

Approximate Pseudoinverse Solutions to Ill-Conditioned Linear Systems¹

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Abstract. A new method for the numerical solution to ill-conditioned systems of linear equations based on the matrix pseudoinverse is presented. Some illustrative numerical results are provided.

1. Introduction

If a system of linear equations

$$Ax = b \quad (1)$$

is ill-conditioned, its numerical solution becomes difficult, since small errors in the vector b may lead to large errors in the solution vector x . Such unstable systems arise in many contexts, e.g., fitting high-degree polynomials to data by least squares and sequential digital filtering. Since in practice roundoff introduces errors, numerical solutions of ill-conditioned systems are often distorted. This may interfere with the use of digital computers to process large quantities of data.

The computed solution to a perturbation of (1) less sensitive to errors in b may be more useful than that computed from (1) itself. The perturbed system

$$A_\epsilon x = b \quad (2)$$

can be solved iteratively for different parameters ϵ , until a solution is found which meets a physical criterion concerning x or some function of x . In Refs. 1 and 2, such iterative solutions via perturbed systems gave meaningful results when direct solution of the ill-conditioned systems themselves did not.

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In this paper, we present a particular perturbation which is shown to have desirable stability and statistical properties and illustrate its application by examples. This perturbation improves those of Refs. 1 and 2. There, the minimum weighted sum of squared norms of \mathbf{x} or $\mathbf{f}(\mathbf{x})$ and $A\mathbf{x} - \mathbf{b}$ yields an A_ϵ corresponding to the chosen weight. Here, the same two quantities are to have minimum norm, with the stronger requirement described below, which yields the approximate pseudoinverse perturbation. The statistical properties of this perturbation make possible a *matching* of the perturbation to the computer used via a stochastic model of roundoff. This and the relevance of the pseudoinverse to ill-conditioned systems comprise the remaining contributions of this paper.

2. Approximate Pseudoinverse Perturbation

The matrix pseudoinverse A^\dagger (Refs. 3-8) provides a solution to (1) when A is any $m \times n$ matrix of rank $r \leq n \leq m$. Specifically, $A^\dagger \mathbf{b}$ is the unique vector such that

$$\begin{aligned} \|A^\dagger \mathbf{b}\| &= \min_{\mathbf{x} \in M} \|\mathbf{x}\| \\ M &= \{\mathbf{x} \mid \min_y \|A\mathbf{y} - \mathbf{b}\|^2 = \|A\mathbf{x} - \mathbf{b}\|^2\} \end{aligned} \quad (3)$$

In other words, whether A is rectangular, inconsistent, or singular, $\mathbf{x} = A^\dagger \mathbf{b}$ has minimum norm among those \mathbf{x} that minimize $\|A\mathbf{x} - \mathbf{b}\|^2$. (The Euclidean norm is used here and throughout this paper.) Furthermore, $A^\dagger = A^{-1}$ when $r = n = m$.

One definition of the pseudoinverse is (Ref. 3)

$$A^\dagger = \lim_{\epsilon \rightarrow 0} (A' A + \epsilon I)^{-1} A' \quad (4)$$

where prime denotes transpose. Hence, we define the *approximate pseudoinverse* by

$$A_\epsilon^\dagger = (A' A + \epsilon I)^{-1} A' = A_\epsilon^{-1} \quad (5)$$

and note that it is the inverse of a matrix given by

$$A_\epsilon = A + \epsilon(A')^{-1} \quad (6)$$

which we propose to use for the perturbation (2).

The motivation for this particular perturbation is twofold. The limit,

the pseudoinverse, yields a solution with the property (3) for singular systems; one way of describing the instabilities of ill-conditioned systems is to say that they are *almost singular*. The minimum norm property (3) is a desirable one when accumulating errors destroy the usefulness of the numerical result obtained by computing $A^{-1}\mathbf{b}$. Furthermore, it implies that the weighted sum of the squares of $\|\mathbf{x}\|$ and $\|A\mathbf{x} - \mathbf{b}\|$ is a minimum.

3. Properties of the Approximate Pseudoinverse

First, we consider whether $A_\epsilon^+ \mathbf{b} = A_\epsilon^{-1} \mathbf{b}$ is relatively more insensitive to errors in \mathbf{b} than $A^{-1} \mathbf{b}$. This can be put quantitatively by defining the *P-condition number* (Ref. 9) of the nonsingular matrix A as

$$P(A) = \left| \frac{\max_i |\lambda_i|}{\min_i |\lambda_i|} \right| \quad (7)$$

where the symbols $\{\lambda_i\}$ are the eigenvalues of A ; a large *P-condition number* corresponds to an ill-conditioned matrix A . Then, for complex square, nonsingular A , where A^* is the conjugate transpose, we have the following theorem (Brown, Ref. 10):

