CHAPTER 3: INVERSE METHODS BASED ON LENGTH

3.1 Introduction

This chapter is concerned with inverse methods based on the length of various vectors that arise in a typical problem. The two most common vectors concerned are the data-error or misfit vector and the model parameter vector. Methods based on the first vector give rise to classic least squares solutions. Methods based on the second vector give rise to what are known as minimum length solutions. Improvements over simple least squares and minimum length solutions include the use of information about noise in the data and *a priori* information about the model parameters, and are known as weighted least squares or weighted minimum length solutions, respectively. This chapter will end with material on how to handle constraints and on variances of the estimated model parameters.

3.2 Data Error and Model Parameter Vectors

The data error and model parameter vectors will play an essential role in the development of inverse methods. They are given by

$$\text{data error vector} = \mathbf{e} = \mathbf{d}^{\text{obs}} - \mathbf{d}^{\text{pre}} \tag{3.1}$$

and

$$\text{model parameter vector} = \mathbf{m} \tag{3.2}$$

The dimension of the error vector $\mathbf{e}$ is $N \times 1$, while the dimension of the model parameter vector is $M \times 1$, respectively. In order to utilize these vectors, we next consider the notion of the size, or length, of vectors.

3.3 Measures of Length

The *norm* of a vector is a measure of its size, or length. There are many possible definitions for norms. We are most familiar with the Cartesian (L_2) norm. Some examples of norms follow:

$$L_1 = \sum_{i=1}^{N} |e_i| \tag{3.3}$$

$$L_2 = \left[\sum_{i=1}^{N} |e_i|^2 \right]^{1/2} \tag{3.4}$$

$$\vdots$$

$$L_M = \left[\sum_{i=1}^{N} |e_i|^M \right]^{1/M} \tag{3.5}$$

and finally,

$$L_\infty = \max_i \; |e_i| \tag{3.6}$$

Important Notice! Inverse methods based on different norms can, and often do, give different answers!

The reason is that different norms give different *weight* to "outliers." For example, the L_∞ norm gives all the weight to the largest misfit. Low-order norms give more equal weight to errors of different sizes.

The L_2 norm gives the familiar Cartesian length of a vector. Consider the total misfit E between observed and predicted data. It has units of length squared and can be found either as the square of the L_2 norm of **e**, the error vector (Equation 3.1), or by noting that it is also equivalent to the dot (or inner) product of **e** with itself, given by

$$E = \mathbf{e}^{\mathrm{T}}\mathbf{e} = [e_1 \quad e_2 \quad \cdots \quad e_N] \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} = \sum_{i=1}^{N} e_i^2 \tag{3.7}$$

Inverse methods based on the L_2 norm are also closely tied to the notion that errors in the data have Gaussian statistics. They give considerable weight to large errors, which would be considered "unlikely" if, in fact, the errors were distributed in a Gaussian fashion.

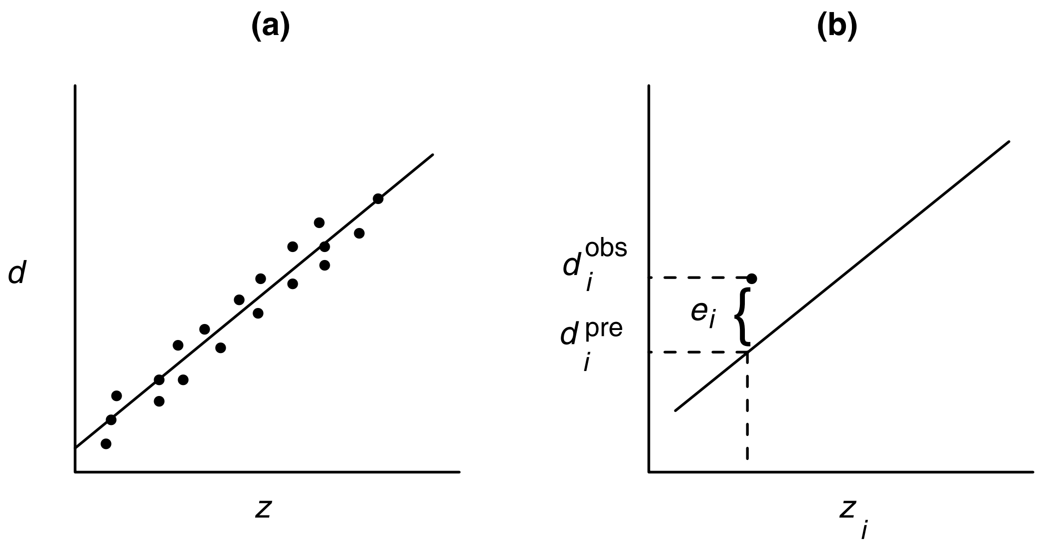
Now that we have a way to quantify the misfit between predicted and observed data, we are ready to define a procedure for estimating the value of the elements in **m**. The procedure is to take the partial derivative of E with respect to each element in **m** and set the resulting equations to zero. This will produce a system of M equations that can be manipulated in such a way that, in general, leads to a solution for the M elements of **m**.

The next section will show how this is done for the least squares problem of finding a best fit straight line to a set of data points.

3.4 Minimizing the Misfit—Least Squares

3.4.1 Least Squares Problem for a Straight Line

Consider the figure below (after Figure 3.1 from Menke, page 36):



(a) Least squares fitting of a straight line to (z, d) pairs. **(b)** The error e_i for each observation is the difference between the observed and predicted datum: $e_i = d_i^{obs} - d_i^{pre}$.

The ith predicted datum d_i^{pre} for the straight line problem is given by

$$d_i^{pre} = m_1 + m_2 z_i \tag{3.8}$$

where the two unknowns, m_1 and m_2, are the intercept and slope of the line, respectively, and z_i is the value along the z axis where the ith observation is made.

For N points we have a system of N such equations that can be written in matrix form as:

$$\begin{bmatrix} d_1 \\ \vdots \\ d_i \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} 1 & z_1 \\ \vdots & \vdots \\ 1 & z_i \\ \vdots & \vdots \\ 1 & z_N \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \tag{3.9}$$

Or, in the by now familiar matrix notation, as

$$\underset{(N \times 1)}{\mathbf{d}} = \underset{(N \times 2)}{\mathbf{G}} \underset{(2 \times 1)}{\mathbf{m}} \tag{1.13}$$

The total misfit E is given by

$$E = \mathbf{e}^{\mathrm{T}}\mathbf{e} = \sum_{i}^{N} \left[d_i^{\text{obs}} - d_i^{\text{pre}} \right]^2 \tag{3.10}$$

$$= \sum_{i}^{N} \left[d_i^{\text{obs}} - (m_1 + m_2 z_i) \right]^2 \tag{3.11}$$

Dropping the "obs" in the notation for the observed data, we have

$$E = \sum_{i}^{N} \left[d_i^2 - 2d_i m_1 - 2d_i m_2 z_i + 2m_1 m_2 z_i + m_1^2 + m_2^2 z_i^2 \right] \tag{3.12}$$

Then, taking the partials of E with respect to m_1 and m_2, respectively, and setting them to zero yields the following equations:

$$\frac{\partial E}{\partial m_1} = 2Nm_1 - 2\sum_{i=1}^{N} d_i + 2m_2 \sum_{i=1}^{N} z_i = 0 \tag{3.13}$$

and

$$\frac{\partial E}{\partial m_2} = -2\sum_{i=1}^{N} d_i z_i + 2m_1 \sum_{i=1}^{N} z_i + 2m_2 \sum_{i=1}^{N} z_i^2 = 0 \tag{3.14}$$

Rewriting Equations (3.13) and (3.14) above yields

$$Nm_1 + m_2 \sum_i z_i = \sum_i d_i \tag{3.15}$$

and

$$m_1 \sum_i z_i + m_2 \sum_i z_i^2 = \sum_i d_i z_i \tag{3.16}$$

Combining the two equations in matrix notation in the form **Am** = **b** yields

$$\begin{bmatrix} N & \sum z_i \\ \sum z_i & \sum z_i^2 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} \sum d_i \\ \sum d_i z_i \end{bmatrix} \tag{3.17}$$

or simply

$$\underset{(2 \times 2)}{\mathbf{A}} \quad \underset{(2 \times 1)}{\mathbf{m}} = \underset{(2 \times 1)}{\mathbf{b}} \tag{3.18}$$

Note that by the above procedure we have reduced the problem from one with N equations in two unknowns (m_1 and m_2) in **Gm = d** to one with two equations in the same two unknowns in **Am = b**.

The matrix equation **Am = b** can also be rewritten in terms of the original **G** and **d** when one notices that the matrix **A** can be factored as

$$\underset{(2 \times 2)}{\begin{bmatrix} N & \sum z_i \\ \sum z_i & \sum z_i^2 \end{bmatrix}} = \underset{(2 \times N)}{\begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \end{bmatrix}} \underset{(N \times 2)}{\begin{bmatrix} 1 & z_1 \\ 1 & z_2 \\ \vdots & \vdots \\ 1 & z_N \end{bmatrix}} = \underset{(2 \times 2)}{\mathbf{G}^{\mathrm{T}}\mathbf{G}} \tag{3.19}$$

Also, **b** above can be rewritten similarly as

$$\begin{bmatrix} \sum d_i \\ \sum d_i z_i \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{bmatrix} = \mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.20}$$

Thus, substituting Equations (3.19) and (3.20) into Equation (3.17), one arrives at the so-called *normal equations* for the least squares problem:

$$\mathbf{G}^{\mathrm{T}}\mathbf{G}\mathbf{m} = \mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.21}$$

The least squares solution $\mathbf{m}_{\mathrm{LS}}$ is then found as

$$\mathbf{m}_{\mathrm{LS}} = [\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{-1}\, \mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.22}$$

assuming that $[\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{-1}$ exists.

In summary, we used the forward problem (Equation 3.9) to give us an explicit relationship between the model parameters (m_1 and m_2) and a measure of the misfit to the observed data, E. Then, we minimized E by taking the partial derivatives of the misfit function with respect to the unknown model parameters, setting the partials to zero, and solving for the model parameters.

