

REGRESSION AND THE MOORE-PENROSE PSEUDOINVERSE

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*To my Father and Mother
on their anniversary*

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PREFACE

For the past ten years, my professional interests have focused on various aspects of regression. It has been my experience that the pseudoinverse is a great unifying concept. It has helped me to understand, remember, and explain many classical results in statistical theory as well as to discover (and rediscover) some new ones.

This book was conceived as a hybrid monograph–textbook. As a text, it would be suitable for the equivalent of a two-quarter course. In teaching such a course, one could fill in the remainder of the year with additional material on (for example) multiple regression, nonlinear regression, large sample theory, and optimal experimental design for regression. For this purpose I have attempted to make the development didactic. On the other hand, most of the material comes from reasonably current periodical literature and a fair amount of the material is my own work (some already published, some not). Virtually all of the material deals with regression either directly (Chapters VI–IX) or as background (Chapters I–V). By restricting the domain of discourse we are able to pursue a leisurely pace and, I hope, to preserve a sense of unity throughout.

At the time the manuscript was completed there were, to my knowledge, no textbook treatments of the pseudoinverse. Since that time, two excellent complementary monographs have appeared containing treatments of the Moore–Penrose pseudoinverse in a more general setting. The first (Boullion and Odell [2]) appeared in early 1971 and concerns itself mainly with algebraic and structural properties of these pseudoinverses. The second (Rao and Mitra [1]) appeared later in 1971 and is extremely comprehensive in its coverage of the then extant pseudoinverse literature. Both volumes contain large bibliographies.

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The index for this book was sorted and alphabetized on our time-share computer terminal. I would like to thank Don Feinberg, who wrote the program, and Nancy Burkey, who fed the necessary information to the computer.

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Part I

**THE GENERAL THEORY
AND COMPUTATIONAL METHODS**

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INTRODUCTION

In 1920, Moore [1] introduced the notion of a generalized inverse for matrices. The idea apparently lay dormant for about 30 years, whereupon a renaissance of interest occurred. As may be appreciated after a brief look through the bibliography, a large and varied literature has appeared since the early 1950s.

At the present time, the theory is elegant, the applications are diverse (e.g., least squares, linear equations, projections, statistical regression analysis, filtering, and linear programming) and most important, a deeper understanding of these topics is achieved when they are studied in the generalized inverse context. The results that we present here are, for the most part, scattered throughout the periodical literature or to be found in out-of-print technical reports. This is the major impetus behind the writing of this monograph.

The level of the material presupposes a familiarity with the notion of "limit" and some of the fundamental properties of finite-dimensional Euclidean spaces. That much will suffice for the first half of the book. The second half is devoted to statistical applications and for these it would be helpful to have had a first course in probability (and/or statistics).

Many exercises are included. (Solution outlines are provided in a separate booklet.) Some of the exercises are supplementary to the material in the monograph, whereas others are lemmas to subsequent theorems. The reader

is urged to do the exercises. They are the key to a thorough understanding of the material.

Sections and equations are numbered according to a decimal system. For example, Eq. (6.3.1) comes after Section (6.2) and before Definition (6.3.1.9). The latter comes before Eq. (6.4). Every effort has been made to maintain the following typographical conventions:

Sets—uppercase script

Matrices—uppercase Latin

Vectors—lowercase Latin

Scalars—lowercase Greek

Vector random variables—lowercase boldface Latin

Real random variables—lowercase boldface Greek.

Bibliographic references are enclosed in square brackets; equation and section numbers are written in parentheses at the left. Sometimes a section or an equation number appears in the middle of a line or at the right side. In this case, the assertion preceding this equation number is a direct consequence of that (previously established) result.

GENERAL BACKGROUND MATERIAL

In this chapter, we will review the key results and definitions from the theory of real linear spaces which are relevant to what follows. This survey is informal and presumes previous exposure of the reader to these notions. (For a more formal review, see Appendix A of Karlin [1]. For a rigorous development, see Halmos [1] or the first half of Bellman [1].)

We begin by reminding the reader that linear transformations from one Euclidean space to another can be represented by matrices, once the coordinate systems for the two spaces have been decided upon. Furthermore, vectors can be represented as long, skinny matrices (having one column). If A is any matrix, we denote the transpose of A by A^T . In our discussions, all matrices, vectors (and scalars) have real entries. Matrix transposition has the following important properties:

$$(AB)^T = B^T A^T, \quad (A^T)^T = A, \quad (A+B)^T = A^T + B^T.$$

If x and y are two vectors having the same number of components, the *inner product* (or scalar product) of x with y is the scalar $x^T y$ (which is the same as $y^T x$). The *norm* of x is $\|x\| = (x^T x)^{1/2}$. Two vectors are said to be *orthogonal* if their inner product vanishes. (The statement, x is orthogonal to y is abbreviated $x \perp y$.)

A *linear manifold* \mathcal{L} is a nonempty subset of a Euclidean space, which is

closed under addition and scalar multiplication (if x and y are elements of \mathcal{L} then for any scalars α and β , $\alpha x + \beta y$ are members of \mathcal{L}).

A vector x is *orthogonal to the linear manifold* \mathcal{L} if x is orthogonal to every vector in \mathcal{L} (abbreviated $x \perp \mathcal{L}$).

The symbol \in will be reserved for set membership ($x \in \mathcal{L}$ means that x is a member of the set \mathcal{L}). The symbol \subseteq denotes set inclusion and \subset denotes proper inclusion.

The following theorem is of fundamental importance in all that follows. We state it without proof:

(2.1) Theorem: Let x be a vector in a finite-dimensional Euclidean space and let \mathcal{L} be a linear manifold in that space. Then there is a unique vector $\hat{x} \in \mathcal{L}$ having the property that $x - \hat{x} \perp \mathcal{L}$.

(2.1.1) *Comment:* An equivalent statement of the theorem is that there is a unique decomposition of x :

$$x = \hat{x} + \tilde{x}$$

where

$$\hat{x} \in \mathcal{L} \quad \text{and} \quad \tilde{x} \perp \mathcal{L}.$$

The vector \hat{x} is called the *projection of x on \mathcal{L}* . It is the vector in \mathcal{L} that is “nearest” to x , as we shall now demonstrate.

(2.2) Theorem: Let x be a vector and \mathcal{L} a linear manifold. If $x = \hat{x} + \tilde{x}$ where $\hat{x} \in \mathcal{L}$ and $\tilde{x} \perp \mathcal{L}$, then

$$\|x - y\| > \|x - \hat{x}\|$$

if

$$y \in \mathcal{L} \quad \text{and} \quad y \neq \hat{x}.$$

Proof: If $y \in \mathcal{L}$ then

$$\begin{aligned} \|x - y\|^2 &= \|\hat{x} + \tilde{x} - y\|^2 = \|(\hat{x} - y) + \tilde{x}\|^2 \\ &= \|\hat{x} - y\|^2 + \|\tilde{x}\|^2 \end{aligned}$$

since $\tilde{x} \perp \mathcal{L}$ and $\hat{x} - y \in \mathcal{L}$. Therefore

$$\|x - y\|^2 \geq \|\tilde{x}\|^2$$

with strict inequality holding unless $\|\hat{x} - y\|^2 = 0$. ■

Theorems (2.1) and (2.2) are “existence theorems.” As a consequence of the next theorem, we can show how to reduce the computation of \hat{x} to the solution

of simultaneous linear equations. First though, we remind the reader that a linear manifold \mathcal{L} is *spanned* by (y_1, y_2, \dots, y_n) if every vector in \mathcal{L} can be expressed as a linear combination of the y_j 's.

(2.3) Theorem: (a) If x is a vector and \mathcal{L} is a linear manifold, then \hat{x} , the projection of x on \mathcal{L} , is the unique vector in \mathcal{L} satisfying the equations

$$(2.3.1) \quad \hat{x}^T y = x^T y \quad \text{for all } y \in \mathcal{L}.$$

(b) If \mathcal{L} is spanned by y_1, y_2, \dots, y_n , \hat{x} is the unique vector in \mathcal{L} satisfying

$$(2.3.2) \quad \hat{x}^T y_j = x^T y_j \quad j = 1, 2, \dots, n.$$

Proof: Part (a) follows directly from (2.1). That \hat{x} satisfies (2.3.2) is a consequence of (a). If x^* is some other vector in \mathcal{L} satisfying

$$x^{*T} y_j = x^T y_j \quad j = 1, 2, \dots, n,$$

then

$$(2.3.3) \quad (x^* - \hat{x})^T y_j = 0 \quad j = 1, 2, \dots, n.$$

Since the y_j 's span \mathcal{L} , any vector in \mathcal{L} is a linear combination of the y_j 's, so that $x^* - \hat{x}$ is orthogonal to *every* vector in \mathcal{L} . Since $x^* - \hat{x} \in \mathcal{L}$, it follows that $(x^* - \hat{x})^T (x^* - \hat{x}) = \|x^* - \hat{x}\|^2 = 0$. Therefore, x^* must coincide with \hat{x} if it lies in \mathcal{L} and satisfies (2.3.2). ■

(2.4) Exercise: If \mathcal{L} is spanned by y_1, y_2, \dots, y_n , then \hat{x} is the unique vector of the form

$$\hat{x} = \sum_{j=1}^n \alpha_j y_j$$

where the α_j 's are any scalars satisfying the simultaneous set of linear equations

$$(2.4.1) \quad \sum_{j=1}^n \alpha_j (y_i^T y_j) = y_i^T x \quad i = 1, 2, \dots, n.$$

(2.5) Exercises

(2.5.1) If \mathcal{L} is spanned by y_1, y_2, \dots, y_n then $x \perp \mathcal{L}$ if x is orthogonal to each of the y_j 's.

(2.5.2) If x and y are vectors in the same Euclidean space, and \mathcal{L} is a linear manifold in that space, then the projection of $\alpha x + \beta y$ on \mathcal{L} is $\alpha \hat{x} + \beta \hat{y}$ where \hat{x} and \hat{y} are the projections of x and y on \mathcal{L} .

If y_1, y_2, \dots, y_n is a set of vectors in the same Euclidean space, we denote

the linear manifold spanned by the y_j 's by $\mathcal{L}(y_1, y_2, \dots, y_n)$. This manifold is the smallest manifold containing all the y_j 's and it consists, exactly, of all those vectors which are expressible as a linear combination of the y_j 's.

(2.5.3) The projection of x on $\mathcal{L}(y)$ is $(x^T y)y/\|y\|^2$ if $y \neq 0$.

If x, y_1, y_2, \dots, y_n is an arbitrary set of vectors in the same Euclidean space, a particularly simple relationship exists between \hat{x}_n , the projection of x on $\mathcal{L}(y_1, \dots, y_n)$, and \hat{x}_{n-1} , the projection of x on $\mathcal{L}(y_1, \dots, y_{n-1})$, provided that y_n is orthogonal to the previous y_j 's:

(2.6) Theorem: If x, y_1, \dots, y_n are vectors in the same Euclidean space and if $y_n \perp \mathcal{L}(y_1, \dots, y_{n-1})$ then

$$(2.6.1) \quad \hat{x}_n = \hat{x}_{n-1} + \begin{cases} 0 & \text{if } y_n = 0 \\ (x^T y_n)y_n/\|y_n\|^2 & \text{otherwise.} \end{cases}$$

Proof: Since $\hat{x}_{n-1} \in \mathcal{L}(y_1, \dots, y_{n-1})$, \hat{x}_n is clearly a member of $\mathcal{L}(y_1, \dots, y_n)$. It is readily verified that the right side of (2.6.1) satisfies (2.3.2), provided y_n is orthogonal to $\mathcal{L}(y_1, \dots, y_{n-1})$ (and in particular, orthogonal to \hat{x}_{n-1}). The conclusion follows from (2.3b). ■

As an immediate consequence we can derive the so-called Fourier expansion theorem:

(2.7) Theorem: If u_1, u_2, \dots, u_n are mutually orthogonal vectors of unit length and x is an arbitrary vector in the same Euclidean space, then \hat{x} , the projection of x on $\mathcal{L}(u_1, \dots, u_n)$ is given by

$$(2.7.1) \quad \hat{x} = \left(\sum_{j=1}^n u_j u_j^T \right) x,$$

$$(2.7.2) \quad \hat{x} = \sum_{j=1}^n (u_j^T x) u_j.$$

Comment: If the u_j 's are k -dimensional vectors, the expression $\sum_{j=1}^n u_j u_j^T$ is a $k \times k$ matrix, so that (2.7.1) is a representation of the matrix which projects x onto $\mathcal{L}(u_1, \dots, u_n)$. Equation (2.7.2), on the other hand, is an explicit representation of \hat{x} as a linear combination of the u_j 's.

If \mathcal{L}_1 and \mathcal{L}_2 are linear manifolds and $\mathcal{L}_1 \subseteq \mathcal{L}_2$, define $\mathcal{L}_2 - \mathcal{L}_1$ as the set of vectors in \mathcal{L}_2 which are orthogonal to \mathcal{L}_1 .

(2.7.3) **Exercise:** If $\mathcal{L}_1 \subseteq \mathcal{L}_2$, then $\mathcal{L}_2 - \mathcal{L}_1$ is a linear manifold.

(2.7.4) **Exercise:** Let x be a vector and suppose $\mathcal{L}_1 \subseteq \mathcal{L}_2$. Define \hat{x}_2 to be the projection of x on \mathcal{L}_2 , \hat{x}_{21} to be the projection of \hat{x}_2 on \mathcal{L}_1 , \hat{x}_1 to be the projection of x on \mathcal{L}_1 and \hat{x}_{21} to be the projection of x on $\mathcal{L}_2 - \mathcal{L}_1$.

Then

- (a) $\hat{x}_{21} = \hat{x}_1$. (The projection of x on \mathcal{L}_1 is obtainable by projecting x on \mathcal{L}_2 and then projecting that vector on \mathcal{L}_1).
- (b) $\hat{x}_2 = \hat{x}_1 + \tilde{x}_{21}$.
- (c) $\|x - \hat{x}_1\| \geq \|x - \hat{x}_2\|$ with strict inequality holding if \mathcal{L}_1 is a proper subset of \mathcal{L}_2 unless $x \in \mathcal{L}_1$.

(2.8) The Gram-Schmidt Orthogonalization Procedure

This procedure takes an arbitrary collection of vectors h_1, h_2, \dots, h_n and generates a set of mutually orthogonal vectors u_1, u_2, \dots, u_n , having the properties that

$$(2.8.1) \quad \mathcal{L}(u_1, u_2, \dots, u_j) = \mathcal{L}(h_1, h_2, \dots, h_j) \quad \text{for } j = 1, \dots, n$$

and

$$(2.8.2) \quad \|u_j\| = 1 \quad \text{if } u_j \neq 0 \quad j = 1, 2, \dots, n.$$

The Procedure

$$(2.8.3) \quad u_1 = \begin{cases} h_1 / \|h_1\| & \text{if } h_1 \neq 0 \\ 0 & \text{if } h_1 = 0. \end{cases}$$

For $j = 1, 2, \dots, n-1$, define

$$(2.8.4) \quad \hat{h}_{j+1} = \sum_{k=1}^j (h_{j+1}^T u_k) u_k$$

and

$$(2.8.5) \quad u_{j+1} = \begin{cases} (h_{j+1} - \hat{h}_{j+1}) / \|h_{j+1} - \hat{h}_{j+1}\| & \text{if } h_{j+1} - \hat{h}_{j+1} \neq 0 \\ 0 & \text{otherwise.} \end{cases}$$

The properties (2.8.1) and (2.8.2) are established by induction: The induction hypothesis is that

$$\mathcal{L}(u_1, u_2, \dots, u_j) = \mathcal{L}(h_1, \dots, h_j)$$

and

$$u_{j+1} \perp \mathcal{L}(u_1, \dots, u_j).$$

By definition of u_1 , $\mathcal{L}(u_1) = \mathcal{L}(h_1)$ and by (2.5.3), \hat{h}_2 is the projection of h_2 on $\mathcal{L}(u_1)$. By (2.1), $h_2 - \hat{h}_2 \perp \mathcal{L}(u_1)$ so that u_2 is orthogonal to $\mathcal{L}(u_1)$. This establishes the induction hypothesis for $j = 1$. If it is assumed that the hypothesis is true for all values of j up through k , then since u_{k+1} is a linear

combination of h_{k+1} and \hat{h}_{k+1} [which lies in $\mathcal{L}(u_1, \dots, u_k) = \mathcal{L}(h_1, \dots, h_k)$], we see that any vector which is a linear combination of u_1, \dots, u_{k+1} is also a linear combination of h_1, \dots, h_{k+1} . This means that $\mathcal{L}(u_1, \dots, u_{k+1}) \subseteq \mathcal{L}(h_1, \dots, h_{k+1})$.