Theorem. If A is normal, i.e., $AA^* = A^*A$, then, for all $\epsilon > 0$,

$$[A + \epsilon(A^*)^{-1}] \mathbf{x} = \mathbf{b} \quad (8)$$

is better conditioned than

$$A\mathbf{x} = \mathbf{b} \quad (9)$$

in terms of the *P-condition number*, unless $P(A) = 1$, in which case the condition numbers of the two systems are equal. More precisely,

$$P(A + \epsilon(A^*)^{-1}) < P(A) \quad \text{if } P(A) > 1 \quad (10)$$

$$P(A + \epsilon(A^*)^{-1}) = P(A) \quad \text{if } P(A) = 1 \quad (11)$$

Proof. By Schur's theorem, there exists a matrix T such that $TT^* = I$ and

$$TAT^* = \begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & 0 & \lambda_n \end{bmatrix} = A$$

Thus,

$$TA^*T^* = A^*, \quad I = A^*T(A^*)^{-1}T^*, \quad (A^*)^{-1} = T(A^*)^{-1}T^*$$

But

$$(A^*)^{-1} = \begin{bmatrix} 1/\bar{\lambda}_1 & 0 & 0 & \cdots & 0 \\ 0 & 1/\bar{\lambda}_2 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & 0 & 1/\bar{\lambda}_n \end{bmatrix}$$

where the bar denotes conjugate quantities. Thus,

$$T[A + \epsilon(A^*)^{-1}]T^* = \begin{bmatrix} \lambda_1 + \epsilon/\bar{\lambda}_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 + \epsilon/\bar{\lambda}_2 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & 0 & 0 & \lambda_n + \epsilon/\bar{\lambda}_n \end{bmatrix}$$

Now, $\arg(1/\bar{\lambda}) = \arg \lambda$ and, thus,

$$|\lambda + \epsilon/\bar{\lambda}| = |\lambda| + \epsilon/|\lambda|$$

Let λ_1 and λ_2 be two eigenvalues of A . If $|\lambda_1| = |\lambda_2|$, then

$$\frac{|\lambda_1 + \epsilon/\bar{\lambda}_1|}{|\lambda_2 + \epsilon/\bar{\lambda}_2|} = 1$$

If $|\lambda_1| > |\lambda_2|$, then

$$|\lambda_1|/|\lambda_2| > 1 > |\lambda_2|/|\lambda_1|$$

Therefore,

$$\begin{aligned} |\lambda_1| \cdot |\lambda_2| + \epsilon/|\lambda_2| &> |\lambda_1| \cdot |\lambda_2| + \epsilon/|\lambda_1| \\ |\lambda_1| [|\lambda_2| + \epsilon/|\lambda_2|] &> |\lambda_2| [|\lambda_1| + \epsilon/|\lambda_1|] \\ \frac{|\lambda_1|}{|\lambda_2|} &> \frac{|\lambda_1 + \epsilon/\bar{\lambda}_1|}{|\lambda_2 + \epsilon/\bar{\lambda}_2|} \end{aligned}$$

On the other hand, if $|\lambda_1| < |\lambda_2|$, then

$$\begin{aligned} |\lambda_2|^2 + \epsilon &> |\lambda_1|^2 + \epsilon \\ |\lambda_2| \cdot [|\lambda_2| + \epsilon/|\lambda_2|] &> |\lambda_1| \cdot [|\lambda_1| + \epsilon/|\lambda_1|] \\ \frac{|\lambda_2|}{|\lambda_1|} &> \frac{|\lambda_1 + \epsilon/\bar{\lambda}_1|}{|\lambda_2 + \epsilon/\bar{\lambda}_2|} \end{aligned}$$

This concludes the proof.

The approximative pseudoinverse solution is also a meaningful statistical quantity. Consider the following formulation based on the original linear system³:

Proposition. If \mathbf{x} and \mathbf{v} are zero mean Gaussian random vectors with covariance matrices $\epsilon^{-1}I$ and I , respectively, and

$$A\mathbf{x} + \mathbf{v} = \mathbf{b} \quad (12)$$

then

$$\mathbf{x}_\epsilon = A_\epsilon^+ \mathbf{b} = (A'A + \epsilon I)^{-1} A' \mathbf{b} \quad (13)$$

is the conditional expectation of \mathbf{x} for given \mathbf{b} , i.e.,

$$\mathbf{x}_\epsilon = A_\epsilon^+ \mathbf{b} = E(\mathbf{x} | \mathbf{b}) \quad (14)$$

The implication is that, if the roundoff error is represented by addition of the random vector \mathbf{v} and the randomness of \mathbf{x} , the relative variances can be estimated to select a range of values of ϵ for the approximate pseudoinverse perturbations.⁴

4. Numerical Example

Newman (Ref. 9) gives the following ill-conditioned system with $P(A) \approx 3000$:

$$A\mathbf{x} = \begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 32 \\ 23 \\ 33 \\ 31 \end{bmatrix} = \mathbf{b} \quad (15)$$

the corresponding inverse and solution:

$$A^{-1} = \begin{bmatrix} 25 & -41 & 10 & -6 \\ -41 & 68 & -17 & 10 \\ 10 & -17 & 5 & -3 \\ -6 & 10 & -3 & 2 \end{bmatrix}, \quad \mathbf{x} = A^{-1}\mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad (16)$$

³ See Albert and Sittler, Ref. 3, p. 390. The proposition was stated without proof.

