Lecture Notes on

Nonlinear Inversion and Tomography:

I. Borehole Seismic Tomography

From a Series of Lectures by

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Chapter 4

Algorithms for Linear Inversion

In Chapter 3, much of our effort was expended showing that least-squares methods generally produce *infeasible models* in traveltime inversion, *i.e.*, models that violate at least one and often many of the physical constraints imposed on the slowness model by the data through Fermat's principle. Having ruined the reputation of least-squares methods in this way, we try to recover and arrive at a new understanding of the true significance of least-squares methods for inversion problems in this section. Two main points should be stressed: (1) The least-squares methods and generalized inverses are intimately related and, in principle, lead to the same results. (2) Iterative methods for inversion based on least-squares criteria fall into the class of "exterior" methods for nonlinear programming, *i.e.*, at each step of the iteration sequence the "best estimate" of the solution is infeasible so this method approaches the solution (lying on the boundary) from outside the set of feasible models.

In linear inversion with block models, we must solve the linear system of equations given by

$$\mathbf{Ms} = \mathbf{t}, \tag{4.1}$$

where we recall that $\mathbf{M}$ is a known $m \times n$ ray-path matrix, $\mathbf{s}$ is an unknown n-vector of slowness values, and $\mathbf{t}$ is a known m-vector of traveltimes.

Three major difficulties arise in solving (4.1):

1. $\mathbf{M}$ is *not* a square matrix;

2. $\mathbf{M}$ is often rank deficient;

3. $\mathbf{M}$ is often poorly conditioned.

Because of these three difficulties, we cannot simply solve (4.1) in terms of an inverse matrix of $\mathbf{M}$, because such an inverse does not exist. The inverse of an $n \times n$ square matrix $\mathbf{A}$ is defined as the unique matrix $\mathbf{X}$ such that

$$\mathbf{XA} = \mathbf{I} = \mathbf{AX}, \tag{4.2}$$

where $\mathbf{I}$ is the $n \times n$ identity matrix. The standard notation for the matrix inverse is $\mathbf{X} = \mathbf{A}^{-1}$. It is clear from the definition of the inverse (4.2) that $\mathbf{X}$ must also be an

$n \times n$ square matrix. Thus, the fact that $\mathbf{M}$ is not square is sufficient to guarantee that the standard definition of an inverse cannot be applied to our problem. It might still be possible to generalize the concept of inverse so that the equation

$$\mathbf{XM} = \mathbf{I} \tag{4.3}$$

uniquely defines a meaningful $n \times m$ inverse matrix $\mathbf{X}$ associated with $\mathbf{M}$. When $n < m$ and the discretized mathematical problem is *overdetermined*, setting

$$\mathbf{X} = \left(\mathbf{M}^T\mathbf{M}\right)^{-1}\mathbf{M}^T \tag{4.4}$$

gives a formal solution to (4.3) if the inverse $(\mathbf{M}^T\mathbf{M})^{-1}$ exists. We will see that this approach may succeed, but its success is tempered by the second and third difficulties: $\mathbf{M}$ is usually rank deficient, or poorly conditioned, or both. The rank of a matrix is the dimension of the subspace spanned by its columns (or rows) and cannot exceed the smaller of the two dimensions of the matrix. Letting r be the rank of our m by n matrix $\mathbf{M}$, if $r = \min(m, n)$ we say $\mathbf{M}$ has *full rank.* If $r < m, n$ then $\mathbf{M}$ is *rank deficient.* If $\mathbf{M}$ is rank deficient, then $(\mathbf{M}^T\mathbf{M})^{-1}$ does not exist and more sophisticated solutions than (4.4) are required. A similar difficulty arises if $m < n$, so the discretized problem is *underdetermined.* A matrix is *poorly conditioned* if the ratio of largest to smallest nonzero eigenvalue $\lambda_1/\lambda_r >> 1$. For example, this ratio is commonly found equal to 100 or 1000, or even more. Computing an accurate pseudoinverse for a poorly conditioned matrix is difficult. If $\mathbf{M}$ is very poorly conditioned, it may be difficult to compute the smallest eigenvalues accurately enough to obtain satisfactory results from the SVD approach for computing $\mathbf{M}^\dagger$. Then, other numerical techniques for iteratively computing the solution of (4.1) may be preferred.

Two techniques for handling the first difficulty ($\mathbf{M}$ not square) are *completing the square* and *Moore-Penrose pseudoinverses* [Moore, 1920; Penrose, 1956a]. Two techniques for handling the second difficulty (rank deficiency) are *regularization* and *pseudoinverses.* Thus, the Moore-Penrose pseudoinverse is a common solution for both of these problems. Regularization is usually accomplished either (i) by altering the rank deficient square matrix $\mathbf{M}^T\mathbf{M}$ in a way that produces an invertible matrix, or (ii) by performing a singular value decomposition on $\mathbf{M}$ and using formulas for the SVD of $\mathbf{M}^\dagger$ to construct the pseudoinverse.

There are a number of numerical algorithms for solving the system (4.1) and some of these are especially useful when $\mathbf{M}$ is poorly conditioned. These methods include:

1. standard tomographic reconstruction methods (e.g., ART and SIRT),
2. iterative matrix methods (e.g., Gauss-Seidel and Jacobi's method),
3. conjugate direction/gradient methods,
4. simple iteration,
5. a "neural network" method.

These methods may be analyzed most conveniently in terms of their convergence to the pseudoinverse.

Since the pseudoinverse plays such a central role in all these problem/solution pairs, we begin our discussion by deriving and analyzing $\mathbf{M}^\dagger$. Then, we discuss regularization techniques and finally analyze various numerical techniques for solving (4.1).

4.1 Moore-Penrose Pseudoinverse and SVD

Any nonsymmetric (and/or nonsquare) matrix $\mathbf{M}$ of real numbers can be decomposed in terms of a set of positive eigenvalues and two sets of orthonormal eigenvectors. Let r be the rank of $\mathbf{M}$. There exist r solutions to the eigenvalue problem

$$\mathbf{M}\mathbf{z} = \lambda\mathbf{y}, \tag{4.5}$$
$$\mathbf{M}^T\mathbf{y} = \lambda\mathbf{z}, \tag{4.6}$$

such that $\lambda > 0$ and $\mathbf{y}^T\mathbf{y} = \mathbf{z}^T\mathbf{z} = 1$. Letting λ_i, $\mathbf{y}_i$, $\mathbf{z}_i$, $i = 1, \ldots, r$, denote the solutions, then

$$\mathbf{y}_i^T\mathbf{M}\mathbf{M}^T\mathbf{y}_j = (\lambda_i^2\mathbf{y}_i^T)\mathbf{y}_j = \mathbf{y}_i^T(\lambda_j^2\mathbf{y}_j), \tag{4.7}$$

and

$$\mathbf{z}_i^T\mathbf{M}^T\mathbf{M}\mathbf{z}_j = (\lambda_i^2\mathbf{z}_i^T)\mathbf{z}_j = \mathbf{z}_i^T(\lambda_j^T\mathbf{z}_j), \tag{4.8}$$

so that

$$(\lambda_j^2 - \lambda_i^2)\mathbf{y}_i^T\mathbf{y}_j = 0 = (\lambda_j^2 - \lambda_i^2)\mathbf{z}_i^T\mathbf{z}_j, \tag{4.9}$$

for all combinations of i, j. Furthermore,

$$\lambda_i\mathbf{y}_i^T\mathbf{y}_i = \mathbf{y}_i^T\mathbf{M}\mathbf{z}_i = \mathbf{z}_i^T\mathbf{M}^T\mathbf{y}_i = \lambda_i\mathbf{z}_i^T\mathbf{z}_i, \tag{4.10}$$

showing that

$$\mathbf{y}_i^T\mathbf{y}_i = \mathbf{z}_i^T\mathbf{z}_i, \tag{4.11}$$

for all $1 \le i \le r$. Then, after normalizing the eigenvectors, it follows from (4.9) and (4.11) that

$$\mathbf{y}_i^T\mathbf{y}_j = \mathbf{z}_i^T\mathbf{z}_j = \delta_{ij}. \tag{4.12}$$

The vectors $\mathbf{y}_i$ and $\mathbf{z}_i$, respectively, are left- and right-hand eigenvectors of $\mathbf{M}$ corresponding to the eigenvalue λ_i. Multiple eigenvectors associated with the same eigenvalue are not necessarily orthogonal to each other, but they do form a subspace that is orthogonal to all other eigenvectors with different eigenvalues.

4.1.1 Resolution and completeness

The model space is n-dimensional while the data space is m-dimensional. Any slowness vector in the model space can be expanded in terms of a complete orthonormal set of vectors $\{\mathbf{z}_j\}$ as

$$\mathbf{s} = \sum_{j=1}^{n}\sigma_j\mathbf{z}_j = \sum_{j=1}^{r}\sigma_j\mathbf{z}_j + \mathbf{s}_0, \tag{4.13}$$

and similarly for a data vector

$$\mathbf{t} = \sum_{i=1}^{m} \tau_i \mathbf{y}_i = \sum_{i=1}^{r} \tau_i \mathbf{y}_i + \mathbf{t}_0, \tag{4.14}$$

when expanded in the basis set $\{\mathbf{y}_i\}$. The vectors $\mathbf{s}_0$ and $\mathbf{t}_0$ are respectively arbitrary vectors from the right and left null spaces of $\mathbf{M}$. *Completeness* implies that the identity matrix can be represented in terms of these sets of vectors by taking sums of outer products according to

$$\mathbf{I}_n = \sum_{j=1}^{n} \mathbf{z}_j \mathbf{z}_j^T \tag{4.15}$$

and

$$\mathbf{I}_m = \sum_{i=1}^{m} \mathbf{y}_i \mathbf{y}_i^T. \tag{4.16}$$

Then, for example,

$$\mathbf{I}_n \mathbf{s} = \sum_{jk}^{n} \mathbf{z}_j (\mathbf{z}_j^T \sigma_k \mathbf{z}_k) = \sum_{j=1}^{n} \sigma_j \mathbf{z}_j = \mathbf{s}. \tag{4.17}$$

In each space, only the first r of these vectors can be eigenvectors of $\mathbf{M}$ with $\lambda > 0$. The remaining $n - r$ and $m - r$ vectors necessarily lie in the right and left null spaces of $\mathbf{M}$.

The completeness relation can be written using any complete set of vectors; using the eigenvectors of $\mathbf{M}$ is a choice made as a convenience for the SVD analysis of $\mathbf{M}$.

Now we define *resolution matrices* for the two vector spaces based on *partial sums* of the completeness relations

$$\mathcal{R}_n = \sum_{j=1}^{r} \mathbf{z}_j \mathbf{z}_j^T \tag{4.18}$$

and

$$\mathcal{R}_m = \sum_{i=1}^{r} \mathbf{y}_i \mathbf{y}_i^T. \tag{4.19}$$

Note that for a real, square, and symmetric matrix, there is only one resolution matrix.

Applying the resolution matrices to $\mathbf{s}$ and $\mathbf{t}$, we find

$$\mathcal{R}_n \mathbf{s} = \sum_{j=1}^{r} \sigma_j \mathbf{z}_j \tag{4.20}$$

and

$$\mathcal{R}_m \mathbf{t} = \sum_{i=1}^{r} \tau_i \mathbf{y}_i. \tag{4.21}$$

Thus, the resolution matrices strip off the parts of $\mathbf{s}$ and $\mathbf{t}$ lying in the right and left null spaces of $\mathbf{M}$, respectively.

The full significance of the resolution matrices will become apparent as we develop the generalized inverse, and particularly when we examine the relationship between least-squares methods and the pseudoinverse.

PROBLEMS

PROBLEM 4.1.1 *Show that* $\mathcal{R}_n^2 = \mathcal{R}_n$ *and* $\mathcal{R}_m^2 = \mathcal{R}_m$.

PROBLEM 4.1.2 *Show that* $Tr(\mathcal{R}_n) = Tr(\mathcal{R}_m)$.

4.1.2 Completing the square

These results are most easily derived and understood by using a technique of Lanczos [1961] for completing the square. We define a real, square, and symmetric $(m+n)\times(m+n)$ matrix

$$\mathbf{H} = \begin{pmatrix} 0 & \mathbf{M} \\ \mathbf{M}^T & 0 \end{pmatrix}. \tag{4.22}$$

Then, (4.5)–(4.6) becomes

$$\mathbf{H}\begin{pmatrix} \mathbf{y}_i \\ \mathbf{z}_i \end{pmatrix} = \lambda_i \begin{pmatrix} \mathbf{y}_i \\ \mathbf{z}_i \end{pmatrix}. \tag{4.23}$$

Clearly, for each positive eigenvalue λ_i with eigenvector $(\mathbf{y}_i^T, \mathbf{z}_i^T)^T$, there is a corresponding negative eigenvalue $-\lambda_i$ with eigenvector $(\mathbf{y}_i^T, -\mathbf{z}_i^T)^T$.

PROBLEM

PROBLEM 4.1.3 *Show that* $\mathbf{H}$ *is rank deficient if* $m+n$ *is odd.*

4.1.3 Finding the generalized inverse

The *singular value decomposition* (SVD) of $\mathbf{M}$ is given by

$$\mathbf{M} = \sum_{i=1}^{r} \lambda_i \mathbf{y}_i \mathbf{z}_i^T. \tag{4.24}$$

The Moore-Penrose pseudoinverse of $\mathbf{M}$ can be expressed as

$$\mathbf{M}^\dagger = \sum_{i=1}^{r} \lambda_i^{-1} \mathbf{z}_i \mathbf{y}_i^T. \tag{4.25}$$

Our goal in this section is to derive (4.25). Also, notice that this definition implies

$$\mathbf{M}^\dagger\mathbf{M} = \sum_{i=1}^{r} \mathbf{z}_i \mathbf{z}_i^T = \mathcal{R}_n \tag{4.26}$$

and

$$\mathbf{M}\mathbf{M}^\dagger = \sum_{i=1}^{r} \mathbf{y}_i \mathbf{y}_i^T = \mathcal{R}_m, \tag{4.27}$$

thus making the connection to the resolution matrices.

Completing the square permits us to find a simple and intuitive derivation of the uniqueness conditions required for a meaningful generalized inverse giving rise to the formula (4.25). First, we find the generalized inverse for the square matrices appearing in $\mathbf{H}^2$. Then, we use these results to derive (4.25).

