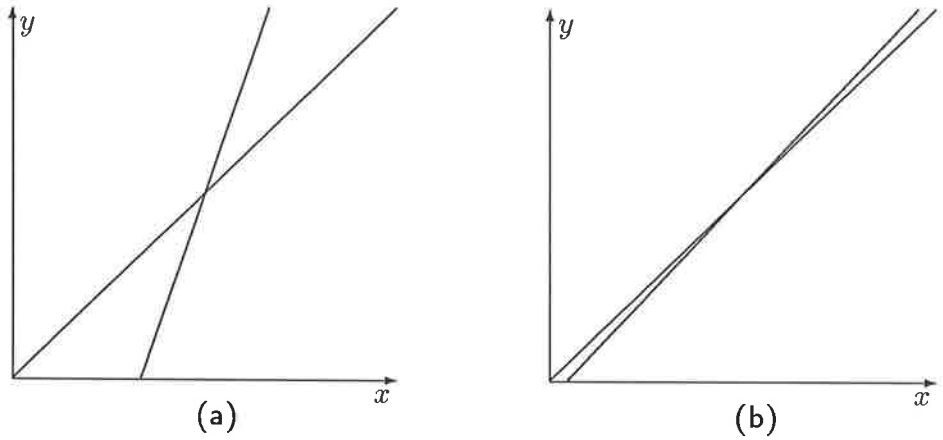


Figure 3.1: (a) Well Conditioned and (b) ill-conditioned system of two linear equations in two unknowns

The following sections introduce some concepts and methods of use for recognizing ill-conditioned systems.

3.3 Vector and matrix norms

In order to recognize an ill-conditioned system, it is necessary to have a measure of some characteristic of vectors and matrices which can be used to compare different systems.

Norms give a measure of the "size" (in some sense) of vectors and matrices, which can be used for this purpose.

3.3.1 Vector norms

The introduction of vector norms is the process of associating a scalar with a vector, this scalar being a measure of the magnitude or length of that vector *in some sense*—in an identical way that a non-negative real number $|\alpha|$ is defined as the magnitude of a complex number α. This measure can then be used to compare different vectors.

Definition 3.2 *A norm of a vector $\mathbf{x} \in C^n$ (complex vectors), denoted by $||\mathbf{x}||$, is any non-negative real scalar function which satisfies the following :*

1. $||\mathbf{x}|| > 0$ *if* $\mathbf{x} \neq \mathbf{0}$ *(positivity)*
2. $||\alpha\mathbf{x}|| = |\alpha| \; ||\mathbf{x}||$ *for any scalar* α *(homogeneity)*
3. $||\mathbf{x} + \mathbf{y}|| \leq ||\mathbf{x}|| + ||\mathbf{y}||$ *for all vectors* $\mathbf{x}, \mathbf{y} \in C^n$ *(triangular inequality)*

One of the most frequently used vector norms is the *Hölder norm* which is given by :

$$||\mathbf{x}||_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{\frac{1}{p}} \tag{3.3}$$

where p is a positive integer, and x_i is the ith component of the vector $\mathbf{x}$. In practice, the most widely used values of p are 1 and 2. The 2-norm (which is also referred to as the Euclidean norm, or the length of the vector $\mathbf{x}$ in the space C^n) is a well known measure of the size or magnitude of a vector.

3.3.2 Matrix norms

Vector norms provide a measure, in some sense, of the magnitude of a vector. In a similar fashion, matrix norms can be defined which provide a measure of the magnitude of a matrix.

Definition 3.3 *A norm of a square matrix* $\mathbf{A}$ *denoted by* $||\mathbf{A}||$, *is any non-negative real scalar function which satisfies the following :*

- $||\mathbf{A}|| > 0$ *if* $\mathbf{A} \neq 0$
- $||\alpha\mathbf{A}|| = |\alpha|\ ||\mathbf{A}||$ *for any scalar* α
- $||\mathbf{A} + \mathbf{B}|| \leq ||\mathbf{A}|| + ||\mathbf{B}||$ *for any* $\mathbf{A}, \mathbf{B} \in C^{nn}$
- $||\mathbf{AB}|| \leq ||\mathbf{A}||\ ||\mathbf{B}||$

There are many matrix norms which satisfy the above relations, of which one of the most important are matrix Hölder norms subordinate to Hölder vector norms :

$$||\mathbf{A}||_p = \max_{\mathbf{x} \neq 0} \frac{||\mathbf{Ax}||_p}{||\mathbf{x}||_p} \tag{3.4}$$

One advantage of using the Hölder matrix norm is that :

$$||\mathbf{Ax}||_p \leq ||\mathbf{A}||_p\ ||\mathbf{x}||_p \text{ for all } \mathbf{A} \in C^{nn} \text{ and } \mathbf{x} \in C^n \tag{3.5}$$

The most widely used Hölder matrix norms are :

- The 1-norm :

$$||\mathbf{A}||_1 = \max_{\mathbf{x}} \frac{||\mathbf{Ax}||_1}{||\mathbf{x}||_1} = \max_j \sum_{i=1}^{n} |a_{ij}|$$

- The 2 norm, or spectral norm :

$$||\mathbf{A}||_2 = \max_{\mathbf{x}} \frac{||\mathbf{Ax}||_2}{||\mathbf{x}||_2}$$

- The ∞-norm :

$$||\mathbf{A}||_\infty = \max_{\mathbf{x}} \frac{||\mathbf{Ax}||_\infty}{||\mathbf{x}||_\infty} = \max_i \sum_{j=1}^{n} |a_{ij}|$$

3.3.2.1 The Spectral Norm

The spectral matrix norm of a general matrix $\mathbf{A}$ may be expressed using the maximum magnitude eigenvalue of the matrix $\mathbf{A}^T\mathbf{A}$:

$$||\mathbf{A}||_2 = \max\sqrt{|\lambda_i(\mathbf{A}^T\mathbf{A})|} \tag{3.6}$$

Usmani (1987, pp. 167-168) gives a proof of this result.

3.4 The Condition Number

Definition 3.4 *The condition number of a matrix* $\mathbf{A}$ *is given by :*

$$\kappa_p(\mathbf{A}) = \frac{\max ||\mathbf{Au}||_p}{\min ||\mathbf{Av}||_p} \qquad ||\mathbf{u}||_p = ||\mathbf{v}||_p = 1 \tag{3.7}$$

The condition number is the maximum possible ratio of Hölder norms of transformed vector lengths, given that the untransformed vectors had a Hölder norm equal to unity. The minimum possible value for a condition number is unity.

The condition number, given in Equation 3.7, may be rewritten using Equation 3.5 as :

$$\kappa_p(\mathbf{A}) = ||\mathbf{A}||_p ||\mathbf{A}^{-1}||_p \tag{3.8}$$

which expresses the condition number in terms of Hölder norms of the matrix of interest and of its inverse.

3.4.1 Use of the condition number

The usefulness of the condition number arises from :

$$\frac{||\mathbf{x}_d||_p}{||\mathbf{x}||_p} \leq \kappa_p(\mathbf{A}) \left(\frac{||\mathbf{A}_d||_p}{||\mathbf{A}||_p} + \frac{||\mathbf{b}_d||_p}{||\mathbf{b}||_p} \right) \tag{3.9}$$

(A proof of this result is given by Deif (1982, pp. 202-204)) *i.e.* the relative change in the solution vector, introduced by errors $\mathbf{A}_d$ and $\mathbf{b}_d$ and defined in terms of the appropriate Hölder vector norm, has an upper limit which is directly related to the condition number, defined in terms of the corresponding Hölder matrix norm. A large condition number implies that the linear system may be ill-conditioned (as in Definition 3.1), whilst a small condition number excludes this possibility[1]. A large condition number does *not* imply that a linear system is ill-conditioned—only that it may be. As described in Section 3.1.1, errors incurred in solving the linear equations may cancel each other out, therefore the errors in

[1] Strictly speaking, a small condition number does not exclude the possibility that the linear system is ill-conditioned, as in Definition 3.1. The discussion throughout this chapter implicitly assumes that the solution algorithm exhibits some form of stability. The topic of stability will be examined more closely in Section 5.2.

the final result may not be as great as expected. As a result, condition numbers may be unnecessarily pessimistic.

It is well known, *e.g.* Wilkinson (1961, 63, 65), that in the error analysis of elimination methods for positive definite matrices that the condition number is characteristic of possible amplification of single round-off errors.

3.4.2 The Spectral Condition Number

The value of $||\mathbf{A}||_2$, the spectral matrix norm, has been given in Section 3.3.2.1. In order to be able to make use of Equation 3.8 in the case $p = 2$ to obtain a spectral condition number it is necessary to have a value for $||\mathbf{A}^{-1}||_2$. This value may be obtained from Equation 2.6 :

$$||\mathbf{A}^{-1}||_2 = \frac{1}{\sqrt{|\lambda_{min}(\mathbf{A}^T\mathbf{A})|}} \tag{3.10}$$

where the notation $\lambda_{min}(\mathbf{M})$ represents the eigenvalue of the matrix $\mathbf{M}$ with minimum magnitude. In a similar fashion, the notation $\lambda_{max}(\mathbf{M})$ will be used to represent the eigenvalue of the matrix M with maximum magnitude. The matrix $\mathbf{A}^T\mathbf{A}$ is real and symmetric for all real matrices, $\mathbf{A}$, therefore all eigenvalues of $\mathbf{A}^T\mathbf{A}$ are real (Section 2.3).

Substituting Equations 3.6 and 3.10 into Equation 3.9 (with $p = 2$), the spectral condition number, for a general matrix $\mathbf{A}$, may be written as :

$$\kappa_2(\mathbf{A}) = \sqrt{\frac{|\lambda_{max}(\mathbf{A}^T\mathbf{A})|}{|\lambda_{min}(\mathbf{A}^T\mathbf{A})|}} \tag{3.11}$$

It is common practice to describe a matrix with a large spectral condition number as "ill-conditioned". This practice will be followed throughout this thesis, although it should be noted that an "ill-conditioned" matrix does not necessarily imply an ill-conditioned linear system, as defined in Definition 3.1. This is discussed further in Section 3.5.

Throughout the remaining chapters of this thesis, unless otherwise stated, the term "condition number" will be used to refer to the spectral condition number. The expression $\kappa(\mathbf{A})$ will refer to the spectral condition number of the matrix $\mathbf{A}$, which has been represented in this chapter as $\kappa_2(\mathbf{A})$.

3.4.2.1 Spectral results for symmetric matrices

If the matrix $\mathbf{A}$ is symmetric, the spectral norms and condition numbers may be simplified as follows :

1. Equation 3.6 for the spectral matrix norm may be rewritten as :

$$||\mathbf{A}||_2 = |\lambda_{max}(\mathbf{A})| \tag{3.12}$$

2. Equation 3.10 may be reduced to :

$$||\mathbf{A}^{-1}||_2 = \frac{1}{|\lambda_{min}(\mathbf{A})|} \tag{3.13}$$

3. The spectral condition number given in Equation 3.11 simplifies to :

$$\kappa_2(\mathbf{A}) = \frac{|\lambda_{max}(\mathbf{A})|}{|\lambda_{min}(\mathbf{A})|} \tag{3.14}$$

3.5 Further considerations

Ill-conditioning as in Definition 3.1 is qualitative rather than quantitative—the definition of an ill-conditioned system is subjective. Several measures of ill-conditioning have been proposed (of which the condition number is one) but common usage is still qualitative. Some other symptoms of ill-conditioning are described by many texts on numerical analysis (*e.g.* Young and Gregory (1972), Ralston and Rabinowitz (1978), Kreyszig (1988)). These could be used to define quantitative measurements. Some examples are :

1. If $|det\ \mathbf{A}|$ is small in comparison with the maximum magnitude of the elements a_{ij} of the matrix $\mathbf{A}$ or the elements b_i of the vector $\mathbf{b}$, then the system $\mathbf{Ax} = \mathbf{b}$ will often be ill-conditioned.

2. If the magnitudes of elements of $\mathbf{A}^{-1}$ are large in comparison with the magnitude of elements of the solution, the system will often be ill-conditioned.

3. If the principal diagonal elements are large in comparison with the off-diagonal elements (*i.e.* the matrix is diagonally dominant), the system is usually well-conditioned, or at least less ill-conditioned than a similar system which is not diagonally dominant.

Unfortunately, no symptoms or measurements are totally indicative of whether or not a given system is ill-conditioned. Cases may be found for each which one or more of these tests indicate the linear system to be ill-conditioned, when it is, in fact, well-conditioned. This is because different matrix systems have different properties (*e.g.* symmetric vs. non-symmetric, positive-definiteness, band nature, etc) which affect the results of some of these tests. More significantly, different solution or inversion algorithms have different numerical properties. No symptom or measurement of ill-conditioning should be used alone, unless the numerical properties of a given matrix class are known when solution is attempted with a given algorithm.

In practice, a number of the quantities used to indicate ill-conditioning are difficult to extract numerically. For example, the condition number, defined in Equations 3.11 and 3.14, involves calculation of the maximum and minimum magnitude eigenvalues of a symmetric matrix. Calculation of these eigenvalues, discussed briefly in Section 2.4, involves a significant computational effort, so performing this test will increase computing costs. Also, small magnitude eigenvalues, which will often occur when the system is ill-conditioned and may occur even if it is well conditioned, are often difficult to extract numerically due to the accumulation of rounding errors in the process (Parlett (1980)).

Because of the problems outlined above, a complete package to test for ill-conditioning is not feasible in practice. However, other, more approximate, tests may be feasible if their results provide an indication of ill-conditioning at a reasonable cost. Case studies may also be performed. These can give valuable insights which may be applied in practice.

Different solution methods have different numerical properties, even though they are attempting to solve the same problem. For example, Gaussian elimination, which reduces the coefficient matrix to triangular form, introduces less numerical error than Gauss-Jordan elimination, which reduces the coefficient matrix to the identity matrix. As discussed in Section 2.2.1, both these methods are based on the same row reduction and pivoting tech-

niques. However, because Gauss-Jordan elimination requires more arithmetic operations to achieve its aim, solution time and the effect of numerical rounding errors is increased. Other methods are also available—for example, in the seismic deconvolution problem, the Conjugate Gradient Method has received attention (Treitel and Wang (1976)) as a method having desirable numerical properties, in addition to reducing processing costs under certain circumstances. These examples demonstrate that ill-conditioning must also be expressed in terms of the solution algorithm used.

The matrix equation may be altered in some way so that the resultant system is less ill-conditioned. Pre-whitening, discussed in Section 4.5, is one such method. Whilst the solution of a pre-whitened system differs from that of the original system, the pre-whitened system is substantially less ill-conditioned.

3.6 Conditioning of the eigenvalue problem

The spectral condition number of a general real matrix $\mathbf{A}$ is expressed in Equation 3.11 in terms of the eigenvalues of maximum and minimum magnitude of the square matrix $\mathbf{A}^T\mathbf{A}$. This section considers how reliably these eigenvalues may be computed.

Parlett (1980) has shown that the eigenvalue problem for symmetric matrices is always well conditioned in the sense that eigenvalues obtained numerically for a symmetric matrix $\mathbf{B}$ will always be those of a matrix :

$$\mathbf{B}+\mathbf{H}$$

where $||\mathbf{H}||_2$ is small in comparison with $||\mathbf{B}||_2$. He also demonstrated that eigenvalues of small magnitude are difficult to evaluate accurately due to round-off. This is essentially because the smallest eigenvalue of $\mathbf{B}$ may be small in comparison with $||\mathbf{H}||_2$. Evaluating the largest magnitude eigenvalue(s) to working accuracy may hinder, or even prevent, the calculation of eigenvalues of small magnitude to an acceptable accuracy.

These conclusions do not hold for general matrices—the process of calculating eigenvalues of a general matrix may be ill-conditioned—computed eigenvalues of a general matrix $\mathbf{B}$ are not necessarily those of $\mathbf{B}+\mathbf{H}$ where $||\mathbf{H}||_2$ is small in comparison with $||\mathbf{B}||_2$.

Chapter 4

Conditioning of deconvolution

Treitel and Wang (1976) observed that autocorrelation matrices, used for time-domain design of digital deconvolution filters, are ill-conditioned in certain cases. They present an example, in which the solution of such a system of linear equations results in significantly different filter points, when the solution is performed on different computers.

This chapter addresses a number of aspects relating to conditioning of autocorrelation matrices, and is an extension of work published by the author, O'Dowd (1990). Early sections present a survey of causes of ill-conditioning from a mathematical point of view. Later, properties of Toeplitz determinants are employed to derive a lower bound for the spectral condition number of symmetric positive definite Toeplitz matrices. This result means that the Wiener-Levinson Algorithm is capable of providing an indication of whether or not it is severely affected by rounding errors when solving the normal equations. Prewhitening is then discussed in detail, and it is seen that prewhitening will always result in a less ill-conditioned autocorrelation matrix. Chapter 5 is devoted towards case studies to illustrate concepts discussed in this chapter and to examine the performance of tests of conditioning which may be formulated from them.

4.1 Spectral Properties

As observed in Section 1.4.1, the autocorrelation matrix, $\mathbf{R}$, is symmetric, Toeplitz, and positive definite in most practical cases. Treitel and Wang (1976) noted that the spectral condition number of a matrix is a measure of conditioning, but did not discuss its physical meaning. The physical meaning of the condition number, $\kappa(\mathbf{R})$ may be determined by considering the meaning of the maximum and minimum eigenvalues. It was proved by Grenander and Szego (1958, Chapter 3) that, defining p and P, respectively, as the smallest and largest values of the power spectrum, we have :

$$p \leq \lambda_{min} \leq \lambda_{max} \leq P \tag{4.1}$$

where λ_{min} and λ_{max} are, respectively, the smallest and largest eigenvalues of the autocorrelation matrix, $\mathbf{R}$. From this it may be seen that :

$$\kappa(\mathbf{R}) = \frac{\lambda_{max}}{\lambda_{min}} \leq \frac{P}{p} \tag{4.2}$$

Related results are given by Ekstrom (1973). Korvin (1978) has also given a derivation of Equation 4.1 using much simpler arguments than are used by these previous authors.

These results indicate that small values of the power spectrum, in comparison with the maximum value, for certain frequencies, may be expected to result in ill-conditioning of the deconvolution problem. Such a conclusion is consistent with the fact, described in Section 1.4.2, that deconvolution in the time domain may be expressed as a division in the frequency domain. This means that zeros in the power spectrum will be an indication that exact deconvolution must fail. Using arguments of continuity, it may be expected that small power values will result in numerical difficulty due to ill-conditioning in the time domain (conversely, extremely large peaks in power, which may be associated with resonance in a wave guide, may also be expected to result in ill-conditioning). Furthermore, aliasing results in an increase in observed values of the spectrum due to additive mapping of higher frequencies to lower values in the discretely obtained spectrum. This allows the interesting conclusion that a poor sampling, which may result in a greater degree of aliasing, may result in an inherently less ill-conditioned autocorrelation matrix than will a much better

sampling. It will be noted in later sections that this effect means that striving for higher resolution by increasing sampling may result in numerical difficulty when deconvolution is performed, thereby offsetting gains provided by the higher resolution.

4.2 Fredholm integrals

A Fredholm integral equation of the first kind is an equation of the form :

$$y(\tau) = \int_{t_s}^{t_e} x(\tau, t) f(t) dt \ \forall \tau_s \leq \tau \leq \tau_e \tag{4.3}$$

If the functions $y(\tau)$ and $x(\tau, t)$ are known, the problem is to find the function $f(t)$. To solve the problem numerically, the interval $[t_s, t_e]$ may be subdivided into n points and the interval $[\tau_s, \tau_e]$ may be subdivided into m points. Equation 4.3 may therefore be approximated as :

$$y(\tau_k) \approx \sum_{j=0}^{n-1} x(\tau_k, t_j) q_j f(t_j) \ \ \forall 0 \leq k \leq m-1 \tag{4.4}$$

where the values q_j are a set of appropriate quadrature weights. Equation 4.4 may be written in vector-matrix form as :

$$\mathbf{X}\mathbf{w} = \mathbf{y} \tag{4.5}$$

where $y_k = y(\tau_k)$, $x_{kj} = x(\tau_k, t_j)$, and $w_j = q_j f(t_j)$.

4.2.1 Linear Dependence of Columns

Hunt (1972) has shown that as the function $x(\tau, t)$ becomes smoother (in the sense that it can be reasonably approximated by a finite Taylor series expansion), or (equivalently) more continuous, that the $(k+1)$th row of $\mathbf{X}$ becomes more nearly a linear combination of rows k and $k-1$ for $k+1 = 2 \ldots m-1$. As described in Section 3.2, this means that Equation 4.5 may be expected to become progressively more ill-conditioned as the function $x(\tau, t)$ becomes more continuous. It may also be expected that as the order of the matrix system is increased and Equation 4.4 becomes a better approximation of Equation 4.3,

the matrix system becomes progressively more ill-conditioned. This is an effect noted by Rust and Burrus (1972).

These results may be applied to deconvolution described previously by noting that the convolution of functions $a(\tau)$ and $f(\tau)$ may be written as :

$$y(\tau) = x * f = \int_{-\infty}^{\infty} x(\tau - t)f(t)dt \quad \forall -\infty \leq \tau \leq \infty \tag{4.6}$$

where the "$*$" is the standard notation for convolution. By setting the function $f(t)$ to be zero outside the range $[t_s, t_e]$ this reduces to :

$$y(\tau) = x * f = \int_{t_s}^{t_e} x(\tau - t)f(t)dt \quad \forall \tau_s \leq \tau \leq \tau_e \tag{4.7}$$

The right hand side of this equation is a special case of Equation 4.3. The coefficient matrix $\mathbf{X}$ of Equation 4.5 reduces to the form :

$$\mathbf{X} = \begin{pmatrix} x_0 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & 0 \\ x_{m-1} & & & x_0 \\ 0 & \ddots & & \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & x_{m-1} \end{pmatrix} \tag{4.8}$$

This matrix is a Toeplitz n by m matrix. Furthermore, it may be seen that $\mathbf{R}_c$, the autocorrelation matrix with values for all possible lags, may be written as :

$$\mathbf{R}_c = \beta \mathbf{X}^T \mathbf{X}$$

where β is simply a constant scale factor. The autocorrelation matrix $\mathbf{R}$ employed in deconvolution is simply a principal submatrix of $\mathbf{R}_c$. Equation 1.5, given for digital convolution, may be obtained by a discrete sampling of Equation 4.7. Therefore, a continuous seismic trace is more likely to result in an ill-conditioned autocorrelation matrix than one which is not as continuous.

4.2.2 Deconvolution is incorrectly posed

The solution of Fredholm integral equations of the first kind, as given in Equation 4.3, would be said to be correctly posed if :

- for every function $y(t)$ there corresponds a solution $f(s)$ to the problem.
- the solution $f(s)$ is unique for any given $y(t)$.
- the solution $f(s)$ is continuous with respect to $y(t)$.

As stated by Tihonov (1963a), it is not generally true that a solution $f(s)$ may be produced for any given $y(t)$ for equations of this type. So there may be no function,$f(s)$, which, when convolved with a given filter, x, will yield a desired output $y(t)$. This means that the solution of Fredholm integral equations, and therefore deconvolution, is incorrectly posed. This has also been observed by Rice (1962) in relation to inverse filtering. In the language of that paper, $f(s)$ and $y(t)$ would be termed "incompatible" if any of the above conditions do not hold.

If the left hand side of Equation 4.7 is only known to a finite accuracy, the different numerical methods to solve Equation 4.7 lead to quite erratic results. Phillips (1962) presents some interesting numerical examples, and attributes this phenomenon to the fact that the integral operator with kernel $x(t,s)$ generally has no bounded inverse. Franklin (1970) noted these effects, and discussed the use of stochastic processes to provide information about ill-posed linear problems.

The phenomenon, in which it is not necessarily true that a solution is able to be produced, may be understood by converting Equation 4.6 into the frequency domain :

$$Y(\omega) = X(\omega)F(\omega)$$

If the kernel $x(t)$ is such that $X(\omega_1)$ is zero for some frequency ω_1, whilst the chosen function $y(t)$ is such that $Y(\omega_1)$ is non-zero, then $F(\omega_1)$ can not exist, and the function f also can not exist. Geophysical inverse theory, discussed in Appendix D, may be used to account for this phenomenon in a physical sense.

4.3 Remark about ill-conditioned autocorrelation matrices

Previous sections have given a survey of a number of causes of ill-conditioned matrices from a mathematical point of view. It must be noted that ill-conditioning of an autocorrelation matrix may be regarded as an approach towards some limit in the properties of that matrix. For example, ill-conditioning of the autocorrelation matrix may be associated with the occurrence of relatively small values in a power spectrum for some frequencies. This is an approach towards a limit in which zeros occur in the power spectrum. Alternatively, an ill-conditioned autocorrelation matrix is symptomatic of the case when rows of the matrix $\mathbf{X}$ are approaching linear dependence.

All discussion so far has ignored cases in which the autocorrelation matrix is positive indefinite because, in practice (*e.g.* Robinson (1967a)), the autocorrelation matrix is assumed to be positive definite, and the possibility of positive indefinite autocorrelation matrices is not considered. However, it must be noted that a positive indefinite (singular) autocorrelation matrix is the limit which is being approached when ill-conditioning is being observed. Korvin (1978) gives a proof that the autocorrelation matrix is positive indefinite in general.

4.4 Prediction Error Variances and Conditioning

The Wiener-Levinson algorithm is commonly employed to solve the normal equations arising in seismic deconvolution. Numerical errors may be expected to occur due to finite word length provided by a computer. This section focuses on an approach for detecting cases in which the autocorrelation matrix may be sufficiently ill-conditioned to produce significant errors in computed Wiener filters, when solution is performed using the Wiener-Levinson algorithm.

4.4.1 Toeplitz determinants

Properties of the autocorrelation matrix, $\mathbf{R}$, were discussed in Section 1.4.1. This section introduces properties of the determinant of the autocorrelation matrix, which are given by Robinson (1967a, pp. 133–144), and will be used in later sections.

The $(k+1)$th principal sub-matrix of the autocorrelation matrix may be written as :

$$\mathbf{R}(k) = \begin{pmatrix} r_0 & r_1 & \dots & r_k \\ r_1 & r_0 & \dots & r_{k-1} \\ \vdots & & \ddots & \vdots \\ r_k & r_{k-1} & \dots & r_0 \end{pmatrix} \tag{4.9}$$

and its determinant as :

$$D(k) = det\,(\mathbf{R}(k)) \tag{4.10}$$

Consider the case where the right hand side of the $(k+1)$th order Wiener equation is a positive spike :

$$\begin{pmatrix} r_0 & r_1 & \dots & r_k \\ r_1 & r_0 & \dots & r_{k-1} \\ & & \vdots & \\ r_k & r_{k-1} & \dots & r_0 \end{pmatrix} \begin{pmatrix} 1 \\ a_1(k) \\ \vdots \\ a_k(k) \end{pmatrix} = \begin{pmatrix} \nu_k \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{4.11}$$

where $\nu_k > 0$, is the corresponding *prediction error variance*. As discussed in Section 2.2.3.1, these terms are fundamental to the workings of the Wiener-Levinson algorithm). On solving Equation 4.11, it may be seen that :

$$\nu_k = \frac{D(k)}{D(k-1)} \tag{4.12}$$

Therefore, the determinant of the n by n coefficient matrix of Equation 1.10 may be expressed as :

$$D(n-1) = \prod_{k=0}^{n-1} \nu_k \tag{4.13}$$

for $n \geq 1$ and where it may be seen that :

$$\nu_0 = D(0) = r_0 \tag{4.14}$$

As seen in Section 2.2.3.1 prediction error variances are fundamental to the solution of linear equations involving symmetric Toeplitz coefficient matrices. Specifically, prediction error variances are intermediate results of the Wiener-Levinson algorithm.

4.4.2 Condition numbers and prediction error variances

As noted in Section 3.6, eigenvalues of small magnitude may be difficult to evaluate to working accuracy due to round-off. This means that the spectral condition number (which may be defined in terms of the maximum and minimum magnitude eigenvalues of a symmetric matrix) may exhibit quite large error, even though the eigenvalue problem is well conditioned. It may be reasonably expected that any computed upper bounds for the spectral condition number will also exhibit large error. For this reason, this section has a different emphasis — a lower bound to the spectral condition number will be evaluated. This lower bound offers the advantage that it is written in terms of prediction error variances, which are intermediate results of the Wiener-Levinson algorithm.

If the autocorrelation matrix, $\mathbf{R}$ is symmetric and positive definite, the determinants of all principal submatrices are positive :

$$D(k) > 0 \ \forall k = 0, \ldots, n-1$$

(Bellman (1960)), from which it may be concluded that :

$$\nu_k > 0 \ \forall k = 0, \ldots, n-1.$$

Properties of eigenvalues of a matrix, described in Section 2.3.3, may be used to show that :

$$D(n-1) = \prod_{k=1}^{n} \lambda_k \tag{4.15}$$

$$\sum_{k=1}^{n} \lambda_k = nr_0 \tag{4.16}$$

where λ_i are the eigenvalues of $\mathbf{R}$, which are real and positive, as discussed in Section 2.3.2. Properties of prediction error variance, provided by Claerbout (1976, pp. 55-57), may be

used to show that :

$$r_0 = \nu_0 \geq \nu_1 \geq \ldots \geq \nu_{n-1} > 0 \tag{4.17}$$

Considering, without loss of generality, the eigenvalues to be ordered :

$$\lambda_n \geq \lambda_{n-1} \geq \ldots \geq \lambda_1 > 0 \tag{4.18}$$

the spectral condition number may be written :

$$\kappa(\mathbf{R}) = \frac{\lambda_{max}}{\lambda_{min}} = \frac{\lambda_n}{\lambda_1}$$

and from Equation 4.16 it may be seen that :

$$0 < \lambda_1 \leq r_0 \tag{4.19}$$

The lower bound in this equation arises directly from the last inequality in Equation 4.18. The upper bound may be obtained using a contradiction argument. Substituting an assumption that $\lambda_1 > r_0$ into Equation 4.16 gives :

$$\sum_{k=2}^{n} \lambda_k < (n-1)r_0$$

There are $n-1$ terms in the summation of the left hand side of this equation. This means that at least one of the eigenvalues, other than λ_1, must be less than r_0, violating the assumption of Equation 4.18. Arguments of a similar nature also give rise to :

$$r_0 \leq \lambda_n < nr_0 \tag{4.20}$$

The vector on the left hand side of Equation 4.11 for the case $k+1 = n$ may be expressed as a linear combination of eigenvectors, $\mathbf{v}_k$, of the autocorrelation matrix :

$$\begin{pmatrix} 1 \\ a_1(n) \\ \vdots \\ a_n(n) \end{pmatrix} = \sum_{k=1}^{n} c_i \mathbf{v}_k$$

Examining the first element of this vector, it may be seen that :

$$\sum_{k=1}^{n} c_i v_{i_1} = 1$$

Substituting into Equation 4.11 gives :

$$\nu_{n-1} = \sum_{k=1}^{n} \lambda_i c_i v_{i_1} \geq \sum_{k=1}^{n} \lambda_1 c_i v_{i_1} = \lambda_1 \sum_{k=1}^{n} c_i v_{i_1} = \lambda_1 \tag{4.21}$$

Equations 4.19 to 4.21 may be combined to obtain :

$$\lambda_n \geq \nu_0 = r_0 \geq \nu_{n-1} \geq \lambda_1 \tag{4.22}$$

from which a lower bound for the spectral condition number, $\kappa(\mathbf{R})$, may be written :

$$\kappa(\mathbf{R}) = \frac{\lambda_n}{\lambda_1} \geq \frac{\nu_0}{\nu_{n-1}} \tag{4.23}$$

This means that intermediate results of the Wiener-Levinson Algorithm may be employed to give an indication of the conditioning of the autocorrelation matrix, $\mathbf{R}$. From Equation 4.17, the lower bound of Equation 4.23 will increase with the order of the matrix. This is consistent with (but is *not* a proof of) a result proven by Bunch (1985) : a positive definite symmetric matrix is at least as ill-conditioned as any of its principal submatrices. This lower bound is sharp in theory, being attained trivially for the n by n identity matrix, $\mathbf{I}$. This result means that small prediction error variances, in comparison with the maximum prediction error variance, may be considered an indication of ill-conditioning. It must be noted, however, that, for general symmetric, Toeplitz, positive definite matrices, this lower bound may be extremely conservative.

Referring to Equation 4.17, it may be seen that all prediction error variances should be positive. Ill-conditioning may be associated with the presence of eigenvalues of relatively small magnitude, in comparison with the eigenvalue of maximum magnitude. As noted in Section 3.6, numerical errors may cause negative computed eigenvalues to occur (this effect was, in fact, observed by Treitel and Wang (1976)). Equation 4.23 indicates that ill-conditioning may, in addition, be associated with the occurrence of prediction error variances of relatively small magnitude, in comparison with the one of maximum value. Just as negative computed eigenvalues may be considered indicative of ill-conditioning, the occurrence of prediction error variances which are negative, due to accumulated round-off error, may be considered a symptom of ill-conditioning. This means that any prediction

error variances, computed in the course of the Wiener-Levinson Algorithm, which are negative provide an indication of ill-conditioning (or, more precisely, that the computed solution may be severely affected by rounding error).

The use of intermediate results of a solution algorithm to gauge effects of round-off error is not unique. The implementation of the Cholesky Decomposition given by Martin et al. (1971b) tests whether or not the numerically obtained determinant of the matrix is positive, and indicates an error if it is not. The results of this section indicate that a similar test may be applied in the Wiener-Levinson Algorithm (and, by extension, other related Toeplitz algorithms) when solving a linear system with a symmetric, positive definite, Toeplitz coefficient matrix.

Cybenko (1980) obtained bounds for condition numbers, defined in terms of the 1-norms of Section 3.3.2, of symmetric, Toeplitz, positive definite matrices. These bounds are written in terms of "partial correlation coefficients" (which are referred to as reflection coefficients in seismic theory) and prediction error variances.

4.4.3 Uses of the error bound

From Equation 4.17 it may be seen that prediction error variances are positive valued and decrease monotonically towards zero. It was shown in Section 4.4.2 that ill-conditioning of the normal equations may be associated with prediction error variances of relatively small value. It was also argued that numerical errors may cause small prediction error variances to be computed with negative values. This means the Wiener-Levinson algorithm may be considered to be severely affected by rounding error when :

- computed prediction error variances are negative,
- computed prediction error variances increase with order of the matrix.

The recursive nature of the Wiener-Levinson algorithm, described in Section 2.2.3.1, also allows the observation that a computed filter $\mathbf{f}_k$, of length $k+1$, is dependent upon prediction error variances $\nu_i, i = 0 \ldots k$, which correspond to solutions of order $i = 1 \ldots k+$

1, but is unaffected by values $\nu_i, i = k+1 \ldots$ which arise when obtaining solutions of higher order systems. Furthermore, the prediction error variance ν_k is computed prior to elements of the filter $\mathbf{f}_k$. This means that, if a filter $\mathbf{f}_n$ for some arbitrary n, is desired, intermediate results of the Wiener-Levinson algorithm may be employed in two possible approaches, which are fundamentally very similar :

- provide an indication that the filter $\mathbf{f}_n$ may be adversely affected by rounding error. An algorithm of this nature is listed in Appendix C.
- stop computation after a filter $\mathbf{f}_k$ $(k < n)$ has been computed, and the prediction error variance ν_{k+1} exhibits one of the above forms of behaviour which would indicate that rounding error would significantly affect the computed filter $\mathbf{f}_{k+1}$.

