The Problem

If the matrix M of ray-path lengths through the cells has been predetermined, our basic inversion problem looks like this:

$$Ms = t,$$

having the formal solution

$$s = M^{-1}t.$$

Of course, if life were this simple, we would *not* be having this summer school.

Why We Must Work Hard

The problems are these:

1. If M is square, it is usually not invertible (i.e., it is singular).

2. More commonly M is not square, so some generalized inverse is required.

The Least Squares Formulation

By far the most common approach to solving these types of data inversion probelms is Least Squares. First, we define a nonnegative functional

$$\mathcal{F}(s) = (t - Ms)^T(t - Ms),$$

where we think of the term Ms as the vector of predicted data, while t is the vector of real data. So $\mathcal{F}(s)$ is the sum of the squares of the discrepancies (errors). If $\mathcal{F} \equiv 0$, then we may have solved our problem. If $\mathcal{F} \neq 0$, then we have not solved our problem, but for small enough $\mathcal{F}$ we might be close to solving it.

The Least Squares Solution

Taking the derivative of $\mathcal{F}$ with respect to s, we can find the choice of s giving the minimum value of the squared error, which is determined by:

$$M^T M s = M^T t.$$

This expression is commonly known as the normal equation for least-squares, and the matrix $M^T M$ the normal matrix for the least-squares problem. Note that this formula still does not give us a direct formula for s. We still need to solve a matrix inversion problem, and the normal matrix may still be singular. But at least it is square!

Two Important Cases

There are two important case to consider at first for finding the solution of the normal equation:
(1) $m > n$ and (2) $m < n$.

In the first case we have more data (m) than unknowns (n). In the second case we have more unknowns (n) than data (m). These situations are often referred to as being "overdetermined" and "underdetermined," respectively. The conditions (1) and (2) are in fact "sufficient" to guarantee that the problem is over- or underdetermined, but not necessary.

More Precise Language

In truth the language "overdetermined" and "underdetermined" should be made more precise. Bill Symes will introduce some more sophisticated language in the next lecture. We will try to clarify the issue by pointing out that the number of data may be "insufficient" to determine the model in the "underdetermined" case, and that "inconsistent" data certainly exist in the data space when the problem is "overdetermined." For example, consider fitting a straight line to 1, 2, or 3 data points.

Inconsistent Data

A separate but important issue is that the measured data may themselves be "inconsistent," by which we mean that no model within the chosen model parameterization may be able to result in this data.

Consequences of Being Over-/Underdetermined

Overdetermined:

When $m > n$, we must have the $m \times m$ matrix

$$MM^T \text{ being singular.}$$

Underdetermined:

When $m < n$, we must have the $n \times n$ matrix

$$M^TM \text{ being singular.}$$

It appears that the underdetermined case is always a problem, because the normal matrix is singular.

For the Sake of Argument:

Let us assume for the moment that the one or the other of the inverses

$$[M^T M]^{-1}$$

$$[M M^T]^{-1}$$

exists. This does not have to be true for real problems and, in fact, it is fair to say that this usually is not true. In typical problems, neither inverse exists.

Formal Solutions for Least Squares

Formal solutions can be given to both types of these least-squares problems.

$$\text{Overdetermined: } s = [M^T M]^{-1} M^T t$$
$$\text{Underdetermined: } s = M^T [M M^T]^{-1} t$$

Note that the solution for the overdetermined case solves just the normal equations, while the solution for the underdetermined case is also a formal solution for the original problem: $Ms = t$.