Let $\mathbf{A} = \mathbf{M}^T\mathbf{M}$ so that

$$\mathbf{A} = \sum_{i=1}^{r} \lambda_i^2 \mathbf{z}_i \mathbf{z}_i^T. \tag{4.28}$$

Then, $\mathbf{A}$ is real symmetric and therefore has real eigenvalues. Since the $\mathbf{z}_i$s are assumed to be an orthonormal and complete set of vectors, any generalized inverse for $\mathbf{A}$ can be written in the form

$$\mathbf{A}^\dagger = \sum_{ij}^{r} \alpha_{ij} \mathbf{z}_i \mathbf{z}_j^T, \tag{4.29}$$

where the coefficients $\alpha_{ij} = \mathbf{z}_i^T \mathbf{A}^\dagger \mathbf{z}_j$ are to be determined and the upper limit on the sum has been taken as r for the sake of simplifying this derivation. Consistency conditions are

$$\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger\mathbf{A} = \sum_{i=1}^{r} \mathbf{z}_i \mathbf{z}_i^T = \mathcal{R}_n, \tag{4.30}$$

which are the conditions intuition[1] suggests are the right ones for the generalized inverse of a square matrix. The final expression in (4.30) is just the completeness relation within the subspace orthogonal to the null space of $\mathbf{A}$. Equation (4.30) implies that $\mathbf{A}^\dagger$ is the unique matrix satisfying the conditions

$$\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}, \tag{4.31}$$

$$\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger. \tag{4.32}$$

It follows easily from (4.28)–(4.30) that

$$\alpha_{ij} = \delta_{ij}/\lambda_i^2. \tag{4.33}$$

Thus, the generalized inverse of this symmetric square matrix is just

$$\mathbf{A}^\dagger = \sum_{i=1}^{r} \mathbf{z}_i \mathbf{z}_i^T / \lambda_i^2. \tag{4.34}$$

[1] Compare (4.2).

To find the needed relation for the nonsymmetric/nonsquare matrix $\mathbf{M}$, again consider the square matrix $\mathbf{H}$. We find easily that

$$\mathbf{H}^2 = \begin{pmatrix} \mathbf{M}\mathbf{M}^T & 0 \\ 0 & \mathbf{M}^T\mathbf{M} \end{pmatrix}. \tag{4.35}$$

Then, for consistency we suppose

$$\mathbf{H}^\dagger = \mathbf{H}(\mathbf{H}^2)^\dagger = (\mathbf{H}^2)^\dagger \mathbf{H}, \tag{4.36}$$

from which it follows that

$$\mathbf{H}^\dagger = \begin{pmatrix} 0 & \mathbf{M}(\mathbf{M}^T\mathbf{M})^\dagger \\ \mathbf{M}^T(\mathbf{M}\mathbf{M}^T)^\dagger & 0 \end{pmatrix} = \begin{pmatrix} 0 & (\mathbf{M}\mathbf{M}^T)^\dagger\mathbf{M} \\ (\mathbf{M}^T\mathbf{M})^\dagger\mathbf{M}^T & 0 \end{pmatrix}. \tag{4.37}$$

Equation (4.37) implies that

$$\mathbf{M}^\dagger = \mathbf{M}^T(\mathbf{M}\mathbf{M}^T)^\dagger = (\mathbf{M}^T\mathbf{M})^\dagger\mathbf{M}^T. \tag{4.38}$$

Using (4.34) in (4.38) then finally yields (4.25). Thus, we have completed one derivation of the pseudoinverse.

A more direct derivation comes from (4.34) by writing down the equivalent expansion for $\mathbf{H}^\dagger$. First, expand $\mathbf{H}$ in terms of the eigenvectors as

$$\mathbf{H} = \frac{1}{2}\sum_{i=1}^{r} \lambda_i \left[\begin{pmatrix} \mathbf{y}_i \\ \mathbf{z}_i \end{pmatrix} (\mathbf{y}_i^T \quad \mathbf{z}_i^T) - \begin{pmatrix} \mathbf{y}_i \\ -\mathbf{z}_i \end{pmatrix} (\mathbf{y}_i^T \quad -\mathbf{z}_i^T) \right] \tag{4.39}$$

$$= \sum_{i=1}^{r} \lambda_i \left[\begin{pmatrix} 0 \\ \mathbf{z}_i \end{pmatrix} (\mathbf{y}_i^T \quad 0) + \begin{pmatrix} \mathbf{y}_i \\ 0 \end{pmatrix} (0 \quad \mathbf{z}_i^T) \right]. \tag{4.40}$$

[The factor of one-half in (4.39) arises from the fact that the norm of the eigenvectors of $\mathbf{H}$ (as defined here) is 2.] Then, from (4.39) and (4.34), we obtain

$$\mathbf{H}^\dagger = \sum_{i=1}^{r} \lambda_i^{-1} \left[\begin{pmatrix} 0 \\ \mathbf{z}_i \end{pmatrix} (\mathbf{y}_i^T \quad 0) + \begin{pmatrix} \mathbf{y}_i \\ 0 \end{pmatrix} (0 \quad \mathbf{z}_i^T) \right] = \begin{pmatrix} 0 & (\mathbf{M}^T)^\dagger \\ \mathbf{M}^\dagger & 0 \end{pmatrix}, \tag{4.41}$$

and (4.25) again follows, thus completing another derivation.

We observe two special cases in which $\mathbf{M}$ is of full rank. If $r = n \le m$ so the problem is either determined or overdetermined but $\mathbf{M}$ is of full rank, then $\mathbf{s}_0$ — the vector from the right null space — is necessarily zero. Further, we can write

$$\mathbf{M}^\dagger = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T = \mathbf{M}^T(\mathbf{M}\mathbf{M}^T)^\dagger. \tag{4.42}$$

Second, if $r = m \le n$ so the problem is either determined or underdetermined but $\mathbf{M}$ is of full rank, then $\mathbf{t}_0$ — the vector from the left null space — vanishes and

$$\mathbf{M}^\dagger = \mathbf{M}^T(\mathbf{M}\mathbf{M}^T)^{-1} = (\mathbf{M}^T\mathbf{M})^\dagger\mathbf{M}^T. \tag{4.43}$$

A subcase of both cases is $r = m = n$ so the problem is just determined and $\mathbf{M}$ is of full rank. $\mathbf{M}$ is then also square and invertible. Since in this case $(\mathbf{M}^T\mathbf{M})^{-1} = \mathbf{M}^{-1}(\mathbf{M}^T)^{-1}$ and $(\mathbf{M}\mathbf{M}^T)^{-1} = (\mathbf{M}^T)^{-1}\mathbf{M}^{-1}$, (4.42) and (4.43) reduce to

$$\mathbf{M}^\dagger = \mathbf{M}^{-1}, \tag{4.44}$$

consistent with the intuitive derivation of the generalized inverse given here.

Example 4.1.1 *Consider a* 2×2 *model with the layout*

s_1	s_2
s_3	s_4

Suppose the ray-path matrix is

$$\mathbf{M} = \begin{pmatrix} 1.00 & 1.00 & 0 & 0 \\ 1.05 & 1.05 & 0 & 0 \end{pmatrix},$$

corresponding to two ray paths going through cells 1 and 2 at slightly different angles. The SVD of $\mathbf{M}$ *is*

$$\mathbf{M} = \begin{pmatrix} 1.00 \\ 1.05 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 0 \end{pmatrix},$$

with the single nonzero eigenvalue $\lambda = \sqrt{4.205}$. *Then, the generalized inverse of* $\mathbf{M}$ *is*

$$\mathbf{M}^\dagger = \frac{1}{\sqrt{4.205}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1.00 & 1.05 \end{pmatrix}.$$

The corresponding resolution matrices are

$$\mathcal{R}_4 = \mathbf{M}^\dagger \mathbf{M} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1/2 & 1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.45}$$

and

$$\mathcal{R}_2 = \mathbf{M}\mathbf{M}^\dagger = \frac{1}{2.1025} \begin{pmatrix} 1.00 \\ 1.05 \end{pmatrix} \begin{pmatrix} 1.00 & 1.05 \end{pmatrix} = \frac{1}{2.1025} \begin{pmatrix} 1.00 & 1.05 \\ 1.05 & 1.1025 \end{pmatrix}. \tag{4.46}$$

Equation (4.45) shows that the two ray paths contain equivalent information about the two cells 1 and 2, but no information about cells 3 and 4. Equation (4.46) shows that, even though the two ray paths do in fact have the same information about the model, the longer ray path is treated as more reliable simply because it is longer. (It is this sort of contradictory result that leads us to consider using other weighting schemes in Section 3.5.*) Another way of displaying the information in the resolution matrix* R_4 *is to exhibit the diagonal values of the matrix on the grid of the slowness cells as*

$\frac{1}{2}$	$\frac{1}{2}$
0	0

This display has nothing to do with the actual slowness values *computed in the inversion, but it does have something to do with the relative reliability of the values computed. We should have more confidence in the computed values of slowness in those cells with the higher diagonal resolution.*

Example 4.1.2 *Using the same layout as the preceding example, consider the ray-path matrix*

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \end{pmatrix}.$$

This matrix corresponds to having one horizontal ray (through cells 1 and 2) and one vertical ray (through cells 1 and 3). The symmetric matrix

$$\mathbf{M}\mathbf{M}^T = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} = \frac{3}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\begin{pmatrix} 1 & -1 \end{pmatrix},$$

showing that the left-eigenvectors of $\mathbf{M}$ *are* $(1,1)$ *and* $(1,-1)$ *with eigenvalues* $\sqrt{3}$ *and 1, respectively. Thus,* $\mathbf{M}$ *is of full rank. Multiplying* $\mathbf{M}$ *on the left by the left-eigenvectors determines the right-eigenvectors and shows that*

$$\mathbf{M} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 2 & 1 & 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\begin{pmatrix} 0 & 1 & -1 & 0 \end{pmatrix},$$

which is easily verified. The generalized inverse is then

$$\mathbf{M}^{\dagger} = \frac{1}{6}\begin{pmatrix} 2 \\ 1 \\ 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & -1 \end{pmatrix}.$$

The resolution matrices are therefore

$$\mathcal{R}_4 = \mathbf{M}^{\dagger}\mathbf{M} = \begin{pmatrix} 2/3 & 1/3 & 1/3 & 0 \\ 1/3 & 2/3 & -1/3 & 0 \\ 1/3 & -1/3 & 2/3 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.47}$$

and

$$\mathcal{R}_2 = \mathbf{M}\mathbf{M}^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.48}$$

The diagonal values of the model resolution matrix are displayed in

$\frac{2}{3}$	$\frac{2}{3}$
$\frac{2}{3}$	0

.

The data resolution matrix is the identity because the ray-path matrix $\mathbf{M}$ *is of full rank, and* $r = m = 2$.

Example 4.1.3 *Consider a* 3×2 *model with the layout*

s_1	s_2
s_3	s_4
s_5	s_6

.

Consider the ray-path matrix

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & \sqrt{2} & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix},$$

corresponding to horizontal rays through the three horizontal pairs of cells and one diagonal ray cutting through cells 2 and 3. The symmetric matrix

$$\mathbf{M}\mathbf{M}^T = \begin{pmatrix} 2 & 0 & \sqrt{2} & 0 \\ 0 & 2 & \sqrt{2} & 0 \\ \sqrt{2} & \sqrt{2} & 4 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

has the eigenvalues $\lambda = 2$ (twice) and $\lambda = 3 \pm \sqrt{5}$, so $\mathbf{M}$ is again of full rank. The corresponding left-eigenvectors of $\mathbf{M}$ are

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ \frac{1}{\sqrt{2}}(1+\sqrt{5}) \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ \frac{1}{\sqrt{2}}(1-\sqrt{5}) \\ 0 \end{pmatrix}.$$

Except for normalization, the right-eigenvectors of $\mathbf{M}$ for the nonzero eigenvalues are then found to be

$$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 2+\sqrt{5} \\ 2+\sqrt{5} \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 2-\sqrt{5} \\ 2-\sqrt{5} \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

The resolution matrices are

$$\mathcal{R}_6 = \mathbf{M}^\dagger\mathbf{M} = \begin{pmatrix} 3/4 & 1/4 & -1/4 & 1/4 & 0 & 0 \\ 1/4 & 3/4 & 1/4 & -1/4 & 0 & 0 \\ -1/4 & 1/4 & 3/4 & 1/4 & 0 & 0 \\ 1/4 & -1/4 & 1/4 & 3/4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 1/2 & 1/2 \end{pmatrix} \tag{4.49}$$

and

$$\mathcal{R}_4 = \mathbf{M}\mathbf{M}^\dagger = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{4.50}$$

The diagonal elements of the model resolution matrix are displayed in

$\frac{3}{4}$	$\frac{3}{4}$
$\frac{3}{4}$	$\frac{3}{4}$
$\frac{1}{2}$	$\frac{1}{2}$

The data resolution matrix is again the identity matrix in this example because the ray-path matrix $\mathbf{M}$ *is of full rank and* $r = m = 4$.

Problems

PROBLEM 4.1.4 *Using (4.26) and (4.27) show that* $Tr(\mathcal{R}_n) = Tr(\mathcal{R}_m) = rank(\mathbf{M})$.

PROBLEM 4.1.5 *If* $\{\mathbf{z}_j\}_n$ *is an orthonormal, complete set of* n*-vectors and* $\{\mathbf{y}_i\}_m$ *is an orthonormal, complete set of* m*-vectors, define the* $n \times n$ *matrix*

$$\mathbf{Z} = \begin{pmatrix} \mathbf{z}_1 & \mathbf{z}_2 & \cdots & \mathbf{z}_n \end{pmatrix}$$

and the $m \times m$ *matrix*

$$\mathbf{Y} = \begin{pmatrix} \mathbf{y}_1 & \mathbf{y}_2 & \cdots & \mathbf{y}_m \end{pmatrix}.$$

Let $\mathbf{O}_{m,n}$ *be an* $m \times n$ *matrix of zeroes. Then, the matrix* $\mathbf{\Lambda}$ *is the* $m \times n$

$$\mathbf{\Lambda} = \left(\begin{array}{cccc:c} \lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \ddots & & \mathbf{O}_{r,n-r} \\ & & & \lambda_r & \\ \hdashline & & \mathbf{O}_{m-r,r} & & \mathbf{O}_{m-r,n-r} \end{array}\right).$$

where the first r *components of* $\mathbf{\Lambda}$ *along the diagonal are the first rp eigenvalues of* $\mathbf{M}$. *Then, if the first* r *vectors in the two sets are the right and left eigenvectors of* $\mathbf{M}$, *show that (4.24) can be rewritten as*

$$\mathbf{M} = \mathbf{Y}\mathbf{\Lambda}\mathbf{Z}^T.$$

Show that

$$\mathbf{M}^\dagger = \mathbf{Z}\mathbf{\Lambda}^\dagger\mathbf{Y}^T,$$

where the $n \times m$ *matrix* $\mathbf{\Lambda}^\dagger$ *is given by*

$$\mathbf{\Lambda}^\dagger = \left(\begin{array}{cccc:c} \lambda_1^{-1} & & & & \\ & \lambda_2^{-1} & & & \\ & & \ddots & & \mathbf{O}_{r,m-r} \\ & & & \lambda_r^{-1} & \\ \hdashline & & \mathbf{O}_{n-r,r} & & \mathbf{O}_{n-r,m-r} \end{array}\right).$$

Show that

$$\mathcal{R}_n = \mathbf{M}^\dagger \mathbf{M} = \mathbf{Z}\mathbf{Z}^T$$

and

$$\mathcal{R}_m = \mathbf{M}\mathbf{M}^\dagger = \mathbf{Y}\mathbf{Y}^T.$$

PROBLEM 4.1.6 *If* $\mathbf{A}$ *is real and symmetric, prove that its eigenvalues are real.*

PROBLEM 4.1.7 *Derive (4.25) from (4.24), (4.34), and (4.38).*

PROBLEM 4.1.8 *Show that (4.38) implies* $(\mathbf{M}\mathbf{M}^T)^\dagger = (\mathbf{M}^T)^\dagger \mathbf{M}^\dagger$.

