



THE NUMERICAL SOLUTION OF ILL-CONDITIONED SYSTEMS OF LINEAR EQUATIONS

Michael T. Heath

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Michael T. Heath

JULY 1974

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University of Tennessee M.S. Thesis.

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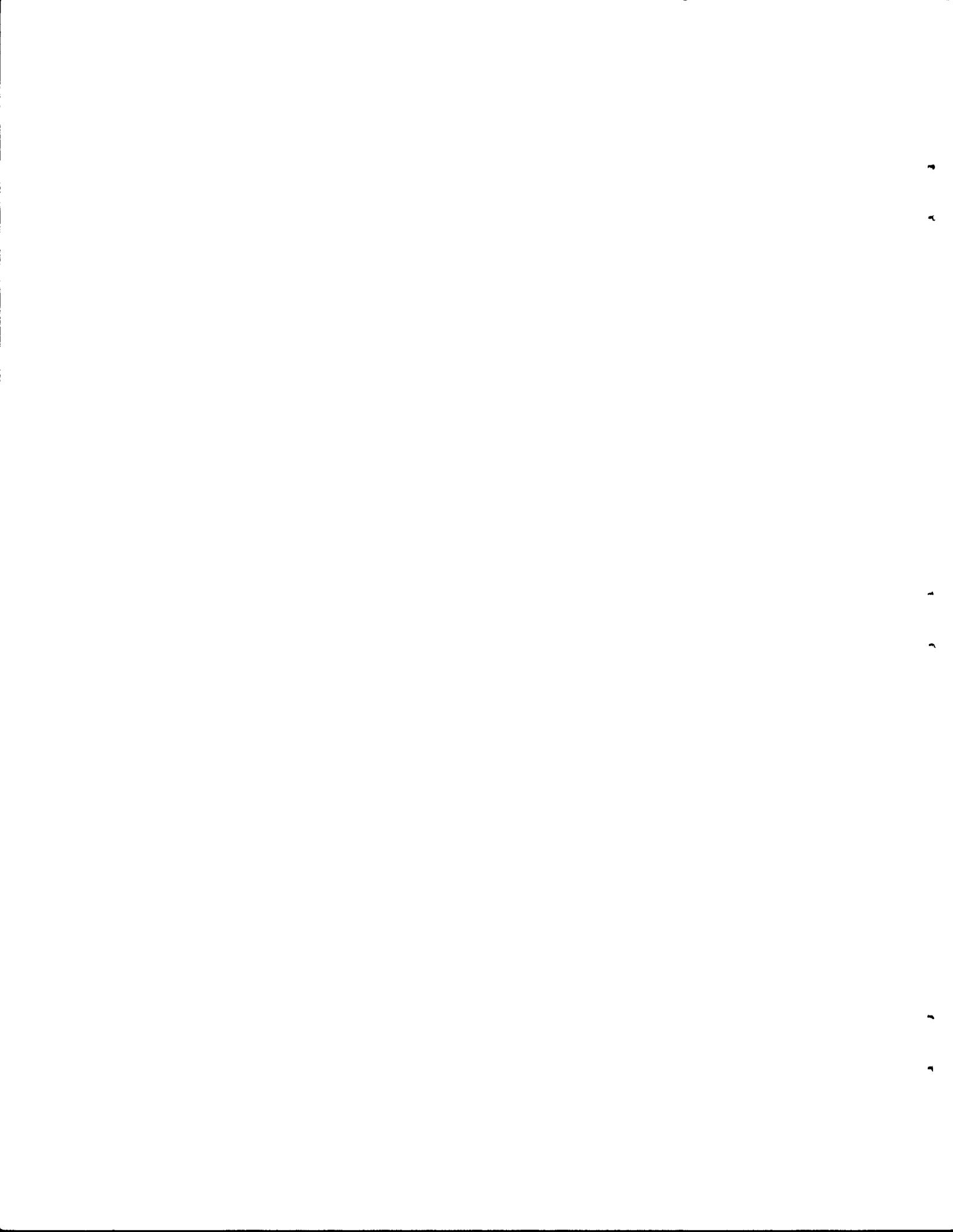
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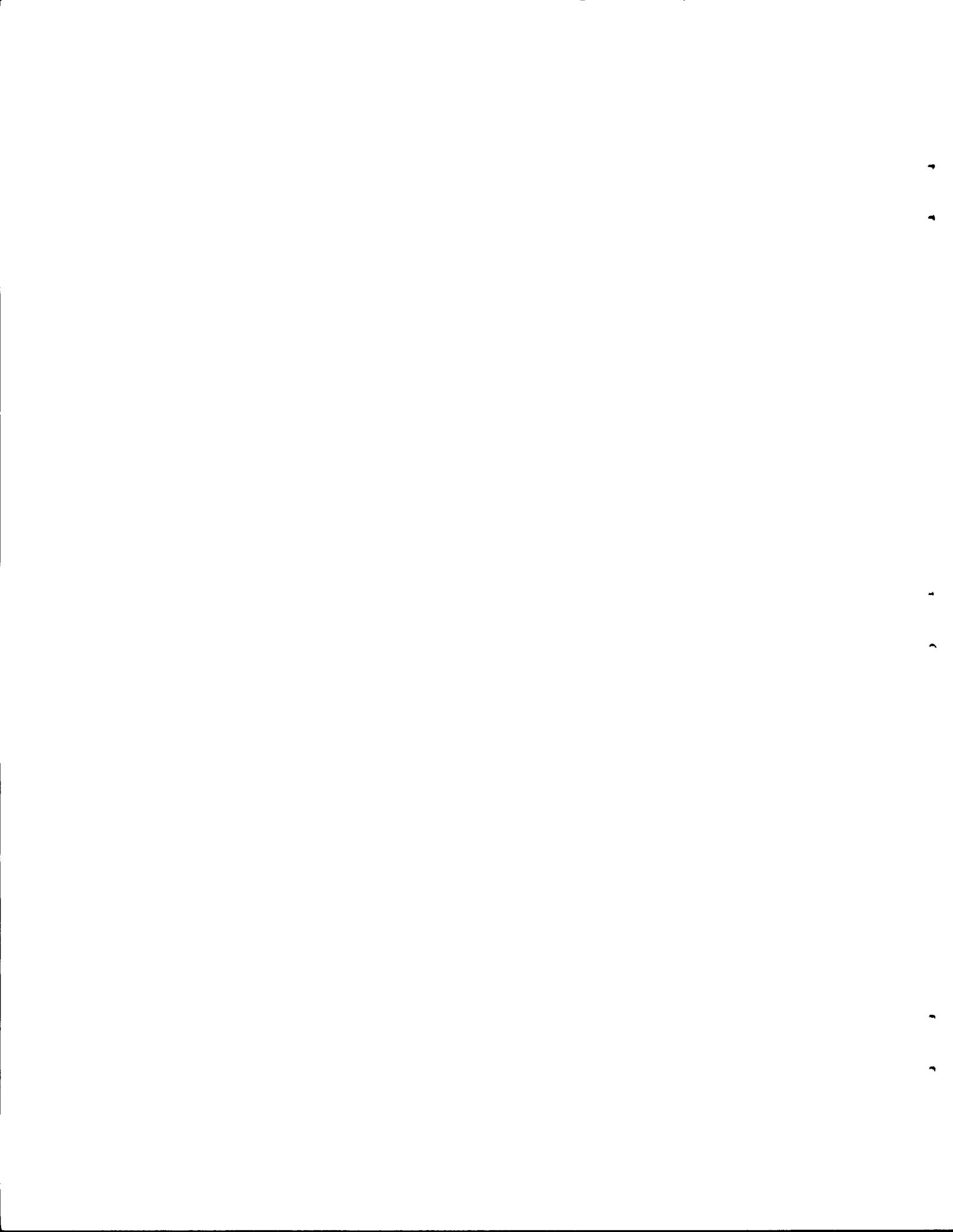
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ABSTRACT

The physical origins of ill-posed problems are discussed, and the computational difficulties involved in their solution are examined. An iterative suboptimal constrained estimation method for solving such problems is presented and several related methods are surveyed. An extensive bibliography is included.

INTRODUCTION

This paper is concerned with the numerical solution of ill-conditioned systems of linear equations. Such systems commonly arise in science and engineering from experiments or problems that are ill-posed. This does not necessarily mean that the problem is ill-conceived, a result of caprice or poor design. Rather, ill-posed problems usually stem from fundamental physical limitations on the accessibility of information about an object or process under study.

