

## MINIMUM PRINCIPLES FOR ILL-POSED PROBLEMS\*

JOEL N. FRANKLIN†

**Abstract.** Ill-posed problems  $Ax = h$  are discussed in which  $A$  is Hermitian and positive definite; a bound  $\|Bx\| \leq \beta$  is prescribed. A minimum principle is given for an approximate solution  $\hat{x}$ . Comparisons are made with the least-squares solutions of K. Miller, A. Tikhonov, et al. Applications are made to deconvolution, the backward heat equation, and the inversion of ill-conditioned matrices. If  $A$  and  $B$  are positive-definite, commuting matrices, the approximation  $\hat{x}$  is shown to be about as accurate as the least-squares solution and to be more quickly and accurately computable.

**1. Introduction.** This paper discusses ill-posed problems of the form

$$(1.1) \quad Ax = h,$$

where  $A$  is a positive-definite Hermitian operator mapping a Hilbert space  $H$  into itself. Although we assume  $(Ax, x) > 0$  if  $x \neq 0$ , we often assume also that  $\|Au\|$  may be arbitrarily near zero on the unit sphere  $\|u\| = 1$ . Then  $A$  cannot have a bounded inverse, and the problem (1.1) is ill-posed because the solution  $x$ , if it exists, is unstable: arbitrarily small perturbations of the data,  $h$ , can produce arbitrarily large perturbations of the solution,  $x$ . Typical of such problems is the Fredholm integral equation of the first kind:

$$(1.2) \quad \int_0^1 A(s, t)x(t) dt = h(s) \quad (0 < s < 1),$$

where  $A(s, t)$  is bounded, integrable, self-adjoint, and positive definite.

We shall also consider equations of the form (1.1) where  $A$  is an  $n \times n$  positive-definite Hermitian matrix, and where the data  $h$  and the solution  $x$  lie in the  $n$ -dimensional vector space. In practice, this problem is ill-posed if  $A$  has a large condition number, which is defined as the ratio of largest to smallest eigenvalues. Here a bounded inverse  $A^{-1}$  does exist in theory, but the solution  $x = A^{-1}h$  is numerically unstable because the relative error

$$(1.3) \quad \frac{\|\delta x\|}{\|x\|} \div \frac{\|\delta h\|}{\|h\|}$$

may become large. In fact, the maximum value of the relative error equals the condition number.

Let  $x^0$  be the unknown solution, and let  $h$  be numerical or other approximate data satisfying

$$(1.4) \quad \|Ax^0 - h\| \leq \varepsilon,$$

where  $\varepsilon$  is small but positive. Here we have replaced the equation  $Ax = h$  by an inequality, which is more realistic because it admits the possibility of a nonzero data error. As originally shown by C. Pucci [16], such a problem can often be regularized by additional information in the form of a prescribed bound

$$(1.5) \quad \|Bx^0\| \leq \beta.$$

Here the operator  $B$  and the finite bound  $\beta$  are known. This is new, given information, which is independent of the original information (1.4).

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† Firestone Laboratory, California Institute of Technology, Pasadena, California 91125.

Keith Miller [14] has considered the problem (1.4), (1.5), in which the linear operators  $A$  and  $B$  are not required to be Hermitian, but are required to be bounded. For such problems he has given several very useful numerical methods based on the least-squares principle

$$(1.6) \quad \|Ax - h\|^2 + \lambda^2 \|Bx\|^2 = \text{minimum.}$$

If  $\varepsilon$  and  $\beta$  are known explicitly, the preferred choice of  $\lambda$  is  $\lambda = \varepsilon/\beta$ . The minimal solution is

$$(1.7) \quad x^1 = (A^*A + \lambda^2 B^*B)^{-1} A^*h,$$

which is the solution by Miller's Method 1.

For the problem of inverting ill-conditioned matrices similar formulas, making use of a prescribed bound, have been used since 1959 or earlier; see references [4] through [8], [12], [13], [15], and the book by C. Lawson and R. Hanson [10, pp. 188–194].

For the ill-posed Fredholm equation (1.2) A. N. Tikhonov [17] developed a least-squares method. Here the prescribed bound takes the form

$$(1.8) \quad \Omega^2(x) \equiv \int_0^1 [x^2(t) + \dot{x}^2(t)] dt \leq \beta^2.$$

Or one may use any other Sobolev norm for  $\Omega(x)$ . Tikhonov's minimum principle for an approximate solution is this:

$$(1.9) \quad \|Ax - h\|^2 + \lambda^2 \Omega^2(x) = \text{minimum.}$$

Error analysis in general and for certain applications has been given in [3].