3.4.2 Derivation of the General Least Squares Solution

We start with any system of linear equations which can be expressed in the form

$$\underset{(N \times 1)}{\mathbf{d}} = \underset{(N \times M)}{\mathbf{G}} \; \underset{(M \times 1)}{\mathbf{m}} \tag{1.13}$$

Again, let $E = \mathbf{e}^{\mathrm{T}}\mathbf{e} = [\mathbf{d} - \mathbf{d}^{\mathrm{pre}}]^{\mathrm{T}}[\mathbf{d} - \mathbf{d}^{\mathrm{pre}}]$

$$E = [\mathbf{d} - \mathbf{Gm}]^{\mathrm{T}}[\mathbf{d} - \mathbf{Gm}] \tag{3.23}$$

$$E = \sum_{i=1}^{N} \left[d_i - \sum_{j=1}^{M} G_{ij} m_j \right] \left[d_i - \sum_{k=1}^{M} G_{ik} m_k \right] \tag{3.24}$$

As before, the procedure is to write out the above equation with all its cross terms, take partials of E with respect to each of the elements in **m**, and set the corresponding equations to zero. For example, following Menke, page 40, Equations (3.6)–(3.9), we obtain an expression for the partial of E with respect to m_q:

$$\frac{\partial E}{\partial m_q} = 2\sum_{k=1}^{M} m_k \sum_{i=1}^{N} G_{iq} G_{ik} - 2\sum_{i=1}^{N} G_{iq} d_i = 0 \tag{3.25}$$

We can simplify this expression by recalling Equation (2.4) from the introductory remarks on matrix manipulations in Chapter 2:

$$C_{ij} = \sum_{k=1}^{M} a_{ik} b_{kj} \tag{2.4}$$

Note that the first summation on i in Equation (3.25) looks similar in form to Equation (2.4), but the subscripts on the first **G** term are "backwards." If we further note that interchanging the subscripts is equivalent to taking the transpose of **G**, we see that the summation on i gives the qkth entry in $\mathbf{G}^{\mathrm{T}}\mathbf{G}$:

$$\sum_{i=1}^{N} G_{iq} G_{ik} = \sum_{i=1}^{N} [G^{\mathrm{T}}]_{qi} G_{ik} = [\mathbf{G}^{\mathrm{T}}\mathbf{G}]_{qk} \tag{3.26}$$

Thus, Equation (3.25) reduces to

$$\frac{\partial E}{\partial m_q} = 2\sum_{k=1}^{M} m_k [\mathbf{G}^{\mathrm{T}}\mathbf{G}]_{qk} - 2\sum_{i=1}^{N} G_{iq} d_i = 0 \tag{3.27}$$

Now, we can further simplify the first summation by recalling Equation (2.6) from the same section

$$d_i = \sum_{j=1}^{M} G_{ij} m_j \tag{2.6}$$

To see this clearly, we rearrange the order of terms in the first sum as follows:

$$\sum_{k=1}^{M} m_k [\mathbf{G}^{\mathrm{T}}\mathbf{G}]_{qk} = \sum_{k=1}^{M} [\mathbf{G}^{\mathrm{T}}\mathbf{G}]_{qk} m_k = [\mathbf{G}^{\mathrm{T}}\mathbf{G}\mathbf{m}]_q \tag{3.28}$$

which is the qth entry in $\mathbf{G}^{\mathrm{T}}\mathbf{G}\mathbf{m}$. Note that $\mathbf{G}^{\mathrm{T}}\mathbf{G}\mathbf{m}$ has dimension $(M \times N)(N \times M)(M \times 1) = (M \times 1)$. That is, it is an M-dimensional vector.

In a similar fashion, the second summation on i can be reduced to a term in $[\mathbf{G}^{\mathrm{T}}\mathbf{d}]_q$, the qth entry in an $(M \times N)(N \times 1) = (M \times 1)$ dimensional vector. Thus, for the qth equation, we have

$$0 = \frac{\partial E}{\partial m_q} = 2[\mathbf{G}^{\mathrm{T}}\mathbf{G}\mathbf{m}]_q - 2[\mathbf{G}^{\mathrm{T}}\mathbf{d}]_q \tag{3.29}$$

Dropping the common factor of 2 and combining the q equations into matrix notation, we arrive at

$$\mathbf{G}^{\mathrm{T}}\mathbf{G}\mathbf{m} = \mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.30}$$

The least squares solution for $\mathbf{m}$ is thus given by

$$\mathbf{m}_{\mathrm{LS}} = [\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.31}$$

The least squares operator, $\mathbf{G}_{\mathrm{LS}}^{-1}$, is thus given by

$$\mathbf{G}_{\mathrm{LS}}^{-1} = [\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}} \tag{3.32}$$

Recalling basic calculus, we note that $\mathbf{m}_{\mathrm{LS}}$ above is the solution that minimizes E, the total misfit. Summarizing, setting the q partial derivatives of E with respect to the elements in $\mathbf{m}$ to zero leads to the least squares solution.

We have just derived the least squares solution by taking the partial derivatives of E with respect to m_q and then combining the terms for $q = 1, 2, \ldots, M$. An alternative, but equivalent, formulation begins with Equation (3.2) but is written out as

$$E = [\mathbf{d} - \mathbf{G}\mathbf{m}]^{\mathrm{T}}[\mathbf{d} - \mathbf{G}\mathbf{m}] \tag{3.23}$$

$$= [\mathbf{d}^{\mathrm{T}} - \mathbf{m}^{\mathrm{T}}\mathbf{G}^{\mathrm{T}}][\mathbf{d} - \mathbf{G}\mathbf{m}]$$

$$= \mathbf{d}^{\mathrm{T}}\mathbf{d} - \mathbf{d}^{\mathrm{T}}\mathbf{G}\mathbf{m} - \mathbf{m}^{\mathrm{T}}\mathbf{G}^{\mathrm{T}}\mathbf{d} + \mathbf{m}^{\mathrm{T}}\mathbf{G}^{\mathrm{T}}\mathbf{G}\mathbf{m} \tag{3.33}$$

Then, taking the partial derivative of E with respect to $\mathbf{m}^{\mathrm{T}}$ turns out to be equivalent to what was done in Equations (3.25)–(3.30) for m_q, namely

$$\partial E/\partial \mathbf{m}^T = -\mathbf{G}^T\mathbf{d} + \mathbf{G}^T\mathbf{G}\mathbf{m} = 0 \tag{3.34}$$

which leads to

$$\mathbf{G}^T\mathbf{G}\mathbf{m} = \mathbf{G}^T\mathbf{d} \tag{3.30}$$

and

$$\mathbf{m}_{LS} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d} \tag{3.31}$$

It is also perhaps interesting to note that we could have obtained the same solution without taking partials. To see this, consider the following four steps.

Step 1. We begin with

$$\mathbf{G}\mathbf{m} = \mathbf{d} \tag{1.13}$$

Step 2. We then premultiply both sides by $\mathbf{G}^T$

$$\mathbf{G}^T\mathbf{G}\mathbf{m} = \mathbf{G}^T\mathbf{d} \tag{3.30}$$

Step 3. Premultiply both sides by $[\mathbf{G}^T\mathbf{G}]^{-1}$

$$[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{G}\mathbf{m} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d} \tag{3.35}$$

Step 4. This reduces to

$$\mathbf{m}_{LS} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d} \tag{3.31}$$

as before. The point is, however, that this way does not show why $\mathbf{m}_{LS}$ is the solution which minimizes E, the misfit between the observed and predicted data.

All of this assumes that $[\mathbf{G}^T\mathbf{G}]^{-1}$ exists, of course. We will return to the existence and properties of $[\mathbf{G}^T\mathbf{G}]^{-1}$ later. Next, we will look at two examples of least squares problems to show a striking similarity that is not obvious at first glance.

3.4.3 Two Examples of Least Squares Problems

Example 1. Best-Fit Straight-Line Problem

We have, of course, already derived the solution for this problem in the last section. Briefly, then, for the system of equations

$$\mathbf{d} = \mathbf{G}\mathbf{m} \tag{1.13}$$

given by

$$\begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} 1 & z_1 \\ 1 & z_2 \\ \vdots & \vdots \\ 1 & z_N \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \tag{3.9}$$

we have

$$\mathbf{G}^{\mathrm{T}}\mathbf{G} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \end{bmatrix} \begin{bmatrix} 1 & z_1 \\ 1 & z_2 \\ \vdots & \vdots \\ 1 & z_N \end{bmatrix} = \begin{bmatrix} N & \sum z_i \\ \sum z_i & \sum z_i^2 \end{bmatrix} \tag{3.36}$$

and

$$\mathbf{G}^{\mathrm{T}}\mathbf{d} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} \sum d_i \\ \sum d_i z_i \end{bmatrix} \tag{3.37}$$

Thus, the least squares solution is given by

$$\begin{bmatrix} m_1 \\ m_2 \end{bmatrix}_{\mathrm{LS}} = \begin{bmatrix} N & \sum z_i \\ \sum z_i & \sum z_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum d_i \\ \sum d_i z_i \end{bmatrix} \tag{3.38}$$

Example 2. Best-Fit Parabola Problem

The *i*th predicted datum for a parabola is given by

$$d_i = m_1 + m_2 z_i + m_3 z_i^2 \tag{3.39}$$

where m_1 and m_2 have the same meanings as in the straight line problem, and m_3 is the coefficient of the quadratic term. Again, the problem can be written in the form:

$$\mathbf{d} = \mathbf{G}\mathbf{m} \tag{1.13}$$

where now we have

$$\begin{bmatrix} d_1 \\ \vdots \\ d_i \\ \vdots \\ d_N \end{bmatrix} = \begin{bmatrix} 1 & z_1 & z_1^2 \\ \vdots & \vdots & \vdots \\ 1 & z_i & z_i^2 \\ \vdots & \vdots & \vdots \\ 1 & z_N & z_N^2 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} \tag{3.40}$$

and

$$\mathbf{G}^{\mathrm{T}}\mathbf{G} = \begin{bmatrix} N & \sum z_i & \sum z_i^2 \\ \sum z_i & \sum z_i^2 & \sum z_i^3 \\ \sum z_i^2 & \sum z_i^3 & \sum z_i^4 \end{bmatrix}, \qquad \mathbf{G}^{\mathrm{T}}\mathbf{d} = \begin{bmatrix} \sum d_i \\ \sum d_i z_i \\ \sum d_i z_i^2 \end{bmatrix} \tag{3.41}$$

As before, we form the least squares solution as

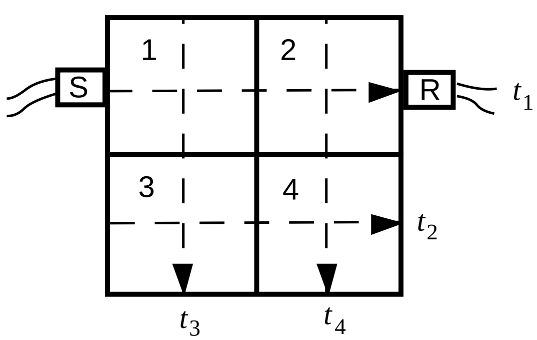
$$\mathbf{m}_{\mathrm{LS}} = [\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.31}$$

Although the forward problems of predicting data for the straight line and parabolic cases look very different, the least squares solution is formed in a way that emphasizes the fundamental similarity between the two problems. For example, notice how the straight-line problem is buried within the parabola problem. The upper left hand 2×2 part of $\mathbf{G}^{\mathrm{T}}\mathbf{G}$ in Equation (3.41) is the same as Equation (3.36). Also, the first two entries in $\mathbf{G}^{\mathrm{T}}\mathbf{d}$ in Equation (3.41) are the same as Equation (3.37).

Next we consider a four-parameter example.