In addition to presenting a new method for handling these problems, an attempt is made to survey other techniques and relate them to the present approach. Although the methods discussed are applicable to a wide variety of problems arising from different circumstances, indirect measuring processes are singled out as a paradigm to illustrate the computational difficulties caused by ill-conditioning and to motivate the proposed cures.

The bibliography is meant to be fairly comprehensive with two exceptions. There is little mention of the voluminous Russian literature on regularization. Only a small sampling of applications is given, just enough to indicate some of the flavor and variety of concrete ways ill-posed problems crop up in practice. Many well known concepts and results from linear algebra and matrix theory are used freely without specific reference. For clarification or further information on such matters, one of the several excellent books in this area [20, 35, 59, 84, 106] should be consulted.

I. ILL-POSED PROBLEMS

1. Measurement

In ordinary life the act of measuring seems completely transparent, devoid of any subtlety. For instance, when one measures the length of a desk with a ruler, there is no reason to suspect that the result is significantly different from the physical reality of the object measured. Suppose, however, one is trying to determine the size of soot particles in a smokestack or fog droplets in a cooling tower. The ruler is of no use. One must resort to some indirect scheme of measuring, such as the scattering of light when the particles are illuminated. Now the quantity actually read on the device might be a voltage in an electrical circuit. The relationship of the voltage readings to the particle sizes present may not be at all simple. Even with the best electronic and optical equipment available a 10 micron particle may sometimes produce a voltage reading expected of a 100 micron particle, and vice versa. Furthermore, the instrument may be completely insensitive to particles in certain size ranges.

While this situation is far removed from ordinary experience, it is common in science and engineering. This is particularly true of experimental or observational sciences where measurements must often be made with imperfect instruments or through significant obscuration. The particle size distribution problem [38, 96, 105, 112-116] is of particular importance because of its relevance to controlling air pollution. Spectroscopists [14, 49, 57] try to determine the energy distribution of incident particles (e.g., neutrons, photons, etc.) from scintillation counts in the voltage bins of a multichannel analyzer.

Similar circumstances occur in physics [50, 91, 93], meteorology [53, 98, 99, 103, 104], astronomy [11, 15, 44, 47, 94], optics [19, 31, 79], geophysics [4-7, 37, 41, 63, 81], medicine [29], and many other fields.

2. Mathematical Model

The above kinds of measurement processes can perhaps best be modeled mathematically by an integral equation in which the kernel represents the characteristics of the instrument, the known function is the observed data, and the desired unknown function reflects the actual phenomenon taking place. Probably the most common cases are linear Fredholm integral equations of the first kind. These have the form

$$\int_a^b K(s,t)f(t)dt = g(s),$$

where f , g , and K are real valued functions defined, respectively, on $[a,b] \subseteq \mathbb{R}^1$, $[c,d] \subseteq \mathbb{R}^1$, and $[c,d] \times [a,b] \subseteq \mathbb{R}^2$.

In the examples given above, the function g would represent counts as a function of voltage, K the response function of the instrument determined by calibration, and f the unknown true particle distribution as a function of size or energy. The response function K can be thought of as a transition probability; that is, $K(s,t)$ is the probability that a particle of size or energy t will produce a voltage reading s .

In this model a perfect instrument is one having the response of a Dirac delta distribution $K(s,t) = \delta(s-t)$. Then

$$g(s) = \int_a^b \delta(s-t)f(t)dt = f(s),$$

where for simplicity we take f and g to be defined on the same interval. This means that the instrument provides direct measurement of the quantity of interest.

For the complex objects of study in science, such an ideal device is usually technologically impossible. At best one must settle for a broadened response, such as a Gaussian distribution which, as a function of t , peaks on the diagonal $s=t$ and drops sharply to zero on either side. Although such a function roughly approximates a delta response, it necessarily smooths or smears the function f somewhat, causing a loss of information in the measured function g . This can be seen, for example, from Riemann's lemma, which implies that for integrable K

$$\lim_{n \rightarrow \infty} \int_a^b K(s,t) \sin(nt) dt = 0.$$

Thus an arbitrarily high frequency component of f has a very small effect on g .

A good many instruments used in actual practice exhibit little or no peaking response at all and are characterized by wide plateaus of complete insensitivity. Such an instrument suffers even more severely from blurring and biasing effects and reduces still further the information content of measured data.

The recovery of this information and determination of the unknown function f is variously known as inversion, unfolding, and unscrambling. This is a classical ill-posed problem in the sense of Hadamard. According to his definition, a problem is well-posed if the solution exists, is unique, and depends continuously on the data. As evidenced by Riemann's lemma, unfolding problems do not meet this definition since a small change in the data g can correspond to an arbitrarily large change in the solution f . In Hilbert space terminology one would say that the integral operator does not have a bounded inverse.

3. Discretization

A standard approach for obtaining a numerical solution to an integral equation is to replace the integral by a quadrature formula and the continuous variables by discrete mesh points. If the weights for the quadrature formula are denoted by w_j , $j=1, \dots, n$, and the mesh points chosen are

$$a \cong t_1 \cong t_2 \cong \dots \cong t_n \cong b,$$

$$c \cong s_1 \cong s_2 \cong \dots \cong s_m \cong d,$$

then the original integral equation is replaced by the approximate equation

$$g(s_i) \cong \sum_{j=1}^n K(s_i, t_j) f(t_j) w_j, \quad i=1, \dots, m.$$

This can be more compactly written in matrix notation as $Ax \cong b$, where the $m \times n$ matrix A and the vectors $x \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$ are defined elementwise by

$$\left. \begin{aligned} a_{ij} &= K(s_i, t_j) w_j \\ x_j &= f(t_j) \\ b_i &= g(s_i) \end{aligned} \right\} \begin{array}{l} i=1, \dots, m; \\ j=1, \dots, n. \end{array}$$

A solution vector x for the matrix equation is taken to be a discrete approximation to a solution function for the integral equation. It should be noted that the validity of this process depends on both approximations: the replacement of infinite dimensional function spaces by finite dimensional vector spaces and the replacement of the integral operator by a summing matrix. In the sequel it will be assumed that these approximations are adequate and attention will be devoted to solving the resulting system of linear algebraic equations.

4. Ill-Conditioning

If the matrix formulation is of primary interest here, it might be wondered why the problem was not stated as such at the outset. This is because a knowledge of the physical source and underlying mathematical theory of ill-posed problems is important in trying to understand the computational difficulties they present and suggests possible approaches to their successful solution.

Physically ill-posed problems lead to computationally ill-conditioned problems. This means that the solution is extremely sensitive to error. There are many possible sources for error in any computation: inaccuracies in the data as originally recorded, truncation error in entering it into the finite word length of machine memory format, accumulation of rounding errors during the course of calculations. In explicit recognition of at least part of this error, the matrix equation might be written

$$Ax = b + e,$$

where $e \in \mathbb{R}^m$ is a vector of errors in the measured data b . When the matrix A is ill-conditioned, the error e in the data b can so contaminate the computed solution x that it is wildly oscillatory, bearing little or no resemblance to any physical quantity it may represent. Indeed, if straightforward matrix inversion techniques are applied to the system as it stands, a nonsensical, physically impossible computed solution is a likely result [107].

