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SOLUTION OF UNDERDETERMINED SYSTEMS OF EQUATIONS

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August 1977

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Prepared for the U.S. Energy Research and Development Administration under the sponsorship of the Associated Western Universities.
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ABSTRACT

The application of generalized inverses in obtaining least squares solutions of underdetermined systems of equations which approximate the true solutions of physical problems giving rise to such systems of equations is examined. Arguments are presented which dispute the use of the least squares solution of minimum norm as an approximation to the true solution. An alternative least squares solution is presented which is based on a priori information. Simple examples are given which "appear" to support the claim that without further information, the new choice of least squares solution will be better than the least squares solution of minimum norm.
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APPLICATION OF GENERALIZED INVERSES IN THE SOLUTION OF UNDERDETERMINED SYSTEMS OF EQUATIONS.

1.0 INTRODUCTION

1.1 Scope. The primary purpose of this paper is to investigate the use of generalized inverses in obtaining least squares solutions to underdetermined systems of equations. The non-uniqueness of such solutions is stressed and the subsequent difficulties associated with using the least squares solution of minimum norm as an approximation to the "actual" solution of a physical problem are discussed. For a certain class of physical problems leading to underdetermined systems of equations, an alternate choice of least squares solution is presented. An argument is given for the use of this type of approximation in place of the least squares approximation of minimum norm, and in conclusion, a couple of examples are given to support the argument in which both types of least squares solution are compared.

1.2 Description of the Problem and Associated Terminology. Throughout the following discussion, \( \mathbb{R}^n \) will denote the set of all n-tuples of real numbers and \( \mathbb{C}^n \) will denote the set of all n-tuples of complex numbers. The elements of \( \mathbb{R}^n \) or \( \mathbb{C}^n \) will be considered as row vectors or column vectors, whichever is convenient in a given discussion. The symbol \( \mathbb{R}^{mxn} \) will be used to denote the set of all \( mxn \) real matrices while \( \mathbb{C}^{mxn} \) will denote the set of complex matrices. The symbol \( \in \) will stand for the phrase "is a member of."

In order to be quite precise in the material which will follow, three definitions are given.

1.2.1 Definition. If \( M \in \mathbb{C}^{mxn} \) and \( b \in \mathbb{C}^m \), then the solution set of the matrix equation \( Mx = b \) is the set

\[
S = \{ x : x \in \mathbb{C}^n \text{ and } Mx = b \}.
\]

1.2.2 Definition. Two matrix equations \( M_1 x = b_1 \) and \( M_2 x = b_2 \) are equivalent if they have the same solution set.
For example, the matrix equations

\[
\begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2
\end{bmatrix}
= 
\begin{bmatrix}
1 \\
1
\end{bmatrix}
\]

and

\[
\begin{bmatrix}
1 & 1 \\
1 & -1 \\
2 & 2
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2
\end{bmatrix}
= 
\begin{bmatrix}
1 \\
1 \\
2
\end{bmatrix}
\]

are equivalent since they have the same solution set, namely the singleton set

\[S = \{ \begin{bmatrix} 1 \\ 0 \end{bmatrix} \} .\]

1.2.3 Definition. A matrix equation \( Mx = b \) is underdetermined if it is equivalent to a matrix equation \( M_1x = b \), where \( M_1 \in \mathbb{C}^{m \times n} \) and \( m < n \).

In view of the definition given above, unless stated to the contrary, it will be assumed that underdetermined systems are of the form \( Mx = b \), where \( M \in \mathbb{C}^{m \times n} \), \( b \in \mathbb{C}^m \), and \( m < n \).

Consider the underdetermined system

(1) \[ Mx = b, \]

where \( M \in \mathbb{R}^{m \times n} \), \( x \in \mathbb{R}^n \), \( b \in \mathbb{R}^m \), and \( m < n \). It is known that if the null space of \( M \) is \( N(M) \), which is defined by

\[ N(M) = \{ y : My = 0 \}, \]
and if \( x_0 \) is a solution of (1), then the set \( S \) of all solutions of (1) is given by

\[
S = \{ x_0 + y : y \in \mathcal{N}(M) \}.
\]

Since \( m < n \), the dimension \( \dim \mathcal{N}(M) \) of the null space of \( M \) satisfies the inequality

\[
\dim \mathcal{N}(M) \geq n - m > 0,
\]

and consequently \( \mathcal{N}(M) \) consists of infinitely many distinct vectors. Hence, the solution set \( S \) of (1) is either \( \emptyset \), which is the empty set and which would occur if (1) had no solution, or \( S \) consists of infinitely many distinct vectors.