Another possible approach would be to correct computed prediction error variances, in some way, when an indication occurs that significant rounding error may occur. The major difficulty which would occur with this approach may be illustrated using the fact that each element of a computed filter $\mathbf{f}$, which is a solution of the normal equations (Equation 1.11), may be written in the form :

$$f_i = \frac{|\mathbf{B}_i|}{|\mathbf{R}|}$$

where :

- $\mathbf{R}$ is the autocorrelation matrix,
- $\mathbf{B}_i$ is a matrix which is equivalent to $\mathbf{R}$, except that $\mathbf{g}$, the right-hand side of Equation 1.11, is substituted for the ith column.

This form of the solution is an expression of Cramer's rule, described in most elementary texts *e.g.* Kreyszig (1988). It means that a significant error in a computed determinant of $\mathbf{R}$ may be expected to indicate significant error in the computed solution to the normal equations. From Equation 4.13, this determinant may be written as the product of *all* prediction error variances. This means that any correction of prediction error variances may be expected to significantly affect the computed value of the determinant, and therefore

affect the computed solution. For this reason, it may be considered that the main value of Equation 4.23 would be in recognition of cases in which rounding error may significantly affect computed solutions, rather than in trying to correct for effects of rounding error. Once this recognition has occurred, other approaches (*e.g.* different solution algorithms, or treatments such as prewhitening) may be preferred.

4.5 Prewhitening

Prewhitening is a process which is commonly employed in seismic processing (*e.g.* Yilmaz (1987)) for the purposes of improving numerical stability. Mathematically, it amounts to the replacement of r_0, the diagonal element of the autocorrelation matrix, $\mathbf{R}$, by the quantity $r_0(1+\epsilon)$ where ϵ is a small positive constant, in practice generally of the order of 0.01.

4.5.1 Prewhitening and Conditioning

Treitel and Wang (1976) observed, without proof, that prewhitening significantly reduces the spectral condition number of the coefficient matrix, with subsequent gains in numerical stability.

The linear system being solved after prewhitening is :

$$(\mathbf{R} + d\mathbf{I})\,\mathbf{w} = \mathbf{g} \tag{4.24}$$

(where $d = r_0\epsilon$) instead of :

$$\mathbf{R}\mathbf{w} = \mathbf{g}$$

as given in Equation 1.11. As discussed in Section 2.3, the eigenvalues $\lambda_i\ i = 1 \ldots n$ of the matrix $\mathbf{R}$ are the solutions of the determinantal equation :

$$det\,(\mathbf{R} - \lambda\mathbf{I}) = 0$$

In a similar fashion, the eigenvalues λ_i' of the matrix $\mathbf{R} + d\mathbf{I}$ are solutions of the determinantal equation :

$$det\left([\mathbf{R} + d\mathbf{I}] - \lambda'\mathbf{I}\right) = 0$$

which may be rewritten as :

$$det\left(\mathbf{R} - [\lambda' - d]\,\mathbf{I}\right) = 0$$

which results in the conclusion that :

$$\lambda_i' = \lambda_i + d$$

When $\mathbf{R}$ is symmetric and positive definite the condition number for the prewhitened coefficient matrix is therefore :

$$\kappa(\mathbf{R} + d\mathbf{I}) = \frac{\lambda_n + d}{\lambda_1 + d} \tag{4.25}$$

This function is a monotonic decreasing function of d, for positive d, resulting in the conclusion that any level of prewhitening will result in a decrease in the spectral condition number.

This is not, however, a sufficient reason to make d arbitrarily large. In particular, Equation 4.24 may be rewritten, for positive d as :

$$\left(\frac{1}{d}\mathbf{R} + \mathbf{I}\right)\mathbf{w} = \frac{1}{d}\mathbf{g}$$

In practice, $\mathbf{R}$ and $\mathbf{g}$ have elements which are finite. It may therefore be seen that $\mathbf{w} \rightarrow 0$ as $d \rightarrow \infty$. This means that information is lost by the deconvolution process if the prewhitening level is too high.

Any level of prewhitening, however small, will result in a less ill-conditioned autocorrelation matrix. It is interesting to note that prewhitening will have a much smaller (relative) effect on the maximum eigenvalue than on the smallest eigenvalue (this is, in fact, the reason why the condition number monotonically decreases with prewhitening level). This means that the beneficial effect of an arbitrarily small level of prewhitening will increase as the autocorrelation matrix becomes more ill-conditioned. For this reason, it is not possible to identify an "optimal" level of prewhitening to reduce the effects of ill-conditioning.

4.5.2 Smoothing the Wiener filter

After prewhitening, the linear system being solved has a different solution to the original system. This leaves open the question of what the solution of a prewhitened system actually represents. In this section, we consider the prediction problem, with prediction distance α and filter length n. A derivation of the normal equations is given by Robinson (1967a). Here, we simply start with the prewhitened normal equations and perform the reverse of that derivation. The approach for other desired Wiener filters is identical to that for the prediction filter.

The prewhitened normal equations, given in matrix form in Equation 4.24 may be written as :

$$\sum_{i=0}^{n-1} w_i r_{j-i} + dw_j = r_{\alpha+j} \ \ (\forall j = 0, \ldots, n-1) \tag{4.26}$$

where $r_j = E\{x_{t+j}x_t\}$ is the autocorrelation function of the seismic trace, x_t. These equations may be expanded to obtain :

$$E\left\{\left[x_{t+\alpha} - \sum_{i=0}^{n-1} w_i x_{t-i}\right] x_{t-j}\right\} + dw_j = 0 \ \forall j = 0 \ldots n-1 \tag{4.27}$$

Multiplying each side of each equation by 2, integrating, and combining the results, it may be seen that prewhitening may be interpreted as the minimization of an expression :

$$I' = E\left\{(x_{t+\alpha} - y_t)^2\right\} + d\sum_{j=0}^{n-1} w_j^2 \tag{4.28}$$

where

$$y_t = \sum_{j=0}^{n-1} w_j x_{t-j}$$

is the estimate obtained of $x_{t+\alpha}$. The first term on the right hand side of Equation 4.28 is the error variance which is being minimized by the Wiener filter without prewhitening, and the second term is a (discrete) "regularizing functional" in the sense of Tihonov (1963a, b). This regularizing functional has the effect of imposing a "smoothing constraint" on the computed filter, reducing the class of possible filters which may be produced as a solution of the normal equations *i.e.* prewhitening results in the production of a smoother filter. As noted by Treitel and Wang (1976), an ill-conditioned system may be expected to produce

a set of filter elements which vary widely in magnitude. Such a smoothing of the filter, as discussed here, may be expected to alleviate this problem. It should also be noted that the regularizing term is equivalent to the introduction of a filter energy constraint, as discussed by Treitel and Lines (1982).

4.5.3 Prewhitening in the frequency domain

It is noted in a number of geophysical texts, *e.g.* Yilmaz (1987), that zero values in an amplitude spectrum (which would cause frequency domain deconvolution, discussed in Section 1.4.2, to fail) are unlikely, due to effects such as uncorrelated noise in the data, and that prewhitening has the effect of improving numerical stability when solving the normal equations.

Prewhitening is mathematically equivalent to the addition of uncorrelated white noise, n_t with the following properties :

$$\begin{aligned} E\{x_t n_t\} &= 0 \\ E\{n_t\} &= 0 \\ E\left\{n_t^2\right\} &= N^2 \ll E\left\{x_t^2\right\} = r_0 \end{aligned}$$

This means that the autocorrelation of $x_t + n_t$ is represented by :

$$r_t{}' = \begin{cases} r_t & t \neq 0 \\ r_0\left(1 + \frac{N^2}{r_0}\right) & t = 0 \end{cases}$$

This autocorrelation function is identical to the replacement of r_0 by the quantity $r_0(1+\epsilon)$ with $\epsilon = \frac{N^2}{r_0}$.

It is well known (*e.g.* Bracewell (1978)) that an impulse function, expressed mathematically as the delta function :

$$\delta(t) = \begin{cases} 1 & \text{if } t = 0, \\ 0 & \text{otherwise.} \end{cases}$$

has a constant valued Fourier Transform :

$$\delta(t) \leftrightarrow \Delta(\omega) = k(> 0)$$

This means that prewhitening in the time domain has the effect of adding a constant to all values of the power spectrum, decreasing the ratio of maximum to minimum in the power spectrum. As observed in Section 4.1, this means that the autocorrelation matrix must become less ill-conditioned.

4.6 Conclusions

Causes of ill-conditioned autocorrelation matrices are intimately related to the fact that digital deconvolution is a discretization of a physical/mathematical problem which, in general, may have either no solution or multiple solutions. Properties of the underlying system must have an effect on the least-squares approach. Numerical difficulty in time domain deconvolution may be related back to small (or zero) values in the frequency domain. Obtaining more data, therefore better approximating the underlying physical system, may result in an ill-conditioned deconvolution problem, offsetting any gains produced by higher resolution.

The Wiener-Levinson algorithm is commonly employed to solve the normal equations which appear when performing least-squares deconvolution. It has been shown here that intermediate results of the algorithm may be used to provide an indication of when the computed Wiener filter may exhibit significant error. When the computed intermediate results indicate that the computed filter has been adversely affected by rounding errors, a more reliable approach (*e.g.* computing in higher precision, an more numerically reliable solution method, or a moderate level of prewhitening) may be desirable. Another approach suggested is a reduction in the length of the filter computed, in which intermediate results may be employed to determine when rounding error may significantly affect computed filters of a greater length.

Chapter 5

A study of deconvolution

A number of causes of ill-conditioning of autocorrelation matrices were discussed in Chapter 4. This chapter examines examples of ill-conditioned and well-conditioned autocorrelation matrices. The objective is to determine which, if any, concepts may be employed to recognize the occurrence of an ill-conditioned autocorrelation matrix. Results obtained when solving the normal equations via different algorithms are discussed. To determine whether or not prediction error variances may be employed to recognize ill-conditioning of the autocorrelation matrix, condition numbers of all principal submatrices of the autocorrelation matrix, and corresponding prediction error variances, are examined.

5.1 An ill-conditioned autocorrelation matrix

In this section, a theoretical example is considered. A sequence of 128 uniformly distributed random numbers between 0 and 1 was generated. In order to ensure that a number of small values, in comparison with the maximum, occur, each odd numbered value, as determined by the number of calls to the random number generating function, was multiplied by 10^{-6} if it was greater than the next value in the sequence. The 64 odd-numbered values were considered, for the purposes of this study, to represent a "synthetic power spectrum" and converted to a "synthetic autocorrelation" using the cosine transform described by Robinson (1967a). By reapplying the cosine transform, computed power

spectra were obtained from the synthetic autocorrelation. These computed powers were obtained using both single and double precision[1], for the purposes of determining whether or not a computed power spectrum may be employed to gain an indication of ill-conditioning. Spiking filters produced using different solution algorithms are also examined.

The synthetic autocorrelation, synthetic power spectrum, and computed power spectra are illustrated in Figure 5.1. It may be observed that the computed power spectra, in single or double precision, show a similar form to that of the synthetic power spectrum. Unfortunately, referring to Table 5.1, it may be seen that the power spectrum computed using single precision exhibits 12 values which are non-positive, a result which (apparently) violates the condition that all values in the power spectrum be positive (Ford and Hearne (1966), Robinson (1967a), Usmani (1987)). The negative values are of a very small magnitude so they are not resolved in Figure 5.1. One zero value also

	Simulated	Double prec.	Single prec.
Minimum value	1.762×10^{-8}	1.159×10^{-8}	-8.598×10^{-7}
Maximum value	0.8234	0.8234	0.8234
Minimum magnitude	1.762×10^{-8}	1.159×10^{-8}	0
Maximum magnitude	0.8234	0.8234	0.8234
Max:min magnitude	4.674×10^{7}	7.102×10^{7}	∞
# of values ≤ 0	0	0	12

Table 5.1: Comparison of different precision power spectra.

occurs, so the ratio of maximum to minimum magnitude values in the power spectrum (which, as discussed in Section 4.1, is an upper bound for the spectral condition number) is infinite. This would also have bearing in frequency domain deconvolution, as discussed in Section 1.4.2. In the power spectrum computed using double precision, the smallest magnitude value exhibits a relative error of the order of 50%, so the computed ratio of maximum to minimum power also exhibits a similar error. Whilst it is true that such a range of power values may be indicative of ill-conditioning, it also demonstrates that the

[1]The meaning of single and double precision, as it applies in this study, is discussed in Appendix A.

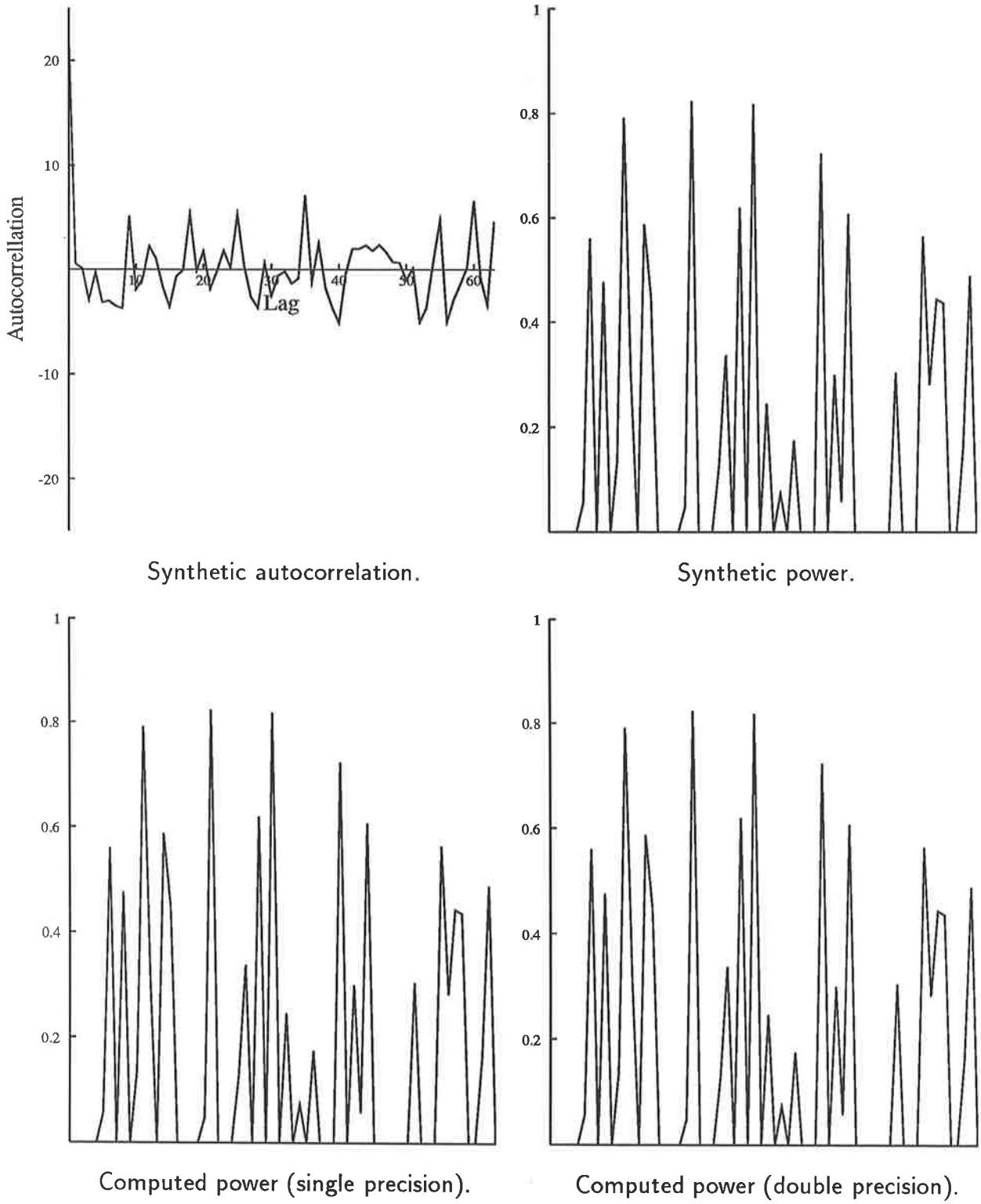


Figure 5.1: Synthetic autocorrelation and computed power spectra (random sequence).

bound on the condition number provided by computed power spectra may be very pessimistic. This is so even if computations are performed in higher precision, due to the error involved when estimating small power values. The observed error in small power values may be attributed to Gibb's phenomenon, described in most texts of Fourier analysis (*e.g.* Bracewell (1978)), but rarely discussed in geophysical literature, Meyerhoff (1968a, b, c) being a notable exception. Gibb's phenomenon is an effect in which computed large values in a discrete spectrum, exhibiting a discontinuous nature, may be larger than actual values, and small computed values may be less than the actual values, due to an overshoot associated with discontinuities. This effect may result in numerical difficulty in computing relatively small values of a spectrum, in a fashion analogous to the difficulty encountered when computing small magnitude eigenvalues of a matrix, as discussed in Section 3.6. Ford and Hearne (1966) previously noted, without explanation, this difficulty with calculations of power spectra, and stated that it may be alleviated by prewhitening. This statement is supported by arguments of Section 4.5.3.

The condition number of the 64 by 64 autocorrelation matrix has been computed to a value of 9.905×10^6.

5.1.1 Results from different solution algorithms

A number of different algorithms may be employed to compute least squares filters. This section compares the quality of results produced by solving the normal equations when the right-hand side is a unit impulse :

$$\begin{pmatrix} r_0 & r_1 & \cdots & r_{n-1} \\ r_1 & r_0 & \cdots & r_{n-2} \\ & & \ddots & \\ r_{n-1} & r_{n-2} & \cdots & r_0 \end{pmatrix} \begin{pmatrix} s_0 \\ s_1 \\ \vdots \\ s_{n-1} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

For the purposes of comparison, a solution was obtained using Gaussian Elimination in double precision. This solution will be referred to as the "double precision filter". This filter is not necessarily exact—it is merely guaranteed correct to a larger number of significant

figures, as discussed in Appendix A. The following algorithms, discussed in Section 2.2, are considered :

- Gaussian elimination.
- Wiener-Levinson algorithm.
- Conjugate Gradient algorithm. For the purposes of comparison, the number of iterations chosen was 64, which is the order of the coefficient matrix. The initially selected starting vector was the 64-length zero vector.
- Trench's algorithm. This is an algorithm which inverts a Toeplitz matrix. For the purpose of comparison, the first column of the inverse matrix was chosen (which is the right-hand side of the linear system of interest).

The double precision filter is illustrated in Figure 5.2, and filters produced by the different algorithms are shown in Figure 5.3. Comparing the graphs in these two figures, it may be

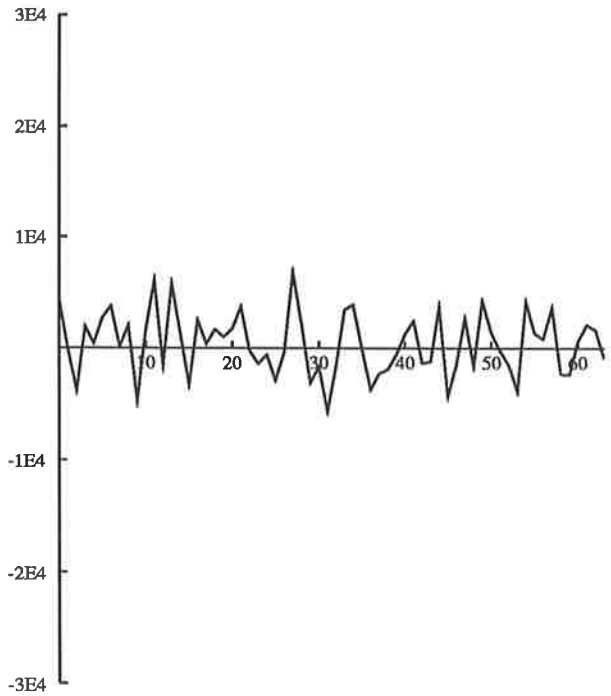


Figure 5.2: Double precision filter produced from "synthetic autocorrelation".

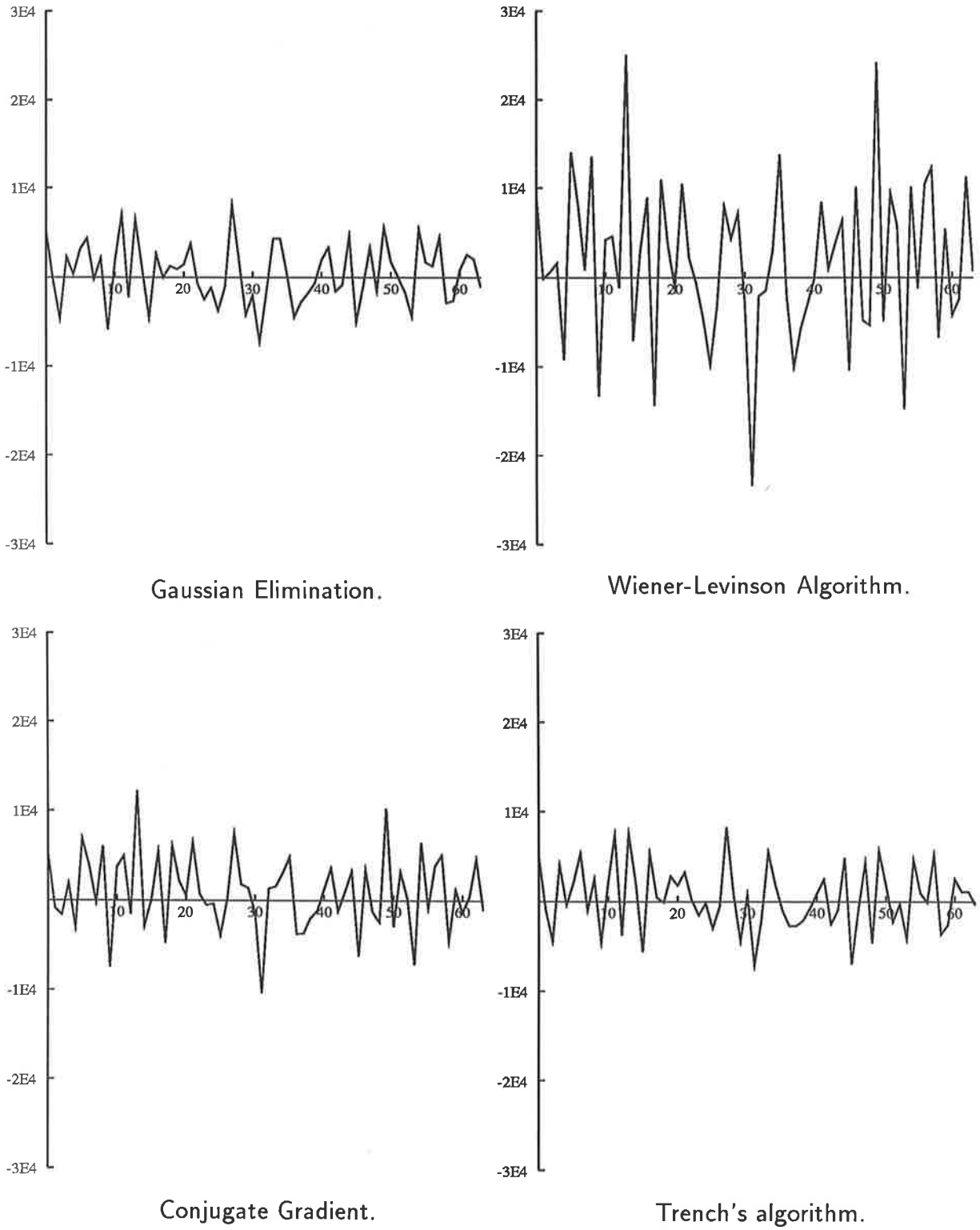


Figure 5.3: Filters produced by various algorithms working in single precision.

observed that the filter produced by Gaussian elimination is visually the most similar to the double precision filter. This is a strong indication that Gaussian elimination has produced a filter with less error than have the other algorithms. The filter produced by Trench's algorithm also closely resembles the double precision filter, although there are observable differences. Visually, the conjugate gradient algorithm has produced poorer quality results, which exhibit a more erratic variation in amplitude, than have Gaussian elimination or Trench's algorithm. This effect may be expected because the Conjugate gradient method is an iterative scheme which minimizes an error norm. Therefore, in this ill-conditioned example, this algorithm may be expected to produce a filter exhibiting significant error. However, the most disturbing result is that produced by the Wiener-Levinson algorithm, which exhibits a more erratic behaviour, and a much larger apparent error relative to the double precision solution, than have solutions produced by the other approaches, despite the fact that the Wiener-Levinson algorithm is a direct method, and is most frequently employed in seismic processing. These observations also apply to summary statistics given in Table 5.2. In this table the following conventions are employed :

- $||\ldots||$ denotes the Euclidean norm, defined in Section 3.3.1,
- $\mathbf{f}_a$ denotes a spiking filter produced by a given solution algorithm, a. The elements of this vector are denoted as f_i.
- $\mathbf{f}_d$ denotes the "double precision filter" *i.e.* $\mathbf{f}_a$ produced by Gaussian elimination in double precision.

Most interesting of these statistics is the norm of the computed error relative to the norm of the double precision solution. In terms of observed quality, the different methods may be ranked in the same order as that determined previously by a visual examination of the filters. The Wiener-Levinson algorithm, which produced a solution exhibiting an error of the order of 264%, has performed very poorly in comparison with the other methods. In this example, as in all later examples, spiking filters computed using double precision have been confirmed to be minimum phase by checking that zeros of the z-transform lie inside

	Algorithm, a				
	Double prec.	Gauss.	C-G	Trench	W-L
$\|\|\mathbf{f}_a\|\|$	2.234×10^4	2.681×10^4	3.436×10^4	2.854×10^4	7.165×10^4
$\|\|\mathbf{f}_a - \mathbf{f}_d\|\|$	0	5196	2.171×10^4	1.042×10^4	6.019×10^4
$\frac{\|\|\mathbf{f}_a - \mathbf{f}_d\|\|}{\|\|\mathbf{f}_d\|\|}$	0	0.2326	0.9716	0.4665	2.694
$\min f_i$	-5631	-7285	-1.035×10^4	-7087	-2.339×10^4
$\max f_i$	6783	8067	1.226×10^4	8301	2.503×10^4

Table 5.2: Summary statistics for filters of Figure 5.3.

the unit circle. This check has not been performed for spiking filters computed using single precision because of their associated error.

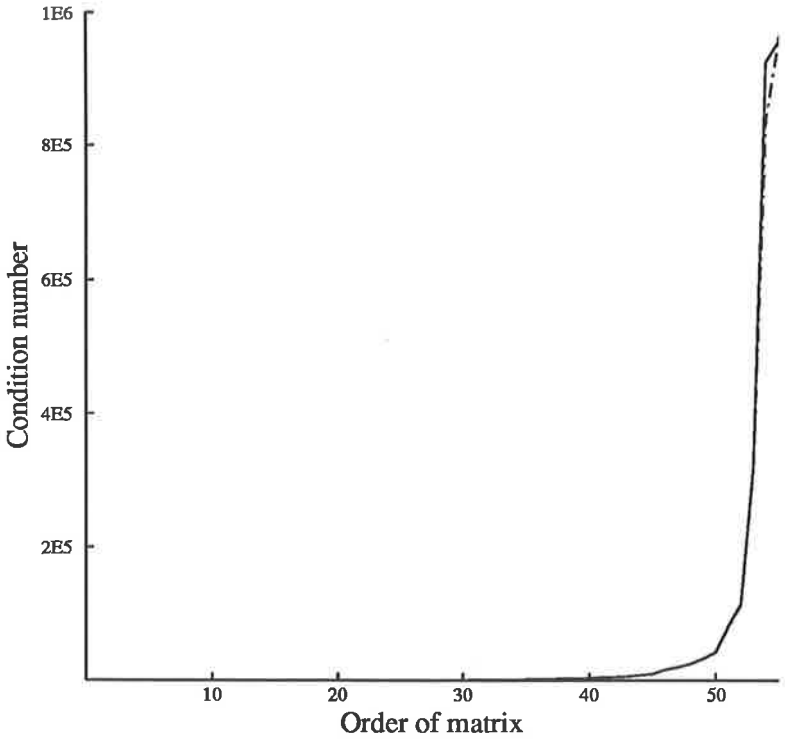
5.1.2 Condition numbers and prediction error variances

It has been shown in Section 4.4.2 that prediction error variances, which are intermediate results of the Wiener-Levinson algorithm, may be used to provide a lower bound for the spectral condition number of a symmetric, positive-definite Toeplitz matrix. Because the Wiener-Levinson algorithm has a recursive nature, described in Section 2.2.3.1, it is of interest to discuss condition numbers and prediction error variances for systems as the order of the matrix is increased.

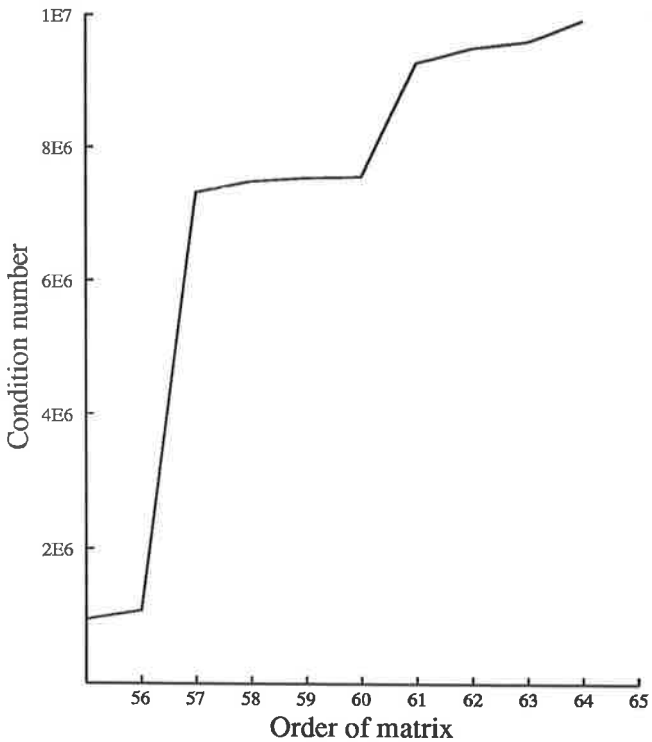
Figure 5.4 illustrates condition numbers for principal submatrices of the autocorrelation matrix, computed using a variant of the QR algorithm described by Martin et al. (1971a). This algorithm assumes a upper Hessenberg matrix. For this reason, the autocorrelation matrix was balanced using the procedure of Parlett and Reinsch (1971) and reduced to Hessenberg form using the procedure of Martin and Wilkinson (1971). Condition numbers computed using the Jacobi-type approach described by Rutishauser (1971) show little difference to those computed using the QR algorithm.

Observations which may be made concerning these condition numbers are as follows :

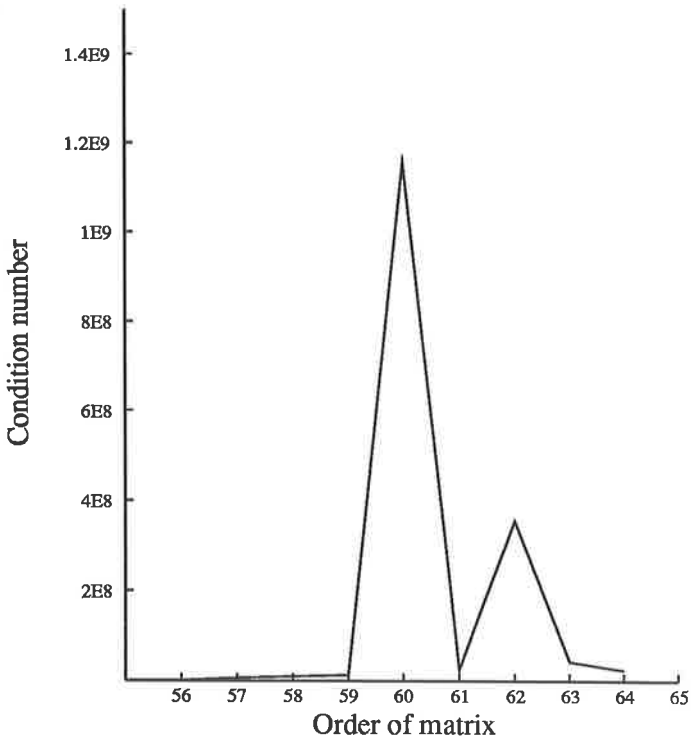
- as the order of the submatrix increases there is little discrepancy between results



Low order (dashed = DP).



Double precision (high order).



Single precision (high order).

Figure 5.4: Condition numbers calculated using different precision arithmetic.

produced using single precision and those produced using double precision.

- for larger order sub-matrices (> 54) the condition numbers show significant discrepancy between single and double precision.

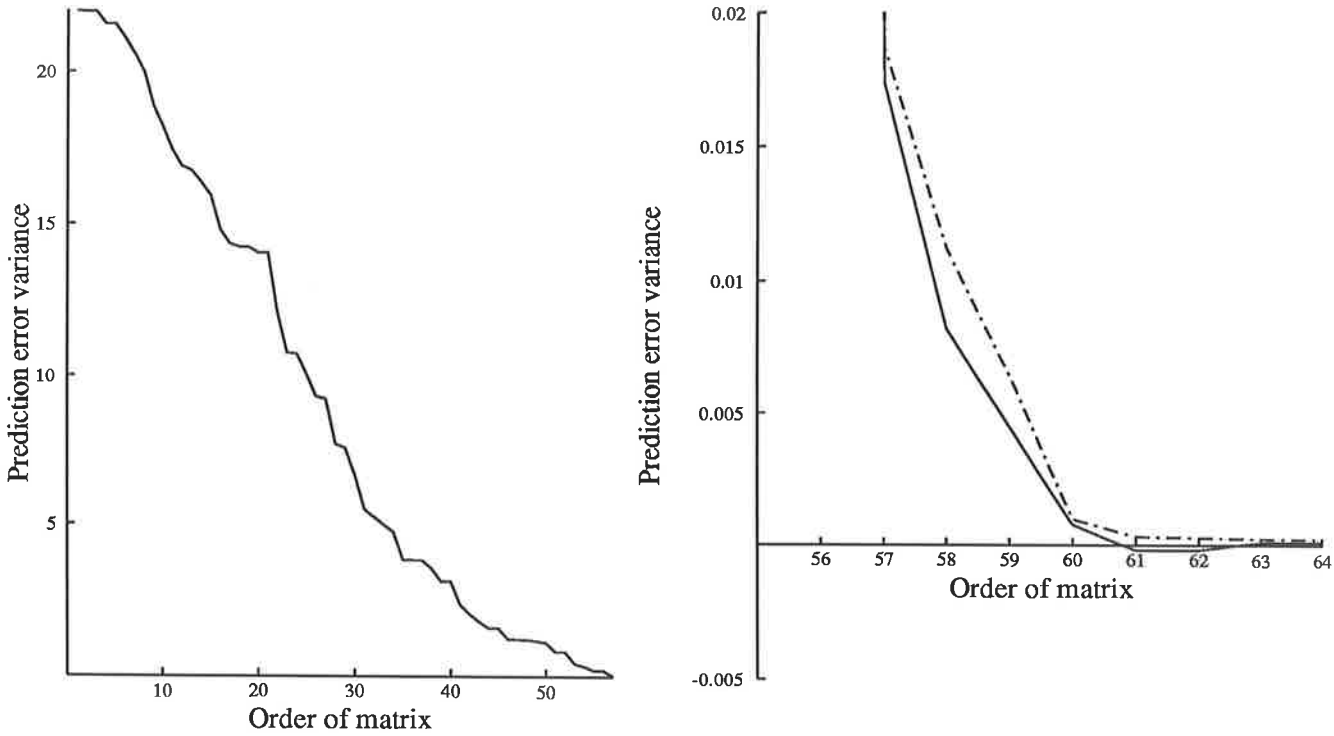
The condition numbers computed using single precision at higher order are associated with the occurrence of negative computed eigenvalues, which do not occur in the corresponding double precision results. This difference may be attributed to difficulty associated with computation of eigenvalues of small magnitude.

