Int. J. Engng Ed. Vol. 12, No. 4, p. 309–314, 1996
Printed in Great Britain.

0949-149X/91 $3.00+0.00

A Note on Pseudo-inverse*

KAI MING YU
Department of Manufacturing Engineering, Hong Kong Polytechnic, Hong Kong

Undergraduate engineering mathematical courses oftentimes emphasize algorithms leading to solutions of particular problems. One such algorithm that is implemented aims to obtain solutions for a linear system of equations. The mathematical background addressing properly constrained, under-constrained and over-constrained conditions may not be studied in depth with respect to how these situations effect their respective solutions. As an example we consider the solutions of non-homogeneous systems where the number of equations can exceed or equal or is less than the number of unknowns. The three cases will be discussed in detail for the homogeneous and non-homogeneous systems. The pseudo-inverse for a matrix will be introduced and implemented extensively to solve the non-homogeneous system. Two principle applications of the pseudo-inverse will be developed. First, we will compute the conversion matrix for Euler operators implemented in geometric modelling; secondly, will be an alternate proof for the least square error property.

AUTHOR QUESTIONNAIRE

1. The paper discusses materials for a course in:
   Engineering Mathematics, Geometric Modelling (Euler operator section), and Machine Vision (least square error section).
2. Students of the following departments are taught in this course:
   General engineering discipline (mechanical, industrial, electrical, electronic, civil and structural).
3. Level of the course (year):
   First year undergraduate and master.
4. Mode of presentation:
   Lecture.
5. Is the material presented in a regular or elective course:
   Regular for undergraduate engineering mathematics, elective for master courses (Geometric modelling & machine vision).
6. Class or hours required to cover the material:
   1–2 hours. This depends on the subject lecturer.
7. Student homework or revision hours required for the materials:
   Nil. This depends on the subject lecturer.
8. Description of the novel aspects presented in your paper:
   Give a complete picture of solving systems of linear equation with pseudo-inverse.
9. The standard text recommended in the course, in addition to author's notes:
   E. Kreyszig, Advanced Engineering Mathematics, 7/e, John Wiley & Sons 1993.
10. The material is/is not covered in the text.
    The material in the paper is not covered in the text.

INTRODUCTION

SYSTEMS of linear equations play an important role in engineering problem solving. This is because non-linear models of the physical world are usually solved by approximate linear models, and the system characteristics are usually described by more than one variable. Examples include: solving multiple-input–multiple-output systems in modern control; finding optimal solutions; data fitting for reverse engineering; and calibrating cameras for machine vision, etc. In the undergraduate engineering mathematics courses, skills needed to solve a system of linear equations are taught under the linear algebra topic and usually stress techniques such as the Gaussian elimination method. The inter-relation between the properly constrained, under-constrained and over-constrained situations may not be covered in sufficient detail to allow the students to have an overall view. For example, solution of non-homogeneous systems with different numbers of equations and unknowns is sometimes avoided. This paper discusses how to obtain a complete range of the skills needed for solving a system of linear equations, including: homogeneous and non-homogeneous cases, and equal and different numbers of equations and unknowns. Two particular cases of applying the pseudo-inverse to solve non-homogeneous systems with different numbers of equations and unknowns are then explained in detail. The first case demonstrates how to obtain

* Accepted November 10, 1995

the conversion matrix for Euler operators in geometric modelling. A more natural solution based on the pseudo-inverse can be derived. A system of linear equations may be purposely over-constrained in practice, say in minimizing measurement errors by taking more than enough data. The second case gives an alternate proof of the least-squares error property of the pseudo-inverse. This proof, however, does not require the students to have a rich knowledge of linear algebra.

