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CONSTRAINED LEAST SQUARES INTERVAL ESTIMATION*

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Abstract. We extend the classical least squares method for estimating confidence intervals to the rank deficient case, stabilizing the estimate by means of *a priori* side constraints. In order to avoid quadratic programming, we develop a suboptimal method which is in some ways similar to ridge regression but is quite different in that it provides an unambiguous criterion for the choice of the arbitrary parameter. We develop a method for choosing that parameter value and illustrate the procedure by applying it to an example problem.

Key words. confidence intervals, constrained least squares, deconvolution, first kind integral equations, ill-conditioned linear systems, interval estimation, regularization, unfolding

1. Introduction. In this paper we shall be concerned with the problem of obtaining confidence interval estimates from linear regression models with rank deficient or nearly rank deficient matrices. We assume that the model has the standard form

$$\mathbf{y} = \mathbf{K}\mathbf{x} + \mathbf{e} \tag{1.1}$$

where $\mathbf{K}$ is the known $m \times n$ matrix, $\mathbf{x}$ is the unknown solution vector, $\mathbf{y}$ is the vector of observations, and $\mathbf{e}$ is a stochastic error vector satisfying

$$E(\mathbf{e}) = \mathbf{0}, \qquad E(\mathbf{e}\mathbf{e}^T) = \mathbf{S}^2, \tag{1.2}$$

where E denotes the expectation operator. We assume, without loss of generality, that the covariance matrix $\mathbf{S}^2$ is diagonal. In most applications $\mathbf{y}$ is considered to be a sample from a multivariate normal distribution with unknown mean $\bar{\mathbf{y}}$ which satisfies $\mathbf{K}\mathbf{x} = \bar{\mathbf{y}}$. We shall not be overly concerned here with the exact form of the $\mathbf{y}$-distribution, assuming only that the equi-probability contours are ellipsoidal and that for any confidence level $\alpha < 1$ we can find a corresponding constant μ so that the expression

$$(\bar{\mathbf{y}} - \mathbf{y})^T \mathbf{S}^{-2} (\bar{\mathbf{y}} - \mathbf{y}) \leqq \mu^2 \tag{1.3}$$

defines an α-level confidence ellipsoid for the unknown $\bar{\mathbf{y}}$.

The classical linear estimation problem is to find, for a given n-vector $\mathbf{w}$, the best linear, unbiased estimator for the linear function

$$\phi(\mathbf{x}) = \mathbf{w}^T \mathbf{x}. \tag{1.4}$$

Assuming that rank $(\mathbf{K}) = n$, the solution is

$$\hat{\phi} = \mathbf{w}^T \hat{\mathbf{x}}$$

where $\hat{\mathbf{x}}$ is the least squares solution vector defined by

$$\hat{\mathbf{x}} = (\mathbf{K}^T \mathbf{S}^{-2} \mathbf{K})^{-1} \mathbf{K}^T \mathbf{S}^{-2} \mathbf{y}. \tag{1.5}$$

An α-level confidence interval $[\phi_{lo}, \phi^{up}]$ for ϕ is obtained from

$$\phi_{lo}^{up} = \mathbf{w}^T \hat{\mathbf{x}} \pm \sqrt{(\mu^2 - r_0)\mathbf{w}^T (\mathbf{K}^T \mathbf{S}^{-2} \mathbf{K})^{-1} \mathbf{w}} \tag{1.6}$$

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where $\mathbf{r}_0$ is the minimum of the sum of squared residuals, i.e.,

$$r_0 = \min_{\mathbf{x}} \{(\mathbf{y}-\mathbf{K}\mathbf{x})^T\mathbf{S}^{-2}(\mathbf{y}-\mathbf{K}\mathbf{x})\} = (\mathbf{y}-\mathbf{K}\hat{\mathbf{x}})^T\mathbf{S}^{-2}(\mathbf{y}-\mathbf{K}\hat{\mathbf{x}}).$$

Since (1.3) defines a confidence ellipsoid in $\mathbf{y}$-space, it follows that

$$(\mathbf{K}\mathbf{x}-\mathbf{y})^T\mathbf{S}^{-2}(\mathbf{K}\mathbf{x}-\mathbf{y}) \leqq \mu^2$$

or, equivalently,

$$(\mathbf{x}-\hat{\mathbf{x}})^T\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}(\mathbf{x}-\hat{\mathbf{x}}) \leqq \mu^2 - r_0, \tag{1.7}$$

defines a confidence ellipsoid in $\mathbf{x}$-space. The confidence bounds ϕ_{lo}, ϕ^{up} are just the values attained by $\phi(\mathbf{x})$ on the two support planes of this latter confidence ellipsoid which are orthogonal to the vector $\mathbf{w}$ (cf. [14, Appendix III]).

In the case rank $(\mathbf{K}) < n$ the ellipsoid (1.7) is unbounded in some directions and the confidence intervals become $(-\infty, +\infty)$ for any vector $\mathbf{w}$ having a nonzero component in the null space of $\mathbf{K}$. In most applications it is not practical to pick $\mathbf{w}$ without such a component, and in fact it is not even possible to unambiguously determine rank $(\mathbf{K})$. Therefore it is necessary to add some a priori side constraints to the problem in order to obtain nontrivial interval estimates. In this paper we shall add side constraints of the form

$$p_j \leqq x_j \leqq q_j, \qquad j = 1, \cdots, n, \tag{1.8}$$

where the p_j and q_j are known bounds obtained from external considerations.