Figure 5.5 illustrates computed prediction error variances. A similar (but reversed) effect to that noted for condition numbers is observed for prediction error variances :

- the difference between prediction error variances computed for lower order systems, in different precision, is negligible.

- prediction error variances, computed using single precision for higher order systems, exhibit a much larger relative discrepancy relative to their double precision counterparts. Some prediction error variances, computed using single precision are negative, an effect which also (apparently) violates the condition that the matrix is positive definite.

These results indicate that values of prediction error variances may be employed to provide an indication of when the Wiener-Levinson algorithm is overcome by rounding errors. As prediction error variances are computed as intermediate results of the algorithm, they may be extracted at little additional cost when solving the linear system. This is in contrast with a scheme involving explicit extraction of eigenvalues of a matrix, which involves a much greater computing cost.



Low order systems. High order systems (dashed line = DP).

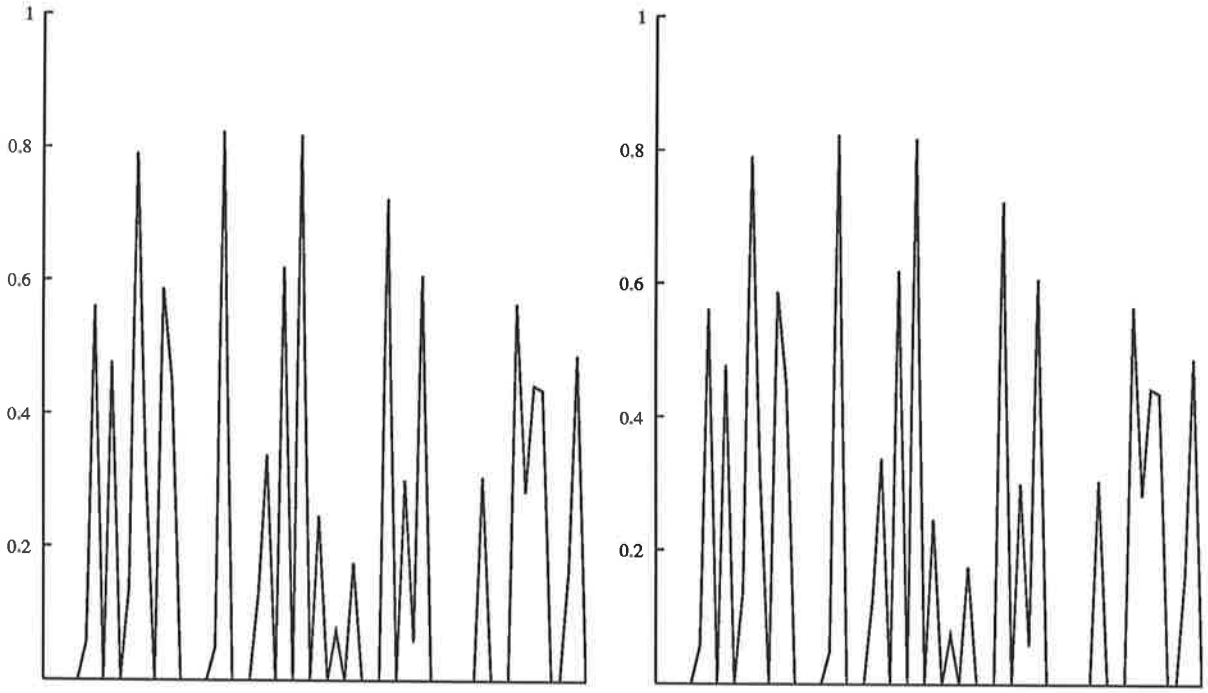
Figure 5.5: Prediction error variances calculated using different precision arithmetic.

5.1.3 The effect of prewhitening

It has been seen in previous sections that an ill-conditioned autocorrelation matrix may cause difficulties when computing a power spectrum, or when solving the normal equations. This section considers the effect of 0.1% prewhitening on computed results—*i.e.* the diagonal element, r_0, of the autocorrelation matrix is increased by 0.1%. As discussed in Section 4.5.3, this treatment is equivalent to the addition of a constant positive value to all values in the power spectrum.

5.1.3.1 Power spectra

Power spectra, computed after prewhitening, are illustrated in Figure 5.6. Visually, there is little difference between these spectra and those illustrated in Figure 5.1. Differences



Computed power (single precision). Computed power (double precision).

Figure 5.6: Computed prewhitened power spectra (random sequence).

between the spectra are more apparent in summary statistics for Figures 5.1 and 5.6 which are given in Table 5.3. Significantly, spectra for the prewhitened autocorrelation show little difference between single and double precision. Prewhitening has had little effect on the maximum computed power value, but has had the effect of eliminating the negative value which arose when computing the spectrum in single precision. This may be interpreted as a consequence of increasing the minimum power value.

The condition number of the prewhitened 64 by 64 autocorrelation matrix has been computed to a value of 3162, which is a significant improvement over the value of 9.905×10^6 reported previously.

	Double precision		Single precision	
	$p.w. = 0$	$p.w. = 0.01\%$	$p.w. = 0$	$p.w. = 0.01\%$
Minimum value	1.159×10^{-8}	1.731×10^{-4}	-8.598×10^{-7}	1.723×10^{-4}
Maximum value	0.8234	0.8236	0.8234	0.8236
Min. magnitude	1.159×10^{-8}	1.731×10^{-4}	0	1.723×10^{-4}
Max. magnitude	0.8234	0.8236	0.8234	0.8236
Max:min magnitude	7.102×10^{9}	4757	∞	4781
# of values ≤ 0	0	0	12	0

Table 5.3: Comparison of power spectra with prewhitening.

5.1.3.2 Results from different solution algorithms

Figures 5.7 and 5.8 illustrate the spiking filters computed using different approaches, after prewhitening. These filters do not appear significantly different to each other, in contrast with results of Figures 5.2 and 5.3. This effect is also apparent in summary statistics of Table 5.4, where it may be observed that all algorithms have produced solutions with small error. The Conjugate Gradient scheme has produced results exhibiting the least error, in terms of norms.

	Algorithm, a				
	Double prec.	Gauss.	C-G	Trench	W-L
$\|\|\mathbf{f}_a\|\|$	9.048	9.049	9.048	9.050	9.048
$\|\|\mathbf{f}_a - \mathbf{f}_d\|\|$	0	6.004×10^{-4}	3.132×10^{-4}	2.022×10^{-3}	8.837×10^{-4}
$\frac{\|\|\mathbf{f}_a - \mathbf{f}_d\|\|}{\|\|\mathbf{f}_d\|\|}$	0	6.635×10^{-5}	3.462×10^{-5}	2.235×10^{-4}	9.766×10^{-5}
$\min f_i$	-2.150	-2.151	-2.150	-2.151	-2.150
$\max f_i$	2.565	2.565	2.565	2.566	2.565

Table 5.4: Summary statistics for filters of Figure 5.7.

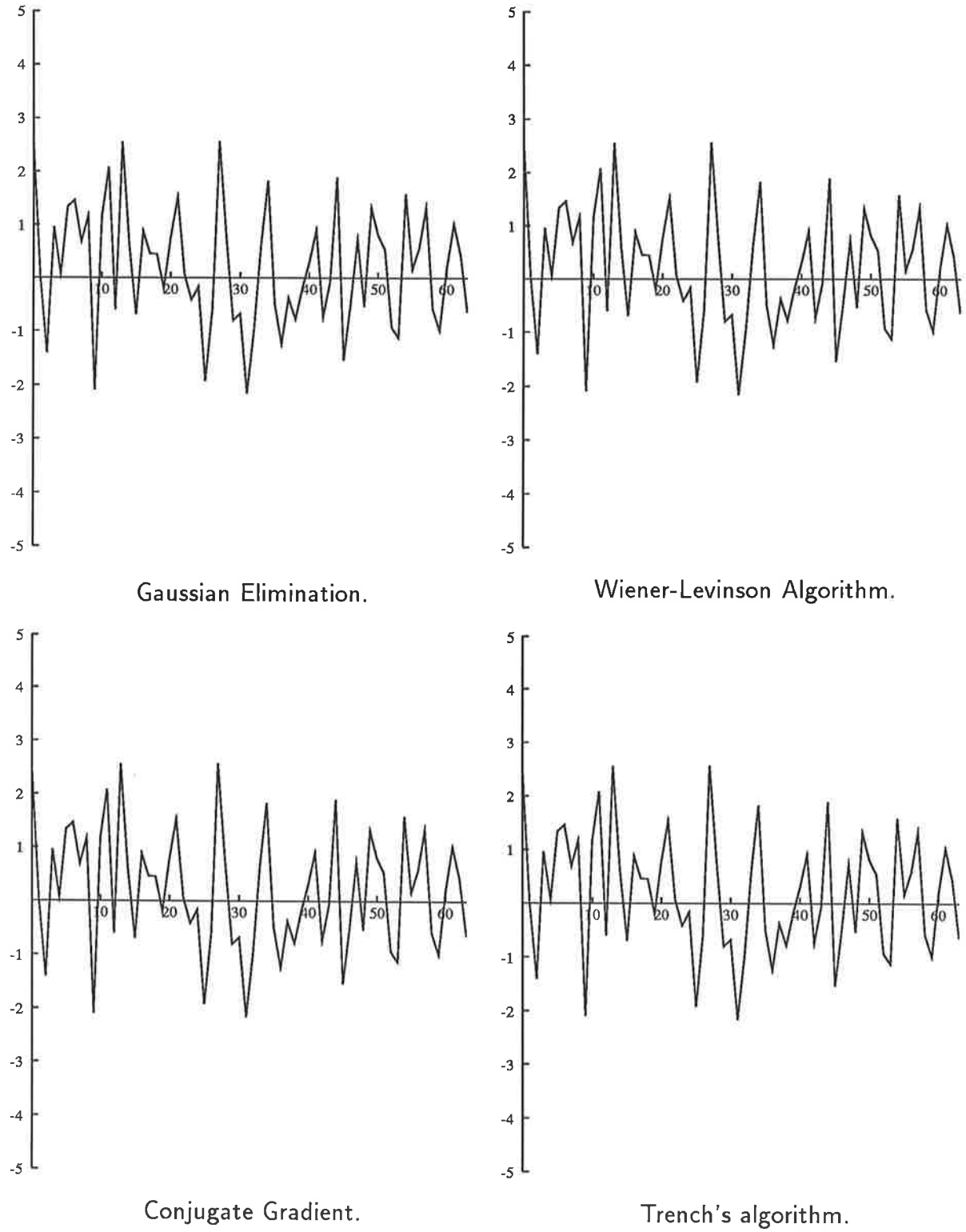


Figure 5.7: Filters produced by various algorithms working in single precision after 0.1% prewhitening.

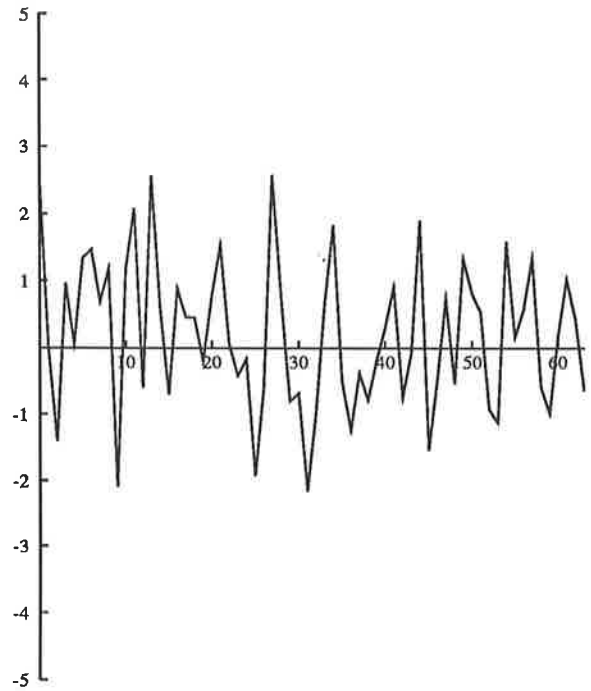


Figure 5.8: Double precision filter produced with 0.1% prewhitening.

5.2 Stability of direct methods for linear systems

Results of Section 5.1 indicate that Gaussian elimination with partial pivoting, Trench's algorithm, and the Wiener-Levinson algorithm possess different stability properties. Concepts of stability of an algorithm, and conditioning of a matrix, as discussed in Chapter 3, are intimately involved with the works of Wilkinson (1961, 63, 65). There has been discrepancy in literature relating to stability of direct algorithms for Toeplitz systems, with some authors (*e.g.* Cornyn (1974), Cybenko (1980)) claiming that various algorithms are stable, and others (*e.g.* Tukey (1967)) claiming they are unstable. Bunch (1985) has observed that algorithms based on partitioning of the matrix, are unstable when applied to any linear system involving a Toeplitz coefficient matrix which is either not symmetric or not positive definite. Cybenko (1980) claimed that the Levinson-Durbin algorithm (a term which refers to the basic approach applied by the algorithms of Levinson (1946),

Trench (1964), and Zohar (1974) (not discussed further in this thesis)) is stable for the class of symmetric, positive definite, Toeplitz matrices, allowing the conclusion that related algorithms are also stable. However, a backward error analysis, in the sense of the works of Wilkinson, was not given. This resulted in some controversy, which has been addressed by Bunch (1987), whose approach will be summarized in the remainder of this section.

5.2.1 Weak and Strong stability

Given that there is controversy surrounding the stability of direct algorithms for solution of linear equations involving Toeplitz coefficient matrices, it is necessary to define concepts of stability. The definitions given here are those of Bunch (1987).

Definition 5.1 *An algorithm for solving linear equations is weakly stable for a class of matrices $\mathcal{A}$ if for each well-conditioned matrix $\mathbf{A} \in \mathcal{A}$ and for each right-hand side vector $\mathbf{b}$ the computed solution $\mathbf{x}_c$ to $\mathbf{Ax} = \mathbf{b}$ is such that $||\mathbf{x} - \mathbf{x}_c||/||\mathbf{x}||$ is small.*

This definition means that an algorithm is described as weakly stable if, when applied to solve a linear system with a well-conditioned coefficient matrix, it computes a solution exhibiting little error. If an algorithm is not weakly stable for a given matrix class $\mathcal{A}$, then it is unstable. For example, Gaussian elimination performed without pivoting may produce a solution exhibiting large error, or fail entirely to produce a solution, even if the coefficient matrix is well-conditioned. Examples of this type of behaviour are given in many basic texts, *e.g.* Gerald and Wheatley (1984), as a justification for the use of pivoting. This means that Gaussian elimination without pivoting is unstable, unlike Gaussian elimination with partial or complete pivoting. An unstable algorithm introduces an exception to the statement, made in Section 3.4.1, that a small condition number excludes the possibility of numerical instability. A linear system may be described as ill-conditioned, as in Definition 3.1, even for a well-conditioned matrix, if the solution algorithm is unstable. The discussion throughout Chapter 3 relates primarily to the effect of perturbations in either the coefficient matrix or the right hand side vector. The use of condition numbers for determining whether or not a

numerically computed solution exhibits a large error implicitly assumes that the algorithm is at least weakly stable.

Definition 5.1 is weaker than the definition of stability of Wilkinson (1961, 63, 65), given in Definition 5.2 :

Definition 5.2 *An algorithm for solving linear equations is stable for a class of matrices $\mathcal{A}$ if for each matrix $\mathbf{A} \in \mathcal{A}$ and for each right-hand side vector $\mathbf{b}$ the computed solution $\mathbf{x}_c$ to $\mathbf{Ax} = \mathbf{b}$ satisfies an equation $\hat{\mathbf{A}}\mathbf{x}_c = \hat{\mathbf{b}}$ where $\hat{\mathbf{A}}$ is close to $\mathbf{A}$ and $\hat{\mathbf{b}}$ is close to $\mathbf{b}$.*

In this definition "$\hat{\mathbf{A}}$ is close to $\mathbf{A}$" means that $||\hat{\mathbf{A}} - \mathbf{A}||$ is small, for some matrix norm of interest (*e.g.* the spectral norm). An analogous meaning applies to "$\hat{\mathbf{b}}$ is close to $\mathbf{b}$".

The vector $\mathbf{x}_c$ is a solution of an infinite number of possible equations of the form $\hat{\mathbf{A}}\mathbf{x}_c = \hat{\mathbf{b}}$. Definition 5.2 requires that, in at least one of those systems, the matrix $\hat{\mathbf{A}}$ is close to $\mathbf{A}$ and the vector $\hat{\mathbf{b}}$ is close to $\mathbf{b}$. If an algorithm is stable it is also weakly stable. This definition of stability does not require that the matrix $\hat{\mathbf{A}}$ be in the matrix class $\mathcal{A}$, to which $\mathbf{A}$ belongs. For example, if $\mathbf{A}$ is a Toeplitz matrix, there is no requirement that $\hat{\mathbf{A}}$ also be Toeplitz. Therefore Definition 5.2 may be restricted even further :

Definition 5.3 *An algorithm for solving linear equations is strongly stable for a class of matrices $\mathcal{A}$ if for each matrix $\mathbf{A} \in \mathcal{A}$ and for each right-hand side vector $\mathbf{b}$ the computed solution $\mathbf{x}_c$ to $\mathbf{Ax} = \mathbf{b}$ satisfies $\hat{\mathbf{A}}\mathbf{x}_c = \hat{\mathbf{b}}$ where $\hat{\mathbf{A}} \in \mathcal{A}$, $\hat{\mathbf{A}}$ is close to $\mathbf{A}$, and $\hat{\mathbf{b}}$ is close to $\mathbf{b}$.*

If an algorithm is strongly stable for a given matrix class $\mathcal{A}$, it is also stable (and therefore also weakly stable) on that matrix class. Definition 5.3 is equivalent to the definition for stability given by Stewart (1973).

Weak stability is desirable because it guarantees that a reasonably accurate solution is produced when the matrix $\mathbf{A}$ is well-conditioned. However, weak stability allows no assurances as $\mathbf{A}$ becomes more ill-conditioned. Stability and strong stability are more desirable properties for a solution algorithm to possess because they guarantee that large

error can occur only when the condition number is large, but a large condition number does not necessarily imply large errors in the solution.

5.2.2 Stability of different algorithms

Given the definitions of Section 5.2.1, the following results, stated by Bunch (1987), may be proven :

- Gaussian elimination, with partial or complete pivoting, is strongly stable on the class of non-singular matrices.
- Gaussian elimination, with partial or complete pivoting, is stable on the classes of symmetric matrices, and of symmetric positive definite matrices

The distinction between the two statements of stability of Gaussian elimination with pivoting is subtle. If the class of non-singular matrices are considered, Gaussian elimination is strongly stable. However, by restricting the class of matrices further to symmetric, or symmetric positive definite, matrices, Gaussian elimination is stable. This is because, for matrices in these classes, the approximate matrix $\hat{\mathbf{A}}$ may be non-singular, but not necessarily symmetric or symmetric positive definite. It does not follow from error analyses that Gaussian elimination is strongly stable on these symmetric matrix classes. Note that this does *not* imply that Gaussian elimination is not strongly stable on these matrix classes, it is merely an indication that current error analyses are unable to determine whether or not it is.

5.2.3 Stability of Toeplitz algorithms

We now reach the conclusion of Bunch (1987) which motivated this discussion. In terms of the above definitions, Cybenko (1980) proved that the Levinson-Durbin algorithm, the Wiener-Levinson algorithm, and Trench's algorithm are *weakly stable* on the class of symmetric, positive definite, Toeplitz matrices. This result does not exclude the possibility

that any of these algorithms are stable (or even strongly stable), but such results remain to be proven or disproven.

This discussion allows some light to be thrown on observations made in Section 5.1.1. The ranking of quality of results observed indicates that, of the direct algorithms, Gaussian elimination has behaved in the most stable fashion, followed in order by Trench's algorithm, and the Wiener-Levinson algorithm. The results for Gaussian elimination and Trench's algorithm may indicate that these algorithms have conformed with a more restrictive definition of stability than has the Wiener-Levinson algorithm, on the class of symmetric positive-definite Toeplitz matrices. The filters produced by these algorithms exhibited measurable error, which may be attributed to the ill-conditioning of the problem, rather than to limitations in the algorithms themselves. It must be stressed that this merely supports the possibility that these algorithms may be stable on this matrix class, and in no way constitutes a proof that they are.

Any algorithm may produce a solution with significant error if the coefficient matrix is sufficiently ill-conditioned. The observed poor quality results produced by the Wiener-Levinson algorithm may, in addition to indicating ill-conditioning of the autocorrelation matrix, be an indication that it conforms to a weaker form of stability on the class of symmetric, positive definite, Toeplitz matrices than do Gaussian elimination or Trench's algorithm.

The Wiener-Levinson algorithm is weakly stable, therefore it is guaranteed to produce a reliable solution if the coefficient matrix is well-conditioned, symmetric, and positive definite. Results of Section 5.1 indicate that reliable solutions are not necessarily produced if the coefficient matrix is ill-conditioned. In relation to Wiener filtering, this means that the Wiener-Levinson algorithm is guaranteed to produce filters exhibiting small error when the autocorrelation matrix is well-conditioned. However, when the autocorrelation matrix is ill-conditioned, the filters produced may not be reliable, as exhibited in the example of Section 5.1. A test, which involves examination of prediction error variances, is of value because an indication may be provided when numerical difficulties are encountered.

Observations of this section indicate that poor results of the Wiener-Levinson algorithm

may be due to limitations of that algorithm. The comparatively higher quality results of the conjugate gradient algorithm, observed in Section 5.1, and noted previously by Treitel and Wang (1976), may be interpreted as being due to limitations of the Wiener-Levinson algorithm when applied to ill-conditioned problems, rather than to virtues of the conjugate gradient algorithm, which was the conclusion of Treitel and Wang (1976).

5.3 A synthetic vibroseis cross-correlation

Results of Section 5.1 provide insights into the manifestations—in terms of computed power spectra, prediction error variances, and accuracy of computed Wiener spiking filters—which are introduced when the autocorrelation matrix is ill-conditioned. However, the previous example provides no indication of the behaviour of computed prediction operators, and no indication of effects introduced when erroneous operators are applied in the computation of deconvolved traces.

A synthetic vibroseis cross-correlation with a 4 millisecond sampling increment, is illustrated in Figure 5.9. It was generated, from the wavelet and impulse response described in Appendix B, as follows :

1. the minimum phase wavelet of Figure B.1 was convolved with the impulse response of Figure B.3 to produce a synthetic trace.

2. the trace produced in Step 1 was convolved with a linear vibroseis sweep signal of constant amplitude, which was employed as a 25-85 Hertz chirp wave form (Kulhanek (1976)) with a four second duration.

3. the vibroseis trace produced by Step 2 was cross-correlated with the vibroseis sweep signal. This procedure is in accordance with common practice, as described by Yilmaz (1987).

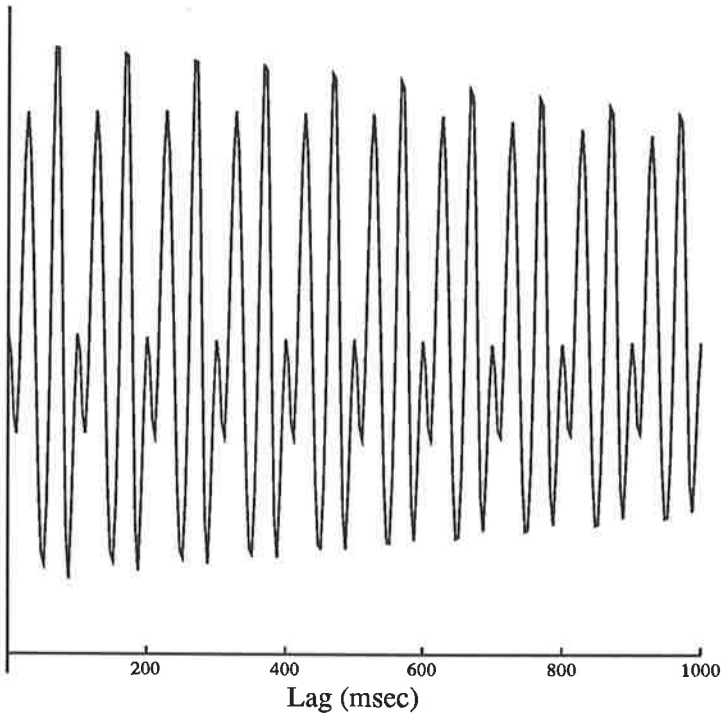


Figure 5.9: First 1000 millisecond window of the vibroseis cross correlation (25-85 Hz, 4 second sweep).

The first 1000 millisecond window of the normalized autocorrelation of the vibroseis cross-correlation is illustrated in Figure 5.10. The most striking feature of this autocorrelation is that it exhibits an approximately periodic nature, with little loss of amplitude at larger lags. Such a form of behaviour indicates that the frequency content of the autocorrelation is dominated by a small number of frequencies, which means that the power spectrum contains values which are significantly different in magnitude. Such an effect is observed in the computed power spectra of Figure 5.11. This figure illustrates spectra obtained by applying cosine transforms to autocorrelation functions. Two cases are considered here :

- the spectrum is computed using the entire autocorrelation function
- the spectrum is computed using the first fifty lags of the autocorrelation function. This function has been presented with the purpose of determining whether or not a

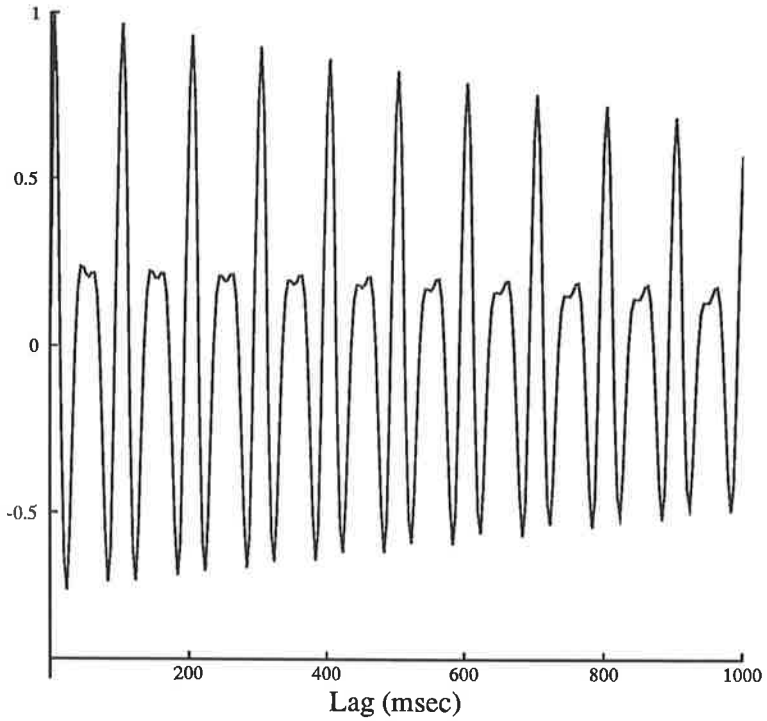


Figure 5.10: First 1000 millisecond window of the normalized autocorrelation function.

cosine transform on the first 50 lags may be employed to determine when the 50 by 50 normal equations are ill-conditioned. It was noted in Section 1.4.2.2 that some windowing function is desirable when truncating a series to compute a spectrum. The truncated spectra illustrated in this chapter have had no such window applied. Results were found to exhibit similar effects, whether or not such a window is applied, therefore results obtained for different window schemes are not reported here.

For comparison these two spectra were computed using single and double precision arithmetic. It is interesting to note that the spectra computed using the first fifty lags exhibit negative values in both single and double precision. The peaks which occur in the spectra computed using 50 autocorrelation values are significantly wider than those computed using the complete autocorrelation. This behaviour would be affected by choice of window functions.

Summary statistics for the different spectra are given in Table 5.5. It may be seen that negative values occur in both spectra computed using single precision, and zeros occur in

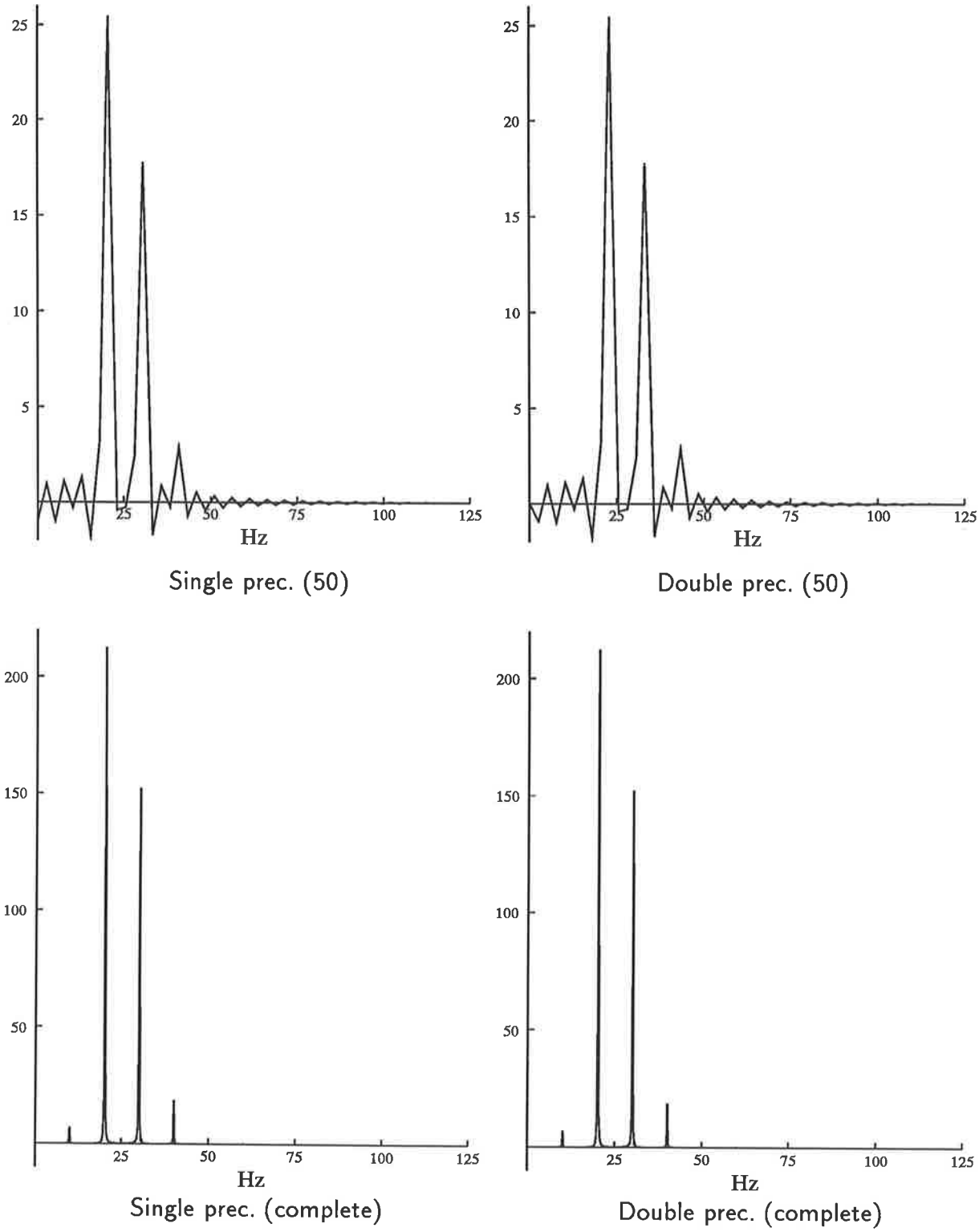


Figure 5.11: Computed power spectra of the signal of Figure 5.9.

Precision	Double		Single	
Length of sequence	50	complete	50	complete
Minimum value	-1.725	0	-1.725	-2.411×10^{-5}
Maximum value	25.47	212.4	25.47	212.4
Minimum magnitude	0	0	1.621×10^{-3}	1.008×10^{-8}
Maximum magnitude	25.47	212.4	25.47	212.4
Max:min magnitude	∞	∞	1.1571×10^{4}	2.108×10^{10}
# of values ≤ 0	25	1	25	140

Table 5.5: Summary statistics of power spectra of the synthetic cross-correlation

both spectra computed using double precision. As in Section 5.1, this behaviour may be interpreted as being due to ill-conditioning of the autocorrelation, but a test based on this result may be too pessimistic.

The condition number of the autocorrelation matrix of order 50 is approximately 7.053×10^{6}. The fact that the ratio of maximum to minimum magnitude values computed from 50 lags of the autocorrelation, in single precision, is less than either of these condition numbers violates the condition of Section 4.1. However, the occurrence of a number of negative values of significant magnitude in the spectrum, in this case, means that this ratio has little real meaning.