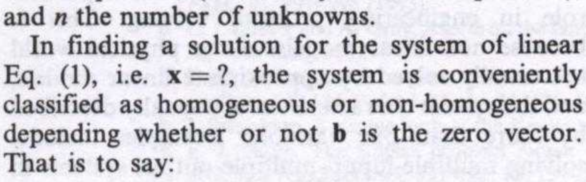
COMPLETE PICTURE OF SOLVING SYSTEM OF LINEAR EQUATIONS

A system of linear equations can be represented in matrix form,

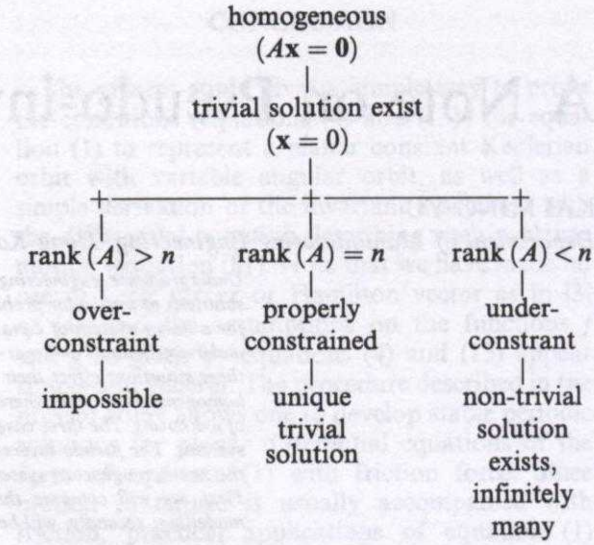
$$A\mathbf{x} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} = \mathbf{b},$$

where A is an $m \times n$ rectangular matrix, x is an $m \times 1$ column vector and $\mathbf{b}$ is an $m \times 1$ column vector. When A is square, i.e. $m = n$, vectors $\mathbf{x}$ and $\mathbf{b}$ will have the same number of rows, i.e. $m \times 1$. In addition, one can consider m as the number of linear equations (which may not be independent), and n the number of unknowns.

In finding a solution for the system of linear Eq. (1), i.e. $\mathbf{x} = ?$, the system is conveniently classified as homogeneous or non-homogeneous depending whether or not $\mathbf{b}$ is the zero vector. That is to say:



Homogeneous systems always have a trivial solution. Whether the trivial solution is unique or not depends on the rank of the matrix A. We recall the **rank** of a matrix A, denoted rank (A), is defined to be the maximum number of linearly independent row vectors of the matrix A. (The rank of zero matrix is defined to be zero.) An immediate property is that the rank of any matrix A cannot be greater than the number of rows, i.e. $\text{rank}(A) \leq m$. Thus, we use rank (A), the maximum number of **linearly independent** equations, rather than m, to differentiate the properly or over- and under-constraint cases. It can be proved that $\text{rank}(A) = \text{rank}(A^T)$ where A^T is the transpose of A [2: p. 158, Problem 10]. Since $\text{rank}(A^T) \leq n$, it follows that $\text{rank}(A) \leq n$. As a result, the over-constraint case with more independent equations than unknowns has no solution as $\text{rank}(A) > n$ is impossible.

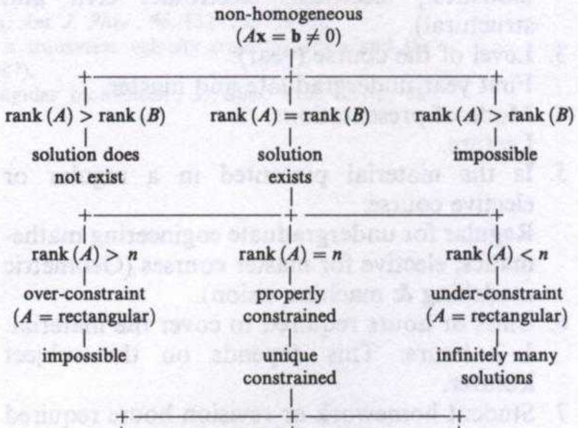


In the above diagram, matrix A is not classified as square or rectangular, as the solution method is determined by its rank. In the case when A is square, one can use its mathematical determinant to establish whether its inverse exists or not.

In solving non-homogeneous system, we need to form the augmented matrix, B, as

$$B = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} & b_m \end{bmatrix}.$$

Thus, the solution can be depicted as follows:



When rank $(A) = n$, it is clear that the case $m < n$ is impossible since $\text{rank}(A) \leq m$ in all situations. Moreover, as in the homogeneous system, there is no solution for the over-constrained case.