The method that will be described here is basically a generalization and extension of the FERDOR method of radiation spectrum unfolding which was developed at Oak Ridge National Laboratory in the 1960's by Walter R. Burrus and his colleagues. The problem addressed by FERDOR is to give confidence interval estimates of quantities of the form

$$\int_a^b w(\mathscr{E})x(\mathscr{E})\, d\mathscr{E},$$

where $x(\mathscr{E})$ is an unknown radiation energy spectrum which is related to a measured pulse height spectrum y_i by

$$\int_a^b K_i(\mathscr{E})x(\mathscr{E})\, d\mathscr{E} = y_i + e_i, \qquad i = 1, \cdots, m. \tag{1.9}$$

The $K_i(\mathscr{E})$ are the response functions of the measuring instrument, and the e_i are random measuring errors. The functions $w(\mathscr{E})$, which are designed to exhibit the various desired aspects of the unknown spectrum, are called window functions, and we shall often refer to the vector $\mathbf{w}$ as a window vector.

The FERDOR method has enjoyed great success in spite of the lack, until rather recently, of adequate, coherent documentation. A succinct description of the method has been given by Burrus et al. [4] in a paper which also briefly outlines the history of its development and gives references to earlier published descriptions. The method assumes that $K_i(\mathscr{E}) \geqq 0$, $i = 1, \cdots, m$ and $x(\mathscr{E}) \geqq 0$ for all energies $\mathscr{E}$. The basic discrete problems that must be solved are

$$\phi_{lo} = \min_{\mathbf{x}} \{\mathbf{w}^T\mathbf{x} | (\mathbf{K}\mathbf{x}-\mathbf{y})^T\mathbf{S}^{-2}(\mathbf{K}\mathbf{x}-\mathbf{y}) \leqq \mu^2, \mathbf{x} \geqq \mathbf{0}\}, \tag{1.10}$$

$$\phi^{up} = \max_{\mathbf{x}} \{\mathbf{w}^T\mathbf{x} | (\mathbf{K}\mathbf{x}-\mathbf{y})^T\mathbf{S}^{-2}(\mathbf{K}\mathbf{x}-\mathbf{y}) \leqq \mu^2, \mathbf{x} \geqq \mathbf{0}\}. \tag{1.11}$$

In [13, Chapt. 5], it is shown that each of these problems can be solved by parametric quadratic programming, but because of the excessive amount of computation required, this is an expensive approach for most applications which require a large number of window vectors. The FERDOR approach is suboptimal in that it gives interval estimates that are wider than the optimally narrow intervals obtained from the quadratic programming procedures. The suboptimal estimates are obtained by an augmented least squares procedure which is similar in approach to ridge regression, and it is necessary to choose the value of an arbitrary parameter. The main contribution of the present work is to provide a procedure for the optimum choice of that parameter value. We also extend the previous work to allow different types of a priori side constraints and by iterating the procedure to obtain improved suboptimal bounds. In the next section we develop the new procedure without considering the statistical details which are described at length in [13, Chapt. 6].

2. Development of the method. Given an n-vector $\mathbf{w}$ and an $m \times n$ matrix $\mathbf{K}$, we wish to find bounds for $\phi(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$, where

$$\mathbf{y} = \mathbf{K}\mathbf{x} + \mathbf{e}$$

and $\mathbf{y}$ lies in the error ellipsoid

$$(\mathbf{y} - \mathbf{K}\mathbf{x})^T\mathbf{S}^{-2}(\mathbf{y} - \mathbf{K}\mathbf{x}) \leqq \mu^2, \tag{2.1}$$

with $\mathbf{S}^{-2}$ a positive definite diagonal matrix, and μ any constant such that

$$\mu^2 \geqq r_0 = \min_{\mathbf{x}} (\mathbf{y} - \mathbf{K}\mathbf{x})^T\mathbf{S}^{-2}(\mathbf{y} - \mathbf{K}\mathbf{x}).$$

The problems are then

$$\text{Find} \quad \begin{matrix} \max \\ \min \end{matrix} \left\{ \mathbf{w}^T\mathbf{x} \middle| (\mathbf{K}\mathbf{x} - \mathbf{y})^T\mathbf{S}^{-2}(\mathbf{K}\mathbf{x} - \mathbf{y}) \leqq \mu^2 \right\}. \tag{2.2}$$

Often $\mathbf{w}$ is taken successively as $(1, 0, \cdots, 0)^T$, $(0, 1, \cdots, 0)^T$, $\cdots$, $(0, \cdots, 1)^T$, so that the quantities $\mathbf{w}^T\mathbf{x}$ are estimates of the components of $\mathbf{x}$. If $\mathbf{K}$ is an ill-conditioned matrix, the error ellipsoid (2.1), which we will call the S-ellipsoid, is greatly elongated in the directions of the eigenvectors corresponding to the small eigenvalues of $\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}$. (See Fig. 2.1.) The principal axes have the same directions as the eigenvectors of $\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}$, and their lengths are inversely proportional to the corresponding eigenvalues.

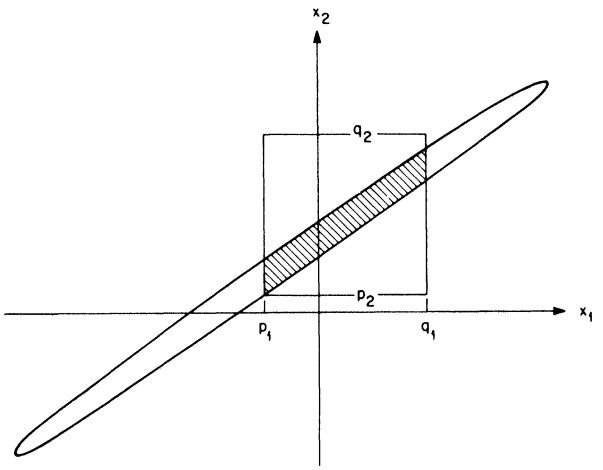

FIG. 2.1. *The* S*-ellipsoid and the* Q*-box.*

If $\mathbf{w}$ has a component in the direction of one of the long axes of the S-ellipsoid, the bounds on $\mathbf{w}^T\mathbf{x}$ will be very wide. We seek to improve these bounds by incorporating into the problem a priori knowledge of bounds on the components of $\mathbf{x}$, $p_j \leqq x_j \leqq q_j$, $j = 1, \cdots, n$ as shown in Fig. 2.1. The problems may now be stated as follows:

$$\text{(2.3)} \quad \text{Find} \quad \phi_{lo}^{up} = \begin{matrix}\max \\ \min\end{matrix} \left\{ \mathbf{w}^T\mathbf{x} \middle| (\mathbf{Kx}-\mathbf{y})^T\mathbf{S}^{-2}(\mathbf{Kx}-\mathbf{y}) \leqq \mu^2,\ p_j \leqq x_j \leqq q_j,\ j = 1, \cdots, n \right\}.$$