Tikhonov's minimum principle (1.9) can be put in Miller's form (1.6) if  $B$  is suitably defined, but now  $B$  is unbounded. For example, we may define  $B$  on the domain of functions

$$(1.10) \quad x(t) = \sum_{n=0}^{\infty} a_n \cos n\pi t \quad (0 < t < 1),$$

where  $\sum n^2 a_n^2 < \infty$ . Then we define

$$(1.11) \quad Bx(t) = \sum_{n=0}^{\infty} (1 + n^2 \pi^2)^{1/2} a_n \cos n\pi t.$$

This makes  $B$  positive definite and unbounded, with domain dense in the real Hilbert space  $L^2$ ; and

$$(1.12) \quad \int_0^1 [x^2(t) + \dot{x}^2(t)] dt = \|Bx\|^2 = a_0^2 + \frac{1}{2} \sum_1^{\infty} (1 + n^2 \pi^2) a_n^2.$$

Now the Tikhonov principle (1.9) takes Miller's form (1.6), and Tikhonov's minimal solution is given by (1.7).

In the present paper, we will analyze a different minimum principle for the ill-posed problem (1.4) with prescribed bound (1.5). Though  $A$  is bounded, we allow  $B$  to be unbounded (as it must be to include Tikhonov's regularizations); but we require  $B^{-1}$  to be bounded. We define  $\hat{x}$  to be the solution of this problem:

$$(1.13) \quad (Ax, x) - 2\text{Re}(h, x) + \lambda(Bx, x) = \text{minimum},$$

where  $\lambda = \varepsilon/\beta$ . The solution has the simple form

$$(1.14) \quad \hat{x} = (A + \lambda B)^{-1}h.$$

This principle is less generally applicable than Miller's, since it applies only to ill-posed problems  $Ax = h$  in which  $A$  is Hermitian and positive definite. But the simple form of the solution  $\hat{x}$  has advantages in numerical analysis, particularly in the inversion of ill-conditioned matrices.

For matrices, both principles are examples of least squares; see Lawson and Hanson [10]. The principle (1.6) comes from the least-squares problem

$$(1.15) \quad \begin{pmatrix} A \\ \lambda B \end{pmatrix} x = \begin{pmatrix} h \\ 0 \end{pmatrix}.$$

The principle (1.13) comes from the least-squares problem

$$(1.16) \quad \begin{pmatrix} L \\ \sqrt{\lambda}R \end{pmatrix} x = \begin{pmatrix} (L^*)^{-1}h \\ 0 \end{pmatrix}$$

where  $L$  and  $R$  appear in the Cholesky factorizations  $L^*L = A$ ,  $R^*R = B$ .

**2. Error estimates.** Let  $\langle x \rangle$  be a seminorm on the Hilbert space  $H$ . If  $x^0$  is the unknown solution of the inequalities

$$(2.1) \quad \|Ax^0 - h\| \leq \varepsilon, \quad \|Bx^0\| \leq \beta,$$

and if  $x$  is an approximate solution, then  $\langle x - x^0 \rangle$  is a measure of the error. Miller [14] defines these quantities:

$$(2.2) \quad \mathcal{M}(\varepsilon, \beta) = \sup \{ \langle x \rangle : \|Ax\| \leq \varepsilon, \|Bx\| \leq \beta \},$$

$$(2.3) \quad \mathcal{M}_1(\varepsilon, \beta) = \sup \{ \langle x \rangle : \|Ax\|^2 + \lambda^2 \|Bx\|^2 \leq 2\varepsilon^2 \}$$

where  $\lambda = \varepsilon/\beta$ . In his Lemma 3, he proves

$$(2.4) \quad \mathcal{M}(\varepsilon, \beta) \leq \mathcal{M}_1(\varepsilon, \beta) \leq \sqrt{2} \mathcal{M}(\varepsilon, \beta)$$

(I have changed his notation by using  $\beta$  instead of  $E$ .)

The quantity  $\mathcal{M}$  shows how much the information  $\|Bx\| \leq \beta$  restricts  $\langle x \rangle$  if you know  $\|Ax\| \leq \varepsilon$ . This is important because in an ill-posed problem  $Ax = h$ , the norm  $\|Au\|$  may tend to zero on the unit sphere,  $\|u\| = 1$ ; therefore,  $\|x\|$ —and perhaps  $\langle x \rangle$ —may be very large even if  $\|Ax\| \leq \varepsilon$ .

Miller presents four numerical methods based on least squares. If both  $\varepsilon$  and  $\beta$  are known explicitly (and are not just known to exist), the preferred method is Method 1; and this is the method we shall use for purposes of comparison. Miller's minimum principle and its solution,  $x^1$ , appear in our formulas (1.6), (1.7). In his Lemma 4, he gives this error estimate:

$$(2.5) \quad \langle x^1 - x^0 \rangle \leq \mathcal{M}_1(\varepsilon, \beta).$$

Our purpose is to examine the minimum principle (1.13) and the solution,  $\hat{x}$ , given in (1.14). We assume that  $A$  is bounded, Hermitian, and positive definite. We are concerned with ill-posed problems, in which  $A^{-1}$  is unbounded or very large in norm. We assume  $B$  is Hermitian and positive definite, with a bounded inverse  $B^{-1}$ ; we assume that the domain of  $B$  is dense in the Hilbert space, but we do not assume  $B$  is bounded.