3.4.4 Four-Parameter Tomography Problem

Finally, let's consider a four-parameter problem, but this one based on the concept of tomography.



$$\begin{aligned} t_1 &= h\left(\frac{1}{v_1}\right) + h\left(\frac{1}{v_2}\right) = h(s_1 + s_2) \\ t_2 &= h\left(\frac{1}{v_3}\right) + h\left(\frac{1}{v_4}\right) = h(s_3 + s_4) \\ t_3 &= h\left(\frac{1}{v_1}\right) + h\left(\frac{1}{v_3}\right) = h(s_1 + s_3) \\ t_4 &= h\left(\frac{1}{v_2}\right) + h\left(\frac{1}{v_4}\right) = h(s_2 + s_4) \end{aligned} \tag{3.42}$$

$$\begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ t_4 \end{bmatrix} = h \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \end{bmatrix} \tag{3.43}$$

or

$$\mathbf{d} = \mathbf{Gm} \tag{1.13}$$

$$\mathbf{G}^{\mathrm{T}}\mathbf{G} = h^2 \begin{bmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} = h^2 \begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 2 & 0 & 1 \\ 1 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix} \tag{3.44}$$

$$\mathbf{G}^{\mathrm{T}}\mathbf{d} = h \begin{bmatrix} t_1 + t_3 \\ t_1 + t_4 \\ t_2 + t_3 \\ t_2 + t_4 \end{bmatrix} \tag{3.45}$$

So, the normal equations are

$$\mathbf{G}^{\mathrm{T}}\mathbf{Gm} = \mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.21}$$

$$h \begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 2 & 0 & 1 \\ 1 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \end{bmatrix} = \begin{bmatrix} t_1 + t_3 \\ t_1 + t_4 \\ t_2 + t_3 \\ t_2 + t_4 \end{bmatrix} \tag{3.46}$$

or

$$h \left(\begin{bmatrix} 2 \\ 1 \\ 1 \\ 0 \end{bmatrix} s_{1+} \begin{bmatrix} 1 \\ 2 \\ 0 \\ 1 \end{bmatrix} s_{2+} \begin{bmatrix} 1 \\ 0 \\ 2 \\ 1 \end{bmatrix} s_{3+} \begin{bmatrix} 0 \\ 1 \\ 1 \\ 2 \end{bmatrix} s_4 \right) = \begin{bmatrix} t_1 + t_3 \\ t_1 + t_4 \\ t_2 + t_3 \\ t_2 + t_4 \end{bmatrix} \tag{3.47}$$

Example: $s_1 = s_2 = s_3 = s_4 = 1$, $h = 1$; then $t_1 = t_2 = t_3 = t_4 = 2$

By inspection, $s_1 = s_2 = s_3 = s_4 = 1$ is a solution, *but* so is $s_1 = s_4 = 2$, $s_2 = s_3 = 0$, or $s_1 = s_4 = 0$, $s_2 = s_3 = 2$.

Solutions are nonunique! Look back at **G**. Are all of the columns or rows independent? No! What does that imply about **G** (and $\mathbf{G}^T\mathbf{G}$)? Rank < 4. What does that imply about $(\mathbf{G}^T\mathbf{G})^1$? It does not exist. So does $\mathbf{m}_{LS}$ exist? No.

Other ways of saying this: The vectors $\mathbf{g}_i$ do not span the space of **m**. Or, the experimental set-up is not sufficient to uniquely determine the solution. Note that this analysis can be done without any data, based strictly on the experimental design.

Another way to look at it: Are the columns of **G** independent? No. For example, coefficients –1, +1, +1, and –1 will make the equations add to zero. What pattern does that suggest is not resolvable?

Now that we have derived the least squares solution, and considered some examples, we next turn our attention to something called the determinancy of the system of equations given by Equation (1.13):

$$\mathbf{d} = \mathbf{G}\mathbf{m} \tag{1.13}$$

This will begin to permit us to classify systems of equations based on the nature of **G**.

3.5 Determinancy of Least Squares Problems

(See Pages 46–52, Menke)

3.5.1 Introduction

We have seen that the least squares solution to **d** = **Gm** is given by

$$\mathbf{m}_{LS} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d} \tag{3.31}$$

There is no guarantee, as we saw in Section 3.4.4, that the solution even exists. It fails to exist when the matrix $\mathbf{G}^T\mathbf{G}$ has no mathematical inverse. We note that $\mathbf{G}^T\mathbf{G}$ is square ($M \times M$), and it is at least mathematically possible to consider inverting $\mathbf{G}^T\mathbf{G}$. (N.B. The dimension of $\mathbf{G}^T\mathbf{G}$ is $M \times M$, independent of the number of observations made). Mathematically, we can say the $\mathbf{G}^T\mathbf{G}$ has an inverse, and it is unique, when $\mathbf{G}^T\mathbf{G}$ has rank M. The rank of a matrix was considered in Section 2.2.3. Essentially, if $\mathbf{G}^T\mathbf{G}$ has rank M, then it has enough information in it to "resolve" M things (in this case, model parameters). This happens when all M rows (or equivalently, since $\mathbf{G}^T\mathbf{G}$ is square, all M columns) are independent. Recall also that independent means you cannot write any row (or column) as a linear combination of the other rows (columns).

$\mathbf{G}^T\mathbf{G}$ will have rank < M if the number of observations N is less than M. Menke gives the example (pp. 45–46) of the straight-line fit to a single data point as an illustration. If $[\mathbf{G}^T\mathbf{G}]^{-1}$ does not exist, an infinite number of estimates will all fit the data equally well. Mathematically, $\mathbf{G}^T\mathbf{G}$ has rank < M if $|\mathbf{G}^T\mathbf{G}| = 0$, where $|\mathbf{G}^T\mathbf{G}|$ is the determinant of $\mathbf{G}^T\mathbf{G}$.

Now, let us introduce Menke's nomenclature based on the nature of $\mathbf{G}^T\mathbf{G}$ and on the prediction error. In all cases, the number of model parameters is *M* and the number of observations is *N*.

3.5.2 Even-Determined Problems: *M* = *N*

If a solution exists, it is unique. The prediction error $[\mathbf{d}^{obs} - \mathbf{d}^{pre}]$ is identically zero. For example,

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 5 & -1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \tag{3.48}$$

for which the solution is $\mathbf{m} = [1, 3]^T$.

3.5.3 Overdetermined Problems: Typically, *N* > *M*

With more observations than unknowns, typically one cannot fit all the data exactly. The least squares problem falls in this category. Consider the following example:

$$\begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 5 & -1 \\ -3 & 1 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \tag{3.49}$$

This overdetermined case consists of adding one equation to Equation (3.48) in the previous example. The least squares solution is $[1.333, 4.833]^T$. The data can no longer be fit exactly.

3.5.4 Underdetermined Problems: Typically, *M* > *N*

With more unknowns than observations, **m** has no unique solution. A special case of the underdetermined problem occurs when you can fit the data exactly, which is called the *purely underdetermined* case. The prediction error for the purely underdetermined case is exactly zero (i.e., the data can be fit exactly). An example of such a problem is

$$[1] = [2 \quad 1] \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} \tag{3.50}$$

Possible solutions include $[0, 1]^T$, $[0.5, 0]^T$, $[5, -9]^T$, $[1/3, 1/3]^T$ and $[0.4, 0.2]^T$. The solution with the minimum length, in the L_2 norm sense, is $[0.4, 0.2]^T$.

The following example, however, is also underdetermined, but no choice of m_1, m_2, m_3 will produce zero prediction error. Thus, it is not purely underdetermined.

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} \tag{3.51}$$

(You might want to verify the above examples. Can you think of others?)

Although I have stated that overdetermined (underdetermined) problems typically have $N > M$ ($N < M$), it is important to realize that this is not always the case. Consider the following:

$$\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 2 & 2 \end{bmatrix} \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} \tag{3.52}$$

For this problem, m_1 is *overdetermined*, (that is, no choice of m_1 can exactly fit both d_1 and d_2 unless d_1 happens to equal d_2), while at the same time m_2 and m_3 are *underdetermined*. This is the case even though there are two equations (i.e., the last two) in only two unknowns (m_2, m_3). The two equations, however, are not independent, since two times the next to last row in **G** equals the last row. Thus this problem is both *overdetermined* and *underdetermined* at the same time.

For this reason, I am not very satisfied with Menke's nomenclature. As we will see later, when we deal with vector spaces, the key will be the single values (much like eigenvalues) and associated eigenvectors for the matrix **G**.

3.6 Minimum Length Solution

The minimum length solution arises from the purely underdetermined case ($N < M$, and can fit the data exactly). In this section, we will develop the minimum length operator, using Lagrange multipliers and borrowing on the basic ideas of minimizing the length of a vector introduced in Section 3.4 on least squares.

3.6.1 Background Information

We begin with two pieces of information:

1. First, $[\mathbf{G}^T\mathbf{G}]^{-1}$ does not exist. Therefore, we cannot calculate the least squares solution $\mathbf{m}_{LS} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d}$.

2. Second, the prediction error $\mathbf{e} = \mathbf{d}^{obs} - \mathbf{d}^{pre}$ is exactly equal to zero.

To solve *underdetermined* problems, we must *add* information that is not already in **G**. This is called *a priori* information. Examples might include the constraint that density be greater than zero for rocks, or that v_n, the seismic *P*-wave velocity at the Moho falls within the range $5 < v_n < 10$ km/s, etc.

Another *a priori* assumption is called "solution simplicity." One seeks solutions that are as "simple" as possible. By analogy to seeking a solution with the "simplest" misfit to the data (i.e., the smallest) in the least squares problem, one can seek a solution which minimizes the total length of the model parameter vector, **m**. At first glance, there may not seem to be any reason to do this. It does make sense for some cases, however. Suppose, for example, that the unknown model parameters are the velocities of points in a fluid. A solution that minimized the length of **m** would also minimize the kinetic energy of the system. Thus, it would be appropriate in this case to minimize **m**. It also turns out to be a nice property when one is doing nonlinear problems, and the **m** that one is using is actually a vector of changes to the solution at the previous step. Then it is nice to have small step sizes. The requirement of solution simplicity will lead us, as shown later, to the so-called minimum length solution.

3.6.2 Lagrange Multipliers (See Page 50 and Appendix A.1, Menke)

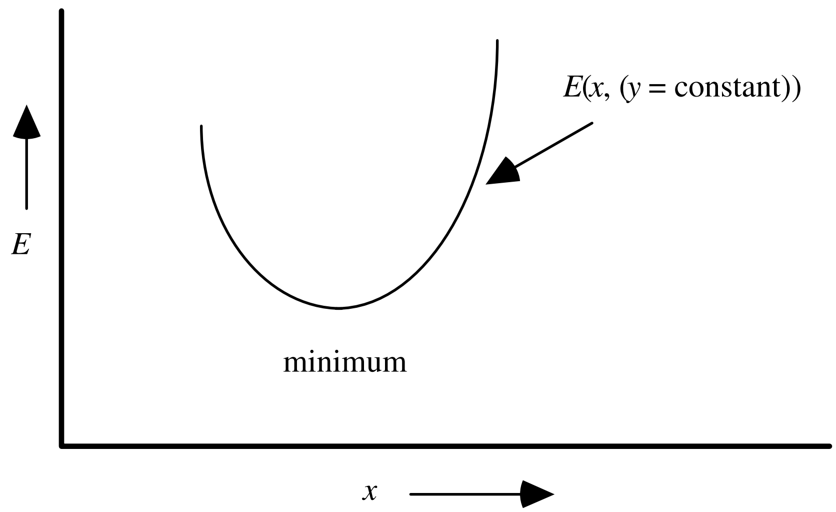
Lagrange multipliers come to mind whenever one wishes to solve a problem subject to some constraints. In the purely underdetermined case, these constraints are that the data misfit be zero. Before considering the full purely underdetermined case, consider the following discussion of Lagrange Multipliers, mostly after Menke.

Lagrange Multipliers With 2 Unknowns and 1 Constraint

Consider $E(x, y)$, a function of two variables. Suppose that we want to minimize $E(x, y)$ subject to some constraint of the form $\phi(x, y) = 0$.