Geometrically, the constraint region is the intersection of the S-ellipsoid and an interval in R^n, which we call the Q-box. Since the calculation of a solution cannot easily be done using the intersection of an ellipsoid and a box, we replace the Q-box by an ellipsoid which circumscribes it, namely,

$$\frac{1}{n}(\mathbf{x}-\mathbf{d})^T\mathbf{Q}^{-2}(\mathbf{x}-\mathbf{d}) \leqq 1,$$

where

$$\mathbf{d} = \left(\frac{p_1+q_1}{2}, \frac{p_2+q_2}{2}, \cdots, \frac{p_n+q_n}{2} \right)^T, \quad \text{and} \quad \mathbf{Q} = \operatorname{diag}\left(\frac{q_1-p_1}{2}, \cdots, \frac{q_n-p_n}{2} \right).$$

We call this ellipsoid the Q-ellipsoid and remark here that, unless a mistake has been made in the analysis of the problem, the S- and Q-ellipsoids have a nonempty intersection.

The intersection of two ellipsoids is no easier to handle computationally than the intersection of a box and an ellipsoid. One strategy is to find another ellipsoid which contains the intersection of the S and Q ellipsoids. W. Kahan [9] has defined a "tight" circumscribing ellipsoid about the intersection of two ellipsoids with common centers, but there is no guarantee that the S- and Q-ellipsoids have that property. Consequently, we make one more suboptimizing step and take a convex linear combination of the S- and Q-ellipsoids. The problems now become:

$$\text{(2.4)} \quad \phi_{lo}^{up} = \begin{matrix}\max \\ \min\end{matrix} \left\{ \mathbf{w}^T\mathbf{x} \middle| \eta \cdot \frac{1}{\mu^2}(\mathbf{Kx}-\mathbf{y})^T\mathbf{S}^{-2}(\mathbf{Kx}-\mathbf{y}) + (1-\eta)\cdot\frac{1}{n}(\mathbf{x}-\mathbf{d})^T\mathbf{Q}^{-2}(\mathbf{x}-\mathbf{d}) \leqq 1 \right\}, \quad 0 \leqq \eta \leqq 1,$$

where η determines how much of each ellipsoid is taken. It can be shown that every such convex combination of the S- and Q-ellipsoids is an ellipsoid which contains the original constraint region, i.e., the intersection of the S-ellipsoid and the Q-box. The constraint in (2.4) can be written

$$(\mathbf{Ax}-\mathbf{p})^T \begin{pmatrix} \frac{\eta}{\mu^2}\mathbf{S}^{-2} & 0 \\ 0 & \frac{1-\eta}{n}\mathbf{Q}^{-2} \end{pmatrix} (\mathbf{Ax}-\mathbf{p}) \leqq 1,$$

where

$$\mathbf{A} = \begin{pmatrix} \mathbf{K} \\ \mathbf{I} \end{pmatrix}, \qquad \mathbf{p} = \begin{pmatrix} \mathbf{y} \\ \mathbf{d} \end{pmatrix}.$$

Now define new parameters

$$\tau = \left(\frac{1-\eta}{\eta} \right)\mu^2 \quad \text{and} \quad \mathbf{V}^{-2}(\tau) = \begin{pmatrix} \mathbf{S}^{-2} & 0 \\ 0 & \frac{\tau}{n}\mathbf{Q}^{-2} \end{pmatrix}.$$

The constraint can then be rewritten as

$$(\mathbf{Ax}-\mathbf{p})^T\mathbf{V}^{-2}(\tau)(\mathbf{Ax}-\mathbf{p}) \leqq \tau+\mu^2,$$

with τ chosen from the interval $[0, +\infty)$. Note that the matrix $\mathbf{V}^{-2}(\tau)$ would be rank deficient only if one or more of the x_j were completely determined by a priori information. We assume in the following that any such x_j have been removed from the problem. By conventional least squares,

$$\rho_0 = \min_{\mathbf{x}} (\mathbf{Ax}-\mathbf{p})^T\mathbf{V}^{-2}(\tau)(\mathbf{Ax}-\mathbf{p}) \tag{2.5}$$

is attained at

$$\tilde{\mathbf{x}} = [\mathbf{A}^T\mathbf{V}^{-2}(\tau)\mathbf{A}]^{-1}\mathbf{A}^T\mathbf{V}^{-2}(\tau)\mathbf{p},$$

or

$$\tilde{\mathbf{x}} = \left[\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}+\frac{\tau}{n}\mathbf{Q}^{-2}\right]^{-1}\left[\mathbf{K}^T\mathbf{S}^{-2}\mathbf{y}+\frac{\tau}{n}\mathbf{Q}^{-2}\mathbf{d}\right].$$

Notice here the similarity to ridge regression (cf. [7], [8], [10]), where

$$\mathbf{x}^* = [\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}+\lambda\mathbf{I}]^{-1}\mathbf{K}^T\mathbf{S}^{-2}\mathbf{y}$$

would be the ridge estimate of $\mathbf{x}$.