If  $\langle x \rangle$  is any seminorm, we define these quantities:

$$(2.6) \quad \mathcal{N}(\varepsilon, \beta) = \sup \{ \langle x \rangle : (Ax, x) \leq \varepsilon \|x\|, (Bx, x) \leq \beta \|x\| \},$$

$$(2.7) \quad \mathcal{N}_1(\varepsilon, \beta) = \sup \{ \langle x \rangle : (Ax, x) + \lambda (Bx, x) \leq 2\varepsilon \|x\| \},$$

where  $\varepsilon > 0, \beta > 0$ , and  $\lambda = \varepsilon/\beta$ . These quantities are practically the same, namely,

$$(2.8) \quad \mathcal{N}(\varepsilon, \beta) \leq \mathcal{N}_1(\varepsilon, \beta) \leq 2\mathcal{N}(\varepsilon, \beta).$$

The reason for defining both of them is that sometimes one is easier to compute than the other. The last three formulas are comparable to Miller's formulas that we have numbered (2.2), (2.3), and (2.4); we will obtain quantitative comparisons later. First we will estimate the error  $\langle \hat{x} - x^0 \rangle$ .

**THEOREM 1.** *Let  $A$  and  $B$  satisfy the preceding assumptions. Let  $x^0$  satisfy (2.1), and let  $\hat{x} = (A + \lambda B)^{-1}h$ . Then  $\hat{x}$  uniquely solves the minimum problem (1.13), and*

$$(2.9) \quad \langle \hat{x} - x^0 \rangle \leq \mathcal{N}_1(\varepsilon, \beta).$$

*Proof.* The operator  $(A + \lambda B)$  has a bounded inverse because

$$(2.10) \quad ((A + \lambda B)x, x) \geq \lambda (Bx, x) \geq \lambda \|B^{-1}\|^{-1} \|x\|^2.$$

Then, since  $\hat{x} = (A + \lambda B)^{-1}h$ ,

$$(2.11) \quad \begin{aligned} (Ax, x) - 2\text{Re}(h, x) + \lambda (Bx, x) \\ = ((A + \lambda B)(x - \hat{x}), (x - \hat{x})) - ((A + \lambda B)\hat{x}, \hat{x}) \\ \geq -((A + \lambda B)\hat{x}, \hat{x}) = -(h, \hat{x}) \end{aligned}$$

with equality if and only if  $x = \hat{x}$ . This proves that  $\hat{x}$  is the unique solution of the minimum problem (1.13).

Let  $\varphi = x - \hat{x}$ . Then

$$\begin{aligned} (A\varphi, \varphi) + \lambda (B\varphi, \varphi) &= ((A + \lambda B)(x - \hat{x}), \varphi) \\ &= ((A + \lambda B)x - h, \varphi). \end{aligned}$$

Thus, for all  $x$  we have the identity

$$(2.12) \quad (A\varphi, \varphi) + \lambda (B\varphi, \varphi) = (Ax - h, \varphi) + \lambda (Bx, \varphi).$$

Set  $x = x^0$ . Then  $\|Ax - h\| \leq \varepsilon$  and  $\lambda \|Bx\| \leq \varepsilon$ , and so

$$(2.13) \quad (A\varphi, \varphi) + \lambda (B\varphi, \varphi) \leq 2\varepsilon \|\varphi\| \quad (\varphi = x^0 - \hat{x}).$$

This gives the error estimate (2.9).  $\square$

**3. Comparisons.** Now we will compare the minimum principles (1.6) and (1.13).

For all  $\lambda \geq 0$  the expression (1.6) is  $\geq 0$  and therefore has the finite lower bound 0. This is not always true of the expression (1.13). If  $\lambda = 0$ , it becomes

$$(3.1) \quad (Ax, x) - 2\text{Re}(h, x).$$

If  $h$  lies outside the range of  $A$ , this expression may tend to  $-\infty$  as  $x$  varies. But of course this cannot happen if  $\lambda > 0$  in (1.13), since we have assumed  $\|B^{-1}\| < \infty$ .

As an example of (3.1), let  $H$  be the Hilbert space of vectors  $x$  with real components satisfying

$$\|x\|^2 = \sum_{n=1}^{\infty} x_n^2 < \infty.$$

Let (3.1) take the form

$$(3.2) \quad \sum_{n=1}^{\infty} n^{-1}x_n^2 - 2 \sum_{n=1}^{\infty} n^{-1}x_n.$$

If we set  $x_n = 1$  for  $n = 1, \dots, N$  and set  $x_n = 0$  for  $n > N$ , the expression (3.2) equals

$$(3.3) \quad - \sum_{n=1}^N n^{-1} \rightarrow -\infty \quad \text{as } N \rightarrow \infty.$$

Now let us compare the quantities  $\mathcal{M}_1(\varepsilon, \beta)$  and  $\mathcal{N}_1(\varepsilon, \beta)$ , which are the upper bounds for the errors  $\langle x^1 - x^0 \rangle$ .