PROBLEM 4.1.9 *It was implicitly assumed in (4.36) that*

$$(\mathbf{H}^2)^\dagger = (\mathbf{H}^\dagger)^2. \tag{4.51}$$

Show that (4.51) follows from (4.34). Then, verify that (4.38) is consistent with (4.51).

PROBLEM 4.1.10 *Find the pseudoinverse and the resolution matrix of*

$$\mathbf{A} = \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}.$$

PROBLEM 4.1.11 *Find the pseudoinverse and the resolution matrix of*

$$\mathbf{A} = \begin{pmatrix} 5/4 & -1/2 & -3/4 \\ -1/2 & 1 & -1/2 \\ -3/4 & -1/2 & 5/4 \end{pmatrix}.$$

PROBLEM 4.1.12 *Find the pseudoinverse and the resolution matrices of*

$$\mathbf{M} = \begin{pmatrix} 3/5 & 6/5 & 3/5 & 0 \\ 3/5 & 0 & 3/5 & 6/5 \end{pmatrix}.$$

PROBLEM 4.1.13 *Suppose that* $\mathbf{A}$ *is nonsingular,* $\mathbf{w}$ *is some normalized vector, and* ϵ *is a positive scalar. Show that*

$$\left[\mathbf{A} + \epsilon \mathbf{w}\mathbf{w}^T\right]^{-1} = \mathbf{A}^{-1} - \epsilon \frac{\mathbf{A}^{-1}\mathbf{w}\mathbf{w}^T\mathbf{A}^{-1}}{1 + \epsilon \mathbf{w}^T\mathbf{A}^{-1}\mathbf{w}}. \tag{4.52}$$

Then, use (4.52) to show that, if

$$\mathbf{B} = \mathbf{A} - \lambda \mathbf{w}\mathbf{w}^T \quad \textit{and} \quad \mathbf{B}\mathbf{w} = 0,$$

then

$$\mathbf{B}^\dagger = \mathbf{A}^{-1} - \frac{1}{\lambda}\mathbf{w}\mathbf{w}^T.$$

PROBLEM 4.1.14 *Suppose* $\mathbf{A}$ *is real and symmetric with SVD given by* $\mathbf{A} = \sum_{i=1}^{n} \rho_i \mathbf{z}_i \mathbf{z}_i^T$ *where* $\rho_i > 0$ *for* $1 \le i \le r$ *and* $\rho_i = 0$ *for* $r+1 \le i \le n$. *Show that*

$$\mathbf{A}^\dagger = \left[\mathbf{A} + \mu \sum_{i=r+1}^{n} \mathbf{z}_i \mathbf{z}_i^T \right]^{-1} - \frac{1}{\mu} \sum_{i=r+1}^{n} \mathbf{z}_i \mathbf{z}_i^T \tag{4.53}$$

for any $\mu > 0$.

PROBLEM 4.1.15 *Suppose that (4.29) is replaced by*

$$\mathbf{A}^\dagger \equiv \sum_{i,j}^{n} \alpha_{ij} \mathbf{z}_i \mathbf{z}_j^T,$$

where the upper limit on the sum is taken to be the size of the model vector space. Repeat the derivation of the pseudoinverse and explain the differing results.

PROBLEM 4.1.16 *Show that the four equations*

$$\boxed{\begin{array}{rcl} \mathbf{MXM} &=& \mathbf{M}, \\ \mathbf{XMX} &=& \mathbf{X}, \\ (\mathbf{MX})^T &=& \mathbf{MX}, \\ (\mathbf{XM})^T &=& \mathbf{XM}, \end{array}}$$

have a unique solution $\mathbf{X}$ *for any real matrix* $\mathbf{M}$. *Show that* $\mathbf{X} = \mathbf{M}^\dagger$. *Then show directly that* $(\mathbf{M}^T\mathbf{M})^\dagger = \mathbf{M}^\dagger(\mathbf{M}^\dagger)^T$. *[Penrose, 1955a]*

PROBLEM 4.1.17 *If* $\mathbf{A}$ *is real, square, and symmetric, then show that the equations*

$$\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger\mathbf{A} = \mathcal{R}_n$$

are equivalent to the set of uniqueness conditions in PROBLEM 4.1.16 *for* $\mathbf{A}^\dagger$.

PROBLEM 4.1.18 *Show that, if* $\mathbf{X}$ *is a real, square, and symmetric matrix satisfying* $\mathbf{X}^2 = \mathbf{X}$, *then* $\mathbf{X}^\dagger = \mathbf{X}$. *Does* $\mathbf{X}^\dagger = \mathbf{X}$ *imply* $\mathbf{X}^2 = \mathbf{X}$*?*

PROBLEM 4.1.19 *Use the defining equations for* $\mathbf{M}^\dagger$ *in* PROBLEM 4.1.16 *to show directly that* $\mathbf{M}^\dagger = \mathbf{M}^T(\mathbf{M}\mathbf{M}^T)^\dagger = (\mathbf{M}^T\mathbf{M})^\dagger\mathbf{M}$ *thus verifying (4.38). [Hint: Use the defining equations three times, once each for* $(\mathbf{M}^T\mathbf{M})^\dagger$, *for* $(\mathbf{M}\mathbf{M}^T)^\dagger$, *and for* $\mathbf{M}^\dagger$.*]*

PROBLEM 4.1.20 *If* r *is the rank of* $\mathbf{M}$, *show that* $\mathbf{M}$ *can be factored into a product of an* $m \times r$ *matrix* $\mathbf{L}$ *and an* $r \times n$ *matrix* $\mathbf{R}$ *such that*

$$\mathbf{M} = \mathbf{LR},$$

where $\mathbf{L}$ *and* $\mathbf{R}$ *are each of rank* r. *Show that the generalized inverse* $\mathbf{M}^\dagger$ *may be written*

$$\mathbf{M}^\dagger = \mathbf{R}^T(\mathbf{R}\mathbf{R}^T)^{-1}(\mathbf{L}^T\mathbf{L})^{-1}\mathbf{L}^T. \tag{4.54}$$

Use (4.54) to show that $\mathbf{M}^\dagger = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T$ *when* $r = n$ *and that* $\mathbf{M}^\dagger = \mathbf{M}^T(\mathbf{M}\mathbf{M}^T)^{-1}$ *when* $r = m$. *[Smith and Franklin, 1969]*

PROBLEM 4.1.21 *Any real matrix* $\mathbf{M}$ *can be partitioned into the form*

$$\mathbf{M} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{C}\mathbf{A}^{-1}\mathbf{B} \end{pmatrix} \tag{4.55}$$

after some rearrangement of the rows and columns.

1. *If* $\mathbf{A}$ *is a nonsingular submatrix of* $\mathbf{M}$ *whose rank is equal to that of* $\mathbf{M}$, *then verify that*

$$\mathbf{M}^{\dagger} = \begin{pmatrix} \mathbf{A}^T\mathbf{P}\mathbf{A}^T & \mathbf{A}^T\mathbf{P}\mathbf{C}^T \\ \mathbf{B}^T\mathbf{P}\mathbf{A}^T & \mathbf{B}^T\mathbf{P}\mathbf{C}^T \end{pmatrix}, \tag{4.56}$$

where $\mathbf{P} = (\mathbf{A}\mathbf{A}^T + \mathbf{B}\mathbf{B}^T)^{-1}\mathbf{A}(\mathbf{A}^T\mathbf{A} + \mathbf{C}^T\mathbf{C})^{-1}$. *[Hint:* $\mathbf{M} = \begin{pmatrix} \mathbf{I}_r \\ \mathbf{C}\mathbf{A}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{A} & \mathbf{B} \end{pmatrix}$*]*

2. *How do we know the inverses in the definition of* $\mathbf{P}$ *exist?*

[Penrose, 1955b]

PROBLEM 4.1.22 *Rao and Mitra [1971] and Barnett [1990] discuss variations of the generalized inverse obtained by relaxing the constraints on its definition given in* PROBLEM 4.1.16.

1. *Give an example of a generalized inverse* $\mathbf{X}$ *satisfying*

$$\mathbf{M}\mathbf{X}\mathbf{M} = \mathbf{M}, \tag{4.57}$$

but not satisfying at least one of the remaining conditions.

2. *Show that all generalized inverses satisfying (4.57) may be expressed in the form*

$$\mathbf{X} = \mathbf{X}_0 + \mathbf{Y} - \mathbf{X}_0\mathbf{M}\mathbf{Y}\mathbf{M}\mathbf{X}_0,$$

where $\mathbf{X}_0$ *is a particular matrix satisfying condition (4.57) and* $\mathbf{Y}$ *is an arbitrary* $n \times m$ *matrix. Explain this result using singular value decomposition.*

3. *Show that, if* $\mathbf{M}$ *is rearranged as in (4.55), then one choice of* $\mathbf{X}$ *in (4.57) is*

$$\mathbf{X} = \begin{pmatrix} \mathbf{A}^{-1} & -\mathbf{A}^{-1}\mathbf{B}\mathbf{Z} \\ 0 & \mathbf{Z} \end{pmatrix},$$

where $\mathbf{Z}$ *is an arbitrary matrix having the proper dimensions.*

PROBLEM 4.1.23 *Consider the stochastic inverse*

$$\mathbf{X} = \mathcal{C}_{st}\mathcal{C}_{tt}^{-1}.$$

introduced in PROBLEM 3.4.5. *If the noise* $\mathbf{N}$ *is negligible so that* $\mathbf{M}\mathbf{S} = \mathbf{T}$ *but* $\mathcal{C}_{tt}$ *is still invertible, show that* $\mathbf{X}$ *satisfies the first three of the Moore-Penrose conditions (see* PROBLEM 4.1.16*) for the generalized inverse. Show that this matrix is a special case of*

$$\mathbf{X} = \mathbf{Z}\left[\mathbf{M}\mathbf{Z}\right]^{-1}, \tag{4.58}$$

where $\mathbf{Z}$ *is an arbitrary* $n \times m$ *matrix except that* $\mathbf{M}\mathbf{Z}$ *must be invertible. What are the conditions on* $\mathbf{Z}$ *needed to guarantee that the third Moore-Penrose condition is satisfied? What is the matrix* $\mathbf{Z}$ *if* $\mathbf{X}$ *satisfies all four conditions?*

4.1.4 Relation to least-squares

Now we can solve the least-squares problem using the SVD of $\mathbf{M}$. To see this, we will let $w_i = 1$ for simplicity. To begin, first recognize that $\mathbf{s}$ and $\mathbf{t}$ may be expanded in terms of the left- and right-eigenvectors:

$$\mathbf{t} = \sum_{i=1}^{r} \tau_i \mathbf{y}_i + \mathbf{t}_0, \tag{4.59}$$

$$\mathbf{s} = \sum_{i=1}^{r} \sigma_i \mathbf{z}_i + \mathbf{s}_0, \tag{4.60}$$

where

$$\mathbf{z}_i^T \mathbf{s}_0 = \mathbf{y}_i^T \mathbf{t}_0 = 0 \quad \text{for all} \quad i = 1, \ldots, r, \tag{4.61}$$

and

$$\tau_i = \mathbf{y}_i^T \mathbf{t}, \tag{4.62}$$

$$\sigma_i = \mathbf{z}_i^T \mathbf{s}. \tag{4.63}$$

In terms of the expansion coefficients and unit weights, we have

$$\Psi(\mathbf{s}) = (\mathbf{M}\mathbf{s} - \mathbf{t})^T(\mathbf{M}\mathbf{s} - \mathbf{t}) \tag{4.64}$$

$$= \mathbf{t}_0^T \mathbf{t}_0 + \sum_{i=1}^{r} (\lambda_i \sigma_i - \tau_i)^2. \tag{4.65}$$

For nonzero eigenvalues, setting

$$\lambda_i \sigma_i = \tau_i \tag{4.66}$$

minimizes Ψ by eliminating the sum in (4.65). Then,

$$\mathbf{s} = \mathbf{s}_0 + \sum_{i=1}^{r} \lambda_i^{-1} \tau_i \mathbf{z}_i. \tag{4.67}$$

The vector $\mathbf{s}_0$ is an arbitrary vector from the right null space of $\mathbf{M}$. We can minimize $\mathbf{s}^T\mathbf{s}$ by setting $\mathbf{s}_0 = 0$. Thus, we obtain the minimum-norm least-squares model:

$$\hat{\mathbf{s}}_{\mathrm{LS}} = \sum_{i=1}^{r} \lambda_i^{-1} \tau_i \mathbf{z}_i. \tag{4.68}$$

The reader can easily verify that

$$\hat{\mathbf{s}}_{\mathrm{LS}} = \mathbf{M}^{\dagger} \mathbf{t}. \tag{4.69}$$

It is a general result that the Moore-Penrose pseudoinverse solves the least-squares problem. We will make use of this fact later when we attempt to construct methods of solving the inversion problem that are both fast and easy to implement.

Problems

Problem 4.1.24 *Verify (4.69).*

Problem 4.1.25 *Define* $\mathbf{Z}_0$ *to be a "best approximate solution" of the matrix equation* $\mathbf{MZ} = \mathbf{Y}$ *if for all* $\mathbf{Z}$, *either*

1. $||\mathbf{MZ} - \mathbf{Y}|| > ||\mathbf{MZ}_0 - \mathbf{Y}||$, *or*
2. $||\mathbf{MZ} - \mathbf{Y}|| = ||\mathbf{MZ}_0 - \mathbf{Y}||$ *and* $||\mathbf{Z}|| = ||\mathbf{Z}_0||$,

where $||\mathbf{A}||^2 \equiv Tr(\mathbf{A}^T\mathbf{A})$. *Then, show that* $\mathbf{Z} = \mathbf{M}^\dagger\mathbf{Y}$ *is the unique best approximate solution of* $\mathbf{MZ} = \mathbf{Y}$. *[Penrose, 1955b]*

Problem 4.1.26 *Let* $\mathbf{Z}_0 = \mathbf{M}^\dagger\mathbf{Y}$ *and*

$$\mathbf{Z} = \mathbf{Z}_0 + \sum_{i=r+1}^{n} \alpha_i \mathbf{z}_i \mathbf{y}_i^T \mathbf{Y},$$

where the α_i*s are scalars and the* $\mathbf{z}_i$*s and* $\mathbf{y}_i$*s for* $r+1 \le i \le n$ *are vectors from the right and left null spaces of* $\mathbf{M}$. *Then, which condition in* Problem 4.1.25 *does* $\mathbf{Z}$ *violate? Under what circumstances is the "best approximate solution" defined in* Problem 4.1.25 *really the best?*

Problem 4.1.27 *Show that*

$$\hat{\mathbf{s}}_{\mathrm{LS}} = \mathcal{R}_n \mathbf{s},$$

where $\mathcal{R}_n = \mathbf{M}^\dagger\mathbf{M}$ *is the model space resolution matrix. [Backus and Gilbert, 1968; 1970; Jackson, 1972]*

Problem 4.1.28 *Show that*

$$\mathbf{M}\hat{\mathbf{s}}_{\mathrm{LS}} = \mathcal{R}_m \mathbf{t},$$

where $\mathcal{R}_m = \mathbf{M}\mathbf{M}^\dagger$ *is the data space resolution matrix. [Wiggins, 1972; Jackson, 1972]*

4.2 Scaling Methods

Given $\mathbf{M}$ we define two diagonal matrices based on row and column sums of its elements, l_{ij}. Let $\mathbf{L}$ and $\mathbf{C}$ be diagonal matrices such that

$$L_{ii} = \sum_{j=1}^{n} l_{ij}, \quad i = 1, \dots m, \tag{4.70}$$

$$C_{jj} = \sum_{i=1}^{m} l_{ij}, \quad j = 1, \dots, n. \tag{4.71}$$

L_{ii} is the length of the ith ray path, obtained by summing the lengths of its intersection with all cells. C_{jj}, on the other hand, is the total length of ray segments intersecting the jth cell. C_{jj} (or its minor variations) is known variously as the *illumination*, *hit parameter*, or *coverage* of cell j.