As shown in the previous diagram, the properly constrained case will have a unique solution. When A is a square matrix, the solution is $\mathbf{x} = A^{-1}\mathbf{b}$ where $A^{-1}\mathbf{b}$ is the inverse matrix.

When A is a rectangular matrix an alternate method can be implemented by introducing the

pseudo-inverse matrix or sometimes termed to be the **generalized inverse**. The pseudo-inverse is defined to be $A^+ = (A^TA)^{-1}A^T$ and it is immediate that $\mathbf{x} = (A^TA)^{-1}A^T\mathbf{b} = A^+\mathbf{b}$.

It can be verified by multiplying both sides of $\mathbf{x} = A^+\mathbf{b}$ with $(AA^T)^{-1}AA^TA$ to obtain $A\mathbf{x} = \mathbf{b}$. The pseudo-inverse exists if the inverse $(A^TA)^{-1}$ exists or if rank $(A^TA) = n$ (or the determinant of A^TA is non-zero). It can be proved that [2: pp. 158, 484, Problem 11] rank $(A^T) = n \Rightarrow$ rank $(A^TA) = n$. Since rank (A) = rank (A^T), rank (A) is used in the check for both the square and rectangular matrix cases. Note that the solution with the generalized pseudo-inverse can be found in references on applied linear algebra [2, 3].

CONVERSION MATRIX FOR EULER OPERATORS

In computer-aided design and manufacturing, boundary representation is one popular scheme used to represent solid models of physical objects. The topological information of the boundary model is represented by shells which are a composite of faces that bound a volume, faces, rings which are a composite of edges that bound a hole-area on faces, edges, vertices and through-holes or handles. The total number of these topological entities in a solid are denoted by S, F, R, E, V and H respectively and are found to obey the Euler–Poincaré equation: $V - E + F - R = 2(S - H)$ [4]. During a geometric modelling session, a valid topology is created or destroyed by performing Euler operations that are based on the Euler–Poincaré equation.

The Euler–Poincaré equation can be regarded as an equation of a hyperplane in a six-dimensional space. In the hyperspace, the coordinate tuple of any point is $\mathbf{P} = (V, E, F, R, S, G)$. The hyperplane can be seen to pass through the origin $\mathbf{O}$. Let $f(\mathbf{P}) = V - E + F - R - 2S + 2H = 0$ and the normal of the hyperplane is $\nabla \mathbf{f}$, then

$$V - E + F - R - 2S + 2H = \begin{bmatrix} V \\ E \\ F \\ R \\ S \\ H \end{bmatrix}^T \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \\ -1 \\ 2 \end{bmatrix}$$

$$= (\mathbf{P} - \mathbf{O}) \cdot \nabla \mathbf{f} = \mathbf{P}\nabla \mathbf{f} = 0.$$

Since only integral coordinates are possible, the hyperplane and hyperspace used are discrete grid and lattice, respectively.

To obtain the transition for creating or destroying a valid object, one needs to differentiate or take variation on the Euler equation, i.e.

$$\Delta V - \Delta E + \Delta F - \Delta R - 2\Delta S + 2\Delta H$$

$$= \begin{bmatrix} \Delta V \\ \Delta E \\ \Delta F \\ \Delta R \\ \Delta S \\ \Delta H \end{bmatrix}^n \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \\ -2 \\ 2 \end{bmatrix} = \Delta \mathbf{P} \cdot \nabla \mathbf{f} = 0.$$

The transition in a topological entity, $\Delta \mathbf{P}$, is restricted to the shortest displacement involving a null transition, unit increment or unit decrement along each axis, i.e. $\Delta = -1, 0, 1$.

As a 6-D hyperspace will have a 5-D hyperplane, five span vectors are needed to span the hyperplane. In other words, five primitive Euler operations are required to maintain the validity of the Euler–Poincaré equation.