**THEOREM 2.** *Let  $\mathcal{M}_1$  and  $\mathcal{N}_1$  be defined as in (2.3) and (2.7). Then for every seminorm  $\langle x \rangle$ ,*

$$(3.4) \quad \mathcal{M}_1(\varepsilon, \beta) \leq \mathcal{N}_1(\varepsilon, \beta).$$

*Moreover, the ratio  $\mathcal{M}_1/\mathcal{N}_1$  may be arbitrarily near zero. But if  $A$  and  $B$  commute, and if  $\langle x \rangle = \|x\|$ , then*

$$(3.5) \quad \mathcal{N}_1(\varepsilon, \beta) \leq \sqrt{2} \mathcal{M}_1(\varepsilon, \beta).$$

In many ill-posed problems with prescribed bounds,  $A$  and  $B$  do commute. Then this theorem shows that the errors in the two methods,  $\|x^1 - x^0\|$  and  $\|\hat{x} - x^0\|$ , have practically the same upper bound.

*Proof of the theorem.* If

$$\|Ax\|^2 + \lambda^2 \|Bx\|^2 \leq 2\varepsilon^2$$

then

$$(3.6) \quad \begin{aligned} (Ax, x) + \lambda (Bx, x) &\leq (\|Ax\| + \lambda \|Bx\|)\|x\| \\ &\leq \sqrt{2}(\|Ax\|^2 + \lambda^2 \|Bx\|^2)^{1/2} \|x\| \\ &\leq 2\varepsilon \|x\|. \end{aligned}$$

That proves the inequality (3.4).

Next we will show that  $\mathcal{M}_1/\mathcal{N}_1$  may go to zero. For an example, we will use the real Euclidian vector space  $H$  with  $n$  dimensions. We define the diagonal matrix

$$(3.7) \quad A = B = n^{1/2} \text{diag}(1, 2^{-1/2}, 3^{-1/2}, \dots, n^{-1/2}).$$

We define the seminorm  $\langle x \rangle = \|Ax\|$ . Let  $\lambda = 1$ . Then our definitions become

$$(3.8) \quad \mathcal{M}_1(\varepsilon, \beta) = \sup \{ \|Ax\| : 2\|Ax\|^2 \leq 2\varepsilon^2 \}$$

$$(3.9) \quad \mathcal{N}_1(\varepsilon, \beta) = \sup \{ \|Ax\| : 2(Ax, x) \leq 2\varepsilon \|x\| \}.$$

Then  $\mathcal{M}_1 = \varepsilon$ , but

$$(3.10) \quad \mathcal{N}_1 = \varepsilon \max \frac{\|Ax\| \|x\|}{(Ax, x)}.$$

Let  $x_k = n^{-1/2}(k = 1, \dots, n)$ . Then as  $n \rightarrow \infty$

$$\begin{aligned} \|x\|^2 &= 1, \\ (3.11) \quad \|Ax\|^2 &= \sum_{k=1}^n k^{-1} \sim \log n, \\ (Ax, x) &= n^{-1/2} \sum_{k=1}^n k^{-1/2} \rightarrow 2. \end{aligned}$$

Therefore, for fixed  $\varepsilon > 0$ ,  $\mathcal{N}_1 \rightarrow \infty$  as  $n \rightarrow \infty$ ; and so  $\mathcal{M}_1/\mathcal{N}_1 \rightarrow 0$ .

Now suppose  $\langle x \rangle \equiv \|x\|$ . Then

$$\begin{aligned} (3.12) \quad \mathcal{M}_1 &= \sup \{ \|x\| : \|Ax\|^2 + \lambda^2 \|Bx\|^2 \leq 2\varepsilon^2 \} \\ &= \sup \{ \|x\| : ((A^2 + \lambda^2 B^2)x, x) \leq 2\varepsilon^2 \} \\ &= \sqrt{2} \varepsilon \|(A^2 + \lambda^2 B^2)^{-1}\|^{1/2}. \end{aligned}$$

Similarly, we find

$$\begin{aligned} (3.13) \quad \mathcal{N}_1 &= \sup \{ \|x\| : ((A + \lambda B)x, x) \leq 2\varepsilon \|x\| \} \\ &= 2\varepsilon \|(A + \lambda B)^{-1}\|. \end{aligned}$$

If  $A$  and  $B$  commute, then the bounded operators  $A$  and  $(\lambda B)^{-1}$  have spectral representations

$$\begin{aligned} (3.14) \quad A &= \int \rho_v dE_v, \\ (\lambda B)^{-1} &= \int \sigma_v^{-1} dE_v \end{aligned}$$

where  $dE_v$  is a common projection operator, and where

$$(3.15) \quad 0 \leq \rho_v \leq \|A\|, \quad 0 \leq \sigma_v^{-1} \leq \lambda^{-1} \|B^{-1}\|.$$

(If  $A$  and  $B$  are matrices, then  $\rho_v$  and  $\sigma_v$  are eigenvalues of  $A$  and  $\lambda B$  belonging to a common eigenvector.)