5.3.1 Prediction filters

In order to compare results produced by different solution algorithms, prediction filters for a prediction distance of 3 lag values, which corresponds to the first zero crossing of the autocorrelation, are given using the same algorithms as in Section 5.1.1, with the exception of Trench's algorithm. The filters computed using different approaches are illustrated in Figure 5.12. It may be observed that, as for the example of Section 5.1, the conjugate gradient algorithm and the Wiener-Levinson algorithm have produced filters which differ significantly (*e.g.* larger range of values, more oscillatory behaviour) from

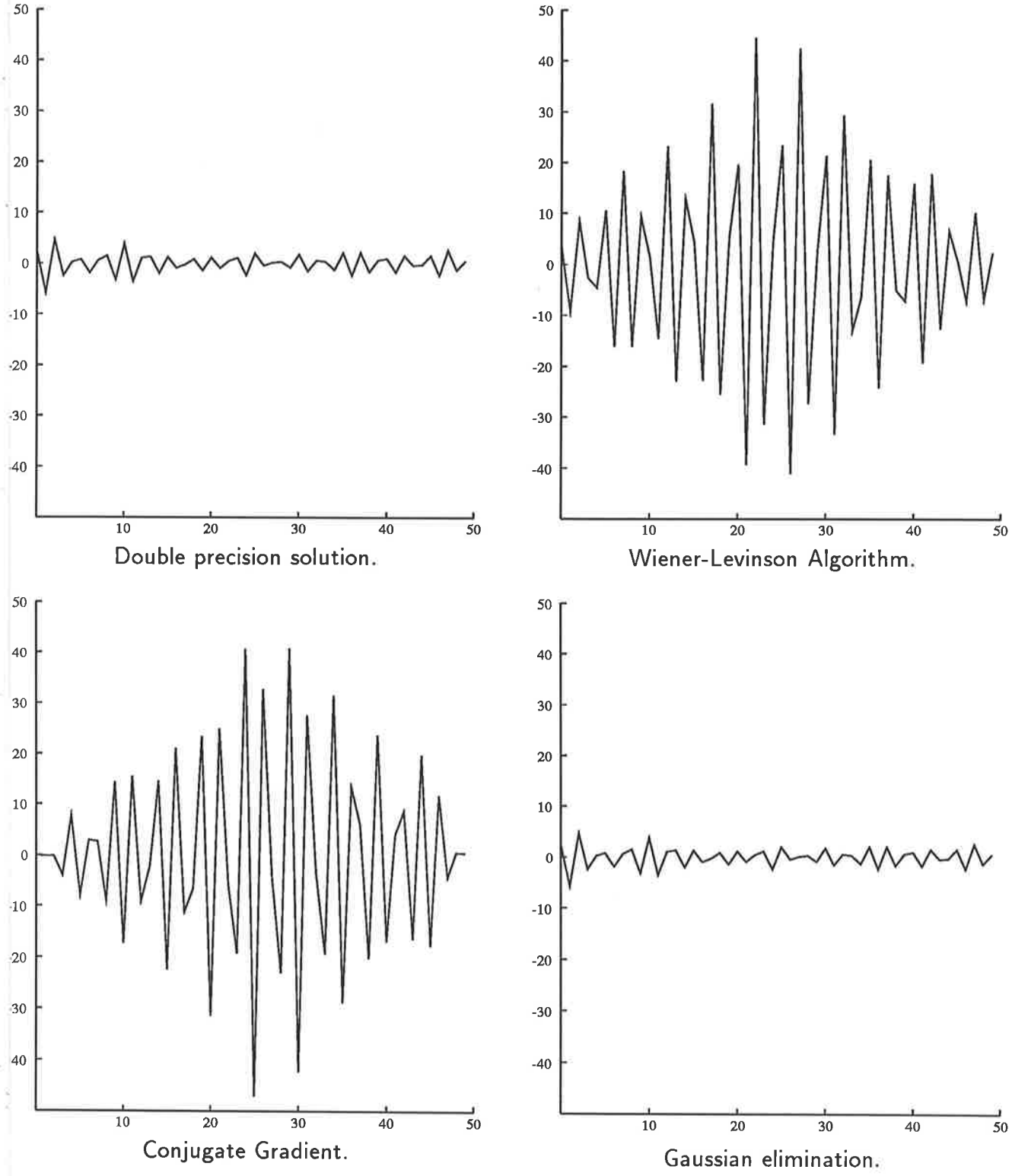


Figure 5.12: Filters produced by different approaches.

the double precision solution, whilst Gaussian elimination has produced a filter which exhibits little difference from the double precision solution. In this particular example, the Wiener-Levinson algorithm has produced a filter which appears to be of similar accuracy to that produced by the conjugate gradient scheme, in contrast to the observation of Section 5.1 that the conjugate gradient scheme produces a significantly more accurate filter than does the Wiener-Levinson algorithm. Summary statistics of Table 5.6 allow the observation that the Wiener-Levinson algorithm has produced results which are slightly more accurate than those of the conjugate gradient scheme. Both exhibit a relative error in terms of norms of the order of 1000% which means they have produced a much poorer solution than has Gaussian elimination, which exhibits an error of slightly less than 1%. Treitel and Wang (1976) presented an example in which the conjugate gradient algorithm produces more accurate filters than does the Wiener-Levinson algorithm. This observation is not supported here, and means that, whilst the conjugate gradient algorithm is capable of producing solutions superior to those of the Wiener-Levinson algorithm when solving ill-conditioned normal equations, there is no general guarantee that it will do so. The observation that the Wiener-Levinson algorithm produces a filter of much poorer accuracy than does Gaussian elimination lends support to the possibility that the Wiener-Levinson algorithm may not be stable, in the sense of Definition 5.2, as is Gaussian elimination, on the class of symmetric, positive definite Toeplitz matrices.

	Algorithm, a			
	Double precision (d)	Gaussian Elimination	Conjugate Gradient	Wiener Levinson
$\|\|\mathbf{f}_a\|\|$	13.54	13.53	139.9	141.4
$\|\|\mathbf{f}_a - \mathbf{f}_d\|\|$	0	0.1289	146.8	137.8
$\frac{\|\|\mathbf{f}_a - \mathbf{f}_d\|\|}{\|\|\mathbf{f}_d\|\|}$	0	0.009525	10.84	10.18
$\min f_i$	−5.728	−5.725	− 47.05	− 41.03
$\max f_i$	4.622	4.618	40.76	44.49

Table 5.6: Summary statistics for prediction filters.

5.3.2 Prediction error variances

Table 5.7 lists computed prediction error variances, obtained as intermediate results of the Wiener-Levinson algorithm. The occurrence of negative prediction error variances, the first of which is ν_{30} (corresponding to a system of order 31), indicates that conditioning of the normal equations may be affecting the accuracy of computed Wiener filters of greater order. In cases where negative prediction error variances occur when solving the

Prediction Error Variance	
ν_0	1
ν_{29}	2.758×10^{-4}
ν_{30}	-5.278×10^{-4}
ν_{31}	1.651×10^{-3}
ν_{32}	7.333×10^{-5}
ν_{33}	-2.293×10^{-2}
ν_{34}	1.466×10^{-3}
ν_{35}	7.575×10^{-4}
ν_{36}	2.368×10^{-4}
ν_{37}	-2.716×10^{-3}
ν_{38}	9.798×10^{-4}
ν_{39}	1.619×10^{-4}
ν_{40}	-3.962×10^{-3}
ν_{41}	9.239×10^{-4}
ν_{42}	-1.073×10^{-4}
ν_{43}	1.235×10^{-2}
ν_{44}	1.319×10^{-3}
ν_{45}	7.477×10^{-4}
ν_{46}	2.796×10^{-4}
ν_{47}	-1.439×10^{-3}
ν_{48}	1.108×10^{-3}
ν_{49}	4.430×10^{-4}

Table 5.7: Some computed prediction error variances for the previous example.

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normal equations, other, more reliable, approaches (*e.g.* Gaussian elimination, or higher precision solutions) may be desirable. Alternatively, prewhitening, which produces a coefficient matrix which is less ill-conditioned than the original autocorrelation matrix, may be employed.

5.3.3 Deconvolved outputs

Deconvolved outputs, produced by applying prediction error filters, obtained from prediction filters of Section 5.3.1, are illustrated in Figure 5.13. It may be observed that prediction error filters produced from the prediction filters of the Wiener-Levinson and conjugate gradient algorithms have been much less effective than that of Gaussian elimination. This means that ill-conditioning in the normal equations may be expected to propagate through computations, resulting in a relatively poor quality deconvolved output.

5.3.4 The effect of prewhitening

It was observed in Section 5.1.3 that prewhitening significantly improves the conditioning of an autocorrelation matrix, with subsequent improvement in quality of solution of the normal equations, and beneficial effects with computations of power spectra. The purpose of this section is to examine the effect of a moderate level of prewhitening (0.01%) on results obtained for the synthetic vibroseis cross-correlation, in a similar fashion to the discussion of Section 5.1.3, and to examine the effect of prewhitening on deconvolved outputs. The condition number of the 50 by 50 autocorrelation matrix in this case is approximately 1.437×10^5 which is an improvement of an order of magnitude over the condition number without prewhitening. This demonstrates the fact that any level of prewhitening results in a less ill-conditioned autocorrelation matrix.

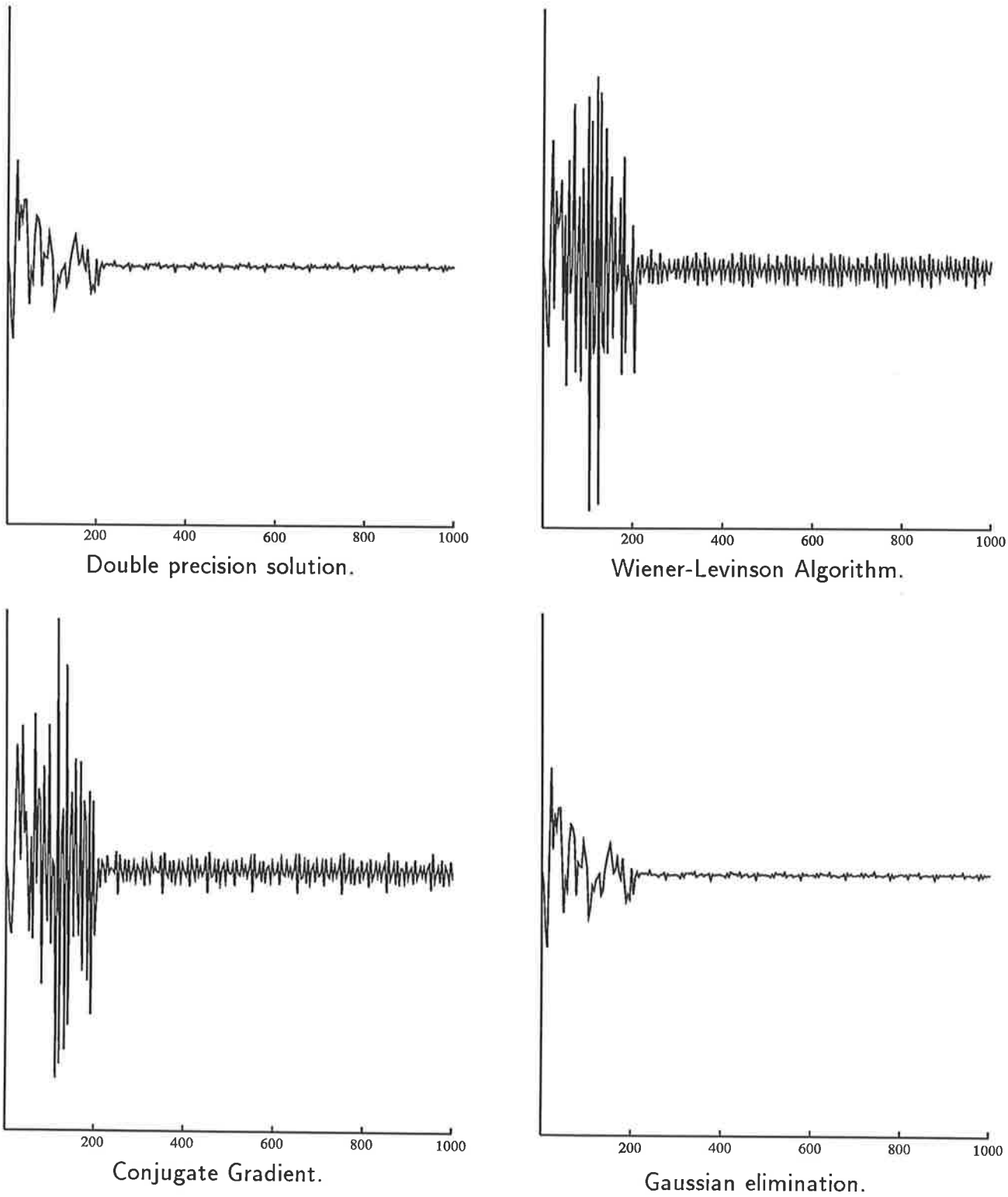


Figure 5.13: First 1000 millisecond window of the deconvolved outputs.

5.3.4.1 Power spectra

Figure 5.14 illustrates power spectra, computed in the same fashion as those in Figure 5.11, after prewhitening. It may be observed that spectra computed using the first 50 lags of the autocorrelation still exhibit a number of negative values with significant magnitude, and that the magnitude of negative values has not been significantly affected in comparison with graphs in Figure 5.11. This means that quite a large level of prewhitening would be necessary to eliminate negative values in this spectrum, and that the spectrum computed from the first 50 lags of the autocorrelation function has provided little indication about of conditioning of the 50 by 50 normal equations. In order to gain any useful information about conditioning of the normal equations from a power spectrum, it is necessary to consider the entire computed autocorrelation.

Table 5.8 gives summary statistics for all the spectra. It is interesting to note that the power spectrum computed from the entire autocorrelation exhibits a zero in double precision, but none in single precision. This behaviour could be related to the ill-conditioning of the normal equations. However, it will be seen in later sections that the prewhitened normal equations in this case appear reasonably well-conditioned.

These results mean that power spectra may be employed to gain an indication of ill-

Precision	Double		Single	
Length of sequence	50	complete	50	complete
Minimum	-1.725	0	-1.725	7.591×10^{-5}
Maximum	25.47	212.4	25.47	212.4
Minimum magnitude	0	0	1.521×10^{-3}	7.591×10^{-5}
Maximum magnitude	25.47	212.4	25.47	212.4
Max:min magnitude	∞	∞	1.674×10^{4}	2.798×10^{6}
# of values ≤ 0	25	1	25	0

Table 5.8: Summary statistics of power spectra of the synthetic cross-correlation after prewhitening

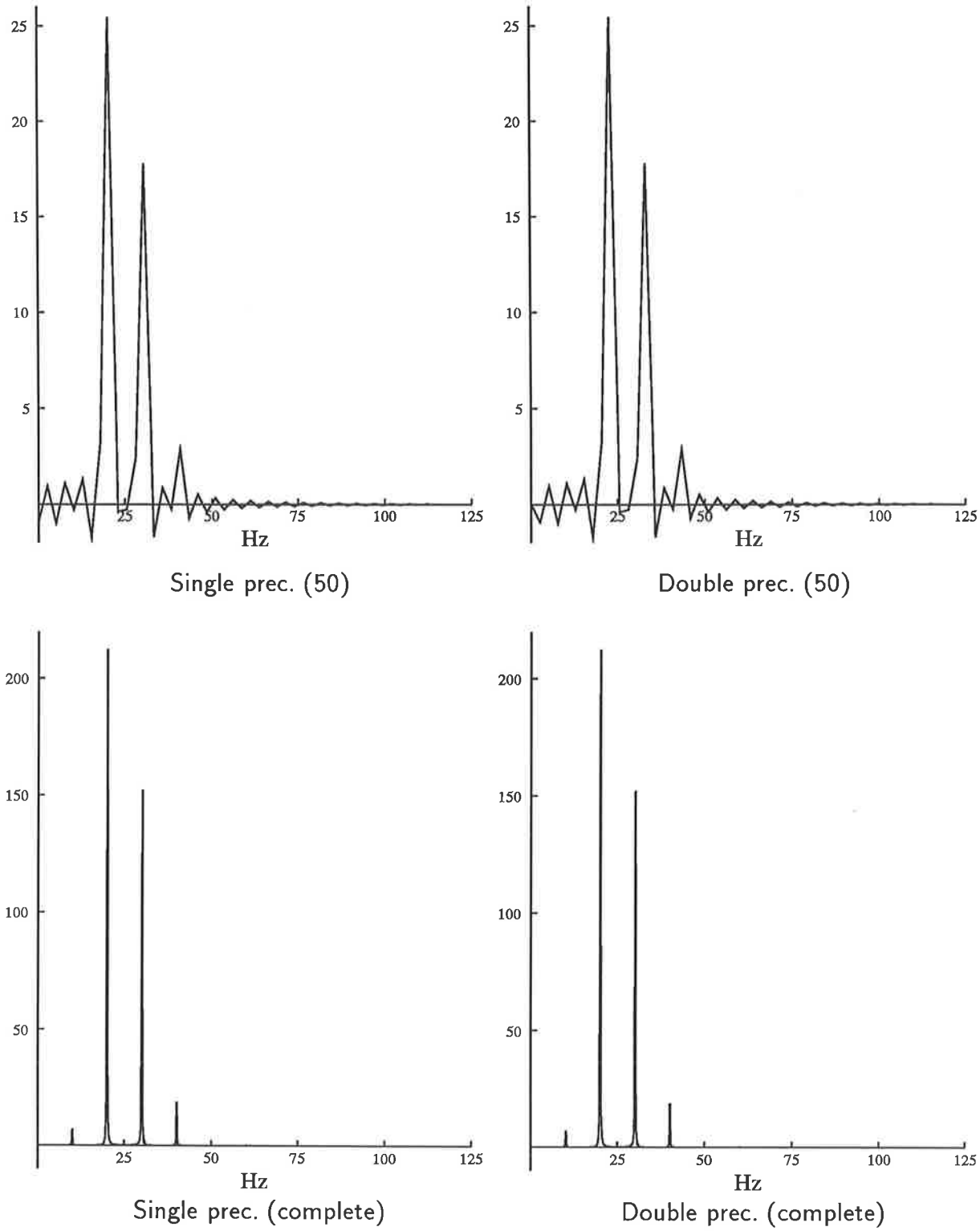


Figure 5.14: Computed power spectra of the signal of Figure 5.9 after prewhitening.

conditioning in the normal equations, although this indication is unnecessarily pessimistic. Based on the fact that values in the power spectrum provide an upper bound for the condition number, this is a result which may be expected. The occurrence of negative or zero values in the computed spectra, in single or double precision may, as in Section 5.1, be attributed to Gibb's phenomenon.

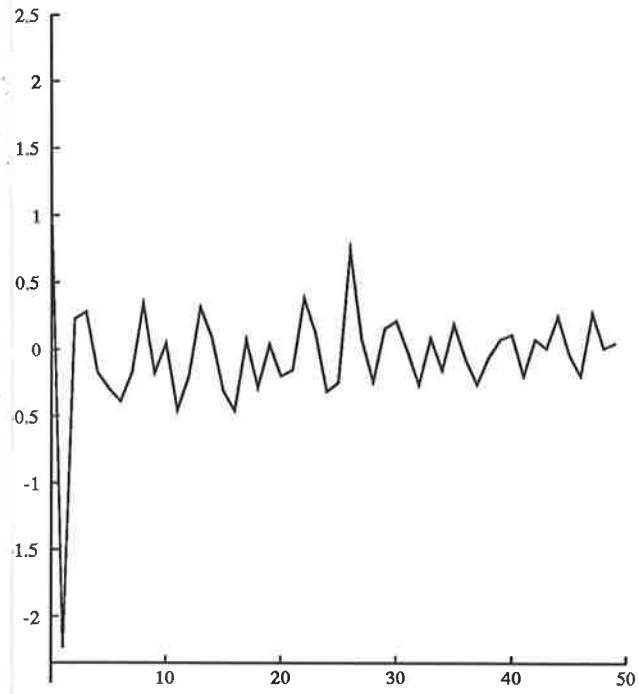
5.3.4.2 Prediction filters

Figure 5.15 illustrates prediction filters obtained by the different algorithms being considered. It may be observed that the filters produced by all algorithms, other than the conjugate gradient algorithm, show strong agreement with each other and with the double precision solution. The filter produced by the conjugate gradient algorithm exhibits more error than those produced by the other approaches. This observation also applies to summary statistics of Table 5.9.

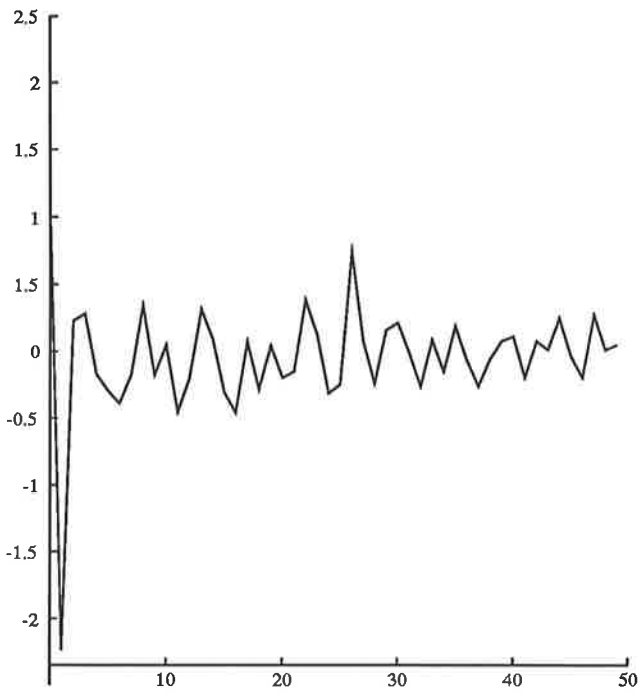
	Algorithm, a			
	Double precision (d)	Gaussian Elimination	Conjugate Gradient	Wiener Levinson
$\|\|\mathbf{f}_a\|\|$	2.980	2.979	2.867	2.980
$\|\|\mathbf{f}_a - \mathbf{f}_d\|\|$	0	1.329×10^{-3}	1.537	2.843×10^{-3}
$\frac{\|\|\mathbf{f}_a - \mathbf{f}_d\|\|}{\|\|\mathbf{f}_d\|\|}$	0	4.461×10^{-4}	0.5157	9.543×10^{-4}
$\min f_i$	-2.235	-2.235	-1.959	-2.236
$\max f_i$	1.013	1.013	0.8760	1.013

Table 5.9: Summary statistics for prediction filters after prewhitening.

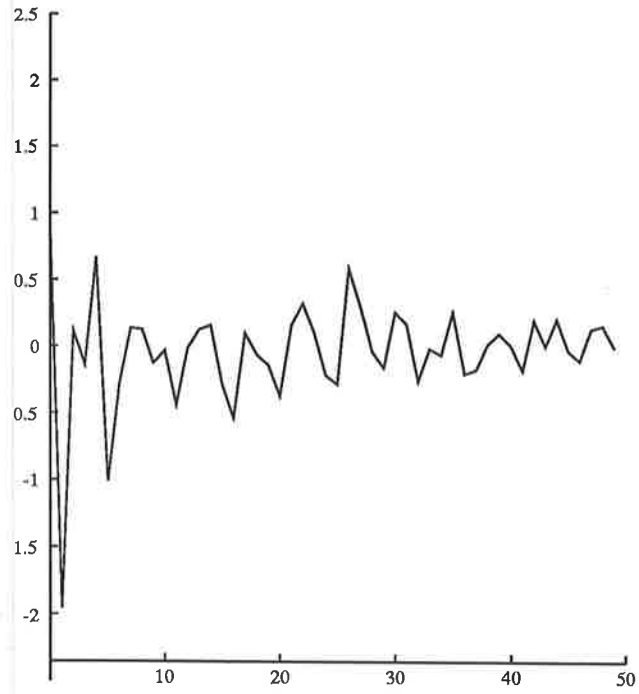
The spurious behaviour of the conjugate gradient algorithm may be related to the fact that the autocorrelation matrix in this case, with a condition number of 1.437×10^5, may still be considered somewhat ill-conditioned. This example shows that the conjugate gradient algorithm may be significantly affected by rounding error, even in cases where the Wiener-Levinson algorithm is not. As noted in Section 4.5, the spectral condition number



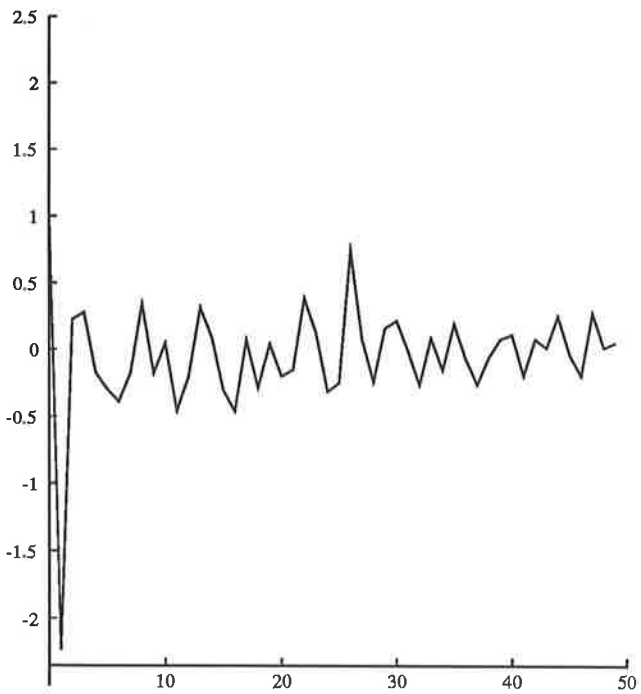
Double precision solution.



Wiener-Levinson Algorithm.



Conjugate Gradient.



Gaussian elimination.

Figure 5.15: Filters produced by different approaches after prewhitening.

is a monotonically decreasing function of prewhitening levels. This means that a higher level of prewhitening than considered here may be expected to reduce the error encountered when solution is performed with the conjugate gradient algorithm.

5.3.4.3 Prediction error variances

It was noted in Section 5.3.2 that some prediction error variances, produced as intermediate results of the Wiener-Levinson algorithm, were negative. In this case, in which the computed prediction filter exhibited little error, no negative prediction error variances were observed, and the values decreased monotonically from $\nu_0 = 1.0001$ to $\nu_{49} = 1.767 \times 10^{-3}$. This means that Equation 4.17, describing the behaviour of prediction error variances, is satisfied. This is a result which may be expected because the Wiener-Levinson algorithm produced filters exhibiting little error.

5.3.4.4 Deconvolved outputs

Deconvolved outputs, produced by applying prediction error filters obtained from prediction filters of Section 5.3.4.2, are illustrated in Figure 5.16. It may be observed that the deconvolved outputs in this case all show a much stronger similarity to each other than do the outputs illustrated in Figure 5.13. Additionally, these deconvolved outputs, particularly at lower lags, show a resemblance to the deconvolved outputs obtained using double precision without prewhitening (Figure 5.13). This means that, for interpretation purposes, the results produced by the conventional Wiener-Levinson algorithm, after prewhitening, may be considered to be as useful as those produced by using Gaussian elimination (which introduces more cost) without prewhitening.

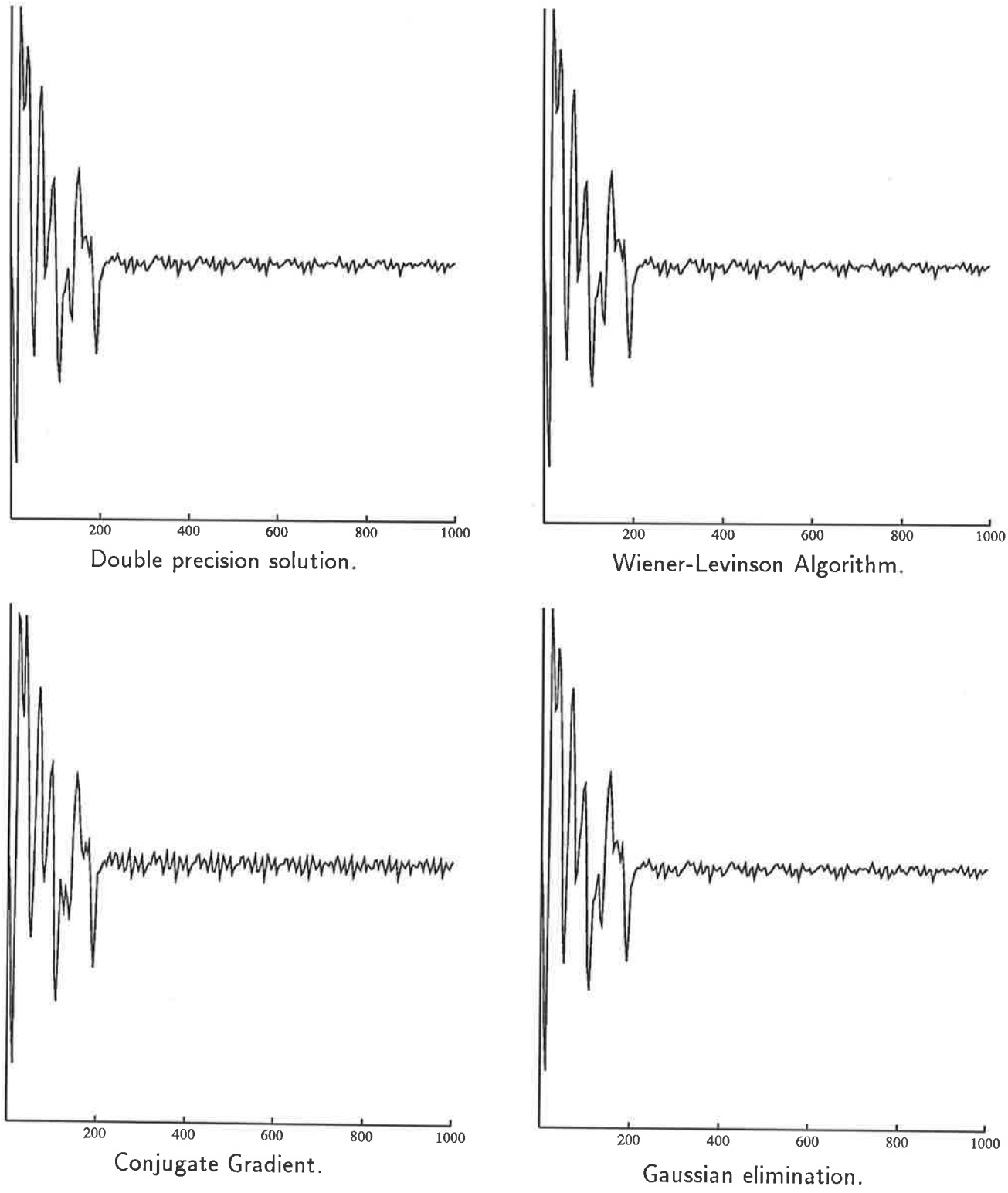


Figure 5.16: First 1000 millisecond window of the deconvolved outputs after prewhitening.

5.4 The effect of interpolating to a smaller sample increment

It was noted in Section 4.2.1 that a smooth trace will result in a more ill-conditioned autocorrelation matrix than one which is not as smooth. This section examines the effect of interpolating a synthetic trace from a 4 millisecond sampling interval to a 2 millisecond sampling interval. The trace examined in this section is illustrated in Figure 5.17. It was generated by convolving the trace of Figure B.1 with the impulse response of Figure B.3. For the purposes of this study, this trace was interpolated to a two millisecond sampling interval using a Newton-Gregory interpolating polynomial of degree 5. The procedure employed is that given by Gerald and Wheatley (1984, pp. 212-213). As discussed in Section 4.2.1, results similar to those presented here may be expected for any interpolation technique. The normalised autocorrelation for the interpolated trace is illustrated in Figure 5.18. The

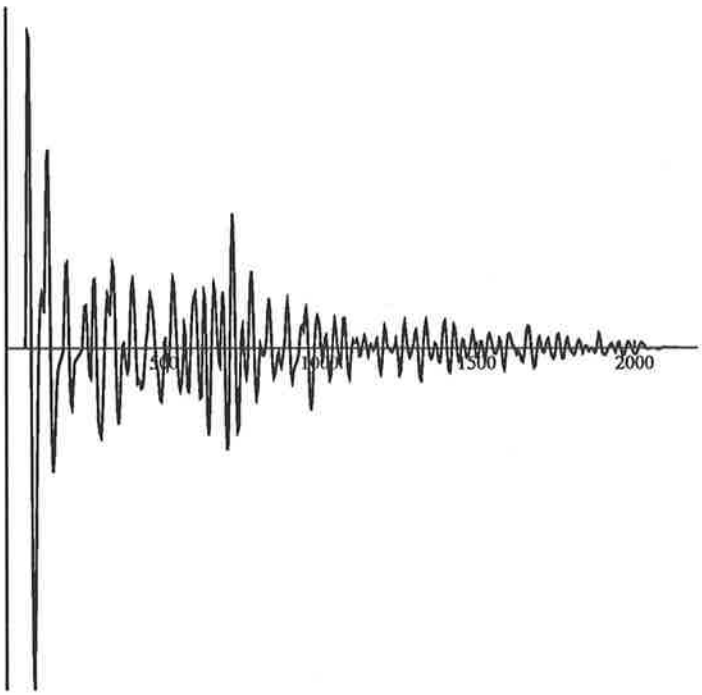


Figure 5.17: Synthetic trace.

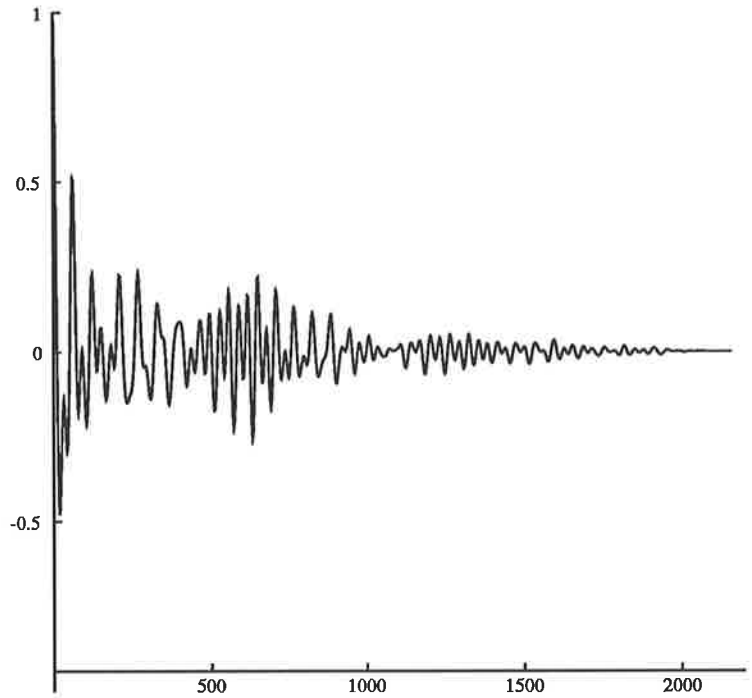
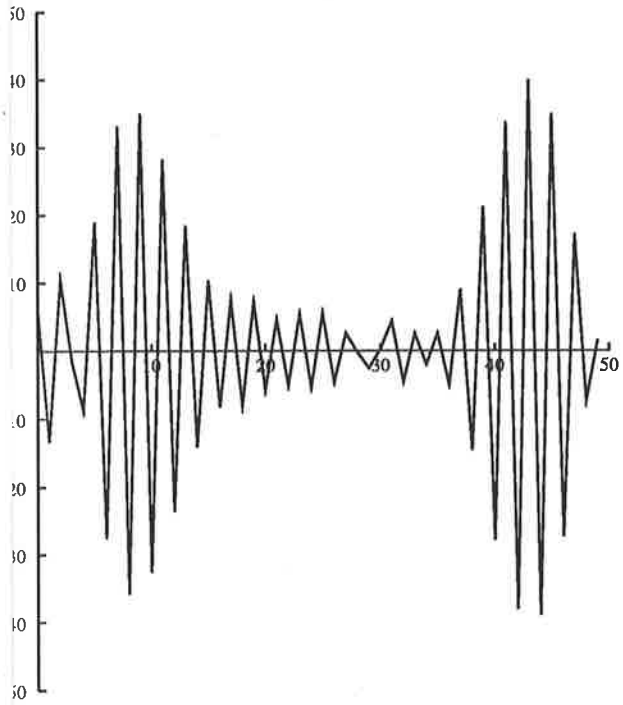


Figure 5.18: Autocorrelation of the interpolated trace.