Let A be a matrix of transition per Euler operation, $\mathbf{n}$ the vector representing the number of Euler operators being applied, and $\mathbf{t}$ the total resulted transition. Then, we have

$$A\mathbf{n} = \sum_{j=1}^{5} \begin{bmatrix} \Delta V_j \\ \Delta E_j \\ \Delta F_j \\ \Delta R_j \\ \Delta S_j \\ \Delta H_j \end{bmatrix} n_j$$

$$= \begin{bmatrix} \Delta V_1 & \Delta V_2 & \Delta V_3 & \Delta V_4 & \Delta V_5 \\ \Delta E_1 & \Delta E_2 & \Delta E_3 & \Delta E_4 & \Delta E_5 \\ \Delta F_1 & \Delta F_2 & \Delta F_3 & \Delta F_4 & \Delta F_5 \\ \Delta R_1 & \Delta R_2 & \Delta R_3 & \Delta R_4 & \Delta R_5 \\ \Delta S_1 & \Delta S_2 & \Delta S_3 & \Delta S_4 & \Delta S_5 \\ \Delta H_1 & \Delta H_2 & \Delta H_3 & \Delta H_4 & \Delta H_5 \end{bmatrix} \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \end{bmatrix}$$

$$= \begin{bmatrix} \Delta V \\ \Delta E \\ \Delta F \\ \Delta R \\ \Delta S \\ \Delta H \end{bmatrix} = \mathbf{t}.$$

Thus $\mathbf{n} = (A^TA)^{-1}A^T\mathbf{t}$ as A is rectangular where $(A^TA)^{-1}A^T$ is the pseudo-inverse.

Traditionally, people add the Euler–Poincaré equation to the last column of the transition matrix A to make it square. In this case, $\mathbf{n} = A^{-1}\mathbf{t}$ where A^{-1} is the inverse. We then have

$$An = \begin{bmatrix} \Delta V_1 & \Delta V_2 & \Delta V_3 & \Delta V_4 & \Delta V_5 & 1 \\ \Delta E_1 & \Delta E_2 & \Delta E_3 & \Delta E_4 & \Delta E_5 & -1 \\ \Delta F_1 & \Delta F_2 & \Delta F_3 & \Delta F_4 & \Delta F_5 & 1 \\ \Delta R_1 & \Delta R_2 & \Delta R_3 & \Delta R_4 & \Delta R_5 & -1 \\ \Delta S_1 & \Delta S_2 & \Delta S_3 & \Delta S_4 & \Delta S_5 & -2 \\ \Delta H_1 & \Delta H_2 & \Delta H_3 & \Delta H_4 & \Delta H_5 & 2 \end{bmatrix} \times \begin{bmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \\ 0 \end{bmatrix} = \begin{bmatrix} \Delta V \\ \Delta E \\ \Delta F \\ \Delta R \\ \Delta S \\ \Delta H \end{bmatrix} = \mathbf{t}.$$

For instance, if the set of Euler operators used is {MVFS, MVE, MEF, MEKR, MFKRH} [5] where M, K stands for makes (+1) and neutralized by (−1) respectively, then the transition matrix A can be written as

$$A = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \end{bmatrix}$$

or

$$A = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & -1 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & -1 & -1 & -1 \\ 0 & 0 & 1 & 0 & 0 & -2 \\ 0 & 0 & 0 & -1 & 0 & 2 \end{bmatrix}.$$

Note that rectangular A is properly constrained, i.e., $m = 6$, $n = 5$ and rank $(A) = 5$.

The pseudo-inverse and the inverse matrix are found to be

$$(A^T A)^{-1} A^T = \frac{1}{12} \begin{bmatrix} 9 & 3 & -3 & 3 & -6 & -6 \\ -5 & 5 & 7 & 5 & -2 & 2 \\ 2 & -2 & 2 & -2 & 8 & 4 \\ 2 & -2 & 2 & -2 & -4 & -8 \\ -3 & 3 & -3 & -9 & 6 & 6 \end{bmatrix}$$

and

$$A^{-1} = \frac{1}{12} \begin{bmatrix} 9 & 3 & -3 & 3 & -6 & -6 \\ -5 & 5 & 7 & 5 & -2 & 2 \\ 2 & -2 & 2 & -2 & 8 & 4 \\ 2 & -2 & 2 & -2 & -4 & -8 \\ -3 & 3 & -3 & -9 & 6 & 6 \\ 1 & -1 & 1 & -1 & -2 & 2 \end{bmatrix}.$$