The operators  $(A + \lambda B)^{-1}$  and  $(A^2 + \lambda^2 B^2)^{-1}$  are bounded, since the constant  $\lambda$  is positive. They have these spectral representations:

$$\begin{aligned} (3.16) \quad (A + \lambda B)^{-1} &= \int (\rho_v + \sigma_v)^{-1} dE_v, \\ (A^2 + \lambda^2 B^2)^{-1} &= \int (\rho_v^2 + \sigma_v^2)^{-1} dE_v. \end{aligned}$$

Then

$$\begin{aligned} (3.17) \quad \|(A + \lambda B)^{-1}\| &= \sup (\rho_v + \sigma_v)^{-1}, \\ \|(A^2 + \lambda^2 B^2)^{-1}\| &= \sup (\rho_v^2 + \sigma_v^2)^{-1}. \end{aligned}$$

But for all positive  $\rho$  and  $\sigma$

$$(\rho + \sigma)^{-1} \leq (\rho^2 + \sigma^2)^{-1/2},$$

and so

$$(3.18) \quad \|(A + \lambda B)^{-1}\| \leq \|(A^2 + \lambda^2 B^2)^{-1}\|^{1/2}.$$

Now (3.12) and (3.13) imply  $\mathcal{N}_1 \leq \sqrt{2} \mathcal{M}_1$ .  $\square$

*Note 1.* Our proof of the inequality  $\mathcal{N}_1 \leq \sqrt{2} \mathcal{M}_1$  assumes that  $A$  and  $B$  commute. If  $A$  and  $B$  do not commute, the inequality may be false. For example, let  $\lambda = 1$  and let

$$A = \begin{pmatrix} 1 & -2 \\ -2 & 5 \end{pmatrix}, \quad B = \begin{pmatrix} 5 & -2 \\ -2 & 1 \end{pmatrix}.$$

Then

$$A + B = \begin{pmatrix} 6 & -4 \\ -4 & 6 \end{pmatrix}, \quad A^2 + B^2 = \begin{pmatrix} 34 & -24 \\ -24 & 34 \end{pmatrix}.$$

The minimum eigenvalues of these two matrices are

$$\lambda_{\min}(A + B) = 2, \quad \lambda_{\min}(A^2 + B^2) = 10.$$

Therefore,

$$\|(A + B)^{-1}\| = 1/2 > \|(A^2 + B^2)^{-1}\|^{1/2} = 1/\sqrt{10}.$$

Thus, for this example the inequality (3.18) is false, and  $\mathcal{N}_1 > \sqrt{2} \mathcal{M}_1$ .

*Note 2.* In Miller's assumption  $\|Bx^0\| \leq \beta$ , where he takes  $B$  to be bounded, we make no loss of generality by assuming  $B = B^*$ , since we can always replace  $B$  by the Hermitian operator  $B_1 = (B^*B)^{1/2}$  and then assume  $\|B_1x^0\| \leq \beta$ .

*Note 3.* If  $A$  has an inverse, the principle (1.13) can be put in the form (1.6). If we define

$$A_1 = A^{1/2}, \quad g = A^{-1/2} h, \quad \lambda_1 = \lambda^{1/2}, \quad B_1 = B^{1/2}$$

then the principle

$$(Ax, x) - 2\operatorname{Re}(h, x) + \lambda(Bx, x) = \text{minimum}$$

takes the form

$$\|A_1x - g\|^2 + \lambda_1^2 \|B_1x\|^2 = \text{minimum}.$$

But this form cannot be used if  $A$  lacks a bounded inverse, which is the case if the original problem  $Ax = h$  is ill-posed.

**4. Deconvolution.** We will now apply our results to the real convolution equation

$$(4.1) \quad \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} a(z - y)u(y) dy = h(z) \quad (-\infty < z < \infty).$$

(Here we have called the unknown  $u$  instead of  $x$ .) Let the function  $a(z)$  have the Fourier transform

$$(4.2) \quad A(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega z} a(z) dz \quad (-\infty < \omega < \infty),$$

and let  $u$  and  $h$  have the Fourier transforms  $U$  and  $H$ . Then the convolution equation (4.1) becomes

$$(4.3) \quad A(\omega)U(\omega) = H(\omega).$$

As a rule, this equation is ill-posed. A data error  $\delta H(\omega)$  produces a solution error

$$(4.4) \quad \delta U(\omega) = A^{-1}(\omega) \delta H(\omega).$$

If the transform  $A(\omega) \rightarrow 0$  as  $\omega \rightarrow \pm\infty$ , then a data error at high frequencies is greatly magnified when it is multiplied by  $A^{-1}(\omega)$ .

We shall suppose  $A(\omega) > 0$ . This means that the original convolution operator in (4.1) is positive definite, since

$$(4.5) \quad \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u(z) a(z-y) u(y) dy dz = \int_{-\infty}^{\infty} A(\omega) |U(\omega)|^2 d\omega.$$

Although  $A(\omega) > 0$ , we shall usually have  $A(\omega) \rightarrow 0$  as  $\omega \rightarrow \pm\infty$ .