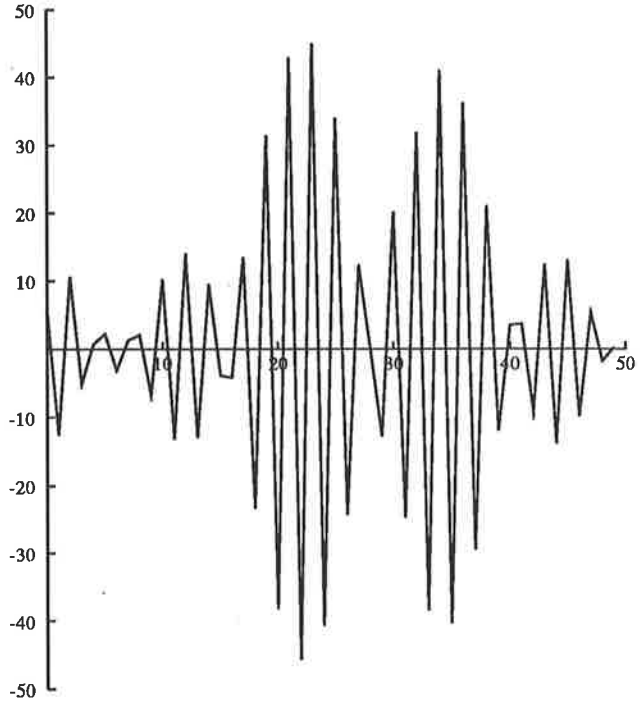
condition numbers of the autocorrelation matrices of order 50 have been computed to a value of 2.138×10^4 for the original trace, and to a value of 1.012×10^{11} for its interpolated counterpart. The relatively small value of the condition number in the uninterpolated case means that it may be considered relatively well-conditioned, and little error would be expected in computed prediction filters. This is, in fact, what occurs. For this reason, this section focuses exclusively on prediction filters obtained for the interpolated trace.

5.4.1 Prediction filters

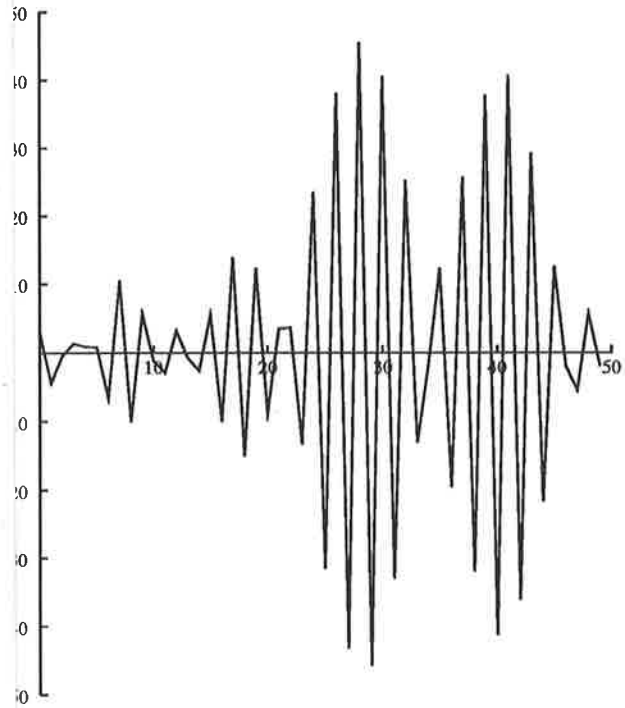
Prediction filters of length 50 elements have been computed for a prediction distance of 12 milliseconds, corresponding to 6 sampling increments. Computed prediction filters for the different approaches are illustrated in Figure 5.19 and summary statistics are presented in Table 5.10. It may be observed that, in this example, the Wiener-Levinson algorithm has



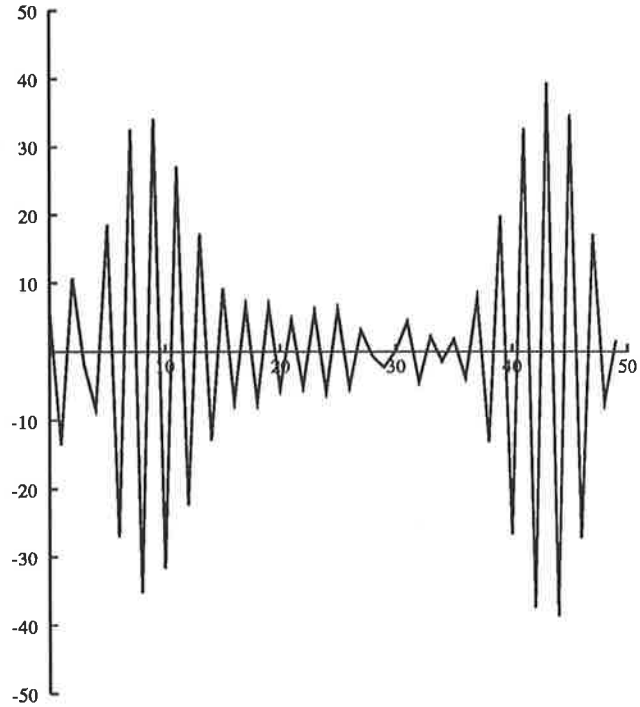
Double precision solution.



Wiener-Levinson Algorithm.



Conjugate Gradient.



Gaussian elimination.

Figure 5.19: Prediction filters produced by different approaches.

produced a filter which exhibits larger error than have the other approaches. The conjugate gradient algorithm has produced a filter which exhibits larger error than has Gaussian elimination, but less error than has the Wiener-Levinson algorithm (compare, for example, filter elements 20 to 30). This is in accordance with observations of Treitel and Wang (1976) but not with results of Section 5.3. The large errors in the prediction filters may be expected to result in poor quality deconvolved outputs, as occurred in Section 5.3.3.

	Algorithm, a			
	Double precision (d)	Gaussian Elimination	Conjugate Gradient	Wiener Levinson
$\|\|\mathbf{f}_a\|\|$	135.0	131.7	154.2	156.0
$\|\|\mathbf{f}_a - \mathbf{f}_d\|\|$	0	5.021	157.3	199.1
$\frac{\|\|\mathbf{f}_a-\mathbf{f}_d\|\|}{\|\|\mathbf{f}_d\|\|}$	0	3.720×10^{-2}	1.165	1.475
$\min f_i$	−38.94	−38.65	−45.71	−45.71
$\max f_i$	39.83	39.37	45.54	44.94

Table 5.10: Summary statistics for prediction filters for the interpolated trace.

5.5 Discussion

Examples have been presented which demonstrate a number of factors which affect conditioning and numerical stability. It has been seen that very small values in a power spectrum, relative to the largest value, may be expected to result in an ill-conditioned autocorrelation matrix. However, a test based on performing a cosine transform on the autocorrelation to obtain a power spectrum may be expected to be of little value because of the behaviour of computed power spectra, which may be attributed to Gibb's phenomenon. Truncation of an autocorrelation series may also be expected to affect a test of this nature.

In the ill-conditioned examples presented, the Wiener-Levinson algorithm and conjugate gradient algorithm produced Wiener filters of much poorer quality than did Gaussian elimination. The poor quality results produced by the Wiener-Levinson algorithm suggest that stability properties of that algorithm are inferior to those of Gaussian elimination.

This demonstrates that the use of the Wiener-Levinson algorithm, in preference to Gaussian elimination, involves a trade-off between computer times (*e.g.* n^2 vs. n^3 arithmetic operations) and accuracy of the solution which may be obtained using Gaussian elimination. In this chapter, solutions obtained by the conjugate gradient scheme were produced by applying n iterations to solve normal equations of order n. Treitel and Wang (1976) applied an error criterion to determine when the conjugate gradient scheme had converged on a solution, obtained convergence after a smaller number of iterations than employed here, and observed that the conjugate gradient scheme had produced solutions exhibiting less error than had the Wiener-Levinson algorithm. In examples presented in this chapter, it was observed that the Wiener-Levinson algorithm may produce filters superior to those produced by the conjugate gradient algorithm, but there is no general guarantee that it will do so. This means that no general statement may be made comparing the errors in solution computed using the Wiener-Levinson algorithm with those computed by the conjugate gradient scheme.

It is interesting to note that the example of Treitel and Wang (1976) was based on a vibroseis cross-correlation which had been interpolated from a 4 millisecond to a 2 millisecond sampling increment for static correction purposes. Results of this chapter and of Treitel and Wang (1976) could be used to suggest that, when a trace is interpolated to a smaller sampling increment, the Wiener-Levinson algorithm may produce Wiener filters which are inferior to those produced by other approaches, such as the conjugate gradient algorithm. However this can not be considered to be a general result, and more numerical experimentation would be warranted in this area.

Prediction error variances, which are produced as intermediate results of the Wiener-Levinson algorithm, may be employed to detect when the Wiener-Levinson algorithm produces Wiener filters exhibiting significant error. Results of this chapter suggest that such a test may be expected to provide a more reliable indication, at insignificant cost, than would a test involving computed power spectra. When error is indicated using prediction error variances, a more reliable algorithm such as Gaussian elimination may be desirable, or a treatment such as prewhitening may be preferred.

Chapter 6

Conditioning of Geostatistical Methods

The determination of kriging or co-kriging weights involves the solution of a set of linear equations. Because a significant number of points (10–25 say) are often used to perform the estimation, some computational approach is often employed to obtain the operator. Consequently, the kriging approach may be susceptible to rounding errors in the solution process. Co-kriging, which uses an even larger coefficient matrix, also may be susceptible to computational error. The major aim of this chapter is to extend discussion of Chapter 4 to apply to ordinary kriging, where the kriging equations are considered to be written in terms of the covariance function. Results for ordinary kriging are extended to apply to co-kriging.

6.1 Robustness

Some attention (*e.g.* Brooker (1977), Cressie and Hawkins (1980), Armstrong (1984), Bardossy (1988), Posa (1989)) has been directed towards the topic of robustness in geostatistics. "Robustness" is a statistical term which, rather ambiguously, refers to insensitivity to small perturbations in data, assumptions, or models (*e.g.* Huber (1982)). Comparing this concept with Definition 3.1, it may be seen that conditioning and robustness are closely

related.

Some approaches and case studies have been presented, in geostatistical literature, which either examine robustness in some sense, or some transformation of data which introduces robustness. Examples include :

- the change in estimation variance introduced by a change in variogram parameters *e.g.* Brooker (1985, 86),
- changes in dispersion variances due to inaccurately modelled semivariograms *e.g.* Brooker (1988)
- the effect of extreme values on the experimental semivariogram *e.g.* Journel (1984), Sullivan (1984),

This section describes one form of robustness, defined by Armstrong and Diamond (1984a), which is based on conditioning of the kriging matrix.

6.1.1 The neighbourhood of a semivariogram

Let $\mathcal{S}$ denote the set of valid semivariogram functions, in the sense that conditions of Section 1.5.6 are satisfied. Also let $\gamma(h) \in \mathcal{S}$ be the function which truly describes some phenomenon of interest, and let $g(h) \in \mathcal{S}$ be a model which has been fitted to an experimental semivariogram in order to characterize that phenomenon. Let $\mathbf{x}$ be the solution vector obtained for $\gamma(h)$ from Equation 1.27, and $\mathbf{\Delta x}$ be the error vector introduced by using the model $g(h)$ instead of the true function $\gamma(h)$.

The relative difference between the true function $\gamma(h)$ and the estimating function $g(h)$ may be written as :

$$\Delta(h) = \left| \frac{\gamma(h) - g(h)}{\gamma(h)} \right|$$

The δ-neighbourhood of the semivariogram function $\gamma(h)$ may be defined as :

$$\mathcal{N}_\delta(\gamma) = \left\{ g \in \mathcal{S} : \left| \frac{\gamma(h) - g(h)}{\gamma(h)} \right| < \delta \quad \forall\, h \right\} \tag{6.1}$$

If the most desirable situation is that the relative error in the solution vector is less than some value ϵ :

$$\frac{||\mathbf{\Delta x}||}{||\mathbf{x}||} \leq \epsilon$$

it is desirable to know the neighbourhood of semivariogram models, $\mathcal{N}_\delta(\gamma)$, in which this will occur. Armstrong and Diamond (1984a) have shown that this neighbourhood is the one for which :

$$\delta \leq \frac{\epsilon}{(2+\epsilon)\kappa(\mathbf{A})} \tag{6.2}$$

where $\mathbf{A}$ is the coefficient matrix for the kriging system and $\kappa(\mathbf{A})$ is its condition number. A larger value of δ represents a larger neighbourhood for which the solution is considered to be valid, and is therefore indicative of a more robust semivariogram model in this sense. It may be seen in Equation 6.2 that a large condition number indicates that the system is more sensitive to error (as would be expected from discussion in Chapter 3), and that the kriging system is less robust in the sense that a small relative error in the semivariogram model can produce a large relative change in the computed kriging operator which is obtained as the solution to Equation 1.22.

In geostatistical practice, models are fitted to experimental semivariograms (or, equivalently, the covariances). This notion of robustness is important—if a fitted model does not adequately describe the phenomenon of interest, results from kriging may not be reliable. The condition number, because it provides a direct (albeit pessimistic) indication of sensitivity of the kriging process to errors, is also an important consideration in a study of robustness. Even if a semivariogram or covariance model is accurately modelled, the respective kriging system may be very sensitive to errors if the condition number is large.

6.2 Kriging

This section focuses attention on the conditioning of kriging matrices which may be obtained when kriging is performed using covariance functions. A number of properties of the kriging matrix are discussed, and the effect of conditioning of the covariance matrix on the kriging matrix is discussed.

6.2.1 Kriging matrices

The coefficient matrix of Equation 1.24 may be written in partitioned matrix form as :

$$\mathbf{K}_c = \left(\begin{array}{c|c} \mathbf{C} & \mathbf{v} \\ \hline \mathbf{v}^T & 0 \end{array}\right) \tag{6.3}$$

where :

- $\mathbf{C}$ is the n by n covariance matrix. Elements of this matrix are values of the covariance function, $C(h)$: $C_{ij} = C(|\mathbf{x}_i - \mathbf{x}_j|)$, where $\mathbf{x}_i$ and $\mathbf{x}_j$ denote locations of data points,
- $\mathbf{v}$ denotes the n-length vector with all elements equal to 1.

In a similar fashion, the coefficient matrix in Equation 1.28, may be written as :

$$\mathbf{K}_\gamma = \left(\begin{array}{c|c} \mathbf{\Gamma} & \mathbf{v} \\ \hline \mathbf{v}^T & 0 \end{array}\right) \tag{6.4}$$

where $\mathbf{\Gamma}$ will be referred to as the "semivariogram matrix". The elements of this matrix are values of the semivariogram function $\gamma(h) = C(0) - C(h)$: $\Gamma_{ij} = \gamma(|\mathbf{x}_i - \mathbf{x}_j|)$. The value $C(0)$ is referred to as the sill.

Under an assumption of stationarity the solutions of Equations 1.24 and 1.28 are identical. This means that the matrices $\mathbf{K}_c$ and $\mathbf{K}_\gamma$ could both be referred to as a kriging matrix. Throughout the remainder of this thesis, unless specified otherwise, the term "kriging matrix" refers to the matrix $\mathbf{K}_c$. The remainder of this chapter considers properties of $\mathbf{K}_c$. It will be observed in Chapter 7 that $\mathbf{K}_\gamma$ exhibits some effects of a similar nature.

6.2.2 Effects of Data Configuration

Using different data configurations to obtain a kriging estimate, assuming a particular semivariogram or covariance model, will affect elements of the kriging matrix, and therefore

affect conditioning. This section introduces some simple considerations which will be applied throughout the remainder of this thesis.

6.2.2.1 The effect of ordering data

Given that n fixed data locations are to be employed to obtain a kriging estimate, one question which may be posed is whether or not changing the order in which data points are employed has any beneficial effect on conditioning. For example, given three data locations in a line at locations $x_1 = 0$, $x_2 = 1$, and $x_3 = 2$, the kriging matrix may be expressed as :

$$\begin{pmatrix} C(0) & C(1) & C(2) & 1 \\ C(1) & C(0) & C(1) & 1 \\ C(2) & C(1) & C(0) & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

where $C(h)$ denotes the covariance function. The question being posed is whether or not any affect on conditioning occurs if the data is ordered differently, for example $x_1' = 1$, $x_2' = 0$, $x_3' = 2$. The kriging matrix which would be obtained with this new ordering is :

$$\begin{pmatrix} C(0) & C(1) & C(1) & 1 \\ C(1) & C(0) & C(2) & 1 \\ C(1) & C(2) & C(0) & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Such different ordering may be applied because different solution algorithms may take advantage of any properties of the coefficient matrix to produce a solution more rapidly. The actual weights produced when solving the linear equations provided by these different orderings will be the same (neglecting effects such as rounding error).

The effect of changing the order in which two data points are employed is mathematically represented as the swapping of respective rows and columns of the kriging matrix. In the above example, rows 1 and 2 are swapped and columns 1 and 2 are swapped. On general kriging matrices, the operation of swapping rows i and j, then columns i and j, may be expressed as :

$$\mathbf{K'}_c = \mathbf{P}^{-1}\mathbf{K}_c\mathbf{P}$$

where $\mathbf{P}$ is a permutation matrix obtained by swapping rows i and j of the identity matrix, $\mathbf{I}$. As noted in Section 2.4.1, such a relationship between $\mathbf{K'}_c$ and $\mathbf{K}_c$ means that both have the same eigenvalues, and therefore the same condition numbers. This means that the spectral condition number is not affected by changing the order of data used to perform the kriging estimate. Therefore any advantages (*e.g.* more rapid solution) offered by an algorithm which requires a special ordering of data are not offset by an effect in which the condition number increases. Any differences in computed kriging weights will be due to properties of respective algorithms, and not because the linear system being solved becomes any more or less ill-conditioned. Additionally, only one possible ordering of data needs to be considered in a discussion of conditioning of kriging matrices.

6.2.2.2 The effect of changing data configuration

Whereas different ordering of data has no effect on the conditioning of kriging matrices, changing the configuration of data may have a more serious effect.

Duplication of data locations results in a singular kriging matrix, having an infinite condition number, because the respective rows/columns are duplicated. Using arguments of continuity, it may then be expected that as data spacing is reduced towards zero, there must eventually be an increase of the condition number. Data which contains some samples which are close to each other may be described as clustered. This means that data containing clusters is more likely to result in an ill-conditioned kriging matrix than is data not containing clusters.

Another important consideration is the effect of adding or removing a data point. It has already been shown than permutations of the data have no effect on conditioning. This means that, without loss of generality, the covariance matrix may be permuted so that a data point to be removed is represented only in the last row and column of the covariance matrix. The covariance matrix obtained after removing this data point is simply a principal sub-matrix of the original. Bunch (1985) used the Cauchy interlace theorem, described by Wilkinson (1965) and Parlett (1980), to show that the spectral condition number of a symmetric, positive definite matrix is at least that of any of its principal submatrices. This

means that the removal of a data point results in an equally ill-conditioned or a less ill-conditioned covariance matrix. It will be shown in Section 6.2.4 that a stationary kriging matrix is at least as ill-conditioned as the corresponding stationary covariance matrix. Therefore the kriging matrix may be expected to become more ill-conditioned as more data is employed to perform the kriging estimate.

6.2.3 Indefiniteness of the Kriging Matrix

Davis and Grivet (1984) observed that the kriging matrix, $\mathbf{K}_c$, is not positive definite, and inferred that this results in numerical instability when solving the kriging equations. The argument employed used the fact that an indefinite matrix has a non-positive eigenvalue, while other eigenvalues are positive, and this was taken to mean that one eigenvalue may be zero, or close to zero, which will result in numerical instability when solving linear equations. However, an observation that an eigenvalue of a matrix is not positive, while other eigenvalues are, is insufficient reason to conclude that any eigenvalue of that matrix is almost zero. If an eigenvalue is not close to zero, the possibility of numerical instability is discounted, unless the solution algorithm being applied is unstable, in the sense of Section 5.2.1, on the class of matrices to which the coefficient matrix belongs. This means that the observation that the kriging matrix is not positive definite is insufficient to explain any observed numerical instability. The fact that an indefinite matrix need not be ill-conditioned is demonstrated by the fact that the condition number of Equation 3.14 is dependent upon the magnitudes of the extreme eigenvalues, and not on their sign.

Posa (1989) has shown that the kriging matrix, $\mathbf{K}_c$, is non-singular and indefinite, with exactly one negative eigenvalue, when the covariance matrix is assumed to be positive definite. The issue of indefiniteness vs. ill-conditioning has also been mentioned by Jiahua and Xinxing (1987). A lack of positive definiteness of a matrix does not imply that it is ill-conditioned, unless the matrix is known in advance to be positive definite, and numerical results indicate otherwise *e.g.* the implementation of the Cholesky Decomposition given by Martin et al. (1971b) assumes a real positive definite symmetric matrix and

indicates an error if this is not true. As the kriging matrix is known to be indefinite, the kriging system can not be solved using algorithms, such as the Cholesky Decomposition, which assume positive definite coefficient matrices.

6.2.4 Conditioning of the Kriging Matrix

By case study Posa (1989) illustrated that the type of semivariogram or covariance model may dramatically affect the conditioning of the kriging matrix. In particular, it was demonstrated that the Gaussian model gives much larger condition numbers than do the exponential or spherical models. This is an indication that properties of the covariance matrix may affect the conditioning of the kriging matrix.

The kriging matrix, $\mathbf{K}_c$, is real, symmetric and indefinite, with one negative eigenvalue. There is no reason, in general, to believe that the negative eigenvalue is the one with either maximum or minimum magnitude, so it is not possible to directly draw conclusions about the conditioning of $\mathbf{K}_c$. However, the matrix $\mathbf{K}_c^2$ is real, symmetric and positive definite as :

$$\lambda_i(\mathbf{K}_c^2) = \lambda_i^2(\mathbf{K}_c)$$

The matrix $\mathbf{K}_c^2$ may be written, as in Section 6.2.1, in partitioned form :

$$\mathbf{K}_c^2 = \left(\begin{array}{c|c} \mathbf{C}^2 + \mathbf{v}^T\mathbf{v} & \mathbf{Cv} \\ \hline \mathbf{v}^T\mathbf{C} & \mathbf{v}^T\mathbf{v} \end{array}\right)$$

where the matrix

$$\mathbf{U} = \mathbf{v}^T\mathbf{v}$$

is simply an n by n matrix in which all elements are unity.

$\mathbf{K}_c^2$ is real, symmetric and positive definite, so the matrix $\mathbf{C}^2 + \mathbf{U}$ must also be positive definite (Bellman (1960)), and the eigenvalues of both these matrices must be real and positive. Applying the Cauchy interlace theorem, described by Wilkinson (1965)

and Parlett (1980), it may be seen that :

$$\begin{aligned} \lambda_{min}(\mathbf{K}_c^2) &\leq \lambda_{min}(\mathbf{C}^2 + \mathbf{U}) \\ \lambda_{max}(\mathbf{K}_c^2) &\geq \lambda_{max}(\mathbf{C}^2 + \mathbf{U}) \end{aligned}$$

from which it may be seen that :

$$\kappa(\mathbf{K}_c^2) \geq \kappa(\mathbf{C}^2 + \mathbf{U}) \tag{6.5}$$

As noted in Section 1.6.1, ordinary kriging may be viewed as an extended form of deconvolution, and the autocorrelation and covariance functions are closely related. As a result of this relationship, the covariance function in one dimension may be expressed as a convolution :

$$C(h) = x(-h) * x(h)$$

where $x(h)$ represents data with zero mean. The autocorrelation of the covariance function may be written as :

$$q(h) = C(-h) * C(h) = x(h) * x(-h) * x(h) * x(-h)$$

Elements of the matrix $\mathbf{C}^2$ are values of the function $q(h)$, in the same fashion as the discrete autocorrelation may be expressed as a matrix multiplication. Applying a Fourier transform, these convolutions may be expressed as multiplications in the frequency domain. These arguments, which apply to one-dimensional data, may be readily extended to apply to more general cases by considering concepts such as multi-dimensional Fourier transforms, described by Bracewell (1978), amongst others.

The matrix $\mathbf{C}^2 + \mathbf{U}$ has elements which are values of the function :

$$q(h) + 1$$

Converting into the frequency domain it may be seen that :

$$q(h) + 1 \leftrightarrow Q(\omega) + \delta(\omega)$$

where :

- $Q(h)$ is the Fourier Transform of $q(h)$ (*i.e.* the square of the spectrum of $x(h)$),
- $\delta(h)$ is the delta, or impulse function, described in Section 4.5.3

Dietrich (1989) notes that, in geostatistical practice, fitted covariance functions are square integrable and monotonically decay towards zero as lag, h, increases. This means that the corresponding spectra also decay towards zero. Therefore, the maximum value of the function $Q(\omega) + \delta(\omega)$ is greater than the maximum value of $Q(\omega)$, while all other values of these functions are identical. Results given in Section 4.1 allow the conclusion that :

$$\kappa(\mathbf{C}^2 + \mathbf{U}) > \kappa(\mathbf{C}^2) \tag{6.6}$$

Combining Equations 6.5 and 6.6 allows the conclusions that the kriging matrix is at least as ill-conditioned as the corresponding stationary covariance matrix :

$$\kappa(\mathbf{K}_c) > \kappa(\mathbf{C}) \tag{6.7}$$

and that an ill-conditioned stationary covariance matrix implies an ill-conditioned kriging matrix.

The observation that an ill-conditioned stationary covariance matrix results in an ill-conditioned kriging matrix means that numerical difficulty may be observed when solving the kriging equations if the covariance matrix is ill-conditioned. From the perspective of robustness, kriging may be expected to be non-robust if the covariance matrix is ill-conditioned.

6.2.5 Conditioning of covariance matrices

Discussion given in Sections 1.6.1 and 6.2.4 means that all results discussed in Chapter 4 may be applied, with some extension, to conditioning of covariance and kriging matrices.

When data is acted upon by a kriging operator to produce a kriged estimate, the kriging operator is applied as a (generalized) convolution process. Kriging, as commonly practiced, introduces two factors not present in deconvolution : the unbias constraint and the fact

that the experimental covariance is fitted with some functional form. This modelling of the covariance (or semivariogram) constrains the type of function employed.

It was noted in Section 6.2.4 that, in geostatistical practice, fitted covariance functions are square integrable and monotonically decay towards zero. This means that the corresponding spectra also decay towards zero. As discussed in Section 4.1, small values in a power spectrum, in comparison with the maximum value, may be expected to result in ill-conditioning of autocorrelation matrices. By analogy, a similar effect may be expected to occur with the covariance matrix. This means that the covariance matrix may be expected to become more ill-conditioned as the spectrum of the covariance function decays more rapidly to zero. Dietrich (1989) considered kriging operators as the discretization of integral operators, and noted that the Fourier transform of a Gaussian function is also a Gaussian function. Therefore, the eigenvalues of the corresponding integrable operator decay exponentially towards zero. Behaviour of this nature may be compared with that which occurs when the kernel of the integral operator is a Green's function (*i.e.* the inverse of a differential operator), in which the eigenvalues can only decay algebraically, as is the case with the spherical model, which occurs in examples of Chapter 7. More information on integral operators is provided by texts such as Anselone (1971), Hochstadt (1973), and Zabreyko et al. (1975).

Extending arguments of Section 4.2 it may be seen that, if a given covariance model is a function which is the covariance of a smooth function Z, in the sense that it may be reasonably approximated with a finite Taylor's series expansion, then the corresponding covariance matrix may expected to be ill-conditioned. This is also indicated by arguments of Dietrich (1989). Another measure of smoothness which could be employed is the derivative of the covariance function at zero lag :

$$\left.\frac{dC(h)}{dh}\right|_{h=0}$$

For example, a Gaussian covariance function may be written in the form :

$$C(h) = e^{-h^2}$$

has a derivative of 0 at $h = 0$, while a spherical covariance function may be written in the form :

$$C(h) = \frac{1}{2}h^3 - \frac{3}{2}h$$

which has a non-zero derivative at $h = 0$. The Gaussian function may be considered to represent a greater degree of smoothness than does the spherical function, in this sense. Therefore, covariance matrices derived from a Gaussian model may be expected to be more ill-conditioned than covariance matrices derived from a spherical model, as will be observed in examples of Chapter 7.

The process of prewhitening of autocorrelation matrices amounts to the addition of uncorrelated white noise. In geostatistical texts, *e.g.* Journel and Huijbregts (1978), the addition of uncorrelated white noise is referred to as the addition of a nugget effect to covariance models. The arguments applied for prewhitening of autocorrelation matrices in Section 4.5 may therefore be applied to account for observations by Dietrich (1989) and Posa (1989) who noted that the presence of a nugget effect results in less ill-conditioned covariance and kriging matrices.

6.3 Co-kriging

In this section, conditioning of co-kriging using two variables will be considered. The coefficient matrix produced in this case, when co-kriging is performed using cross-covariance functions may be expressed as :

$$\mathbf{K}_{ck} = \left(\begin{array}{c|c|c|c} \mathbf{C}_{11} & \mathbf{C}_{12} & \mathbf{v}_{n_1} & \mathbf{0}_{n_1} \\ \hline \mathbf{C}_{12}^T & \mathbf{C}_{22} & \mathbf{0}_{n_2} & \mathbf{v}_{n_2} \\ \hline \mathbf{v}_{n_1}^T & \mathbf{0}_{n_2}^T & 0 & 0 \\ \hline \mathbf{0}_{n_1}^T & \mathbf{v}_{n_2}^T & 0 & 0 \end{array}\right) \tag{6.8}$$

where :

- $\mathbf{v}_n$ denotes a n-length vector whose elements are all unity,
- $\mathbf{0}_n$ denotes a n-length vector whose elements are all zero,
- n_i is the number of samples of variable number i,
- $\mathbf{C}_{ij}$ is the cross-covariance matrix between variables number i and j. The elements of this matrix are written in terms of the corresponding cross-covariance function. The covariance matrices $\mathbf{C}_{ii}$ are in general symmetric and positive indefinite. In all following discussion, unless otherwise stated, the covariance matrices will be assumed positive definite, removing the possibility of singular covariance matrices. The matrices $\mathbf{C}_{ij}$ $i \neq j$ are, in general, rectangular.
- the matrix $\mathbf{K}_{ck}$ will be referred to as the "co-kriging matrix".

The co-kriging matrix may be readily seen to be indefinite, because it has two zero values on the diagonal. The matrix may be permuted to place these values on the upper left of the matrix, in which case the determinants of the 1 by 1 and 2 by 2 principal submatrices

are not positive, violating a condition of positive-definiteness given by Bellman (1960). It must also be noted that the positive definite constraints of Section 1.5.9 imply that the matrix :

$$\left(\begin{array}{c|c} \mathbf{C}_{11} & \mathbf{C}_{12} \\ \hline \mathbf{C}_{12}^T & \mathbf{C}_{22} \end{array}\right)$$

is positive definite.

The co-kriging matrix, $\mathbf{K}_{ck}$, is indefinite. Using arguments similar to those of Section 6.2.4, it may be seen that the matrix :

$$\mathbf{K}_{ck}^2 = \left(\begin{array}{c|c|c|c} \mathbf{C}_{11}^2 + \mathbf{C}_{12}\mathbf{C}_{12}^T + \mathbf{v}_{n_1}\mathbf{v}_{n_1}^T & \mathbf{C}_{11}\mathbf{C}_{12}^T + \mathbf{C}_{12}\mathbf{C}_{22} & \mathbf{C}_{11}\mathbf{v}_{n_1} & \mathbf{C}_{12}\mathbf{v}_{n_2} \\ \hline \mathbf{C}_{12}^T\mathbf{C}_{11} + \mathbf{C}_{22}\mathbf{C}_{12}^T & \mathbf{C}_{12}^T\mathbf{C}_{12} + \mathbf{C}_{22}^2 + \mathbf{v}_{n_2}\mathbf{v}_{n_2}^T & \mathbf{C}_{12}^T\mathbf{v}_{n_1} & \mathbf{C}_{22}\mathbf{v}_{n_2} \\ \hline \mathbf{v}_{n_1}^T\mathbf{C}_{11} & \mathbf{v}_{n_1}^T\mathbf{C}_{12} & n_1 & 0 \\ \hline \mathbf{v}_{n_2}^T\mathbf{C}_{12}^T & \mathbf{v}_{n_2}^T\mathbf{C}_{22} & 0 & n_2 \end{array}\right) \tag{6.9}$$

is positive definite.

The focus of Sections 6.3.1 and 6.3.2 is the case in which all variables are sampled at all locations. Such a scenario is employed in probability kriging, a non-parametric method discussed by Journel (1984), Sullivan (1984) and Isaaks (1984). In this case $n_1 = n_2(= n)$

and the matrix $\mathbf{C}_{12}$ is symmetric. Equation 6.9 may then be rewritten as :

$$\mathbf{K}^2_{ck} = \left(\begin{array}{c|c|c|c} \mathbf{C}_{11}^2 + \mathbf{C}_{12}^2 + \mathbf{U} & \mathbf{C}_{11}\mathbf{C}_{12} + \mathbf{C}_{12}\mathbf{C}_{22} & \mathbf{C}_{11}\mathbf{v} & \mathbf{C}_{12}\mathbf{v} \\ \hline \mathbf{C}_{12}\mathbf{C}_{11} + \mathbf{C}_{22}\mathbf{C}_{12} & \mathbf{C}_{12}^2 + \mathbf{C}_{22}^2 + \mathbf{U} & \mathbf{C}_{12}\mathbf{v} & \mathbf{C}_{22}\mathbf{v} \\ \hline \mathbf{v}^T\mathbf{C}_{11} & \mathbf{v}^T\mathbf{C}_{12} & n & 0 \\ \hline \mathbf{v}^T\mathbf{C}_{12} & \mathbf{v}^T\mathbf{C}_{22} & 0 & n \end{array}\right) \tag{6.10}$$

where $\mathbf{U} = \mathbf{v}\mathbf{v}^T$ is an n by n matrix with all elements unity. Section 6.3.3 extends results of Sections 6.3.1 and 6.3.2 towards more general cases in which all data is not necessarily sampled at all locations.