The following question now arises. If the underdetermined matrix equation (1) has been obtained in trying to solve some physical problem, then is there a "best" solution to the physical problem which can be found satisfying (1) and which is based only on the information contained in (1)? The remainder of this paper will be devoted to examining this question and trying to provide a satisfactory solution using generalized inverses.

2.0 LEAST SQUARES SOLUTIONS

2.1 Motivation. In looking for "the best" or "an admissible" solution to an underdetermined matrix equation

\[
(1) \quad Mx = b,
\]

which has resulted in trying to solve a given physical problem, we recall that (1) may not even have a solution. This brings to mind a similar type of problem which is encountered when we try to find a curve out of a given collection of curves which
is the "best fit" in some sense to a given graph consisting of a finite number of points. This type of problem generally leads to an overdetermined system

\[ My = c, \]

where \( M \in \mathbb{R}^{m \times n}, y \in \mathbb{R}^n, c \in \mathbb{R}^m, m > n \) (recall that \( m < n \) for an underdetermined system), and \( y \) is vector whose coordinates represent parameters of the class of curves under consideration. Furthermore, the system (2) is usually inconsistent; that is, it has no solution. If the matrix equation is inconsistent, then the next thing which comes to mind is to try to find a vector \( y \) such that \( ||My - c|| \) is a minimum, where \( || \cdot || \) is some norm on \( \mathbb{R}^m \). It has been found that the ordinary Euclidean norm defined by

\[ ||(x_1, x_2, \ldots, x_m)|| = (x_1^2 + x_2^2 + \ldots + x_m^2)^{1/2} \]

is the easiest to deal with mathematically in this problem and there will be a unique vector \( y \) such that \( ||My - c|| \) is a minimum provided that \( M \) is of rank \( n \). In this case, it is known that

\[ y = (M^T M)^{-1} M^T c, \]

where \( M^T \) is the transpose of \( M \). This solution is called "the least squares solution of (2)". Furthermore, for a good number of classes of curves which are of practical importance in curve fitting, it can be shown that for the corresponding overdetermined systems (2), the matrix \( M \) will always be of rank \( n \) and hence have a unique least squares solution \( y \) of the form (3).

Perhaps we could hope to find a unique least squares solution of some type to the underdetermined system (1) which would be "the best" such solution in some sense to our given physical problem. In order to study the more general problem of finding the least squares solutions of

\[ Mx = b \]

with no restrictions on \( M \), the idea of a generalized inverse must be introduced.
3.0 GENERALIZED INVERSES

3.1 Introduction. There are many different types of generalized inverses (see [1]). Extensive bibliographies on the subject are included in [1], [3], [4], and [5], and a modern treatment of generalized inverses of linear operators on Hilbert spaces is given in [6], which also includes a lengthy bibliography. Rather than surveying several types of generalized inverses and their corresponding properties, we shall concentrate on one such inverse, the so-called Moore-Penrose generalized inverse. This generalized inverse is selected in place of the alternatives mainly because it possesses more properties pertinent to the solution of the generalized least squares problem than do the others.

3.2 Definition. Let $M \in \mathbb{C}^{m \times n}$. Then $M^+$ is a generalized inverse for $M$ if $M^+$ satisfies the following four equations which were introduced by Penrose in [2].

(i) $MM^+M = M$
(ii) $M^+MM^+ = M^+
(iii) (MM^+)^* = MM^+
(iv) (M^+M)^* = M^+M$.

In the above, $^*$ denotes conjugate transpose. It can now be shown ([1] or [2]) for any $M \in \mathbb{C}^{m \times n}$, there is one and only one matrix $M^+$ satisfying conditions (i) - (iv). That is, for any complex matrix $M$, $M^+$ exists and is unique. If $M$ is of rank $m$ and $m = n$, then $M^+ = M^{-1}$. A general method for computing $M^+$ for arbitrary matrices $M$ is discussed in [7]. Two theorems which are useful in computing generalized inverses of special classes of matrices are as follows.

3.2.1 Theorem. If $M \in \mathbb{C}^{m \times n}$ and rank $M = n$, then

$$M^+ = (M^*M)^{-1}M^*.$$ 

This result is well known, and therefore, no proof is offered.

3.2.2 Theorem. If $M \in \mathbb{C}^{m \times n}$ and rank $M = n$, then

$$M^+ = M^*(M^*M)^{-1}.$$
Proof. It is known that \((M^\dagger)^* = (M^*)^+\) (see [2]). Furthermore, \(M^*\) is an \(n\times m\) matrix of rank \(m\), and hence the preceding theorem can be used to obtain
\[
(M^*)^+ = (M^*)^* (M^*)^{-1} (M^*)^*
= (MM^*)^{-1} M.
\]
Or,
\[
(M^\dagger)^* = (MM^*)^{-1} M,
\]
and by taking conjugate transpose of each side of the equation above, we find
\[
M^\dagger = M^* ((MM^*)^{-1})^*
= M^* ((M^*)^* M^*)^{-1}
= M^* (MM^*)^{-1}.
\]
Q.E.D.