We look for an unknown solution  $U_0(\omega)$ . We replace the equation (4.3) by an inequality

$$(4.6) \quad \|A(\omega)U_0(\omega) - H(\omega)\| \leq \varepsilon.$$

This permits a nonzero data error  $\delta H(\omega)$  with  $L^2$  norm  $\leq \varepsilon$ .

The problem is still ill-posed; to make sense of it we need some new given information. We shall suppose this information takes the form of a prescribed bound

$$(4.7) \quad \|B(\omega)U_0(\omega)\| \leq \beta,$$

where  $B(\omega) > 0$  and  $B(\omega)$  has a positive lower bound. In fact, we shall usually have  $B(\omega) \rightarrow \infty$  as  $\omega \rightarrow \pm\infty$ . In any case, the inverse  $B^{-1}(\omega)$  is bounded.

The least-squares approach to the extended problem (4.6), (4.7) is to solve

$$(4.8) \quad \|AU - H\|^2 + \lambda^2 \|BU\|^2 = \text{minimum},$$

where  $\lambda = \varepsilon/\beta$ . The solution is

$$(4.9) \quad U_1(\omega) = \frac{A(\omega)H(\omega)}{A^2(\omega) + \lambda^2 B^2(\omega)}.$$

This is the approach taken by Miller, although we have here allowed  $B$  to be unbounded. The inverse transform

$$(4.10) \quad u_1(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iz\omega} U_1(\omega) d\omega$$

is an approximate solution of the original convolution equation (4.1).

A second approach to (4.6), (4.7) is to solve

$$(4.11) \quad (AU, U) - 2(U, H) + \lambda (BU, U) = \text{minimum},$$

where the inner product is defined by

$$(4.12) \quad (F, G) = \int_{-\infty}^{\infty} F(\omega)\bar{G}(\omega) d\omega.$$

(The expression (4.11) is real-valued, since we assume  $U(\omega)$  and  $H(\omega)$  are the transforms of real-valued functions  $u(z)$  and  $h(z)$ .) The solution of (4.11) is

$$(4.13) \quad \hat{U}(\omega) = \frac{H(\omega)}{A(\omega) + \lambda B(\omega)}.$$

The inverse transform  $\hat{u}(z)$  is a second approximate solution of (4.1).

A third approach is to use what Miller calls the method of *partial eigenfunction expansion*. This is not a minimum principle, but it is useful for comparison; and it is

often a good numerical method. Define the set

$$(4.14) \quad \Omega = \{\omega : A(\omega) \geq \lambda B(\omega)\},$$

and let  $\Omega'$  be its complement. Then define the *cutoff* solution

$$(4.15) \quad U_c(\omega) = \begin{cases} A^{-1}(\omega)H(\omega) & \text{on } \Omega, \\ 0 & \text{on } \Omega'. \end{cases}$$

We now have three approximate solutions  $U(\omega)$ , and we can compare their errors  $\|U - U_0\|$ , where  $U_0$  is the unknown true solution of (4.6), (4.7). In the present application, the general formulas (3.12) and (3.13) imply

$$(4.16) \quad \mathcal{M}_1(\varepsilon, \beta) = \frac{\sqrt{2}\varepsilon}{\inf_{\omega} [A^2(\omega) + \lambda^2 B^2(\omega)]^{1/2}},$$

$$(4.17) \quad \mathcal{N}_1(\varepsilon, \beta) = \frac{2\varepsilon}{\inf_{\omega} [A(\omega) + \lambda B(\omega)]},$$

and formulas (3.4) and (3.5) state

$$(4.18) \quad \mathcal{M}_1 \leq \mathcal{N}_1 \leq \sqrt{2}\mathcal{M}_1.$$

For the approximation  $U_1(\omega)$  Miller's error bound is

$$(4.19) \quad \|U_1 - U_0\| \leq \mathcal{M}_1(\varepsilon, \beta).$$

For the approximation  $\hat{U}(\omega)$  our error bound is

$$(4.20) \quad \|U_2 - U_0\| \leq \mathcal{N}_1(\varepsilon, \beta).$$

For the cutoff approximation,  $U_c(\omega)$ , Miller's error bound is

$$(4.21) \quad \|U_c - U_0\| \leq \sqrt{2}\mathcal{M}(\varepsilon, \beta) \leq \sqrt{2}\mathcal{M}_1(\varepsilon, \beta),$$

where

$$\mathcal{M}(\varepsilon, \beta) = \sup \{\|F\| : \|AF\| \leq \varepsilon, \|BF\| \leq \beta\}.$$

The last estimate appears in Miller's Lemma 8 in [14]. He proves it by the theory of spectral representation for commuting bounded operators. Since in our application  $B$  is usually unbounded, we should give a separate proof. We will prove

$$(4.22) \quad \|A(U_c - U_0)\| \leq \sqrt{2}\varepsilon,$$

$$(4.23) \quad \|B(U_c - U_0)\| \leq \sqrt{2}\beta.$$

These inequalities directly imply (4.21).