For a discussion of the technique of ridge regression, see Hoerl and Kennard [7] who point out that the variance of the estimate of $\mathbf{x}$ is reduced, at the cost of some bias, the bias squared being a continuous monotonically increasing function of λ. Unfortunately, as Brown and Beattie show in [2], the bias produced by ridge regression can be large, and since the expression for squared bias involves $\mathbf{x}$, bias cannot be accurately estimated. One advantage of the interval estimation technique is that for any $\tau \in [0, \infty)$ the interval $[\phi_{lo}, \phi^{up}]$ contains $\mathbf{w}^T\mathbf{x}$ with at least the same confidence level as that associated with the original error ellipsoid. Also, there is no universally accepted way to choose the λ of ridge regression, but the interval estimation strategy provides a criterion for choosing τ. *Since all values of τ produce valid confidence intervals, one should choose that value which yields the narrowest interval.*

The problems now are: Find

$$\begin{aligned}\max_{\min}\left\{\mathbf{w}^T\mathbf{x} \middle| (\mathbf{Ax}-\mathbf{p})^T\mathbf{V}^{-2}(\mathbf{Ax}-\mathbf{p}) \leqq \tau+\mu^2\right\} \\ = \max_{\min}\left\{\mathbf{w}^T\mathbf{x} \middle| (\mathbf{x}-\tilde{\mathbf{x}})^T(\mathbf{A}^T\mathbf{V}^{-2}\mathbf{A})(\mathbf{x}-\tilde{\mathbf{x}}) \leqq \tau+\mu^2-\rho_0\right\}.\end{aligned}$$

The solutions, using Lagrange multipliers, are

$$\phi_{lo}^{up} = \mathbf{w}^T\tilde{\mathbf{x}} \pm \sqrt{\tau+\mu^2-\rho_0}\sqrt{\mathbf{w}^T(\mathbf{A}^T\mathbf{V}^{-2}\mathbf{A})^{-1}\mathbf{w}}. \tag{2.6}$$

Note that $\tilde{\mathbf{x}}$, ρ_0 and $\mathbf{V}^{-2}$, and hence ϕ^{up} and ϕ_{lo} are dependent on the choice of τ. We wish to choose a τ (if one exists) giving the minimum interval width. Let

$$\mathscr{L}^2 = (\tau+\mu^2-\rho_0)\mathbf{w}^T(\mathbf{A}^T\mathbf{V}^{-2}\mathbf{A})^{-1}\mathbf{w}.$$

We take $\partial\mathscr{L}^2/\partial\tau$ and solve the equation

$$\frac{\partial\mathscr{L}^2}{\partial\tau} = 0 \quad \text{for } \tau.$$

Recall that $\mathbf{A}^T\mathbf{V}^{-2}\mathbf{A}=\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}+(\tau/n)\mathbf{Q}^{-2}$, so that when $\tau=0$, the problem reduces to the one corresponding to the S-ellipsoid, while as τ increases, the S-ellipsoid becomes insignificant compared to the Q-ellipsoid. For a typical ill-conditioned problem, we might expect graphs of $\mathscr{L}^2$ versus τ and $\partial\mathscr{L}^2/\partial\tau$ versus τ to look somewhat like the ones in Fig. 2.2. The shapes of the graphs have been verified by trial examples.

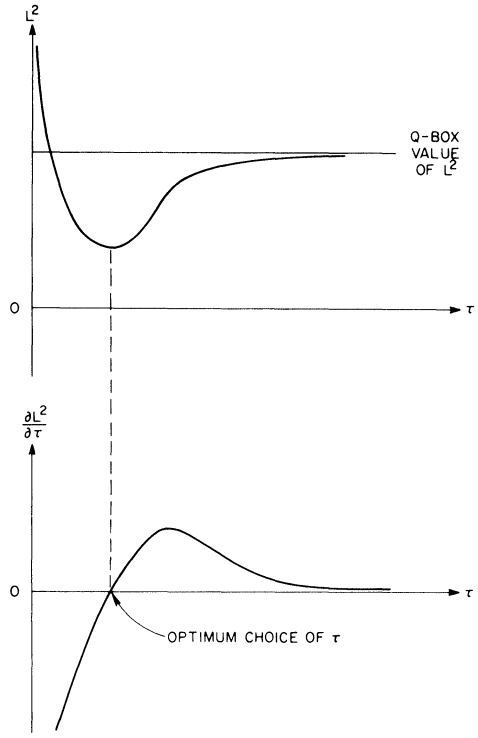

FIG. 2.2. *Choice of* τ.

To solve $\partial\mathscr{L}^2/\partial\tau=0$, we need to invert $\mathbf{A}^T\mathbf{V}^{-2}\mathbf{A}=\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}+(\tau/n)\mathbf{Q}^{-2}$. It is convenient to make the following change of variables. Let

$$\mathbf{x}'=\mathbf{Q}^{-1}\mathbf{x}.$$

We then have

$$\mathbf{A}\mathbf{x}=\begin{pmatrix}\mathbf{K}\\ \mathbf{I}\end{pmatrix}\mathbf{Q}\mathbf{x}'=\begin{pmatrix}\mathbf{K}\mathbf{Q}\\ \mathbf{Q}\end{pmatrix}\mathbf{x}',$$

and the least squares solution of (2.5) is

$$\tilde{\mathbf{x}}'=\left(\mathbf{Q}\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}\mathbf{Q}+\frac{\tau}{n}\mathbf{I}\right)^{-1}\left(\mathbf{Q}\mathbf{K}^T\mathbf{S}^{-2}\mathbf{y}+\frac{\tau}{n}\mathbf{Q}^{-1}\mathbf{d}\right).$$