3.2.3. Example. Since \(M = \begin{bmatrix} 1 & 0 & i \\ 0 & 1 & 0 \end{bmatrix}\) is a \(2 \times 3\) matrix of rank 2, the hypothesis of theorem 3.2.2. is satisfied and
\[
M^\dagger = M^* (MM^*)^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -i & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & i \\ 0 & 1 & 0 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ -i & 0 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -i & 0 \end{bmatrix} 1/2 \begin{bmatrix} 1 & 0 \\ 0 & 2 \\ -i & 0 \end{bmatrix} = 1/2 \begin{bmatrix} 1 & 0 \\ 0 & 2 \\ -i & 0 \end{bmatrix}.
\]

3.3. USING GENERALIZED INVERSES IN EXAMINING THE GENERALIZED LEAST SQUARES PROBLEM.

In [1] and [2], we find the following theorem.
3.3.1 Theorem. Suppose that $M \in \mathbb{C}^{m \times n}$ and $b \in \mathbb{C}^m$. Then the set of all least squares solutions to

$$Mx = b$$

is the set

$$\{x : x = M^+ b + (I_n - M^+ M)y, \, y \in \mathbb{C}^n\},$$

where $I_n$ denotes the $n \times n$ identity matrix.

A theorem not noted in either [1] or [2] which gives further insight on the composition of the least squares solution set given above is the following.

3.3.2 Theorem. The null space of $M \in \mathbb{C}^{m \times n}$ is

$$N(M) = \{(I_n - M^+ M)y : y \in \mathbb{C}^n\}.$$

Proof. Recall that $N(M) = \{y : My = 0\}$. Set

$$S = \{(I_n - M^+ M)y : y \in \mathbb{C}^n\}.$$

If $z = (I_n - M^+ M)y \in S$, then

$$Mz = M(I_n - M^+ M)y$$
$$= My - MM^+ My$$
$$= My - My$$
$$= 0,$$

so that $S \subseteq N(M)$. Conversely if $x \in N(M)$, then $Mx = 0$ and

$$x = (I_n - M^+ M)x$$
$$= x - (M^+ M)x$$
$$= x - M^+(Mx)$$
$$= x - M^+(0)$$
$$= x$$

implies that $x \in S$ and hence $N(M) \subseteq S$. Therefore, $S \subseteq N(M)$ and $N(M) \subseteq S$ gives

$S = N(M)$. 

Q.E.D.
This theorem implies that if x and y are two least squares solutions of (1), then \( Mx = My \). It does not mean \( x = y \) or even that \( x \) and \( y \) are of the "same general shape."

It is clear from these results that there will be a **unique** least squares solution if and only if \( N(M) = \{0\} \), where \( 0 \) represents the n-tuple consisting of all coordinates 0. This will be true if, and only if \( \text{rank } M = n \). For an underdetermined system, \( \text{rank } M \leq m \leq n \), and consequently, for any underdetermined system, there will be infinitely many distinct least squares solutions of (1). In order to further clarify this result, an example will be given.

3.3.3 Example. Consider the system of equations

\[
\begin{align*}
x_1 + x_2 &= 2 \\
x_2 + x_3 &= 2 \\
x_1 + 2x_2 + x_3 &= 5.
\end{align*}
\]

This system is inconsistent since adding the first and second equations together gives an equation which is in disagreement with the third. The system of equations can be written in matrix form as \( Mx = b \), where

\[
M = \begin{bmatrix}
1 & 1 & 0 \\
0 & 1 & 1 \\
1 & 2 & 1
\end{bmatrix}, \quad
x = \begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}, \quad
\text{and } b = \begin{bmatrix}
2 \\
2 \\
5
\end{bmatrix}
\]

The generalized inverse of \( M \), which was computed using the general method given in [7], is

\[
M^+ = \frac{1}{9} \begin{bmatrix}
5 & -4 & 1 \\
1 & 1 & 2 \\
-4 & 5 & 1
\end{bmatrix}.
\]

Also,

\[
M^+M = \frac{1}{9} \begin{bmatrix}
5 & -4 & 1 \\
1 & 1 & 2 \\
-4 & 5 & 1
\end{bmatrix} \begin{bmatrix}
1 & 1 & 0 \\
0 & 1 & 1 \\
1 & 2 & 1
\end{bmatrix}
\]
The least squares solution of minimum norm is \( x = \frac{7}{9} (1, 2, 1) \). Another least squares solution having positive coefficients (there are infinitely many of these) is \( x = \frac{7}{9} (2, 1, 2) \), which is obtained by setting \( \alpha = \frac{7}{9} \). Either of these distinct vectors \( x \) gives the same vector \( Mx \) so that \( ||Mx - b|| \) is the same in either case, and as mentioned earlier, this is the minimum obtainable value for \( ||Mx - b|| \).