On the other hand,

$$h_{k+1} = \|h_{k+1} - \hat{h}_{k+1}\| u_{k+1} + \hat{h}_{k+1}$$

the right side being a linear combination of the nonzero members of $\{u_1, u_2, \dots, u_{k+1}\}$. Since $\mathcal{L}(h_1, \dots, h_k) = \mathcal{L}(u_1, \dots, u_k)$ under the induction hypothesis, any vector which is expressible as a linear combination of h_1, \dots, h_{k+1} is also expressible as a linear combination of u_1, \dots, u_{k+1} . Therefore, $\mathcal{L}(h_1, \dots, h_{k+1}) \subseteq \mathcal{L}(u_1, \dots, u_{k+1})$. This establishes the first half of the induction hypothesis for $j = k + 1$.

The second half follows since \hat{h}_{k+2} is the projection of h_{k+2} on $\mathcal{L}(u_1, \dots, u_{k+1})$, (2.7.2). By (2.1), $h_{k+2} - \hat{h}_{k+2} \perp \mathcal{L}(u_1, \dots, u_{k+1})$ and therefore, so is u_{k+2} . ■

(2.8.6) **Exercise:** $u_j = 0$ if and only if h_j is a linear combination of (h_1, \dots, h_{j-1}) .

In what follows, two special linear manifolds will be of particular interest: If H is any matrix, the *null space* of H , denoted by $\mathcal{N}(H)$, is the set of vectors which H maps into zero:

$$\mathcal{N}(H) = \{x: Hx = 0\}.$$

[The null space of H , $\mathcal{N}(H)$, always has at least one element, namely the null vector 0.]

The *range* of H , denoted by $\mathcal{R}(H)$, is the set of vectors which are after-images of vectors in the Euclidean space which serves as the domain of H :

$$\mathcal{R}(H) = \{z: z = Hx \text{ for some } x\}$$

It is easy to see that $\mathcal{N}(H)$ and $\mathcal{R}(H)$ are linear manifolds.

(2.9) Exercises

(2.9.1) Let the column vectors of H be denoted by h_1, h_2, \dots, h_n . Show that $\mathcal{R}(H) = \mathcal{L}(h_1, h_2, \dots, h_n)$.

(2.9.2) Show that H^T is the *adjoint* of H . That is to say, if H is an $n \times m$ matrix, then for any m -dimensional vector, x and any n -dimensional vector y , the inner product of x with Hx is the same as the inner product of y with $H^T x$.

If \mathcal{L} is a linear manifold in a Euclidean space \mathcal{E} , the *orthogonal complement*

of \mathcal{L} (denoted by \mathcal{L}^\perp) is defined to be the set of vectors in \mathcal{E} which are (each) orthogonal to \mathcal{L} .

It is easy to see that \mathcal{L}^\perp is itself a linear manifold.

$$(2.9.3) \quad (\mathcal{L}^\perp)^\perp = \mathcal{L}.$$

$$(2.9.4) \quad \text{If } x \text{ is a vector in } \mathcal{E} \text{ and } x^\top y = 0 \text{ for all } y \in \mathcal{E}, \text{ then } x = 0.$$

The null space of a matrix is related to the range space of its transpose. In fact, the next theorem shows that the null space of H consists of those vectors which are orthogonal to the column vectors of H^\top (i.e., the rows of H) which is just another way of saying

(2.10) Theorem: For any matrix H , $\mathcal{N}(H) = \mathcal{R}^\perp(H^\top)$.

Proof: $x \in \mathcal{N}(H)$ if and only if $Hx = 0$. Therefore, $x \in \mathcal{N}(H)$ if and only if $y^\top Hx = 0$ for all y (having the correct number of components, of course). [Use (2.9.4).] Since $y^\top Hx = (H^\top y)^\top x$, we see that $Hx = 0$ if and only if x is orthogonal to all vectors of the form $H^\top y$. These vectors, collectively, make up $\mathcal{R}(H^\top)$, thus proving the assertion. ■

By applying the projection theorem (2.1), we deduce as an immediate consequence of (2.10), that every vector z (having the correct number of components) has a unique decomposition as the sum of two terms, one lying in $\mathcal{R}(H)$ and one lying in $\mathcal{N}(H^\top)$:

(2.11) Theorem: If H is an $n \times m$ matrix and z is an n -dimensional vector, we can uniquely decompose z :

$$z = \hat{z} + \tilde{z}$$

where $\hat{z} \in \mathcal{R}(H)$ and $\tilde{z} \in \mathcal{N}(H^\top)$.

(2.11.1) Exercise: In (2.11), \hat{z} is the projection of z on $\mathcal{R}(H)$ and \tilde{z} is the projection of z on $\mathcal{N}(H^\top)$. Consequently $H^\top z = H^\top \hat{z}$.

A matrix is said to be *symmetric* if it is equal to its transpose. Obviously, symmetric matrices are square.

(2.11.2) Exercise: Matrices of the form $H^\top H$ and HH^\top are always symmetric.

By virtue of (2.10),

$$(2.11.3) \quad \mathcal{N}(A) = \mathcal{R}^\perp(A) \quad \text{and} \quad \mathcal{R}(A) = \mathcal{N}^\perp(A)$$

if A is symmetric.

Moreover, if H is any matrix, then

(2.12) Theorem: $\mathcal{R}(H) = \mathcal{R}(HH^T)$, $\mathcal{R}(H^T) = \mathcal{R}(H^TH)$, $\mathcal{N}(H) = \mathcal{N}(H^TH)$, and $\mathcal{N}(H^T) = \mathcal{N}(HH^T)$.

Proof: It suffices to prove that $\mathcal{N}(H^T) = \mathcal{N}(HH^T)$ and $\mathcal{N}(H) = \mathcal{N}(H^TH)$. Then apply (2.10) and (2.9). To prove that $\mathcal{N}(H^T) = \mathcal{N}(HH^T)$, we note that $HH^Tx = 0$ if $H^Tx = 0$. On the other hand, if $HH^Tx = 0$, then $x^THH^Tx = 0$ so that $\|H^Tx\|^2 = 0$ which implies that $H^Tx = 0$. Thus $H^Tx = 0$ if and only if $HH^Tx = 0$. The same proof applies to show that $\mathcal{N}(H) = \mathcal{N}(H^TH)$. ■

A square matrix is *nonsingular* if its null space consists only of the zero vector. If a square matrix is not nonsingular, it is called *singular*.

(2.12.1) Exercise: If the row vectors of H are linearly independent, then the null space of H^T consists of the zero vector.

(2.12.2) Exercise: Let h_1, h_2, \dots, h_n be a linearly independent set of vectors. Let G be the $n \times n$ matrix whose $(i-j)$ th entry is $h_i^T h_j$ (G is known as a *Grammian*). Show that G is nonsingular. [Hint: $G = HH^T$ where H is the matrix whose rows are $h_1^T, h_2^T, \dots, h_n^T$. Now apply (2.12.1) and (2.12).]

If A is a nonsingular matrix, there is a unique matrix, A^{-1} , which is the left and right inverse of A :

$$A(A^{-1}) = (A^{-1})A = I$$

where I is the identity matrix.

(2.13) Theorem: If H is any matrix and δ is nonzero, then $H^TH + \delta^2 I$ is nonsingular.

Proof: If $(H^TH + \delta^2 I)x = 0$, then $0 = x^T(H^TH + \delta^2 I)x \stackrel{?}{=} \|Hx\|^2 + \delta^2 \|x\|^2$ which can only occur if $x = 0$. ■

We close this chapter with a statement of the celebrated diagonalization theorem for symmetric matrices. The proof may be found in Bellman [1].

A (possibly complex) number λ is called an *eigenvalue* of the (square) matrix A if $A - \lambda I$ is singular.

(2.13.1) Exercise: If A is real and symmetric, its eigenvalues are real. [Hint: If $(A - \lambda I)x = 0$, then $(A - \bar{\lambda} I)\bar{x} = 0$, where $\bar{\lambda}$ and \bar{x} are the complex conjugates of λ and x .]

(2.14) Theorem: If A is real and symmetric with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$,

then there is a matrix T such that $T^T = T^{-1}$ and

$$T^T A T = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n).$$

[The term $\text{diag}(\lambda_1, \dots, \lambda_n)$ refers to a diagonal matrix with entries $\lambda_1, \dots, \lambda_n$. If $T^T = T^{-1}$, T is said to be an *orthogonal* matrix.]

(2.14.1) **Exercise:** If T is an orthogonal matrix, the rows of T are mutually orthogonal and have unit length. So too, are the columns.

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GEOMETRIC AND ANALYTIC PROPERTIES OF THE MOORE-PENROSE PSEUDOINVERSE

We begin our treatment of the pseudoinverse by characterizing the minimum norm solution to the classical least squares problem:

(3.1) Theorem: Let z be an n -dimensional vector and let H be an $n \times m$ matrix.

(a) There is always a vector, in fact a unique vector \hat{x} of minimum norm, which minimizes

$$\|z - Hx\|^2.$$

(b) \hat{x} is the unique vector in $\mathcal{R}(H^T)$ which satisfies the equation

$$Hx = \hat{z}$$

where \hat{z} is the projection of z on $\mathcal{R}(H)$.

Proof: By (2.11) we can write

$$z = \hat{z} + \tilde{z}$$

where \tilde{z} is the projection of z on $\mathcal{N}(H^T)$. Since $Hx \in \mathcal{R}(H)$ for every x , it follows that

$$\hat{z} - Hx \in \mathcal{R}(H) \quad \text{and since} \quad \tilde{z} \in \mathcal{R}^\perp(H), \quad \tilde{z} \perp \hat{z} - Hx.$$

Therefore

$$\|z - Hx\|^2 = \|\hat{z} - Hx + \tilde{z}\|^2 = \|\hat{z} - Hx\|^2 + \|\tilde{z}\|^2 \geq \|\tilde{z}\|^2.$$

This lower bound is attainable since \hat{z} , being in the range of H , is the after-image of some x_0 :

$$\hat{z} = Hx_0.$$

Thus, for this x_0 , the bound is attained:

$$\|z - Hx_0\|^2 = \|z - \hat{z}\|^2 = \|\tilde{z}\|^2.$$

On the other hand, we just showed that

$$\|z - Hx\|^2 = \|\hat{z} - Hx\|^2 + \|\tilde{z}\|^2$$

so that the lower bound is attained at x^* only if x^* is such that $Hx^* = \hat{z}$. For any such x^* , we can decompose it via (2.11) into two orthogonal vectors:

$$x^* = \hat{x}^* + \tilde{x}^*$$

where

$$\hat{x}^* \in \mathcal{R}(H^T) \quad \text{and} \quad \tilde{x}^* \in \mathcal{N}(H).$$

Thus

$$Hx^* = H\hat{x}^* \quad \text{so that} \quad \|z - Hx^*\|^2 = \|z - H\hat{x}^*\|^2$$

and

$$\|x^*\|^2 = \|\hat{x}^*\|^2 + \|\tilde{x}^*\|^2 \geq \|\hat{x}^*\|^2$$

with strict inequality unless $x^* = \hat{x}^*$ [i.e., unless x^* coincides with its projection on $\mathcal{R}(H^T)$ —which is to say, unless $x^* \in \mathcal{R}(H^T)$ to begin with].

So far, we have shown that x_0 minimizes $\|z - Hx\|^2$ if and only if $Hx_0 = \hat{z}$, and that, among those vectors which minimize $\|z - Hx\|^2$, any vector of minimum norm must lie in the range of H^T . To demonstrate the uniqueness of this vector, suppose that \hat{x} and x^* both are in $\mathcal{R}(H^T)$ and that

$$H\hat{x} = Hx^* = \hat{z}.$$

Then

$$x^* - \hat{x} \in \mathcal{N}(H^T).$$

But

$$H(x^* - \hat{x}) = 0$$

so that

$$x^* - \hat{x} \in \mathcal{N}(H) = \mathcal{R}^\perp(H^T) \quad \text{as well.} \quad (2.10)$$

Thus $x^* - \hat{x}$ is orthogonal to itself, which means that $\|x^* - \hat{x}\|^2 = 0$ (i.e., $x^* = \hat{x}$). ■

(3.1.1) *Comment:* An alternate statement of (3.1) which is equivalent, but perhaps more illuminating is this:

There is always an n -dimensional vector y such that

$$\|z - HH^T y\|^2 = \inf_x \|z - Hx\|^2.$$

If

$$\|z - Hx_0\|^2 = \inf_x \|z - Hx\|^2$$

then $\|x_0\| \geq \|H^T y\|$, with strict inequality holding unless $x_0 = H^T y$. y satisfies the equation

$$HH^T y = \hat{z}$$

where \hat{z} is the projection of z on $\mathcal{R}(H)$.

(3.1.2) **Exercise:** $\|z - Hx\|^2$ is minimized by x_0 if and only if $Hx_0 = \hat{z}$, where \hat{z} is the projection of z on $\mathcal{R}(H)$.

The minimal least squares solution alluded to in (3.1) can be characterized as a solution to the so-called *normal equations*:

(3.2) **Theorem:** Among those vectors x , which minimize $\|z - Hx\|^2$, \hat{x} , the one having minimum norm, is the unique vector of the form

$$(3.2.1) \quad \hat{x} = H^T y$$

which satisfies

$$(3.2.2) \quad H^T Hx = H^T z.$$

Comment: The theorem says that \hat{x} can be obtained by finding any vector y_0 which satisfies the equation

$$H^T HH^T y = H^T z$$

and then taking

$$\hat{x} = H^T y_0.$$

Proof: By (2.12), $\mathcal{R}(H^T) = \mathcal{R}(H^T H)$. Since $H^T z$ is in the range of H^T , it must therefore be in the range of $H^T H$ and so, must be the afterimage of some x under the transformation $H^T H$. In other words, (3.2.2) always has at least one solution in x . If x is a solution to (3.2.2), so then is \hat{x} , the projection of x on $\mathcal{R}(H^T)$, since $Hx = H\hat{x}$, (2.11.1). Since $\hat{x} \in \mathcal{R}(H^T)$, it is the afterimage of some vector y under H^T :

$$\hat{x} = H^T y.$$

So far we have shown that there is at least one solution to (3.2.2) of the form (3.2.1). To show uniqueness, suppose

$$\hat{x}_1 = H^T y_1 \quad \text{and} \quad \hat{x}_2 = H^T y_2$$

both satisfy (3.2.2). Then

$$H^T H (H^T y_1 - H^T y_2) = 0$$

so that

$$H^T (y_1 - y_2) \in \mathcal{N}(H^T H) = \mathcal{N}(H) \quad (2.12)$$

which implies that

$$H H^T (y_1 - y_2) = 0.$$

Thus

$$(y_1 - y_2) \in \mathcal{N}(H H^T) = \mathcal{N}(H^T) \quad (2.12)$$

and so

$$\hat{x}_1 = H^T y_1 = H^T y_2 = \hat{x}_2.$$

Thus, there is *exactly one* solution to (3.2.2) of the form (3.2.1). If we can show that this solution also satisfies the equation

$$Hx = \hat{z}$$

where \hat{z} is the projection of z on $\mathcal{R}(H)$ then, by virtue of (3.1b) we will be done.

But, in (2.11.1) we showed that

$$(3.2.3) \quad H^T z = H^T \hat{z}.$$

In Theorem (3.1), we showed that there is a unique solution in $\mathcal{R}(H^T)$ to the equation

$$(3.2.4) \quad Hx = \hat{z}.$$

This (unique) solution therefore satisfies the equation

$$H^T Hx = H^T \hat{z}$$

as well. Since $H^T z = H^T \hat{z}$, (3.2.3), we see that the (unique) solution to (3.2.4) which lies in $\mathcal{R}(H^T)$ must coincide with \hat{x} , the unique solution to (3.2.2) which lies in $\mathcal{R}(H^T)$. In summary, the vector \hat{x} alluded to in the statement of (3.2) coincides exactly with the vector \hat{x} alluded to in (3.1). ■

We are now in a position to exhibit an explicit representation for the minimum norm solution to a least squares problem. A preliminary lemma is needed which, for the sake of continuity, is stated here and proven later:

(3.3) Lemma: For any real symmetric matrix A ,

$$P_A = \lim_{\delta \rightarrow 0} (A + \delta I)^{-1} A = \lim_{\delta \rightarrow 0} A(A + \delta I)^{-1}$$

always exists. For any vector z ,

$$\hat{z} = P_A z$$

is the projection of z on $\mathcal{R}(A)$.

(3.4) Theorem: For any $n \times m$ matrix H ,

$$(3.4.1) \quad H^+ = \lim_{\delta \rightarrow 0} (H^T H + \delta^2 I)^{-1} H^T$$

$$(3.4.2) \quad = \lim_{\delta \rightarrow 0} H^T (H H^T + \delta^2 I)^{-1}$$

always exists. For any n -vector z ,

$$\hat{x} = H^+ z$$

is the vector of minimum norm among those which minimize

$$\|z - Hx\|^2.$$

Comment: Henceforth, we use the symbol I to represent the identity matrix, whose dimensionality is to be understood from the context. For example, in the expression $H^T H + I$, we refer to the $m \times m$ identity, whereas in $H H^T + I$, we refer to the $n \times n$ identity.