As in (2.6), we have

$$\phi_{lo}^{up}=\mathbf{w}^T(\mathbf{Q}\tilde{\mathbf{x}}')\pm\sqrt{\tau+\mu^2-\rho_0}\,\sqrt{\mathbf{w}^T\mathbf{Q}\left(\mathbf{Q}\mathbf{K}^T\mathbf{S}^{-2}\mathbf{K}\mathbf{Q}+\frac{\tau}{n}\mathbf{I}\right)^{-1}\mathbf{Q}\mathbf{w}}. \tag{2.6'}$$

Now it can be seen how the change of variables helps in writing the inverse. Consider

the singular value decomposition of $\mathbf{S}^{-1}\mathbf{KQ}$,

$$\mathbf{S}^{-1}\mathbf{KQ} = \mathbf{L}\Sigma\mathbf{R}^T,$$

where $\mathbf{L}$ is an $m \times m$ orthogonal matrix, $\mathbf{R}$ is an $n \times n$ orthogonal matrix, and Σ is the $m \times n$ singular value matrix. Using the singular value decomposition,

$$\left(\mathbf{QK}^T\mathbf{S}^{-2}\mathbf{KQ} + \frac{\tau}{n}\mathbf{I}\right) = \mathbf{R}\left(\Sigma^T\Sigma + \frac{\tau}{n}\mathbf{I}\right)\mathbf{R}^T.$$

Notice that $\Sigma^T\Sigma = \operatorname{diag}(\sigma_1^2, \cdots, \sigma_n^2)$, where some of the σ_j may be 0. Now the inverse can easily be written:

$$\left[\mathbf{QK}^T\mathbf{S}^{-2}\mathbf{KQ} + \frac{\tau}{n}\mathbf{I}\right]^{-1} = \mathbf{R}\operatorname{diag}\left(\frac{n}{n\sigma_1^2+\tau}, \cdots, \frac{n}{n\sigma_n^2+\tau}\right)\mathbf{R}^T.$$

It is now straightforward, but tedious, to calculate the partial derivative $\partial\mathscr{L}^2/\partial\tau$, where

$$\mathscr{L}^2 = (\tau + \mu^2 - \rho_0)\left[\mathbf{w}^T\mathbf{Q}\left(\mathbf{QK}^T\mathbf{S}^{-2}\mathbf{KQ} + \frac{\tau}{n}\mathbf{I}\right)^{-1}\mathbf{Qw}\right].$$

The result is

$$\frac{\partial\mathscr{L}^2}{\partial\tau} = -\frac{(\tau+\mu^2-\rho_0)}{n}\sum_{j=1}^{n}\frac{v_j^2}{(\sigma_j^2+\tau/n)^2} + \left\{1 - \frac{1}{n}\sum_{j=1}^{n}\frac{(z_j+\tau r_j/n)^2}{(\sigma_j^2+\tau/n)^2} + \frac{2}{n}\sum_{j=1}^{n}\frac{(z_j+\tau r_j/n)r_j}{(\sigma_j^2+\tau/n)} - \frac{1}{n}\sum_{j=1}^{n} r_j^2\right\}\sum_{j=1}^{n}\frac{v_j^2}{(\sigma_j^2+\tau/n)},$$

where

$$\mathbf{r} = \mathbf{R}^T\mathbf{Q}^{-1}\mathbf{d}, \quad \mathbf{v} = \mathbf{R}^T\mathbf{Qw}, \quad \mathbf{z} = \Sigma^T\mathbf{L}^T\mathbf{S}^{-1}\mathbf{y}.$$

An equation solver may be used to seek values of τ at which this derivative is zero. We supply lower and upper bounds for τ and use an adaptation of Brent's ZERO ([1, Chapt. 4]). In conventional ridge regression, the columns of $\mathbf{K}$ would be normalized to have zero means and unit variances; we choose initial bounds for τ in terms of the norms of the columns of $\mathbf{S}^{-1}\mathbf{KQ}$. If the problem is a well-conditioned one, ZERO may fail to find an axis crossing because $\partial\mathscr{L}^2/\partial\tau > 0$ for all τ (see Fig. 2.3a). In that case, we set $\tau = 0$ and solve the unconstrained problem. If the a priori bounds are the best obtainable, ZERO also fails since $\partial\mathscr{L}^2/\partial\tau < 0$ for all τ, indicating that the Q-box provides the best bounds. (See Fig. 2.3b.)

Notice that $\mathbf{w}$ does not enter into the singular value decomposition of $\mathbf{S}^{-1}\mathbf{KQ}$, so that τ can be found for any number of window vectors $\mathbf{w}$ without doing the *SVD* again. In particular, $\mathbf{w}$ can successively be taken to be $(1, 0, \cdots, 0)^T$, $(0, 1, 0, \cdots, 0)^T, \cdots,$ $(0, 0, \cdots, 1)^T$ to find new bounds on $x_1, \cdots, x_n$. The bounds thus obtained define a new interval in R^n which is guaranteed to contain the intersection of the S-ellipsoid with the original a priori constraint region. Hopefully the new bounds are all better than the original ones. If they are not better for some of the x_j, then the original bounds are retained in those cases. The new vector interval can then be used to define a new $\mathbf{Q}$-matrix and $\mathbf{d}$-vector and the whole process can be iterated to improve the bounds further. At each step of the iteration the current Q-box is not necessarily a 100% guaranteed vector interval for the solution $\mathbf{x}$, but it is guaranteed to contain the intersection of the original 100% a priori constraint box with the S-ellipsoid, so it defines confidence intervals for the x_j with confidence levels that are at least as great as those of the S-ellipsoid. The idea in iterating this type of calculation was first