A quantitative measure of the conditioning of a matrix is given by the condition number defined by

$$\text{Cond}(A) = \|A\|_2 \|A^\dagger\|_2,$$

where $\|\cdot\|_2$ denotes the Euclidean norm and " \dagger " denotes the Moore-Penrose pseudoinverse. A theoretical upper bound for the relative error in the computed solution is given by [84]

$$(1.1) \quad \frac{\|x - \bar{x}\|_2}{\|x\|_2} \leq \text{Cond}(A) \frac{\|e\|_2}{\|b\|_2},$$

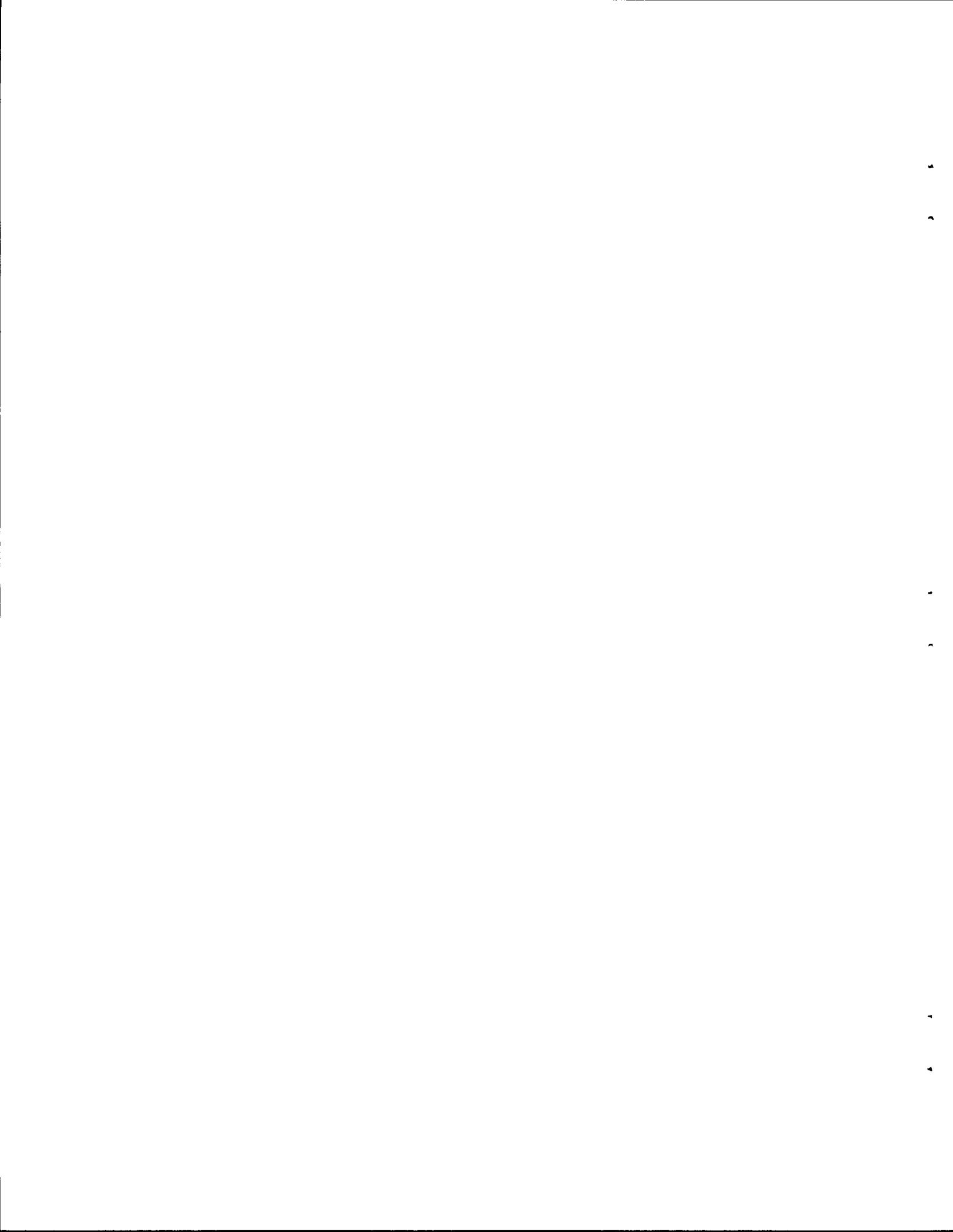
where $x = A^\dagger b$ is the solution to the original system and $\bar{x} = A^\dagger(b + e)$ is the solution to the perturbed system. Thus, ill-conditioning is associated with a large value for $\text{Cond}(A)$, since in this case the bound on the error in x is very large. Practically speaking, this allows undesirably wide variation and great uncertainty in the calculated solution even when $\|e\|_2$ is small. This behavior corresponds to the unboundedness of the inverse of the integral operator from which A is obtained.

There are other ways of looking at ill-conditioning which lead to similar conclusions. For instance, if A is considered constant and assumed nonsingular, then the partial derivatives of the components of the solution with respect to the components of the data are given by

$$\frac{\partial x_i}{\partial b_j} = a'_{ij},$$

where $\{a'_{ij}\} = A^{-1}$. Here again the large magnitudes of the elements of the inverse matrix indicate great sensitivity of the solution to the data. Mendelsohn [54, 55] discusses several interesting properties and simple examples of ill-conditioned matrices.

It should be noted that matrices arising from ill-posed problems such as first-kind integral equations are inherently ill-conditioned, regardless of the particular discretization employed (so long as it is reasonably faithful in approximating the integral). For example, Gautschi [24] has studied the effect of a great variety of different quadrature formulas on the conditioning of the kernel matrix resulting from Laplace transform inversion ($K(s,t) = e^{-st}$). He shows that while some are better than others, they are all poorly conditioned.



II. PREVIOUS METHODS

1. Constraints

The fundamental difficulty with ill-posed problems is the lack of sufficient information from response measurements to infer the correct solution. This is reflected mathematically in the fact that the system matrix tends to be underdetermined (rank deficient) even if it is formally overdetermined (more rows than columns). An obvious approach, then, is to augment the data provided by the instrument with any additional knowledge of the nature of the quantity being measured in order to make the computed solution at least physically meaningful and possibly even correct. Mathematically this amounts to building up the rank of the matrix or reducing the solution space so as to yield a unique solution which satisfies all constraints known to obtain a priori. Such constraints usually take the form of inequalities or equations, perhaps with tolerances, imposed on the solution.

2. Smoothing

In contrast to the wildly oscillatory behavior typically resulting from applying simple matrix inversion algorithms to ill-conditioned equations, most natural processes are smooth. This notion has given rise to a family of techniques which require the computed solution to be smooth, in some sense, by a process variously known as damping [51, 52, 87, 88, 101], smoothing [68, 95, 9, 80], regularization [89, 90], relaxation [76], or stabilization [78, 82].

The central idea of such methods is to replace the minimization problem

$$\min_x \{ \|Ax - b\| \}$$

by the problem

$$(2.1) \quad \min_x \left\{ \|Ax - b\| + \lambda \|x\|' \right\},$$

where $\|\cdot\|'$ is possibly a different norm from $\|\cdot\|$, and the positive scalar λ is a relative weighting factor. By simultaneously minimizing the residual and some norm of the solution, oscillations in the solution tend to be damped out, giving a smoothed solution which still satisfies the original equations to some degree.

The amount of smoothing is controlled by the choice of norm $\|\cdot\|'$ as well as the scalar λ . Norms usually employed are of the Sobolev type, involving finite differences of the elements of the solution vector x , or derivatives if applied directly to the original integral equation. The usual central difference operators

$$\Delta_1 = \begin{pmatrix} -1 & 1 & & & \\ 0 & \cdot & \cdot & \cdot & \circ \\ \circ & \cdot & \cdot & \cdot & \cdot \\ \circ & \cdot & \cdot & \cdot & 1 \\ 0 & & & & -1 \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} -1 & 1 & & & \\ 1 & -2 & \cdot & \cdot & \circ \\ \circ & \cdot & \cdot & \cdot & \cdot \\ \circ & \cdot & \cdot & \cdot & -2 \\ 1 & & & & -1 \end{pmatrix}, \text{ etc.,}$$

lead to the norms $\|x\|' = \|\Delta_1 x\|_2$, and the minimization problem (2.1) becomes

$$\min_x \left\{ \|Ax - b\|_2 + \lambda \|\Delta_1 x\|_2 \right\}.$$

The normal equations for this least squares problem are given by

$$(A^T A + \lambda^2 \Delta_1^T \Delta_1) x = A^T b.$$

However, explicit formation of the matrix $A^T A$ can be avoided by employing the equivalent partitioned matrix formulation

$$\begin{pmatrix} A \\ \lambda \Delta_1 \end{pmatrix} x = \begin{pmatrix} b \\ 0 \end{pmatrix},$$

which can then be solved by orthogonalization. Note that this approach subsumes the case where the Euclidean norm is employed for both the residual and the solution by simply taking $\Delta_0 = I_n$, the $n \times n$ identity matrix. More complicated Sobolev norms consisting of linear combinations of higher differences can be handled computationally by stacking the difference matrices, for example,

$$\begin{pmatrix} A \\ \lambda_0 \Delta_0 \\ \lambda_1 \Delta_1 \end{pmatrix} x = \begin{pmatrix} b \\ 0 \\ 0 \end{pmatrix},$$

where λ_0, λ_1 are independent scalar weights.

