necessary. (For "unsticking" procedures, see [10].) The uniqueness of the solution is also not well understood, although for two-dimensional images of reasonable complexity it is believed to be unique.

Deterministic constraints can be incorporated, via projection operators, into iterative methods of linear regularization. In particular, rearranging terms somewhat, we can write the iteration (18.5.21) as

$$\widehat{\mathbf{u}}^{(k+1)} = [\mathbf{1} - \epsilon \lambda \mathbf{H}] \cdot \widehat{\mathbf{u}}^{(k)} + \epsilon \mathbf{A}^T \cdot (\mathbf{b} - \mathbf{A} \cdot \widehat{\mathbf{u}}^{(k)})$$
(18.5.27)

If the iteration is modified by the insertion of projection operators at each step

$$\widehat{\mathbf{u}}^{(k+1)} = (\mathcal{P}_1 \mathcal{P}_2 \cdots \mathcal{P}_m) [\mathbf{1} - \epsilon \lambda \mathbf{H}] \cdot \widehat{\mathbf{u}}^{(k)} + \epsilon \mathbf{A}^T \cdot (\mathbf{b} - \mathbf{A} \cdot \widehat{\mathbf{u}}^{(k)})$$
(18.5.28)

(or, instead of \mathcal{P}_i 's, the \mathcal{T}_i operators of equation 18.5.26), then it can be shown that the convergence condition (18.5.22) is unmodified, and the iteration will converge to minimize the quadratic functional (18.5.6) subject to the desired nonlinear deterministic constraints. See [7] for references to more sophisticated, and faster converging, iterations along these lines.

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18.6 Backus-Gilbert Method

The *Backus-Gilbert method* [1,2] (see, e.g., [3] or [4] for summaries) differs from other regularization methods in the nature of its functionals \mathcal{A} and \mathcal{B} . For \mathcal{B} , the method seeks to maximize the *stability* of the solution $\hat{u}(x)$ rather than, in the first instance, its smoothness. That is,

$$\mathcal{B} \equiv \operatorname{Var}[\widehat{u}(x)] \tag{18.6.1}$$

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(C) 1986-1992 by Numerical Recipes Software.
To order Numerical Recipes books, diskettes, or CDROMs COMPUTING (ISBN 0-521 -43064-X is used as a measure of how much the solution $\hat{u}(x)$ varies as the data vary within their measurement errors. Note that this variance is not the expected deviation of $\hat{u}(x)$ from the true u(x) — that will be constrained by \mathcal{A} — but rather measures the expected experiment-to-experiment scatter among estimates $\hat{u}(x)$ if the whole experiment were to be repeated many times.

For \mathcal{A} the Backus-Gilbert method looks at the relationship between the solution $\hat{u}(x)$ and the true function u(x), and seeks to make the mapping between these as close to the identity map as possible in the limit of error-free data. The method is linear, so the relationship between $\hat{u}(x)$ and u(x) can be written as

$$\widehat{u}(x) = \int \widehat{\delta}(x, x') u(x') dx'$$
(18.6.2)

for some so-called *resolution function* or *averaging kernel* $\hat{\delta}(x, x')$. The Backus-Gilbert method seeks to minimize the width or *spread* of $\hat{\delta}$ (that is, maximize the resolving power). \mathcal{A} is chosen to be some positive measure of the spread.

While Backus-Gilbert's philosophy is thus rather different from that of Phillips-Twomey and related methods, in practice the differences between the methods are less than one might think. A *stable* solution is almost inevitably bound to be *smooth*: The wild, unstable oscillations that result from an unregularized solution are always exquisitely sensitive to small changes in the data. Likewise, making $\hat{u}(x)$ close to u(x) inevitably will bring error-free data into agreement with the model. Thus \mathcal{A} and \mathcal{B} play roles closely analogous to their corresponding roles in the previous two sections.

The principal advantage of the Backus-Gilbert formulation is that it gives good control over just those properties that it seeks to measure, namely stability and resolving power. Moreover, in the Backus-Gilbert method, the choice of λ (playing its usual role of compromise between \mathcal{A} and \mathcal{B}) is conventionally made, or at least can easily be made, *before* any actual data are processed. One's uneasiness at making a *post hoc*, and therefore potentially subjectively biased, choice of λ is thus removed. Backus-Gilbert is often recommended as the method of choice for designing, and predicting the performance of, experiments that require data inversion.

Let's see how this all works. Starting with equation (18.4.5),

$$c_i \equiv s_i + n_i = \int r_i(x)u(x)dx + n_i \tag{18.6.3}$$

and building in linearity from the start, we seek a set of *inverse response kernels* $q_i(x)$ such that

$$\widehat{u}(x) = \sum_{i} q_i(x)c_i \tag{18.6.4}$$

is the desired estimator of u(x). It is useful to define the integrals of the response kernels for each data point,

$$R_i \equiv \int r_i(x) dx \tag{18.6.5}$$

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Substituting equation (18.6.4) into equation (18.6.3), and comparing with equation (18.6.2), we see that

$$\widehat{\delta}(x,x') = \sum_{i} q_i(x) r_i(x') \tag{18.6.6}$$

We can require this averaging kernel to have unit area at every x, giving

$$1 = \int \widehat{\delta}(x, x') dx' = \sum_{i} q_i(x) \int r_i(x') dx' = \sum_{i} q_i(x) R_i \equiv \mathbf{q}(x) \cdot \mathbf{R} \quad (18.6.7)$$

where $\mathbf{q}(x)$ and \mathbf{R} are each vectors of length N, the number of measurements.