The following question now arises. For an underdetermined system of equations obtained in trying to solve a physical problem, is there any one of the infinitely many least squares solutions which can be used as a reliable estimate to the true
solution of the physical problem? We might hope that the following theorem found in [1] provides the answer.

3.3.4 Theorem. (Penrose [2]) There is a unique least squares solution to $Mx = b$ which is of minimum norm, and this solution is given by

\[ x = M^+ b. \]

With the above theorem, it is an attractive idea to hope that the least squares solution of minimum norm will be of good approximation to the solution of an underdetermined system arising as a result of a given physical problem. By "solution" in the preceding statement, we mean of course the actual solution of the physical problem.

In order to examine this possibility, some comments are in order. First, if $Mx = b$ is consistent, then this is still a least squares problem in which least squares solutions will in fact be solutions. Second, for a fixed positive integer n, we expect that of all consistent underdetermined systems $Mx = b$ involving mxn matrices $M$, the ones having the most "well-behaved" solution sets will be those with $\text{rank } M = m = n - 1$. Third, it is conceivable that any such system may have arisen in trying to solve some physical problem. Whether or not the minimum norm solution is a good approximation to the solution of the given physical problem without additional information will depend on the solution set of the system. The following theorem shows that in general, for underdetermined systems, there is no assurance that the least squares solution of minimum norm will be anything like the desired solution to the given physical problem. This is a consequence of the theorem which demonstrates that situations can arise where there are two different solutions to the same matrix equation. These solutions are of completely different shape and size, and yet either of these solutions might have been the one we were looking for in solving a given physical problem. Furthermore, the least squares solution of minimum norm must be noticeably different from at least one of the two solutions just mentioned.

3.3.5 Theorem. Let $n$ be a positive integer and let $z_1 = (y_1, y_2, \ldots, y_n)$ and $z_2 = (w_1, w_2, \ldots, w_n)$ be any two vectors in $\mathbb{R}^n$. Then there is a system of $n - 1$ linearly independent equations in $n$ unknowns having both $z_1$ and $z_2$ as solutions.
Proof. The proof will be broken into three distinct cases.

Case I. If $z_1$ and $z_2$ are both 0, then the system

$$
\begin{align*}
  x_1 &= 0 \\
  x_2 &= 0 \\
  &\quad \vdots \\
  x_{n-1} &= 0
\end{align*}
$$

will suffice.

Case II. If $z_1$ and $z_2$ are dependent and $z_1$ is non-zero, extend $\{z_1\}$ to a basis $\beta$ for $\mathbb{R}^n$. Set $Tz_1 = 0$ and $Tz = z$ for $z \in \beta - \{z_1\}$, and then extend $T$ linearly to all of $\mathbb{R}^n$. Let $M$ be the matrix representing $T$ with respect to the standard basis for $\mathbb{R}^n$. Since $\dim R(T) = n - 1$, it follows that $n - 1$ rows of $M$ are linearly independent. If $Mx = 0$ is interpreted as a system of equations and a dependent row is omitted, then $n - 1$ independent equations remain. Furthermore, $x = z_1$ and $x = z_2$ are solutions of this new system of $n - 1$ linearly independent equations in $n$ unknowns.

Case III. Suppose that $z_1$ and $z_2$ are linearly independent. Set $w = z_2 - z_1$. Then $w$ and $z_1$ are independent since if they were dependent, it would follow that $w = \alpha z_1$ for some scalar $\alpha \neq 0$, and hence

$$
  z_2 = z_1 + w = z_1 + \alpha z_1 = (1 + \alpha) z_1,
$$

contradicting the fact that $z_1$ and $z_2$ are independent. Extend $\{z_1, w\}$ to a basis $\beta$ for $\mathbb{R}^n$. Define $T: \mathbb{R}^n \to \mathbb{R}^n$ by setting $Tz_1 = z_1$, $Tw = 0$, $Tz = z$ for $z \in \beta - \{z_1, w\}$, and extend $T$ linearly to all of $\mathbb{R}^n$. Since $\dim R(T) = n - 1$, it follows that $M$ has $n - 1$ linearly independent rows. Select $n - 1$ such rows and delete the other row from the system of equations

$$
  Mx = z_1.
$$

Since $z_1$ and $z_2 = z_1 + w$ satisfy the equation above, it follows that both $z_1$ and $z_2$ satisfy the new system of $n - 1$ linearly independent equations in $n$ unknowns, which completes the proof.
The following example is now presented in order to illustrate the preceding theorem. If $T: \mathbb{R}^n \to \mathbb{R}^n$ and $\beta_1$ and $\beta_2$ are bases for $\mathbb{R}^n$, then $M(T; \beta_1, \beta_2)$ will represent the matrix of $T$ with respect to $\beta_1$ and $\beta_2$, where it will be assumed that the elements of the domain are expressed in terms of the basis $\beta_1$ while members of the codomain are expressed in terms of the basis $\beta_2$. The phrase "$M$ is the matrix of $T$ with respect to the basis $\beta$" will mean $M = M(T; \beta, \beta)$.