The role played by the weighting factor λ in these methods is crucial. If λ is chosen too small, then the problem is still poorly conditioned and the solution still oscillatory. However, if λ is taken too large, then the solution is excessively damped and the original equation to be solved has little influence on it. The arbitrariness of seeking a mediating value for λ is the chief drawback of these methods. Even if the solution obtained is made physically reasonable, there is no indication how much the solution could vary and still remain within the smoothness constraint and error tolerance of the original data.

3. Singular Value Expansion

The singular value decomposition of the matrix A is given by the factorization

$$A = U \begin{pmatrix} D \\ 0 \end{pmatrix} V^T,$$

where $U^T U = I_m$, $V^T V = I_n$, and $D = \text{diag}(\delta_1, \dots, \delta_n)$, with $\delta_1 \geq \delta_2 \geq \dots \geq \delta_n \geq 0$. The diagonal entries δ_i of D , called the singular values of A , are the nonnegative square roots of the eigenvalues of $A^T A$ and the columns of U and V are orthonormal eigenvectors of AA^T and $A^T A$, respectively. The conditioning of the matrix A can be characterized in terms of this decomposition. If δ_k is the smallest nonzero singular value of A , then $\text{Cond}(A) = \delta_1/\delta_k$. Thus, a poorly conditioned matrix is one with a great variation in the magnitudes of its singular values.

To see how this affects the solution of the equation $Ax = b$, the factorization is substituted in to obtain

$$U \begin{pmatrix} D \\ 0 \end{pmatrix} V^T x = b,$$

or

$$x = V(D^\dagger, 0)U^T b,$$

where $D^\dagger = \text{diag}(\delta_1^{-1}, \dots, \delta_k^{-1}, 0, \dots, 0)$. The expansion becomes clearer if the summation is written out explicitly

$$(2.2) \quad x = \sum_{i=1}^k \frac{u_i^T b}{\delta_i} v_i,$$

where u_i and v_i denote column vectors of U and V , respectively. Thus, the smaller singular values entering into the denominator of the terms of the expansion tend to greatly magnify any error in the data vector b ,

about the solution. A very flexible and informative objective function is an arbitrary linear functional of the solution, $\varphi(x) = w^T x$, obtained by taking an arbitrary vector $w \in \mathbb{R}^n$. To pick out an individual component of the solution vector x , the vector w is chosen to be the corresponding coordinate basis vector.

Sometimes the true data vector b is known to lie within a polytope determined by an interval of uncertainty about each of its components. This would be true with rounding or truncation error in recording or entering the data, in which case the interval width might be, say, one digit in the last decimal place. A natural norm for such a problem is one whose unit ball is a polytope, such as the max-norm $\|\cdot\|_\infty$ or the sum-norm $\|\cdot\|_1$. Under these circumstances one may consider any solution equally acceptable which satisfies the equation within the tolerance of the data,

$$|Ax - b| \leq |e|.$$

Determining the extrema of a linear functional $\varphi(x) = w^T x$ is then a linear programming problem of the standard form [60-62, 70, 73]

$$\min_x \{w^T x\} \quad \text{subject to } x \geq 0,$$

$$Ax \geq b - |e|, \quad -Ax \geq -b - |e|$$

and

$$\max_x \{w^T x\} \quad \text{subject to } x \geq 0,$$

$$Ax \leq b + |e|, \quad -Ax \leq -b + |e|.$$

Any of the previously discussed constraints can be imposed, either by change of variable or by incorporating additional side constraints directly into the tableau. The form of the problem is retained, but

the solution obtained satisfies whatever conditions are desired. The preceding formulation can be modified to allow negative x by introducing nonnegative variables u and v and setting $x = u - v$.

A far more realistic and common experimental situation is for the measured data b to be drawn as a sample from some population with a random error of observation due to counting statistics or other source of uncertainty. Such a probabilistic interpretation not only models instrumental behavior better but also makes available a rigorous statistical error analysis. As will be seen in greater detail below, an ellipsoidal norm, such as the Euclidean norm, is the logical choice here. This leads to an optimization problem of the form

$$\max_x \{w^T x\} \quad \text{or} \quad \min_x \{w^T x\}$$

$$\text{subject to } \|Ax - b\|_2 \leq \|e\|_2$$

plus other possible constraints. Unfortunately this is the reverse of the standard quadratic programming problem [2, 3, 92, 93, 39] which has a quadratic objective and linear constraints. It can be converted to a parametric problem [75] of the standard type, but this can be prohibitively expensive computationally. It is therefore the aim of the next section to develop methods for the quadratic problem which, like the smoothing and singular value methods discussed earlier, require little more work than simple matrix inversion techniques but, unlike those methods, produce error bounds as well.

III. CONSTRAINED ESTIMATION

1. Classical Regression

The measured data vector b is assumed to be centered in an ellipsoidal measurement error region $E_m \subseteq R^m$ defined by

$$E_m = \left\{ y \in R^m : (y - b)^T S^{-2} (y - b) \leq \mu^2 \right\},$$

where S^{-2} is a positive definite matrix and μ^2 is a positive real constant. For example, the surface of this ellipsoid might represent a probability isopleth for a multivariate normal statistical distribution with covariance matrix S^2 . Estimates are sought for the upper and lower bounds of an arbitrary linear functional $\varphi(x) = w^T x$ of the solution vector $x \in R^n$ subject to the constraint $Ax \in E_m$. From the ellipsoid E_m the matrix A induces another ellipsoid $E_n \subseteq R^n$ defined by

$$E_n = \left\{ x \in R^n : (Ax - b)^T S^{-2} (Ax - b) \leq \mu^2 \right\}.$$

Thus the problem is to estimate

$$\varphi_{\text{up}} = \max_{x \in E_n} \left\{ w^T x \right\} \quad \text{and} \quad \varphi_{\text{lo}} = \min_{x \in E_n} \left\{ w^T x \right\}.$$

From the theory of linear regression it is well known that the minimum residual

$$r_0 = \min_x \left\{ (Ax - b)^T S^{-2} (Ax - b) \right\} \leq \mu^2$$

is attained when

$$\hat{x} = (A^T S^{-2} A)^{\dagger} A^T S^{-2} b.$$

Furthermore, provided φ is an estimable function (i.e., w lies in the row space of A), the upper and lower bounds for φ are just the values assumed by $w^T x$ on the two support planes of E_n which are orthogonal to w .

To determine these values note that the covariance matrix of the solution x is $(A^T S^{-2} A)^\dagger$ and therefore the variance of φ is given by $w^T (A^T S^{-2} A)^\dagger w$. Thus, defining

$$\delta = \left[(\mu^2 - r_0) w^T (A^T S^{-2} A)^\dagger w \right]^{\frac{1}{2}},$$

the bounds are given by

$$\varphi_{\text{up}} = w^T \hat{x} + \delta, \quad \varphi_{\text{lo}} = w^T \hat{x} - \delta.$$

For more information about confidence ellipsoids and their planes of support, as well as other statistical concepts employed in this paper, see Scheffé [77]. For the use of the Moore-Penrose pseudoinverse in this context, consult Price [69].

2. Suboptimal Estimation

The classical procedure outlined above completely solves the problem when φ is estimable; and this is always the case if the rank r of the matrix A is full, $r = n$. But if $r < n$ and w does not lie in the column space of $A^T S^{-2} A$, then the above bounds become infinite. To see why this is true geometrically, observe that the ellipsoid E_n has its axes in the directions of the eigenvectors of $A^T S^{-2} A$ and their respective lengths are proportional to the reciprocals of the corresponding eigenvalues. As a result, even though E_m may be well behaved, if $A^T S^{-2} A$ is singular, then the axes of E_n determined by eigenvectors corresponding to zero eigenvalues have infinite extent. Thus if w has a nonzero projection in any of these directions, its variance becomes infinite, hence the name inestimable. Near singularity is just as disastrous computationally because the great elongation of E_n due to very small eigenvalues gives very large bounds for φ

for some choices of w . Unfortunately rank deficiency, near singularity and severe ill-conditioning are the rule rather than the exception in problems arising from the discretization of integral equations.

Many an experimentalist has been rudely initiated to this behavior upon finding that seemingly innocent variations within E_m allow solutions obtained to roam far afield from expected results and yet remain within E_n .