The steps, using Lagrange multipliers, are as follows (next page):

Step 1. At the minimum in E, small changes in x and y lead to no change in E:



$$\therefore\, dE = \frac{\partial E}{\partial x}dx + \frac{\partial E}{\partial y}dy = 0 \tag{3.53}$$

Step 2. The constraint equation, however, says that dx and dy cannot be varied independently (since the constraint equation is independent, or different, from E). Since $\phi(x, y) = 0$ for all x, y, then so must $d\phi(x, y) = 0$. But,

$$d\phi = \frac{\partial \phi}{\partial x}dx + \frac{\partial \phi}{\partial y}dy = 0 \tag{3.54}$$

Step 3. Form the weighted sum of (3.53) and (3.54) as

$$dE + \lambda d\phi = \left(\frac{\partial E}{\partial x} + \lambda\frac{\partial \phi}{\partial x}\right)dx + \left(\frac{\partial E}{\partial y} + \lambda\frac{\partial \phi}{\partial y}\right)dy = 0 \tag{3.55}$$

where λ is a constant. Note that (3.55) holds for arbitrary λ.

Step 4. If λ is chosen, however, in such a way that

$$\frac{\partial E}{\partial x} + \lambda\frac{\partial \phi}{\partial x} = 0 \tag{3.56}$$

then it follows that

$$\frac{\partial E}{\partial y} + \lambda\frac{\partial \phi}{\partial y} = 0 \tag{3.57}$$

since at least one of dx, dy (in this case, dy) is arbitrary (i.e., dy may be chosen nonzero).

When λ has been chosen as indicated above, it is called the Lagrange multiplier. Therefore, (3.55) above is equivalent to minimizing $E + \lambda\phi$ without any constraints, i.e.,

$$\frac{\partial}{\partial x}(E + \lambda\phi) = \frac{\partial E}{\partial x} + \lambda \frac{\partial \phi}{\partial x} = 0 \tag{3.58}$$

and

$$\frac{\partial}{\partial y}(E + \lambda\phi) = \frac{\partial E}{\partial y} + \lambda \frac{\partial \phi}{\partial y} = 0 \tag{3.59}$$

Step 5. Finally, one must still solve the constraint equation

$$\phi(x, y) = 0 \tag{3.60}$$

Thus, the solution for (x, y) that minimizes E subject to the constraint that $\phi(x, y) = 0$ is given by (3.58), (3.59), and (3.60).

That is, the problem has reduced to the following three equations:

$$\frac{\partial E}{\partial x} + \lambda \frac{\partial \phi}{\partial x} = 0 \tag{3.56}$$

$$\frac{\partial E}{\partial y} + \lambda \frac{\partial \phi}{\partial y} = 0 \tag{3.57}$$

and

$$\phi(x, y) = 0 \tag{3.60}$$

in the three unknowns (x, y, λ).

Extending the Problem to M Unknowns and N Constraints

The above procedure, used for a problem with two variables and one constraint, can be generalized to M unknowns in a vector $\mathbf{m}$ subject to N constraints $\phi_j(m) = 0$, $j = 1, \ldots, N$. This leads to the following system of M equations, $i = 1, \ldots, M$:

$$\frac{\partial E}{\partial m_i} + \sum_{j=1}^{N} \lambda_j \frac{\partial \phi_j}{\partial m_i} = 0 \tag{3.61}$$

with N constraints of the form

$$\phi_j(m) = 0 \tag{3.62}$$

3.6.3 Application to the Purely Underdetermined Problem

With the background we now have in Lagrange multipliers, we are ready to reconsider the purely underdetermined problem. First, we pose the following problem: find **m** such that $\mathbf{m}^{\mathrm{T}}\mathbf{m}$ is minimized subject to the N constraints that the data misfit be zero.

$$e_i = d_i^{\mathrm{obs}} - d_i^{\mathrm{pre}} = d_i^{\mathrm{obs}} - \sum_{j=1}^{M} G_{ij} m_j = 0, \; i = 1, \ldots, N \tag{3.63}$$

That is, minimize

$$\psi(\mathbf{m}) = \mathbf{m}^{\mathrm{T}}\mathbf{m} + \sum_{i=1}^{N} \lambda_i e_i \tag{3.64}$$

with respect to the elements m_i in **m**. We can expand the terms in Equation (3.64) and obtain

$$\psi(\mathbf{m}) = \sum_{k=1}^{M} m_k^2 + \sum_{i=1}^{N} \lambda_i \left[d_i - \sum_{j=1}^{M} G_{ij} m_j \right] \tag{3.65}$$

Then, we have

$$\frac{\partial \psi}{\partial m_q} = 2\sum_{k=1}^{M} \frac{\partial m_k}{\partial m_q} m_k - \sum_{i=1}^{N} \lambda_i \sum_{j=1}^{M} G_{ij} \frac{\partial m_j}{\partial m_q} \tag{3.66}$$

but

$$\frac{\partial m_k}{\partial m_q} = \delta_{kq} \qquad \text{and} \qquad \frac{\partial m_j}{\partial m_q} = \delta_{jq} \tag{3.67}$$

where δ_{ij} is the Kronecker delta, given by

$$\delta_{ij} = \begin{cases} 1, i = j \\ 0, i \neq j \end{cases}$$

Thus

$$\frac{\partial \psi}{\partial m_q} = 2m_q - \sum_{i=1}^{N} \lambda_i G_{iq} = 0 \qquad q = 1, 2, \ldots, M \tag{3.68}$$

In matrix notation over all q, Equation (3.68) can be written as

$$2\mathbf{m} - \mathbf{G}^{\mathrm{T}}\boldsymbol{\lambda} = \mathbf{0} \tag{3.69}$$

where $\boldsymbol{\lambda}$ is an $N \times 1$ vector containing the N Lagrange Multipliers λ_i, $i = 1, \ldots, N$. Note that $\mathbf{G}^T\boldsymbol{\lambda}$ has dimension $(M \times N)$ x $(N \times 1) = M \times 1$, as required to be able to subtract it from **m**.

Now, solving explicitly for **m** yields

$$\mathbf{m} = \tfrac{1}{2}\ \mathbf{G}^T\boldsymbol{\lambda} \tag{3.70}$$

The constraints in this case are that the data be fit exactly. That is,

$$\mathbf{d} = \mathbf{Gm} \tag{1.13}$$

Substituting (3.70) into (1.13) gives

$$\mathbf{d} = \mathbf{Gm} = \mathbf{G}(\tfrac{1}{2}\mathbf{G}^T\boldsymbol{\lambda}) \tag{3.71}$$

which implies

$$\mathbf{d} = \tfrac{1}{2}\mathbf{G}\mathbf{G}^T\boldsymbol{\lambda} \tag{3.72}$$

where $\mathbf{GG}^T$ has dimension $(N \times M) \times (M \times N)$, or simply $N \times N$. Solving for $\boldsymbol{\lambda}$, when $[\mathbf{GG}^T]^{-1}$ exists, yields

$$\boldsymbol{\lambda} = 2[\mathbf{GG}^T]^{-1}\mathbf{d} \tag{3.73}$$

The Lagrange Multipliers are not ends in and of themselves. But, upon substitution of Equation (3.73) into (3.70), we obtain

$$\mathbf{m} = \tfrac{1}{2}\mathbf{G}^T\boldsymbol{\lambda} = \tfrac{1}{2}\mathbf{G}^T\{2[\mathbf{GG}^T]^{-1}\}\mathbf{d} \tag{3.9}$$

Rearranging, we arrive at the *minimum length solution*, $\mathbf{m}_{\mathrm{ML}}$:

$$\mathbf{m}_{\mathrm{ML}} = \mathbf{G}^T[\mathbf{GG}^T]^{-1}\mathbf{d} \tag{3.74}$$

where $\mathbf{GG}^T$ is an $N \times N$ matrix and the minimum length operator, $\mathbf{G}^{-1}_{\mathrm{ML}}$, is given by

$$\mathbf{G}^{-1}_{\mathrm{ML}} = \mathbf{G}^T[\mathbf{GG}^T]^{-1} \tag{3.75}$$

The above procedure, then, is one that determines the solution which has the minimum length (L_2 norm = $[\mathbf{m}^T\mathbf{m}]^{1/2}$) amongst the infinite number of solutions that fit the data exactly. In practice, one does not actually calculate the values of the Lagrange multipliers, but goes directly to (3.74) above.

The above derivation shows that the length of **m** is minimized by the minimum length operator. It may make more sense to seek a solution that deviates as little as possible from some prior estimate of the solution, $<\mathbf{m}>$, rather than from zero. The zero vector is, in fact, the prior estimate $\langle \mathbf{m} \rangle$ for the minimum length solution given in Equation (3.74). If we wish to explicitly include $\langle \mathbf{m} \rangle$, then Equation (3.74) becomes

$$\mathbf{m}_{\mathrm{ML}} = \langle \mathbf{m} \rangle + \mathbf{G}^{\mathrm{T}}[\mathbf{G}\mathbf{G}^{\mathrm{T}}]^{-1}[\mathbf{d} - \mathbf{G}\langle \mathbf{m} \rangle]$$

$$= \langle \mathbf{m} \rangle + \mathbf{G}_{\mathrm{ML}}^{-1}[\mathbf{d} - \mathbf{G}\langle \mathbf{m} \rangle] = \mathbf{G}_{\mathrm{ML}}^{-1}\mathbf{d} + [\mathbf{I} - \mathbf{G}_{\mathrm{ML}}^{-1}\mathbf{G}]\langle \mathbf{m} \rangle \tag{3.76}$$

We note immediately that Equation (3.76) reduces to Equation (3.74) when $\langle \mathbf{m} \rangle = \mathbf{0}$.

3.6.4 Comparison of Least Squares and Minimum Length Solutions

In closing this section, it is instructive to note the similarity in form between the minimum length and least squares solutions:

Least Squares:
$$\mathbf{m}_{\mathrm{LS}} = [\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{d} \tag{3.31}$$

with
$$\mathbf{G}_{\mathrm{LS}}^{-1} = [\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}} \tag{3.32}$$

Minimum Length:
$$\mathbf{m}_{\mathrm{ML}} = \langle \mathbf{m} \rangle + \mathbf{G}^{\mathrm{T}}[\mathbf{G}\mathbf{G}^{\mathrm{T}}]^{-1}[\mathbf{d} - \mathbf{G}\langle \mathbf{m} \rangle] \tag{3.76}$$

with
$$\mathbf{G}_{\mathrm{ML}}^{-1} = \mathbf{G}^{\mathrm{T}}[\mathbf{G}\mathbf{G}^{\mathrm{T}}]^{-1} \tag{3.75}$$

The minimum length solution exists when $[\mathbf{G}\mathbf{G}^{\mathrm{T}}]^{-1}$ exists. Since $\mathbf{G}\mathbf{G}^{\mathrm{T}}$ is $N \times N$, this is the same as saying when $\mathbf{G}\mathbf{G}^{\mathrm{T}}$ has rank N. That is, when the N rows (or N columns) are **independent**. In this case, your ability to "predict" or "calculate" each of the N observations is independent.