3.3.6 Example. Suppose we wish to find two linearly independent equations in three unknowns which have both $(0, 5, 10)$ and $(10, -5, 0)$ as solutions. These two vectors are independent. Set

$$w = (10, -5, 0) - (0, 5, 10)$$

$$= (10, -10, -10).$$

The set $\beta = \{(1, 0, 0), (0, 5, 10), (10, -10, -10)\}$ forms a basis for $\mathbb{R}^3$. Set

$$T(10, -10, -10) = 0$$

and

$$t z = z$$

for $z \in \beta - \{(10, -10, -10)\}$, and extend $T$ linearly to all of $\mathbb{R}^3$. The matrix $\tilde{M} = M(T; \beta, S)$ of $T$ with respect to $\beta$ and the standard basis $S$ for $\mathbb{R}^3$ is

$$\tilde{M} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 10 & 0 \end{bmatrix}. $$

The matrix $M(I; \beta, S)$ of the identity map with respect to $\beta$ and the standard basis $S$ for $\mathbb{R}^3$ is given by

$$M(I; \beta, S) = \begin{bmatrix} 1 & 0 & 10 \\ 0 & 5 & -10 \\ 0 & 10 & -10 \end{bmatrix}. $$
consequently,

\[
M(I; S, \beta) = \frac{1}{50} \begin{bmatrix}
50 & 100 & -50 \\
0 & -10 & 10 \\
0 & -10 & 5
\end{bmatrix}
\]

\[
= \frac{1}{10} \begin{bmatrix}
10 & 20 & -10 \\
0 & -2 & 2 \\
0 & -2 & 1
\end{bmatrix}
\]

If M represents the matrix of T with respect to S, then

\[
M = \frac{1}{10} \begin{bmatrix}
1 & 0 & 0 \\
0 & 5 & 0 \\
0 & 10 & 0
\end{bmatrix}
\begin{bmatrix}
10 & 20 & -10 \\
0 & -2 & 2 \\
0 & -2 & 1
\end{bmatrix}
\]

\[
= \frac{1}{10} \begin{bmatrix}
10 & 20 & -10 \\
0 & -10 & 10 \\
0 & -20 & 20
\end{bmatrix}
\]

\[
= \begin{bmatrix}
1 & 2 & -1 \\
0 & -1 & 1 \\
0 & -2 & 2
\end{bmatrix}
\]

Note that the second and third rows of the matrix M are linearly dependent and therefore, omit the third row of the system of equations determined by

\[
\begin{bmatrix}
1 & 2 & -1 \\
0 & -1 & 1 \\
0 & -2 & 2
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
= \begin{bmatrix}
0 \\
5 \\
10
\end{bmatrix}
\]

obtaining the system

\[
x_1 + 2x_2 - x_3 = 0 \\
-x_2 + x_3 = 5,
\]

which consists of two linearly independent equations in three unknowns having both (10, -5, 0) and (0, 5, 10) as solutions. Of course, there are infinitely many other
solutions to the system of equations since the solution set is

$$ S = \{(0, 5, 10) + \alpha (10, -10, -10) : \alpha \in \mathbb{R}\}, $$

but the important thing to notice is that given the original two 3-tuples, we were able to come up with two linearly independent equations in three unknowns having the original two vectors as solutions.

4.0 MODELS USED TO SOLVE UNDERDETERMINED SYSTEMS

4.1 The Problem. Consider again the problem of finding a least squares solution of

(1) \[ M x = b \]

which best approximates the actual solution of a physical problem giving rise to this system of equations when the system is underdetermined. The last theorem developed above strongly suggests that the least squares solution of minimum norm is not necessarily a good guess in general. What might be better? Certainly whichever solution is chosen should be a least squares solution, but which one? If nothing more is known about the problem, then there is clearly not much more one can do. However, there are classes of problems for which something more can be proposed. Suppose that after parameters determining an ideal geometry or ideal kinetic rates for a physical problem are fixed, an underdetermined matrix equation of the form (1) is derived in trying to obtain the actual solution of the problem. The fixed parameters are assumed to determine a vector \( x_0 \) which is obtained by theoretical or statistical considerations, and then a vector \( b_0 = M x_0 \) can be computed using the known vector \( x_0 \) and the known matrix \( M \). It is assumed that if an experiment is performed from which the data \( b \) are determined, then the matrix equation