What is needed is to cut E_n down to size by utilizing any "ball park" knowledge one may have of the solution. A method for doing this is presented below. It is an iterative extension of a suboptimal technique first given in [74], which is reviewed here for motivation and to fix notation. Suppose one can give reasonable lower bounds p and upper bounds q for the solution. These intervals for the components of x define a polytope

$$B = \{x \in \mathbb{R}^n : p \leq x \leq q\}.$$

Assuming that the solution must lie in $B \cap E_n$ narrows the interval $[\varphi_{lo}, \varphi_{up}]$. The polytope B is difficult to treat analytically when using the ℓ^2 norm, so it is replaced by the circumscribing ellipsoid of least volume. Defining the vector $d = \frac{1}{2}(p + q)$ and the matrix $Q = \text{diag}(d)$, this circumscribing ellipsoid is given by

$$C = \{x \in \mathbb{R}^n : (x - d)^T Q^{-2} (x - d) \leq n\}.$$

Since $B \subseteq C$ the solution is contained in $C \cap E_n$, but the price paid for convenience is that the interval for φ is somewhat widened due to the increase in size of the constraint region.

The intersection of two ellipsoids does not have a smooth surface; so still another suboptimal approximation is made, this time replacing $C \cap E_n$ by a convex combination of C and E_n . Such a combination is itself an ellipsoid having the form

$$D = \left\{ x \in \mathbb{R}^n : \eta \cdot \frac{1}{\mu^2} (Ax - b)^T S^{-2} (Ax - b) + (1 - \eta) \cdot \frac{1}{n} (x - d)^T Q^{-2} (x - d) \leq 1 \right\},$$

where $0 \leq \eta \leq 1$. Note that $C \cap E_n \subseteq D$, so that $D \neq \emptyset$ whenever $C \cap E_n \neq \emptyset$. The ellipsoid D can be represented more compactly in partitioned matrix form by defining

$$R = \begin{pmatrix} A \\ I_n \end{pmatrix}, \quad y = \begin{pmatrix} b \\ d \end{pmatrix},$$

$$\tau^2 = \left(\frac{1 - \eta}{\eta} \right) \mu^2, \quad V^{-2} = \begin{pmatrix} S^{-2} & \circ \\ \circ & \frac{\tau^2}{n} Q^{-2} \end{pmatrix}$$

so that

$$D = \left\{ x \in \mathbb{R}^n : (Rx - y)^T V^{-2} (Rx - y) \leq \tau^2 + \mu^2 \right\}.$$

The new parameter τ^2 varies from 0 to ∞ as η varies from 1 to 0 and can be considered a relative weighting factor between the two ellipsoids, $\tau^2 = 0$ giving E_n and $\tau^2 = \infty$ corresponding to C . Assume for the moment that a specific value of τ^2 has been chosen. Strategies for making this choice judiciously will be discussed later.

The new suboptimal problem has now been reduced to the form of a classical linear regression

$$\varphi_{\text{up}} = \max_{x \in D} \{ w^T x \}, \quad \varphi_{\text{lo}} = \min_{x \in D} \{ w^T x \}$$

and can be solved in the same way as previously demonstrated. Specifically, the minimum residual

$$\rho_0 = \min_{\mathbf{x}} \left\{ (\mathbf{R}\mathbf{x} - \mathbf{y})^T \mathbf{V}^{-2} (\mathbf{R}\mathbf{x} - \mathbf{y}) \right\} \leq \tau^2 + \mu^2$$

is attained when

$$\hat{\mathbf{x}} = (\mathbf{R}^T \mathbf{V}^{-2} \mathbf{R})^{-1} \mathbf{R}^T \mathbf{V}^{-2} \mathbf{y} .$$

Note that \mathbf{R} is necessarily full rank if $\tau^2 \neq 0$. Thus, the indicated inverse exists, the normal equations have a unique solution, and every linear functional φ is estimable. The resulting bounds are again given by

$$\varphi_{\text{up}} = \mathbf{w}^T \hat{\mathbf{x}} + \delta \quad , \quad \varphi_{\text{lo}} = \mathbf{w}^T \hat{\mathbf{x}} - \delta$$

with

$$\delta = \left[(\tau^2 + \mu^2 - \rho_0) \mathbf{w}^T (\mathbf{R}^T \mathbf{V}^{-2} \mathbf{R})^{-1} \mathbf{w} \right]^{\frac{1}{2}} .$$

In a practical computational algorithm one would not explicitly invert $\mathbf{R}^T \mathbf{V}^{-2} \mathbf{R}$ but would instead use an orthogonalization technique, such as modified Gram-Schmidt or Householder transformations, to factor

$$(3.1) \quad \mathbf{V}^{-1} \mathbf{R} = \mathbf{W} \begin{pmatrix} \mathbf{U} \\ \mathbf{0} \end{pmatrix}$$

with \mathbf{W} orthogonal and \mathbf{U} upper triangular. Then, with $\mathbf{z} = \mathbf{W}^T (\mathbf{V}^{-1} \mathbf{y})$, this would easily yield

$$\hat{\mathbf{x}} = (\mathbf{U}^{-1}, \mathbf{0}) \mathbf{z},$$

$$\rho_0 = \mathbf{y}^T \mathbf{V}^{-2} \mathbf{y} - \mathbf{z}^T \begin{pmatrix} \mathbf{I}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \mathbf{z},$$

$$\delta = \left[(\tau^2 + \mu^2 - \rho_0) \mathbf{w}^T \mathbf{U}^{-1} \mathbf{U}^{-T} \mathbf{w} \right]^{\frac{1}{2}}$$

in an efficient and stable manner.

3. Iterative Procedure

At this point an interval bound $[\varphi_{lo}, \varphi_{up}]$ has been obtained for $w^T x$. Successively taking w equal to the n coordinate basis vectors produces interval estimates for the individual components of the solution vector. At least some of these are hopefully sharper than the original values p and q . This provides the basis for an iterative procedure. After the first step any improvements in the bounds can be incorporated into the estimates p and q and the process repeated. This can be carried on so long as any one of the $2n$ bounds continues to change. In practice the convergence of this process is assured, since one simply would not accept the new iterate for a given component bound if it were not an improvement. Thus, monotonic bounded sequences would result, and convergence necessarily follows.

The object is to successively shrink the bounding region so as to yield the narrowest possible interval estimate. Because of the suboptimality of the ellipsoidal approximations made along the way, the ultimate theoretical bounds resulting from a linear constraint can never quite be reached. However, this deficiency is minimized by the fact that the convex combination ellipsoid produces the tightest possible fit [42].

After the first step subsequent iterations are not as expensive computationally, since the orthogonalization (3.1) does not have to be repeated in its entirety. This is true because only the last n rows of the matrix $V^{-1}R$ change from one iteration to the next. Thus, the first m rows, $S^{-1}A$, are orthogonalized only once, stored, and then the successive sets of the last n rows treated as updates. Furthermore, since

these lower rows are nonzero only on the diagonal, a simpler orthogonalization technique, such as Givens transformations, can be employed to complete the factorization. It should also be noted that using all n basis vectors as values for w is hardly a problem computationally, since this merely amounts to picking out the diagonal elements of the matrix $U^{-1} U^{-T}$. After obtaining the smallest bounding region one may then want to estimate $[\varphi_{10}, \varphi_{up}]$ for some other w , and the orthogonal factorization from the last iteration is available for that purpose.

Initial estimates p and q for the bounds on the solution are needed to begin the iteration. If these are unavailable explicitly from physical considerations, useful starting values can sometimes be generated from other a priori information. It is often the case that A , x , and b are known to have all their elements nonnegative. This automatically gives $p \geq 0$. If in addition the matrix $S = \text{diag}(\sigma_1, \dots, \sigma_m)$, or the problem has been transformed so that S is diagonalized, then the inequalities [74]

$$x_j \leq \min_{1 \leq i \leq m} \left\{ \frac{(Ax)_i}{a_{ij}} \right\}, \quad j = 1, \dots, n$$

for any vector $x \geq 0$ give the bounds

$$(3.2) \quad x_j \leq \min_{1 \leq i \leq m} \left\{ \frac{b_i + \mu \sigma_i}{a_{ij}} \right\}, \quad j = 1, \dots, n$$

for the components of the solution vector x , and these can be used to define the starting value for q .