3.6.5 Example of Minimum Length Problem

Recall the four-parameter, four-observation tomography problem we introduced in Section 3.4.4. At that time, we noted that the least squares solution did not exist because $[\mathbf{G}^{\mathrm{T}}\mathbf{G}]^{1}$ does not exist, since **G** does not contain enough information to solve for 4 model parameters. In the same way, **G** does not contain enough information to fit an arbitrary 4 observations, and $[\mathbf{G}\mathbf{G}^{\mathrm{T}}]^{-1}$ does not exist either for this example. The basic problem is that the four paths through the structure do not provide independent information. However, if we eliminate any one observation (let's say the fourth), then we reduce the problem to one where the minimum length solution exists. In this new case, we have three observations and four unknown model parameters, and hence $N < M$. **G**, which still has enough information to determine three observations uniquely, is now given by

$$\mathbf{G} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \tag{3.77}$$

And $\mathbf{GG}^T$ is given by

$$\mathbf{GG}^T = \begin{bmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \tag{3.78}$$

Now $[\mathbf{GG}^T]^{-1}$ does exist, and we have

$$\mathbf{G}^T[\mathbf{GG}^T]^{-1} = \begin{bmatrix} 0.25 & -0.25 & 0.5 \\ 0.75 & 0.25 & -0.5 \\ -0.25 & 0.25 & 0.5 \\ 0.25 & 0.75 & -0.5 \end{bmatrix} \tag{3.79}$$

If we assume a true model given by $\mathbf{m} = [1.0, 0.5, 0.5, 0.5]^T$, then the data are given by $\mathbf{d} = [1.5, 1.0, 1.5]^T$. The minimum length solution $\mathbf{m}_{ML}$ is given by

$$\mathbf{m}_{ML} = \mathbf{G}^T[\mathbf{GG}^T]^{-1}\mathbf{d} = [0.875, 0.625, 0.625, 0.375]^T \tag{3.80}$$

Note that the minimum length solution is not the "true" solution. This is generally the case, since the "true" solution is only one of an infinite number of solutions that fit the data exactly, and the minimum length solution is the one of shortest length. The length squared of the "true" solution is 1.75, while the length squared of the minimum length solution is 1.6875. Note also that the minimum length solution varies from the "true" solution by $[-0.125, 0.125, 0.125, -0.125]^T$. This is the same direction in model space (i.e., $[-1, 1, 1, -1]^T$) that represents the linear combination of the original columns of **G** in the example in Section 3.4.4 that add to zero. We will return to this subject when we have introduced singular value decomposition and the partitioning of model and data space.

3.7 Weighted Measures of Length

3.7.1 Introduction

One way to improve our estimates using either the least squares solution

$$\mathbf{m}_{LS} = [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d} \tag{3.31}$$

or the minimum length solution

$$\mathbf{m}_{ML} = \langle\mathbf{m}\rangle + \mathbf{G}^T[\mathbf{GG}^T]^{-1}[\mathbf{d} - \mathbf{G}\langle\mathbf{m}\rangle] \tag{3.76}$$

is to use *weighted* measures of the misfit vector

$$\mathbf{e} = \mathbf{d}^{\text{obs}} - \mathbf{d}^{\text{pre}} \tag{3.81}$$

or the model parameter vector **m**, respectively. The next two subsections will deal with these two approaches.

3.7.2 Weighted Least Squares

Weighted Measures of the Misfit Vector **e**

We saw in Section 3.4 that the least squares solution $\mathbf{m}_{\text{LS}}$ was the one that minimized the total misfit between predicted and observed data in the L_2 norm sense. That is, E in

$$E = \mathbf{e}^{\text{T}}\mathbf{e} = \begin{bmatrix} e_1 & e_2 & \cdots & e_N \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_N \end{bmatrix} = \sum_{i=1}^{N} e_i^2 \tag{3.7}$$

is minimized.

Consider a new E, defined as follows:

$$E = \mathbf{e}^{\text{T}}\mathbf{W}_e\mathbf{e} \tag{3.82}$$

and where $\mathbf{W}_e$ is an, as yet, unspecified $N \times N$ weighting matrix. $\mathbf{W}_e$ can take any form, but one convenient choice is

$$\mathbf{W}_e = [\text{cov}\ \mathbf{d}]^{-1} \tag{3.83}$$

where $[\text{cov}\ \mathbf{d}]^{-1}$ is the inverse of the covariance matrix for the data. With this choice for the weighting matrix, data with large variances are weighted less than ones with small variances. While this is true in general, it is easier to show in the case where $\mathbf{W}_e$ is diagonal. This happens when [cov **d**] is diagonal, which implies that the errors in the data are uncorrelated. The diagonal entries in $[\text{cov}\ \mathbf{d}]^{-1}$ are then given by the reciprocal of the diagonal entries in [cov **d**]. That is, if

$$[\text{cov}\,\mathbf{d}] = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \sigma_N^2 \end{bmatrix} \tag{3.84}$$

then

$$[\mathrm{cov}\,\mathbf{d}]^{-1} = \begin{bmatrix} \sigma_1^{-2} & 0 & \cdots & 0 \\ 0 & \sigma_2^{-2} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \sigma_N^{-2} \end{bmatrix} \tag{3.85}$$

With this choice for $\mathbf{W}_e$, the weighted misfit becomes

$$E = \mathbf{e}^{\mathrm{T}}\mathbf{W}_e\mathbf{e} = \sum_{i=1}^{N}\left[e_i \sum_{j=1}^{N} W_{ij} e_j \right] \tag{3.86}$$

But,

$$W_{ij} = \delta_{ij} \frac{1}{\sigma_i^2} \tag{3.87}$$

where δ_{ij} is the Kronecker delta. Thus, we have

$$E = \sum_{i=1}^{N} \frac{1}{\sigma_i^2} e_i^2 \tag{3.88}$$

If the *i*th variance σ_i^2 is large, then the component of the error vector in the *i*th direction, e_i^2, has little influence on the size of *E*. This is not the case in the unweighted least squares problem, where an examination of Equation (3.4) clearly shows that each component of the error vector contributes equally to the total misfit.

Obtaining the Weighted Least Squares Solution $\mathbf{m}_{\mathrm{WLS}}$

If one uses $E = \mathbf{e}^{\mathrm{T}}\mathbf{W}_e\mathbf{e}$ as the weighted measure of error, we will see below that this leads to the weighted least squares solution:

$$\mathbf{m}_{\mathrm{WLS}} = [\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{d} \tag{3.89}$$

with a weighted least squares operator $\mathbf{G}_{\mathrm{WLS}}^{-1}$ given by

$$\mathbf{G}_{\mathrm{WLS}}^{-1} = [\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{W}_e \tag{3.90}$$

While this is true in general, it is easier to arrive at Equation (3.89) in the case where $\mathbf{W}_e$ is a diagonal matrix and the forward problem $\mathbf{d} = \mathbf{Gm}$ is given by the least squares problem for a best-fitting straight line [see Equation (3.9)].

Step 1.

$$E = \mathbf{e}^{\mathrm{T}}\mathbf{W}_e\mathbf{e} = \sum_{i=1}^{N}\left[e_i\sum_{j=1}^{N}W_{ij}e_j\right] = \sum_{i=1}^{N}W_{ii}e_i^2 \tag{3.91}$$

$$= \sum_{i=1}^{N}W_{ii}\left(d_i^{\mathrm{obs}} - d_i^{\mathrm{pre}}\right)^2 = \sum_{i=1}^{N}W_{ii}\left[d_i - \sum_{j=1}^{M}G_{ij}m_j\right]^2 \tag{3.92}$$

$$= \sum_{i=1}^{N}W_{ii}\left(d_i^2 - 2m_1d_i - 2m_2d_iz_i + m_1^2 + 2m_1m_2z_i + m_2^2z_i^2\right) \tag{3.93}$$

Step 2. Then

$$\frac{\partial E}{\partial m_1} = -2\sum_{i=1}^{N}d_iW_{ii} + 2m_1\sum_{i=1}^{N}W_{ii} + 2m_2\sum_{i=1}^{N}z_iW_{ii} = 0 \tag{3.94}$$

and

$$\frac{\partial E}{\partial m_2} = -2\sum_{i=1}^{N}d_iz_iW_{ii} + 2m_1\sum_{i=1}^{N}z_iW_{ii} + 2m_2\sum_{i=1}^{N}z_i^2W_{ii} = 0 \tag{3.95}$$

This can be written in matrix form as

$$\begin{bmatrix} \sum_{i=1}^{N}W_{ii} & \sum_{i=1}^{N}z_iW_{ii} \\ \sum_{i=1}^{N}z_iW_{ii} & \sum_{i=1}^{N}z_i^2W_{ii} \end{bmatrix}\begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N}d_iW_{ii} \\ \sum_{i=1}^{N}z_id_iW_{ii} \end{bmatrix} \tag{3.96}$$

Step 3. The left-hand side can be factored as

$$\begin{bmatrix} \sum W_{ii} & \sum z_iW_{ii} \\ \sum z_iW_{ii} & \sum z_i^2W_{ii} \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \end{bmatrix}\begin{bmatrix} W_{11} & 0 & \cdots & 0 \\ 0 & W_{22} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & W_{NN} \end{bmatrix}\begin{bmatrix} 1 & z_1 \\ 1 & z_2 \\ \vdots & \vdots \\ 1 & z_N \end{bmatrix} \tag{3.97}$$

or simply

$$\begin{bmatrix} \sum W_{ii} & \sum z_iW_{ii} \\ \sum z_iW_{ii} & \sum z_i^2W_{ii} \end{bmatrix} = \mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G} \tag{3.98}$$

Similarly, the right-hand side can be factored as

$$\begin{bmatrix} \sum d_i W_{ii} \\ \sum d_i z_i W_{ii} \end{bmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ z_1 & z_2 & \cdots & z_N \end{bmatrix} \begin{bmatrix} W_{11} & 0 & \cdots & 0 \\ 0 & W_{22} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & W_{NN} \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_N \end{bmatrix} \tag{3.99}$$

or simply

$$\begin{bmatrix} \sum d_i W_{ii} \\ \sum d_i z_i W_{ii} \end{bmatrix} = \mathbf{G}^{\mathrm{T}} \mathbf{W}_e \mathbf{d} \tag{3.100}$$

Step 4. Therefore, using Equations (3.98) and (3.100), Equation (3.96) can be written as

$$\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G}\mathbf{m} = \mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{d} \tag{3.101}$$

The weighted least squares solution, $\mathbf{m}_{\mathrm{WLS}}$ from Equation (3.89) is thus

$$\mathbf{m}_{\mathrm{WLS}} = [\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G}]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{d} \tag{3.102}$$

assuming that $[\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G}]^{-1}$ exists, of course.

3.7.3 Weighted Minimum Length

The development of a weighted minimum length solution is similar to that of the weighted least squares problem. The steps are as follows.