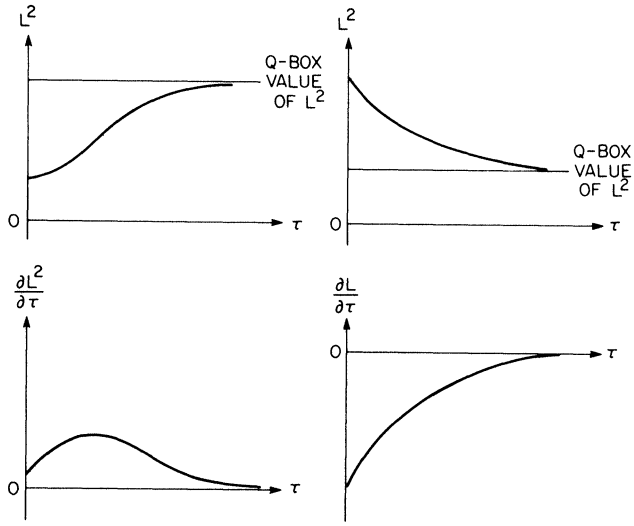

FIG. 2.3. a. *Well-conditioned problem.* b. *A priori bounds best obtainable.*

suggested by W. R. Burrus [3, Chapt. 9] and was briefly discussed by M. T. Heath [6, Chapt. 3]. The iteration process is expensive in our procedure because the singular value decomposition must be repeated at each step. This is not a prohibitive disadvantage, however, because the iteration converges very quickly. Two or three iterations have been sufficient for every problem we have tried. A referee suggested reducing the calculations by using a bidiagonalization of $\mathbf{S}^{-1}\mathbf{KQ}$ (cf. Elden [5]) rather than the full singular value decomposition.

It is possible to use extra knowledge about the solution vector $\mathbf{x}$ to improve the bounds even more. For example, suppose $0 \leqq x_1 \leqq \cdots \leqq x_n$. Then $\mathbf{x}$ can be written

$$\mathbf{x} = \mathbf{Pu}, \qquad \mathbf{u} \geqq \mathbf{0},$$

where

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

The initial bounds on the u_j can be obtained from

$$p_1 \leqq u_1 \leqq q_1, \quad p_j - q_{j-1} \leqq u_j \leqq q_j - p_{j-1}, \quad j = 2, 3, \cdots, n.$$

Now suppose that we want to find $\min^{\max}(x_1 + x_4)$. Then $\mathbf{w}^T = (1, 0, 0, 1, 0, \cdots, 0)$, and $\mathbf{w}^T\mathbf{x} = \mathbf{w}^T\mathbf{Pu}$. The matrix $\mathbf{P}$ is essentially a "shape" matrix, incorporating a priori knowledge of the shape of the solution. The vector $\mathbf{w}$ is a "window" vector determining which linear combination of components of $\mathbf{x}$ we look at. The final problems are then:

find

$$\min^{\max}\left\{(\mathbf{w}^T\mathbf{P})\mathbf{u} \middle| (\mathbf{KPu} - \mathbf{y})^T\mathbf{S}^{-2}(\mathbf{KPu} - \mathbf{y}) \leqq \mu^2\right\}.$$

We replace $\mathbf{K}$ by $\mathbf{K}' = \mathbf{KP}$, and the initial bounds on the $\mathbf{u}$ are used to form a matrix

$\mathbf{Q}'$ analogous to the $\mathbf{Q}$ in the original problem. The transformation of variables is then $\mathbf{u}' = (\mathbf{Q}')^{-1}\mathbf{u}$.

3. An example. We now present a well-known integral equation problem as an example illustrating the method and the use of a priori constraints on the solution $\mathbf{x}$. The problem was originally given by Phillips [11], and was discussed by Rust and Burrus ([13, § 1.5]). The problem is to solve

$$\int_{-6}^{6} K(t, s)x(s)\,ds = y(t), \qquad |t| \leqq 6,$$

where

$$K(t, s) = \begin{cases} 1 + \cos\dfrac{\pi(s-t)}{3}, & |s-t| \leqq 3, \quad |t| \leqq 6, \\ 0, & |s-t| \geqq 3, \quad |t| \leqq 6, \end{cases}$$

and

$$y(t) = (6 - |t|)\left[1 + \frac{1}{2}\cos\frac{\pi t}{3}\right] + \frac{9}{2\pi}\sin\frac{\pi|t|}{3}, \qquad |t| \leqq 6.$$

The solution is

$$x(s) = \begin{cases} 1 + \cos\left(\dfrac{\pi s}{3}\right), & |s| \leqq 3, \\ 0, & |s| > 3. \end{cases}$$

We present a 60×41 discretization of the problem. Let

$$s_j = -3 + \tfrac{3}{20}(j-1), \quad j = 1, \cdots, 41,$$

$$t_i = -6 + \tfrac{1}{5}(i - .5), \quad i = 1, \cdots, 60,$$

$$K_{ij} = \begin{cases} \left[1 + \cos\left(\dfrac{\pi}{3}(s_j - t_i)\right)\right]\omega_j, & |s_j - t_i| \leqq 6, \quad |t_i| \leqq 6, \\ 0, & \text{otherwise}, \end{cases}$$

where the ω_j are the quadrature weights for the implied integration. Using Simpson's rule, those weights become

$$\omega_1 = \omega_{41} = \tfrac{1}{20},$$

$$\omega_{2k} = \tfrac{1}{5}, \quad k = 1, 2, \cdots, 20, \qquad \omega_{2k+1} = \tfrac{1}{10}, \quad k = 1, 2, \cdots, 19.$$

The discretized right-hand side becomes

$$y_i = (6 - |t_i|)\left(1 + \frac{1}{2}\cos\left(\frac{\pi}{3}t_i\right)\right) + \frac{9}{2\pi}\sin\left(\left|\frac{\pi}{3}t_i\right|\right),$$

and the discretized solution is

$$x_j = \begin{cases} 1 + \cos\left(\dfrac{\pi s_j}{3}\right), & |s_j| \leqq 3, \\ 0, & |s_j| \geqq 3. \end{cases}$$

Note that K_{ij} and x_j are always nonnegative and that $\mathbf{x}$ is symmetric about $s = 0$, $x_1 \leqq x_2 \leqq \cdots \leqq x_{20} \leqq x_{21} \geqq \cdots \geqq x_{41}$. Even if we did not know the true solution $x(s)$, we could deduce that it must be symmetric because $y(t)$ is symmetric and the shape

of the kernel, considered as a function of s, is the same for all values of t. In order to derive the initial upper bounds for the x_j, we can use the following technique which works for any problem with all of the K_{ij} and x_j nonnegative (see [12, Chapt. 2]).