Proof: Since

$$(H^T H H^T + \delta^2 H^T) = H^T (H H^T + \delta^2 I) = (H^T H + \delta^2 I) H^T$$

and since $(H H^T + \delta^2 I)$ and $(H^T H + \delta^2 I)$ have inverses when $\delta^2 > 0$, (2.13), it is clear that the right sides of (3.4.1) and (3.4.2) are equal if either exists.

Let z be a given n -dimensional vector, and decompose z into its projections on $\mathcal{R}(H)$ and $\mathcal{N}(H^T)$ according to (2.11);

$$z = \hat{z} + \tilde{z}.$$

Since

$$H^T z = H^T \hat{z} \quad (2.11.1)$$

and since $\hat{z} \in \mathcal{R}(H)$ must be the afterimage of some vector x_0 under H , we see that

$$(3.4.3) \quad \begin{aligned} (H^T H + \delta^2 I)^{-1} H^T z &= (H^T H + \delta^2 I)^{-1} H^T \hat{z} \\ &= (H^T H + \delta^2 I)^{-1} H^T H x_0. \end{aligned}$$

The limit of the last expression always exists and coincides with \hat{x}_0 , the projection of x_0 on $\mathcal{R}(H^T H)$, by virtue of (3.3). Since $\mathcal{R}(H^T) = \mathcal{R}(H^T H)$, (2.12), and since

$$\begin{aligned}\hat{z} &= Hx_0 \\ &= H\hat{x}_0\end{aligned}\tag{2.11.1}$$

we conclude that

$$\hat{x}_0 \equiv \lim_{\delta \rightarrow 0} (H^T H + \delta^2 I)^{-1} H^T z$$

always exists, is an element of $\mathcal{R}(H^T)$, and satisfies the relation

$$H\hat{x}_0 = \hat{z}$$

where \hat{z} is the projection of z on $\mathcal{R}(H)$. The desired conclusion follows directly from (3.1). ■

(3.5) Corollary: For any vector z , HH^+z is the projection of z on $\mathcal{R}(H)$ and $(I - HH^+)z$ is the projection of z on $\mathcal{N}(H^T)$. For any vector x , H^+Hx is the projection of x on $\mathcal{R}(H^T)$ and $(I - H^+H)x$ is the projection of x on $\mathcal{N}(H)$.

Proof: By (3.4.2), $HH^+ = \lim_{\delta \rightarrow 0} HH^T(HH^T + \delta^2 I)^{-1}$ and by (3.4.1), $H^+H = \lim_{\delta \rightarrow 0} (H^T H + \delta^2 I)^{-1} H^T H$. (3.3) tells us that HH^+z is therefore the projection of z on $\mathcal{R}(HH^T)$, which coincides with the projection of z on $\mathcal{R}(H)$, (2.12). Similarly, (3.3) and (2.12) imply that H^+Hx is the projection of x on $\mathcal{R}(H^T H) = \mathcal{R}(H^T)$.

Since $z - \hat{z}$ is the projection of z on $\mathcal{N}(H^T)$ if \hat{z} is the projection of z on $\mathcal{R}(H)$, (2.11), it follows that

$$z - HH^+z \quad \text{is the projection of } z \text{ on } \mathcal{N}(H^T).$$

By the same token,

$$(I - H^+H)x \quad \text{is the projection of } x \text{ on } \mathcal{N}(H). \quad \blacksquare$$

The matrix H^+ , which we explicitly define in (3.4), is the so-called “Moore–Penrose generalized inverse for H .” We will usually refer to it more familiarly as “the pseudoinverse of H .”

Corollary (3.5) is tremendously important and should be noted carefully. It expresses the four most fundamental projection operators in terms of pseudoinverses. The results of (3.4) are attributed (via a slightly different method of proof) to den Broeder and Charnes [1].

(3.5.1) Exercise: $H^+ = H^{-1}$ if H is square and nonsingular.

(3.5.2) **Exercise:** $H^+ = H^T(HH^T)^{-1}$ if the rows of H are linearly independent. [*Hint:* Apply (2.12.2) to show (HH^T) has an inverse. Then use (3.4.2).]

(3.5.3) **Exercise:** $H^+ = (H^TH)^{-1}H^T$ if the columns of H are linearly independent.

Before proceeding to the light task of milking these results for all they are worth, we pause to furnish the proof for Lemma (3.3), as promised:

Proof of (3.3): If A is any symmetric matrix and δ_0 is a nonzero scalar whose magnitude is less than the magnitude of A 's smallest nonzero eigenvalue, then for any δ with

$$0 < |\delta| < |\delta_0|$$

$(A + \delta I)$ is nonsingular and hence, for all such δ 's, $(A + \delta I)^{-1}$ exists.

If z is any vector, we write

$$z = \hat{z} + \tilde{z}$$

where

$$\hat{z} \in \mathcal{R}(A) \quad \tilde{z} \in \mathcal{N}(A) \quad (2.11)$$

and

$$Az = A\hat{z}. \quad (2.11.1)$$

Since $\hat{z} \in \mathcal{R}(A)$, we can write $\hat{z} = Ax_0$ for some x_0 and so

$$\begin{aligned} (A + \delta I)^{-1}Az &= (A + \delta I)^{-1}A\hat{z} \\ &= (A + \delta I)^{-1}A(Ax_0). \end{aligned}$$

From (2.14), the diagonalization theorem, we conclude that

$$A = TDT^T$$

where

$$D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$$

is the diagonal matrix of A 's eigenvalues and T is an orthogonal matrix:

$$T^T = T^{-1}.$$

Thus

$$(A + \delta I)^{-1}Az = (A + \delta I)^{-1}A^2x_0 = T(D + \delta I)^{-1}D^2T^Tx_0.$$

Element-by-element, it is plain to see that

$$\lim_{\delta \rightarrow 0} (D + \delta I)^{-1}D^2 = D$$

so that

$$\lim_{\delta \rightarrow 0} (A + \delta I)^{-1} A z = T D T^T x_0 = A x_0 = \hat{z}$$

the projection of z on $\mathcal{R}(A)$.

The same argument works for $\lim_{\delta \rightarrow 0} A(A + \delta I)^{-1} z$. ■

In (3.5.1)–(3.5.3), formulas for H^+ in terms of inverses were given for the case where the rows and/or the columns of H are linearly independent. There are cases though where these conditions need not obtain:

$$H = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

In such cases, H^+ does not have a simple formula in terms of inverses. However, a better understanding of H^+ can be had by treating, in turn, the following cases: H a 1×1 matrix, H diagonal, H symmetric, H rectangular:

If H is a 1×1 (scalar) matrix, then

$$H^+ = \lim_{\delta^2 \rightarrow 0} (H^2 + \delta^2 I) H = \begin{cases} 0 & \text{if } H = 0 \\ 1/H & \text{if } H \neq 0. \end{cases}$$

If H is diagonal:

$$H = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_m)$$

then

$$H^+ = \text{diag}(\lambda_1^+, \lambda_2^+, \dots, \lambda_m^+)$$

where

$$\lambda_j^+ = \begin{cases} 0 & \text{if } \lambda_j = 0 \\ 1/\lambda_j & \text{if } \lambda_j \neq 0. \end{cases}$$

In terms of least squares, this makes sense, for if

$$z = \begin{pmatrix} \zeta_1 \\ \vdots \\ \zeta_n \end{pmatrix} \quad H = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$$

and

$$x = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix}$$

is to be chosen to minimize

$$\|z - Hx\|^2 = \sum_{j=1}^n (\zeta_j - \lambda_j \xi_j)^2$$

it is clear that the choice

$$\xi_j^* = \begin{cases} \zeta_j/\lambda_j & \text{if } \lambda_j \neq 0 \\ \text{arbitrary} & \text{if } \lambda_j = 0 \end{cases}$$

will minimize the sum of squares, and that

$$\|x^*\|^2 = \sum_{j=1}^n \xi_j^{*2}$$

is made smallest when

$$\xi_j^* = 0 \quad \text{if } \lambda_j = 0.$$

Thus, the minimum norm solution for the case of a diagonal H is

$$\hat{x} = \begin{pmatrix} \hat{\xi}_1 \\ \vdots \\ \hat{\xi}_n \end{pmatrix}$$

where

$$\hat{\xi}_j = \lambda_j^+ \zeta_j; \quad \text{i.e.,} \quad \hat{x} = H^+ z.$$

(3.6) The Special Case of Symmetric Matrices

If H is a symmetric $m \times m$ matrix, the diagonalization theorem allows us to write

$$H = TDT^T$$

where T is an orthogonal matrix and D is diagonal.

By (3.4),

$$\begin{aligned} H^+ &= \lim_{\delta \rightarrow 0} T(D^2 + \delta^2 I)^{-1} DT^T \\ &= T[\lim_{\delta \rightarrow 0} (D^2 + \delta^2 I)^{-1} D] T^T \\ &= TD^+ T^T. \end{aligned}$$

Thus, the pseudoinverse for a symmetric matrix is obtained by pseudo-inverting the diagonal matrix of its eigenvalues. Since H is nonsingular if and only if its eigenvalues are nonzero (in which case $D^+ = D^{-1}$), we see that

$$H^+ = TD^{-1}T^T$$

if H is symmetric and nonsingular: Since $TT^T = T^T T = I$, it is easy to see that $HH^+ = H^+H = I$ in this case, so that $H^+ = H^{-1}$.

The last result can be expressed in a different notation, and gives rise to various so-called spectral representation theorems [cf. (3.15)]: If the column vectors of T are denoted by t_i ($i = 1, \dots, m$), so that we can write T as a partitioned matrix,

$$T = (t_1 \vdots t_2 \vdots \cdots \vdots t_m)$$

the diagonalization theorem states that

$$(3.6.1) \quad H = TDT^T \equiv \sum_{j=1}^m \lambda_j t_j t_j^T.$$

Furthermore, since

$$T^T T = I$$

this tells us that

$$t_i^T t_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

so that the columns of T are *orthonormal* (mutually orthogonal with unit length). Furthermore,

$$HT = TDT^T T = TD$$

which can be read column by column as

$$Ht_j = \lambda_j t_j \quad j = 1, 2, \dots, m.$$

Thus, each t_j is an *eigenvector* of H associated with the eigenvalue λ_j . If the λ_j 's are not all distinct, the t_j 's are mutually orthogonal nonetheless.

The fact that

$$H^+ = TD^+ T^T$$

can be expressed as

$$(3.6.2) \quad H^+ = \sum_{j=1}^m \lambda_j^+ t_j t_j^T.$$

(3.7) Exercises

(3.7.1) Let H be an $m \times m$ symmetric matrix and suppose the nonzero eigenvalues of H are $\lambda_1, \lambda_2, \dots, \lambda_k$ ($k \leq m$).

(a) Show that there is a representation for H of the form

$$H = TDT^T$$

where

$$D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_k, \overbrace{0, \dots, 0}^{m-k \text{ zeros}})$$

and T is an orthogonal matrix. (*Hint*: If D is not arranged properly, use a permutation matrix, which is always orthogonal, to do so.)

(b) If the columns of T are denoted by t_1, t_2, \dots, t_m , show that

$$\mathcal{R}(H) = \mathcal{L}(t_1, \dots, t_k) \quad \text{and} \quad \mathcal{N}(H) = \mathcal{L}(t_{k+1}, \dots, t_m).$$

(3.7.2) Without appealing to the diagonalization theorem, show directly that if H is symmetric and if $Hx = \lambda_1 x$ and $Hy = \lambda_2 y$ then $x \perp y$ if $\lambda_1 \neq \lambda_2$.

The representation (3.6.2) is particularly interesting since it clearly shows the radically discontinuous nature of pseudoinversion. Two matrices may be very close to each other element by element. However, if their ranks differ (e.g., if one is singular, while the other is nonsingular) their pseudoinverses usually differ greatly. For example, the diagonal matrices

$$D_1 = \begin{pmatrix} 4 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad D_2 = \begin{pmatrix} 4 & 0 \\ 0 & 10^{-10} \end{pmatrix}$$

are close to each other, but

$$D_1^+ = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad D_2^+ = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & 10^{10} \end{pmatrix}$$

differ greatly. In terms of (3.6.2), it is easy to understand why, since the transformation

$$\lambda^+ = \begin{cases} 1/\lambda & \text{if } \lambda \neq 0 \\ 0 & \text{if } \lambda = 0 \end{cases}$$

exhibits an infinite discontinuity at $\lambda = 0$. This characteristic induces serious computational difficulties which we will discuss at the appropriate time.

In (3.8), we will see that the pseudoinverse of an arbitrary rectangular matrix is expressible in terms of the pseudoinverse of symmetric matrices:

$$\begin{aligned} H^+ &= (H^T H)^+ H^T \\ &= H^T (H H^T)^+ \end{aligned}$$

so that one can, in theory, diagonalize symmetric matrices (for which well-known algorithms are available) and proceed directly to pseudoinversion from there. However, there are other, less tedious methods for computing H^+ (Chapter V). The problem of round-off is quite serious, as the reader may have already come to appreciate.

(3.7.3) Let H be an $n \times m$ matrix and let x_1, x_2, \dots, x_r , $r \leq m$ be an orthonormal set of n -dimensional vectors such that

$$\mathcal{R}(H) = \mathcal{L}(x_1, x_2, \dots, x_r).$$

Then

$$HH^+ = \sum_{j=1}^r x_j x_j^T.$$

[Hint: Use (3.5) and (2.7).]

A symmetric matrix P is called a *projection matrix* if it is idempotent (i.e., $P^2 = P$).

(3.7.4) The eigenvalues of a projection matrix are either zero or unity.

(3.7.5) If P is a projection matrix, $P^+ = P$ and Px is the projection of x on $\mathcal{R}(P)$. If $x \in \mathcal{R}(P)$, then $Px = x$.

(3.7.6) HH^+ , H^+H , $I - HH^+$, and $I - H^+H$ are projection matrices.

(3.7.7) If P_1, P_2, \dots, P_n are projection matrices having the property that $P_i P_j = 0$ if $i \neq j$ and if P is another projection such that

$$\mathcal{R}(P) = \mathcal{R}\left(\sum_{j=1}^n P_j\right) \quad \text{then} \quad P = \sum_{j=1}^n P_j.$$

[Hint: First show that $Q \equiv \sum_{j=1}^n P_j$ is a projection matrix. Then $Q^+ = Q$ and so $QQ^+x = Qx$ which is the projection of x on $\mathcal{R}(Q)$. On the other hand, $PP^+x = Px$ is the projection of x on the range of P . Since $\mathcal{R}(P) = \mathcal{R}(Q)$, we have $Px = Qx$ for all x .]

(3.7.8) Let h_1, h_2, \dots, h_n be a set of vectors and let \hat{H} be the matrix whose column vectors are h_1, h_2, \dots, h_n . Then for any x , $\hat{H}\hat{H}^+x$ is the projection of x on $\mathcal{L}(h_1, h_2, \dots, h_n)$.

(3.7.9) If H is any matrix, then $Hx = 0$ if and only if $x = (I - H^+H)y$ for some y .

(3.7.10) If H is any matrix, then $z \in \mathcal{R}(H)$ if and only if $z = HH^+u$ for some u .

We now turn our attention to an exploration of the most important properties of H^+ .

(3.8) Theorem: For any matrix H ,

$$(3.8.1) \quad H^+ = (H^T H)^+ H^T$$

$$(3.8.2) \quad (H^T)^+ = (H^+)^T$$

$$(3.8.3) \quad H^+ = H^T(HH^T)^+.$$

Proof

$$(H^T H)^+ H^T = \{\lim_{\delta \rightarrow 0} [(H^T H)^2 + \delta^2 I]^{-1} (H^T H)\} H^T$$

and

$$H^+ = \lim_{\delta \rightarrow 0} [H^T H + \delta^2 I]^{-1} H^T. \quad (3.4)$$

By (2.11), any vector z can be written as

$$z = Hx_0 + \tilde{z} \quad \text{for some } x_0$$

where

$$H^T \tilde{z} = 0.$$

Thus

$$(3.8.4) \quad (H^T H)^+ H^T z = \lim_{\delta \rightarrow 0} [(H^T H)^2 + \delta^2 I]^{-1} (H^T H)^2 x_0$$

and

$$(3.8.5) \quad H^+ z = \lim_{\delta \rightarrow 0} [H^T H + \delta^2 I]^{-1} H^T H x_0.$$

Using the diagonalization theorem (2.14), we write

$$H^T H = T D T^T$$

where D is diagonal and T is orthogonal. Equation (3.8.4) takes the form

$$(H^T H)^+ H^T z = T \{\lim_{\delta \rightarrow 0} [D^2 + \delta^2 I]^{-1} D^2\} T^T x_0$$

while (3.8.5) takes the form

$$H^T z = T \{\lim_{\delta \rightarrow 0} [D + \delta^2 I]^{-1} D\} T^T x_0.$$

For diagonal D 's, the matrices in braces are the same, which proves (3.8.1).