6.3.1 Intrinsic co-regionalization

Intrinsic coregionalization of two variables may be described as a situation in which :

$$\begin{aligned} \mathbf{C}_{11} &= \mathbf{C} \\ \mathbf{C}_{12} &= k_{12}\mathbf{C} \\ \mathbf{C}_{22} &= k_{22}\mathbf{C} \ (k_{22} > |k_{12}|) \end{aligned}$$

The condition on k_{22} ensures that the positive definiteness conditions of Section 1.5.9 are satisfied. In this case, the matrix $\mathbf{K}^2_{ck}$ may be written as :

$$\mathbf{K}^2_{ck} = \left(\begin{array}{c|c|c|c} (k_{12}^2 + 1)\mathbf{C}^2 + \mathbf{U} & k_{12}(k_{22} + 1)\mathbf{C}^2 & \mathbf{C}\mathbf{v} & k_{12}\mathbf{C}\mathbf{v} \\ \hline k_{12}(k_{22} + 1)\mathbf{C}^2 & (k_{12}^2 + k_{22}^2)\mathbf{C}^2 + \mathbf{U} & k_{12}\mathbf{C}\mathbf{v} & k_{22}\mathbf{C}\mathbf{v} \\ \hline \mathbf{v}^T\mathbf{C} & k_{12}\mathbf{v}^T\mathbf{C} & n & 0 \\ \hline k_{12}\mathbf{v}^T\mathbf{C} & k_{22}\mathbf{v}^T C & 0 & n \end{array}\right) \tag{6.11}$$

This matrix is positive definite, which means that the Cauchy interlace theorem may be applied, as in Section 6.2.4, to show that the condition number of any principal submatrix is at least that of any other principal submatrices of lower order. Therefore it may be concluded that :

$$\kappa(\mathbf{K}_{ck}^2) \geq \kappa\left(\left[k_{12}^2 + 1\right]\mathbf{C}^2 + \mathbf{U}\right)$$

By rearranging rows and columns, it may also be seen that :

$$\kappa(\mathbf{K}_{ck}^2) \geq \kappa\left(\left[k_{12}^2 + k_{22}^2\right]\mathbf{C}^2 + \mathbf{U}\right)$$

Using arguments similar to those of Section 6.2.4 it may therefore be seen that

$$\kappa(\mathbf{K}_{ck}) > \kappa(\mathbf{C})$$

i.e. the co-kriging matrix in this case is at least as ill-conditioned as the covariance matrix of interest.

6.3.2 More general co-regionalizations

It was concluded in the previous section that, when all variables are sampled at all locations and co-regionalization is intrinsic, the coefficient matrix of co-kriging is at least as ill-conditioned as the underlying covariance matrix of interest. Unfortunately, as noted in Section 1.5.7, this case is of little interest in practice because co-kriging produces no more information than does ordinary kriging. In this section, we consider the effect of more general co-regionalizations, still focusing on the scenario in which all variables are sampled at all locations.

The matrix $\mathbf{K}_{ck}$ may be permuted (by changing the location of rows and columns for

the unbias constraint in Equation 6.8) into the form :

$$\mathbf{K}'_{ck} = \left(\begin{array}{c|c|c|c} \mathbf{C}_{11} & \mathbf{v} & \mathbf{C}_{12} & \mathbf{0} \\ \hline \mathbf{v}^T & 0 & \mathbf{0}^T & 0 \\ \hline \mathbf{C}_{12}^T & \mathbf{0} & \mathbf{C}_{22} & \mathbf{v} \\ \hline \mathbf{0}^T & 0 & \mathbf{v}^T & 0 \end{array}\right)$$

which may be expressed more simply as :

$$\mathbf{K}'_{ck} = \left(\begin{array}{c|c} \mathbf{K}_c(1) & \mathbf{A} \\ \hline \mathbf{A} & \mathbf{K}_c(2) \end{array}\right)$$

where $\mathbf{K}_c(i)$ represents the kriging matrix which would be obtained when ordinary kriging is performed on variable i, and $\mathbf{A}$ is given by :

$$\mathbf{A} = \left(\begin{array}{c|c} \mathbf{C}_{12} & \mathbf{0} \\ \hline \mathbf{0}^T & 0 \end{array}\right)$$

Using this representation, it may be seen that :

$$\mathbf{K}'^2_{ck} = \left(\begin{array}{c|c} \mathbf{K}_c^2(1) + \mathbf{A}^2 & \mathbf{K}_c(1)\mathbf{A} \\ \hline \mathbf{A}\mathbf{K}_c(1) & \mathbf{K}_c^2(2) + \mathbf{A}^2 \end{array}\right)$$

Using arguments of Section 6.2.4 it may therefore be seen that :

$$\kappa\left(\mathbf{K}_{ck}^2\right) \geq \kappa\left(\mathbf{K}_c^2(i) + \mathbf{A}^2\right) \quad i = 1, 2 \tag{6.12}$$

These bounds arise because the condition number of a positive definite matrix is at least that of any of its principal sub-matrices. It may be seen that $\mathbf{K}_c^2(1) + \mathbf{A}^2$ may be written in partitioned matrix form as :

$$\left(\begin{array}{c|c} \mathbf{C}_{11}^2 + \mathbf{C}_{12}^2 + \mathbf{U} & \mathbf{C}_{11}\mathbf{v} \\ \hline \mathbf{C}_{11}\mathbf{v}^T & n \end{array}\right)$$

The matrix $\mathbf{K}_c^2(2) + \mathbf{A}^2$ may also be expressed in a similar fashion.

Elements of the cross-covariance matrix, $\mathbf{C}_{12}$, are values of the cross-covariance function. The only difference between the covariance and cross-covariance functions is that the cross-covariance function may either be positive or negative. In all other respects, however, the cross-covariance function has an identical character to a covariance function—it is square integrable in most practical cases and its spectrum decays towards zero. The above partitioned matrix form is independent of the sign of the cross-covariance, and sign of the cross-covariance therefore has no effect on conditioning of the co-kriging matrix.

Minimum and maximum values in the spectra of $\mathbf{C}_{ij}^2$ may be denoted respectively as m_{ij} and M_{ij}. Using results discussed in Section 4.1 for values of the power spectra, it may be seen that :

$$m_{ij} \leq \lambda_{min}\left(\mathbf{C}_{ij}^2\right) \leq \lambda_{max}\left(\mathbf{C}_{ij}^2\right) \leq M_{ij} \tag{6.13}$$

were $\lambda_{min}()$ and $\lambda_{max}()$ denote eigenvalues of minimum and maximum magnitude respectively. As all covariance and cross-covariance models decay towards zero, it may be seen that :

$$m_{11} + m_{12} \leq \lambda_{min}\left(\mathbf{C}_{11}^2 + \mathbf{C}_{12}^2\right) \leq \lambda_{max}\left(\mathbf{C}_{11}^2 + \mathbf{C}_{12}^2\right) \leq M_{11} + M_{12} \tag{6.14}$$

Combining Equations 6.13 and 6.14 it may then be seen that :

$$\kappa\left(\mathbf{C}_{11}^2 + \mathbf{C}_{12}^2\right) \geq \min\left(\kappa\left(\mathbf{C}_{11}^2\right), \kappa\left(\mathbf{C}_{12}^2\right)\right)$$

As $\kappa(\mathbf{M}^2) = \kappa^2(\mathbf{M})$ for any symmetric matrix $\mathbf{M}$, arguments similar to those of Section 6.2.4 may be employed to see that :

$$\kappa\left(\mathbf{K}_{ck}\right) > \min\left(\kappa\left(\mathbf{C}_{11}\right), \kappa\left(\mathbf{C}_{12}\right)\right)$$

Similar considerations may be made concerning the matrix $\mathbf{K}_c^2(2) + \mathbf{A}^2$ to observe that :

$$\kappa\left(\mathbf{K}_{ck}\right) > \min\left(\kappa\left(\mathbf{C}_{22}\right), \kappa\left(\mathbf{C}_{12}\right)\right)$$

which means that the co-kriging matrix is more ill-conditioned than at least one of its component stationary cross-covariance matrices.

The arguments of this section may be readily extended to the case when a larger number of variables are employed to obtain a co-kriging estimate, when all variables are sampled at all locations. In these cases it may be concluded that at least one of the condition numbers of component cross-covariance matrices provides a lower bound for the condition number of the co-kriging matrix.

6.3.3 More general data configurations

In this section the previous assumption that all variables are sampled at all locations is abandoned. In the general case, the covariance matrices $\mathbf{C}_{11}$ and $\mathbf{C}_{22}$ are of different orders, n_1 and n_2, and the matrix $\mathbf{C}_{12}$ is rectangular. However, similar arguments to those of Section 6.3.2 may be applied to show that :

$$\begin{aligned}\kappa\left(\mathbf{K}_{ck}\right) &> \min\left(\kappa\left(\mathbf{C}_{11}\right), \kappa\left(\mathbf{C}_{12}^T\right)\right) \\ \kappa\left(\mathbf{K}_{ck}\right) &> \min\left(\kappa\left(\mathbf{C}_{22}\right), \kappa\left(\mathbf{C}_{12}\right)\right)\end{aligned}$$

which means that properties of all covariance and cross-covariance matrices *and their transposes* affect the conditioning of the co-kriging matrix. The need to refer to transposes of cross covariance matrices arises from the fact, described by Equation 3.11, that the spectral condition number of a general matrix $\mathbf{A}$ is expressed in terms of the eigenvalues of $\mathbf{A}^T\mathbf{A}$.

One additional lower bound on the $\kappa(\mathbf{K}_{ck})$ may be obtained by permuting to place the two last rows and columns of Equation 6.9 in the upper left positions. It may then be seen that :

$$\kappa(\mathbf{K}_{ck}) \geq \sqrt{\frac{\max(n_1, n_2)}{\min(n_1, n_2)}}$$

which means that, if the numbers of samples of different variables are significantly different, conditioning may be affected. This final constraint has little bearing in practice—in order to raise the possibility of significant ill-conditioning or non-robustness of co-kriging the relative numbers of data points must be much larger than would normally be seen in practice. This constraint is included here mainly for completeness.

The constraints of this section may also be extended to apply to cases in which a larger number of variables are used to perform the co-kriging estimation.

6.4 Discussion

It has been shown that the kriging matrix is at least as ill-conditioned as the corresponding stationary covariance matrix. It must be stressed that this result depends on the assumption of covariance models of the type most commonly employed in geostatistical practice—the experimental covariance is modelled as a monotonic decreasing, square integrable function. There is no guarantee that a kriging matrix derived from a more arbitrary covariance matrix will be more ill-conditioned than that covariance matrix. Similar results have been derived for co-kriging matrices. What has not been examined closely in this chapter is the effect of the presence of unbias constraints upon conditioning—the results of this chapter allow only observations relating to effects of properties of the covariance and cross-covariance on conditioning of ordinary kriging and co-kriging.

Properties of covariance and cross-covariance functions/matrices which have been assumed throughout this chapter are :

- functions, which are fitted to experimentally obtained covariances and/or cross-covariances, are square integrable and monotonically decay towards zero,
- covariance matrices are positive definite. Cross-covariance functions/matrices are chosen to ensure that the positive definiteness conditions of Section 1.5.9 are satisfied.

When elements of the coefficient matrices (other than elements introduced by the presence

of unbias constraints) solved in ordinary kriging and co-kriging are values of covariance or cross-covariance functions, properties of these functions affect conditioning of the coefficient matrices in the fashion described in this chapter.

Chapter 7 examines, via numerical experiments, a number of effects of model parameters on conditioning of ordinary kriging, considering cases in which the kriging system is expressed in terms of either covariance or semivariogram functions. Observed behaviour, when semivariogram functions are employed, is of a similar nature to that which occurs when covariance functions are employed. Examples of co-kriging systems are also considered.

Chapter 7

A study in geostatistics

A number of theoretical aspects relating to conditioning of kriging and co-kriging, performed using covariance and cross-covariance functions, were examined in Chapter 6. In this chapter a number of these theoretical aspects are examined via numerical experiment. The experiments also consider the conditioning of kriging and co-kriging performed using semivariogram and cross-variogram functions, which were not examined in Chapter 6.

7.1 Conditioning of Kriging with a Pure Nugget Effect

In Section 6.2.4, it was shown that an ill-conditioned stationary covariance matrix results in an ill-conditioned kriging matrix. In this section, it is demonstrated that this is a sufficient, but not a necessary, condition—the kriging matrix may be ill-conditioned, even if the stationary covariance matrix is not. The conditioning of kriging performed with a

pure nugget effect is considered :

$$\mathbf{K}_c = \begin{pmatrix} c & 0 & \dots & 0 & 1 \\ 0 & c & \dots & 0 & 1 \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & c & 1 \\ 1 & \dots & 1 & 1 & 0 \end{pmatrix}$$

$$\mathbf{K}_\gamma = \begin{pmatrix} 0 & c & \dots & c & 1 \\ c & 0 & \dots & c & 1 \\ \vdots & & \ddots & \vdots & \vdots \\ c & \dots & c & 0 & 1 \\ 1 & \dots & 1 & 1 & 0 \end{pmatrix}$$

where $c > 0$ is referred to as the sill. Results in this section are independent of data configuration (other than assuming that duplication of data is avoided, in which case the above equations do not apply). It is also important to note that the condition number of the covariance matrix obtained from a pure nugget effect is always unity. Thus effects described in this section relate to the effects of scaling the model when the covariance matrix is well-conditioned. Conditioning of the coefficient matrices obtained when kriging, using either covariances or semivariograms, are considered.

To evaluate the eigenvalues of $\mathbf{K}_c$ consider the matrix :

$$\mathbf{K}_c - c\mathbf{I} = \begin{pmatrix} & & & 1 \\ & \phi & & \vdots \\ & & & 1 \\ 1 & \dots & 1 & -c \end{pmatrix}$$

and note that the first n rows are all the vector $(0, 0 \dots, 0, 1)$, where $n > 1$ is the number of data points being used to perform the kriging estimation. It may therefore be seen that $\mathbf{K}_c - c\mathbf{I}$ has rank 2 or, equivalently, $n-1$ of its eigenvalues are zero. Non-zero eigenvalues may be obtained by expanding :

$$(\mathbf{K}_c - c\mathbf{I}) \begin{pmatrix} x_1 \\ \vdots \\ x_{n+1} \end{pmatrix} = \lambda \begin{pmatrix} x_1 \\ \vdots \\ x_{n+1} \end{pmatrix} \ (\lambda \neq 0)$$

to obtain :

$$x_{n+1} = \lambda x_i \quad \forall i = 1 \ldots n$$

$$\sum_{j=1}^{n} x_j - c x_{n+1} = \lambda x_{n+1}$$

It may then be seen that $x_1 = x_2 = \ldots = x_n$ and :

$$\lambda^2 + c\lambda - n = 0$$

and the non-zero eigenvalues of $\mathbf{K}_c - c\mathbf{I}$ are :

$$\frac{-c + \sqrt{c^2 + 4n}}{2}, \frac{-c - \sqrt{c^2 + 4n}}{2}$$

therefore, the eigenvalues of $\mathbf{K}_c$ are :

$$c, \frac{c + \sqrt{c^2 + 4n}}{2}, \frac{c - \sqrt{c^2 + 4n}}{2}$$

where the eigenvalue c is repeated $n - 1$ times.

In a similar fashion, by considering the matrix $\mathbf{K}_\gamma + c\mathbf{I}$, it may be shown that the eigenvalues of $\mathbf{K}_\gamma$ are :

$$-c, \frac{(n-1)c + \sqrt{(n-1)^2 c^2 + 4n}}{2}, \frac{(n-1)c - \sqrt{(n-1)^2 c^2 + 4n}}{2}$$

with the eigenvalue $-c$ being repeated $n - 1$ times.

From the above results, the spectral condition numbers may be written :

$$\kappa(\mathbf{K}_c) = \frac{|\lambda_{max}(\mathbf{K}_c)|}{|\lambda_{min}(\mathbf{K}_c)|} = \begin{cases} \frac{c+\sqrt{c^2+4n}}{2c} & \text{if } c < \sqrt{\frac{n}{2}}. \\ \frac{c^2+2n+c\sqrt{c^2+4n}}{2n} & \text{if } c \geq \sqrt{\frac{n}{2}}. \end{cases}$$

$$\kappa(\mathbf{K}_\gamma) = \frac{|\lambda_{max}(\mathbf{K}_\gamma)|}{|\lambda_{min}(\mathbf{K}_\gamma)|} = \begin{cases} \frac{(n-1)c+\sqrt{(n-1)^2c^2+4n}}{2c} & \text{if } c < 1. \\ \frac{(n-1)^2c^2+2n+(n-1)c\sqrt{(n-1)^2c^2+4n}}{2n} & \text{if } c \geq 1. \end{cases}$$

These condition numbers allow some interesting conclusions :

- for a sill, c, large in comparison with the number of data points, n, the condition numbers of both types of kriging matrix are approximately quadratic with c :

$$\begin{aligned} \kappa(\mathbf{K}_c) &\approx \frac{c^2}{n} \\ \kappa(\mathbf{K}_\gamma) &\approx nc^2 \end{aligned} \tag{7.1}$$

- as the sill decreases to zero, the condition number increases. This may also be readily seen by noting that both $\mathbf{K}_c$ and $\mathbf{K}_\gamma$ are singular for $c = 0$. As eigenvalues of a matrix are continuous functions of its elements, so is the spectral condition number.

In the case being considered here, the covariance matrix is a scaled version of the n by n identity matrix. Therefore, the condition number of the covariance matrix is unity, which, as stated in Section 3.4, is the minimum possible value for a condition number. The results of this section indicate that the presence of the unbias constraint introduces a scaling effect on the spectral condition number, demonstrating that the kriging matrix may be ill-conditioned even when the corresponding stationary covariance matrix is well-conditioned. Similar effects are indicated for coefficient matrices defined in terms of semivariogram functions. This means that kriging is not guaranteed to be robust, even if the covariance matrix is well-conditioned.

7.2 Data configuration to be considered in later sections

The remainder of this chapter is devoted to numerical experiments in kriging and co-kriging. For these purposes, one particular data configuration will be employed, this being illustrated in Figure 7.1. This data configuration consists of 25 points on a square 5 by 5 grid, where the grid spacing is considered to be one unit of distance. In examples which involve solving kriging equations to obtain kriging weights and Lagrange multipliers, it is considered that kriging is being employed to estimate the mean of the block at the centre of the grid (*i.e.* the block is centred on the origin in Figure 7.1).

Two semivariogram model types are considered at various times in this chapter. The first is the spherical function :

$$sph(h) = \begin{cases} 0 & h = 0 \\ c_0 + c_1 \left(\frac{3}{2}\frac{h}{a} - \frac{1}{2}\left(\frac{h}{a}\right)^3 \right) & 0 < h \leq a \\ c_0 + c_1 & h > a \end{cases} \tag{7.2}$$

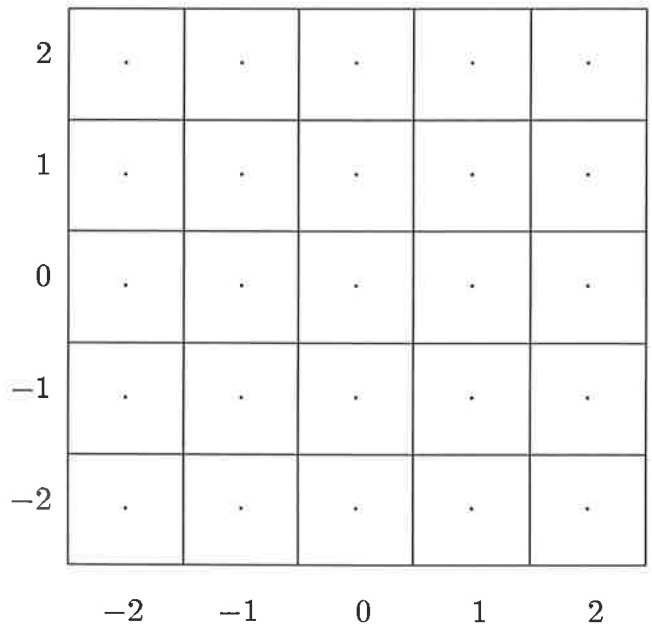


Figure 7.1: Data configuration employed in examples.

where :

- a represents the range,
- c_0 represents the nugget effect,
- $c = c_0 + c_1$ represents the sill,
- $\frac{c_0}{c}$ represents the relative nugget,
- the corresponding covariance function is $sph_c(h) = c - sph(h)$.

The second function considered is the Gaussian :

$$gauss(h) = \begin{cases} 0 & h = 0 \\ c_0 + c_1 \left(1 - e^{-(h/a)^2}\right) & h > 0 \end{cases} \tag{7.3}$$

These equations define semivariogram functions of interest, which will be used to define elements of semivariogram and covariance matrices.

Examples in co-kriging are restricted to the scenario in which two variables are being employed to perform the co-kriging estimate, and both variables are sampled at all locations of Figure 7.1. Co-kriging weights and Lagrange multipliers are computed. For simplicity, the data sets are indexed 1 and 2, where data set number 1 is the data set being estimated using the co-kriging process (*i.e.* variable k_0 in Section 1.5.7) and data set number 2 is being used to provide more information for the purposes of performing the co-kriging estimation. Parameters, such as cross-variogram models/matrices and Lagrange multipliers, are indexed in a similar fashion *e.g.* the covariance matrix for data set number 1 will be referred to as $\mathbf{C}_{11}$ and the cross-covariance matrix between the two data sets referred to as $\mathbf{C}_{12}$. This notation is consistent with that employed in discussion of Section 6.3.

7.3 The effect of model parameters

In this section, spherical semivariogram models, having a range not greater than ten sampling units, are considered. Posa (1989) has demonstrated that the spherical function results in relatively well-conditioned kriging matrices, in comparison with other models such as the Gaussian. It may then be concluded that effects observed in this section are an extension of results of Section 7.1.

A graph of $\kappa(\mathbf{K}_c)$ vs. sill is given in Figure 7.2. The semivariogram function has a range of two units, and no nugget effect (*i.e.* $c_0 = 0$). Similar effects are observed when models with different range and relative nugget values are considered. It may be observed that the condition number is approximately quadratic with sill, as was seen in Section 7.1. The observed behaviour of $\kappa(\mathbf{K}_\gamma)$ is similar to that of $\kappa(\mathbf{K}_c)$.

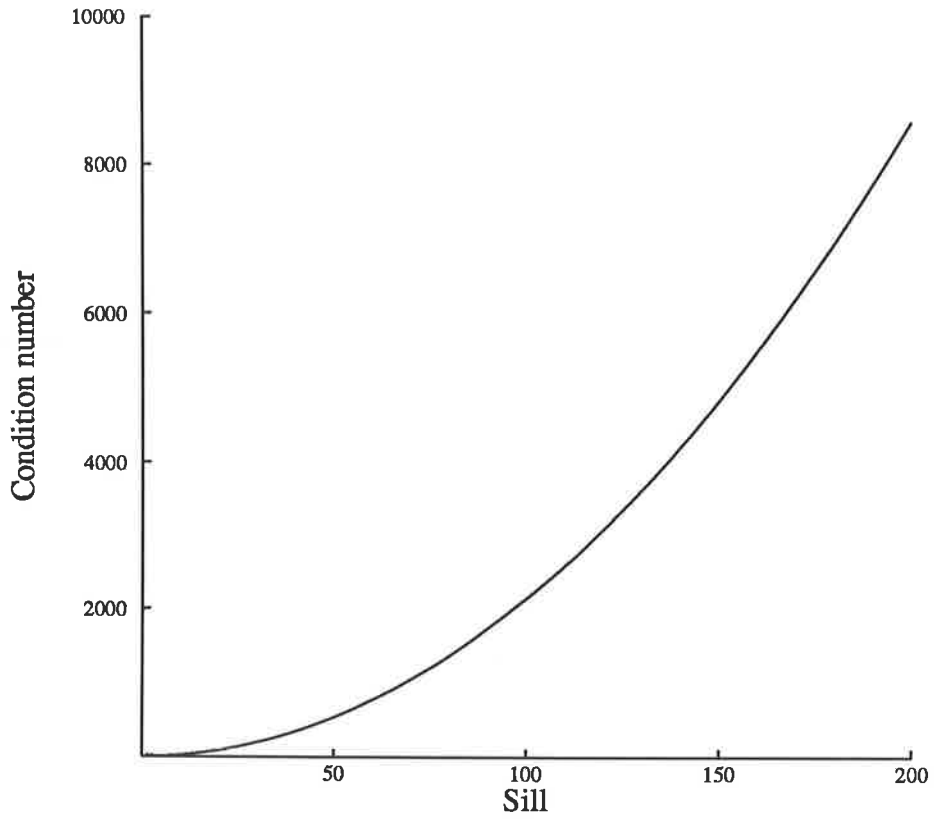


Figure 7.2: $\kappa(\mathbf{K}_c)$ vs. sill ($a = 2, c_0 = 0$).

In Figure 7.3, the focus is placed on smaller values of sill, and it may be seen that $\kappa(\mathbf{K}_c)$ increases sharply as the sill approaches zero, as was found in Section 7.1 *i.e.* extremely small values of sill result in a ill-conditioned kriging system. Again, the observed behaviour of $\kappa(\mathbf{K}_\gamma)$ is similar to that of $\kappa(\mathbf{K}_c)$.

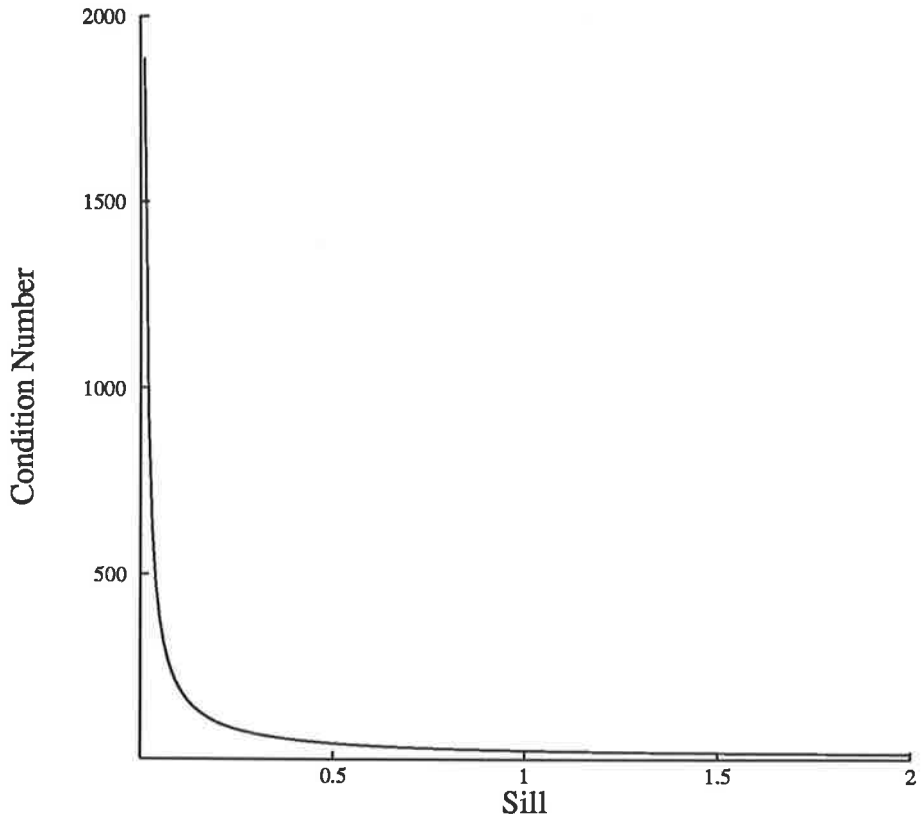


Figure 7.3: $\kappa(\mathbf{K}_c)$ vs. sill for small sill values ($a = 2, c_0 = 0$).

The effects of range and relative nugget on $\kappa(\mathbf{K}_c)$ are illustrated in Figure 7.4. It may be seen that $\kappa(\mathbf{K}_c)$ decreases with relative nugget and increases with range. Similar behaviour is exhibited at different sill values, although the magnitude of values changes markedly.

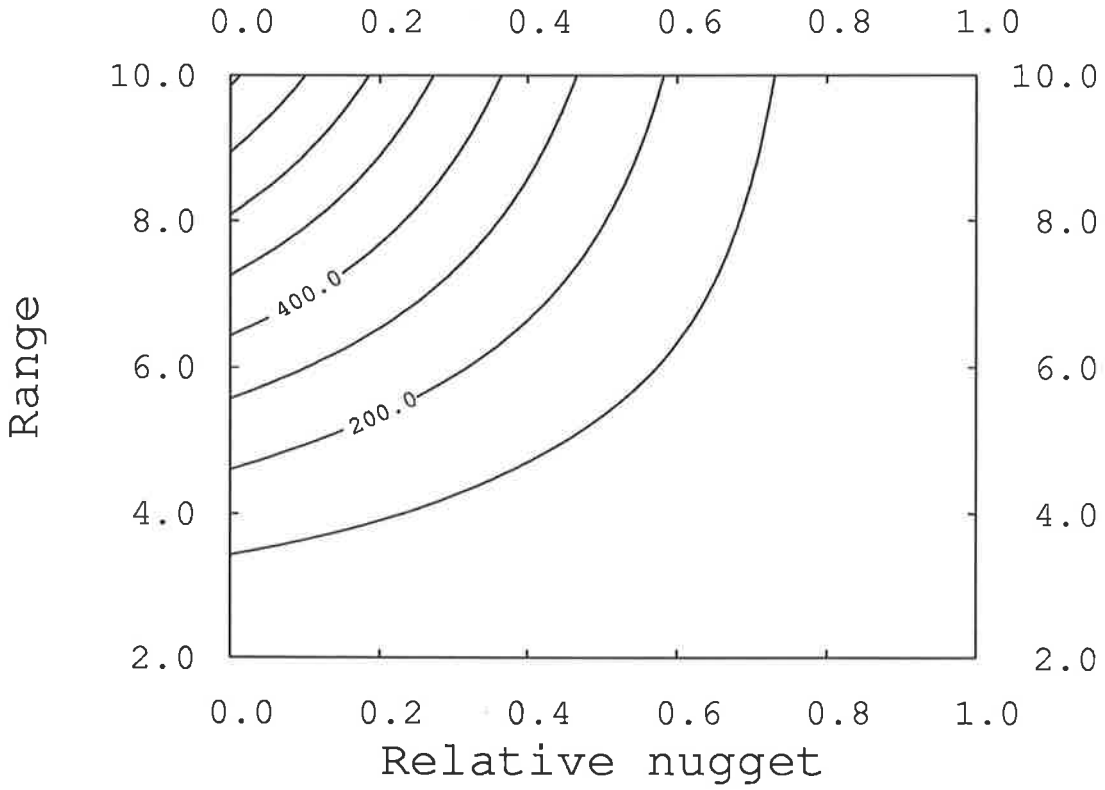


Figure 7.4: $\kappa(\mathbf{K}_c)$ vs. range and relative nugget (sill=10).

As seen in Figure 7.5, when the sill value is 1, $\kappa(\mathbf{K}_\gamma)$ behaves similarly to $\kappa(\mathbf{K}_c)$—it increases with range and decreases with relative nugget. However, when the sill is larger, as in Figure 7.6, this effect is reversed *i.e.* $\kappa(\mathbf{K}_\gamma)$ decreases with range and increases with relative nugget. This effect illustrates the strong scaling effect on the condition number introduced by changing the sill value.

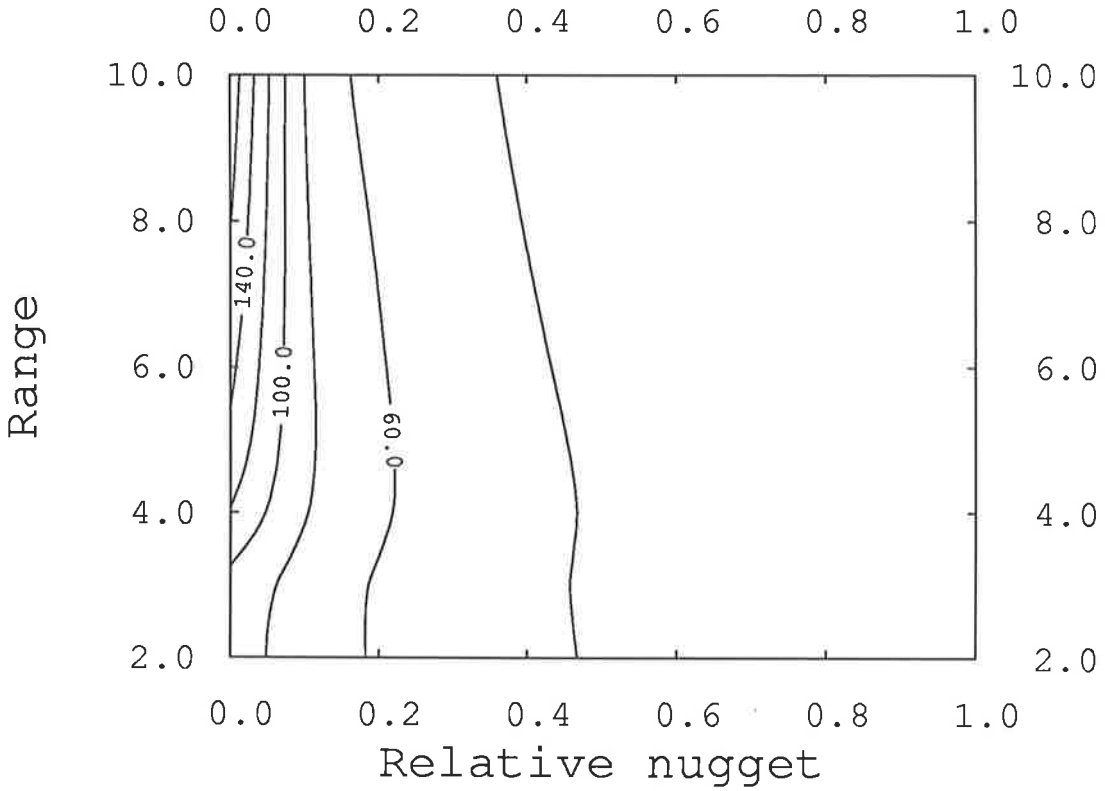


Figure 7.5: $\kappa(\mathbf{K}_\gamma)$ vs. range and relative nugget (sill=1).

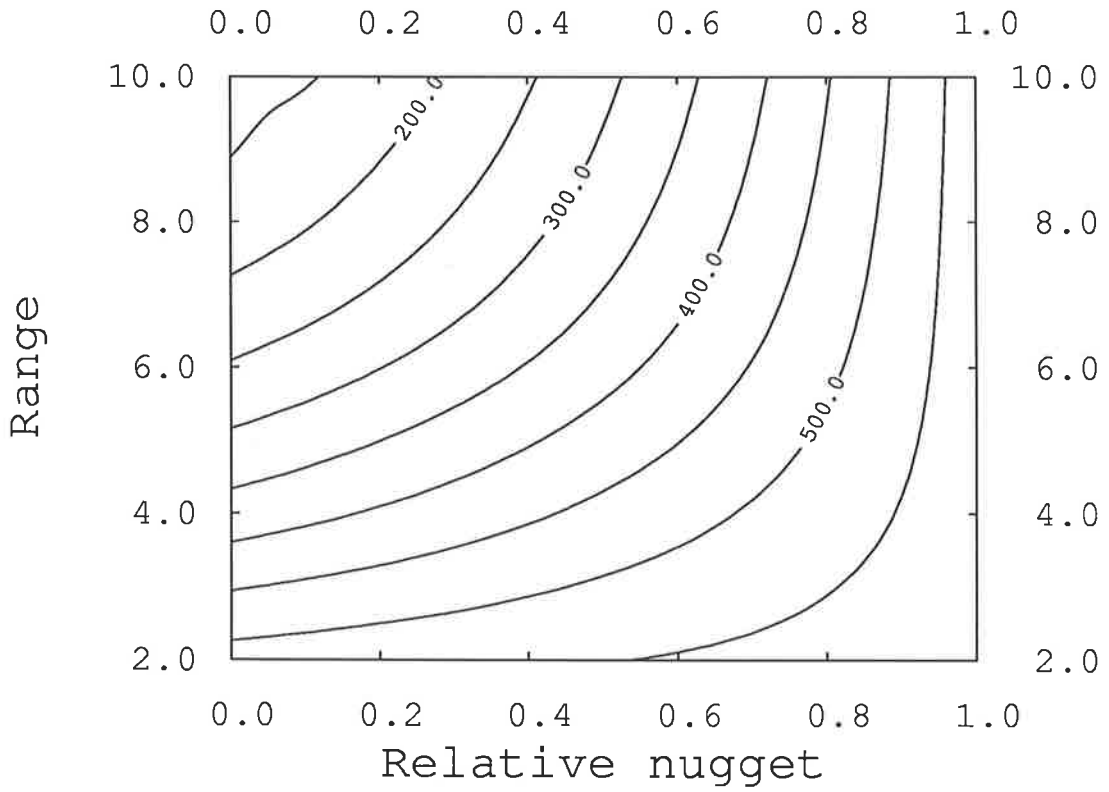


Figure 7.6: $\kappa(\mathbf{K}_\gamma)$ vs. range and relative nugget (sill=5).