For us, the operators  $A$  and  $B$  are just ordinary positive functions, and the proofs are easy. For any  $F(\omega)$ , we have

$$(4.24) \quad \begin{aligned} \|F\|^2 &\equiv \int_{-\infty}^{\infty} |F|^2 d\omega = \int_{\Omega} |F|^2 d\omega + \int_{\Omega'} |F|^2 d\omega \\ &\equiv \|F\|_{\Omega}^2 + \|F\|_{\Omega'}^2. \end{aligned}$$

With this notation, we find

$$(4.25) \quad \begin{aligned} \|A(U_c - U_0)\|^2 &= \|A(U_c - U_0)\|_{\Omega}^2 + \|A(U_c - U_0)\|_{\Omega'}^2 \\ &= \|H - AU_0\|_{\Omega}^2 + \|AU_0\|_{\Omega'}^2. \end{aligned}$$

Since  $A < \lambda B$  on  $\Omega'$ , we find

$$(4.26) \quad \|AU_0\|_{\Omega'} \leq \lambda \|BU_0\|_{\Omega'} \leq \lambda \beta = \varepsilon.$$

Now (4.26) yields (4.22). Similarly,

$$(4.27) \quad \begin{aligned} \|B(U_c - U_0)\|^2 &= \|B(U_c - U_0)\|_{\Omega}^2 + \|B(U_c - U_0)\|_{\Omega'}^2 \\ &\leq \lambda^{-2} \|A(U_c - U_0)\|_{\Omega}^2 + \|BU_0\|^2 \leq 2\beta^2. \end{aligned}$$

This proves (4.23), and now (4.21) follows.

All three approximations have the same form, namely,

$$(4.28) \quad U(\omega) = (1 + [\lambda B(\omega)A^{-1}(\omega)]^p)^{-1} A^{-1}(\omega)H(\omega).$$

We get  $U_1(\omega)$ ,  $\hat{U}(\omega)$ ,  $U_c(\omega)$  for  $p = 2, 1, \infty$ .

*Example.* We will consider the backward heat equation with prescribed bound at a previous time. Let the temperature  $\varphi(z, t)$  solve

$$(4.29) \quad \frac{\partial \varphi}{\partial t} = \frac{\partial^2 \varphi}{\partial z^2} \quad (-\infty < z < \infty).$$

If  $\tau > 0$  is fixed, and if  $\varphi(z, \tau)$  is given, we wish to compute the initial temperature  $\varphi(z, 0)$ . This problem is ill-posed.

If we set  $h(z) = \varphi(z, \tau)$  and  $u(z) = \varphi(z, 0)$ , we can state this problem as a convolution equation (4.1) by defining the kernel

$$(4.30) \quad a(z) = \frac{1}{\sqrt{2\tau}} e^{-z^2/(4\tau)} \quad (-\infty < z < \infty).$$

Or we can use the equation (4.3) for the transforms:

$$(4.31) \quad e^{-\tau\omega^2} U(\omega) = H(\omega).$$

More realistically, we look for a solution  $U_0(z)$  to an inequality:

$$(4.32) \quad \|e^{-\tau\omega^2} U_0(\omega) - H(\omega)\| \leq \varepsilon.$$

In the extended problem we have additional information: at a previous time,  $t = -\sigma < 0$ , we have

$$(4.33) \quad \|\varphi(z, -\sigma)\| \leq \beta.$$

In terms of Fourier transforms, this says

$$(4.34) \quad \|e^{\sigma\omega^2} U(\omega)\| \leq \beta.$$

In this example,

$$(4.35) \quad A(\omega) = e^{-\tau\omega^2}, \quad B(\psi) = e^{\sigma\omega^2}.$$

The three approximations are (with  $\lambda = \varepsilon/\beta$ )

$$(4.36) \quad U_1(\omega) = \frac{e^{-\tau\omega^2} H(\omega)}{e^{-2\tau\omega^2} + \lambda^2 e^{2\sigma\omega^2}},$$

$$(4.37) \quad U(\omega) = \frac{H(\omega)}{e^{-\tau\omega^2} + \lambda e^{\sigma\omega^2}},$$

and

$$(4.38) \quad U_c(\omega) = \begin{cases} e^{\tau\omega^2} H(\omega) & \text{if } |\omega| \leq \omega_c, \\ 0 & \text{if } |\omega| > \omega_c, \end{cases}$$

where the cutoff frequency  $\omega_c$  is the positive root of the equation

$$(4.39) \quad e^{-\tau\omega_c^2} = \lambda e^{\sigma\omega_c^2}.$$

As we have seen, all the error estimates are about the same; they appear in formulas (4.19), (4.20), (4.21). For definiteness, we will use the last. If  $\|AF\| \leq \varepsilon$  and  $\|BF\| \leq \beta$ , then

$$(4.40) \quad \begin{aligned} \int e^{-2\tau\omega^2} |F|^2 d\omega &\leq \varepsilon^2, \\ \int e^{2\sigma\omega^2} |F|^2 d\omega &\leq \beta^2 = \lambda^{-2} \varepsilon^2. \end{aligned}$$