To prove (3.8.2), notice that $(HH^T + \delta^2 I)^{-1}$ is symmetric so by (3.4.1),

$$\begin{aligned} (H^T)^+ &= \lim_{\delta \rightarrow 0} (HH^T + \delta^2 I)^{-1} H \\ &= \lim_{\delta \rightarrow 0} [H^T (HH^T + \delta^2 I)^{-1}]^T \\ &= (H^+)^T. \end{aligned} \quad (3.4.2)$$

To prove (3.8.3), we use (3.8.2) to establish that

$$(3.8.6) \quad [(H^T)^+]^T = H^+$$

and (3.8.1) to establish that

$$(3.8.7) \quad (H^T)^+ = (HH^T)^+ H.$$

Since $(HH^T)^+$ is symmetric, (3.8.3) follows from (3.8.6) after taking transposes in (3.8.7). ■

In his paper of 1955, which was probably responsible for the rebirth of interest in the topic of generalized inverses, Penrose [1], characterized the pseudoinverse as the (unique) solution to a set of matrix equations. The pseudoinverse H^+ that we have been investigating satisfies the Penrose conditions:

(3.9) Theorem: For any matrix H , $B = H^+$ if and only if

$$(3.9.1) \quad HB \text{ and } BH \text{ are symmetric}$$

$$(3.9.2) \quad HBH = H$$

$$(3.9.3) \quad BHB = B.$$

Proof of necessity

$$HH^+ = \lim_{\delta \rightarrow 0} HH^T(HH^T + \delta^2 I)^{-1}$$

and

$$H^+H = \lim_{\delta \rightarrow 0} (H^TH + \delta^2 I)^{-1} H^TH. \quad (3.4)$$

Both are symmetric. This shows that H^+ satisfies (3.9.1). By (3.5), HH^+ is the projection on $\mathcal{R}(H)$. Since $Hx \in \mathcal{R}(H)$ for all x , (3.7.5) assures that $(HH^+)(Hx) = Hx$. This shows that H^+ satisfies (3.9.2). By (3.8.1),

$$(3.9.4) \quad H^+H = (H^TH)^+(H^TH).$$

By (3.8.1) and (3.9.2)

$$\begin{aligned} H^+ &= (H^TH)^+ H^T = (H^TH)^+ [H(H^+H)]^T \\ &= (H^TH)^+ H^T (HH^+)^T. \end{aligned}$$

Since HH^+ is symmetric, (3.7.6),

$$H^+ = (H^TH)^+ H^T (HH^+) = (H^TH)^+ (H^TH) H^+$$

and by (3.9.4), the last is equal to

$$(H^+H)H^+.$$

This establishes (3.9.3).

Proof of sufficiency: Suppose B satisfies (3.9.1)–(3.9.3):
Since

$$\begin{aligned} BH &= (BH)^T \quad \text{and} \quad H = HBH \\ H &= HBH = HH^T B^T. \end{aligned}$$

Since

$$\begin{aligned} HH^+ H &= H \\ H^+ H &= H^+ (HH^T B^T) = [H(H^+ H)]^T B^T \end{aligned}$$

and so

$$(3.9.5) \quad H^+ H = H^T B^T = BH.$$

Since $B = BHB$ and since HB is symmetric,

$$(3.9.6) \quad B^T = HBB^T.$$

Premultiplying (3.9.6) by HH^+ , we find that

$$HH^+ B^T = HH^+ HBB^T = HBB^T \quad (3.9.2)$$

and by (3.9.6) the last is equal to B^T . Thus

$$(3.9.7) \quad B^T = (HH^+) B^T.$$

Taking transposes in (3.9.7), we find that

$$B = B(HH^+)^T = (BH) H^+$$

and by (3.9.5) we finally conclude that

$$B = H^+ HH^+.$$

Since $H^+ HH^+ = H^+$, we see that

$$B = H^+. \quad \blacksquare$$

The Penrose characterization for pseudoinverses is extremely useful as a method for proving identities. For instance, if one thinks that a certain expression coincides with the pseudoinverse of a certain matrix H , a handy way of deciding is to run the expression through conditions (3.9.1)–(3.9.3) and observe whether or not they hold.

(3.10) Exercise: If A and B are nonsingular, it is well known that $(AB)^{-1} = B^{-1}A^{-1}$. Use (3.9) to show that it is not generally true that $(AB)^+ = B^+A^+$. Where do the conditions break down? Exhibit a counterexample. [See (4.10)–(4.16) for a detailed study of this problem.]

(3.11) Exercise: Prove the following:

$$(3.11.1) \quad (H^+)^+ = H.$$

$$(3.11.2) \quad (H^T H)^+ = H^+ (H^T)^+ \quad \text{and} \quad (H H^T)^+ = (H^T)^+ H^+.$$

$$(3.11.3) \quad \text{If } A \text{ is symmetric and } \alpha > 0, \text{ then } (A^\alpha)^+ = (A^+)^{\alpha} \\ \text{and } A^\alpha (A^\alpha)^+ = (A^+)^{\alpha} A^\alpha = A A^+.$$

$$(3.11.4) \quad (H^T H)^+ = H^+ (H H^T)^+ H = H^T (H H^T)^+ (H^T)^+.$$

$$(3.11.5) \quad \mathcal{R}(H^+) = \mathcal{R}(H^+ H) = \mathcal{R}(H^T); \\ \mathcal{N}(H) = \mathcal{N}(H^+ H) = \mathcal{N}[(H^T H)^+].$$

$$(3.11.6) \quad \text{If } A \text{ is symmetric, } A A^+ = A^+ A.$$

$$(3.11.7) \quad H H^+ = (H H^T)(H H^T)^+ = (H H^T)^+ (H H^T) \\ \text{and } H^+ H = (H^T H)(H^T H)^+ = (H^T H)^+ (H^T H).$$

$$(3.11.8) \quad \text{If } A \text{ is symmetric and } \alpha > 0, \quad A^+ A^\alpha = A^\alpha A^+.$$

$$(3.11.9) \quad \text{If } H \text{ is a nonzero } n \times 1 \text{ matrix (a column vector) } H^+ = H^T / H^T H \\ \text{and } H H^+ = H H^T / \|H\|^2.$$

The properties of pseudoinverses and projections which we have developed can be readily applied to the theory of least squares subject to constraints. But first, we summarize the general results for unconstrained least squares and the related theory of linear equations, in the language of pseudoinverses:

(3.12) Theorem: (a) x_0 minimizes

$$(3.12.1) \quad \|z - Hx\|^2$$

if and only if x_0 is of the form

$$(3.12.2) \quad x_0 = H^+ z + (I - H^+ H)y$$

for some y .

(b) The value of x which minimizes (3.12.1) is unique if and only if $H^+ H = I$. The last is true if and only if zero is the only null vector of H .

(c) The equation

$$(3.12.3) \quad Hx = z$$

has a solution if and only if

$$H H^+ z = z.$$

The last is true if and only if $z \in \mathcal{R}(H)$. x_0 is a solution to (3.12.3) if and only if it is of the form (3.12.2). Equation (3.12.3) has a unique solution ($= H^+ z$) if and only if $H H^+ z = z$ and $H^+ H = I$.

Proof: (a) $\|z - Hx\|^2$ is minimized by x_0 if and only if $Hx_0 = \hat{z}$, where \hat{z} is the projection of z on $\mathcal{R}(H)$, (3.12). By (3.4), H^+z minimizes $\|z - Hx\|^2$ so that $Hx_0 = H(H^+z)$. This means that $x_0 - H^+z$ is a null vector of H if x_0 minimizes (3.12.1). The last is true if and only if

$$x_0 - H^+z = (I - H^+H)y \quad \text{for some } y. \quad (3.7.9)$$

Conversely, if x_0 has the form (3.12.2), then $Hx_0 = H(H^+z)$ since $H(I - H^+H) = 0$, (3.9.2). This proves part (a).

(b) The value of x which minimizes (3.12.1) is unique if and only if $(I - H^+H)y$ vanishes for all y . This can only happen if the projection of all vectors on $\mathcal{N}(H)$ is zero, which means that $\mathcal{N}(H)$ consists only of the zero vector. $(I - H^+H)y = 0$ for all y , by the way, if and only if $H^+H = I$. This proves (b).

(c) Equation (3.12.3) has a solution if and only if z is the afterimage of some x under H . This is, by definition, the same as saying $z \in \mathcal{R}(H)$. By virtue of (3.7.10), the last holds true if and only if

$$z = HH^+u$$

for some u . Since HH^+ is a projection, (3.7.6), it follows that

$$HH^+z = (HH^+)^2u = HH^+u = z.$$

When (3.12.3) has a solution x_0 , this solution must minimize $\|z - Hx\|^2$ (the minimal value in this case being zero) and so x_0 must be of the form (3.12.2). The solution is unique if and only if $H^+H = I$ [part (b)] and these conclusions collectively serve to establish (c). ■

(3.12.4) **Corollary:** Let G be a rectangular matrix and suppose u is a vector in $\mathcal{R}(G)$. Then

(a) $\mathcal{S} = \{x: Gx = u\}$ is nonempty and x_0 minimizes $\|z - Hx\|^2$ over \mathcal{S} if and only if

$$x_0 = G^+u + \bar{H}^+\bar{z} + (I - G^+G)(I - \bar{H}^+\bar{H})y$$

for some y , where

$$\bar{z} = z - HG^+u \quad \text{and} \quad \bar{H} = H(I - G^+G).$$

(b) The vector of minimum norm among those which minimize $\|z - Hx\|^2$ over \mathcal{S} is

$$G^+u + \bar{H}^+\bar{z}.$$

Proof: (a) If $u \in \mathcal{R}(G)$ then by (3.12), \mathcal{S} is nonempty and

$$\mathcal{S} = \{x: x = G^+u + (I - G^+G)v \text{ for some } v\}.$$

Therefore

$$\min_{x \in \mathcal{S}} \|z - Hx\| = \min_v \|\bar{z} - \bar{H}v\|.$$

The latter minimum occurs at v_0 if and only if

$$v_0 = \bar{H}^+ \bar{z} + (I - \bar{H}^+ \bar{H})y \quad \text{for some } y \quad (3.12a)$$

so that x_0 minimizes $\|z - Hx\|$ over \mathcal{S} if and only if

$$x_0 = G^+u + (I - G^+G)[\bar{H}^+ \bar{z} + (I - \bar{H}^+ \bar{H})y] \quad \text{for some } y.$$

Since

$$\bar{H}^+ = \bar{H}^T(\bar{H}\bar{H}^T)^+ \quad (3.8.3)$$

and since

$$(I - G^+G)^2 = (I - G^+G) = (I - G^+G)^T \quad (3.7.6)$$

it follows that

$$(3.12.4.1) \quad (I - G^+G)\bar{H}^+ = (I - G^+G)^2\bar{H}^T(\bar{H}\bar{H}^T)^+ = \bar{H}^+$$

and so it is clear that any value of x which minimizes $\|z - Hx\|$ over \mathcal{S} is of the form

$$x_0 = G^+u + \bar{H}^+ \bar{z} + (I - G^+G)(I - \bar{H}^+ \bar{H})y$$

for some y .

(b) $[(I - G^+G)(I - \bar{H}^+ \bar{H})y]^T G^+u = y^T(I - \bar{H}^+ \bar{H})(I - G^+G)G^+u$ since $(I - G^+G)$ and $I - \bar{H}^+ \bar{H}$ are symmetric. The last is zero since $(I - G^+G)G^+ = G^+ - G^+GG^+ = 0$. Thus

$$(3.12.4.2) \quad (I - G^+G)(I - \bar{H}^+ \bar{H})y \perp G^+u.$$

On the other hand,

$$\begin{aligned} [(I - G^+G)(I - \bar{H}^+ \bar{H})y]^T \bar{H}^+ \bar{z} &= y^T(I - \bar{H}^+ \bar{H})(I - G^+G)\bar{H}^+ \bar{z} \\ &= y^T(I - \bar{H}^+ \bar{H})\bar{H}^+ \bar{z}. \end{aligned} \quad (3.12.4.1)$$

Since $\bar{H}^+ - \bar{H}^+ \bar{H}\bar{H}^+ = 0$, we see that $(I - G^+G)(I - \bar{H}^+ \bar{H})y \perp \bar{H}^+ \bar{z}$ as well, so that if x_0 minimizes $\|z - Hx\|^2$ over \mathcal{S} , then

$$\begin{aligned} \|x_0\|^2 &= \|G^+u + \bar{H}^+ \bar{z}\|^2 + \|(I - G^+G)(I - \bar{H}^+ \bar{H})y\|^2 \\ &\geq \|G^+u + \bar{H}^+ \bar{z}\|^2 \end{aligned}$$

with strict inequality holding unless

$$x_0 = G^+u + \bar{H}^+ \bar{z}. \quad \blacksquare$$

(3.12.5) **Exercise:** (a) The equation $Hx = z$ has a solution for all z if the rows of H are linearly independent.

(b) If the equation $Hx = z$ has a solution, the solution is unique if and only if the columns of H are linearly independent.

(3.12.6) **Exercise:** Let H be an $n \times m$ matrix with linearly independent columns. For any $k \times m$ matrix G , let $\bar{H} = H(I - G^+G)$. Show that $(I - G^+G)(I - \bar{H}^+\bar{H}) = 0$. [Hint: If $w = (I - G^+G)(I - \bar{H}^+\bar{H})v$, then $Hw = 0$. Apply (2.12.1).]

Comment: If the columns of H are linearly independent and u is in the range of G , then (3.12.6) and (3.12.4) together, imply that there is a unique vector which minimizes $\|z - Hx\|^2$ over \mathcal{S} . In general, though, the minimizing vector is not unique. However, the vector, $\hat{x}_0 = G^+u + \bar{H}^+\bar{z}$, has minimum norm among those which minimize $\|z - Hx\|^2$ over \mathcal{S} . The vector $\bar{x} = \bar{H}^+\bar{z}$ is the vector of minimum norm among those which minimize $\|\bar{z} - \bar{H}x\|^2$ subject to no constraints. \bar{x} and \hat{x}_0 differ by G^+u , the minimum norm vector in \mathcal{S} .

(3.12.7) **Exercise:** [Refer to (3.12.4).] If \mathcal{S} is empty, then $x^* = G^+u + \bar{H}^+\bar{z}$ is the vector of minimum norm which minimizes $\|z - Hx\|$ over \mathcal{S}^* where $\mathcal{S}^* = \{x: \|Gx - u\|^2 \text{ is minimized}\}$. [Hint: $\mathcal{S}^* = \{x: x = G^+u - (I - G^+G)v \text{ for some } v.\}$ The proof of (3.12.4) carries over word for word.]

(3.12.8) **Application to Linear Programming** (Ben-Israel and Charnes [2], also Ben-Israel *et al.* [1])

Let a , b , and c be specified n -vectors and let A be a given $m \times n$ matrix. Consider the problem of minimizing $c^T x$ with respect to x , subject to the constraints

$$a \leq Ax \leq b$$

(where the vector inequality is to be interpreted componentwise).

Following the conventional terminology, the problem is said to be *feasible* if the constraint set is nonempty, and *bounded* if the minimal value of $c^T x$ on the constraint set is finite.

Assuming that the problem is feasible, it follows readily that the problem is bounded if and only if $A^+Ac = c$. To see this, suppose first that the problem is bounded. If $\mathcal{N}(A) = \{0\}$ then $I - A^+A = 0$, (3.5), and so $A^+Ac = c$. Otherwise, if $0 \neq y \in \mathcal{N}(A)$, and if x_0 is in the constraint set, so is $x_0 + \alpha y$ for every scalar α . Hence

$$\min_{a \leq Ax \leq b} c^T x \leq c^T(x_0 + \alpha y) = c^T x_0 + \alpha c^T y$$

which can be made arbitrarily small and negative unless c is orthogonal to every null vector of A . Thus, the problem is bounded if and only if

$$c \in \mathcal{N}^\perp(A) = \mathcal{R}(A^T). \quad (2.10)$$

Since

$$A^+Ac \text{ is the projection of } c \text{ on } \mathcal{R}(A^T) \quad (3.5)$$

we see that boundedness implies $A^+Ac = c$.

Conversely, if $A^+Ac = c$, then $c \in \mathcal{R}(A^T)$ so that $c = A^Tz$ for some z . Thus $c^Tx = z^TAx$. Each component of Ax is bounded below on the constraint set so that z^TAx is bounded below as x ranges over the constraint set. Henceforth, we assume that $c \in \mathcal{R}(A^T)$.