For all values j^* of the subscript j and all i, we have

$$K_{ij^*}x_{j^*} \leqq \sum_{j=1}^{n} K_{ij}x_j = (Kx)_i.$$

Dividing by K_{ij^*}, we get

$$x_{j^*} \leqq \frac{(Kx)_i}{K_{ij^*}} \quad \text{for all } i,$$

and hence

$$x_j \leqq \min_{1 \leqq i \leqq m} \frac{(Kx)_i}{K_{ij}}. \tag{3.1}$$

We now need to find upper bounds for the $(Kx)_i$. From the error ellipsoid (2.1), we have

$$(\mathbf{Kx}-\mathbf{y})^T\mathbf{S}^{-2}(\mathbf{Kx}-\mathbf{y}) \leqq \mu^2,$$

where

$$\mathbf{S}^{-2} = \operatorname{diag}\left(\frac{1}{s_1^2}, \cdots, \frac{1}{s_m^2}\right).$$

In this example, we let $s_i = .0001\, y_i$. Equation (2.1) can be written in the form

$$\sum_{i=1}^{m} \frac{[(\mathbf{Kx}-\mathbf{y})_i]^2}{s_i^2} \leqq \mu^2,$$

hence

$$\frac{(\mathbf{Kx}-\mathbf{y})_i^2}{s_i^2} \leqq \mu^2 \quad \text{for all } i = 1, \cdots, m,$$

or

$$(\mathbf{Kx})_i \leqq y_i + \mu s_i.$$

Substituting in (3.1), we have

$$x_j \leqq \min_{1 \leqq i \leqq m} \left\{\frac{y_i + \mu s_i}{K_{ij}}\right\}, \qquad j = 1, \cdots, n.$$

In this way we obtain the initial upper bounds q_j of § 2, and we set $p_j = 0$, $j = 1, \cdots, n$. Note that the bounds $[p_j, q_j]$ in this case are not guaranteed to contain the x_j with 100% confidence but they are guaranteed to contain the intersection of the error ellipsoid with the positive orthant, and that intersection is the basic constraint region for this example. In practice, initial bounds computed by this method are always extremely conservative and in fact do provide 100% confidence boxes. In addition to using a priori constraints and initial bounds on $\mathbf{x}$, we can try to improve the bounds by solving a slightly less ambitious problem. Instead of solving for bounds on all of the x_j, we find bounds for an average of the x_j's. For example,

$$\bar{x}_j \sim \frac{1}{2\Delta s} \int_{s_{j-1}}^{s_{j+1}} x(s)\, ds.$$

The integral may be approximated by using a 3-point Simpson's rule, yielding

$$\bar{x}_{2j} \cong \tfrac{1}{6}(x_{2j-1} + 4x_{2j} + x_{2j+1}), \qquad j = 1, \cdots, 20.$$

For a 60×41 example, we let the jth window vector $\mathbf{w}_j = \frac{1}{6}(0, \cdots, 1, 4, 1, \cdots 0)^T$, with the 4 in the $2j$th place, and estimate $\bar{x}_2, \bar{x}_4, \cdots, \bar{x}_{40}$. Figure 3.1 compares the pointwise estimates with 3-point Simpson averaging for the 60×41 problem with a symmetric hump constraint (see below). As can be seen from the graphs, averaging greatly improves bounds in this case. Next, we observe the effect of a priori knowledge of $\mathbf{x}$ by solving the 60×41 problem three ways with Simpson 3-point averaging.

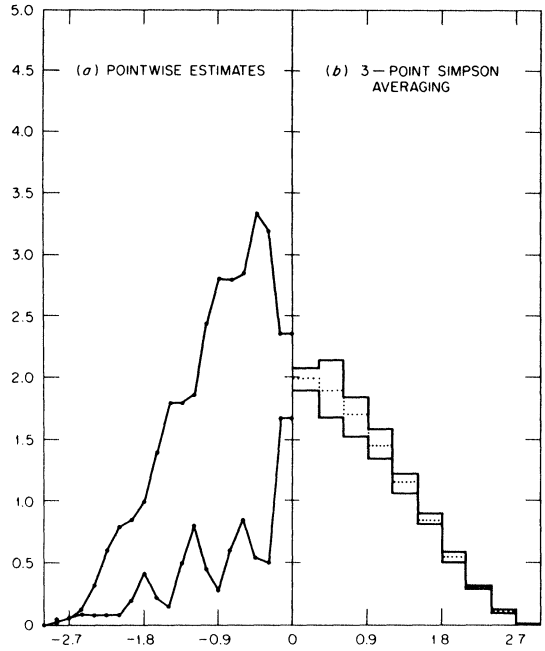

FIG. 3.1. 60×41, *symmetric hump constraint.*

We first solve the problem using no knowledge of $\mathbf{x}$ except the initial bounds. Next, we incorporate the knowledge of a "hump" in $\mathbf{x}$, $0 < x_1 \leqq \mathbf{x}_2 \leqq \cdots \leqq x_{21}$, $x_{22} \geqq x_{23} \geqq \cdots \geqq x_{41}$, but we do not assume symmetry. For this case the 41×41 "shape" matrix is the following:

$$\mathbf{P} = \begin{pmatrix} \mathbf{T} & \mathbf{0} \\ \mathbf{0} & \mathbf{U} \end{pmatrix},$$

where $\mathbf{T}$ and $\mathbf{U}$ are 21×21 and 20×20 triangular matrices, respectively, of the form

$$\mathbf{T} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ 1 & 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}, \qquad \mathbf{U} = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 & 1 & 1 \\ 1 & 1 & 1 & \cdots & 1 & 1 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & & & & \vdots \\ 1 & 0 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix}.$$