First, recall that the minimum length solution minimizes $\mathbf{m}^{\mathrm{T}}\mathbf{m}$. By analogy with weighted least squares, we can choose to minimize

$$\mathbf{m}^{\mathrm{T}}\mathbf{W}_m\mathbf{m} \tag{3.103}$$

instead of $\mathbf{m}^{\mathrm{T}}\mathbf{m}$. For example, if one wishes to use

$$\mathbf{W}_m = [\mathrm{cov}\ \mathbf{m}]^{-1} \tag{3.104}$$

then one must replace **m** above with

$$\mathbf{m} - \langle\mathbf{m}\rangle \tag{3.105}$$

where **<m>** is the expected, or *a priori*, estimate for the parameter values. The reason for this is that the variances must represent fluctuations about zero. In the weighted least squares problem, it is assumed that the error vector **e** which is being minimized has a mean of zero. Thus, for the weighted minimum length problem, we replace **m** by its departure from the expected value **<m>**. Therefore, we introduce a new function L to be minimized:

$$L = [\mathbf{m} - \langle\mathbf{m}\rangle]^T \mathbf{W}_m [\mathbf{m} - \langle\mathbf{m}\rangle] \tag{3.106}$$

If one then follows the procedure in Section 3.6 with this new function, one eventually (as in "It is left to the student as an exercise!!") is led to the weighted minimum length solution $\mathbf{m}_{\mathrm{WML}}$ given by

$$\mathbf{m}_{\mathrm{WML}} = \langle\mathbf{m}\rangle + \mathbf{W}_m^{-1}\mathbf{G}^T[\mathbf{G}\mathbf{W}_m^{-1}\mathbf{G}^T]^{-1}[\mathbf{d} - \mathbf{G}\langle\mathbf{m}\rangle] \tag{3.107}$$

and the weighted minimum length operator, $\mathbf{G}_{\mathrm{WML}}^{-1}$, is given by

$$\mathbf{G}_{\mathrm{WML}}^{-1} = \mathbf{W}_m^{-1}\mathbf{G}^T[\mathbf{G}\mathbf{W}_m^{-1}\mathbf{G}^T]^{-1} \tag{3.108}$$

This expression differs from Equation (3.38), page 54 of Menke, which uses $\mathbf{W}_m$ rather than $\mathbf{W}_m^{-1}$. I believe Menke's equation is wrong. Note that the solution depends explicitly on the expected, or *a priori*, estimate of the model parameters **<m>**. The second term represents a departure from the *a priori* estimate **<m>**, based on the inadequacy of the forward problem **G<m>** to fit the data **d** exactly.

Other choices for $\mathbf{W}_m$ include:

1. $\mathbf{D}^T\mathbf{D}$, where **D** is a derivative matrix (a measure of the flatness of **m**) of dimension $(M - 1) \times M$:

$$\mathbf{D} = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{bmatrix} \tag{3.109}$$

2. $\mathbf{D}^T\mathbf{D}$, where **D** is an $(M - 2) \times M$ roughness (second derivative) matrix given by

$$\mathbf{D} = \begin{bmatrix} 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 & -2 & 1 \end{bmatrix} \tag{3.110}$$

Note that for both choices of **D** presented, $\mathbf{D}^T\mathbf{D}$ is an $M \times M$ matrix of rank less than M (for the first-derivative case, it is of rank $M - 1$, while for the second it is of rank $M - 2$). This means that $\mathbf{W}_m$ does not have a mathematical inverse. This can introduce some nonuniqueness into the solution, but does not preclude finding a solution. Finally, note that many choices for $\mathbf{W}_m$ are possible.

3.7.4 Weighted Damped Least Squares

In Sections 3.7.2 and 3.7.3 we considered weighted versions of the least squares and minimum length solutions. Both unweighted and weighted problems can be very unstable if the matrices that have to be inverted are nearly singular. In the weighted problems, these are

$$\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G} \tag{3.111}$$

and

$$\mathbf{G}\mathbf{W}_m^{-1}\,\mathbf{G}^{\mathrm{T}} \tag{3.112}$$

respectively, for least squares and minimum length problems. In this case, one can form a weighted penalty, or cost function, given by

$$E + \varepsilon^2 L \tag{3.113}$$

where E is from Equation (3.91) for weighted least squares and L is from Equation (3.106) for the weighted minimum length problem. One then goes through the exercise of minimizing Equation (3.113) with respect to the model parameters $\mathbf{m}$, and obtains what is known as the weighted, damped least squares solution $\mathbf{m}_{\mathrm{WD}}$. It is, in fact, a weighted mix of the weighted least squares and weighted minimum length solutions.

One finds that $\mathbf{m}_{\mathrm{WD}}$ is given by either

$$\mathbf{m}_{\mathrm{WD}} = <\mathbf{m}> + [\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G} + \varepsilon^2\mathbf{W}_m]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{W}_e[\mathbf{d} - \mathbf{G}<\mathbf{m}>] \tag{3.114}$$

or

$$\mathbf{m}_{\mathrm{WD}} = <\mathbf{m}> + \mathbf{W}_m^{-1}\,\mathbf{G}^{\mathrm{T}}[\mathbf{G}\mathbf{W}_m^{-1}\,\mathbf{G}^{\mathrm{T}} + \varepsilon^2\mathbf{W}_e^{-1}]^{-1}[\mathbf{d} - \mathbf{G}<\mathbf{m}>] \tag{3.115}$$

where the weighted, damped least squares operator, $\mathbf{G}_{\mathrm{WD}}^{-1}$, is given by

$$\mathbf{G}_{\mathrm{WD}}^{-1} = [\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G} + \varepsilon^2\mathbf{W}_m]^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{W}_e \tag{3.116}$$

or

$$\mathbf{G}_{\mathrm{WD}}^{-1} = \mathbf{W}_m^{-1}\,\mathbf{G}^{\mathrm{T}}[\mathbf{G}\mathbf{W}_m^{-1}\,\mathbf{G}^{\mathrm{T}} + \varepsilon^2\mathbf{W}_e^{-1}]^{-1} \tag{3.117}$$

The two forms for $\mathbf{G}_{\mathrm{WD}}^{-1}$ can be shown to be equivalent. The ε^2 term has the effect of damping the instability. As we will see later in Chapter 6 using *singular-value decomposition*, the above procedure minimizes the effects of small singular values in $\mathbf{G}^{\mathrm{T}}\mathbf{W}_e\mathbf{G}$ or $\mathbf{G}\mathbf{W}_m^{-1}\,\mathbf{G}^{\mathrm{T}}$.

In the next section we will learn two methods of including *a priori* information and constraints in inverse problems.

3.8 *A Priori* Information and Constraints
(See Menke, Pages 55–57)

3.8.1 Introduction

Another common type of *a priori* information takes the form of *linear equality constraints*:

$$\mathbf{Fm} = \mathbf{h} \tag{3.118}$$

where $\mathbf{F}$ is a $P \times M$ matrix, and P is the number of linear constraints considered. As an example, consider the case for which the mean of the model parameters is known. In this case with only one constraint, we have

$$\frac{1}{M}\sum_{i=1}^{M} m_i = h_1 \tag{3.119}$$

Then, Equation (3.118) can be written as

$$\mathbf{Fm} = \frac{1}{M}\begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix}\begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_M \end{bmatrix} = h_1 \tag{3.120}$$

As another example, suppose that the jth model parameter m_j is actually known in advance. That is, suppose

$$m_j = h_1 \tag{3.121}$$

Then Equation (3.118) takes the form

$$\mathbf{Fm} = \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{bmatrix}\begin{bmatrix} m_1 \\ \vdots \\ m_j \\ \vdots \\ m_M \end{bmatrix} = h_1 \tag{3.122}$$

$$\Uparrow$$

jth column

Note that for this example it would be possible to remove m_j as an unknown, thereby reducing the system of equations by one. It is often preferable to use Equation (3.122), even in this case, rather than rewriting the forward problem in a computer code.

3.8.2 A First Approach to Including Constraints

We will consider two basic approaches to including constraints in inverse problems. Each has its strengths and weaknesses. The first includes the constraint matrix **F** in the forward problem, and the second uses Lagrange multipliers. The steps for the first approach are as follows.

Step 1. Include **Fm** = **h** as rows in a new **G** that operates on the original **m**:

$$\underset{(N+P)\times M}{\begin{bmatrix} \mathbf{G} \\ \mathbf{F} \end{bmatrix}} \quad \underset{M \times 1}{\begin{bmatrix} m_1 \\ m_2 \\ \vdots \\ m_M \end{bmatrix}} = \underset{(N+P)\times 1}{\begin{bmatrix} \mathbf{d} \\ \mathbf{h} \end{bmatrix}} \tag{3.123}$$

Step 2. The new $(N + P) \times 1$ misfit vector **e** becomes

$$\mathbf{e} = \underset{(N+P)\times 1}{\begin{bmatrix} \mathbf{d}^{\text{obs}} \\ \mathbf{h} \end{bmatrix}} - \underset{(N+P)\times 1}{\begin{bmatrix} \mathbf{d}^{\text{pre}} \\ \mathbf{h}^{\text{pre}} \end{bmatrix}} \tag{3.124}$$

Performing a least squares inversion would minimize the new $\mathbf{e}^{\text{T}}\mathbf{e}$, based on Equation (3.124). The difference

$$\mathbf{h} - \mathbf{h}^{\text{pre}} \tag{3.125}$$

which represents the misfit to the constraints, may be small, but it is unlikely that it would vanish, which it must if the constraints are to be satisfied.

Step 3. Introduce a weighted misfit:

$$\mathbf{e}^{\text{T}}\mathbf{W}_e\mathbf{e} \tag{3.126}$$

where $\mathbf{W}_e$ is a diagonal matrix of the form

$$W_e = \left[\begin{array}{cccc|cccc} 1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & & 0 & 0 & 0 & & 0 \\ \vdots & & \ddots & \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & \cdots & 0 & (\text{big}\ \#) & 0 & \cdots & 0 \\ 0 & 0 & & 0 & 0 & (\text{big}\ \#) & & \vdots \\ \vdots & & \ddots & \vdots & \vdots & & \ddots & 0 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & (\text{big}\ \#) \end{array}\right] \begin{array}{c} \uparrow \\ N \\ \downarrow \\ \uparrow \\ P \\ \downarrow \end{array} \tag{3.127}$$

That is, it has relatively large values for the last P entries associated with the constraint equations. Recalling the form of the weighting matrix used in Equation (3.83), one sees that Equation (3.127) is equivalent to assigning the constraints very small variances. Hence, a weighted least squares approach in this case will give large weight to fitting the constraints. The size of the big numbers in $\mathbf{W}_e$ must be determined empirically. One seeks a number that leads to a solution that satisfies the constraints acceptably, but does not make the matrix in Equation (3.111) that must be inverted to obtain the solution too poorly conditioned. Matrices with a large range of values in them tend to be poorly conditioned.