Let $\mathbf{v}$ be the n-vector whose components are each 1:

$$\mathbf{v} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}. \tag{4.72}$$

Similarly, let $\mathbf{u}$ be the analogous m-vector. Then $\mathbf{Mv}$ is the m-vector containing the ray lengths. We can also infer that $\mathbf{Lu}$ is the same vector. Analogously, $\mathbf{M}^T\mathbf{u}$ and $\mathbf{Cv}$ are both the n-vector containing the cell coverages. That is,

$$\mathbf{Mv} = \mathbf{Lu}, \tag{4.73}$$

$$\mathbf{M}^T\mathbf{u} = \mathbf{Cv}. \tag{4.74}$$

This implies that $\lambda = 1$, $\mathbf{y} = \mathbf{u}$, $\mathbf{z} = \mathbf{v}$ is a solution to the eigenvalue problem

$$\mathbf{Mz} = \lambda\mathbf{Ly}, \tag{4.75}$$

$$\mathbf{M}^T\mathbf{y} = \lambda\mathbf{Cz}. \tag{4.76}$$

This problem is a generalization of our earlier eigenvalue problem (4.5)–(4.6) in that it incorporates positive definite weighting matrices $\mathbf{L}$ and $\mathbf{C}$. In place of the orthonormality conditions (4.12), we require the *conjugacy* conditions

$$\mathbf{y}_i^T\mathbf{L}\mathbf{y}_j = \mathbf{z}_i^T\mathbf{C}\mathbf{z}_j = \delta_{ij}. \tag{4.77}$$

With these conditions, the generalized eigenvalue problem can be converted to the standard form of (4.5)–(4.6) using the (*preconditioning*) transformations

$$\mathbf{M}' = \mathbf{L}^{-1/2}\mathbf{M}\mathbf{C}^{-1/2}, \tag{4.78}$$

$$\mathbf{y}' = \mathbf{L}^{1/2}\mathbf{y}, \tag{4.79}$$

$$\mathbf{z}' = \mathbf{C}^{1/2}\mathbf{z}. \tag{4.80}$$

Whenever $\mathbf{L}^{-\frac{1}{2}}$ and $\mathbf{C}^{-\frac{1}{2}}$ appear in the formulas, we make the implicit assumption that all the diagonal elements of both these matrices are nonzero. A zero diagonal component of $\mathbf{L}$ would correspond to a ray path with no length, which is clearly unphysical. However, a zero diagonal component of $\mathbf{C}$ corresponds to a cell with no ray coverage, which clearly can and does happen in practice. If so, then we assume that this cell is removed from the inversion problem.[2]

By construction, the eigenvalues of $\mathbf{M}$ and $\mathbf{M}'$ are the same, but for different eigenvalue problems: (4.75)–(4.76) and

$$\mathbf{M}'\mathbf{z}' = \lambda\mathbf{y}', \tag{4.81}$$

$$\mathbf{M}'^T\mathbf{y}' = \lambda\mathbf{z}'. \tag{4.82}$$

[2]Some methods for doing so are discussed in Section 6.

PROPOSITION 4.2.1 *The eigenvalues of* $\mathbf{M}'$ *lie in the interval [-1,1].*

Proof: Recall that the eigenvalues come in pairs: if $\lambda, \mathbf{y}', \mathbf{z}'$ solves the eigenvalue problem, so does $-\lambda, \mathbf{y}', -\mathbf{z}'$. Then, we may (without loss of generality) restrict the discussion to eigenvalues satisfying $\lambda \geq 0$.

Let λ, $\mathbf{y}$, $\mathbf{z}$ be any solution to (4.75)–(4.76) with $\lambda > 0$. Then, in components,

$$\sum_j l_{ij} z_j = \lambda L_{ii} y_i, \tag{4.83}$$

$$\sum_i l_{ij} y_i = \lambda C_{jj} z_j. \tag{4.84}$$

Let $y_{\max}$ be the largest absolute component of $\mathbf{y}$, i.e., $y_{\max} = \max_i |y_i|$. Similarly, let $z_{\max} = \max_j |z_j|$. Since $l_{ij} \geq 0$, we can infer

$$z_{\max} \sum_j l_{ij} \geq \lambda L_{ii} |y_i|, \tag{4.85}$$

$$y_{\max} \sum_i l_{ij} \geq \lambda C_{jj} |z_j|. \tag{4.86}$$

Recalling the definitions of C_{jj} and L_{ii} given by (4.70) and (4.71), this implies

$$z_{\max} \geq \lambda |y_i|, \tag{4.87}$$

$$y_{\max} \geq \lambda |z_j|, \tag{4.88}$$

which must hold for all i and j; thus

$$z_{\max} \geq \lambda y_{\max}, \tag{4.89}$$

$$y_{\max} \geq \lambda z_{\max}. \tag{4.90}$$

Thus, we have $z_{\max} \geq \lambda^2 z_{\max}$, which implies $\lambda^2 \leq 1$ and therefore $-1 \leq \lambda \leq 1$. ∎

PROBLEMS

PROBLEM 4.2.1 *Show that the eigenvectors of* $\mathbf{M}'$ *having eigenvalue* $\lambda = 1$ *are* $\mathbf{y}' = \mathbf{L}^{\frac{1}{2}}\mathbf{u}$ *and* $\mathbf{z}' = \mathbf{C}^{\frac{1}{2}}\mathbf{v}$. *What are the eigenvectors of* $(\mathbf{M}')^\dagger$ *having unit eigenvalue?*

PROBLEM 4.2.2 *Using* $\mathbf{M}\mathbf{M}^\dagger\mathbf{M} = \mathbf{M}$ *and (4.70), demonstrate the general result*

$$\mathbf{M}\mathbf{M}^\dagger\mathbf{L}\mathbf{u} = \mathcal{R}_m\mathbf{L}\mathbf{u} = \mathbf{L}\mathbf{u}. \tag{4.91}$$

Thus, $\mathbf{Lu}$ *is an eigenvector of the data resolution matrix* $\mathcal{R}_m$, *having unit eigenvalue.*

PROBLEM 4.2.3 *Using* $\mathbf{M}\mathbf{M}^\dagger\mathbf{M} = \mathbf{M}$ *and (4.71), derive the general result that*

$$\mathbf{v}^T\mathbf{C}\mathbf{M}^\dagger\mathbf{M} = \mathbf{v}^T\mathbf{C}\mathcal{R}_n = \mathbf{v}^T\mathbf{C}. \tag{4.92}$$

Thus, $\mathbf{v}^T\mathbf{C}$ *is an eigenvector of the model resolution matrix* $\mathcal{R}_n$, *having unit eigenvalue.*

PROBLEM 4.2.4 *Three examples of data resolution matrices are presented in (4.46), (4.48), and (4.50). Check to see if they agree with (4.91).*

PROBLEM 4.2.5 *Three examples of model resolution matrices are presented in (4.45), (4.47), and (4.49). Check to see if they agree with (4.92).*

PROBLEM 4.2.6 *Use the definition of the pseudoinverse in* PROBLEM 4.1.16 *to show that, if*

$$\mathbf{M}' = \mathbf{L}^{-\frac{1}{2}}\mathbf{M}\mathbf{C}^{-\frac{1}{2}},$$

then

$$\mathbf{X} = \mathbf{C}^{-\frac{1}{2}}(\mathbf{M}')^{\dagger}\mathbf{L}^{-\frac{1}{2}}, \tag{4.93}$$

where $\mathbf{X}$ *is an approximate generalized inverse satisfying the first two conditions (*$\mathbf{MXM} = \mathbf{M}$ *and* $\mathbf{XMX} = \mathbf{X}$*). Use (4.93) to show that the SVDs of* $\mathbf{M}$ *and* $\mathbf{X}$ *have the form*

$$\mathbf{M} = \frac{\mathbf{L}\mathbf{u}\mathbf{v}^T\mathbf{C}}{\mathbf{u}^T\mathbf{L}\mathbf{u}} + \dots$$

and

$$\mathbf{X} = \frac{\mathbf{v}\mathbf{u}^T}{\mathbf{u}^T\mathbf{L}\mathbf{u}} + \dots, \tag{4.94}$$

where the terms not shown are for eigenvectors of $\mathbf{M}'$ *with eigenvalues* $\lambda < 1$*. Treat (4.94) as an approximate inverse, and compare the resulting estimate of* $\mathbf{s}$ *to (3.42). What can be said about the accuracy of this approximate inverse?*

PROBLEM 4.2.7 *Use (4.93) and (4.94) to show that*

$$\mathbf{u}^T\mathbf{MX} = \mathbf{u}^T, \tag{4.95}$$

for a ray-path matrix $\mathbf{M}$*. Thus,* $\mathbf{u}$ *is a left eigenvector of the approximate data resolution matrix* $\mathbf{MX}$*, having unit eigenvalue. What restrictions (if any) are there on the validity of (4.95)?*

PROBLEM 4.2.8 *Use (4.93) and (4.94) to show that*

$$\mathbf{XMv} = \mathbf{v}, \tag{4.96}$$

for a ray-path matrix $\mathbf{M}$*. Thus,* $\mathbf{v}$ *is a right eigenvector of the approximate model resolution matrix* $\mathbf{XM}$*, having unit eigenvalue. What restrictions (if any) are there on the validity of (4.96)?*

4.3 Weighted Least-Squares, Regularization, and Effective Resolution

In weighted least-squares, a good choice of weighting matrix is $\mathbf{L}^{-1}$, that is, the inverse of the ray length matrix. In Section 3.5, we discussed the physical arguments for using such a weight matrix. Here we will show that mathematical arguments based on stability and regularization lead to the same choice of weight matrix.

4.3.1 General weights and objective functionals

There is an inherent arbitrariness to the choice of weight matrix in a least-squares minimization. Let $\mathbf{F}$ and $\mathbf{G}$ be two positive, diagonal weight matrices, $m \times m$ and $n \times n$ respectively. Then define the scaled inversion problem so that

$$\mathbf{M}' = \mathbf{F}^{-\frac{1}{2}}\mathbf{M}\mathbf{G}^{-\frac{1}{2}}, \quad \mathbf{s}' = \mathbf{G}^{\frac{1}{2}}\mathbf{s}, \quad \mathbf{t}' = \mathbf{F}^{-\frac{1}{2}}\mathbf{t}. \tag{4.97}$$

The (unweighted) damped least-squares minimization problem associated with (4.97) is to minimize the functional

$$\Psi'(\mathbf{s}') = (\mathbf{t}' - \mathbf{M}'\mathbf{s}')^T(\mathbf{t}' - \mathbf{M}'\mathbf{s}') + \mu(\mathbf{s}' - \mathbf{s}'_0)^T(\mathbf{s}' - \mathbf{s}'_0), \tag{4.98}$$

with respect to $\mathbf{s}'$. The normal equations resulting from (4.98) are

$$(\mathbf{M}'^T\mathbf{M}' + \mu\mathbf{I})(\mathbf{s}' - \mathbf{s}'_0) = \mathbf{M}'^T(\mathbf{t}' - \mathbf{M}'\mathbf{s}'_0). \tag{4.99}$$

The result for the untransformed $\mathbf{s}$ is exactly the same whether we use the functional (4.98) or the weighted least-squares functional

$$\Psi(\mathbf{s}) = (\mathbf{t} - \mathbf{M}\mathbf{s})^T\mathbf{F}^{-1}(\mathbf{t} - \mathbf{M}\mathbf{s}) + \mu(\mathbf{s} - \mathbf{s}_0)^T\mathbf{G}(\mathbf{s} - \mathbf{s}_0). \tag{4.100}$$

In either case, the result is

$$\mathbf{s} = \mathbf{s}_0 + (\mathbf{M}^T\mathbf{F}^{-1}\mathbf{M} + \mu\mathbf{G})^{-1}\mathbf{M}^T\mathbf{F}^{-1}(\mathbf{t} - \mathbf{M}\mathbf{s}_0). \tag{4.101}$$

In truth, every least-squares method is a special case of the general weighted least-squares method — the more common ones just have unit weights everywhere.

The minimum of (4.100) is achieved by the slowness model given in (4.101) as long as the matrix $\mathbf{M}^T\mathbf{F}^{-1}\mathbf{M} + \mu\mathbf{G}$ is invertible. Thus, some relaxation of the conditions placed on the weight matrix $\mathbf{G}$ is possible. One common choice is to make the regularization term correspond to minimizing the gradient or curvature of the model. Then, the matrix $\mathbf{G} = \mathbf{K}^T\mathbf{K}$, where $\mathbf{K}\mathbf{s}$ is either the gradient of the model or its Laplacian. Such a weight matrix is neither diagonal nor positive. In fact, a constant model vector lies in the null space of such a $\mathbf{G}$. The combined matrix $\mathbf{M}^T\mathbf{F}^{-1}\mathbf{M} + \mu\mathbf{G}$ may still be invertible however, since the null spaces of the two terms are generally orthogonal.