We now make the additional assumption that the rows of A are linearly independent. In this case, the equation $Ax = z$ has a solution for every m -dimensional vector z , (3.12.5), and so

$$\min_{a \leq Ax \leq b} c^Tx = \min_{a \leq z \leq b} \min_{z = Ax} c^Tx.$$

The set of x 's for which $z = Ax$ is of the form

$$A^+z + (I - A^+A)y$$

where y is free to vary unrestricted over n space, (3.12). Since $c \in \mathcal{R}(A^T) = \mathcal{N}^\perp(A)$, we see that c is orthogonal to all null vectors of A [of which $(I - A^+A)y$ is one] so that

$$c^Tx = c^TA^+z \quad \text{if } Ax = z.$$

Consequently,

$$\begin{aligned} \min_{a \leq Ax \leq b} c^Tx &= \min_{a \leq z \leq b} c^TA^+z \\ &= \min_{a \leq z \leq b} (A^{+T}c)^Tz \end{aligned}$$

and if \tilde{z} minimizes the right side, any x of the form

$$\tilde{x} = A^+\tilde{z} + (I - A^+A)y$$

will minimize the left side over the constraint set.

The minimization of the right side is trivial: Denote the components of a , b , $A^{+T}c$, and z by α_i , β_i , γ_i , and ζ_i , respectively. Then

$$\min_{a \leq z \leq b} (A^{+T}c)^Tz = \min_{\substack{\alpha_i \leq \zeta_i \leq \beta_i \\ i=1, \dots, n}} \sum_{i=1}^n \gamma_i \zeta_i$$

and the components of the solution vector are clearly

$$\tilde{\zeta}_i = \begin{cases} \beta_i & \text{if } \gamma_i < 0 \\ \alpha_i & \text{if } \gamma_i > 0 \\ \text{anything between} \\ \alpha_i \text{ and } \beta_i \text{ (inclusive)} & \text{if } \gamma_i = 0. \end{cases}$$

The present solution depends crucially upon the assumption that the rows of A are linearly independent. If this assumption is violated, a modified procedure (more complicated) must be resorted to in order to solve the problem (Ben-Israel and Robers [1]).

(3.13) Exercises

(3.13.1) If A and B are matrices with the same number of rows, then

$$\mathcal{R}(A) \subseteq \mathcal{R}(B) \quad \text{if and only if} \quad BB^+A = A.$$

(3.13.2) If A and B are matrices with the same number of rows, the matrix equation

$$BX = A$$

has a solution if and only if $\mathcal{R}(A) \subseteq \mathcal{R}(B)$. In this case, any matrix of the form

$$X = B^+A + (I - B^+B)Y$$

(where Y has the same number of rows and columns as X) is a solution.

The solution is unique if and only if $B^+B = I$ [i.e., $\mathcal{N}(B) = \{0\}$].

(3.13.3) If M is nonsingular and A is rectangular with the same number of rows then

$$(MA)^+(MA) = A^+A.$$

If N is nonsingular and A is rectangular with the same number of columns,

$$(AN)(AN)^+ = AA^+.$$

(3.13.4) The matrix equation

$$AXB = C$$

has a solution in X if and only if

$$AA^+CB^+B = C.$$

In this case, the general solution is

$$X = A^+CB^+ + M - A^+AMB B^+$$

where M is arbitrary (same number of rows and columns as X).

(3.13.5) For any matrix A ,

$$A^+ = WAY$$

where W and Y are, respectively, any solutions to

$$WAA^T = A^T$$

and

$$A^TAY = A^T$$

(Decell, [1]).

(3.13.6) A matrix is said to be normal if it commutes with its transpose. In this case, show that

$$A^+A = AA^+.$$

(3.13.7) If T is orthogonal, $(AT)^+ = T^TA^+$.

(3.13.8) If $\mathcal{R}(B) \subseteq \mathcal{R}(A)$, then among those matrices X that satisfy

$$AX = B,$$

the one which minimizes the trace of X^TX is $\hat{X} = A^+B$.

If $AZ = B$, then

$$\text{trace}(Z^TZ) > \text{trace}(\hat{X}^T\hat{X}) \quad \text{if } Z \neq \hat{X}.$$

(3.13.9) The following conditions are equivalent:

- (a) $XH^+ = 0$,
- (b) $XH^T = 0$,
- (c) $XH^+H = 0$.

(3.13.10) If P is a projection, and if H is any rectangular matrix (having the right number of columns) then

$$(\bar{H}^T\bar{H})^+ = P(\bar{H}^T\bar{H})^+ = (\bar{H}^T\bar{H})^+P, \quad P\bar{H}^+ = \bar{H}^+,$$

and

$$\bar{H}^+ = (\bar{H}^T\bar{H})^+H^T$$

where

$$\bar{H} = HP.$$

(3.14) Exercises

(3.14.1) Let $h_1, h_2, \dots, h_n, \dots$ be any collection of vectors and define

$$A_0 = I$$

$$A_n = \begin{cases} A_{n-1} & \text{if } h_n \text{ is a linear combination of } h_1, h_2, \dots, h_{n-1} \\ A_{n-1} - \frac{(A_{n-1} h_n)(A_{n-1} h_n)^T}{h_n^T A_{n-1} h_n} & \text{otherwise.} \end{cases}$$

Show that for each n

- (a) A_n is the projection on $\mathcal{L}^\perp(h_1, \dots, h_n)$.
- (b) $A_n h_{n+1}$ is the (unnormalized) $(n+1)$ st vector in the Gram-Schmidt orthogonalization of h_1, h_2, \dots, h_{n+1} .

(3.14.2) Stationary Probability for a Markov Chain

A matrix P is called a stochastic matrix if its entries are nonnegative and its row sums are unity. Such matrices can be used to represent the one step transition probabilities for homogeneous Markov chains. If the process is *ergodic* (a condition which can be deduced by visual inspection of the transition matrix, Feller [1, Chap. XV]) then

$$\lim_{n \rightarrow \infty} (P^T)^n = (x \vdots x \vdots \cdots \vdots x)$$

where x is the unique *probability vector* (a vector having nonnegative components which sum to unity) satisfying

$$P^T x = x.$$

This probability vector is the *steady state* probability distribution for the Markov chain. The i th component of x represents the (steady state) probability that the process is in state i at any given instant.

Using these facts as a starting point, show that

- (a) $y = P^T y$ only if y is a multiple of x .
- (b) The row vectors of $I - P^T$ are linearly dependent.

Denoting the columns of $I - P$ by q_1, q_2, \dots, q_N , show that

- (c) q_1, q_2, \dots, q_{N-1} are linearly independent.
- (d) If $A_0 = I$,

$$A_n = A_{n-1} - (A_{n-1} q_n)(A_{n-1} q_n)^T / q_n^T A_{n-1} q_n \quad n = 1, 2, \dots, N-1$$

and u is the N -dimensional vector whose components are all ones, then

$$x = A_{N-1} u / u^T A_{N-1} u.$$

[Hint: A_{N-1} is the projection on $\mathcal{L}^\perp(q_1, q_2, \dots, q_{N-1})$; cf. Decell and Odell [1].]

In (3.6.1) and (3.6.2) we showed how a symmetric matrix and its pseudo-inverse can be represented in terms of its eigenvalues and eigenvectors. Using the theory which we have developed thus far, we can deduce an analogous result for an arbitrary rectangular matrix A in terms of the eigenvalues and eigenvectors of $A^T A$ and AA^T (see Good [1]).

We begin by reminding the reader that any matrix of the form $A^T A$ has a unique symmetric square root, which has the explicit representation

$$(A^T A)^{1/2} = T D^{1/2} T^T$$

where T is the orthogonal matrix which reduces $A^T A$ to the diagonal matrix D ,

$$A^T A = T D T^T$$

and $D^{1/2}$ is obtained by taking the (positive) square root of D 's (nonnegative) diagonal entries. [D 's entries are clearly nonnegative since

$$D = T^T A^T A T$$

so that for any x

$$x^T D x = \|A T x\|^2 \geq 0.$$

In particular, if $D = \text{diag}(d_1, \dots, d_n)$ and x has all zero components except for a 1 in the j th place, $x^T D x = d_j \geq 0$.]

(3.15) Theorem: Let A be an $n \times m$ matrix and let L be the $r \times r$ diagonal matrix of (AA^T) 's nonzero eigenvalues arranged in arbitrary order.

Then there is an $n \times r$ matrix P and an $r \times m$ matrix Q such that the following conditions hold:

$$(3.15.1) \quad A = P L^{1/2} Q.$$

$$(3.15.2) \quad A A^T = P L P^T.$$

$$(3.15.3) \quad A A^+ = P P^T.$$

$$(3.15.4) \quad P^T P = I.$$

$$(3.15.5) \quad A^T A = Q^T L Q.$$

$$(3.15.6) \quad A^+ A = Q^T Q.$$

$$(3.15.7) \quad Q Q^T = I.$$

Comment: By (3.15.4) and (3.15.7), the columns of P are orthonormal as are the rows of Q . By (3.15.2) and (3.15.4), $AA^T P = PL$ which shows that the columns of P are eigenvectors of AA^T , the j th column being an eigenvector associated with the j th diagonal entry λ_j of L . By (3.15.5) and (3.15.7), the same goes for the j th column of Q^T (which is the j th row of Q). This result is often referred to as the *singular decomposition theorem*.

Proof: By (3.11.3) and (3.11.7)

$$AA^+ = (AA^T)^{1/2}[(AA^T)^{1/2}]^+$$

so by (3.9.2)

$$(3.15.8) \quad A = (AA^T)^{1/2}[(AA^T)^{1/2}]^+ A.$$

By virtue of (3.7.1)

$$(3.15.9) \quad AA^T = TDT^T$$

where

$$D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_r, \overbrace{0, 0, \dots, 0}^{n-r}),$$

$\lambda_j > 0$, and T is an orthogonal matrix. Let us express T and D as partitioned matrices:

$${}^n_n T = {}^n \begin{bmatrix} {}^r P & {}^{n-r} P_0 \end{bmatrix}$$

$$D = \begin{matrix} & {}^r & {}^{n-r} \\ & L & 0 \\ {}^r & \vdots & \vdots \\ {}^{n-r} & 0 & 0 \end{matrix}$$

where

$$L = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_r).$$

Then (3.15.9) can be rewritten as

$$(3.15.10) \quad AA^T = PLP^T$$

which proves (3.15.2). Define

$$(3.15.11) \quad Q = P^T[(AA^T)^{1/2}]^+ A.$$

Since

$$(AA^T)^{1/2} = TD^{1/2}T^T$$

and since

$$D^{1/2} = \begin{bmatrix} L^{1/2} & 0 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix}$$

we can write

$$(3.15.12) \quad (AA^T)^{1/2} = PL^{1/2}P^T.$$

Therefore, by (3.15.11)

$$\begin{aligned} PL^{1/2}Q &= (PL^{1/2}P^T)[(AA^T)^{1/2}]^+A \\ &= A. \end{aligned} \quad (3.15.12) \text{ and } (3.15.8)$$

This proves (3.15.1).

$$\begin{aligned} AA^+ &= (AA^T)(AA^T)^+ \\ &= (TDT^T)(TD^+T^T) = TDD^+T^T \\ &= PP^T \end{aligned} \quad (3.11.7)$$

which proves (3.15.3). Since T is an orthogonal matrix, its columns are orthonormal, so $P^TP = I$ which establishes (3.15.4).

$$Q^TLQ = A^T[(AA^T)^{1/2}]^+PLP^T[(AA^T)^{1/2}]^+A \quad (3.15.11)$$

$$= A^T[(AA^T)^{1/2}]^+(AA^T)[(AA^T)^{1/2}]^+A \quad (3.15.12)$$

$$= A^T[(AA^+)]A \quad (3.11.3) \text{ and } (3.11.7)$$

$$= A^TA$$

which proves (3.15.5).

$$Q^TQ = A^T[(AA^T)^{1/2}]^+PP^T[(AA^T)^{1/2}]^+A. \quad (3.15.11)$$

By virtue of (3.15.9)

$$\begin{aligned} (AA^T)^+ &= TD^+T^T \\ &= PL^{-1}P^T \end{aligned}$$

and so by (3.11.3)

$$[(AA^T)^{1/2}]^+ = [(AA^T)^+]^{1/2} = PL^{-1/2}P^T.$$

Thus

$$\begin{aligned} Q^TQ &= A^T(PL^{-1/2}P^T)(PP^T)(PL^{-1/2}P^T)A \\ &= A^TPL^{-1}P^TA \\ &= A^T(AA^T)^+A \\ &= A^+A. \end{aligned} \quad (3.8.3)$$

This proves (3.15.6). Finally, by (3.15.11)

$$\begin{aligned} QQ^T &= P^T[(AA^T)^{\frac{1}{2}}]^+ AA^T[(AA^T)^{\frac{1}{2}}]^+ P \\ &= P^T(AA^+)P \end{aligned} \quad (3.11.3) \text{ and } (3.11.7)$$

$$= P^T(PP^T)P \quad (3.15.3)$$

$$= I. \quad \blacksquare \quad (3.15.4)$$

(3.15.13) **Exercise:** The nonzero eigenvalues of $A^T A$ and AA^T are identical.

$$(3.15.14) \text{ Exercise: } A^+ = Q^T L^{-\frac{1}{2}} P^T, \quad Q^+ = Q^T, \quad P^+ = P^T.$$

(3.16) **Exercise:** There exists a representation for A of the form (3.16.1)

$$(3.16.1) \quad A = \sum_j \lambda_j^{\frac{1}{2}} p_j q_j^T$$

where the λ_j 's are the nonzero eigenvalues of $A^T A$ (or AA^T) repeated according to their multiplicity,

$$(3.16.2) \quad AA^T p_j = \lambda_j p_j; \quad A^T A q_j = \lambda_j q_j$$

and

$$(3.16.3) \quad p_i^T p_j = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} = q_i^T q_j.$$

The representation is not necessarily unique, but not all such representations [with p_j and q_j satisfying (3.16.2)–(3.16.3)] are valid.

$$(3.17) \text{ Exercise: } A^+ = \sum_j \lambda_j^{-\frac{1}{2}} q_j p_j^T \text{ if } A \text{ satisfies (3.16.1)–(3.16.3).}$$

(3.18) **Exercise:** Any matrix A can be represented as a linear combination of partial isometries:

$$A = \sum \lambda_j^{\frac{1}{2}} U(\lambda_j)$$

where the λ_j 's are the *distinct* nonzero eigenvalues of $A^T A$ and

$$U(\lambda) = \lambda^{-\frac{1}{2}} A \{I - (A^T A - \lambda I)^+ (A^T A - \lambda I)\}$$

satisfy

$$U(\lambda_j)U^T(\lambda_k) = 0 \quad \text{if } k \neq j$$

$$U^T(\lambda_j)U(\lambda_k) = 0 \quad \text{if } k \neq j$$

$$A^+ = \sum_j \lambda_j^{-1/2} U^T(\lambda_j).$$

[Hint: $I - (A^T A - \lambda I)^+ (A^T A - \lambda I)$ is the projection on the null space of $A^T A - \lambda I$, which is spanned by the eigenvectors (if any) of $A^T A$ associated with λ . Then use (3.16.1).] See Ben-Israel and Charnes [1], Penrose [1], and Golub and Kahan [1] for related work.

(3.19) Exercise *Iterative method for finding the dominant eigenvalue and associated eigenvector for AA^T and $A^T A$.*

Let

$$y_0 = Ax_0 / \|Ax_0\|$$

$$x_{n+1} = A^T y_n / \|A^T y_n\|$$

$$y_{n+1} = Ax_{n+1} / \|Ax_{n+1}\| \quad n = 0, 1, \dots$$

Then

$$\lim_{n \rightarrow \infty} x_n = q \quad \text{and} \quad \lim_{n \rightarrow \infty} y_n = p \quad \text{exist}$$

provided that x_0 is not orthogonal to $\mathcal{N}(A^T A - \lambda_1 I)$ where λ_1 is the largest eigenvalue of $A^T A$.