But for all  $\omega$

$$(4.41) \quad \min(e^{-\tau\omega^2}, \lambda e^{\sigma\omega^2}) \geq e^{-\tau\omega_c^2},$$

where  $\omega_c$  solves (4.39):

$$(4.42) \quad \omega_c = [(\sigma + \tau)^{-1} \ln \lambda^{-1}]^{1/2}.$$

Therefore, by the definition of  $\mathcal{M}(\varepsilon, \beta)$ ,

$$(4.43) \quad \|F\| \leq e^{\tau\omega_c^2} \varepsilon = \mathcal{M}(\varepsilon, \beta).$$

By (4.42), this says

$$(4.44) \quad \mathcal{M}(\varepsilon, \beta) = \beta^{\tau/(\sigma+\tau)} \varepsilon^{\sigma/(\sigma+\tau)}.$$

And now (4.21) gives the error estimate

$$(4.45) \quad \|U_c - U_0\| \leq \sqrt{2} \beta^{\tau/(\sigma+\tau)} \varepsilon^{\sigma/(\sigma+\tau)}.$$

This upper bound pertains to the transforms, but it applies to  $u_c(z) - u_0(z)$  since, by Parseval's theorem,  $\|u_c - u_0\| = \|U_c - U_0\|$ . From the logarithmic convexity of solutions of the heat equation, an upper bound like (4.45) is the most we could expect from any numerical method. See, for instance, [1].

For a numerical example, suppose

$$(4.46) \quad \sigma = 1, \quad \tau = 1, \quad \beta = 1, \quad \varepsilon = 10^{-4}.$$

Then (4.45) says  $\|u_c - u_0\| \leq \sqrt{2} \cdot 10^{-2}$ . The approximate solution is easy to compute numerically; it is the finite integral

$$(4.47) \quad u_c(z) = \frac{1}{\sqrt{2\pi}} \int_{-\omega_c}^{\omega_c} e^{-iz\omega} e^{\omega^2} H(\omega) d\omega,$$

where  $\omega_c = 2.146$ . Since  $H(\omega)$  is the transform of the real-valued function  $h(z)$ , we have  $H(-\omega) = \bar{H}(\omega)$ , and (4.47) becomes

$$(4.48) \quad u_c(z) = \sqrt{\frac{2}{\pi}} \int_0^{2.146} e^{\omega^2} \operatorname{Re}(e^{-iz\omega} H(\omega)) d\omega,$$

which can easily be integrated numerically.

For deconvolution in general, the approximate solutions  $u_1(z)$  and  $\hat{u}(z)$  have simple analytic forms, but the cutoff solution  $u_c(z)$  usually has an advantage for numerical analysis: it is an integral over a *finite* interval.

**5. Ill-conditioned matrices.** If  $A$  is positive definite but ill-conditioned, and if  $B$  is positive definite, and if the unknown  $x^0$  satisfies

$$(5.1) \quad \|Ax^0 - h\| \leq \varepsilon, \quad \|Bx^0\| \leq \beta,$$

then the different minimum principles (1.6), (1.13) give the different approximate solutions

$$(5.2) \quad x^1 = (A^2 + \lambda^2 B^2)^{-1} Ah, \quad \hat{x} = (A + \lambda B)^{-1} h,$$

where  $\lambda = \varepsilon/\beta$ . Error estimates appear in § 2.

As  $\varepsilon \rightarrow 0$ , the approximation  $\hat{x}$  has two numerical advantages: 1) it can be computed more quickly; 2) it can be computed more accurately, since the condition numbers of  $A^2 + \lambda^2 B^2$  and  $A + \lambda B$  must approach those of  $A^2$  and  $A$  as  $\lambda \rightarrow 0$ . Thus, if  $\gamma(A)$  is the condition number of  $A$ , as  $\varepsilon \rightarrow 0$

$$(5.3) \quad \gamma(A^2 + \lambda^2 B^2) \rightarrow \gamma(A^2) = [\gamma(A)]^2 > \gamma(A),$$

while

$$(5.4) \quad \gamma(A + \lambda B) \rightarrow \gamma(A).$$

Before the limit  $\lambda = 0$ , the condition numbers are hard to estimate unless  $A$  and  $B$  commute. But if  $A$  and  $B$  commute, and if  $A$  and  $\lambda B$  have the corresponding eigenvalues  $\rho_v$  and  $\sigma_v$ , then of course

$$\rho_v^2 + \sigma_v^2 \leq (\rho_v + \sigma_v)^2 \leq 2(\rho_v^2 + \sigma_v^2).$$

So the condition numbers of  $A + \lambda B$  and  $A^2 + \lambda^2 B^2$  satisfy

$$(5.5) \quad \frac{1}{2} \leq \frac{[\gamma(A + \lambda B)]^2}{\gamma(A^2 + \lambda^2 B^2)} \leq 2.$$

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