PROBLEMS

PROBLEM 4.3.1 *Find explicit expressions for the matrix* $\mathbf{K}$ *such that*

1. $\mathbf{Ks}$ *is the gradient of the slowness model;*

2. $\mathbf{Ks}$ *is the Laplacian of the slowness model.*

PROBLEM 4.3.2 *Suppose the desired weight matrices* $\mathbf{F}$ *and/or* $\mathbf{G}$ *are nonnegative diagonal, (i.e., have some zeroes along the diagonal). Generalize (4.97), replacing these definitions by*

$$\mathbf{M}' = (\mathbf{F}^\dagger)^{\frac{1}{2}}\mathbf{M}(\mathbf{G}^\dagger)^{\frac{1}{2}}, \quad \mathbf{s}' = \mathbf{G}^{\frac{1}{2}}\mathbf{s}, \quad \mathbf{t}' = (\mathbf{F}^\dagger)^{\frac{1}{2}}\mathbf{t},$$

where $\mathbf{F}^\dagger$ *and* $\mathbf{G}^\dagger$ *are the pseudoinverses of* $\mathbf{F}$ *and* $\mathbf{G}$ *respectively. If* $\mathbf{F} = \mathbf{L}$ *and* $\mathbf{G} = \mathbf{C}$ *with some of the cell coverages vanishing, compare the approach using generalized inverses to the usual method of deleting uncovered cells from the inversion problem.*

PROBLEM 4.3.3 *Suppose that the damping parameter* $\mu = 0$ *and the diagonal elements of* $\mathbf{F}$ *are given by*

$$F_{ii} = |(\mathbf{Ms})_i - t_i|\,,^{2-p}$$

where the term in the exponent $p \geq 1$ *(*$p = 2$ *for least-squares). Show that the resulting special case of (4.101) is the slowness minimizing*

$$\Psi_p(\mathbf{s}) = \sum_{i=1}^{m} |(\mathbf{Ms})_i - t_i|\,.^p$$

Assuming that some of the traveltime residuals vanish and $p = 1$*, use the result of* PROBLEM 4.3.2 *to provide an appropriate generalization of (4.101). This method is known as* iteratively reweighted least-squares. *[Claerbout and Muir, 1973; Claerbout, 1976; Scales, Gersztenkorn, and Treitel, 1988]*

4.3.2 Regularization

There are physical reasons for choosing particular weighting schemes and some of these reasons have been discussed in Section 3.5. A sound mathematical reason for choosing a particular scheme [Burkhard, 1980] might be either "convergence" or "regularization." It may be difficult or impossible to compute the result (4.101) unless appropriate weight matrices are used, since $\mathbf{M}^T\mathbf{F}^{-1}\mathbf{M}$ may be poorly conditioned or noninvertible. We will see in our discussion of *simple iteration* (Section 4.4.3) that this method converges if the eigenvalues of the matrix $\mathbf{M}$ (or equivalently $\mathbf{M}'$ here) lie in the range $-\sqrt{2} \leq \lambda_i \leq \sqrt{2}$. So how can we choose the weight matrices to guarantee that the eigenvalues fall in the desired range?

For the sake of argument, suppose that

$$\mathbf{Ms} = \lambda\mathbf{Fr}, \tag{4.102}$$
$$\mathbf{M}^T\mathbf{r} = \lambda\mathbf{Gs}. \tag{4.103}$$

Then, in terms of components, we have

$$\sum_j l_{ij} s_j = \lambda F_{ii} r_i, \tag{4.104}$$

$$\sum_i l_{ij} r_j = \lambda G_{jj} s_i. \tag{4.105}$$

Letting $s_{\max}$ be the magnitude of the largest component of $\mathbf{s}$ and $r_{\max}$ the magnitude of the largest component of $\mathbf{r}$, we have

$$s_{\max} L_{ii} \geq \lambda F_{ii} |r_i|, \tag{4.106}$$

$$r_{\max} C_{jj} \geq \lambda G_{jj} |s_j|. \tag{4.107}$$

It follows that

$$s_{\max} \geq \lambda \frac{F_{ii}}{L_{ii}} r_{\max} \geq \lambda^2 \frac{F_{ii} G_{jj}}{L_{ii} C_{jj}} s_{\max}. \tag{4.108}$$

So, in general, we can guarantee that the eigenvalues λ will be bounded above by unity by requiring that

$$1 \geq \frac{L_{ii} C_{jj}}{F_{ii} G_{jj}}, \quad \text{for all} \quad i, j. \tag{4.109}$$

Many choices of $\mathbf{F}$ and $\mathbf{G}$ are permitted by (4.109), but perhaps the simplest choice is

$$\mathbf{F} = \mathbf{L} \quad \text{and} \quad \mathbf{G} = \mathbf{C}. \tag{4.110}$$

Thus, although the choice (4.110) is certainly not unique, it is nevertheless a good choice for the weight matrices in weighted least-squares, and guarantees that $\lambda^2 \leq 1$ as desired.

In Section 7.2, we find that another choice of weight matrices has the same constraining properties on the eigenvalues, yet has more useful properties in nonlinear tomography algorithms.

4.3.3 Effective resolution

Another way of understanding the significance of formulas such as (4.101) is to reconsider the fundamental relation

$$\mathbf{M}\mathbf{s} = \mathbf{t} \tag{4.111}$$

and its rearrangement

$$\mathbf{M}\Delta\mathbf{s} = \mathbf{t} - \mathbf{M}\mathbf{s}_0, \tag{4.112}$$

where $\Delta\mathbf{s} = \mathbf{s} - \mathbf{s}_0$. Now, view the matrix

$$\mathbf{X} = (\mathbf{M}^T \mathbf{F}^{-1} \mathbf{M} + \mu \mathbf{G})^{-1} \mathbf{M}^T \mathbf{F}^{-1} \tag{4.113}$$

as an approximate generalized inverse of $\mathbf{M}$. Multiplying (4.112) on the left by $\mathbf{X}$, we have

$$\mathbf{XM}\Delta\mathbf{s} = (\mathbf{M}^T\mathbf{F}^{-1}\mathbf{M} + \mu\mathbf{G})^{-1}\mathbf{M}^T\mathbf{F}^{-1}(\mathbf{t} - \mathbf{M}\mathbf{s}_0). \tag{4.114}$$

If $\mathbf{XM} = \mathbf{I}$ were true, then (4.114) and (4.101) would be identical; however, for any $\mu > 0$,

$$\mathbf{XM} = \mathbf{I} - \mu(\mathbf{M}^T\mathbf{F}^{-1}\mathbf{M} + \mu\mathbf{G})^{-1}\mathbf{G} \neq \mathbf{I}. \tag{4.115}$$

Thus, the product $\mathbf{XM}$ is analogous to the resolution matrix $\mathcal{R}_n = \mathbf{M}^\dagger\mathbf{M}$. We will call the product $\mathbf{XM}$ the $n \times n$ *effective resolution matrix*

$$\mathbf{XM} \equiv \mathcal{E}_n, \tag{4.116}$$

and similarly define the product

$$\mathbf{MX} \equiv \mathcal{E}_m, \tag{4.117}$$

as the $m \times m$ effective resolution matrix.

The generalized inverse $\mathbf{M}^\dagger$ gives optimal performance in the sense that no other choice of inverse can produce resolution matrices closer to the identity matrix than $\mathcal{R}_n$ and $\mathcal{R}_m$. To see how well the approximate inverse $\mathbf{X}$ does in this regard, we can compare the effective resolution matrices with the optimal ones. For simplicity, consider the case $\mathbf{F} = \mathbf{G} = \mathbf{I}$. Then, the SVD of $\mathcal{E}_n$ shows that

$$\mathcal{E}_n = (\mathbf{M}^T\mathbf{M} + \mu\mathbf{I})^{-1}\mathbf{M}^T\mathbf{M} = \sum_{j=1}^{r}\left(\frac{\lambda_j^2}{\lambda_j^2 + \mu}\right)\mathbf{z}_j\mathbf{z}_j^T. \tag{4.118}$$

Then, it is easy to see that the effective resolution matrix is closely related to the resolution matrix $\mathcal{R}_n$ by

$$\mathcal{E}_n = \mathcal{R}_n - \sum_{j=1}^{r}\frac{\mu}{\lambda_j^2 + \mu}\mathbf{z}_j\mathbf{z}_j^T. \tag{4.119}$$

If the damping parameter is sufficiently small but still positive ($\mu \to 0^+$), we expect $\mathcal{E}_n \to \mathcal{R}_n$. Similarly, the effective resolution matrix $\mathcal{E}_m$ satisfies

$$\mathcal{E}_m = \mathbf{M}(\mathbf{M}^T\mathbf{M} + \mu\mathbf{I})^{-1}\mathbf{M}^T = \mathcal{R}_m - \sum_{i=1}^{r}\frac{\mu}{\lambda_i^2 + \mu}\mathbf{y}_i\mathbf{y}_i^T. \tag{4.120}$$

and $\mathcal{E}_m \to \mathcal{R}_m$ as $\mu \to 0^+$. We see then that the effective resolution matrices are suboptimal, but approach optimal in the limit that $\mu \to 0^+$. This calculation shows that the approximate inverse $\mathbf{X}$ is biased, but not very strongly biased if very small values of μ are used.

Problem

PROBLEM 4.3.4 *Use (4.119) and (4.120) to show that* $Tr(\mathcal{E}_n) = Tr(\mathcal{E}_m) < rank(\mathbf{M})$ *if* $\mu > 0$.

4.4 Sequential and Iterative Methods

First consider the case where $r = n$. The least-squares solution is then given by

$$\hat{\mathbf{s}}_{\mathrm{LS}} = (\mathbf{M}^T\mathbf{M})^{-1}\mathbf{M}^T\mathbf{t}. \tag{4.121}$$

We begin by summarizing the main ideas behind two matrix inversion methods that work if $\mathbf{M}^T\mathbf{M}$ is invertible. Then, we discuss other methods applicable to more realistic problems in tomography.

Our main focus in this discussion will be to elucidate the general principles behind these methods and to show how they relate to the Moore-Penrose pseudoinverse. A later section will be devoted to evaluating iterative methods and making some jugdments about which algorithms are best for tomography and inversion problems.

4.4.1 Series expansion method

Again letting $\mathbf{A} = \mathbf{M}^T\mathbf{M}$, observe that $\mathbf{A}$ is square and suppose it to be of full rank. In terms of the SVD of $\mathbf{M}$,

$$\mathbf{A} = \sum_{i=1}^{n} \lambda_i^2 \mathbf{z}_i \mathbf{z}_i^T. \tag{4.122}$$

Let $\rho_i = \lambda_i^2$. Then, since $\mathbf{A}$ satisfies its own characteristic polynomial, we have the following matrix identity:

$$(\mathbf{A} - \rho_1\mathbf{I})(\mathbf{A} - \rho_2\mathbf{I})\dots(\mathbf{A} - \rho_n\mathbf{I}) = 0. \tag{4.123}$$

The left-hand side of this equation is simply an nth order matrix polynomial in $\mathbf{A}$, which can be rewritten as

$$\mathbf{A}^n - (\rho_1 + \cdots + \rho_n)\mathbf{A}^{n-1} + \cdots + (-1)^n \rho_1 \cdots \rho_n \mathbf{I} = 0. \tag{4.124}$$

Multiplying through formally by $\mathbf{A}^{-1}$

$$\mathbf{A}^{n-1} - (\rho_1 + \cdots + \rho_n)\mathbf{A}^{n-2} + \cdots + (-1)^n \rho_1 \cdots \rho_n \mathbf{A}^{-1} = 0, \tag{4.125}$$

or

$$\mathbf{A}^{-1} = \frac{(-1)^{n+1}}{\rho_1 \cdots \rho_n}\left[\mathbf{A}^{n-1} - (\rho_1 + \cdots + \rho_n)\mathbf{A}^{n-2} + \cdots + \mathbf{I}\right]. \tag{4.126}$$

This gives a series expansion for $\mathbf{A}^{-1}$ in powers of $\mathbf{A}$ itself. Based on this series, $\mathbf{A}^{-1}\mathbf{M}^T\mathbf{t}$ may be computed recursively if the eigenvalues of $\mathbf{A}$ are known, or at least if the symmetric functions of the eigenvalues that appear in the formulas are known.

This approach clearly fails if $\mathbf{A}$ is not of full rank, since the multiplication leading to (4.125) cannot be performed. The final division by the product of the eigenvalues in (4.126) also cannot be performed.

PROBLEM

PROBLEM 4.4.1 *A real symmetric matrix* $\mathbf{B}$ *has a single vector* $\mathbf{w}$ *in its null space. Use (4.126) to find an expression for the pseudoinverse* $\mathbf{B}^\dagger$.

4.4.2 Conjugate directions and conjugate gradients

In the method of conjugate directions [Hestenes and Stiefel, 1952], a different expansion of $\mathbf{A}^{-1}$ is used. Let $\mathbf{p}_1, \ldots, \mathbf{p}_n$ be a set of vectors such that

$$\mathbf{p}_i^T \mathbf{A} \mathbf{p}_j = \delta_{ij} \mathbf{p}_i^T \mathbf{A} \mathbf{p}_i. \tag{4.127}$$

The vectors $\mathbf{p}_i$ are not necessarily orthogonal with respect to the usual vector dot product, but by construction they are orthogonal relative to the matrix $\mathbf{A}$. The vectors $\mathbf{p}_i$ are said to be conjugate relative to $\mathbf{A}$. Then consider

$$\mathbf{A}' \equiv \sum_{i=1}^{n} \frac{\mathbf{p}_i \mathbf{p}_i^T}{\mathbf{p}_i^T \mathbf{A} \mathbf{p}_i}. \tag{4.128}$$

It follows from (4.127) and (4.128) that

$$\mathbf{A}'(\mathbf{A}\mathbf{p}_j) = \sum_{i=1}^{n} \mathbf{p}_i \delta_{ij} = \mathbf{p}_j, \tag{4.129}$$

and

$$(\mathbf{p}_j^T \mathbf{A})\mathbf{A}' = \sum_{i=1}^{n} \mathbf{p}_i^T \delta_{ij} = \mathbf{p}_j^T, \tag{4.130}$$

which is also just the transpose of (4.129) since $\mathbf{A} = \mathbf{A}^T$. Thus, if the $\mathbf{p}_i$s span the entire vector space (*i.e.*, if they are complete), (4.129) and (4.130) show that

$$\mathbf{A}'\mathbf{A} = \mathbf{I} = \mathbf{A}\mathbf{A}'. \tag{4.131}$$

Uniqueness of the inverse then implies that

$$\mathbf{A}^{-1} = \mathbf{A}'. \tag{4.132}$$

The completeness relation in terms of the $\mathbf{p}_i$s is therefore

$$\mathbf{I} = \sum_{i=1}^{n} \frac{\mathbf{p}_i \mathbf{p}_i^T \mathbf{A}}{\mathbf{p}_i^T \mathbf{A} \mathbf{p}_i} = \sum_{i=1}^{n} \frac{\mathbf{A}\mathbf{p}_i \mathbf{p}_i^T}{\mathbf{p}_i^T \mathbf{A} \mathbf{p}_i}. \tag{4.133}$$

This approach produces a valid and simple formula (4.128) for $\mathbf{A}^{-1}$ when $\mathbf{A}$ is of full rank, and furthermore it is guaranteed to converge in a finite number of steps (see PROBLEM 4.4.5). But, when $\mathbf{A}$ is rank deficient, it must happen that $\mathbf{p}_i^T \mathbf{A} \mathbf{p}_i = 0$ for some $\mathbf{p}_i$ and, therefore, this method also fails in the cases often of most interest in tomography.

Conjugate directions may still be useful for singular $\mathbf{A}$s if care is taken to choose only $\mathbf{p}_i$s orthogonal to the null space of $\mathbf{A}$. Then, this approach may be used to generate the generalized inverse of $\mathbf{A}$.