In addition, the bounds :

$$\kappa(\mathbf{K}_c) \leq 10c^2$$
$$\kappa(\mathbf{K}_\gamma) \leq 25c^2$$

were observed for all values of relative nugget in $[0, 1]$ when the range was less than 10 units and the sill, c, was at least 1. This suggests that the value nc^2 given in Equation 7.1 is an upper bound for both $\kappa(\mathbf{K}_c)$ and $\kappa(\mathbf{K}_\gamma)$ for spherical models with range not exceeding 10 units.

From the preceding results, it may be seen that the spectral condition numbers of kriging matrices, derived from a spherical model, and written in terms of either covariance or semivariogram functions, are dependent primarily on sill. A "large" condition number

implies possible non-robustness or numerical instability when solving the kriging system. This means that it is desirable to avoid large condition numbers. Large condition numbers may be avoided by a simple scaling. There are two possible approaches. The first is to scale the model, to make the condition number small enough to avoid difficulty. For example, most computers provide floating point values in single precision with six to eight decimal places (or, more precisely, about 20 to 30 binary places), which means that a condition number of the order of 10^6 to 10^8 may be interpreted as an indication of ill-conditioning (*e.g.* Appendix A). Scaling the spherical model so that it has a sill value in the range 1 to $1000/\sqrt{n}$ will reduce the condition number to tractable levels, when spherical semivariogram models with range not exceeding 10 units are employed. By noting that the sill effect is equivalent to the variance of the data, it may be seen that this treatment has the same effect as scaling the data. Scaling the covariance or semivariogram model so it has a sill of 1 is equivalent to expressing the kriging system in terms of the correlogram function, described by Journel and Huijbregts (1978), rather than the covariance function.

The second approach is to replace the 1's of Equations 1.24 and 1.28 by a value, β, such that the ratio of β to the sill value is within the range $0.001\sqrt{n}$ to 1. The coefficient matrices produced by this approach differ from those produced in the previous paragraph only by a scale factor.

A large condition number (for discussion here, greater than about 10^6) implies only the possibility of numerical instability. Scalings described here ensure that this possibility is removed without resorting to the more expensive approach of working in higher precision. The above approaches will have an effect on the computed kriging weights, or the Lagrange multiplier, unless similar changes are made to the vector on the right hand sides of the linear equations. The scalings given here assume a regular data configuration, and a spherical model with a range not exceeding 10 units. It will be seen in Section 7.4 that large values of range, or close spacing of the data, have a significant additional effect on conditioning which the scaling procedure given here may not totally remove. Scaling effects, of a similar nature to those discussed here, may be expected to have beneficial effects relating to conditioning when different semivariogram models (*e.g.* a Gaussian function), or more

general data configurations, are employed.

As noted in Section 5.2.1 a large condition number does not necessarily imply numerical instability because properties of a solution algorithm must be taken into account. This means that effects introduced by changing the sill of a covariance model, which can result in a large condition number, will not necessarily affect the accuracy of the computed kriging weights or Lagrange multiplier.

Past case studies in geostatistical robustness (*e.g.* Brooker (1985), Posa (1989)) have assumed models with a fixed sill value and have examined the effect of changing other model parameters. The results of this section and Section 7.1 indicate that values of sill have a dramatic effect on condition number of the respective coefficient matrices. This in turn implies the *possibility* of non-robustness.

The effects observed here may be related directly to optimal scaling, which is discussed, amongst others, by Bauer (1963), Evans and Hatzopoulos (1979). Essentially, an optimal scaling involves multiplying rows or columns by constants chosen in such a fashion as to obtain a relatively small condition number. Elements of the solution vector obtained after such a scaling procedure differ from those of the unscaled solution by only a scale factor. Scaling procedures are easily applied to linear systems because they involve only a trivial transformation of the coefficient matrix.

7.4 The effect of data spacing in kriging

This section focuses on the observation made in Section 6.2.2.2 that close spacing of data may result in ill-conditioning of both $\mathbf{K}_c$ and $\mathbf{K}_\gamma$. An alternative approach is to fix the range and examine the effect of data spacing. This alternative means that behaviour which occurs when the range of a spherical model is large, and data spacing is fixed at one unit, provides information about behaviour when data spacing is small for a fixed range. In Section 6.2.2.2 it was noted small data spacings may be expected to result in ill-conditioned kriging matrices. This in turn means that it may be expected that $\kappa(\mathbf{K}_c)$ and $\kappa(\mathbf{K}_\gamma)$ will exhibit an increase with range, when the data spacing remains at one unit.

In Figure 7.7, $\kappa(\mathbf{K}_c)$ is plotted as a function of range of a spherical function for larger range values than those considered previously. It may be seen that, for large range, $\kappa(\mathbf{K}_c)$ increases approximately linearly with range. A similar behaviour is exhibited by $\kappa(\mathbf{K}_\gamma)$. This means that values of range which are large in comparison with the data spacing result in a large condition number, and illustrates arguments of Section 6.2.2.2. The contradiction of these results with those of Figure 7.6, where $\kappa(\mathbf{K}_\gamma)$ decreases with range, appears to be attributable to the behaviour of $\kappa(\mathbf{K}_\gamma)$ with sill. The behaviour demonstrated here is a limiting effect, and the interaction of values of sill and relative nugget may cause the conclusions here not to hold for certain choices of model parameters.

It should be noted that the values of range studied in this section are extremely high in comparison with data spacing and, as such, would generally be unrealistic in practice.

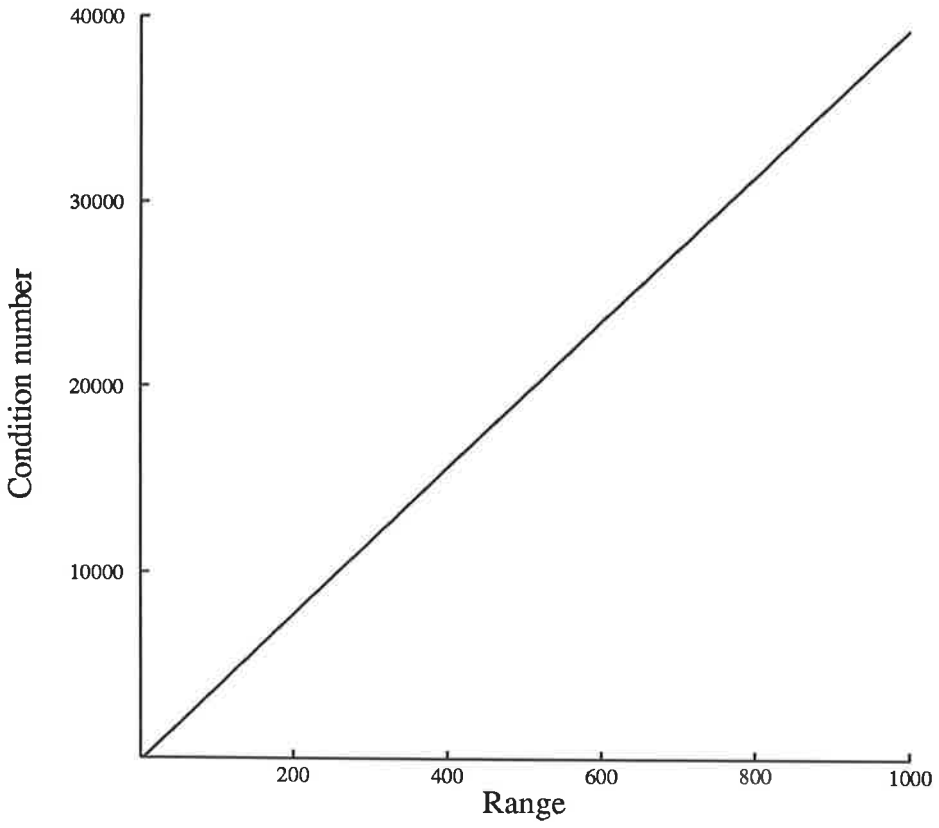


Figure 7.7: $\kappa(\mathbf{K}_c)$ vs. range for large range values ($c = 1, c_0 = 0$).

They are presented here because they provide a simple means of examining some effects of data spacing on conditioning. A large range in a semivariogram model is representative of a smoother set of data values than is a smaller range. Therefore, these results are consistent with those of Section 6.2.5.

7.5 When is conditioning of kriging matrices important ?

Observations so far indicate that ill-conditioning of kriging matrices may be caused by :

- an ill-conditioned covariance matrix.
- a "scaling effect" introduced by the presence of the unbias constraint. This effect can result in an ill-conditioned kriging matrix, even when the covariance matrix is well-conditioned.

A question which may now be posed is : When do any of these effects influence accuracy of computed kriging weights, the Lagrange multiplier, or any other quantity computed from them? In previous discussion, conclusions were drawn assuming that a large condition number results in numerical instability and/or a non-robust kriging system. However, it has been noted in Chapter 5 that properties of the solution algorithm must be considered when determining whether or not a large condition number results in numerical instability, whilst in Section 6.1 it has been noted that the condition number provides only an upper bound as a measure of robustness.

In examples which follow, Gaussian elimination with pivoting is employed to solve the kriging equations. This means that a small condition number excludes the possibility of large errors in the computed solution, and large errors in a computed solution may arise when the condition number is large. The purpose here is to determine cases in which Gaussian elimination produces significant error, as measured in terms of error norms, in the solution vector, which incorporates both the desired kriging operator and the Lagrange multiplier.

Table 7.1 compares the quantities obtained from the kriging equations when the sill of a spherical variogram model is varied, and relative nugget and range are kept constant. The kriging equations solved here were those in which elements of the kriging matrix and right hand side vector were written in terms of semivariogram values (*i.e.* these results are numerical solutions of Equation 1.28). Results of a similar nature are also observed for the solution of kriging equations written in terms of covariance values. It may be observed that the quantities computed using Gaussian elimination, with the sill values considered exhibit little visual difference from the corresponding double precision solutions. This observation also applies to quantities $||\mathbf{e}||/||\mathbf{x}||$ which are reported in this table. The vectors $\mathbf{e}$ and $\mathbf{x}$ are defined as follows :

- $\mathbf{x}$ denotes the solution of Equation 1.28, computed using double precision,
- if $\mathbf{x}_s$ denotes the solution of Equation 1.28 computed using single precision, then $\mathbf{e} = \mathbf{x} - \mathbf{x}_s$.

In this fashion, the quantity $||\mathbf{e}||/||\mathbf{x}||$ denotes a relative error, in terms of norms, with respect to the double precision solution.

The kriging solutions presented in Table 7.1 exhibit little error for all sill values shown, in spite of the fact that the condition numbers corresponding to both the small and large sill values are much larger than that obtained when the sill is one. Because of the data configuration, illustrated in Figure 7.1, it may also be expected that the values of the kriging weights, $w(i,j)$, chosen to correspond to locations (i,j) in Figure 7.1, would show symmetry relations of the form $w(i,j) = w(|i|,|j|) = w(|j|,|i|)$. This symmetry is observed in this example, apart from slight changes in the last reported significant figure in the single precision solutions. The value of the Lagrange multiplier is affected by a scaling due to different sill values.

Table 7.2 presents kriging weights and Lagrange multipliers computed by kriging with a Gaussian semivariogram model. Unlike the spherical function, the Gaussian function can not be analytically integrated. For this reason, the values $\overline{\gamma}(\mathbf{x}_\alpha, R)$ which appear in Equation 1.28 were approximated using a simple numerical integration, in which the region

Zero nugget. Range : 5 $\kappa(\mathbf{\Gamma}) = 124.4$

Double precision results (sill : 1)

−0.002999	−0.004629	−0.007347	−0.004629	−0.002999
−0.004629	0.02611	0.1019	0.02611	−0.004629
−0.007347	0.1019	0.5665	0.1019	−0.007347
−0.004629	0.02611	0.1019	0.02611	−0.004629
−0.002999	−0.004629	−0.007347	−0.004629	−0.002999

Lagrange multiplier : -3.007×10^{-4}

Sill $= 10^{-4}$ $\kappa(\mathbf{K}_\gamma) = 3.780 \times 10^5$

−0.002998	−0.004630	−0.007346	−0.004630	−0.002998
−0.004630	0.02611	0.1019	0.02611	−0.004629
−0.007346	0.1019	0.5665	0.1019	−0.007348
−0.004630	0.02611	0.1019	0.02611	−0.004629
−0.002998	−0.004629	−0.007348	−0.004629	−0.002999

Lagrange multiplier : -3.009×10^{-8} $||\mathbf{e}||/||\mathbf{x}|| = 1.240 \times 10^{-4}$

Sill $= 1$ $\kappa(\mathbf{K}_\gamma) = 134.9$

−0.002999	−0.004629	−0.007346	−0.004629	−0.002999
−0.004629	0.02611	0.1019	0.02611	−0.004629
−0.007347	0.1019	0.5665	0.1019	−0.007346
−0.004623	0.02611	0.1019	0.02611	−0.004629
−0.002999	−0.004629	−0.007346	−0.004629	−0.002999

Lagrange multiplier : -3.007×10^{-4} $||\mathbf{e}||/||\mathbf{x}|| = 1.862 \times 10^{-4}$

Sill $= 10^4$ $\kappa(\mathbf{K}_\gamma) = 1.220 \times 10^9$

−0.002997	−0.004630	−0.007346	−0.004630	−0.002998
−0.004630	0.02611	0.1019	0.02611	−0.004630
−0.007346	0.1019	0.5665	0.1019	−0.007346
−0.004631	0.02611	0.1019	0.02611	−0.004631
−0.002997	−0.004630	−0.007347	−0.004631	−0.002997

Lagrange multiplier : -3.009 $||\mathbf{e}||/||\mathbf{x}|| = 9.246 \times 10^{-4}$

Table 7.1: Effect of sill on computed solutions of kriging equations (spherical semivariogram function).

Zero nugget. Range : 3 $\kappa(\mathbf{\Gamma}) = 2.510 \times 10^7$

Double precision results (Sill : 1)

0.001113	−0.003028	−0.004779	−0.003028	0.001113
−0.003028	0.01087	0.05731	0.01087	−0.0030281
−0.0047789	0.05731	0.7662	0.05731	−0.0047789
−0.0030281	0.01087	0.05731	0.01087	−0.0030281
0.0011126	−0.0030281	−0.0047789	−0.0030281	0.0011126

Lagrange multiplier : 5.570×10^{-5}

Sill $= 10^{-4}$ $\kappa(\mathbf{K}_\gamma) = 1.001 \times 10^{11}$

−0.02232	0.07113	−0.1102	0.07701	−0.02602
0.06652	−0.2091	0.3703	−0.2271	0.07785
−0.09805	0.3526	0.3456	0.3773	−0.1136
0.06446	−0.2030	0.3621	−0.2211	0.07586
−0.02095	0.06710	−0.1048	0.07306	−0.02470

Lagrange multiplier : 1.022×10^{-8} $||\mathbf{e}||/||\mathbf{x}|| = 1.033$

Sill $= 1$ $\kappa(\mathbf{K}_\gamma) = 2.868 \times 10^7$

−0.01008	0.03002	−0.04865	0.02823	−0.008958
0.02937	−0.08419	0.1827	−0.07793	0.02545
−0.04628	0.1782	0.6080	0.1684	−0.04012
0.02474	−0.06936	0.1611	−0.06118	0.01960
−0.006963	0.02008	−0.03421	0.01705	−0.005061

Lagrange multiplier : 6.844×10^{-5} $||\mathbf{e}||/||\mathbf{x}|| = 0.1490$

Sill $= 10^4$ $\kappa(\mathbf{K}_\gamma) = 9.527 \times 10^8$

0.01654	−0.04813	0.05412	−0.04363	0.01361
−0.04921	0.1456	−0.1183	0.1318	−0.04024
0.05651	−0.1210	0.9978	−0.1015	0.04392
−0.04571	0.1345	−0.1024	0.1196	−0.03613
0.01408	−0.04033	0.04294	−0.03513	0.01073

Lagrange multiplier : 0.3698 $||\mathbf{e}||/||\mathbf{x}|| = 0.4708$

Table 7.2: Effect of sill on computed solutions of kriging equations (gaussian semivariogram function).

R was divided into a 16 by 16 grid. The solutions computed using single precision for different sill values show little resemblance to each other. This observation is sufficient to conclude that at least one of these computed solutions exhibits significant error. These solutions may be assessed more rigorously by comparing them to solutions computed using double precision. It may be seen that none of the single precision results closely resemble the corresponding double precision results, and the relative errors, measured in terms of norms, are significantly larger than the relative errors in the example of Table 7.1. This means that, in this case, numerical errors have a significant effect for all sill values. The different behaviours exhibited when kriging using spherical or Gaussian covariance functions has been considered in Section 6.2.5.

These examples illustrate that, when the kriging equations are being solved using Gaussian elimination, the computed solution, which consists of the kriging operator and Lagrange multiplier, does not necessarily exhibit large error if the covariance matrix is well-conditioned, even if the kriging matrix is ill-conditioned due to the sill value. However, when the covariance matrix is ill-conditioned, the effect of sill may become significant. In practice, this gives further support to the conclusion of Posa (1989) who advocated fitting of functions to experimental covariances or semivariograms which result in well-conditioned covariance matrices, in preference to functions which result in ill-conditioned covariance matrices, especially if (as is currently the case in practice) there is no prior information indicating that the function which gives the ill-conditioned covariance matrix is most suitable. The effects given here relate only to Gaussian elimination with pivoting, an algorithm which was noted in Section 5.2 to be one with quite good stability properties. There can be no general guarantee that the effect of sill on condition number will not affect kriging weights if they are computed using a different algorithm, because the type of behaviour described here is dependent upon properties of the respective solution algorithms. Posa (1989) also demonstrated that the use of functions which introduce a nugget effect result in less ill-conditioned kriging matrices than those with no nugget effect, an effect discussed in Section 6.2.5.

7.6 Conditioning of co-kriging

It was seen in Section 6.3 that the minimum value for the condition number of all cross-covariance matrices provides a lower bound for the condition number of the corresponding co-kriging matrix. This effect is analogous to the fashion in which the stationary covariance matrix affects the corresponding kriging matrix. It has been observed previously in this chapter that the presence of unbias constraints in kriging has a significant effect on conditioning of the kriging matrix, but that this effect does not necessarily result in significant error in computed kriging weights or Lagrange multipliers. It may be expected that observed effects in co-kriging will be analogous to those observed for kriging :

1. if *all* covariance or cross-covariance matrices are ill-conditioned, the co-kriging matrix may also be ill-conditioned. However, if at least one is not ill-conditioned, co-kriging may be expected to be substantially less ill-conditioned.

2. scaling effects introduced by unbias constraints may also be expected to occur. Multiplying any of the covariance/cross-covariance models by a constant may be expected to affect the condition number of the co-kriging matrix. However, this effect will not necessarily affect computed co-kriging weights or Lagrange multipliers.

It was observed in Section 6.2.5 that the presence of a nugget effect in the covariance model substantially improves conditioning of the covariance matrix. This means that if any of the (cross-)covariance models exhibit a nugget effect, a substantial improvement in conditioning of co-kriging may be expected. Posa (1989) advocated the modelling of experimental covariances by functions which result in well-conditioned covariance matrices. On the basis of results of Section 6.3, it may be expected that fitting functions to experimental covariance and cross-covariances which result in well-conditioned covariance or cross-covariance matrices will be desirable in co-kriging.

Table 7.3 presents solutions to co-kriging equations in which all semivariogram and cross-variograms are spherical with range 5 units, and no nugget effect. Table 7.4 exhibits corresponding results obtained after the introduction of modest nugget effects to the two

Co-kriging using cross-variograms

Semivariogram and cross-variogram sills : $c_{11} = 100$, $c_{12} = 50$, $c_{22} = 100$

Range of all cross-variograms : 5

Zero nugget effects. $\kappa(\mathbf{\Gamma}) = 124.4$ $\kappa(\mathbf{K}_{ck}) = 2.746 \times 10^5$

Double precision solution

Weights applied to data set #1

-3.000×10^{-3}	-4.628×10^{-3}	-7.348×10^{-3}	-4.628×10^{-3}	-3.000×10^{-3}
-4.628×10^{-3}	2.611×10^{-2}	0.1019	2.611×10^{-2}	-4.628×10^{-3}
-7.348×10^{-3}	0.1019	0.5665	0.1019	-7.348×10^{-3}
-4.628×10^{-3}	2.611×10^{-2}	0.1019	2.611×10^{-2}	-4.628×10^{-3}
-3.000×10^{-3}	-4.628×10^{-3}	-7.348×10^{-3}	-4.628×10^{-3}	-3.000×10^{-3}

Weights applied to data set #2 are all zero

Lagrange multiplier #1 : -3.006×10^2 Lagrange multiplier #2 : -1.503×10^{-2}

Weights applied to data set #1

-2.999×10^{-3}	-4.628×10^{-3}	-7.347×10^{-3}	-4.628×10^{-3}	-2.999×10^{-3}
-4.629×10^{-3}	2.611×10^{-2}	0.1019	2.611×10^{-2}	-4.628×10^{-3}
-7.347×10^{-3}	0.1019	0.5665	0.1019	-7.347×10^{-3}
-4.629×10^{-3}	2.611×10^{-2}	0.1019	2.611×10^{-2}	-4.629×10^{-3}
-2.999×10^{-3}	-4.629×10^{-3}	-7.347×10^{-3}	-4.629×10^{-3}	-2.999×10^{-3}

Weights applied to data set #2

-1.242×10^{-9}	-7.086×10^{-9}	-3.575×10^{-9}	-3.598×10^{-9}	8.597×10^{-9}
0	-1.334×10^{-9}	2.095×10^{-8}	7.743×10^{-9}	-1.297×10^{-8}
0	7.038×10^{-10}	-1.970×10^{-9}	-1.674×10^{-8}	-6.825×10^{-10}
-9.070×10^{-9}	-3.727×10^{-9}	1.468×10^{-8}	0	0
1.012×10^{-8}	-8.783×10^{-9}	2.989×10^{-9}	-4.471×10^{-10}	-3.327×10^{-9}

Lagrange multiplier #1 : -3.007×10^2 Lagrange multiplier #2 : -1.503×10^{-2}

$||\mathbf{e}||/||\mathbf{x}|| = 6.301 \times 10^{-6}$

Table 7.3: Computed solutions of the co-kriging equations (spherical cross-variogram functions, no nugget effects).

Co-kriging using cross-variograms

Semivariogram and cross-variogram sills : $c_{11} = 100$, $c_{12} = 50$, $c_{22} = 100$

Range of all cross-variograms : 5

Relative nugget effects : $c_{0_{11}}/c_{11} = 0.01$, $c_{0_{12}}/c_{12} = 0$, $c_{0_{22}}/c_{22} = 0.01$.

$\kappa(\mathbf{\Gamma}_{11}) = 117.3$, $\kappa(\mathbf{\Gamma}_{12}) = 124.4$ $\kappa(\mathbf{K}_{ck}) = 2.758 \times 10^5$

Double precision solution

Weights applied to data set #1

-3.902×10^{-3}	-4.653×10^{-3}	-6.632×10^{-3}	-4.653×10^{-3}	-3.902×10^{-3}
-4.653×10^{-3}	2.896×10^{-2}	0.1053	2.896×10^{-2}	-4.653×10^{-3}
-6.632×10^{-3}	0.1053	0.5424	0.1053	-6.632×10^{-3}
-4.653×10^{-3}	2.896×10^{-2}	0.1053	2.896×10^{-2}	-4.653×10^{-3}
-3.902×10^{-3}	-4.653×10^{-3}	-6.632×10^{-3}	-4.653×10^{-3}	-3.902×10^{-3}

Weights applied to data set #2

4.479×10^{-4}	-6.422×10^{-6}	-3.780×10^{-4}	-6.422×10^{-6}	4.479×10^{-4}
-6.422×10^{-6}	-1.391×10^{-3}	-1.568×10^{-3}	-1.391×10^{-3}	-6.422×10^{-6}
-3.780×10^{-4}	-1.567×10^{-3}	1.160×10^{-2}	-1.567×10^{-3}	-3.780×10^{-4}
-6.422×10^{-6}	-1.391×10^{-3}	-1.567×10^{-3}	-1.391×10^{-3}	-6.422×10^{-6}
4.479×10^{-4}	-6.422×10^{-6}	-3.780×10^{-4}	-6.422×10^{-6}	4.479×10^{-4}

Lagrange multiplier #1 : -4.763×10^{-2} Lagrange multiplier #2 : -1.462×10^{-2}

Single precision : Gaussian elimination, pivoting on maximum element.

Weights applied to data set #1

-3.903×10^{-3}	-4.653×10^{-3}	-6.632×10^{-3}	-4.653×10^{-3}	-3.902×10^{-3}
-4.653×10^{-3}	2.896×10^{-2}	0.1053	2.896×10^{-2}	-4.652×10^{-3}
-6.632×10^{-3}	0.1053	0.5424	0.1053	-6.633×10^{-3}
-4.653×10^{-3}	2.896×10^{-2}	0.1053	2.896×10^{-2}	-4.653×10^{-3}
-3.902×10^{-3}	-4.652×10^{-3}	-6.633×10^{-3}	-4.652×10^{-3}	-3.902×10^{-3}

Weights applied to data set #2

4.485×10^{-4}	-7.041×10^{-6}	-3.777×10^{-4}	-7.073×10^{-6}	4.486×10^{-4}
-7.157×10^{-6}	-1.390×10^{-3}	-1.567×10^{-3}	-1.390×10^{-3}	-7.209×10^{-6}
-3.777×10^{-4}	-1.567×10^{-3}	1.160×10^{-2}	-1.567×10^{-3}	-3.775×10^{-4}
-6.996×10^{-6}	-1.390×10^{-3}	-1.567×10^{-3}	-1.390×10^{-3}	-7.087×10^{-6}
4.485×10^{-4}	-7.244×10^{-6}	-3.775×10^{-4}	-7.098×10^{-6}	4.485×10^{-4}

Lagrange multiplier #1 : -4.762×10^{-2} Lagrange multiplier #2 : -1.462×10^{-2}

$||\mathbf{e}||/||\mathbf{x}|| = 1.438 \times 10^{-5}$

Table 7.4: Computed solutions of the co-kriging equations (spherical cross-variogram functions, moderate nugget effects).

semivariogram models. It may be observed that, in both these examples, the single precision solutions show a strong resemblance to their double precision counterparts and relative errors in terms of norms, denoted by $||e||/||x||$ are small.

The addition of nugget effects has had little effect on the weights applied to data set number 1, but the weights which apply to data set number 2 have changed substantially. This change is not a result of ill-conditioning. Employing spherical cross-variogram models, which all have no nugget effect, means that intrinsic coregionalization, described in Section 1.5.7, occurs. In the scenario being considered, in which all variables are sampled at all locations, this means that co-kriging provides no more information than would ordinary kriging because the weights being applied to data set number 2 are zero. The computed weights for data set number 2, computed using single precision, are extremely small, and may be considered as (machine) zero. The addition of moderate nugget effects to the two semivariogram models being considered in this example means that intrinsic coregionalization no longer occurs, and weights which apply to data set number 2 are no longer zero.

Table 7.5 illustrates co-kriging weights and Lagrange multipliers obtained using single precision when all semivariogram and cross-variogram models are Gaussian functions with range 3 and no nugget effect, meaning that coregionalization is intrinsic in this case. It is interesting to note that there is little apparent similarity between results produced by solving the co-kriging equations using two different variants of Gaussian elimination. This means that conditioning of the coefficient matrix, in this case, results in significant error in at least one of these computed solutions. Comparing relative errors, in terms of norms, of these single precision solutions with the double precision results illustrated in Table 7.6, it may be seen that the results computed using Gaussian elimination with pivoting on the maximum element exhibits significantly less error than those computed using Gaussian elimination with pivoting of the first non-zero element.

Semivariogram and cross-variogram sills : $c_{11} = 100$, $c_{12} = 50$, $c_{22} = 100$
Range of all cross-variograms : 3

Co-kriging using cross-variograms

$\kappa(\mathbf{\Gamma}) = 2.510 \times 10^{7}$ $\kappa(\mathbf{K}_{ck}) = 7.577 \times 10^{7}$

.....

Algorithm : Gaussian elimination, pivoting on maximum element.

Weights applied to data set #1

9.085×10^{-3}	-2.710×10^{-2}	2.790×10^{-2}	-2.685×10^{-2}	8.928×10^{-3}
-2.664×10^{-2}	8.202×10^{-2}	-3.924×10^{-2}	8.124×10^{-2}	-2.615×10^{-2}
2.711×10^{-2}	-3.875×10^{-2}	0.8965	-3.765×10^{-2}	2.642×10^{-2}
-2.646×10^{-2}	8.146×10^{-2}	-3.844×10^{-2}	8.063×10^{-2}	-2.593×10^{-2}
8.964×10^{-3}	-2.673×10^{-2}	2.737×10^{-2}	-2.644×10^{-2}	8.782×10^{-3}

Weights applied to data set #2

1.329×10^{-7}	-4.246×10^{-7}	6.110×10^{-7}	-4.714×10^{-7}	1.627×10^{-7}
-4.268×10^{-7}	1.352×10^{-6}	-1.931×10^{-6}	1.480×10^{-6}	-5.089×10^{-7}
6.118×10^{-7}	-1.925×10^{-6}	2.734×10^{-6}	-2.084×10^{-6}	7.126×10^{-7}
-4.687×10^{-7}	1.467×10^{-6}	-2.072×10^{-6}	1.570×10^{-6}	-5.341×10^{-7}
1.609×10^{-7}	-5.022×10^{-7}	7.057×10^{-7}	-5.317×10^{-7}	1.797×10^{-7}

Lagrange multiplier #1 : 3.825×10^{-3} Lagrange multiplier #2 : 1.193×10^{-3}

$||\mathbf{e}||/||\mathbf{x}|| = 0.2459$

.....

Algorithm : Gaussian elimination, pivoting on first non-zero element.

Weights applied to data set #1

0.2449	−0.7643	1.063	−0.8040	0.2704
−0.7374	2.302	−3.162	2.429	−0.8189
0.9815	−3.025	5.105	−3.208	1.099
−0.7056	2.212	−3.048	2.353	−0.7964
0.2234	−0.7028	0.9854	−0.7518	0.2548

Weights applied to data set #2

6.858×10^{-7}	-2.134×10^{-6}	3.009×10^{-6}	-2.295×10^{-6}	7.897×10^{-7}
-2.180×10^{-6}	6.767×10^{-6}	-9.532×10^{-6}	7.257×10^{-6}	-2.498×10^{-6}
3.090×10^{-6}	-9.589×10^{-6}	1.350×10^{-5}	-1.027×10^{-5}	3.532×10^{-6}
-2.335×10^{-6}	7.246×10^{-6}	-1.020×10^{-5}	7.754×10^{-6}	-2.661×10^{-6}
7.884×10^{-7}	-2.451×10^{-6}	3.449×10^{-6}	-2.618×10^{-6}	8.957×10^{-7}

Lagrange multiplier #1 : -3.726×10^{-2} Lagrange multiplier #2 : -1.863×10^{-2}

$||\mathbf{e}||/||\mathbf{x}|| = 11.56$

Table 7.5: Computed solutions of the co-kriging equations (Gaussian cross-variogram functions with no nugget effect).

Weights applied to data set #1

3.443×10^{-3}	-1.010×10^{-2}	4.877×10^{-3}	-1.010×10^{-2}	3.443×10^{-3}
-1.010×10^{-2}	3.231×10^{-2}	2.806×10^{-2}	3.231×10^{-2}	-1.010×10^{-2}
4.877×10^{-3}	2.806×10^{-2}	0.8061	2.806×10^{-2}	4.877×10^{-3}
-1.010×10^{-2}	3.231×10^{-2}	2.806×10^{-2}	3.231×10^{-2}	-1.010×10^{-2}
3.443×10^{-3}	-1.010×10^{-2}	4.877×10^{-3}	-1.010×10^{-2}	3.443×10^{-3}

Weights applied to data set #2 are all zero.

Lagrange multiplier #1 : 5.156×10^{-3} Lagrange multiplier #2 : 2.578×10^{-3}

Table 7.6: Double precision counterparts of Table 7.5.

It is also of interest to note that changing the sills of the Gaussian semivariogram functions to $c_{11} = 10^4$ and $c_{22} = 1$, and not changing any other model parameters, causes both Gaussian elimination and Gauss-Jordan elimination, with pivoting on the first non-zero element and working in single precision, to return an error code indicating a zero determinant, and not to produce a solution at all, when elements of the co-kriging matrix are considered to be written in terms of semivariogram and cross-variogram functions. Condition numbers of cross-covariance, cross-variogram, and co-kriging matrices for this example are illustrated in Table 7.7. The condition numbers which occur when $c_{11} = 10^4$ and $c_{22} = 1$ are significantly larger than those which occur when $c_{11} = c_{22} = 100$. In this example, scaling of the models significantly affects the conditioning of coefficient matrices of co-kriging, the quality of computed solutions, and even whether or not different numerical approaches produce any solution.

Model	$\kappa(\mathbf{\Gamma})$	$\kappa(\mathbf{K}_{ck}(\gamma))$	$\kappa(\mathbf{C})$	$\kappa(\mathbf{K}_{ck}(c))$
$c_{11} = 100$, $c_{22} = 100$	2.510×10^7	7.577×10^7	2.664×10^7	7.838×10^7
$c_{11} = 10^4$, $c_{22} = 1$		3.368×10^{11}		3.484×10^{11}

Table 7.7: Effect of sills on conditioning of co-kriging matrices (Gaussian function, range 3, no nugget effects).

Table 7.8 illustrates solutions to the co-kriging equations, obtained using single precision, produced after the introduction of moderate nugget effects to gaussian semivariogram functions of Tables 7.5 and 7.6. Corresponding double precision results are illustrated in Table 7.9. It may be observed that the addition of even these moderate nugget effects has resulted in solutions exhibiting less error than those, illustrated in Tables 7.5 and 7.6, which were computed without a nugget effect. This may be attributed to a significant reduction in the condition number of the co-kriging matrix ($\kappa(\mathbf{K}_{ck})$ has a value of 7.577×10^7 without nugget effects, and 1.972×10^5 after the addition of nugget effects).