The choice of the parameter τ plays an important role in the potential success of the above technique. Since τ determines the convex combination D of the two ellipsoids E_n and C , there is a trade-off between

them as τ varies. If τ is chosen too small, then D is nearly the same as E_n and the problem is still poorly conditioned. On the other hand, if τ is very large, then C dominates the combination and the new bounds for the solution cannot be expected to differ much from the original ones which determine C . Thus an intermediate value for τ is desirable and may be sought by trial and error or determined from detailed knowledge of the error structure of the problem. However, the apparent arbitrariness in choosing τ , which plagues several related methods, can be exploited to good advantage in the present approach. This is because at any stage the best previous information is retained for use in the next step. Thus, τ can be varied as the iterations proceed, making the bounds subject to improvement due to altering τ as well as to the iteration procedure itself. In fact, test cases indicate that bounds for different components of the solution may react best to different values of τ . The author has found this approach particularly useful in an interactive, time-sharing computer environment, since the user can monitor the progress of the iterations and experimentally change τ for the greatest effect.

IV. OTHER METHODS AND PROBLEMS

1. Related Methods

The iterative suboptimal constrained estimation method presented in the previous section has some important similarities and some important differences with other techniques for ill-conditioned linear systems. There is an obvious kinship with the methods (2.1), the parameter τ being analogous to the weighting or damping factor λ . However, the proponents of these methods seem to have been interested only in obtaining a single plausible solution rather than in getting bounds on all possible solutions. This vagueness makes such techniques of questionable rigor. Moreover, they have failed to utilize the geometric interpretation of such methods as a convex combination of ellipsoids. For instance, the Phillips-Twomey method [68, 95]

$$(4.1) \quad x = (A^T A + \lambda H)^{-1} A^T b$$

can be interpreted as taking combinations of E_n and a circle about the origin when $H = I_n$, or a strip along the line $x_1 = x_2 = \dots = x_n$ when $H = \Delta_1^T \Delta_1$. Other related techniques which can be interpreted similarly include the statistical estimation method of Strand and Westwater [85, 86], the stochastic extension method of Franklin [22], and the ridge regression method of Hoerl and Kennard [32-34]. Another technique along these lines was developed by Backus and Gilbert in the context of geophysical inversion problems [4-7]. Many of the ingredients of the Backus-Gilbert approach can be found in earlier work, but these have been combined in a particularly systematic and thorough way, including a penetrating analysis of the trade-off between resolution

and noise reduction. Recent treatments of regularization methods in a more general setting include [36], [40], and [102].

As Rutishauser has pointed out [76], the relaxation methods are related to the singular value decomposition in that they attenuate, rather than truncate, the singular value expansion for the solution. He also goes a step further by defining a doubly relaxed least squares solution, given by

$$[A^T A + \lambda I + \lambda(A^T A + \lambda I)^{-1}]x = A^T b,$$

together with an orthogonalization algorithm for solving this equation.

Riley has proposed the interesting iterative scheme [71, 26]

$$x^{(i+1)} = (A^T A + \lambda I)^{-1} (A^T b + \lambda x^{(i)}).$$

It can easily be shown that for any $\lambda > 0$ this sequence converges to the true least squares solution of $Ax = b$, provided A has full rank.

Practically speaking, for ill-conditioned A the iteration must be treated much like an asymptotic expansion and halted before the oscillatory behavior of the true solution starts to creep into the iterates, a fact which negates somewhat the attractive feature of being (theoretically) independent of λ . A similar iterative scheme is related to the method of steepest descent in [45], [58], and [67].

A number of authors [1, 46, 88] have pointed out the relationship of the damping methods to the Moore-Penrose pseudoinverse summarized by the formula

$$A^\dagger = \lim_{\lambda \rightarrow 0} (A^T A + \lambda I)^{-1} A^T.$$

Wiener filter theory is also relevant in this connection, as shown by Foster [21].

The idea of splitting the solution space into two subspaces, one where the problem is well conditioned and the other where it is poorly conditioned, has been explored in several papers [16, 18, 25, 30] but without conspicuous practical success, unless one includes the truncated singular value expansion as an example of this approach.

Although the viewpoint of this discussion has been exclusively that of solving integral equations, it should be noted that many of the techniques discussed have also been applied to other kinds of ill-posed problems, such as those arising in partial differential equations. For examples see [23], [56], and the bibliography in [64].

2. Errors in the Matrix

Throughout this paper the elements of the matrix A have been tacitly assumed to be sharply defined constants, subject to no uncertainties. However, in an experimental situation the calibration runs which determine the kernel matrix may be as liable to instrumental error as later data gathering runs. Even in a purely mathematical problem, such as integral transform inversion, the quadrature formula and mesh points chosen for the discretization can significantly alter the system matrix. The effects of such uncertainties in the matrix should be adequately assessed if the solution obtained is to be meaningful.

For an ill-conditioned matrix this problem is greatly complicated by the fact that the rank of the matrix is poorly determined numerically and may well change as the matrix varies. Important geometric insight into this phenomenon is given by Kahan [43]. The analog of the

classical error analysis for nonsingular matrices is carried out for the rank deficient case in [10] and [83]. Pereyra [65,66] has extended these considerations into a general notion of stability for linear equations. The problem has also been considered in a linear programming context [60-62, 73]. Kuperman [48] employs several techniques--norms, sensitivities (partial derivatives), linear programming, interval arithmetic, statistical analysis--to determine intervals of uncertainty for the solution due to uncertainties in both the data vector and the matrix under mild ill-conditioning with invariant, full rank. An approach closer in spirit to that of Section III is [17].

Whatever method is used in solving a system of linear equations, ideally one would like to know under what conditions the solution it produces is a continuous function of the matrix elements, as well as a quantitative measure of the possible effects of matrix errors. Too little attention has been given to this aspect of the problem by proposers of techniques for ill-conditioned systems, including the present author. This difficult task should provide ample ground for future research.

V. AN EXAMPLE

In order to illustrate the above concepts and methods, the following example is taken from [110]:

$$A = \begin{pmatrix} .6 \sqrt{1/2} & .8 \sqrt{1/2} \\ .8 \sqrt{1/2} & .6 \sqrt{1/2} \\ \sqrt{1/2} & \sqrt{1/2} \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix},$$

$$S = I, \quad \mu^2 = 0.8636,$$

with the constraint $x \geq 0$. This simple system does not exhibit the extreme degree of ill-conditioning frequently associated with unfolding problems and does not invoke the full power of the methods discussed above. Nevertheless, it still demonstrates the efficacy of these special techniques and affords comparisons between them. Furthermore, having a two-dimensional solution space enables convenient pictorial representation.

The main point of [110] is to explore the relationship between the damped least squares method (4.1) with $H=I$ and the truncated singular value expansion (2.2). To this end the locus of solutions given by each of the two methods is traced as the parameter λ and the rank k , respectively, vary. These loci are shown in Figure 1, which is adapted from [110]. In order to make the latter locus a continuum, a notion of fractional rank is defined by letting the rank $k + \gamma$, with k an integer and $0 \leq \gamma \leq 1$, mean that the solution is obtained by summing the first k terms of the singular value expansion plus the fraction γ of the $k+1$ term. The effect of this is to connect the discrete solutions resulting for integral k by straight line segments.