As an example, to create a tetrahedron from null, the transition required is

$$\mathbf{t} = \begin{bmatrix} 4 \\ 6 \\ 4 \\ 0 \\ 1 \\ 0 \end{bmatrix}.$$

After substitution, the number of Euler operators to be applied is

$$\mathbf{n} = \begin{bmatrix} 3 \\ 3 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad \text{or} \quad \mathbf{n} = \begin{bmatrix} 3 \\ 3 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

That is, one application of MVFS, and three applications of MVE and MEF will construct the three-dimensional simplex.

Note that the addition of the Euler–Poincaré formula to matrix A is artificial. The calculations from square A or rectangular A are the same. In the former case, one needs to ensure that $n_6 = 0$ and then find the inverse of a 6×6 matrix. In the latter case, the formulation of the pseudo-inverse requires inverse of 5×5 square matrix only.

LEAST-SQUARE ERROR PROPERTY OF PSEUDO-INVERSE

In fitting observations $\mathbf{b}$ of order $m \times 1$ by some linear model of an $n \times 1$ parameters $\mathbf{x}$, the prediction is that the linear model will approximate the actual data. Then

$$b_i = \sum_{j=1}^{n} a_{ij} x_j + e_i, \qquad i = 1, m$$

or

$$\mathbf{b} = A\mathbf{x} + \mathbf{e}$$

where e_i are errors and $\mathbf{e}$ is the $m \times 1$ error vector.

In [3: p. 155], two geometric interpretations are used to show that the square error is the minimum one.

The vectors perpendicular to the column space lie in the left nullspace. Thus, the error vector $\mathbf{b} - A\mathbf{x}$ must be in the nullspace of A^T, which is to say:

$$A^T(\mathbf{b} - A\mathbf{x}) = 0.$$

The error vector must be perpendicular to every column of A ($A = [\mathbf{a}_1 \quad \mathbf{a}_2 \quad \cdots \quad \mathbf{a}_n]$) which is to say:

$$\mathbf{a}_1^T(\mathbf{b} - A\mathbf{x}) = 0$$

$$\mathbf{a}_n^T(\mathbf{b} - A\mathbf{x}) = 0$$

or

$$\begin{bmatrix} \mathbf{a}_1^T \\ \vdots \\ \mathbf{a}_n^T \end{bmatrix}(\mathbf{b}-A\mathbf{x}) = A^T(\mathbf{b}-A\mathbf{x}) = 0.$$

Since the magnitude of the error, $\|\mathbf{e}\| = \|\mathbf{b}-A\mathbf{x}\|$, is the distance from $\mathbf{b}$ to the point $A\mathbf{x}$ in the column space, the square of the perpendicular distance or the square error $\mathbf{e}^2 = (\mathbf{b}-A\mathbf{x})^T(\mathbf{b}-A\mathbf{x})$ is minimum.

The above proof is a geometrical one. However, it requires knowledge of vector spaces and in particular geometric interpretations of nullspace, column spaces, etc. An alternative is proposed and explained in detail in this section. Note that this new proof requires knowledge of elementary calculus and matrix algebra only.

First expand the square error equation

$$\begin{aligned}\sum_{i=1}^{m} e_i^2 &= \mathbf{e}^T\mathbf{e} \\ &= (\mathbf{b}-A\mathbf{x})^T(\mathbf{b}-A\mathbf{x}) \\ &= (\mathbf{b}^T-\mathbf{x}^TA^T)(\mathbf{b}-A\mathbf{x}) \\ &= \mathbf{b}^T\mathbf{b}-\mathbf{x}^TA^T\mathbf{b}-\mathbf{b}^TA\mathbf{x}+\mathbf{x}^TA^TA\mathbf{x}.\end{aligned}$$