Standard propagation of errors, and equation (18.6.1), give

$$\mathcal{B} = \operatorname{Var}[\widehat{u}(x)] = \sum_{i} \sum_{j} q_i(x) S_{ij} q_j(x) = \mathbf{q}(x) \cdot \mathbf{S} \cdot \mathbf{q}(x)$$
(18.6.8)

where S_{ij} is the covariance matrix (equation 18.4.6). If one can neglect off-diagonal covariances (as when the errors on the c_i 's are independent), then $S_{ij} = \delta_{ij}\sigma_i^2$ is diagonal.

We now need to define a measure of the width or spread of $\widehat{\delta}(x, x')$ at each value of x. While many choices are possible, Backus and Gilbert choose the second moment of its square. This measure becomes the functional A,

$$\mathcal{A} \equiv w(x) = \int (x' - x)^2 [\widehat{\delta}(x, x')]^2 dx'$$

= $\sum_i \sum_j q_i(x) W_{ij}(x) q_j(x) \equiv \mathbf{q}(x) \cdot \mathbf{W}(x) \cdot \mathbf{q}(x)$ (18.6.9)

where we have here used equation (18.6.6) and defined the *spread matrix* $\mathbf{W}(x)$ by

$$W_{ij}(x) \equiv \int (x' - x)^2 r_i(x') r_j(x') dx'$$
(18.6.10)

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The functions $q_i(x)$ are now determined by the minimization principle

minimize:
$$\mathcal{A} + \lambda \mathcal{B} = \mathbf{q}(x) \cdot \left[\mathbf{W}(x) + \lambda \mathbf{S} \right] \cdot \mathbf{q}(x)$$
 (18.6.11)

subject to the constraint (18.6.7) that $\mathbf{q}(x) \cdot \mathbf{R} = 1$.

The solution of equation (18.6.11) is

$$\mathbf{q}(x) = \frac{[\mathbf{W}(x) + \lambda \mathbf{S}]^{-1} \cdot \mathbf{R}}{\mathbf{R} \cdot [\mathbf{W}(x) + \lambda \mathbf{S}]^{-1} \cdot \mathbf{R}}$$
(18.6.12)

(Reference [4] gives an accessible proof.) For any particular data set c (set of measurements c_i), the solution $\hat{u}(x)$ is thus

$$\widehat{u}(x) = \frac{\mathbf{c} \cdot [\mathbf{W}(x) + \lambda \mathbf{S}]^{-1} \cdot \mathbf{R}}{\mathbf{R} \cdot [\mathbf{W}(x) + \lambda \mathbf{S}]^{-1} \cdot \mathbf{R}}$$
(18.6.13)

(Don't let this notation mislead you into inverting the full matrix $\mathbf{W}(x) + \lambda \mathbf{S}$. You only need to solve for some \mathbf{y} the linear system $(\mathbf{W}(x) + \lambda \mathbf{S}) \cdot \mathbf{y} = \mathbf{R}$, and then substitute \mathbf{y} into both the numerators and denominators of 18.6.12 or 18.6.13.)

Equations (18.6.12) and (18.6.13) have a completely different character from the linearly regularized solutions to (18.5.7) and (18.5.8). The vectors and matrices in (18.6.12) all have size N, the number of measurements. There is no discretization of the underlying variable x, so M does not come into play at all. One solves a different $N \times N$ set of linear equations for each desired value of x. By contrast, in (18.5.8), one solves an $M \times M$ linear set, but only once. In general, the computational burden of repeatedly solving linear systems makes the Backus-Gilbert method unsuitable for other than one-dimensional problems.

How does one choose λ within the Backus-Gilbert scheme? As already mentioned, you can (in some cases *should*) make the choice *before* you see any actual data. For a given trial value of λ , and for a sequence of x's, use equation (18.6.12) to calculate $\mathbf{q}(x)$; then use equation (18.6.6) to plot the resolution functions $\hat{\delta}(x, x')$ as a function of x'. These plots will exhibit the amplitude with which different underlying values x' contribute to the point $\hat{u}(x)$ of your estimate. For the same value of λ , also plot the function $\sqrt{\operatorname{Var}[\hat{u}(x)]}$ using equation (18.6.8). (You need an estimate of your measurement covariance matrix for this.)

As you change λ you will see very explicitly the trade-off between resolution and stability. Pick the value that meets your needs. You can even choose λ to be a function of x, $\lambda = \lambda(x)$, in equations (18.6.12) and (18.6.13), should you desire to do so. (This is one benefit of solving a separate set of equations for each x.) For the chosen value or values of λ , you now have a quantitative understanding of your inverse solution procedure. This can prove invaluable if — once you are processing real data — you need to judge whether a particular feature, a spike or jump for example, is genuine, and/or is actually resolved. The Backus-Gilbert method has found particular success among geophysicists, who use it to obtain information about the structure of the Earth (e.g., density run with depth) from seismic travel time data.

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18.7 Maximum Entropy Image Restoration

Above, we commented that the association of certain inversion methods with Bayesian arguments is more historical accident than intellectual imperative. *Maximum entropy methods*, so-called, are notorious in this regard; to summarize these methods without some, at least introductory, Bayesian invocations would be to serve a steak without the sizzle, or a sundae without the cherry. We should

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