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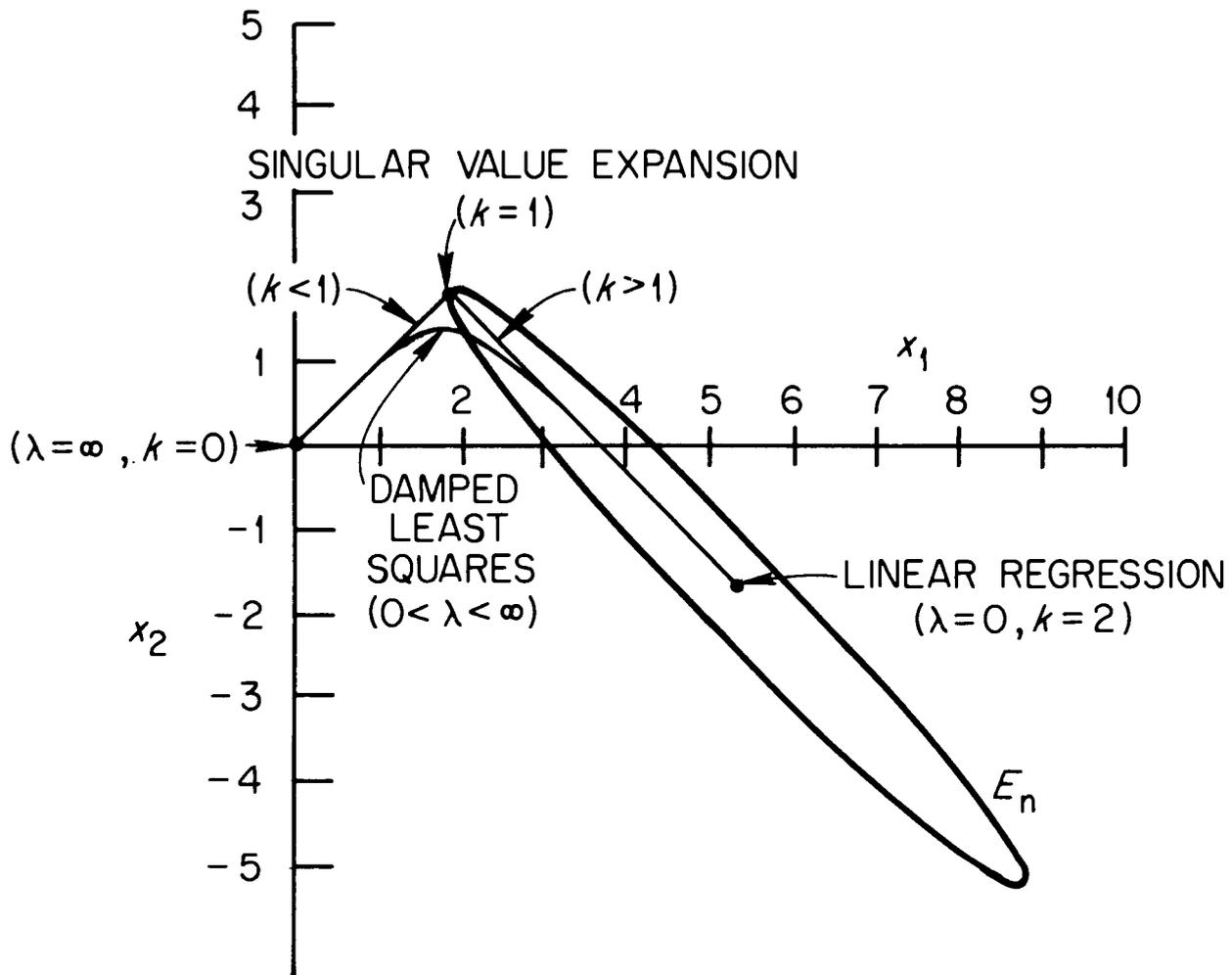


Figure 1. The Loci of Solutions for the Damped Least Squares and Singular Value Methods as Their Respective Parameters Vary.

As seen in the diagram, both of these methods can produce valid solutions which lie in the intersection of the ellipsoid E_n and the positive quadrant. However, both methods also yield "solutions" which lie in only one of the two constraining regions. Furthermore, no distinction is made between these possibilities other than inspecting or testing each candidate individually. Thus there is no rigorous basis for determining an admissible solution or knowing how much the solution could vary and still satisfy the constraints.

These shortcomings are remedied by the method of Section III. First note that the bounds for just the ellipsoid E_n , as obtained by classical linear regression, are

$$p = \begin{pmatrix} 1.804 \\ -5.267 \end{pmatrix}, \quad q = \begin{pmatrix} 8.910 \\ 1.839 \end{pmatrix}.$$

Since nonnegativity places no additional restriction on p_1 or q_2 , the above values are also the optimal values for these bounds, and they can be obtained at any point in the iterative procedure by taking $\tau = 0$. As will be seen, however, it is not necessarily a good idea to do this at the outset.

Independently of these considerations the nonnegativity constraint together with the inequality (3.2) gives the bounds

$$p = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad q = \begin{pmatrix} 4.547 \\ 3.411 \end{pmatrix}$$

and these were used as initial values for the iterative procedure. Since $p_2 = 0$ is already optimal and since optimal values for p_1 and

q_2 can be determined by classical linear regression, the bound of greatest interest is q_1 . The initial value for q_1 is very good and is difficult to improve upon. Extensive trials indicate that the best strategy is to use $\tau=2$ for several iterations, then take $\tau=1.5$ for one iteration, and finally sharpen p_1 and q_2 by taking $\tau=0$. The final values thus obtained are

$$p = \begin{pmatrix} 1.804 \\ 0 \end{pmatrix}, \quad q = \begin{pmatrix} 4.333 \\ 1.839 \end{pmatrix}.$$

The initial and terminal stages of this process are shown in Figure 2.

If a very small or zero value for τ is used initially, then p_1 and q_2 assume their optimal values very quickly, but q_1 never improves beyond its starting value. This behavior is not completely understood at present. However, a guiding principle seems to be that τ should be varied so that all the bounds are improved at about the same rate in order to obtain the best ultimate result. The reason for this is that a radical change in one or two component bounds can cause the approximating ellipsoid to become too eccentric and consequently enclose a great deal of volume outside the bounding polytope.

The final coordinate bounds obtained above are very sharp. However, they can be considered a worst case analysis in the sense that neither the vector p nor q is actually a solution to the problem. To get even more precise limits on the constraint region as a whole, one can estimate still another linear functional, such as $w^T = (1,1)$. This can be done as a simple byproduct of computations already made, and in this case gives the interval estimate $x_1 + x_2 \in [2.932, 4.353]$. Adding this to the previous information gives the final picture shown in Figure 3.

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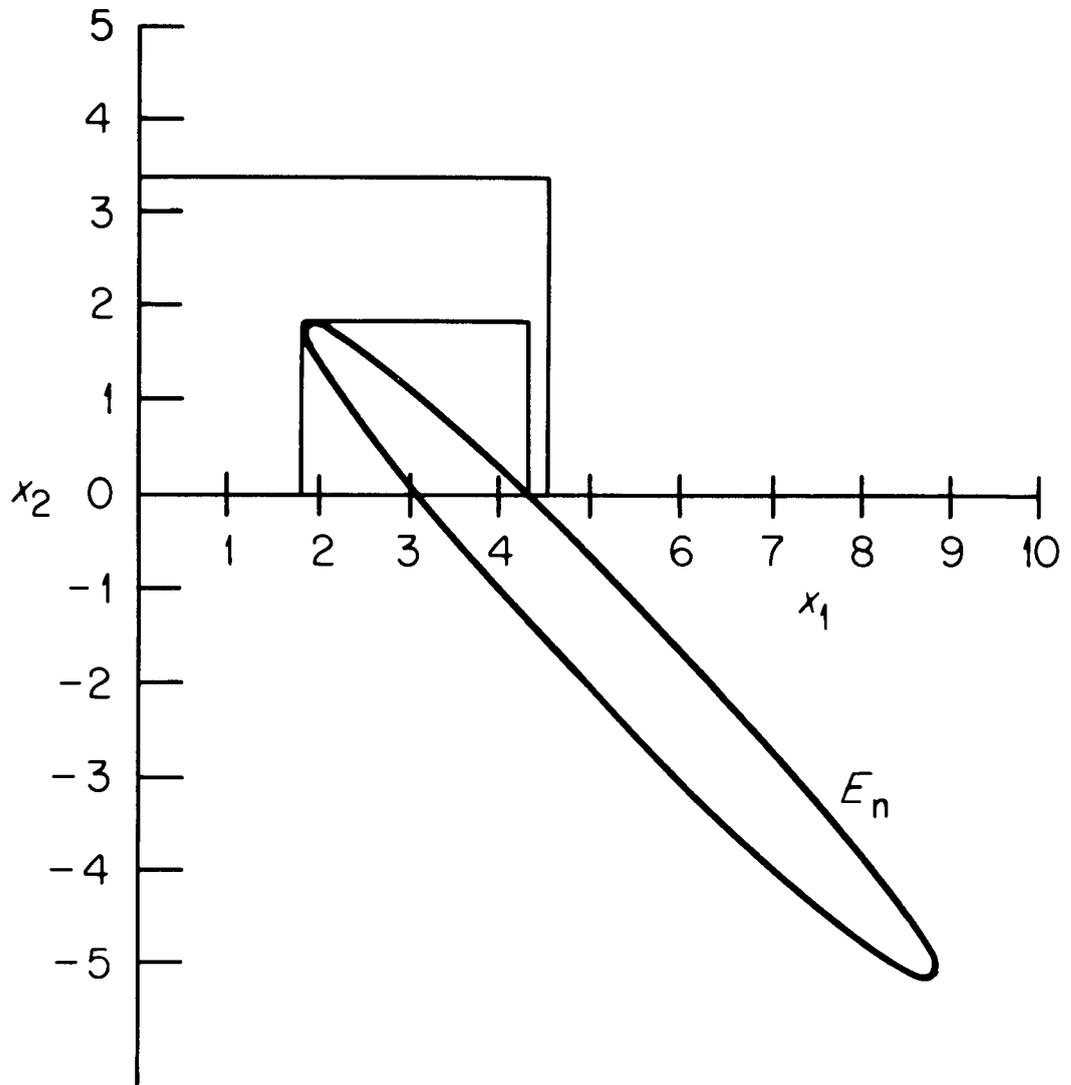


Figure 2. Initial and Final Coordinate Bounds for the Iterative Method of Section III.