To see an example of how this works, consider the method of conjugate gradients [Hestenes and Stiefel, 1952; Golub and Van Loan, 1983; Ashby, Manteuffel, and Saylor, 1990] for solving $\mathbf{M}\mathbf{s} = \mathbf{t}$ in the least-squares sense. The normal equations take the form

$$\mathbf{M}^T \mathbf{M} \mathbf{s} = \mathbf{M}^T \mathbf{t}, \tag{4.134}$$

which may be rewritten for these purposes as

$$\mathbf{As} = \mathbf{b} \tag{4.135}$$

where $\mathbf{A} = \mathbf{M}^T\mathbf{M}$ and $\mathbf{b} = \mathbf{M}^T\mathbf{t}$. Then, starting with the error vector $\mathbf{r}^{(1)} = \mathbf{b} - \mathbf{As}^{(1)}$ equal to the first direction vector $\mathbf{p}^{(1)}$, the conjugate-gradient method uses the iteration scheme

$$\mathbf{s}^{(k+1)} = \mathbf{s}^{(k)} + \frac{(\mathbf{p}^{(k)})^T\mathbf{r}^{(k)}}{(\mathbf{p}^{(k)})^T\mathbf{Ap}^{(k)}}\mathbf{p}^{(k)}, \tag{4.136}$$

$$\mathbf{r}^{(k+1)} = \mathbf{b} - \mathbf{As}^{(k+1)}, \tag{4.137}$$

$$\mathbf{p}^{(k+1)} = \mathbf{r}^{(k+1)} - \frac{(\mathbf{p}^{(k)})^T\mathbf{Ar}^{(k+1)}}{(\mathbf{p}^{(k)})^T\mathbf{Ap}^{(k)}}\mathbf{p}^{(k)}. \tag{4.138}$$

The philosophy of this method is to generate a sequence of directions by taking the latest error vector (4.137) as the primary source and then orthogonalizing (4.138) relative to $\mathbf{A}$ with respect to all previous directions taken (see PROBLEM 4.4.4). Since the error vectors are all of the form $\mathbf{r} = \mathbf{M}^T \times$ *a vector*, this iteration sequence cannot generate vectors in the right null space of $\mathbf{M}$. Thus, in principle, this method can converge to the minimum-norm least-squares solution.

Nevertheless, finite but small eigenvalues can have a large effect through the influence of the denominators appearing in (4.136) and (4.138). Small computational errors get magnified under circumstances of poor conditioning. Regularization of this method can be achieved by terminating the process when the latest direction vector satisfies $(\mathbf{p}^{(k+1)})^T\mathbf{Ap}^{(k+1)} \le \epsilon$ where the scalar ϵ is some preset threshold, or by adding a small positive constant μ to the diagonal elements of $\mathbf{A}$.

PROBLEMS

PROBLEM 4.4.2 *Using definition (4.128), show that*

$$\mathbf{A}'\mathbf{A}\mathbf{A}' = \mathbf{A}'. \tag{4.139}$$

Then, use the positivity of $\mathbf{A}$ *together with (4.128) to show that (4.139) implies*

$$\mathbf{A}'\mathbf{A} = \mathbf{I} = \mathbf{A}\mathbf{A}'.$$

Prove the inverse of a matrix is unique and therefore that $\mathbf{A}' = \mathbf{A}^{-1}$.

PROBLEM 4.4.3 *Show that, if*

$$\mathbf{s}^{(k+1)} = \mathbf{s}^{(k)} + \alpha^{(k)}\mathbf{p}^{(k)}$$

is one in a sequence of iterates to solve $\mathbf{As} = \mathbf{b}$ *for* $\mathbf{s}$ *and if*

$$(\mathbf{p}^{(k)})^T\mathbf{Ap}^{(i)} = 0 \quad \textit{for} \quad i = 1, \dots, k-1,$$

then a residual reducing choice of the scalar $\alpha^{(k)}$ *is*

$$\alpha^{(k)} = \frac{(\mathbf{p}^{(k)})^T[\mathbf{b} - \mathbf{As}^{(k)}]}{(\mathbf{p}^{(k)})^T\mathbf{Ap}^{(k)}}.$$

PROBLEM 4.4.4 *Show that* $\mathbf{p}^{(k+1)}$ *as defined in (4.138) is conjugate to* $\mathbf{p}^{(i)}$ *for* $1 \le i \le k$.

PROBLEM 4.4.5 *Define the matrix*

$$\mathbf{A}'_k = \sum_{i=1}^{k} \frac{\mathbf{p}^{(i)}(\mathbf{p}^{(i)})^T}{(\mathbf{p}^{(i)})^T \mathbf{A} \mathbf{p}^{(i)}}.$$

Show that $\mathbf{A}'_k \mathbf{A} \mathbf{A}'_k = \mathbf{A}'_k$. *Then, show that the iterates obtained in the conjugate-gradient method (4.136)–(4.138) satisfy*

$$\mathbf{s}^{(k+1)} = \mathbf{A}'_k \mathbf{b} + \left(\mathbf{I} - \mathbf{A}'_k \mathbf{A}\right) \mathbf{s}^{(1)}. \tag{4.140}$$

Use this expression to show that the iteration converges to the solution in n *steps if* $\mathbf{A}$ *is an* $n \times n$ *positive matrix. What conditions (if any) are required on the eigenvalues of* $\mathbf{A}$ *for this scheme to converge?*

PROBLEM 4.4.6 *Consider the set of vectors*

$$\mathbf{x}, \mathbf{A}\mathbf{x}, \mathbf{A}^2\mathbf{x}, \ldots, \mathbf{A}^n\mathbf{x},$$

where $\mathbf{x}$ *is not an eigenvector of* $\mathbf{A}$ *but has components along all eigenvectors with nonzero eigenvalues (i.e.,* $\mathbf{x}^T\mathbf{z}_i \neq 0$ *for* $1 \le i \le r$*). Then, use Gram-Schmidt orthogonalization to produce the new set of vectors*

$$\mathbf{x}^{(k+1)} = \left[\mathbf{I} - \sum_{j=1}^{k} \frac{\mathbf{x}^{(j)}(\mathbf{x}^{(j)})^T}{(\mathbf{x}^{(j)})^T \mathbf{x}^{(j)}}\right] \mathbf{A}^{k-1}\mathbf{x}, \tag{4.141}$$

where $\mathbf{x}^{(1)} = \mathbf{x}$, $\mathbf{x}^{(2)} = \mathbf{A}\mathbf{x} - \mathbf{x}(\mathbf{x}^T\mathbf{A}\mathbf{x}/\mathbf{x}^T\mathbf{x})$, ... *How many orthogonal vectors can be produced using this technique? If an arbitrary vector* $\mathbf{x}$ *is chosen, analyze the behavior of this procedure in terms of the eigenvectors of* $\mathbf{A}$.

PROBLEM 4.4.7 *What changes must be made in the conjugate-gradient method in order to solve a weighted least-squares problem?*

PROBLEM 4.4.8 *Use the defining relations of conjugate gradients (4.136)–(4.138) to show that*

$$\frac{(\mathbf{p}^{(k)})^T\mathbf{r}^{(k)}}{(\mathbf{p}^{(k)})^T\mathbf{A}\mathbf{p}^{(k)}} = \frac{(\mathbf{r}^{(k)})^T\mathbf{r}^{(k)}}{(\mathbf{p}^{(k)})^T\mathbf{A}\mathbf{p}^{(k)}} = \frac{(\mathbf{r}^{(k)})^T\mathbf{r}^{(k)}}{(\mathbf{r}^{(k)})^T\mathbf{A}\mathbf{p}^{(k)}} \tag{4.142}$$

and

$$\frac{(\mathbf{p}^{(k)})^T\mathbf{A}\mathbf{r}^{(k+1)}}{(\mathbf{p}^{(k)})^T\mathbf{A}\mathbf{p}^{(k)}} = -\frac{(\mathbf{r}^{(k+1)})^T\mathbf{r}^{(k+1)}}{(\mathbf{r}^{(k)})^T\mathbf{r}^{(k)}}. \tag{4.143}$$

[Hestenes and Stiefel, 1952]

PROBLEM 4.4.9 *Use the results of* PROBLEM 4.4.8 *to show that the following algorithm is a conjugate-gradients algorithm for the traveltime inversion problem:*

$$
\begin{array}{l}
\mathbf{s}^{(0)} = 0; \quad \mathbf{p}^{(0)} = \mathbf{r}^{(0)} = \mathbf{M}^T\mathbf{t}; \\
\textit{for} \quad k = 0, 1, 2, \ldots \\
\{ \\
\quad \alpha_k = \frac{(\mathbf{r}^{(k)})^T\mathbf{r}^{(k)}}{(\mathbf{p}^{(k)})^T\mathbf{M}^T\mathbf{M}\mathbf{p}^{(k)}}; \\
\quad \mathbf{s}^{(k+1)} = \mathbf{s}^{(k)} + \alpha_k\mathbf{p}^{(k)}; \\
\quad \mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha_k\mathbf{M}^T\mathbf{M}\mathbf{p}^{(k)}; \\
\quad \textit{if} \quad |\mathbf{r}^{(k+1)}| \quad \textit{is below threshold then quit}; \\
\quad \beta_k = \frac{(\mathbf{r}^{(k+1)})^T\mathbf{r}^{(k+1)}}{(\mathbf{r}^{(k)})^T\mathbf{r}^{(k)}}; \\
\quad \mathbf{p}^{(k+1)} = \mathbf{r}^{(k+1)} + \beta_k\mathbf{p}^{(k)}; \\
\}
\end{array}
$$

[Hestenes and Stiefel, 1952; van der Sluis and van der Vorst, 1987]

PROBLEM 4.4.10 *Use the result of* PROBLEM 4.4.8 *to show that the following algorithm is also a conjugate-gradients algorithm:*

$$
\begin{array}{l}
\mathbf{s}^{(0)} = 0; \quad \mathbf{t}^{(0)} = \mathbf{t}; \quad \mathbf{p}^{(0)} = \mathbf{r}^{(0)} = \mathbf{M}^T\mathbf{t}; \\
\textit{for} \quad k = 0, 1, 2, \ldots \\
\{ \\
\quad \mathbf{q}^{(k)} = \mathbf{M}\mathbf{p}^{(k)}; \\
\quad \alpha_k = \frac{(\mathbf{r}^{(k)})^T\mathbf{r}^{(k)}}{(\mathbf{q}^{(k)})^T\mathbf{q}^{(k)}}; \\
\quad \mathbf{s}^{(k+1)} = \mathbf{s}^{(k)} + \alpha_k\mathbf{p}^{(k)}; \\
\quad \mathbf{t}^{(k+1)} = \mathbf{t}^{(k)} - \alpha_k\mathbf{q}^{(k)}; \\
\quad \mathbf{r}^{(k+1)} = \mathbf{M}^T\mathbf{t}^{(k+1)}; \\
\quad \textit{if} \quad |\mathbf{r}^{(k+1)}| \quad \textit{is below threshold then quit}; \\
\quad \beta_k = \frac{(\mathbf{r}^{(k+1)})^T\mathbf{r}^{(k+1)}}{(\mathbf{r}^{(k)})^T\mathbf{r}^{(k)}}; \\
\quad \mathbf{p}^{(k+1)} = \mathbf{r}^{(k+1)} + \beta_k\mathbf{p}^{(k)}; \\
\}
\end{array}
$$

Note that this variation on conjugate gradients does not require the formation of the (generally) dense matrix $\mathbf{M}^T\mathbf{M}$*. [Björck and Elfving, 1979; Paige and Saunders, 1982; van der Sluis and van der Vorst, 1987]*

4.4.3 Simple iteration

In simple iteration,[3] we start with an initial model $\mathbf{s}^{(0)}$ and iteratively generate a sequence $\mathbf{s}^{(k)}$, $k = 1, 2, \ldots$ using

$$\mathbf{s}^{(k+1)} = \mathbf{s}^{(k)} + \mathbf{M}^T(\mathbf{t} - \mathbf{M}\mathbf{s}^{(k)}). \tag{4.144}$$

In terms of eigenvector expansion coefficients, the iteration sequence becomes

$$\sigma_i^{(k+1)} = \sigma_i^{(k)} + \lambda_i(\tau_i - \lambda_i\sigma_i^{(k)}). \tag{4.145}$$

To solve this equation, note that it can be rewritten as

$$\sigma_i^{(k+1)} = \lambda_i\tau_i + (1-\lambda_i^2)\sigma_i^{(k)} = \lambda_i\tau_i + (1-\lambda_i^2)[\lambda_i\tau_i + (1-\lambda_i^2)\sigma_i^{(k-1)}]. \tag{4.146}$$

Rearranging the resulting series, we find

$$\sigma_i^{(k+1)} = [1 + (1-\lambda^2) + (1-\lambda^2)^2 + \ldots + (1-\lambda^2)^k]\lambda_i\tau_i + (1-\lambda^2)^{k+1}\sigma_i^{(0)}. \tag{4.147}$$

The series multiplying τ_i can be summed exactly for any value of $\lambda_i \neq 0$ as

$$[1 + (1-\lambda_i^2) + (1-\lambda_i^2)^2 + \ldots + (1-\lambda_i^2)^k] = \frac{1-(1-\lambda_i^2)^{k+1}}{1-(1-\lambda_i^2)} \tag{4.148}$$

from which it follows that

$$\sigma_i^{(k+1)} = \left[\frac{1-(1-\lambda_i^2)^{k+1}}{\lambda_i}\right]\tau_i + (1-\lambda_i^2)^{k+1}\sigma_i^{(0)}. \tag{4.149}$$

If $\lambda_i = 0$, (4.145) shows that $\sigma_i^{(k+1)} = \sigma_i^{(0)}$. If we assume that the eigenvalues, λ_i, are all between $-\sqrt{2}$ and $\sqrt{2}$, the iteration sequence converges. The condition $-\sqrt{2} < \lambda_i < \sqrt{2}$ thus implies that $\sigma_i^{(k)} \to \tau_i/\lambda_i$ as $k \to \infty$. That is, the iteration converges to a least-squares model.

We have already seen in Section 4.2 that the stronger condition $-1 \leq \lambda_i \leq 1$ can be guaranteed with an appropriate preconditioning (prescaling) of the matrix $\mathbf{M}$.

Simple iteration is a good method for solving linear tomography problems, and is much simpler to implement than other methods such as conjugate directions or conjugate gradients. This method has significant computational advantages when the dimensions of $\mathbf{M}$ are large. The method is also closely related to SIRT (Simultaneous Iterative Reconstruction Technique) which will be discussed in Section 4.4.5.

PROBLEMS

[3] Also known as Richardson iteration [Varga, 1962].

PROBLEM 4.4.11 *Repeat the analysis of simple iteration for a damped least-squares objective functional. Show that*

$$\mathbf{s}_\mu^{(k+1)} = \mathbf{s}_\mu^{(k)} + \mathbf{M}^T(\mathbf{t} - \mathbf{M}\mathbf{s}^{(0)}) - (\mathbf{M}^T\mathbf{M} + \mu\mathbf{I})(\mathbf{s}_\mu^{(k)} - \mathbf{s}^{(0)}) \tag{4.150}$$

is a valid iteration scheme. Show that

$$\sigma_i^{(k+1)} = \left[\frac{1-(1-\lambda_i^2-\mu)^{k+1}}{\lambda_i^2+\mu}\right](\lambda_i\tau_i + \mu\sigma_i^{(0)}) + (1-\lambda_i^2-\mu)^{k+1}\sigma_i^{(0)}. \tag{4.151}$$

What restrictions must be placed on the λ_is and μ to guarantee convergence of (4.151)? Find the differences between the asymptotic results for (4.151) and those for the undamped least-squares method.