(1) \[ M x = b \]

will result which may contain errors in the data \( b \). Under "normal" circumstances, we assume that the solution \( x \) to the physical problem and the vector \( x_0 \) will not be drastically different. Unfortunately, the matrix equation (1) is underdetermined, so that even if \( b = b_0 \), taking \( x = M^+ b \) may not give \( x_0 \). It would give \( x_0 \) however if,
in addition, $b = b_0$ and $||x - x_0||$ is required to be a minimum. Furthermore, after a little thought, it would seem that even in cases where there is a true physical deviation between the desired actual solution $x$ and the model vector $x_0$, then, if it could be found, the best estimate for $x$, without further information, would be the least squares solution of (1) which has the property that $||x - x_0||$ is a minimum. We will now introduce terminology and develop an algorithm to implement these ideas.

4.2 TERMINOLOGY AND THEORY

4.2.1 Definition. Suppose $m$ and $n$ are fixed positive integers with $m < n$, $S \subseteq \mathbb{R}^p$, and for each $k$ in $S$ there is an $m \times n$ matrix $M = M_k$ associated with $k$. Define an $M$-problem as any physical problem involving the parameter set $S$ and leading to systems of equations of the form

(1) \[ Mx = b. \]

The $M$-problem is normal if for each $k \in S$ there are vectors $x_0 = (x_0)_k$ and $b_0$ such that $Mx_0 = b_0$, and barring "unexpected" abnormalities, the expected "actual physical solution" of (1) for a given $b$ will not deviate considerably from the model $x_0$ in either size or shape. The vector $x_0 = (x_0)_k$ is a model for $M = M_k$.

Even if an abnormality does occur in $x$, the least squares solution of (1) such that $||x - x_0||$ is a minimum should be the best approximation to the vector $x$ based on the information given.

In order to simplify the statement and development of the following theory, it will be assumed that $M$ is not parameter dependent. The more general theory is developed in exactly the same manner.

4.2.2 Theorem. Let $M \in \mathbb{C}^{m \times n}$ and suppose that $x_0 \in \mathbb{C}^n$ and $b_0 \in \mathbb{C}^m$ are such that $Mx_0 = b_0$. If $b \in \mathbb{C}^m$, then the least squares solution of

(1) \[ Mx = b, \]

with $||x - x_0||$ a minimum, is
where $M^+$ is the Moore-Penrose generalized inverse of $M$.

Proof. Since $M x_0 = b_0$ and therefore, $M x_0 - b_0 = 0$, it follows that for any vector $x \in \mathbb{C}^n$,

$$||M x - b|| = ||M x - b - (M x_0 - b_0)|| = ||M (x - x_0) - (b - b_0)||,$$

so that any vector $x$ minimizing the norm on the right will minimize the norm on the left. With $r = x - x_0$ and $c = b - b_0$, the problem of finding the least squares solution of (1) with $||x - x_0||$ a minimum is equivalent to finding the least squares solution of minimum norm of

$$Mr = c.$$

By theorem 3.3.4,

$$r = M^+ c$$

so that

$$x - x_0 = M^+ (b - b_0),$$

and hence

$$x = x_0 + M^+ (b - b_0).$$

Q.E.D.

When the theorem is restated in terms of $M$-problems, we have the following.

4.2.3 Corollary. If a physical problem is a normal $M$-problem and $x_0$ is a model for $M$, then the least squares solution of $Mx = b$ having $||x - x_0||$ a minimum is

$$x = x_0 + M^+ (b - b_0),$$
where \( b_0 = M x_0 \).

It should be noted here that the least squares solution of (1) of minimum norm and the least squares solution having \( \| x - x_0 \| \) a minimum are actually equal if and only if \( x_0 = M^+ b_0 \), and this condition is not likely to hold true for a given physical problem.

A simple two-dimensional reconstruction problem will now be considered and a comparison of results obtained using the least squares solution of minimum norm and the alternative least squares solution given in this paper will be presented. Data will be altered in order to provide a wider range of tests situations. Noise will not be considered.