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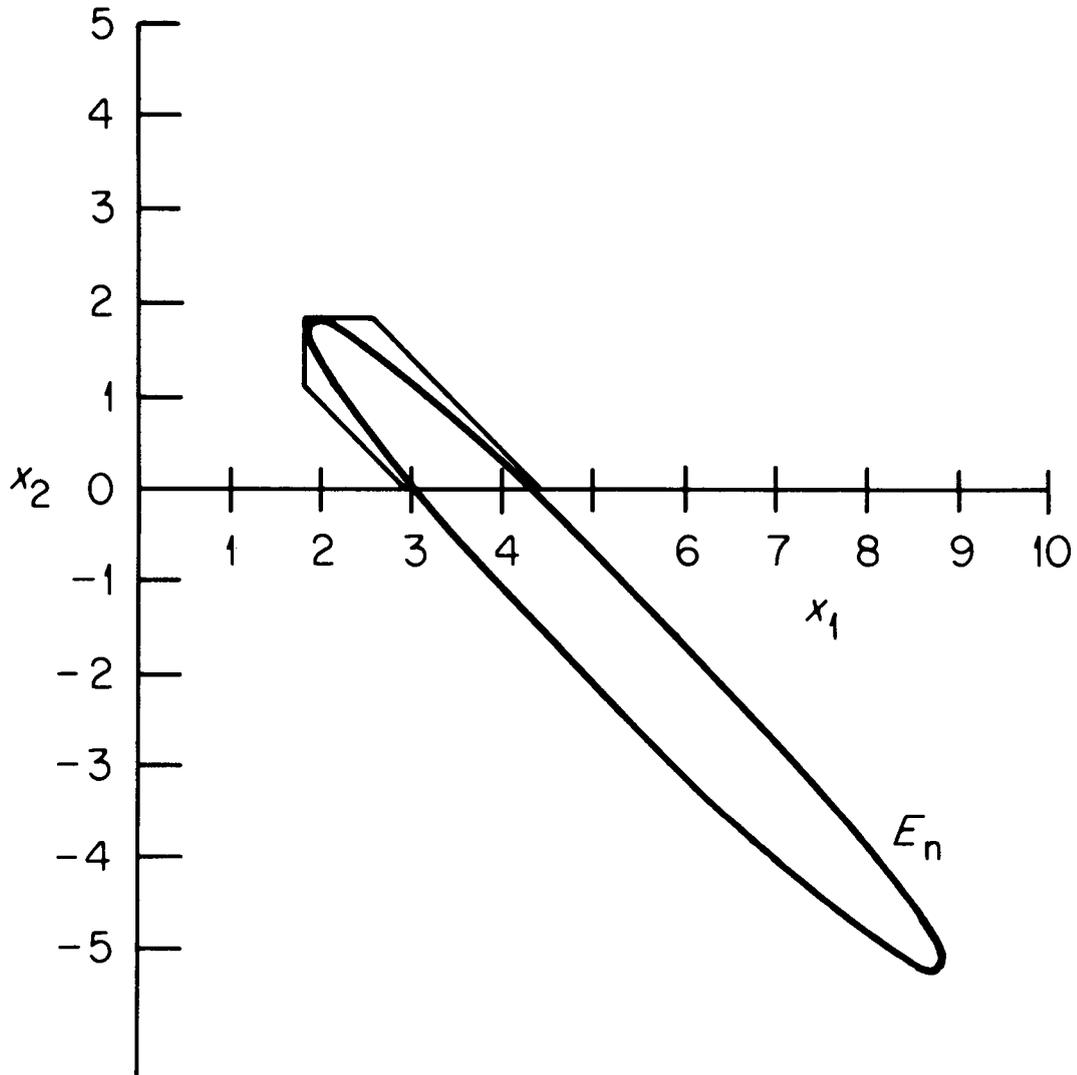


Figure 3. Final Approximation of the Constraint Region Obtained by Estimating the Linear Functional $\varphi(x) = w^T x = x_1 + x_2$.

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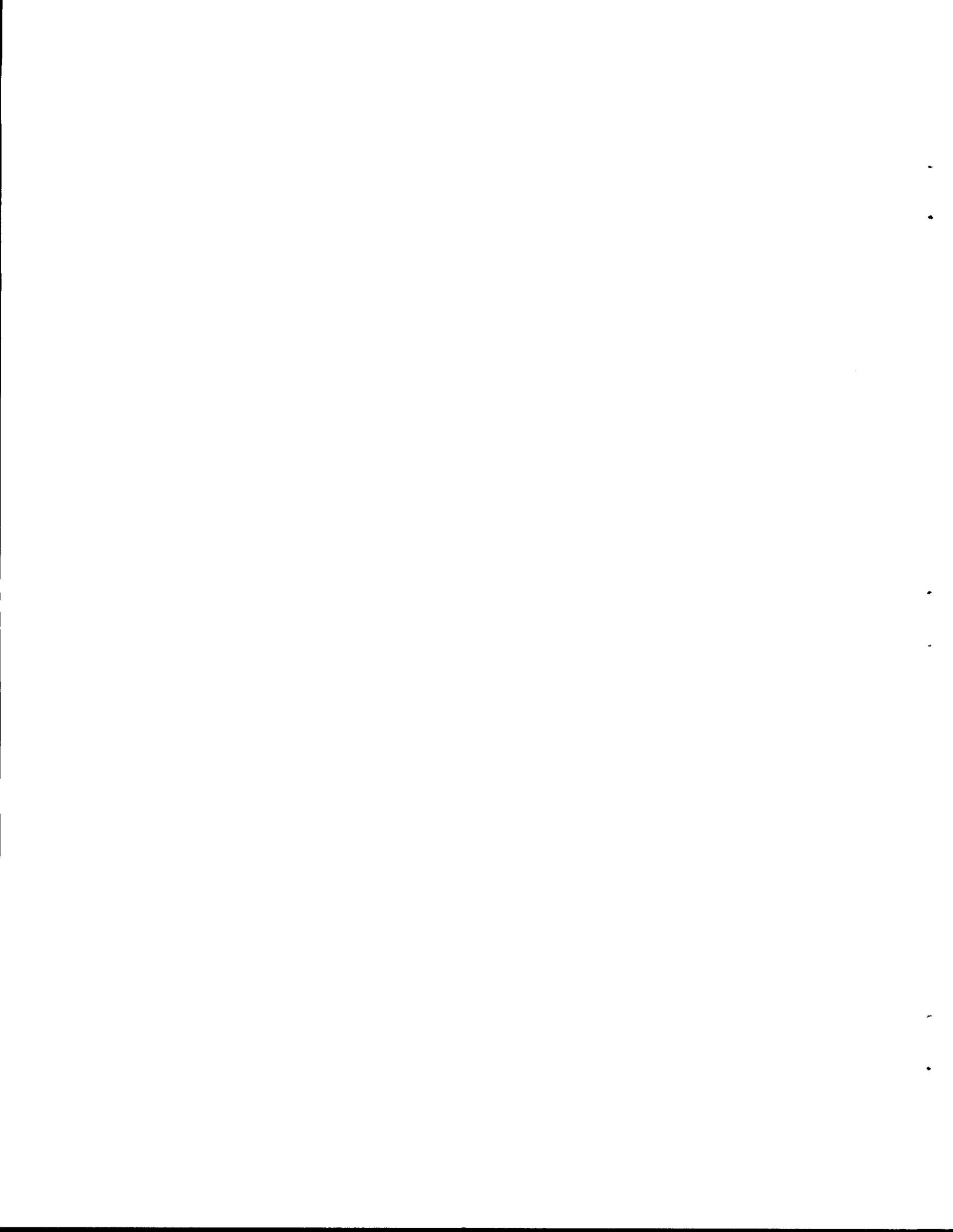
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