Finally, we use all we know about $\mathbf{x}$, namely that $0 \leqq x_1 \leqq x_2 \leqq \cdots \leqq x_{20} \leqq x_{21} \geqq x_{22} \geqq \cdots \geqq x_{41}$ with $x_j = x_{42-j}$, $j = 1, \cdots, 20$. For this "symmetric hump" case, the shape matrix has the form

$$\mathbf{P} = \begin{pmatrix} \mathbf{T} \\ \tilde{\mathbf{U}} \end{pmatrix},$$

with $\mathbf{T}$ as defined above, and $\tilde{\mathbf{U}}$ is the 20×21 matrix formed by adjoining a column of zeros to $\mathbf{U}$, i.e., $\tilde{\mathbf{U}} = (\mathbf{U}|\mathbf{0})$. In this case we have effectively reduced the size of the problem by half. Figure 3.2 compares the nonnegativity only and nonsymmetric hump solutions. For the case of the symmetric hump, refer to Fig. 3.1. From this example, the advantage of incorporating all possible knowledge of $\mathbf{x}$ is clear.

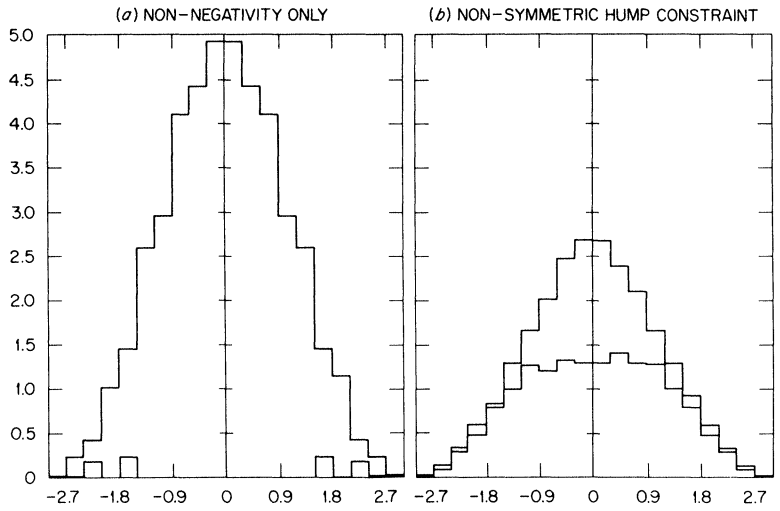

FIG. 3.2. 60×41, *3-point Simpson averaging.*

It is reasonable to hope that the more information put into the problem, the better will be the bounds on an $\mathbf{x}$-vector of a given size. Accordingly, we compare 20×41, 40×41, and 60×41 examples of the problem with 3-point Simpson averaging and symmetric hump constraint. The 20×41 and 40×41 graphs are shown in Fig. 3.3. For the 60×41 example, see Fig. 3.1. From this example, we see that the more information that can be used, the better the result will be. This is true only up to a point, however. If the integration is very crude (n small) compared to the amount of information (m large) the problem becomes inconsistent, due to discretization error. For pointwise estimates the 40×21 and 60×21 examples fail with the quantity $\tau + \mu^2 - \rho_0$, one of the factors of $\mathscr{L}^2$, becoming negative. There was a small discrepancy in all of the pointwise estimates in that the bounds for the first four points did not include the true values, which were all close to zero. We surmise that this was caused by the discretization error in approximating the continuous problem with the quadrature rule.

In all cases, the method was allowed to iterate three times, and in all of the cases, the bounds did not improve after the first iteration. However, the authors have encountered problems where bounds kept improving slightly for several iterations.

The method has been applied to several radiation spectrum unfolding problems using real, measured data. In all cases it has produced useful bounds for the unknown

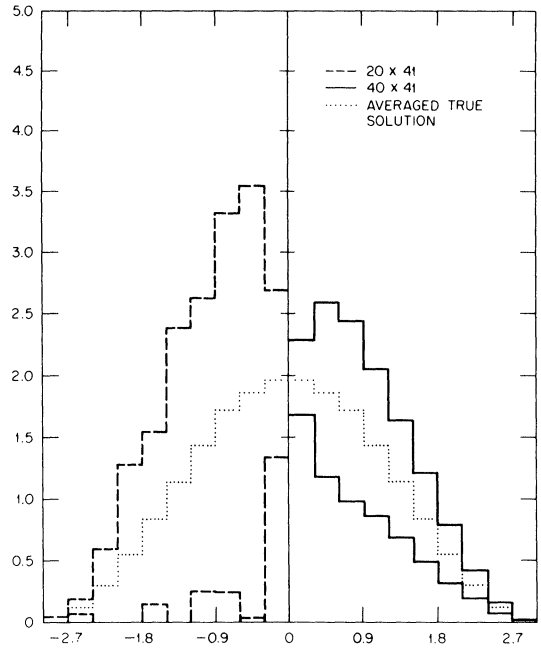

FIG. 3.3. *3-point Simpson averaging, symmetric hump constraint.*

spectrum, and in some of these cases the bounds were so sharp that the effect of suboptimality was scarcely noticeable. In most cases, however, the intervals were noticeably wider than those obtained from the quadratic programming solutions of problems (1.10) and (1.11). In these cases the suboptimal intervals provide good starting estimates for the parametric quadratic programming procedure and significantly reduce the work required to obtain the optimal intervals.

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