Furthermore,

$$AA^T p = \lambda_1 p \quad \text{and} \quad A^T A q = \lambda_1 q$$

so that

$$\begin{aligned} \lambda_1 &= \lim_{n \rightarrow \infty} \|A^T y_n\|^2 \\ &= \lim_{n \rightarrow \infty} \|Ax_n\|^2. \end{aligned}$$

PSEUDOINVERSES OF PARTITIONED MATRICES AND SUMS AND PRODUCTS OF MATRICES

If c_1, c_2, \dots, c_m are a collection of vectors in an n -dimensional space, we can write the $n \times m$ matrix

$$C_m = (c_1 \vdots c_2 \vdots \dots \vdots c_m)$$

whose j th column is c_j , in terms of C_{m-1} and c_m :

$$(4.1) \quad C_m = (C_{m-1} \vdots c_m) \quad (m = 2, 3, \dots).$$

The pseudoinverse of C_1 is easy to compute:

$$(4.2) \quad C_1^+ = c_1^T / c_1^T c_1 \quad (3.11.9)$$

and so, if we can develop a convenient relationship between C_m^+ and C_{m-1}^+ , we will have a nice computational procedure for pseudoinverting a rectangular matrix "a column at a time":

(4.3) Theorem (Greville [2]): If

$$(4.3.1) \quad C_{m+1} = (C_m \vdots c_{m+1})$$

then

$$(4.3.2) \quad C_{m+1}^+ = \left(\frac{C_m^+ [I - c_{m+1} k_{m+1}^T]}{k_{m+1}^T} \right)$$

where

$$(4.3.3) \quad k_{m+1} = \begin{cases} \frac{(I - C_m C_m^+) c_{m+1}}{\|(I - C_m C_m^+) c_{m+1}\|^2} & \text{if } (I - C_m C_m^+) c_{m+1} \neq 0 \\ \frac{C_m^{+T} C_m^+ c_{m+1}}{1 + \|C_m^+ c_{m+1}\|^2} & \text{otherwise.} \end{cases}$$

Comment: $(I - C_m C_m^+) c_{m+1}$ is zero if and only if $C_m C_m^+ c_{m+1} = c_{m+1}$ [i.e., if and only if c_{m+1} is in the range of C_m , (3.7.5)]. The range of C_m is spanned by c_1, \dots, c_m (why?) and so k_{m+1} is defined by the first part of (4.3.3) if and only if c_{m+1} is not a linear combination of c_1, \dots, c_m .

Proof: The proof is a straightforward, though tedious verification that the right side of (4.3.2) satisfies the conditions of (3.9). We leave the details to the reader. (Greville's original proof was constructive. The interested reader will find it instructive, as well.) ■

(4.4) Application to Stepwise Regression

It is very common for an experimentalist to observe samples of a function of an independent variable (e.g., time) whose functional form is not known *a priori* and for him to wish to model the behavior of this function (e.g., for the purpose of prediction). Typically, the experimenter has in mind a family of functions, $\varphi_1(\tau), \varphi_2(\tau), \dots, \varphi_m(\tau)$ and the data is modeled by choosing an appropriate set of weights and representing (approximating) the observed data as a linear combination of the φ 's.

To be more explicit, if the observations denoted by $\zeta_1, \zeta_2, \dots, \zeta_n$ are made at times $\tau_1, \tau_2, \dots, \tau_n$ and if the points (τ_j, ζ_j) are plotted on cartesian coordinates, the problem boils down to choosing a set of scalars $\xi_1, \xi_2, \dots, \xi_m$ so that the graph of the function

$$\sum_{j=1}^m \xi_j \varphi_j(\tau)$$

plotted as a function of τ , comes as close as possible to the given data points.

The most popular method for choosing the weights is (for good cause) the method of least squares, in which the ξ_j 's are chosen to minimize the sums of the squares of the (vertical) distances from the data points to the curve.

In mathematical terms, the ξ_j 's are chosen to minimize

$$(4.4.1) \quad \sum_{k=1}^n \left(\zeta_k - \sum_{j=1}^m \xi_j \varphi_j(\tau_k) \right)^2.$$

If a vector notation is used, so that

$$z = \begin{pmatrix} \zeta_1 \\ \vdots \\ \zeta_n \end{pmatrix} \quad x = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_m \end{pmatrix} \quad c_j = \begin{pmatrix} \varphi_j(\tau_1) \\ \vdots \\ \varphi_j(\tau_n) \end{pmatrix}$$

and

$$C_m = (c_1 \vdots c_2 \cdots \vdots c_m) \quad (\text{an } n \times m \text{ matrix})$$

then the problem of choosing ξ_1, \dots, ξ_m to minimize (4.4.1) is the same as choosing x to minimize

$$(4.4.2) \quad \|z - C_m x\|^2.$$

In (3.4) we showed that

$$(4.4.3) \quad \hat{x}^{(m)} = C_m^+ z$$

always minimizes (4.4.2) and is in fact the vector of minimum norm which does the job. Suppose $\hat{x}^{(m)}$ is computed and that the residual sum of squares

$$\|z - C_m \hat{x}^{(m)}\|^2$$

(which measures the degree of fit between the data and the model) is unacceptably large.

The standard response to such a situation is to augment the family of functions $\varphi_1(\cdot), \varphi_2(\cdot), \dots, \varphi_m(\cdot)$ by adding an $(m+1)$ st function $\varphi_{m+1}(\cdot)$ and then choosing the $m+1$ weights $\xi_1, \xi_2, \dots, \xi_{m+1}$ to minimize the new residual sum of squares

$$\sum_{k=1}^n \left(\zeta_k - \sum_{j=1}^{m+1} \xi_j \varphi_j(\tau_k) \right)^2$$

which can be expressed in vector-matrix notation as

$$\|z - C_{m+1} x\|^2$$

where z is as defined before,

$$C_{m+1} = (C_m \vdots c_{m+1}) \quad c_{m+1} = \begin{pmatrix} \varphi_{m+1}(\tau_1) \\ \vdots \\ \varphi_{m+1}(\tau_n) \end{pmatrix}$$

and x is now an $m+1$ -dimensional vector,

$$x = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_{m+1} \end{pmatrix}.$$

The minimum norm solution is

$$(4.4.4) \quad \hat{x}^{(m+1)} = C_{m+1}^+ z$$

and the results of (4.3) show how $\hat{x}^{(m+1)}$ is related to $\hat{x}^{(m)}$:

$$\begin{aligned} \hat{x}^{(m+1)} = C_{m+1}^+ z &= \left(\frac{C_m^+ z - C_m^+ c_{m+1} (k_{m+1}^T z)}{k_{m+1}^T z} \right) \\ &= \left(\frac{\hat{x}^{(m)} - (k_{m+1}^T z) C_m^+ c_{m+1}}{k_{m+1}^T z} \right). \end{aligned}$$

(4.5) Exercise: Let $\hat{z}^{(m)} = C_m \hat{x}^{(m)}$ and $e^{(m)} = \|z - \hat{z}^{(m)}\|^2$.

(a) $e^{(m+1)} \leq e^{(m)}$ with strict inequality holding unless c_{m+1} is a linear combination of c_1, \dots, c_m or unless $c_{m+1} \perp (z - \hat{z}^{(m)})$.

(b) $e^{(m+1)} = (1 - \rho_{z, m+1|m}^2) e^{(m)}$,

$$\rho_{z, m+1|m} = [(z - \hat{z}^{(m)})^T \tilde{c}_{m+1}] [\|z - \hat{z}^{(m)}\| \cdot \|\tilde{c}_{m+1}\|]^{-1}$$

and

$$\tilde{c}_{m+1} = (I - C_m C_m^+) c_{m+1}.$$

$\rho_{z, m+1|m}$ is called the *partial* correlation coefficient between z and c_{m+1} , given c_1, \dots, c_m . Interpret the partial correlation coefficient geometrically.

(c) $e^{(m)} = [\prod_{j=1}^m (1 - \rho_{z, j|j-1}^2)] \|z\|^2$.

(d) The *multiple* correlation coefficient of z on c_1, \dots, c_m is defined to be

$$r_{z|m} = z^T \hat{z}^{(m)} / (\|z\| \cdot \|\hat{z}^{(m)}\|).$$

Interpret the multiple correlation coefficient geometrically and show that

$$\prod_{j=1}^m (1 - \rho_{z, j|j-1}^2) = 1 - r_{z|m}^2.$$

A word of caution is in order with regard to the interpretation of (4.5a). The object of modeling data is generally predictive in nature. Therefore, the fact that the residual sum of squares can be reduced by the addition of another regressor is not sufficient cause to add regressors *ad infinitum*. A fine line must be tread between parsimonious modeling (using few regressors) and

getting a good fit. In many statistical contexts, underspecifying the number of regressors results in biased estimates. Over specification (too many regressors) results in loss of accuracy. The question, "How many regressors is enough?" is partially answered by the theory of the analysis of variance and covariance, under certain assumptions. The question, "How should I choose my family of regressors to begin with?" is much more difficult and not easily answered in quantitative terms.

The results of (4.3) lead directly to an important representation for pseudo-inverses of certain types of matrix sums:

(4.6) Theorem: Let c_1, c_2, \dots be a collection of n -dimensional vectors and let

$$\begin{aligned} S_m &= \sum_{j=1}^m c_j c_j^T \\ &= C_m C_m^T \quad (m = 1, 2, \dots) \end{aligned}$$

where C_m is as defined in (4.1). Then

$$(4.6.1) \quad S_{m+1}^+ = \begin{cases} S_m^+ + \left[\frac{1 + c_{m+1}^T S_m^+ c_{m+1}}{(c_{m+1}^T A_m c_{m+1})^2} \right] (A_m c_{m+1})(A_m c_{m+1})^T \\ \quad - \frac{(S_m^+ c_{m+1})(A_m c_{m+1})^T + (A_m c_{m+1})(S_m^+ c_{m+1})^T}{c_{m+1}^T A_m c_{m+1}} \\ \quad \text{if } c_{m+1} \text{ is not a linear combination of } c_1, \dots, c_m \\ S_m^+ - \frac{(S_m^+ c_{m+1})(S_m^+ c_{m+1})^T}{1 + c_{m+1}^T S_m^+ c_{m+1}} \quad \text{otherwise} \end{cases}$$

where

$$(4.6.2) \quad A_m = I - S_m S_m^+.$$

Comment: A_m is the projection on $\mathcal{N}(S_m^T) = \mathcal{R}^\perp(S_m)$, (3.5). Since $S_m = C_m C_m^T$ and

$$\mathcal{R}(C_m C_m^T) = \mathcal{R}(C_m) \quad (2.12)$$

$$= \mathcal{L}(c_1, c_2, \dots, c_m) \quad (4.3.4)$$

we see that A_m is the projection on $\mathcal{L}^\perp(c_1, \dots, c_m)$, and so $c_{m+1} \in \mathcal{L}(c_1, \dots, c_m)$ if and only if $A_m c_{m+1} = 0$. Thus, c_{m+1} is *not* a linear combination of c_1, \dots, c_m if and only if $A_m c_{m+1} \neq 0$.

Furthermore, by virtue of (3.14.1), A_m satisfies a recursion of its own [replace h_m by c_m in (3.14.1)].

Proof of (4.6)

$$(4.6.3) \quad \begin{aligned} S_{m+1}^+ &= (C_{m+1} C_m^T)^+ \\ &= (C_{m+1}^+)^T (C_m^+). \end{aligned} \quad (3.11.2) \text{ and } (3.8.2)$$

(4.6.1) results when (4.3.2) and (4.3.3) are combined in (4.6.3) and note is taken of the fact that

$$I - C_m C_m^+ = I - S_m S_m^+ = A_m. \quad \blacksquare$$

(4.6.4) **Exercise** [Extension of (3.14.1)]: Let

$$C_m = (c_1 : c_2 : \cdots : c_m)$$

and

$$D_m = D_0 - D_0 C_m (C_m^T D_0 C_m)^+ C_m^T D_0$$

where D_0 is an arbitrary matrix of the form $D_0 = R^T R$. Then

$$(a) \quad D_m = R^T Q_m R$$

where Q_m is the projection on $\mathcal{L}^\perp(Rc_1, \dots, Rc_m) = \mathcal{R}^\perp(RC_m)$.

$$(b) \quad D_{m+1} = \begin{cases} D_m - \frac{(D_m c_{m+1})(D_m c_{m+1})^T}{c_{m+1}^T D_m c_{m+1}} & \text{if } Rc_{m+1} \text{ is not a l.c.} \\ & \text{(linear combination)} \\ & \text{of } Rc_1, \dots, Rc_m; \\ D_m & \text{otherwise.} \end{cases}$$

(c) If $R^T R$ is nonsingular, Rc_{m+1} is a linear combination of Rc_1, \dots, Rc_m if and only if $D_m c_{m+1} = 0$, so that D_{m+1} is defined by the first half of the recursion if $D_m c_{m+1} \neq 0$, otherwise by the second half.

Comment: If $A_m = I - C_m C_m^+$ then $A_0 = I$ and

$$A_{m+1} = \begin{cases} \frac{A_m - (A_m c_{m+1})(A_m c_{m+1})^T}{c_{m+1}^T A_m c_{m+1}} & \text{if } A_m c_{m+1} \neq 0 \\ A_m & \text{otherwise.} \end{cases} \quad (3.14.1)$$

If $R^T R$ is nonsingular, D_m and A_m satisfy the same recursion. A_m and D_m differ because of the different initial conditions.

(4.6.5) **Exercise:** If A is symmetric, nonsingular and $h^T A^{-1} h \neq -1$, then

$$(A + hh^T)^{-1} = A^{-1} - \frac{(A^{-1} h)(A^{-1} h)^T}{1 + h^T A^{-1} h}.$$

The results of (4.3) and (4.6) can be extended to the case of higher-order partitioning. The proofs are computational in nature, but are basically the

same as (4.3) and (4.6). We state the results without proofs and refer the interested reader to the papers by Cline [2, 3] for details.

(4.7) Theorem

$$(4.7.1) \quad (U;V)^+ = \left(\begin{array}{c} U^+ - U^+ V J \\ \hline J \end{array} \right)$$

where

$$(4.7.2) \quad J = C^+ + (I - C^+ C) K V^T U^{+T} U^+ (I - V C^+)$$

$$(4.7.3) \quad C = (I - U U^+) V$$

and

$$(4.7.4) \quad K = \{I + [U^+ V (I - C^+ C)]^T [U^+ V (I - C^+ C)]\}^{-1}.$$

Comment: Any matrix of the form $I + D^T D$ is nonsingular, (2.13), so K always exists. The dimension of K is the same as the dimension of $C^T C$ which is the same as the dimension of $V^T V$. If U^+ is known, $(U;V)^+$ can be computed at the expense of inverting a square matrix the size of $V^T V$, and finding $I - C^+ C$, the projection on $\mathcal{N}(C)$.

The extension of (4.6) to higher-order partitions is

(4.8) Theorem

$$(4.8.1) \quad \begin{aligned} (UU^T + VV^T)^+ &= (CC^T)^+ + [I - (VC^+)^T] \\ &\quad \times [(UU^T)^+ - (UU^T)^+ V (I - C^+ C) K V^T (UU^T)^+] \\ &\quad \times [I - VC^+] \end{aligned}$$

where C and K are as defined in (4.7).

Comment: We can also write

$$(4.8.2) \quad C = [I - (UU^T)(UU^T)^+] V$$

and

$$(4.8.3) \quad K = \{I + [(I - C^+ C) V^T (UU^T)^+ V (I - C^+ C)]\}^{-1}.$$

Here, U and V can be interchanged throughout the right side of (4.8.1) without altering the validity of the statement, owing to the symmetry of the left side.

$$(4.8.4) \text{ Exercise: } (U;0)^+ = \left(\begin{array}{c} U^+ \\ \hline 0 \end{array} \right).$$

(4.8.5) **Exercise:** In the special case where $U = C_m$ and $V = c_{m+1}$, show that (4.7) and (4.8) yield formulas which coincide with (4.3) and (4.6).

Theorem (4.8) is extremely important if for no other reason than that it allows the development of an explicit perturbation theory for the pseudo-inverse of matrices of the form $A^T A$:

(4.9) Theorem

$$(4.9.1) \quad [H^T H + \lambda^{-2} G^T G]^+ = (\bar{H}^T \bar{H})^+ + \lambda^2 (I - \bar{H}^+ H)(G^T G)^+ (I - \bar{H}^+ H)^T \\ - \lambda^4 (I - \bar{H}^+ H)[H(G^T G)^+]^T \\ \times Q M(\lambda) Q [H(G^T G)^+] (I - \bar{H}^+ H)^T$$

where

$$(4.9.2) \quad \bar{H} = H(I - G^+ G) = H[I - (G^T G)^+ (G^T G)]$$

$$(4.9.3) \quad Q = I - \bar{H} \bar{H}^+$$

and

$$(4.9.4) \quad M(\lambda) = [I + \lambda^2 Q H (G^T G)^+ H^T Q]^{-1}.$$

Proof: Let $U = G^T/\lambda$, $V = H^T$ and apply (4.8):

$$[H^T H + \lambda^{-2} G^T G]^+ = (C C^T)^+ + \lambda^2 [I - (H^T C^+)]^T \\ \times [(G^T G)^+ - \lambda^2 (G^T G)^+ H^T (I - C^+ C) K H (G^T G)^+] \\ \times (I - H^T C^+)$$

where

$$C = (I - G^+ G) H^T = \bar{H}^T, \quad I - C^+ C = Q$$

and

$$K = [I + \lambda^2 Q H (G^T G)^+ H^T Q]^{-1} = M(\lambda).$$

But,

$$(I - H^T C^+)^T = (I - H^T \bar{H}^T)^T = I - \bar{H}^+ H$$

and

$$G^T H^T = (H G^+)^T.$$

Finally, if $I + A$ is nonsingular, then

$$(I + A)^{-1} = I - (I + A)^{-1} A$$

so that

$$(I - C^+ C) K \equiv Q M(\lambda) = Q M(\lambda) Q$$

and (4.9.1) follows directly. ■

A scalar function $\varphi(\cdot)$, of a real variable λ , is said to be $O(\lambda^n)$ as $\lambda \rightarrow 0$ if $\varphi(\lambda)/\lambda^n$ is bounded as $\lambda \rightarrow 0$. A matrix valued function is $O(\lambda^n)$ if each entry of the matrix is $O(\lambda^n)$.