PROBLEM 4.4.12 *Show that, if the maximum eigenvalue is $\lambda_1 = \sqrt{2}$, then convergence of simple iteration is improved by considering $\overline{\mathbf{s}}^{(k+1)} = \frac{1}{2}(\mathbf{s}^{(k+1)} + \mathbf{s}^{(k)})$. [Ivansson, 1983]*

4.4.4 Neural network method

Consider a sequence of models $\mathbf{s}(\eta)$ as a function of a continuous index variable η. We think of η as a measure of the iteration computation time, or as a continuous version of the iteration counter k used in the preceding discussion. The data misfit functional, Ψ, applied to this sequence then is also a function of η. We have

$$\frac{d\Psi}{d\eta} = 2\frac{d\mathbf{s}^T}{d\eta}\nabla_{\mathbf{s}^T}\Psi, \tag{4.152}$$

where

$$\nabla_{\mathbf{s}^T}\Psi = \mathbf{M}^T(\mathbf{M}\mathbf{s} - \mathbf{t}). \tag{4.153}$$

We would like $d\Psi/d\eta < 0$ so that $\mathbf{s}(\eta)$ converges to a model minimizing Ψ as $\eta \to \infty$. It is easy to verify that a negative derivative is achieved by requiring, for some positive scalar $\gamma > 0$,

$$\frac{d\mathbf{s}}{d\eta} = -\gamma\mathbf{M}^T(\mathbf{M}\mathbf{s} - \mathbf{t}). \tag{4.154}$$

Since the differential change in $\mathbf{s}$ is proportional to the local gradient of the objective functional, this choice produces a type of gradient descent method. We thus have a first-order differential equation for $\mathbf{s}(\eta)$. In terms of the expansion coefficients, σ_i, this becomes

$$\frac{d\sigma_i}{d\eta} = \gamma\lambda_i(\tau_i - \lambda_i\sigma_i). \tag{4.155}$$

Using $\sigma_i = 0$ as an initial condition, the solution to (4.155) is given by

$$\sigma_i(\eta) = \lambda_i^{-1}\tau_i\left[1 - e^{-\gamma\lambda_i^2\eta}\right]. \tag{4.156}$$

We see that $\mathbf{s}(\eta)$ does indeed converge to $\mathbf{s}_{\rm LS} = \sum_{i=1}^{r} \lambda_i^{-1}\tau_i \mathbf{z}_i$, with its exponential convergence rate controlled by γ and the magnitudes of the positive eigenvalues λ_i for $i = 1, \ldots, r$.

This approach may be used with other objective functionals. For example, we may compare the results of this approach directly with those of simple iteration by considering the damped least-squares functional

$$\Psi_\mu = (\mathbf{t} - \mathbf{M}\mathbf{s})^T(\mathbf{t} - \mathbf{M}\mathbf{s}) + \mu(\mathbf{s} - \mathbf{s}_b)^T(\mathbf{s} - \mathbf{s}_b), \tag{4.157}$$

where $\mathbf{s}_b$ is the starting model $\mathbf{s}(0) = \mathbf{s}_b$. Then, the same analysis shows that a reasonable equation of motion for $\mathbf{s}(\eta)$ is

$$\frac{d\mathbf{s}}{d\eta} = -\gamma \left[(\mathbf{M}^T\mathbf{M} + \mu\mathbf{I})\mathbf{s} - \mathbf{M}^T\mathbf{t} - \mu\mathbf{s}_b \right], \tag{4.158}$$

where γ is again some positive scalar. Now the coefficients satisfy

$$\frac{d\sigma_i}{d\eta} = \gamma \left[\lambda_i\tau_i + \mu\sigma_i(0) - (\lambda_i^2 + \mu)\sigma_i(\eta) \right], \tag{4.159}$$

which yields upon integration

$$\sigma_i(\eta) = \frac{\lambda_i\tau_i + \mu\sigma_i(0)}{\lambda_i^2 + \mu} \left[1 - e^{-\gamma\lambda_i^2\eta} \right] + \sigma_i(0)e^{-\gamma\lambda_i^2\eta}. \tag{4.160}$$

In the presence of the damping term, the method does not converge to $\mathbf{s}_{\rm LS}$. Instead, it converges exponentially to an approximation with the coefficients $\sigma_i(\infty)$ being weighted averages of the initial value $\sigma_i(0)$ and τ_i/λ_i. The coefficients of the eigenvectors in the null space do not change from their initial values.

Further discussion of this approach together with comparisons to other methods may found in Jeffrey and Rosner [1986a,b] and Lu and Berryman [1990].

Problems

PROBLEM 4.4.13 *Repeat the analysis of the simple iteration and neural network methods assuming the objective functionals are damped and weighted least-squares. Compare the asymptotic results.*

PROBLEM 4.4.14 *Compare the convergence rates of simple iteration and the neural network method.*

4.4.5 ART and SIRT

Probably the two best known methods of solving linear equations for tomographic applications in general geometries are ART and SIRT. ART is the Algebraic Reconstruction Technique [Gordon, Bender, and Herman, 1970; Tanabe, 1971; Herman, Lent, and Rowland, 1973; Natterer, 1986], while SIRT is the Simultaneous Iterative Reconstruction Technique [Gilbert, 1972; Dines and Lytle, 1979; Ivansson, 1983]. ART is closely related to Kaczmarz's iterative projection method of solving linear equations [Kaczmarz, 1937; Gordon, 1974; Guenther et al., 1974]. Our discussion will not distinguish between ART and

Kaczmarz's algorithm, although the term ART is often used to refer to any algebraic reconstruction method including the many variations on Kaczmarz's algorithm [Gordon, 1974]. The discussion of ART presented here is a simplified version of Tanabe's analysis of Kaczmarz's method. The discussion of SIRT follows Ivansson's [1983] analysis of the method developed by Dines and Lytle [1979].

First, we present definitions of two types of projection operators that will be important for the analysis of ART algorithms. Some of the properties of these operators are presented in PROBLEM 4.4.15.

DEFINITION 4.4.1 *A projection operator* $P(\mathbf{a}_i)$ *for a vector* $\mathbf{a}_i$ *is*

$$P(\mathbf{a}_i) \equiv \frac{\mathbf{a}_i\mathbf{a}_i^T}{\mathbf{a}_i^T\mathbf{a}_i}.$$

If a definite set of vectors $\{\mathbf{a}_i\}$ *is under consideration (so no confusion can arise), we shorten the notation to* $P_i = P(\mathbf{a}_i)$.

DEFINITION 4.4.2 *The orthogonal projection operator* $P_\perp(\mathbf{a}_i)$ *for a vector* $\mathbf{a}_i$ *is*

$$P_\perp(\mathbf{a}_i) \equiv \mathbf{I} - P(\mathbf{a}_i).$$

If a definite set of vectors $\{\mathbf{a}_i\}$ *is under consideration, the notation is shortened to* $Q_i = P_\perp(\mathbf{a}_i)$.

Once again, to solve for the slowness model $\mathbf{s}$ given a traveltime vector $\mathbf{t}$ and a ray-path matrix $\mathbf{M}$, we choose to solve $\mathbf{Ms} = \mathbf{t}$ in the least-squares sense (although ART does not require a square matrix) by solving $\mathbf{As} = \mathbf{b}$ where $\mathbf{A} = \mathbf{M}^T\mathbf{M}$ and $\mathbf{b} = \mathbf{M}^T\mathbf{t}$. Now write the matrix $\mathbf{A}$ as

$$\mathbf{A}^T = (\,\mathbf{a}_1 \quad \mathbf{a}_2 \quad \ldots \quad \mathbf{a}_n\,), \tag{4.161}$$

where the $\mathbf{a}_i$s are the n column vectors of the transpose of $\mathbf{A}$. Now suppose that we have an estimate of the slowness vector $\mathbf{s} \simeq \bar{\mathbf{s}}$ and we want to improve the agreement between the data and the estimate of the data by adding an optimal correction in the direction of vector $\mathbf{a}_i$. Then, considering the relation

$$\mathbf{a}_i^T(\bar{\mathbf{s}} + \alpha_i\mathbf{a}_i) = b_i, \tag{4.162}$$

the optimal value of the coefficient α_i is

$$\alpha_i = \frac{b_i - \mathbf{a}_i^T\bar{\mathbf{s}}}{\mathbf{a}_i^T\mathbf{a}_i}. \tag{4.163}$$

Next, we can define an iterative sequence — starting from a guess $\mathbf{s}^{(0)}$ and making use of only one row of $\mathbf{A}$ at a time — given by

$$\mathbf{s}^{(i)} = \mathbf{s}^{(i-1)} + \frac{b_i - \mathbf{a}_i^T\mathbf{s}^{(i-1)}}{\mathbf{a}_i^T\mathbf{a}_i}\mathbf{a}_i. \tag{4.164}$$

Then it is easy to rearrange (4.164) into the form

$$\mathbf{s}^{(i)} = Q_i \mathbf{s}^{(i-1)} + \frac{b_i}{\mathbf{a}_i^T \mathbf{a}_i} \mathbf{a}_i \qquad \text{for} \qquad 1 \le i \le n. \tag{4.165}$$

The significance of (4.165) is that any component of $\mathbf{s}^{(i-1)}$ in the direction $\mathbf{a}_i$ is removed by the orthogonal projection operator Q_i and then the optimal component proportional to $b_i/||\mathbf{a}_i||$ in the direction of the unit vector $\mathbf{a}_i/||\mathbf{a}_i||$ is added in its place.

A single iteration of ART is completed when we have cycled once through all the column vectors of $\mathbf{A}^T$. Then, the slowness $\mathbf{s}^{(n)}$ is the result and this becomes the starting point for the next iteration. In fact, (4.165) may be used for further iterations with only the minor modification that the i subscripts on everything but the slowness estimate should be replaced by $i' = i \bmod n$, except that $i' = n$ if $i \bmod n = 0$.[4] Thus, we have

$$\mathbf{s}^{(i)} = Q_{i'} \mathbf{s}^{(i-1)} + \frac{b_{i'}}{\mathbf{a}_{i'}^T \mathbf{a}_{i'}} \mathbf{a}_{i'} \qquad \text{for} \qquad 1 \le i' \le n, \quad \text{and} \quad 1 \le i, \tag{4.166}$$

and the iteration number is $k = [i/n]$, where the bracket stands for the greatest integer of the argument.

Now it is straightforward to show that

$$\begin{aligned} \mathbf{s}^{(n)} = & \; Q_n Q_{n-1} \cdots Q_1 \mathbf{s}^{(0)} + \frac{b_1}{\mathbf{a}_1^T \mathbf{a}_1} Q_n Q_{n-1} \cdots Q_2 \mathbf{a}_1 \\ & + \frac{b_2}{\mathbf{a}_2^T \mathbf{a}_2} Q_n Q_{n-1} \cdots Q_3 \mathbf{a}_2 + \ldots + \frac{b_n}{\mathbf{a}_n^T \mathbf{a}_n} \mathbf{a}_n, \end{aligned} \tag{4.167}$$

which can be written more compactly as

$$\mathbf{s}^{(n)} = \mathbf{Q}\mathbf{s}^{(0)} + \mathbf{R}\mathbf{b} \tag{4.168}$$

by introducing the matrices

$$\mathbf{Q} = Q_n Q_{n-1} \cdots Q_1 \tag{4.169}$$

and

$$\mathbf{R} = \begin{pmatrix} \frac{Q_n Q_{n-1} \cdots Q_2 \mathbf{a}_1}{\mathbf{a}_1^T \mathbf{a}_1} & \frac{Q_n Q_{n-1} \cdots Q_3 \mathbf{a}_2}{\mathbf{a}_2^T \mathbf{a}_2} & \cdots & \frac{\mathbf{a}_n}{\mathbf{a}_n^T \mathbf{a}_n} \end{pmatrix}. \tag{4.170}$$

It follows easily from (4.168) that

$$\mathbf{s}^{(kn)} = \sum_{p=0}^{k-1} \mathbf{Q}^p \mathbf{R}\mathbf{b} + \mathbf{Q}^k \mathbf{s}^{(0)}, \tag{4.171}$$

[4]The choice of range $1 \le i \le n$ for subscripts made here is typical of Fortran programming conventions. An inversion code written in C would more naturally use the range $0 \le i \le n-1$ and thereby avoid the need for the exception when $i \bmod n = 0$.

where k is the iteration number. Thus, as $k \to \infty$, the iterates $\mathbf{s}^{(kn)} \to \mathbf{s}$, the slowness solving our linear equation if

$$\lim_{k\to\infty} \sum_{p=1}^{k-1} \mathbf{Q}^p\mathbf{R} = \mathbf{A}^\dagger \tag{4.172}$$

and

$$\lim_{k\to\infty} \mathbf{Q}^k\mathbf{s}^{(0)} = \mathbf{n} \quad \text{or} \quad 0, \tag{4.173}$$

where $\mathbf{n}$ is any vector from the right null space of $\mathbf{A}$. However, it has been found that ART may not converge in practice if the data are inconsistent and/or if $\mathbf{A}$ is singular or nearly so [Gilbert, 1972; Gordon, 1974; Dines and Lytle, 1979], which brings us to SIRT.

One common version of the SIRT algorithm [Dines and Lytle, 1979; Ivansson, 1983] may be written in component form as

$$s_j^{(k+1)} = s_j^{(k)} + N_{jj}^{-1} \sum_{i=1}^{m} \frac{(t_i - \sum_{p=1}^{n} l_{ip}s_p^{(k)})l_{ij}}{\sum_{q=1}^{m} l_{iq}^2}, \tag{4.174}$$

where N_{jj} is the number of rays passing through cell j (sometimes known as the hit parameter). In vector notation, this becomes

$$\mathbf{s}^{(k+1)} = \mathbf{s}^{(k)} + \mathbf{N}^{-1}\mathbf{M}^T\mathbf{D}^{-1}(\mathbf{t} - \mathbf{M}\mathbf{s}^{(k)}), \tag{4.175}$$

where $\mathbf{N}$ is the diagonal matrix whose components are N_{jj} and $\mathbf{D}$ is the diagonal matrix whose components are

$$D_{ii} = (\mathbf{M}\mathbf{M}^T)_{ii} = \sum_{j=1}^{n} l_{ij}^2. \tag{4.176}$$

Convergence of this algorithm has been proven by Ivansson [1983]. We present a similar proof.