⁴ Note, however, that

$$\lim_{\epsilon \rightarrow 0} \text{var}[\mathbf{x}_\epsilon] = \lim_{\epsilon \rightarrow 0} (1/\epsilon)I = \begin{bmatrix} \infty & 0 \\ & \ddots \\ 0 & \infty \end{bmatrix}$$

Table 1. Approximate Pseudoinverse Solutions and Sensitivity

ϵ	0	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
$\mathbf{x}_\epsilon = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$	1.024 0.966 1.011 0.995	0.962 1.048 0.994 1.006	1.028 0.956 1.017 0.994	1.006 0.986 1.002 0.9978	1.1113 0.8179 1.0465 0.9727	1.1209 0.79928 1.05058 0.97002	1.12109 0.7973 1.0524 0.96912
$\mathbf{x}_\epsilon^\delta = \begin{bmatrix} x_1^\delta \\ x_2^\delta \\ x_3^\delta \\ x_4^\delta \end{bmatrix}$	9.204 -12.607 4.498 -1.102	9.11 -12.447 4.461 -1.079	8.515 -11.433 4.206 -0.927	5.192 -5.965 2.835 -0.1119	1.8555 -0.4385 1.4457 0.7116	1.1813 0.67667 1.1647 0.87843	1.10967 0.79846 1.12598 0.90306
$\ \mathbf{x}_\epsilon\ $	1.998	2.006	1.998	1.996	1.986	2.036	1.985
$\ \mathbf{x}_\epsilon^\delta\ $	16.282	16.093	14.892	8.402	2.496	1.995	1.988
$\ \mathbf{x}_\epsilon - \mathbf{x}_\epsilon^\delta\ $	16.361	16.275	14.947	8.392	1.536	0.193	0.100
S_ϵ	818.7	811.3	748.0	420.5	77.34	9.475	5.016
S'_ϵ	100.5	101.1	100.4	99.89	61.54	9.668	5.007

and the solution:

$$\mathbf{x}^\delta = A^{-1}\mathbf{b}^\delta = A^{-1} \begin{bmatrix} 32.1 \\ 22.9 \\ 33.1 \\ 30.9 \end{bmatrix} = \begin{bmatrix} 9.2 \\ -12.6 \\ 4.5 \\ -1.1 \end{bmatrix} \quad (17)$$

when ± 0.1 errors are introduced in \mathbf{b} . For this example, we define the scalar sensitivity to errors $\pm \delta$ in \mathbf{b} as

$$S(\delta) = \frac{\|\mathbf{x}^\delta - \mathbf{x}\|}{\|\mathbf{x}\|} \cdot 100\% \quad (18)$$

where the errors are placed as in (17) and \mathbf{x}^δ is obtained from $\mathbf{b}^\delta = [b_1 + \delta, b_2 - \delta, b_3 + \delta, b_4 - \delta]'$.⁵ Then, from (16) and (17), $S(0.1) = 818.7\%$. Alternatively, $S'(0.1) = 100.5\%$, where $S'(\delta)$ is the sensitivity relative to \mathbf{x}^δ , that is, (18) with the roles of \mathbf{x} and \mathbf{x}^δ interchanged (in practical situations, we have no knowledge whether \mathbf{b} or \mathbf{b}^δ is the exact quantity).

⁵ The errors shown yield the worst solution. We could make a more general definition of sensitivity by inserting *supremum over all possible errors* in (18).

The results of the approximate pseudoinverse solutions to $A\mathbf{x} = \mathbf{b}$ and $A\mathbf{x}^\delta = \mathbf{b}^\delta$, \mathbf{x}_ϵ and $\mathbf{x}_\epsilon^\delta$, and the corresponding sensitivities are given in Table 1 for $\epsilon = 0, 10^{-6}, 10^{-5}, \dots, 10^{-1}$. They show that there are three regions for ϵ : (a) large values, where the sensitivity is reduced to an insignificant amount, but the problem is changed so that true solution is $\mathbf{x}_\epsilon \approx [1.12, 0.80, 1.05, 0.97]'$ instead of $\mathbf{x} = (1, 1, 1, 1)'$; (b) small values, where sensitivity and solution tend toward those of the usual solution; and (c) intermediate values ($10^{-4} < \epsilon < 10^{-3}$), where the results are in between for both the sensitivity and the solution. (Solutions and sensitivity versus ϵ could be calculated for several \mathbf{b} vectors likely to give rise to instabilities, and an arbitrary ϵ -value selected from the intermediate range we noted above, based on this detailed *prior* analysis.)

5. Conclusion

The approximate pseudoinverse provides an approach to improving stability for numerical solutions of ill-conditioned linear systems. However, since no *a priori* criterion exists for choosing the degree of perturbation of the original unstable system, and since many ill-conditioned systems become unstable only for certain error vectors, care should be taken in applying the approximate pseudoinverse and interpreting the results it yields.

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