(4.9.5) Corollary

- (a) $M(\lambda) = I + O(\lambda^2)$ as $\lambda \rightarrow 0$.
- (b) $[H^T H + (\lambda^2)^{-1} G^T G]^+ = (\bar{H}^T \bar{H})^+ + \lambda^2 (I - \bar{H}^+ H)(G^T G)^+ \\ \times (I - \bar{H}^+ H)^T + O(\lambda^4) \quad \text{as } \lambda \rightarrow 0.$

Proof: (a) $M(\lambda)$ is obviously $O(1)$, since $\lim_{\lambda \rightarrow 0} M(\lambda) = I$. Since $(I+A)^{-1} = I - A(I+A)^{-1}$, we see that $M(\lambda) - I = -\lambda^2 QH(G^T G)^+ H^T QM(\lambda)$ so that $[M(\lambda) - I]/\lambda^2$ equals a constant matrix times $M(\lambda)$, which is bounded. Thus, $M(\lambda) - I = O(\lambda^2)$, as asserted.

(b) Follows directly. ■

(4.9.6) **Exercise:** Show that $\lim_{\lambda \rightarrow \infty} M(\lambda)$ exists, and calculate the limit. [Hint: Let $\varepsilon = 1/\lambda$ and apply (4.9.5b) to $[I + \varepsilon^{-2} A^T A]^{-1}$, where $A = G^T + H^T Q$.]

(4.9.7) **Exercise:** Under what conditions will $\lim_{\varepsilon \rightarrow 0} (H^T H + \varepsilon^2 G^T G)^+$ exist?

Comment: Exercise (4.9.7) again illustrates the extreme discontinuous nature of pseudoinverses. (See the discussion preceding (3.7.3). Also see Stewart [1] and Ben-Israel [1]).

(4.9.8) **Exercise:** (a) If $U^T U$ is nonsingular and $A(\lambda) = O(1)$ as $\lambda \rightarrow 0$, then $U^T U + \lambda A(\lambda)$ is nonsingular for all suitably small λ , and

$$(b) [U^T U + \lambda A(\lambda)]^{-1} = (U^T U)^{-1} + O(\lambda) \quad \text{as } \lambda \rightarrow 0.$$

(4.9.9) **Exercise:** Let C be an arbitrary symmetric matrix. Then

- (a) $(C + \lambda^2 I)^{-1}$ and $(I + \lambda^2 C^+)^{-1}$ exist whenever λ^2 is suitably large or suitably small and so
- (b) $[I + \lambda^{-2} C]^{-1} = (I - CC^+) + \lambda^2 C^+ (I + \lambda^2 C^+)^{-1}$ if λ^2 is suitably large or suitably small, and
- (c) $(I + \lambda^2 C)^{-1} = (I - CC^+) + C^+ (C^+ + \lambda^2 I)^{-1}$ if λ^2 is suitably large or suitably small.
- (d) $[I + \lambda^{-2} C]^{-1} = (I - CC^+) - \sum_{j=1}^n (-\lambda^2)^j (C^+)^j + O(\lambda^{2n+2})$ as $\lambda \rightarrow 0$.

[Hint: Write $C = T^T D T$ where T is orthogonal and D is diagonal, and use (3.6).]

(4.10) The Concept of Rank

If \mathcal{L} is a linear manifold in a Euclidean n -space, the *dimension of \mathcal{L}* [abbreviated $\dim(\mathcal{L})$] is defined to be the maximum number of vectors in \mathcal{L} that can be chosen linearly independent of one another. A fundamental fact that we shall take for granted is that *any* basis for \mathcal{L} has exactly r linearly independent vectors, where $r = \dim(\mathcal{L})$.

(4.10.1) **Exercise:** If $\mathcal{L}_1 \subseteq \mathcal{L}_2$, then

$$\dim(\mathcal{L}_2 - \mathcal{L}_1) = \dim(\mathcal{L}_2) - \dim(\mathcal{L}_1).$$

If A is any matrix, the *rank of A* [abbreviated $\text{rk}(A)$] is defined to be the dimension of A 's range:

$$\text{rk}(A) = \dim[\mathcal{R}(A)].$$

Several properties of rank play an important role in the theory of pseudoinverses for products and in the statistical applications of Chapter VI. They are straightforward consequences of already established results and are left as exercises:

(4.10.2) Exercise

(a) For any matrix A

$$\text{rk}(A) = \text{rk}(A^T A) = \text{rk}(A^T) = \text{rk}(A A^T).$$

(b) For any matrices A and B (of the right size)

$$\text{rk}(AB) = \text{rk}(A^+ AB) = \text{rk}(ABB^+).$$

(c) $\text{rk}(AB) \leq \min[\text{rk}(A), \text{rk}(B)]$.

(d) If $\text{rk}(A) = \text{rk}(AB)$ then $\mathcal{R}(A) = \mathcal{R}(AB)$ and the equation

$$ABX = A$$

has a solution in X .

(4.10.3) **Exercise:** (a) If P is a projection, $\text{rk}(P) = \text{trace}(P)$.

(b) If P_0, P_1 , and P_2 are projections with $\mathcal{R}(P_1) \subseteq \mathcal{R}(P_0)$, $\mathcal{R}(P_2) \subseteq \mathcal{R}(P_0)$ and $P_1 P_2 = 0$ then

$$P_0 = P_1 + P_2$$

if and only if $\text{rk}(P_0) = \text{rk}(P_1) + \text{rk}(P_2)$ (c.f. Cochran's theorem, Scheffé [1]).

We now turn our attention to the question of pseudoinverses for products of matrixes. If A and B are nonsingular, $(AB)^{-1} = B^{-1}A^{-1}$, but it is not

generally true that $(AB)^+ = B^+A^+$ as evidenced by the example

$$A = \begin{pmatrix} 1 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (AB)^+ = 1 \quad B^+A^+ = \frac{1}{2}.$$

Greville [3] has found necessary and sufficient conditions for $(AB)^+ = B^+A^+$. These we state as the following.

(4.11) Theorem: $(AB)^+ = B^+A^+$ if and only if

$$(4.11.1) \quad \mathcal{R}(BB^T A^T) \subseteq \mathcal{R}(A^T)$$

and

$$(4.11.2) \quad \mathcal{R}(A^T AB) \subseteq \mathcal{R}(B).$$

Proof: Since $A^+A = A^T A^{T+}$, (4.11.1) holds if and only if the equation

$$(4.11.3) \quad A^+ A B B^T A^T = B B^T A^T. \quad (3.13.1)$$

By the same token, (4.11.2) holds if and only if

$$(4.11.4) \quad B B^+ A^T A B = A^T A B.$$

We will show that (4.11.3) and (4.11.4) are necessary and sufficient for $(AB)^+ = B^+A^+$:

Suppose (4.11.3) and (4.11.4) hold. Multiply (4.11.3) on the left by B^+ and on the right by $(AB)^{T+}$:

$$\begin{aligned} B^+ [A^+ A (B B^T A^T)] (B^T A^T)^+ \\ &= B^+ A^+ (AB) [(AB)^+ (AB)]^T \\ &= B^+ A^+ (AB) \end{aligned}$$

while

$$\begin{aligned} B^+ [B B^T A^T] (AB)^{T+} \\ &= B^+ B B^T A^T (AB)^{T+} \\ &= (AB)^T (AB)^{T+} \\ &= (AB)^+ (AB) \end{aligned}$$

so that if (4.11.3) holds

$$(4.11.5) \quad B^+ A^+ (AB) = (AB)^+ (AB).$$

By the same token, if both sides of (4.11.4) are premultiplied by $(AB)^{T+}$ and postmultiplied by A^+ , we find that

$$(4.11.6) \quad (AB) B^+ A^+ = (AB) (AB)^+.$$

The right-hand sides of (4.11.5) and (4.11.6) are symmetric and so B^+A^+ satisfies (3.9.1). We are done if we can show that B^+A^+ satisfies (3.9.2) and (3.9.3) as well:

If (4.11.5) is premultiplied on both sides by AB , we see that B^+A^+ does indeed satisfy (3.9.2). (3.9.3) is a bit more subtle:

Since

$$\begin{aligned} B^+A^+ &= (B^+BB^+)(A^+AA^+) \\ &= (B^+B^{+\top})(B^\top A^\top)(A^{+\top}A^+) \end{aligned}$$

(4.10.2) tells us that

$$(4.11.7) \quad \text{rk}(B^+A^+) \leq \text{rk}(B^\top A^\top) = \text{rk}(AB).$$

On the other hand, (4.10.2b) asserts that

$$\begin{aligned} (4.11.8) \quad \text{rk}(AB) &= \text{rk}[(AB)^+(AB)] \\ &= \text{rk}[(B^+A^+)(AB)] \end{aligned} \quad (4.11.5)$$

$$\leq \text{rk}(B^+A^+). \quad (4.10.2c)$$

If (4.11.7) and (4.11.8) are combined, we find that

$$(4.11.9) \quad \text{rk}(B^+A^+) = \text{rk}(B^+A^+AB)$$

so that the equation

$$(4.11.10) \quad B^+A^+ABX = B^+A^+$$

has a solution in X .

$$(4.10.2d)$$

Premultiply (4.11.10) by AB and apply (4.11.6) to deduce

$$\begin{aligned} (4.11.11) \quad (AB)(B^+A^+)(AB)X &= \\ (AB)(AB)^+(AB)X &= \\ (AB)X &= (AB)(B^+A^+). \end{aligned}$$

Substituting the last expression for ABX in (4.11.10), we see that

$$(B^+A^+)(AB)(B^+A^+) = B^+A^+$$

which establishes (3.9.3) and shows that $B^+A^+ = (AB)^+$ if (4.11.3) and (4.11.4) hold.

To prove the converse, suppose that $(AB)^+ = B^+A^+$: Then

$$\begin{aligned} (AB)^\top &= [(AB)(AB)^+(AB)]^\top \\ &= (AB)^+(AB)(AB)^\top \\ &= B^+A^+(AB)(AB)^\top. \end{aligned}$$

If the left and right sides are premultiplied by $ABB^T B$ and use is made of the identity

$$\begin{aligned} B^T &= (BB^+ B)^T \\ &= B^T BB^+ \end{aligned}$$

we find that

$$ABB^T B(AB)^T = ABB^T BB^+ A^+(AB)(AB)^T$$

or equivalently

$$(4.11.12) \quad ABB^T(I - A^+ A)BB^T A^T = 0.$$

Since $H^T H = 0$ implies $H = 0$, (4.11.2) tells us that

$$(I - A^+ A)BB^T A^T = 0 \quad [\text{take } H = (I - A^+ A)BB^T A^T]$$

which is the same as (4.11.3). Equation (4.11.4) is proved the same way, interchanging A^T and B throughout in the preceding proof. ■

A general representation for $(AB)^+$ was derived by Cline [1].

$$(4.12) \text{ Theorem: } (AB)^+ = B_1^+ A_1^+$$

where

$$(4.12.1) \quad B_1 = A^+ AB$$

and

$$(4.12.2) \quad A_1 = AB_1 B_1^+.$$

Proof: Clearly

$$(4.12.3) \quad AB = A_1 B_1.$$

Furthermore,

$$(4.12.4) \quad B_1 B_1^+ = A^+ A_1$$

since

$$A^+ A_1 = A^+ (AB_1 B_1^+) = (A^+ A)(A^+ A)BB_1^+ = A^+ ABB_1^+.$$

Similarly

$$(4.12.5) \quad A_1^+ A_1 = A^+ A_1$$

because

$$(A_1^+ A_1)(B_1 B_1^+) = A_1^+ (AB_1 B_1^+) B_1 B_1^+ = A_1^+ (AB_1 B_1^+) = A_1^+ A_1$$

from which follows (4.12.5) after transposes are taken and note is made of (4.12.4).

It is now easy to show that A_1 and B_1 satisfy (4.11.3) and (4.11.4):

$$A_1^+ A_1 B_1 (A_1 B_1)^T = (A^+ A_1) B_1 (A_1 B_1)^T \quad (4.12.5)$$

$$= A^+ (AB) (A_1 B_1)^T \quad (4.12.3)$$

$$= B_1 (A_1 B_1)^T \quad (4.12.1)$$

so (4.11.3) holds.

Similarly,

$$B_1 B_1^+ A_1^T (A_1 B_1) = (A^+ A_1) A_1^T (A_1 B_1) \quad (4.12.4)$$

$$= (A_1^+ A_1) (A_1^T) (A_1 B_1) \quad (4.12.5)$$

$$= A_1^T A_1 B_1$$

which proves (4.11.4), so that

$$(A_1 B_1)^+ = B_1^+ A_1^+.$$

The desired conclusion follows from (4.12.3). ■

(4.13) Exercise: If A is $n \times r$ and B is $r \times m$ then

$$(AB)^+ = B^+ A^+$$

if $\text{rk}(A) = \text{rk}(B) = r$.

(4.14) Exercise: $(AB)^+ = B^+ A^+$ if

(a) $A^T A = I$ or

(b) $BB^T = I$ or

(c) $B = A^T$ or

(d) $B = A^+$.

(4.15) Exercise: If H is rectangular and S is symmetric and nonsingular,

$$(SH)^+ = H^+ S^{-1} [I - (QS^{-1})^+ (QS^{-1})]$$

where

$$Q = (I - HH^+).$$

COMPUTATIONAL METHODS

In recent years, a sizable literature relating to the computation of pseudo-inverses has accompanied the rebirth of interest in the theory. In this chapter, we will describe four distinct approaches to the problem. The first method is based upon the Gramm–Schmidt orthogonalization (hereafter abbreviated GSO), the second is a modification of the “old faithful,” Gauss–Jordan elimination, the third is based upon the ideas of gradient projection and the last is an exotic procedure derived from the Cayley–Hamilton theorem.

(5.1) Method I (GSO, Rust, Burrus, and Schneeberger [1])

Let A be an $n \times m$ matrix of rank $k \leq \min(n, m)$. It is always possible to rearrange the columns of A so that the first k columns are linearly independent while the remaining columns are linear combinations of the first k .

This is the same as saying that for some *permutation* matrix, P (a square matrix of zeros and ones with exactly one nonzero entry in each row and column)

$$(5.1.1) \quad AP = (R|S)$$

where R is $n \times k$ and has rank k and the columns of S are linear combinations

of the columns of R :

$$(5.1.2) \quad S = RU \quad \text{for some } U. \quad (3.13.2)$$

P is an orthogonal matrix so that

$$A = (R|RU)P^T,$$

and

$$A^+ = P[R(I|U)]^+. \quad (4.14)$$

The rank of $(I|U)$ is the same as the rank of $(I|U)(I|U)^T = I + UU^T$, (4.10.2a) which is k . Therefore the rows of $(I|U)$ are linearly independent so that

$$[R(I|U)]^+ = (I|U)^+ R^+ \quad (4.13)$$

$$= (I|U)^T(I + UU^T)^{-1} R^+, \quad (3.5.2)$$

hence

$$(5.1.3) \quad A^+ = P(I|U)^T(I + UU^T)^{-1} R^+.$$

The last equation is the starting point for the computational procedure based on GSO; GSO is used to evaluate P , R^+ , U , and $(I + UU^T)^{-1}$:

(a) Evaluation of P

Perform a GSO on the columns of A , but *do not* normalize: i.e., denote the columns of A by a_1, a_2, \dots, a_m , let

$$c_1^* = a_1$$

$$c_j^* = a_j - \sum_{i \in S_j} \frac{a_j^T c_i^*}{\|c_i^*\|^2} c_i^*$$

where

$$S_j = \{i: i \leq j-1 \text{ and } c_i^* \neq 0\}.$$

The vectors c_j^* are mutually orthogonal and

$$\mathcal{L}(c_1^*, c_2^*, \dots, c_i^*) = \mathcal{L}(a_1, a_2, \dots, a_i) \quad \text{for each } i. \quad (2.8.1)$$

If the vectors $c_1^*, c_2^*, \dots, c_m^*$ are permuted so that the nonzero vectors (of which there will be k) come first, the same permutation matrix applied to the vectors a_1, a_2, \dots, a_m will rearrange them so that the first k are linearly independent, while the last $m-k$ are linear combinations of the first k , since $c_j^* = 0$ if and only if a_j is a linear combination of the preceding a 's. So, if P is any matrix for which

$$(5.1.4) \quad (c_1^* | c_2^* | \dots | c_m^*) P = (c_1 | c_2 | \dots | c_m)$$

where

$$\|c_j\| \begin{cases} > 0 & j = 1, 2, \dots, k \\ = 0 & j = k+1, \dots, m \end{cases}$$

then

$$(5.1.5) \quad AP = (a_1 | a_2 | \dots | a_m)P = (R | S)$$

where R is $n \times k$ of rank k and the columns of S are linear combinations of the columns of R .