Consider the example of the smoothing constraint here, $P = M - 2$:

$$\mathbf{Dm} = \mathbf{0} \tag{3.128}$$

where the dimensions of $\mathbf{D}$ =(M – 2) × m, $\mathbf{m}$ = M × 1, and $\mathbf{0}$ = (M – 2) × 1. The augmented equations are

$$\begin{bmatrix} \mathbf{G} \\ \mathbf{D} \end{bmatrix} \mathbf{m} = \begin{bmatrix} \mathbf{d} \\ \mathbf{0} \end{bmatrix} \tag{3.129}$$

Let's use the following weighting matrix:

$$\mathbf{W}_e = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & & & 0 \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \theta^2 & 0 \\ 0 & \cdots & \cdots & 0 & \theta^2 \end{bmatrix} = \left[\begin{array}{c|c} \mathbf{I}_{N\times N} & 0 \\ \hline 0 & \theta^2 \mathbf{I}_{P\times P} \end{array}\right] \tag{3.130}$$

where θ^2 is a constant. This results in the following, with the dimensions of the three matrices in the first set of brackets being $M \times (N + P)$, $(N + P) \times (N + P)$, and $(N + P) \times M$, respectively:

$$\mathbf{m}_{\text{WLS}} = \left\{ \left[\frac{\mathbf{G}}{\mathbf{D}}\right]^{\text{T}} \left[\begin{array}{c|c} \mathbf{I} & \mathbf{0} \\ \hline \mathbf{0} & \theta^2\mathbf{I} \end{array}\right] \left[\frac{\mathbf{G}}{\mathbf{D}}\right] \right\}^{-1} \left[\frac{\mathbf{G}}{\mathbf{D}}\right]^{\text{T}} \left[\begin{array}{c|c} \mathbf{I} & \mathbf{0} \\ \hline \mathbf{0} & \theta^2\mathbf{I} \end{array}\right] \left[\frac{\mathbf{d}}{\mathbf{0}}\right]$$

$$\underbrace{\left[\ \mathbf{G}^{\text{T}}\ \middle|\ \theta^2\mathbf{D}^{\text{T}}\ \right]}_{} \qquad \underbrace{\left[\ \mathbf{G}^{\text{T}}\ \middle|\ \theta^2\mathbf{D}^{\text{T}}\ \right]}_{}$$

The lower matrices having dimensions of $M \times (N+ P\,) \,|\, (N + P) \times 1$.

$$= [\mathbf{G}^{\text{T}}\mathbf{G} + \theta^2\mathbf{D}^{\text{T}}\mathbf{D}]^{-1}\ [\ \mathbf{G}^{\text{T}}\mathbf{d}] \tag{3.131}$$

$$\qquad M \times M \qquad\qquad M \times 1$$

$$= \left\{ \begin{bmatrix} \mathbf{G} \\ \theta\mathbf{D} \end{bmatrix}^{T} \begin{bmatrix} \mathbf{G} \\ \theta\mathbf{D} \end{bmatrix} \right\}^{-1} [\mathbf{G}^{\text{T}}\mathbf{d}] \tag{3.132}$$

The three matrices within (3.132) have dimensions $M \times (N + P)$, $(N + P) \times M$, and $M \times 1$, respectively, which produce an $M \times 1$ matrix when evaluated. In this form we can see this is simply the $\mathbf{m}_{\text{LS}}$ for the problem

$$\begin{bmatrix} \mathbf{G} \\ \theta\mathbf{D} \end{bmatrix} \mathbf{m} = \begin{bmatrix} \mathbf{d} \\ \mathbf{0} \end{bmatrix} \tag{3.133}$$

By varying θ, we can trade off the misfit and the smoothness for the model.

3.8.3 A Second Approach to Including Constraints

Whenever the subject of constraints is raised, Lagrange multipliers come to mind! The steps for this approach are as follows.

Step 1. Form a weighted sum of the misfit and the constraints:

$$\phi(\mathbf{m}) = \mathbf{e}^{\text{T}}\mathbf{e} + [\mathbf{Fm} - \mathbf{h}]^{\text{T}}\boldsymbol{\lambda} \tag{3.134}$$

which can be expanded as

$$\phi(\mathbf{m}) = \sum_{i=1}^{N} \left[d_i - \sum_{j=1}^{M} G_{ij} m_j \right]^2 + 2\sum_{i=1}^{P} \lambda_i \left[\sum_{j=1}^{M} F_{ij} m_j - h_i \right] \tag{3.135}$$

$$\quad\uparrow \qquad\qquad\qquad\qquad\qquad \uparrow$$

where $\uparrow$ indicates a difference from Equation (3.43) on page 56 in Menke, and where there are P linear equality constraints and where the factor of 2 as been added as a matter of convenience to make the form of the final answer simpler.

Step 2. One then takes the partials of Equation (3.135) with respect to all the entries in **m** and sets them to zero. That is,

$$\frac{\partial \phi(\mathbf{m})}{\partial m_q} = 0 \qquad q = 1, 2, \ldots, M \tag{3.136}$$

which leads to

$$2\sum_{i=1}^{M} m_i \sum_{j=1}^{N} G_{jq} G_{ji} - 2\sum_{i=1}^{N} G_{iq} d_i + 2\sum_{i=1}^{P} \lambda_i F_{iq} = 0 \qquad q = 1, 2, \ldots, M \tag{3.137}$$

where the first two terms are the same as the least squares case in Equation (3.25) since they come directly from $\mathbf{e}^{\mathrm{T}}\mathbf{e}$ and the last term shows why the factor of 2 was added in Equation (3.135).

Step 3. Equation (3.137) is not the complete description of the problem. To the *M* equations in Equation (3.137), *P* constraint equations must also be added. In matrix form, this yields

$$\begin{bmatrix} \mathbf{G}^T\mathbf{G} & \mathbf{F}^{\mathrm{T}} \\ \mathbf{F} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{m} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{G}^{\mathrm{T}}\mathbf{d} \\ \mathbf{h} \end{bmatrix} \tag{3.138}$$

$$(M+P) \times (M+P) \qquad (M+P) \times 1 \qquad (M+P) \times 1$$

Step 4. The above system of equations can be solved as

$$\begin{bmatrix} \mathbf{m} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{G}^T\mathbf{G} & \mathbf{F}^{\mathrm{T}} \\ \mathbf{F} & \mathbf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{G}^{\mathrm{T}}\mathbf{d} \\ \mathbf{h} \end{bmatrix} \tag{3.139}$$

As an example, consider constraining a straight line to pass through some point (z', d'). That is, for *N* observations, we have

$$d_i = m_1 + m_2 z_i \qquad i = 1, N \tag{3.140}$$

subject to the single constraint

$$d' = m_1 + m_2 z' \tag{3.141}$$

Then Equation (3.118) has the form

$$\mathbf{Fm} = [1 \quad z'] \begin{bmatrix} m_1 \\ m_2 \end{bmatrix} = d' \tag{3.142}$$

We can then write out Equation (3.139) explicitly, and obtain the following:

$$\begin{bmatrix} m_1 \\ m_2 \\ \lambda \end{bmatrix} = \begin{bmatrix} N & \sum z_i & 1 \\ \sum z_i & \sum z_i^2 & z' \\ 1 & z' & 0 \end{bmatrix}^{-1} \begin{bmatrix} \sum d_i \\ \sum z_i d_i \\ d' \end{bmatrix} \tag{3.143}$$

Note the similarity between Equations (3.143) and (3.36), the least squares solution to fitting a straight line to a set of points without any constraints:

$$\begin{bmatrix} m_1 \\ m_2 \end{bmatrix}_{\mathrm{LS}} = \begin{bmatrix} N & \sum z_i \\ \sum z_i & \sum z_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum d_i \\ \sum z_i d_i \end{bmatrix} \tag{3.36}$$

If you wanted to get the same result for the straight line passing through a point using the first approach with $\mathbf{W}_e$, you would assign

$$W_{ii} = 1 \qquad i = 1, \ldots, N \tag{3.144}$$

and

$$W_{N+1,\, N+1} = \text{big \#} \tag{3.145}$$

which is equivalent to assigning a small variance (relative to the unconstrained part of the problem) to the constraint equation. The solution obtained with Equation (3.103) should approach the solution obtained using Equation (3.143).

Note that it is easy to constrain lines to pass through the origin using Equation (3.143). In this case, we have

$$d' = z' = 0 \tag{3.146}$$

and Equation (3.143) becomes

$$\begin{bmatrix} m_1 \\ m_2 \\ \lambda \end{bmatrix} = \begin{bmatrix} N & \sum z_i & 1 \\ \sum z_i & \sum z_i^2 & 0 \\ 1 & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} \sum d_i \\ \sum z_i d_i \\ 0 \end{bmatrix} \tag{3.147}$$

The advantage of using the Lagrange multiplier approach to constraints is that the constraints will be satisfied exactly. It often happens, however, that the constraints are only approximately known, and using Lagrange multipliers to fit the constraints exactly may not be appropriate. An example might be a gravity inversion where depth to bedrock at one point is known from drilling. Constraining the depth to be exactly the drill depth may be misleading if the depth in the model is an average over some area. Then the exact depth at one point may not be the best estimate of the depth over the area in question. A second disadvantage of the Lagrange multiplier approach is that it adds one equation to the system of equations in Equation (3.143) for each constraint. This can add up quickly, making the inversion considerably more difficult computationally.

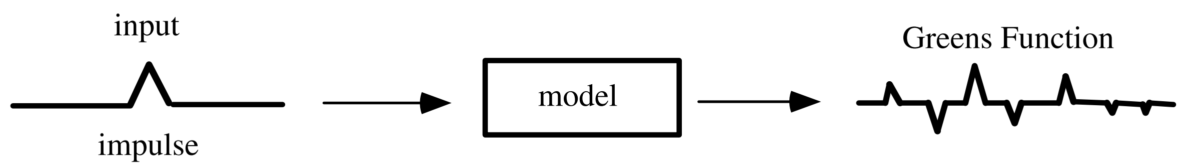
An entirely different class of constraints are called *linear inequality constraints* and take the form

$$\mathbf{Fm} \geq \mathbf{h} \tag{3.148}$$

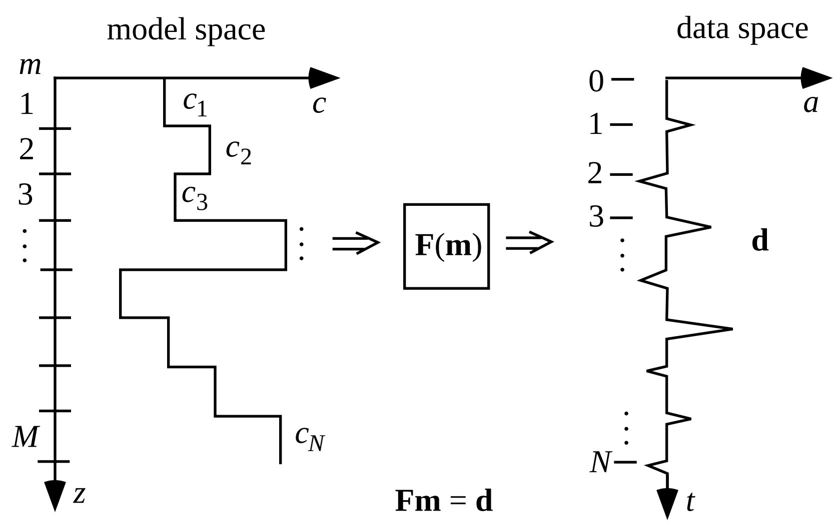
These can be solved using *linear programming* techniques, but we will not consider them further in this class.

3.8.4 Seismic Receiver Function Example

The following is an example of using smoothing constraints in an inverse problem. Consider a general problem in time series analysis, with a delta function input. Then the output from the "model" is the *Greens function* of the system. The inverse problem is this: Given the Greens function, find the parameters of the model.



In a little more concrete form:



If $\mathbf{d}$ is very noisy, then $\mathbf{m}_{LS}$ will have a high-frequency component to try to "fit the noise," but this will not be real. How do we prevent this? So far, we have learned two ways: use $\mathbf{m}_{WLS}$ if we know cov $\mathbf{d}$, or if not, we can place a smoothing constraint on $\mathbf{m}$. An example of this approach using receiver function inversions can be found in Ammon, C. J., G. E. Randall and G. Zandt, On the nonuniqueness of receiver function inversions, *J. Geophys. Res.*, *95*, 15,303-15,318, 1990.

The important points are as follows:

- This approach is used in the real world.
- The forward problem is written

$$d_j = F_j\mathbf{m} \qquad j = 1, 2, 3 \ldots N$$

- This is nonlinear, but after linearization (discussed in Chapter 4), the equations are the same as discussed previously (with minor differences).
- Note the correlation between the roughness in the model and the roughness in the data.
- The way to choose the weighting parameter, σ, is to plot the trade-off between smoothness and waveform fit.