Next, differentiate with respect to $\mathbf{x}$ both sides of the square error equation to obtain

$$\begin{aligned}\nabla(\mathbf{e}^T\mathbf{e}) &= \begin{bmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_n} \end{bmatrix}(\mathbf{e}^T\mathbf{e}) \\ &= \frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}(\mathbf{e}^T\mathbf{e}) \\ &= \frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\mathbf{b}^T\mathbf{b}-\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\mathbf{x}^TA^T\mathbf{b} \\ &\quad -\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\mathbf{b}^TA\mathbf{x}+\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\mathbf{x}^TA^TA\mathbf{x} \\ &= 0\mathbf{b}-IA^T\mathbf{b}-0A\mathbf{x}+IA^TA\mathbf{x} \\ &= -A^T\mathbf{b}+A^TA\mathbf{x}\end{aligned}$$

where 0 is an $n\times m$ zero matrix and I is an $n\times n$ identity matrix.

The least-square error will be the minimum turning point. That is,

$$\begin{cases} \dfrac{\partial}{\partial x_j}\mathbf{e}^T\mathbf{e} = 0 \\[2ex] \dfrac{\partial^2}{\partial x_j^2}\mathbf{e}^T\mathbf{e} > 0, \quad \forall j = 1, n. \end{cases}$$

Setting the gradient of $\mathbf{e}^T\mathbf{e} = 0$ ($n\times 1$ zero vector) implies $\mathbf{x} = A^+\mathbf{b} = (A^TA)^{-1}A^T\mathbf{b}$, where A^+ is the pseudo-inverse of A. To check that the pseudo-inverse will give the least-square error, the second differentiation with respect to $\mathbf{x}$ is taken. Now we have

$$\left(\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}(\mathbf{e}^T\mathbf{e})\right)^T = -\mathbf{b}^TA+\mathbf{x}^TA^TA$$

and therefore

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\left(\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}(\mathbf{e}^T\mathbf{e})\right)^T &= -\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\mathbf{b}^TA+\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\mathbf{x}^TA^TA \\ &= -0A+IA^TA \\ &= A^TA\end{aligned}$$

or

$$\begin{bmatrix} \frac{\partial^2}{\partial x_1^2} & \cdots & \frac{\partial^2}{\partial x_1\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial^2}{\partial x_n\partial x_1} & & \frac{\partial^2}{\partial x_n^2} \end{bmatrix}(\mathbf{e}^T\mathbf{e}) = \begin{bmatrix} \sum_{i=1}^{m} a_{i1}^2 & \cdots & \sum_{i=1}^{m} a_{i1}a_{in} \\ \vdots & \ddots & \vdots \\ \sum_{i=1}^{m} a_{in}a_{i1} & \cdots & \sum_{i=1}^{m} a_{in}^2 \end{bmatrix}.$$

By comparing the diagonal terms, one can see that they are all non-negative. Since none of the column vectors of matrix A is the zero vector, the diagonal terms can only be positive. Hence, the square errors will be the minimum ones.

CONCLUSIONS

The paper explains in detail how to obtain a complete picture of the solution of a system of linear equations. The decision-tree-like schematic diagrams are simple and easy to understand by first-year engineering students. Solution of a system of linear equations is usually taught in first-year engineering mathematics. Two cases to elaborate on the application and property of pseudo-inverses are also given. The first case illustrates the technique for solving a rectangular matrix system without the need to add any dummy column to make the matrix square. The second case provides an alternate proof of the important least-square error property of the pseudo-inverse. The proof assumes the students to have knowledge of elementary calculus rather than having undertaken a comprehensive linear algebra course.

Acknowledgement—The author would like to thank the Department of Manufacturing Engineering, Hong Kong Polytechnic University for assistance provided in the course of preparing this manuscript.

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Dr K. M. Yu graduated in mechanical engineering in 1985 and obtained a PhD in 1991 from the University of Hong Kong. He worked first as a consultant in the Research Center, and then as a Research Associate in the Department of Mechanical Engineering, Hong Kong University of Science and Technology until 1993. He joined the Department of Manufacturing Engineering, Hong Kong Polytechnic University to engage in full-time teaching and research. His research is mainly in the area of computer-aided design and manufacturing, and he has a number of publications in this area.