4.2.4 Example. Consider the simple problem of reconstructing four non-negative values \( x_1, x_2, x_3, \) and \( x_4 \) in a 2 x 2 array from two projections at 0° and 90°.

\[
\begin{array}{c c}
X_1 & X_2 \\
X_3 & X_4 \\
\end{array}
\]

Assuming that the numbers \( b_1, b_2, b_3, \) and \( b_4 \) contain no errors, it follows that the following system of equations is obtained subject to the restriction \( x_1 \geq 0, x_2 \geq 0, x_3 \geq 0, \) and \( x_4 \geq 0 \).

\[
\begin{align*}
x_1 + x_2 &= b_1 \\
x_3 + x_4 &= b_2 \\
x_1 + x_3 &= b_3 \\
x_2 + x_4 &= b_4 .
\end{align*}
\]

The equations are dependent since the fourth equation can be obtained from the first three by subtracting the third equation from the first and then adding the second equation to the result. Consequently, the system of equations consisting of the first three equations is equivalent to the original system, where the notion of equivalence is that of definition 1.2.2 when the systems are thought of in matrix form. Write the equivalent system of equations in matrix form as

\[
M x = b,
\]
where

\[
M = \begin{bmatrix}
1 & 1 & 0 & 0 \\
0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0
\end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}, \quad \text{and} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}.
\]

It should be pointed out that the reduction of the original system to an equivalent system was not necessary but was made only in order to be able to calculate the generalized inverse more easily and make required computations somewhat simpler. Set

\[
y_0 = \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}.
\]

The null space of \( M \) is

\[
N(M) = \{ \alpha y_0 : \alpha \in \mathbb{R} \},
\]

and hence if \( x_0 = z = (z_1, z_2, z_3, z_4)^T \) is a solution of (5) having non-negative coordinates, then the solution set (see definition 1.2.1) of (5), and hence of (4), is

\[
S = \{ x_0 + \alpha y_0 : \alpha \in \mathbb{R} \}.
\]

The requirement that the coordinates of the solution vectors be non-negative is equivalent to \( \alpha \) satisfying the system of inequalities

\[
z_1 + \alpha \geq 0 \\
z_2 - \alpha \geq 0 \\
z_3 - \alpha \geq 0 \\
z_4 + \alpha \geq 0,
\]

which is equivalent to requiring
Set \( \alpha_1 = \max \{-z_1, -z_4\} \) and \( \alpha_2 = \min \{z_2, z_3\} \). Then the set \( T \) of solutions to the original problem having non-negative coordinates is given by

\[
T = \{x_0 + \alpha y_0 : \alpha_1 \leq \alpha \leq \alpha_2\}.
\]

The generalized inverse of \( M \) will also be required in the examples to follow and therefore, will now be computed. Since the rows of \( M \) are linearly independent, the hypothesis of theorem 3.2.2 is satisfied and hence

\[
M^+ = M^T (MM^T)^{-1},
\]

with the transpose in place of the conjugate transpose since \( M \) is a real matrix.

Now,

\[
MM^+ = \begin{bmatrix}
1 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 \\
1 & 0 & 1 & 0
\end{bmatrix} \begin{bmatrix}
1 & 0 & 1 \\
0 & 0 & 0 \\
0 & 1 & 1 \\
0 & 0 & 0
\end{bmatrix}
\]

\[
= \begin{bmatrix}
2 & 0 & 1 \\
0 & 2 & 1 \\
1 & 1 & 2
\end{bmatrix},
\]

so that

\[
(MM^+)^{-1} = \frac{1}{4} \begin{bmatrix}
3 & 1 & -2 \\
1 & 3 & -2 \\
-2 & -2 & 4
\end{bmatrix},
\]

and

\[
M^+ = \frac{1}{4} \begin{bmatrix}
1 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 1 \\
0 & 1 & 0
\end{bmatrix} \begin{bmatrix}
3 & 1 & -2 \\
1 & 3 & -2 \\
-2 & -2 & 4
\end{bmatrix}.
\]
With the matrix $M$ fixed as above, the following table of results is obtained in trying to solve $Mx = b$ using different models $x_0$ for $M$ and different abnormal vectors $x_1$ to generate the observed data set $b$. All results are exact and noise was not incorporated. The vector $b_0$ is equal to $Mx_0$ and the vector $b$ equals $Mx_1$. The problem is to learn how well the distribution $x_0$ can be determined from the observed projection data $b$.

<table>
<thead>
<tr>
<th>model $x_0$</th>
<th>abnormal vector $x_1$</th>
<th>$x = M^*b$</th>
<th>$x = x_0 + M^*(b - b_0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(3, 0, 1, 6)</td>
<td>(3, 1, 2, 8)</td>
<td>(1, 3, 4, 6)</td>
<td>(3, 1, 2, 8)</td>
</tr>
<tr>
<td>(2, 1, 1, 2)</td>
<td>(4, 2, 1, 2)</td>
<td>(3.25, 2.75, 1.75, 1.25)</td>
<td>(3.75, 2.25, 1.25, 1.75)</td>
</tr>
<tr>
<td>(4, 2, 1, 3)</td>
<td>(7, 3, 1, 4)</td>
<td>(5.25, 4.75, 2.75, 2.25)</td>
<td>(6.25, 3.75, 1.75, 3.25)</td>
</tr>
<tr>
<td>(10, 1, 1, 10)</td>
<td>(10, 0, 0, 10)</td>
<td>(5, 5, 5, 5)</td>
<td>(9.5, .5, .5, 9.5)</td>
</tr>
</tbody>
</table>

In all cases, better results were obtained from the least squares solution having $\|x - x_0\|$ a minimum. The first and fourth examples illustrate how much better the results can be. In fact, the vector $x = x_0 + M^*(b - b_0)$ in the first example was equal to $x_0$.