The analysis is very similar to that presented in Section 4.2 on scaling methods. Define

$$\mathbf{M}'' = \mathbf{D}^{-\frac{1}{2}}\mathbf{M}\mathbf{N}^{-\frac{1}{2}}, \tag{4.177}$$

$$\mathbf{y}'' = \mathbf{D}^{\frac{1}{2}}\mathbf{y}, \tag{4.178}$$

$$\mathbf{z}'' = \mathbf{N}^{\frac{1}{2}}\mathbf{z}. \tag{4.179}$$

Then, consider the eigenvalue problem

$$\mathbf{M}''\mathbf{z}'' = \lambda\mathbf{y}'', \tag{4.180}$$

$$\mathbf{M}''^T\mathbf{y}'' = \lambda\mathbf{z}'', \tag{4.181}$$

which is equivalent to

$$\mathbf{M}\mathbf{z} = \lambda \mathbf{D}\mathbf{y}, \tag{4.182}$$

$$\mathbf{M}^T\mathbf{y} = \lambda \mathbf{N}\mathbf{z}. \tag{4.183}$$

We see that, if $\mathbf{y}_i$ and $\mathbf{z}_j$ are eigenvectors for eigenvalues λ_i and λ_j,

$$\mathbf{y}_i^T\mathbf{M}\mathbf{z}_j = \lambda_i \mathbf{y}_i^T\mathbf{D}\mathbf{y}_j = \lambda_i \mathbf{z}_i^T\mathbf{N}\mathbf{z}_j, \tag{4.184}$$

so we are free to normalize the eigenvectors so that

$$(\mathbf{y}_i'')^T\mathbf{y}_j'' = (\mathbf{z}_i'')^T\mathbf{z}_j'' = \delta_{ij}.p \tag{4.185}$$

PROPOSITION 4.4.1 *The eigenvalues of* $\mathbf{M}''$ *lie in the interval [-1,1].*

Proof: The eigenvalue problem (4.180)–(4.181) can be written in components as

$$\sum_{j=1}^{n} \frac{l_{ij}}{(D_{ii}N_{jj})^{\frac{1}{2}}} z_j'' = \lambda y_i'', \tag{4.186}$$

$$\sum_{i=1}^{m} \frac{l_{ij}}{(N_{jj}D_{ii})^{\frac{1}{2}}} y_i'' = \lambda z_j''. \tag{4.187}$$

Now define the sign function as

$$\operatorname{sgn}(l_{ij}) = \begin{cases} +1 & \text{if} \quad l_{ij} > 0, \\ 0 & \text{if} \quad l_{ij} = 0, \\ -1 & \text{if} \quad l_{ij} < 0, \end{cases} \tag{4.188}$$

and note that

$$N_{jj} = \sum_{i=1}^{m} \operatorname{sgn}(l_{ij}), \tag{4.189}$$

since the path lengths are never negative. Considering (4.186) and using Cauchy's inequality for sums, we have

$$\lambda^2 (y_i'')^2 \leq \sum_{p=1}^{n} \frac{l_{ip}^2}{D_{ii}} \sum_{j=1}^{n} \frac{\operatorname{sgn}(l_{ij})(z_j'')^2}{N_{jj}}. \tag{4.190}$$

Using the definition (4.176) of D_{ii} and summing (4.190) over i, we find

$$\lambda^2 \sum_{i=1}^{m} (y_i'')^2 \leq \sum_{i=1}^{m}\sum_{j=1}^{n} \frac{\operatorname{sgn}(l_{ij})(z_j'')^2}{N_{jj}} = \sum_{j=1}^{n} (z_j'')^2. \tag{4.191}$$

Then, the normalization condition (4.185) shows that (4.191) reduces to

$$\lambda^2 \leq 1. \tag{4.192}$$

∎

Thus, an analysis completely analogous to that given previously for simple iteration (see Section 4.4.3) shows that an iteration scheme of the form

$$\mathbf{N}^{\frac{1}{2}}\mathbf{s}^{(k+1)} = \mathbf{N}^{\frac{1}{2}}\mathbf{s}^{(k)} + \mathbf{M}''^{T}\left[\mathbf{D}^{-\frac{1}{2}}\mathbf{t} - \mathbf{M}''\mathbf{N}^{\frac{1}{2}}\mathbf{s}^{(k)}\right], \tag{4.193}$$

is guaranteed to converge to a solution of $\mathbf{M}^T\mathbf{M}\mathbf{s} = \mathbf{M}^T\mathbf{t}$.

Problems

Problem 4.4.15 *Show that*

1. $P(\mathbf{a})\mathbf{a} = \mathbf{a}$; $\mathbf{a}^T P(\mathbf{a}) = \mathbf{a}^T$;
2. $P_\perp(\mathbf{a})\mathbf{a} = 0$; $\mathbf{a}^T P_\perp(\mathbf{a}) = 0$;
3. $P^2(\mathbf{a}) = P(\mathbf{a})$; $P^T(\mathbf{a}) = P(\mathbf{a})$;
4. $P(-\mathbf{a}) = P(\mathbf{a})$; $P(\gamma\mathbf{a}) = P(\mathbf{a})$ *for any scalar* γ;
5. $P(\mathbf{a})P_\perp(\mathbf{a}) = 0 = P_\perp(\mathbf{a})P(\mathbf{a})$;
6. *if* $\mathbf{a}_2^T\mathbf{a}_1 = 0$, *then* $P_1P_2 = P_2P_1$;
7. *if* $\mathbf{a}_2^T\mathbf{a}_1 \neq 0$, *then* $P_1P_2 \neq P_2P_1$ *unless* $\mathbf{a}_2 = \gamma\mathbf{a}_1$ *for some scalar* γ;
8. $P^\dagger(\mathbf{a}) = P(\mathbf{a})$.

Problem 4.4.16 *A beam of light will not pass through a pair of polarizing filters if their axes are crossed at right angles. However, if a third filter is inserted between the first two with its polarizing axis at 45°, then some of the light can get through. Use projection operators for the vectors* $\mathbf{a}_1 = \hat{x}$, $\mathbf{a}_2 = (\hat{x}+\hat{y})/\sqrt{2}$, *and* $\mathbf{a}_3 = \hat{y}$ *to explain this physical effect. Design a product of projection operators that will project a vector* $\hat{x}$ *onto the direction of its reflection* $-\hat{x}$. *What is the smallest number of projection operators that can be used to produce a reflection? [Feynman, Leighton, and Sands, 1963]*

Problem 4.4.17 *Verify (4.167).*

Problem 4.4.18 *Rewrite (4.18) and (4.19) in terms of projection operators.*

Problem 4.4.19 *Rewrite (4.128) in terms of projection operators.*

Problem 4.4.20 *Rewrite the Gram-Schmit orthogonalization procedure (4.141) in terms of projection operators.*

PROBLEM 4.4.21 *Reconsider the conjugate gradients approach (4.136)–(4.138). Show that the iteration scheme can be written as*

$$\mathbf{s}^{(k+1)} = [\mathbf{I} - Q_A^{(k)}]\mathbf{b} + Q_A^{(k)}\mathbf{s}^{(k)}$$

and

$$\mathbf{p}^{(k+1)} = Q_A^{(k)}\left[\mathbf{b} - \mathbf{A}\mathbf{s}^{(k+1)}\right],$$

where

$$Q_A^{(k)} = \mathbf{I} - \frac{(\mathbf{p}^{(k)})^T\mathbf{p}^{(k)}\mathbf{A}}{(\mathbf{p}^{(k)})^T\mathbf{A}\mathbf{p}^{(k)}}.$$

Show that

$$\mathbf{s}^{(k+1)} = [\mathbf{I} - Q_A^{(k)}Q_A^{(k-1)}\cdots Q_A^{(1)}]\mathbf{b} + Q_A^{(k)}Q_A^{(k-1)}\cdots Q_A^{(1)}\mathbf{s}^{(1)}.$$

Compare this result to (4.140).

PROBLEM 4.4.22 *Suppose that* $\mathbf{A}^T = (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4)$. *Show that*

$$\mathbf{R}\mathbf{A} = \mathbf{I} - Q_4Q_3Q_2Q_1$$

if

$$\mathbf{R} = \begin{pmatrix} \frac{Q_4Q_3Q_2\mathbf{a}_1}{\mathbf{a}_1^T\mathbf{a}_1} & \frac{Q_4Q_3\mathbf{a}_2}{\mathbf{a}_2^T\mathbf{a}_2} & \frac{Q_4\mathbf{a}_3}{\mathbf{a}_3^T\mathbf{a}_3} & \frac{\mathbf{a}_4}{\mathbf{a}_4^T\mathbf{a}_4} \end{pmatrix}.$$

Show that

$$\mathbf{A}^\dagger = \sum_{k=0}^{\infty}[Q_4Q_3Q_2Q_1]^k\mathbf{R}.$$

PROBLEM 4.4.23 *What changes must be made in ART and SIRT in order to solve a weighted least-squares problem? Or, a damped and weighted least-squares problem?*

PROBLEM 4.4.24 *Show that ART may be applied directly to the system* $\mathbf{M}\mathbf{s} = \mathbf{t}$ *when the* $m \times n$ *ray-path matrix* $\mathbf{M}$ *is not square by deriving the formula*

$$s_j^{(i)} = s_j^{(i-1)} + \frac{t_{i'} - \sum_{p=1}^{n} l_{i'p}s_p^{(i-1)}}{\sum_{q=1}^{n} l_{i'q}^2}l_{i'j} \tag{4.194}$$

for the iteration sequence in component form.

PROBLEM 4.4.25 *Since* $\mathbf{A} = \mathbf{M}^T\mathbf{M}$ *in the traveltime inversion problem, the components of* $\mathbf{A}$ *are given by*

$$A_{jj'} = \sum_{p=1}^{m} l_{pj}l_{pj'}$$

and the components of the column vector $\mathbf{a}_i$ *are given by*

$$\mathbf{a}_i = \begin{pmatrix} \sum_{p=1}^m l_{pi}l_{p1} \\ \sum_{p=1}^m l_{pi}l_{p2} \\ \vdots \\ \sum_{p=1}^m l_{pi}l_{pn} \end{pmatrix}.$$

Use these facts to write an expression for the ART iteration scheme (4.166) in component form.

PROBLEM 4.4.26 *Do the two forms of ART in* Problems 4.4.24 *and* 4.4.25 *converge to the same slowness value? [Hint: Consider the generalized inverses of* $\mathbf{M}$ *and* $\mathbf{A} = \mathbf{M}^T\mathbf{M}$*.]*

PROBLEM 4.4.27 *The form of SIRT presented in (4.175) is just one of many possibilities. Show that the following alternatives converge and determine their convergence rates:*

1. $\mathbf{X}^{\frac{1}{2}}\mathbf{s}^{(k+1)} = \mathbf{X}^{\frac{1}{2}}\mathbf{s}^{(k)} + \mathbf{X}^{-\frac{1}{2}}\mathbf{M}^T\mathbf{D}^{-1}(\mathbf{t} - \mathbf{M}\mathbf{s}^{(k)})$ *where* $\mathbf{X} = \mathrm{N}/\gamma$ *for* $0 < \gamma < 2$*;*

2. $\overline{\mathbf{D}}^{\frac{1}{2}}\mathbf{s}^{(k+1)} = \overline{\mathbf{D}}^{\frac{1}{2}}\mathbf{s}^{(k)} + \overline{\mathbf{D}}^{-\frac{1}{2}}\mathbf{M}^T\overline{\mathbf{N}}^{-1}(\mathbf{t} - \mathbf{M}\mathbf{s}^{(k)})$ *where* $\overline{\mathbf{D}} = diag(\mathbf{M}^T\mathbf{M})$ *and* $\overline{\mathbf{N}}_{ii} = \sum_{j=1}^n sgn(l_{ij})$ *is the number of cells traversed by the* i*th ray;*

3. $\overline{\mathbf{D}}^{\frac{1}{2}}\mathbf{s}^{(k+1)} = \overline{\mathbf{D}}^{\frac{1}{2}}\mathbf{s}^{(k)} + n^{-1}\overline{\mathbf{D}}^{-\frac{1}{2}}\mathbf{M}^T(\mathbf{t} - \mathbf{M}\mathbf{s}^{(k)})$.

PROBLEM 4.4.28 *Jacobi's method for solving* $\mathbf{A}\mathbf{s} = \mathbf{b}$ *for a square matrix* $\mathbf{A}$ *is*

$$\mathbf{s}^{(k+1)} = \mathbf{s}^{(k)} + \overline{\mathbf{D}}^{-1}(\mathbf{b} - \mathbf{A}\mathbf{s}^{(k)}),$$

where the diagonal matrix

$$\overline{\mathbf{D}} = diag\mathbf{A}.$$

If $\mathbf{s}^{(-1)} = 0$*, compare* $\mathbf{s}^{(0)}$ *to the backprojection estimate (1.16). Show that, in component form, the iterates of Jacobi's method are*

$$s_j^{(k+1)} = \frac{1}{A_{jj}}\left(b_j - \sum_{p=1}^{j-1} A_{jp}s_p^{(k)} - \sum_{p=j+1}^{n} A_{jp}s_p^{(k)}\right) \tag{4.195}$$

for $j = 1, \ldots, n$*. Does this method converge for the traveltime inversion problem? If not, can it be modified to guarantee convergence? Under what circumstances are SIRT and Jacobi's method equivalent?*

PROBLEM 4.4.29 *The Gauss-Seidel method for solving* $\mathbf{A}\mathbf{s} = \mathbf{b}$ *decomposes the square matrix* $\mathbf{A}$ *into*

$$\mathbf{A} = \overline{\mathbf{D}} + \overline{\mathbf{L}} + \overline{\mathbf{U}},$$

where $\overline{\mathbf{D}}$ *is the diagonal of* $\mathbf{A}$ *while* $\overline{\mathbf{L}}$ *and* $\overline{\mathbf{U}}$ *are the lower and upper triangular pieces of* $\mathbf{A}$. *Then, the iteration scheme is given by*

$$(\overline{\mathbf{D}}+\overline{\mathbf{L}})\mathbf{s}^{(k+1)} = \mathbf{b} - \overline{\mathbf{U}}\mathbf{s}^{(k)}.$$

Show that, in component form, the iterates of the Gauss-Seidel method are

$$s_j^{(k+1)} = \frac{1}{A_{jj}}\left(b_j - \sum_{p=1}^{j-1} A_{jp}s_p^{(k+1)} - \sum_{p=j+1}^{n} A_{jp}s_p^{(k)}\right) \tag{4.196}$$

for $j = 1, \ldots, n$. *Compare and contrast (4.195) and (4.196). Does Gauss-Seidel converge for the traveltime inversion problem? If not, can it be modified to guarantee convergence?*

PROBLEM 4.4.30 *To apply the Gauss-Seidel method to* $\mathbf{Ms} = \mathbf{t}$ *when* $\mathbf{M}$ *is not square, define the new* m*-vector* $\mathbf{q}$ *such that* $\mathbf{s} = \mathbf{M}^T\mathbf{q}$. *Then, the Gauss-Seidel approach may be applied directly to*

$$\mathbf{M}\mathbf{M}^T\mathbf{q} = \mathbf{t}.$$

The resulting iteration scheme is

$$q_i^{(k+1)} = \left(t_i - \sum_{p=1}^{i-1}(\mathbf{M}\mathbf{M}^T)_{ip}q_p^{(k+1)} - \sum_{p=i+1}^{m}(\mathbf{M}\mathbf{M}^T)_{ip}q_p^{(k)}\right)/(\mathbf{M}\mathbf{M}^T)_{ii}. \tag{4.197}$$

Write (4.197) in terms of components and compare the result to (4.194). Is ART equivalent to the Gauss-Seidel method?