3.9 Variances of Model Parameters
(See Pages 58–60, Menke)

3.9.1 Introduction

Data errors are mapped into model parameter errors through any type of inverse. We noted in Chapter 2 [Equations (2.61)–(2.63)] that if

$$\mathbf{m}^{\text{est}} = \mathbf{Md} + \mathbf{v} \tag{2.61}$$

and if [cov **d**] is the data covariance matrix which describes the data errors, then the *a posteriori* model covariance matrix is given by

$$[\text{cov}\,\mathbf{m}] = \mathbf{M}[\text{cov}\,\mathbf{d}]\mathbf{M}^{\text{T}} \tag{2.63}$$

The covariance matrix in Equation (2.63) is called the *a posteriori model covariance matrix* because it is calculated after the fact. It gives what are sometimes called the formal uncertainties in the model parameters. It is different from the *a priori* model covariance matrix of Equation (3.85), which is used to constrain the underdetermined problem.

The *a posteriori* covariance matrix in Equation (2.63) shows explicitly the mapping of data errors into uncertainties in the model parameters. Although the mapping will be clearer once we consider the generalized inverse in Chapter 7, it is instructive at this point to consider applying Equation (2.63) to the least squares and minimum length problems.

3.9.2 Application to Least Squares

We can apply Equation (2.63) to the least squares problem and obtain

$$[\text{cov } \mathbf{m}] = \{[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\}[\text{cov } \mathbf{d}]\{[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\}^T \tag{3.149}$$

Further, if [cov **d**] is given by

$$[\text{cov } \mathbf{d}] = \sigma^2\mathbf{I}_N \tag{3.150}$$

then

$$\begin{aligned}[\text{cov } \mathbf{m}] &= [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T[\sigma^2 \mathbf{I}]\{[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\}^T \\ &= \sigma^2 [\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{G}\{[\mathbf{G}^T\mathbf{G}]^{-1}\}^T \\ &= \sigma^2 \{[\mathbf{G}^T\mathbf{G}]^{-1}\}^T \\ &= \sigma^2 [\mathbf{G}^T\mathbf{G}]^{-1}\end{aligned} \tag{3.151}$$

since the transpose of a symmetric matrix returns the original matrix.

3.9.3 Application to the Minimum Length Problem

Application of Equation (2.63) to the minimum length problem leads to the following for the *a posteriori* model covariance matrix:

$$[\text{cov } \mathbf{m}] = \{\mathbf{G}^T[\mathbf{G}\mathbf{G}^T]^{-1}\}[\text{cov } \mathbf{d}]\{\mathbf{G}^T[\mathbf{G}\mathbf{G}^T]^{-1}\}^T \tag{3.152}$$

If the data covariance matrix is again given by

$$[\text{cov } \mathbf{d}] = \sigma^2 \mathbf{I}_N \tag{3.153}$$

we obtain

$$[\text{cov } \mathbf{m}] = \sigma^2 \mathbf{G}^T[\mathbf{G}\mathbf{G}^T]^{-2}\mathbf{G} \tag{3.154}$$

where

$$[\mathbf{G}\mathbf{G}^T]^{-2} = [\mathbf{G}\mathbf{G}^T]^{-1}[\mathbf{G}\mathbf{G}^T]^{-1} \tag{3.155}$$

3.9.4 Geometrical Interpretation of Variance

There is another way to look at the variance of model parameter estimates for the least squares problem that considers the prediction error, or misfit, to the data. Recall that we defined the misfit E as

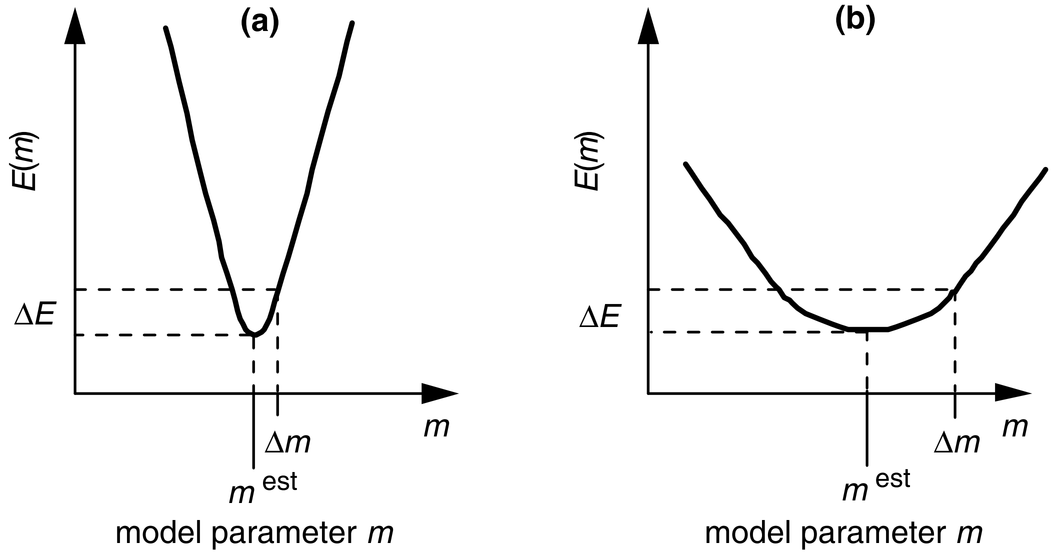
$$\begin{aligned}E = \mathbf{e}^T\mathbf{e} &= [\mathbf{d} - \mathbf{d}^{\text{pre}}]^T[\mathbf{d} - \mathbf{d}^{\text{pre}}] \\ &= [\mathbf{d} - \mathbf{Gm}]^T[\mathbf{d} - \mathbf{Gm}]\end{aligned} \tag{3.23}$$

which explicitly shows the dependence of E on the model parameters $\mathbf{m}$. That is, we have

$$E = E(\mathbf{m}) \tag{3.156}$$

If $E(\mathbf{m})$ has a sharp, well-defined minimum, then we can conclude that our solution $\mathbf{m}_{\mathrm{LS}}$ is well constrained. Conversely, if $E(\mathbf{m})$ has a broad, poorly defined minimum, then we conclude that our solution $\mathbf{m}_{\mathrm{LS}}$ is poorly constrained.

After Figure 3.10, page 59, of Menke, we have (next page),



(**a**) The best estimate m^{est} of model parameter m occurs at the minimum of $E(m)$. If the minimum is relatively narrow, then random fluctuations in $E(m)$ lead to only small errors Δm in m^{est}. (**b**) If the minimum is wide, then large errors in m can occur.

One way to quantify this qualitative observation is to realize that the width of the minimum for $E(\mathbf{m})$ is related to the curvature, or second derivative, of $E(\mathbf{m})$ at the minimum. For the least squares problem, we have

$$\left.\frac{\partial^2 E}{\partial \mathbf{m}^2}\right|_{\mathbf{m}=\mathbf{m}_{\mathrm{LS}}} = \left.\frac{\partial^2}{\partial \mathbf{m}^2}[\mathbf{d}-\mathbf{Gm}]^2\right|_{\mathbf{m}=\mathbf{m}_{\mathrm{LS}}} \tag{3.157}$$

Evaluating the right-hand side, we have for the qth term

$$\frac{\partial^2 E}{\partial m_q^2} = \frac{\partial^2}{\partial m_q^2}[\mathbf{d}-\mathbf{Gm}]^2 = \frac{\partial^2}{\partial m_q^2}\sum_{i=1}^{N}\left[d_i - \sum_{j=1}^{M} G_{ij} m_j\right]^2 \tag{3.158}$$

$$= \frac{\partial^2}{\partial m_q^2} 2\sum_{i=1}^{N}\left[d_i - \sum_{j=1}^{M} G_{ij} m_j\right](-G_{iq}) \tag{3.159}$$

$$= -2\frac{\partial^2}{\partial m_q^2}\sum_{i=1}^{N}\left[G_{iq}d_i - \sum_{j=1}^{M}G_{ij}G_{iq}m_j\right] \tag{3.160}$$

Using the same steps as we did in the derivation of the least squares solution in Equations (3.24)–(3.29), it is possible to see that Equation (3.160) represents the qth term in $\mathbf{G}^T[\mathbf{d} - \mathbf{Gm}]$. Combining the q equations into matrix notation yields

$$\frac{\partial^2}{\partial \mathbf{m}^2}[\mathbf{d}-\mathbf{Gm}]^2 = -2\frac{\partial}{\partial \mathbf{m}}\left\{\mathbf{G}^T[\mathbf{d}-\mathbf{Gm}]\right\} \tag{3.161}$$

Evaluating the first derivative on the right-hand side of Equation (3.161), we have for the qth term

$$\frac{\partial}{\partial m_q}\left\{\mathbf{G}^T[\mathbf{d}-\mathbf{Gm}]\right\} = \frac{\partial}{\partial m_q}\sum_{i=1}^{N}\left[G_{iq}d_i - \sum_{j=1}^{M}G_{ij}G_{iq}m_j\right] \tag{3.162}$$

$$= -\sum_{i=1}^{N}\sum_{j=1}^{M}\frac{\partial}{\partial m_q}\left(G_{ij}G_{iq}m_j\right) \tag{3.163}$$

$$= -\sum_{i=1}^{N}G_{iq}G_{iq} \tag{3.164}$$

which we recognize as the (q, q) entry in $\mathbf{G}^T\mathbf{G}$. Therefore, we can write the $M \times M$ matrix equation as

$$\frac{\partial}{\partial \mathbf{m}}\left\{\mathbf{G}^T[\mathbf{d}-\mathbf{Gm}]\right\} = -\mathbf{G}^T\mathbf{G} \tag{3.165}$$

From Equations (3.150)–(3.158) we can conclude that the second derivative of E in the least squares problem is proportional to $\mathbf{G}^T\mathbf{G}$. That is,

$$\left.\frac{\partial^2 E}{\partial \mathbf{m}^2}\right|_{\mathbf{m}=\mathbf{m}_{\mathrm{LS}}} = (\text{constant})\mathbf{G}^T\mathbf{G} \tag{3.166}$$

Furthermore, from Equation (3.150) we have that [cov **m**] is proportional to $[\mathbf{G}^T\mathbf{G}]^{-1}$. Therefore, we can associate large values of the second derivative of E, given by (3.166) with (1) "sharp" curvature for E, (2) "narrow" well for E, and (3) "good" (i.e., small) model variance.

As Menke points out, [cov **m**] can be interpreted as being controlled either by (1) the variance of the data times a measure of how error in the data is mapped into model parameters or (2) a constant times the curvature of the prediction error at its minimum.

I like Menke's summary for his chapter (page 60) on this material very much. Hence, I've reproduced his closing paragraph for you as follows:

> *The methods of solving inverse problems that have been discussed in this chapter emphasize the data and model parameters themselves. The method of least squares estimates the model parameters with smallest prediction length. The method of minimum length estimates the simplest model parameters. The ideas of data and model parameters are very concrete and straightforward, and the methods based on them are simple and easily understood. Nevertheless, this viewpoint tends to obscure an important aspect of inverse problems. Namely, that the nature of the problem depends more on the relationship between the data and model parameters than on the data or model parameters themselves. It should, for instance, be possible to tell a well-designed experiment from a poorly designed one without knowing what the numerical values of the data or model parameters are, or even the range in which they fall.*

Before considering the relationships implied in the mapping between model parameters and data in Chapter 5, we extend what we now know about linear inverse problems to nonlinear problems in the next chapter.