4.2.5 Example. Suppose $M = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 2 & 1 \end{bmatrix}$, $x_0 = \begin{bmatrix} 6 \\ 2 \\ 4 \end{bmatrix}$, and $b_0 =$

$$Mx_0 = \begin{bmatrix} 8 \\ 6 \\ 14 \end{bmatrix}.$$  Let $x = \begin{bmatrix} 8 \\ 3 \\ 14 \end{bmatrix}$ be abnormal and suppose that the data $b$ in $Mx = \begin{bmatrix} 11 \\ 7 \\ 18 \end{bmatrix}$ is noise or errors in the observed data. The least squares solution of minimum norm for

$Mx = b$
is
\[ x = M^+ b = \frac{1}{9} \begin{bmatrix} 5 & -4 & 1 \\ 1 & 1 & 2 \\ -4 & 5 & 1 \end{bmatrix} \begin{bmatrix} 11 \\ 8 \\ 17 \end{bmatrix} = \frac{1}{9} \begin{bmatrix} 40 \\ 53 \\ 13 \end{bmatrix} \approx \begin{bmatrix} 4.4 \\ 5.9 \\ 1.4 \end{bmatrix}, \]

while the least squares solution with \( ||x - x_0|| \) a minimum is
\[ x = x_0 + M^+ (b - b_0) = \begin{bmatrix} 6 \\ 2 \\ 4 \end{bmatrix} + \frac{1}{9} \begin{bmatrix} 5 & -4 & 1 \\ 1 & 1 & 2 \\ -4 & 5 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 2 \\ 4 \end{bmatrix} + \begin{bmatrix} 10/9 \\ 11/9 \\ 1/9 \end{bmatrix} \approx \begin{bmatrix} 7.1 \\ 3.2 \\ 4.1 \end{bmatrix}. \]

Comparing the results \( x_{\text{true}} = \begin{bmatrix} 8 \\ 3 \\ 4 \end{bmatrix} \), \( x = M^+ b \approx \begin{bmatrix} 4.4 \\ 5.9 \\ 1.4 \end{bmatrix} \), and \( x = x_0 + M^+ (b - b_0) \approx \begin{bmatrix} 7.1 \\ 3.2 \\ 4.1 \end{bmatrix} \), it is clear that the least squares solution with \( ||x - x_0|| \) a minimum is a much better approximation to the true answer than the least squares solution of minimum norm.

5.0 CONCLUSIONS AND CONJECTURES

From the material presented in this paper it appears that for a physical problem leading to an underdetermined system of equations of the form
The least squares solution of minimum norm given by \( x = M^+ b \) may not be a good approximation to the true solution of the physical problem. This is due to the fact that even if the coordinates of \( x \) are restricted to be non-negative, there will still be infinitely many distinct least squares solutions of (1) having non-negative coordinates.

For certain classes of physical problems where a "model" \( x_0 \) can be calculated which is an actual solution of an ideal problem leading to the equation \( Mx_0 = b_0 \) and if \( x_0 \) has the property that its "shape" is representative of the shape of the true physical solutions \( x \) of similar problems involving no abnormalities, then \( x = x_0 + M^+(b - b_0) \) is a least squares solution of (1) which should provide a better approximation to the true solution of the physical problem than \( x = M^+ b \). Furthermore, if "local" abnormalities appear in \( x \), then the least squares solution of (1) having \( \| x - x_0 \| \) a minimum should still be much better than the least squares solution of minimum norm since without further information, the vector \( x \) should not be allowed to deviate any further than is necessary from its ideal or model value. An example of a local abnormality would be a tumor or tumors in a brain in a three-dimensional reconstruction problem. Another example is a local defect in the heart muscle uptake of a radionuclide.

In conclusion, it should be noted that the ideas and conclusions presented in this paper should be tested extensively before reaching any definite conclusion about their reliability in physical experiments involving noise. However, a reasonable conjecture is that the least squares solution having \( \| x - x_0 \| \) a minimum for a given model will almost always be a better estimate of the true solution to a physical problem than the least squares solution of minimum norm. Furthermore, as the number of equations decreases as compared to the number of unknowns, the alternative least squares solution presented in this paper should become even better when compared to the least squares solution of minimum norm.
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Bibliography


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