It must also be noted that relative errors, in terms of norms, reported in Table 7.8 are significantly larger than those reported in Table 7.3, which considered spherical functions. On the basis of this example, it may be concluded that, from a perspective of numerical accuracy, it is desirable to fit spherical functions to experimental cross-variograms instead of Gaussian functions. This supports a more general conclusion that it is desirable to fit cross-variogram and cross-covariance models which result in well-conditioned cross-covariance matrices in preference to models which result in ill-conditioned cross-covariance matrices. Effects which occur for ordinary kriging were noted in Section 7.5 to be of a similar nature, independently of whether the kriging equations being solved were expressed in terms of covariance or semivariogram functions. In an analogous fashion, similar effects are observed in co-kriging independently of whether elements of the coefficient matrix are expressed in terms of cross-covariance or cross-variogram functions.

Co-kriging using cross-variograms

Semivariogram and cross-variogram sills : $c_{11} = 100$, $c_{12} = 50$, $c_{22} = 100$
Relative nuggets : $c_{0_{11}}/c_{11} = 0.01$, $c_{0_{12}}/c_{12} = 0$, $c_{0_{22}}/c_{22} = 0.01$
Range of all cross-variograms : 3

$\kappa(\mathbf{\Gamma}_{11}) = \kappa(\mathbf{\Gamma}_{22}) = 1273$ $\kappa(\mathbf{\Gamma}_{12}) = 2.510 \times 10^7$ $\kappa(\mathbf{K}_{ck}) = 1.972 \times 10^5$

Algorithm : Gaussian elimination, pivoting on maximum element.

Weights applied to data set #1

5.396×10^{-4}	-2.874×10^{-2}	-1.146×10^{-2}	-2.874×10^{-2}	5.410×10^{-4}
-2.874×10^{-2}	7.664×10^{-2}	0.1676	7.665×10^{-2}	-2.876×10^{-2}
-1.146×10^{-2}	0.1676	0.2967	0.1676	-1.146×10^{-2}
-2.874×10^{-2}	7.664×10^{-2}	0.1676	7.665×10^{-2}	-2.875×10^{-2}
5.416×10^{-4}	-2.874×10^{-2}	-1.146×10^{-2}	-2.874×10^{-2}	5.413×10^{-4}

Weights applied to data set #2

9.739×10^{-3}	-5.287×10^{-3}	5.541×10^{-5}	-5.288×10^{-3}	9.740×10^{-3}
-5.281×10^{-3}	-1.031×10^{-2}	4.620×10^{-3}	-1.030×10^{-2}	-5.281×10^{-3}
4.784×10^{-5}	4.618×10^{-3}	2.585×10^{-2}	4.620×10^{-3}	4.609×10^{-5}
-5.281×10^{-3}	-1.030×10^{-2}	4.619×10^{-3}	-1.030×10^{-2}	-5.280×10^{-3}
9.740×10^{-3}	-5.287×10^{-3}	5.507×10^{-5}	-5.287×10^{-3}	9.739×10^{-3}

Lagrange multiplier #1 : 0.3477 Lagrange multiplier #2 : 0.1455

$||\mathbf{e}||/||\mathbf{x}|| = 7.877 \times 10^{-3}$

Algorithm : Gaussian elimination, pivoting on first non-zero element.

Weights applied to data set #1

5.419×10^{-4}	-2.875×10^{-2}	-1.146×10^{-2}	-2.874×10^{-2}	5.470×10^{-4}
-2.875×10^{-2}	7.665×10^{-2}	0.1676	7.662×10^{-2}	-2.874×10^{-2}
-1.146×10^{-2}	0.1676	0.2967	0.1676	-1.148×10^{-2}
-2.875×10^{-2}	7.665×10^{-2}	0.1676	7.659×10^{-2}	-2.870×10^{-2}
5.524×10^{-4}	-2.876×10^{-2}	-1.145×10^{-2}	-2.873×10^{-2}	5.206×10^{-4}

Weights applied to data set #2

9.735×10^{-3}	-5.272×10^{-3}	4.161×10^{-5}	-5.350×10^{-3}	9.785×10^{-3}
-5.277×10^{-3}	-1.032×10^{-2}	4.701×10^{-3}	-1.023×10^{-2}	-5.367×10^{-3}
4.358×10^{-5}	4.636×10^{-3}	2.564×10^{-2}	4.684×10^{-3}	1.047×10^{-4}
-5.288×10^{-3}	-1.026×10^{-2}	4.725×10^{-3}	-1.033×10^{-2}	-5.336×10^{-3}
9.713×10^{-3}	-5.204×10^{-3}	-1.339×10^{-4}	-5.150×10^{-3}	9.716×10^{-3}

Lagrange multiplier #1 : 0.3477 Lagrange multiplier #2 : 0.1457

$||\mathbf{e}||/||\mathbf{x}|| = 0.03087$

Table 7.8: Computed solutions of the co-kriging equations (Gaussian cross-variogram functions with moderate nugget effects).

Weights applied to data set #1

5.563×10^{-4}	-2.876×10^{-2}	-1.144×10^{-2}	-2.876×10^{-2}	5.563×10^{-4}
-2.876×10^{-2}	7.665×10^{-2}	0.1676	7.665×10^{-2}	-2.876×10^{-2}
-1.144×10^{-2}	0.1676	0.2967	0.1676	-1.144×10^{-2}
-2.876×10^{-2}	7.665×10^{-2}	0.1676	7.665×10^{-2}	-2.876×10^{-2}
5.563×10^{-4}	-2.876×10^{-2}	-1.144×10^{-2}	-2.876×10^{-2}	5.563×10^{-4}

Weights applied to data set #2

9.734×10^{-3}	-5.280×10^{-3}	5.017×10^{-5}	-5.280×10^{-3}	9.734×10^{-3}
-5.280×10^{-3}	-1.030×10^{-2}	4.616×10^{-3}	-1.030×10^{-2}	-5.280×10^{-3}
5.017×10^{-5}	4.616×10^{-3}	2.585×10^{-2}	4.616×10^{-3}	5.017×10^{-5}
-5.280×10^{-3}	-1.030×10^{-2}	4.616×10^{-3}	-1.030×10^{-2}	-5.280×10^{-3}
9.734×10^{-3}	-5.280×10^{-3}	5.017×10^{-5}	-5.280×10^{-3}	9.734×10^{-3}

Lagrange multiplier #1 : 0.3476 Lagrange multiplier #2 : 0.1455

Table 7.9: Double precision counterparts of Table 7.8.

7.7 Discussion and conclusions

This chapter has examined a number of effects,relating to conditioning of geostatistical methods, which were discussed in Chapter 6. Some extensions have also been discussed. Effects relating to conditioning of ordinary kriging, discussed in these two chapters, may be summarized as follows :

- when the covariance matrix is ill-conditioned, so are corresponding stationary kriging matrices, whether their elements are written in terms of covariance or semivariogram functions. Effects discussed in Chapter 6, which apply to kriging expressed in terms of covariances, also appear to occur in a similar fashion when the kriging equations are expressed in terms of semivariograms,

- a scaling effect may cause kriging matrices to be ill-conditioned, even if the stationary covariance matrix is well-conditioned. This scaling is primarily dependent upon the sill of the semivariogram function.

- when solution of the kriging equations is performed using Gaussian elimination, ill-conditioning of the kriging matrix has a significant effect only when the stationary covariance is ill-conditioned (*e.g.* the Gaussian model). When the stationary covariance is well conditioned (*e.g.* the spherical model), the scaling effect introduced by changing sill has little bearing on the quality of computed solutions to the kriging equations,

- the introduction of a nugget effect dramatically improves conditioning of the covariance matrix. This has beneficial effects when an experimental covariance is fitted with a function which results in an ill-conditioned covariance matrix.

In practice, these results mean that it is desirable in practice to fit experimental covariances with functions which result in well-conditioned covariance matrices. In conjunction with this, the use of functions incorporating a moderate nugget effect is preferable to the use of a function which introduces no nugget effect. These considerations also apply, with extension, to co-kriging. The use of functions which result in well-conditioned covariance and cross-covariance matrices is supported here.

It must be stressed that properties of covariance or semivariogram models in kriging have the most important effects on conditioning of kriging matrices. This corresponds to past observations in geostatistical literature. In a similar fashion, properties of cross-covariance and cross-variogram models have the most significant effect upon conditioning of co-kriging. It has also been demonstrated here that scaling effects have a damaging effect, on solutions obtained numerically using Gaussian elimination, when the stationary covariance or cross-covariance matrix is ill-conditioned. It must also be noted that, if different solution algorithms are to be employed, scalings discussed in this chapter may have even more important consequences.

Chapter 8

Conclusions

Linear least squares methods involve the solution of a set of linear equations. The accuracy of a computed solution for a linear system is dependent upon a number of factors, including conditioning of the linear system, and stability properties of the algorithm employed to compute the solution. This thesis has examined conditioning of deconvolution, which is employed in seismic processing, and two geostatistical methods, ordinary kriging, and co-kriging. Causes of ill-conditioning have been discussed, and tests of use for recognizing when ill-conditioning occurs have been considered and assessed. Stability properties of some solution algorithms have been considered.

Ill-conditioning in deconvolution may be readily explained in terms of properties of the seismic trace, and the fact that deconvolution is a mathematical problem which may, in general, have no unique solution. Small values in a power spectrum, in comparison with the maximum value, may be expected to result in an ill-conditioned autocorrelation matrix. A consequence of this fact is that negative values in a *computed* power spectrum may be expected to be indicative of ill-conditioning. However, tests based on this result have been seen to be overly pessimistic.

The Wiener-Levinson algorithm, which is commonly employed to solve the normal equations which arise in seismic deconvolution, computes a solution more rapidly than do classical methods such as Gaussian elimination. When the normal equations are ill-conditioned, solutions computed using the Wiener-Levinson exhibit significantly more error than those

produced by the classical Gaussian elimination. Behaviour of this type may be accounted for by considering stability properties of these two algorithms. This computational error may have a significant effect on deconvolved outputs, which may, in turn, be expected to affect any interpretations of those deconvolved outputs. Intermediate results of the Wiener-Levinson algorithm can be employed in a test to determine when a computed filter may show significant error. The conjugate gradient algorithm is an iterative scheme which has received some attention in geophysical literature, with the claim being made that solutions, which exhibit less error than those of the Wiener-Levinson algorithm, may be produced in a relatively small number of iterations. The small number of iterations means that the computational cost associated with this scheme is less than for classical methods. It has been demonstrated in this thesis that, while the conjugate gradient scheme may produce solutions exhibiting less error than those produced using the Wiener-Levinson algorithm, this is not a general result. This means that using either the Wiener-Levinson algorithm or the conjugate gradient algorithm amounts to a trade-off between low computational cost which may be associated with these methods and the accuracy of solutions which could be produced by Gaussian elimination, when solving ill-conditioned normal equations. No general claim can be made comparing the accuracy of solutions produced by the Wiener-Levinson algorithm with those produced by the conjugate gradient scheme.

Conditioning of ordinary kriging may be considered in terms of properties of the covariance or semivariogram functions of interest. Properties of these functions have been discussed in light of the relationship between these functions and the autocorrelation function which is employed in Wiener filtering. It has been shown that an ill-conditioned stationary covariance matrix causes the corresponding kriging matrix to be ill-conditioned. An additional effect, due to the presence of unbias constraints employed with these geostatistical techniques, means that a kriging matrix may exhibit ill-conditioning, even if the covariance is well-conditioned. This effect is directly related to concepts of optimal scaling. Examples have illustrated that solutions to the kriging equations, computed using Gaussian elimination, show little error due to this scaling effect, unless the stationary covariance matrix is ill-conditioned. This means that the use of semivariogram and covariance functions

which result in well-conditioned covariance matrices is desirable in practice. Co-kriging has been seen to exhibit behaviour analogous to that observed for ordinary kriging, and the use of models which result in well-conditioned cross-covariance matrices is supported.

It is important to draw a distinction between effects in conditioning of linear equations which arise due to properties of the equations or due to properties of the particular algorithm being employed to solve them. Depending upon properties of the solution algorithm employed, a computed solution of an ill-conditioned linear system may exhibit little error. This thesis has demonstrated that the Wiener-Levinson algorithm produces a solution, to ill-conditioned normal equations, exhibiting significantly more error than do classical techniques such as Gaussian elimination, and discussed this phenomenon in terms of stability properties of these algorithms. This is a particularly disturbing result in light of the fact that the Wiener-Levinson algorithm is commonly employed in seismic processing. A simple approach, which introduces no extra cost, has been identified to determine cases in which the solution to the normal equations, computed using the Wiener-Levinson algorithm, may exhibit significant numerical error. Solutions to examples of Ordinary Kriging and Co-Kriging equations have been obtained using Gaussian elimination, which is a stable method, and large errors were observed in the computed solutions in some cases, indicating that the properties of the linear equations in question were having a significant effect on the solutions being obtained.

Appendix A

Operational details

In any numerical study, the capabilities of the computing system being employed must be considered. All numerical values presented throughout this thesis were obtained on a VAX/VMS system, and programming was performed using VAX FORTRAN. The VAX FORTRAN compiler provides a number of different types of real number variables, each of which provides a number, t, of significant binary digits. The definition of what constitutes an ill-conditioned matrix depends upon the condition number, the number of binary digits provided by the computer, and the accuracy desired in the solution. Table A.1 presents the different types of floating point variables provided by VAX FORTRAN.

Data type	t	2^t	Approx. # decimal digits
REAL*4 (Single precision)	23	8.387×10^6	7
REAL*8 (Double precision)			
D_floating (default)	55	3.603×10^{16}	16
G_floating	52	4.504×10^{15}	15
REAL*16 (Quad)			
H_floating	112	5.192×10^{33}	32

Table A.1: Significant digits provided by VAX FORTRAN for floating point data types.

A.1 Defining an ill-conditioned linear system

If the spectral condition number of a matrix $\mathbf{A}$, $\kappa(\mathbf{A})$, is approximately 2^m for some value m, then the accuracy of a solution $\mathbf{x}$ of the system :

$$\mathbf{Ax} = \mathbf{b}$$

can only be guaranteed to be accurate to within approximately 2^{t-m}. This means that the solution may be accurate to only $t - m$ binary places. If the solution is desired to an accuracy of greater than $t - m$ binary digits, then the linear equation may be considered to be ill-conditioned. For example, if $\kappa(\mathbf{A}) > 2^t$ then inaccurate results are possible as the solution can not be guaranteed correct to any level of accuracy (Wilkinson (1961)), even when solution is performed with a stable algorithm. This does not mean that greater accuracy is unobtainable, merely that it can not be guaranteed.

A.1.1 Precision of numerical results

Numerical results have been presented in this thesis. In order to assess the various approaches, reported results have been computed using different precision floating point variables, as follows :

- where condition numbers are quoted without referring to precision, they have been calculated using double precision (D_floating) arithmetic to evaluate the eigenvalues.
- all solutions of linear equations, performed for the purpose of studying the different methods, have been produced using single precision arithmetic. This means that a linear system may considered ill-conditioned if $\kappa(\mathbf{A})$ is at least of the order of 10^6 or 10^7, depending upon the accuracy which may be desired in a solution.
- the "correct" or "double precision" results for the purposes of assessing the linear system have been produced using double precision (D_floating) arithmetic. It must be noted that these results are guaranteed to be correct to a higher level of accuracy

than are those computed using single precision. They are not, in fact, necessarily exact solutions.

Results computed using higher precision offer the advantage of greater accuracy than those computed single precision. However, the cost, in terms of computer storage and execution times, is greater.

A.2 Checking precision of solution

Throughout this study, the performance of different solution algorithms are measured by comparing solutions computed using different algorithms with solutions obtained using Gaussian elimination and double precision floating point variables. Comparisons are based upon a visual comparison of single precision and double precision solutions, and/or by means of error norms. When norms have been employed, results reported are of the form :

$$\frac{||\mathbf{x}_d - \mathbf{x}_a||}{||\mathbf{x}_d||}$$

where :

- $\mathbf{x}_a$ denotes the solution computed using an algorithm of interest, with computations being performed in single precision,
- $\mathbf{x}_d$ denotes the solution computed using Gaussian elimination, working in double precision,
- the vertical bars denote the Euclidean norm.

A large value for this ratio is taken to signify a large error, while a small ratio denotes a small error.

One other comparison which could be employed is based on an examination of residuals. The residual associated with a computed solution, $\mathbf{x}_a$, of the system

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

is defined to be the quantity :

$$\mathbf{r} = \mathbf{A}\mathbf{x}_a - \mathbf{b}$$

The norm of the residual, $||\mathbf{r}||$, will be zero if $\mathbf{x}_a = \mathbf{x}$, and small error may be associated with small values of the quantity :

$$\frac{||\mathbf{r}||}{||\mathbf{b}||}$$

Unfortunately, when $\mathbf{A}$ is ill-conditioned, a small value of this ratio does not guarantee that the computed solution $\mathbf{x}_a$ exhibits small error relative to $\mathbf{x}$. For all examples presented in this thesis, the residuals have all being small :

$$\frac{||\mathbf{r}||}{||\mathbf{b}||} \leq 10^{-5}$$

which means that, in all examples, residuals have indicated small error.

Appendix B

Synthetic traces

Synthetic seismic traces used in the study of Chapter 5 were generated using the approximately minimum phase wavelet illustrated in Figure B.1. The reflection coefficient series illustrated in Figure B.2 was used to generate an impulse response series (*i.e.* a multiples plus primaries version of Figure B.2) of two second duration, illustrated in Figure B.3. The trace employed throughout Chapter 5 is the convolution of this impulse response function and the wavelet. Amplitude values for the wavelet and reflection coefficient series are tabulated in Tables B.1 and B.2 respectively. Sample intervals are considered to be four milliseconds throughout the figures and tables of this appendix.

The procedure used to compute autocorrelations of traces is discussed in Section 1.4.1. Power spectra were computed using the cosine transform described by Robinson (1967a). Considerations made in computation of power spectra are discussed in Section 5.3. The power spectra of the wavelet and the impulse response are illustrated in Figures B.4 and B.5 respectively. It may be readily observed that the impulse response does has a number of peaks, and is not white, due to its finite length.

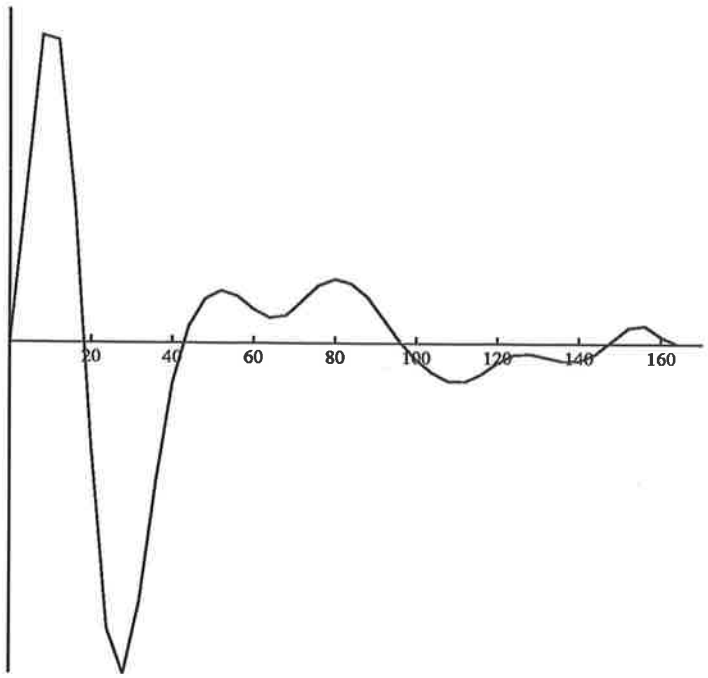


Figure B.1: Synthetic wavelet (approximately minimum phase).

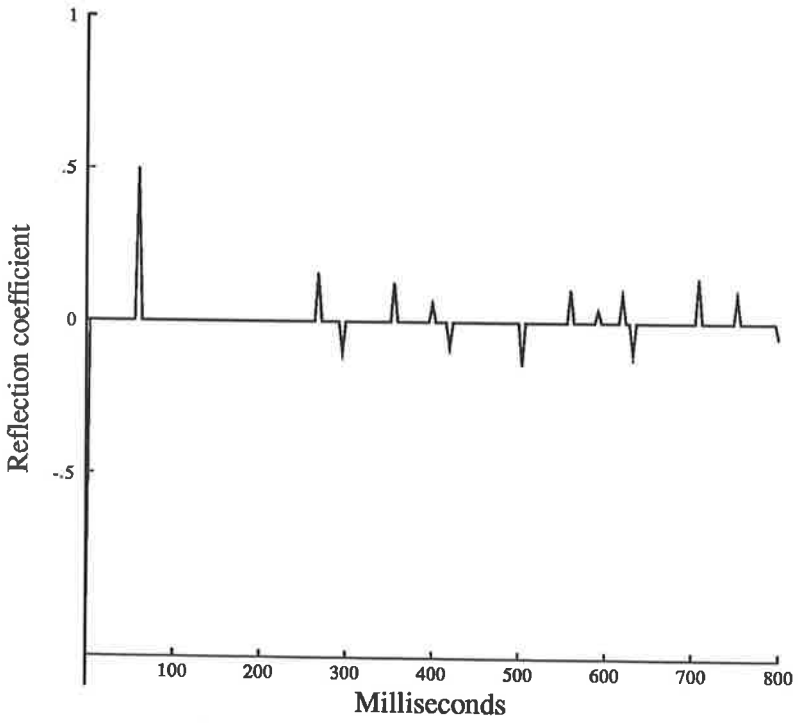


Figure B.2: Reflection coefficient series.

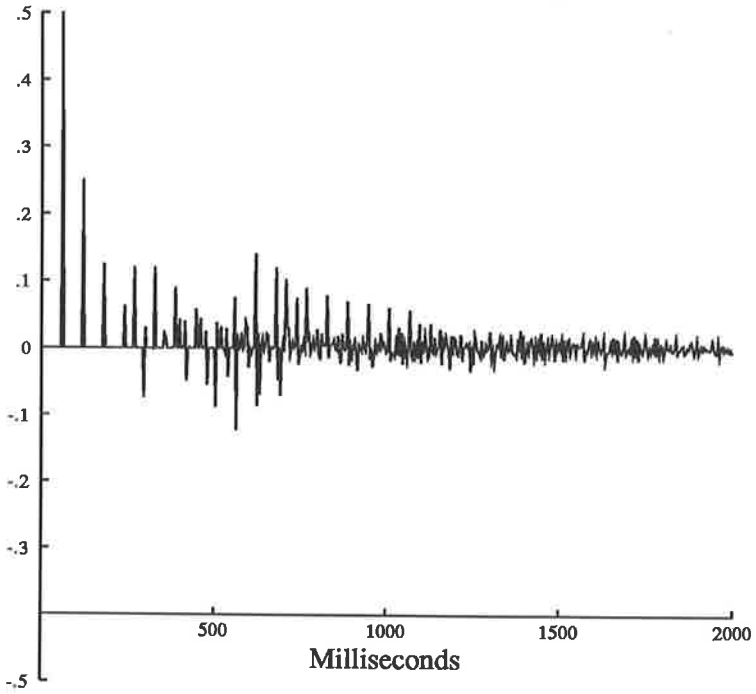


Figure B.3: Impulse response.

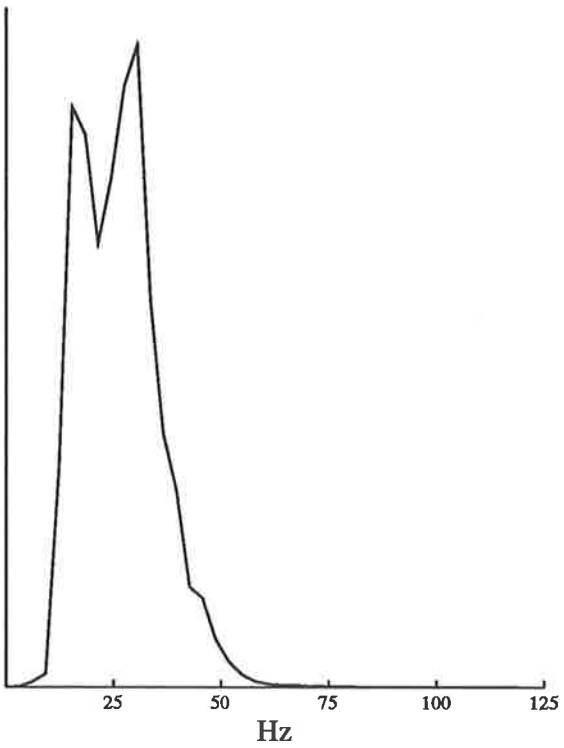


Figure B.4: Power spectrum of the wavelet.

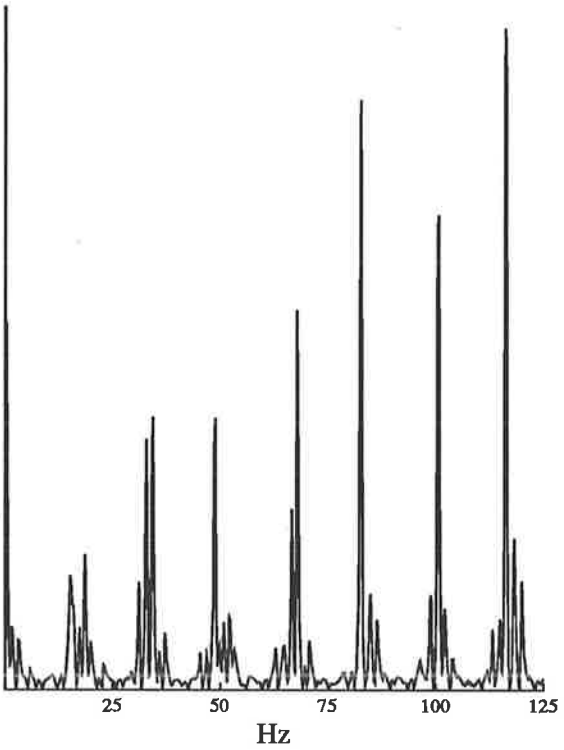


Figure B.5: Power spectrum of the impulse response.

Time (msec)	Amplitude	Time (msec)	Amplitude	Time (msec)	Amplitude
0	0.0	56	14.2	112	−11.5
4	46.8	60	10.4	116	− 9.3
8	92.1	64	7.8	120	− 5.9
12	90.7	68	8.5	124	− 3.4
16	40.7	72	12.8	128	− 3.1
20	− 31.6	76	17.5	132	− 4.2
24	− 86.2	80	19.3	136	− 5.3
28	−100.0	84	18.0	140	− 5.2
32	− 77.8	88	13.9	144	− 3.1
36	− 41.9	92	7.3	148	0.8
40	− 12.2	96	0.4	152	4.9
44	5.2	100	− 5.0	156	5.6
48	13.3	104	− 9.0	160	2.2
52	15.9	108	−11.4	164	0.0

Table B.1: Approximately minimum phase wavelet.

Time (msec)	Coefficient
0	−1.00
60	0.50
268	0.16
296	−0.10
356	0.13
400	0.06
420	−0.08
504	−0.14
560	0.11
592	0.04
620	0.09
632	−0.10
708	0.15
752	0.09
800	−0.05

Table B.2: Reflection coefficient series.

Appendix C

Testing of prediction error variances

The routine listed on the following pages is a modified version of the subroutine EUREKA, given by Robinson (1967a), and is presented to illustrate approaches discussed in Chapters 4 and 5. It solves a set of linear equations involving a symmetric, positive definite, Toeplitz coefficient matrix, returning an error code indicating whether the coefficient matrix is positive definite, indefinite and non-singular, or singular. This test is performed by examining computed prediction error variances. When solving normal equations, in which the coefficient matrix is known to be positive definite, an error code which does not correspond to a positive definite coefficient matrix may be taken as an indication that the computed solution is significantly affected by rounding error. Similar tests, using properties of prediction error variances described in Section 4.4, may also be readily implemented.

```
      SUBROUTINE EUREKA(R,LR,G,F,A,IER)
C
C     This subroutine finds the solution of the single-channel normal
C        equations of the form :
C
C                    RF=G
C
C        where R is a symmetric Toeplitz array
C
C     Arguments
C     =========
C
C     R              First row of Toeplitz array = (R0,R1,...Rm)
C     LR             Dimension of R (= m+1)
C     G              RHS of above Toeplitz system = (G0,G1,...Gm)
C     F              Solution of above system = (F0,F1,...Fm)
C     A              Prediction error operator  = (1,A1,...Am)
C     IER            Error condition
C                         0   No error and R is positive definite.
C                         1   No error and R is not positive definite.
C                              This is an indication of ill-conditioning
C                               if R is known to be positive definite.
C                         2   R is singular (zero prediction error
C                               variance).
C
C                       Error codes 0 and 1 are not terminal (i.e. a
C                         solution is produced). Error code 2 is terminal.
C
      REAL R(1),G(1),F(1),A(1)
      IER=0
      V=R(1)
      D=R(2)
      IF(V.LE.0.000E0) IER=1
      IF(ABS(V).LE.0.0000E0) GOTO 6

      F(1)=G(1)/V
      A(1)=1.0000E0
      Q=F(1)*R(2)

      DO 5 I=2,LR
         A(I)=-D/V
         L=(I-2)/2+1
         DO 2 J=2,L
```

```
         HOLD=A(J)
         K=I-J+1
         A(J)=A(J)+A(I)*A(K)
         A(K)=A(K)+A(I)*HOLD
2     CONTINUE
      IF(2*(I/2).NE.I) A(L+1)=A(L+1)*(1.000E0+A(I))
      V=V+A(I)*D
      IF(V.LE.0.000E0) IER=1
      IF(ABS(V).LE.0.0000E0) GOTO 6
      F(I)=(G(I)-Q)/V
      DO 3 J=1,I-1
         F(J)=F(J)+F(I)*A(I-J+1)
3     CONTINUE
      IF(I.EQ.LR) GOTO 5
      D=0.0000E0
      Q=D
      DO 4 J=1,I
         K=I-J+2
         D=D+A(J)*R(K)
         Q=Q+F(J)*R(K)
4     CONTINUE
5 CONTINUE
  GOTO 7
6 IER=2
7 RETURN
  END
```

Appendix D

Geophysical Inverse Theory

A number of authors *e.g.* Backus and Gilbert (1967, 68), Smith and Franklin (1969), Jordan and Franklin (1971), Parker (1972, 77), Treitel and Lines (1982) have contributed to the development of geophysical inverse theory. Generally, when geophysical measurements are taken, the data is inaccurate or, in some other way, insufficient to enable identification of geological/geophysical features *e.g.* solutions may not be unique (two or more solutions may account for a given set of measurements), or there may be no solution at all. This appendix focuses attention on Least Squares Inversion, a subset of geophysical inverse theory which encompasses all methods considered in this thesis.

D.1 General Linear Systems

Deconvolution, as discussed in Section 1.4.1, may be considered as finding solutions of the equation :

$$\mathbf{X}\mathbf{w} = \mathbf{z} \tag{D.1}$$

where :

- $\mathbf{X}$ is defined in Equation 4.8. If n is the number of samples in the seismic trace, and p is the desired length of the filter, then $\mathbf{X}$ is an n by p matrix
- $\mathbf{w}$ is the desired Wiener filter,

- $\mathbf{z}$ is the arbitrary desired output.

If $n = p$, then the matrix $\mathbf{X}$ is a square matrix. If $\mathbf{X}$ is non-singular, then the solution of Equation D.1 is :

$$\mathbf{w} = \mathbf{X}^{-1}\mathbf{z}$$

and the problem is said to be well posed.

If the length of the seismic trace is greater than the desired length of the filter, *i.e.* $n > p$, then the linear system is said to be over-constrained, and a unique solution of Equation D.1 may not exist. If $n < p$, then the linear system is said to be under-constrained, and there may be many solutions which satisfy Equation D.1. Thus, the fact that deconvolution is incorrectly posed, as discussed in Section 4.2.2, may be accounted for by the observation that problems which arise in geophysical practice may be either over-constrained or under-constrained.

In deconvolution, the length of the seismic trace is generally significantly larger than the desired filter length—thus deconvolution may be considered as the solution of an over-constrained system. The approach which is often adopted, and focused on in this thesis, amounts to the minimization of the expression :

$$||\mathbf{X}\mathbf{w} - \mathbf{z}||^2$$

where the vertical bars denote the Euclidean norm. The vector $\mathbf{w}$ which minimizes this expression is referred to as the least-squares solution. This solution is obtained in Section 1.4.1 by solution of the normal equations.

The normal equations of Equation 1.11 may be expressed, *e.g.* Lines and Treitel (1984), in the form :

$$\mathbf{X}^T\mathbf{X}\mathbf{w} = \mathbf{X}^T\mathbf{z}$$

Thus, in order to compute the Wiener filters using the normal equations, it is necessary to compute the autocorrelation matrix, $\mathbf{R} = \mathbf{X}^T\mathbf{X}$ and the cross-correlation vector, $\mathbf{g} = \mathbf{X}^T\mathbf{z}$. The formation of the autocorrelation matrix and cross-correlation vector involves numerical inaccuracies, which may be troublesome if either n or p are large.

Golub and Reinsch (1970) observed this problem and proposed the solution of least-squares problems by means of the Singular Value Decomposition.

D.2 The Singular Value Decomposition

Lanczos (1961) showed that an n by p matrix, $\mathbf{X}$, may be factorized into the form :

$$\mathbf{X} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T \tag{D.2}$$

where :

- $\mathbf{U}$ is a n by p matrix whose columns are orthonormalized eigenvectors associated with the p largest eigenvalues of $\mathbf{X}\mathbf{X}^T$,
- $\mathbf{\Lambda}$ is a diagonal matrix whose diagonal elements are the singular values of $\mathbf{X}$—the positive square roots of eigenvalues of $\mathbf{X}^T\mathbf{X}$,
- $\mathbf{V}$ is a n by n matrix whose columns are the eigenvectors of $\mathbf{X}^T\mathbf{X}$.

A generalized inverse of $\mathbf{X}$, which exists for any values of n and p, may then be written as :

$$\mathbf{X}^{gen} = \mathbf{V}\mathbf{\Lambda}^{-1}\mathbf{U}^T$$

The desired solution of the least-squares problem, defined in Equation D.1, may then be written as :

$$\mathbf{w} = \mathbf{X}^{gen}\mathbf{z}$$

Golub and Reinsch (1970) provided an efficient algorithm for the Singular Value Decomposition. This approach has a number of advantages over the standard normal equations technique :

1. it is not necessary to compute the matrix $\mathbf{X}^T\mathbf{X}$,
2. solutions produced exhibit less error than those produced by solving the normal equations. See, for example, Treitel and Lines (1982),

3. the method yields information which provides measures of the accuracy of solutions and independence of data elements.

This thesis has focused on accuracy of solutions of the normal equations, using approaches routinely performed in practice. For this reason, the Singular Value Decomposition has not been applied in this thesis. Additionally, the method introduces a number of overheads which would introduce a considerable numerical cost in comparison with techniques considered in this thesis :

1. the method requires computation of the eigenvalues of $\mathbf{X}^T\mathbf{X}$,
2. the method requires a significant working space, and involves a large number of numerical operations.

The numerical accuracy of this approach should not be discounted. As computer technology improves in the future, the overheads associated with the Singular Value Decomposition may become less restrictive, and the method may be feasible for use in large-scale Wiener filtering programs.

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