(b) *Computation of R^+*

The (nonzero) vectors, c_1, c_2, \dots, c_k defined above, represent a GSO of the columns of R . If we let

$$(5.1.6) \quad Q = \left(\frac{c_1}{\|c_1\|} \mid \frac{c_2}{\|c_2\|} \mid \dots \mid \frac{c_k}{\|c_k\|} \right)$$

then

$$\mathcal{R}(Q) = \mathcal{R}(R)$$

so by (3.13.2) there is a $k \times k$ matrix B such that

$$(5.1.7) \quad RB = Q.$$

Indeed since R has rank k , $B = (R^T R)^{-1} R^T Q$. We will derive an algorithm for B in (5.1.16). Since the columns of Q are orthonormal, $Q^T Q = I$ so that B is nonsingular ($Q^T R B = I$), and hence

$$(5.1.8) \quad R = Q B^{-1}.$$

Exercise (4.14) applies again and we find that

$$(5.1.9) \quad R^+ = B Q^+ = B (Q^T Q)^+ Q^T = B Q^T.$$

It remains to evaluate B , U , and $(I + U U^T)^{-1}$.

(c) *Computation of B and U*

Denote the columns of R by r_1, r_2, \dots, r_k and the columns of S by s_1, s_2, \dots, s_{m-k} . The vectors $(c_1, c_2, \dots, c_k, c_{k+1}, \dots, c_m)$ defined in (5.1.4) represent a nonnormalized GSO of $(r_1, r_2, \dots, r_k, s_1, \dots, s_{m-k})$. Indeed

$$(5.1.10) \quad \begin{aligned} c_1 &= r_1 \\ c_j &= r_j - \sum_{i=1}^{j-1} \frac{r_j^T c_i}{\|c_i\|^2} c_i \quad j = 2, \dots, k \end{aligned}$$

and

$$(5.1.11) \quad 0 = c_{k+j} = s_j - \sum_{i=1}^k \frac{s_j^T c_i}{\|c_i\|^2} c_i \quad j = 1, \dots, m-k.$$

From (5.1.10) it is easy to deduce (by induction on j) that

$$(5.1.12) \quad c_j = \sum_{i=1}^j \gamma_{ij} r_i \quad j = 1, 2, \dots, k$$

where

$$(5.1.13) \quad \gamma_{ij} = \begin{cases} 0 & i > j \\ 1 & i = j \\ -\sum_{\alpha=i}^{j-1} \frac{(r_j^T c_\alpha)}{\|c_\alpha\|^2} \gamma_{i\alpha} & i < j. \end{cases}$$

On the other hand, (5.1.11) shows that

$$(5.1.14) \quad s_j = \sum_{i=1}^k \omega_{ij} r_i$$

where ω_{ij} is obtained by substituting (5.1.12) into (5.1.11):

$$(5.1.15) \quad \begin{aligned} s_j &= \sum_{\alpha=1}^k \frac{s_j^T c_\alpha}{\|c_\alpha\|^2} \left(\sum_{i=1}^{\alpha} \gamma_{i\alpha} r_i \right) \\ &= \sum_{i=1}^k \left(\sum_{\alpha=i}^k \frac{s_j^T c_\alpha}{\|c_\alpha\|^2} \gamma_{i\alpha} \right) r_i. \end{aligned}$$

$$(5.1.15) \quad \omega_{ij} = \sum_{\alpha=i}^k \frac{(s_j^T c_\alpha)}{\|c_\alpha\|^2} \gamma_{i\alpha} \quad i = 1, 2, \dots, k; \quad j = 1, \dots, m-k.$$

From (5.1.12) and (5.1.6), we see that

$$Q = \begin{pmatrix} \frac{c_1}{\|c_1\|} & \vdots & \dots & \vdots & \frac{c_k}{\|c_k\|} \end{pmatrix} = RB$$

where B is the $k \times k$ matrix whose (i, j) th entry is

$$(5.1.16) \quad \beta_{ij} = \gamma_{ij} / \|c_j\|$$

while from (5.1.14) we conclude that

$$(5.1.17) \quad S = RU$$

where U is the $k \times m-k$ matrix whose (i, j) th entry is ω_{ij} .

Notice that (5.1.13) defines γ_{ij} in terms of $\gamma_{ij-1}, \gamma_{ij-2}, \dots, \gamma_{ii}$. Computations are conveniently carried out in the following order:

$$\gamma_{11}; \quad \gamma_{22}, \gamma_{12}; \quad \gamma_{33}, \gamma_{23}, \gamma_{13}; \quad \gamma_{44}, \gamma_{34}, \gamma_{24}, \gamma_{14}; \quad \text{etc.}$$

(d) *Evaluation of $(I + UU^T)^{-1}$*

This inversion is achieved via one more GSO:

(5.1.18) **Theorem:** If U is a $k \times r$ matrix and a GSO is performed on the columns of

$$\begin{pmatrix} U \\ I \end{pmatrix},$$

the resulting matrix of orthonormal vectors is

$$V = \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}$$

where

$$V_2 V_2^T = (I + U^T U)^{-1}$$

and

$$I - V_1 V_1^T = (I + UU^T)^{-1}.$$

Comment: The rank of $\begin{pmatrix} U \\ I \end{pmatrix}$ is r since $\begin{pmatrix} U \\ I \end{pmatrix}$ has the same rank as $\begin{pmatrix} U \\ I \end{pmatrix}^T \begin{pmatrix} U \\ I \end{pmatrix} = I + U^T U$ ($r \times r$) which is nonsingular, (2.13), and hence has rank r . Therefore, the GSO, when performed on the columns of $\begin{pmatrix} U \\ I \end{pmatrix}$ will generate only nonzero vectors.

Proof of theorem: Let $H = \begin{pmatrix} U \\ I \end{pmatrix}$. H has rank r [so that $H^+ H = I$, (3.5.3)] and $\mathcal{R}(V) = \mathcal{R}(H)$, so the equation

$$HZ = V$$

has a solution

$$Z = H^+ V. \quad (3.13.2)$$

Since the columns of V are orthonormal, $V^T V = I$, hence $V^+ = (V^T V)^+ V^T = V^T$. Since $\mathcal{R}(V) = \mathcal{R}(H)$,

$$HH^+ = VV^+ = VV^T.$$

Therefore

$$\begin{aligned} ZZ^T &= H^+ (VV^T) H^{+T} = (H^T H)^+ \\ &= (H^T H)^{-1} \quad \text{since } H \text{ has rank } r. \end{aligned} \quad (4.10.2a) \text{ and } (3.5.1)$$

Since

$$HZ = \begin{pmatrix} U \\ -I \end{pmatrix} Z = \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}$$

we have

$$UZ = V_1$$

and

$$Z = V_2.$$

Therefore

$$V_2 V_2^T = ZZ^T = (H^T H)^{-1} = (I + U^T U)^{-1}.$$

The second part of the theorem follows from the identity

$$(I + UU^T)^{-1} = I - U(U^T U + I)^{-1} U^T$$

and the fact that

$$V_1 = UZ = UV_2.$$

Therefore

$$(I + UU^T)^{-1} = I - U(V_2 V_2^T) U^T = I - V_1 V_1^T. \quad \blacksquare$$

Summary of Method I

To find the pseudoinverse of the $n \times m$ matrix A :

1. Perform a GSO on the columns of A . Do not normalize. Call this set of vectors $(c_1^* | \dots | c_m^*)$.
2. Permute the c_j^* 's so that $(c_1 | c_2 | \dots | c_m) = (c_1^* | c_2^* | \dots | c_m^*) P$ where P is a permutation matrix chosen so that

$$\begin{aligned} c_j &\neq 0 & j &= 1, 2, \dots, k \\ c_j &= 0 & j &= k+1, \dots, m. \end{aligned}$$

3. Compute γ_{ij} for $j = i+1, \dots, k$; $i = 1, \dots, k$, according to (5.1.13) ($\gamma_{ii} = 1$, $\gamma_{ij} = 0$ if $i < j$).

4. B is the $k \times k$ matrix whose (i, j) th entry is $\gamma_{ij} / \|c_j\|$, U is the $k \times m-k$ matrix whose (i, j) th entry is ω_{ij} [given by (5.1.15)], $(I + UU^T)^{-1}$ is obtained by performing a (normalized) GSO on the columns of $\begin{pmatrix} U \\ I \end{pmatrix}$ and

$$Q = \begin{pmatrix} \frac{c_1}{\|c_1\|} & \dots & \frac{c_k}{\|c_k\|} \end{pmatrix}.$$

5. $A^+ = P(I \mid U)^T (I + UU^T)^{-1} BQ^T$.

Comment: A FORTRAN listing for this procedure is given in Rust *et al.* [1].

(5.1.19) **Example**

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

$$c_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad c_2 = \begin{pmatrix} -\frac{1}{2} \\ 1 \\ \frac{1}{2} \end{pmatrix}, \quad c_3 = c_4 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

$$k = 2, \quad P = I, \quad R = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix}, \quad S = \begin{pmatrix} 1 & 1 \\ -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

$$\gamma_{11} = 1$$

$$\gamma_{22} = 1 \quad \gamma_{12} = -\frac{1}{2}$$

$$\omega_{11} = 1 \quad \omega_{12} = 1$$

$$\omega_{21} = -1 \quad \omega_{22} = 0.$$

$$\beta_{11} = 1/\sqrt{2}$$

$$\beta_{22} = 2/\sqrt{6} \quad \beta_{12} = -1/\sqrt{6}.$$

$$B = \begin{pmatrix} 1/\sqrt{2} & 0 \\ 2/\sqrt{6} & -1/\sqrt{6} \end{pmatrix}, \quad Q = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{6} \\ 0 & 2/\sqrt{6} \\ 1/\sqrt{2} & 1/\sqrt{6} \end{pmatrix}.$$

$$\begin{pmatrix} U \\ -I \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \xrightarrow{\text{GSO}} V = \begin{bmatrix} 1/\sqrt{3} & 2/\sqrt{15} \\ -1/\sqrt{3} & 1/\sqrt{15} \\ 1/\sqrt{3} & -1/\sqrt{15} \\ 0 & 3/\sqrt{15} \end{bmatrix} = \begin{bmatrix} V_1 \\ V_2 \end{bmatrix}.$$

$$I - V_1 V_1^T = \frac{1}{5} \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix} = (I + U U^T)^{-1}.$$

$$(I + UU^T)^{-1}BQ^T = \frac{1}{15} \begin{pmatrix} 3 & 0 & 3 \\ -1 & 5 & 4 \end{pmatrix}.$$

$$A^+ = \begin{pmatrix} I \\ -\bar{U}^T \end{pmatrix} (I + UU^T)^{-1}BQ^T = \frac{1}{15} \begin{pmatrix} 3 & 0 & 3 \\ -1 & 5 & 4 \\ 4 & -5 & -1 \\ 3 & 0 & 3 \end{pmatrix}.$$

(5.1.20) **Exercise** *Alternate method for inverting $(I + UU^T)$:* Let the columns of U be denoted by u_1, u_2, \dots, u_r . Let

$$W_0 = I$$

$$W_n = W_{n-1} - \frac{(W_{n-1}u_n)(W_{n-1}u_n)^T}{1 + u_n^T W_{n-1}u_n} \quad n = 1, \dots, r.$$

Then for each n ,

$$W_n = \left(I + \sum_{j=1}^n u_j u_j^T \right)^{-1}$$

hence

$$W_r = (I + UU^T)^{-1}.$$

[Hint: Use (4.6.5) or prove directly by induction on n .]

(5.1.21) **Exercise** *Alternate method for the pseudoinversion of $(I|U)$ (Tewarson [2])*

- (a) If P is square and $P^T(I|U) = S^T$ where $S^T S = I$, then $(I|U)^+ = SP^T$.
 (b) If the GSO is applied to the columns of

$$\begin{matrix} k \\ r \end{matrix} \begin{pmatrix} I \\ -\bar{U}^T \end{pmatrix}$$

and the resulting set of orthonormal vectors are denoted by s_1, s_2, \dots, s_k , then there is a $k \times k$ matrix P such that

$$\begin{pmatrix} I \\ -\bar{U}^T \end{pmatrix} P = (s_1 | s_2 | \dots | s_k).$$

- (c) Let $S \equiv (s_1 | s_2 | \dots | s_k)$ be partitioned:

$$S = \begin{matrix} k \\ r \end{matrix} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix}.$$

Then

$$P = S_1 \quad \text{and} \quad (I|U)^+ = SS_1^T.$$

(5.2) Method II (Based on Gauss-Jordan elimination, Ben-Israel and Wersan [1], Noble [1])

If A is an $n \times m$ matrix of rank k , there always exists a nonsingular matrix E and an orthogonal matrix P such that

$$(5.2.1) \quad EA^TAP = \begin{matrix} & k & m-k \\ & \left(\begin{array}{c|c} I & L \\ \hline 0 & 0 \end{array} \right) \\ & m-k & \end{matrix}.$$

Indeed, there are many such E and P . For instance, if P diagonalizes $A^T A$ in such a way that the nonzero eigenvalues of $A^T A$ appear in the upper left-hand corner:

$$P^T A^T A P = \begin{matrix} & k & m-k \\ & \left(\begin{array}{c|c} D & 0 \\ \hline 0 & 0 \end{array} \right) \\ & m-k & \end{matrix}$$

then

$$E = \left(\begin{array}{c|c} D^{-1} & 0 \\ \hline 0 & I \end{array} \right) P^T$$

will do the trick:

$$EA^TAP = \left(\begin{array}{c|c} D^{-1} & 0 \\ \hline 0 & I \end{array} \right) (P^T A^T A P) = \left(\begin{array}{c|c} I & 0 \\ \hline 0 & 0 \end{array} \right)$$

which is a stronger version of (5.2.1). However, the method to be described here only requires that E and P be chosen to satisfy (5.2.1). The present method is based upon the following identity:

(5.2.2) Theorem: If E is nonsingular and P is orthogonal, chosen to satisfy (5.2.1), then

$$A^+ = P(EA^TAP)^+ EA^T.$$

Proof: The equation

$$A^TAX = A^T$$

always has a solution in X , (3.13.1), (3.13.2), hence the equation

$$(5.2.3) \quad A^TAPY = A^T$$

always has a solution in Y since P is nonsingular, hence

$$(5.2.4) \quad EA^TAPY = EA^T$$

always has a solution in Y .

Among all solutions to (5.2.3), the unique matrix which minimizes $\text{tr}(Y^T Y)$ is

$$(5.2.5) \quad \hat{Y} = (EA^TAP)^+ EA^T. \quad (3.13.8)$$

The set of matrices Y satisfying (5.2.4) is the same as the set of matrices satisfying (5.2.3) since E is nonsingular, so \hat{Y} also minimizes

$$\operatorname{tr}(Y^T Y) = \operatorname{tr}[(PY)^T (PY)] \quad (P \text{ is orthogonal})$$

over that class. By (3.13.8),

$$(5.2.6) \quad P \hat{Y} = (A^T A)^+ A^T = A^+$$

and the theorem follows when (5.2.6) and (5.2.5) are combined. ■

(5.2.7) **Corollary:** If E is nonsingular and P is orthogonal and $EA^T AP = \begin{pmatrix} H \\ 0 \end{pmatrix}$ then

$$A^+ = P(H^+ \mid 0)(EA^T).$$

It remains to show how to compute EA^T , H^+ , and P .

(a) *Computation of H , EA^T , and P*

Write down the augmented matrix, ${}_m(A^T A \mid A^T)$, and perform *row operations* on this matrix until the left block is reduced to the point where a permutation of its columns will result in the row echelon form:

$$\begin{aligned} {}_m(A^T A \mid A^T) &\xrightarrow[\text{only (step 1)}]{\text{row operations}} {}_m(EA^T A \mid EA^T) \\ &\xrightarrow[\substack{\text{permute first} \\ m \text{ columns} \\ \text{(step 2)}}]{\text{permute first}} {}_m(EA^T AP \mid EA^T) \\ &= {}_{m-k} \begin{pmatrix} k & m-k \\ I & L \\ 0 & 0 \end{pmatrix} EA^T. \end{aligned}$$

The elementary row operations are reversible so E is nonsingular, as required. The permutation matrix P is orthogonal and is recorded as the columns of $EA^T A$ are permuted to achieve row echelon form. The matrix EA^T occupies the right-hand block of the augmented matrix just after Step 1. The matrix H is $k \times m$ and is given by $(I \mid L)$ after Step 2.

(b) *Computation of H^+*

$$H^+ = (I \mid L)^+ = \begin{pmatrix} I \\ \bar{L}^T \end{pmatrix} (I + LL^T)^{-1}.$$

Evaluate $(I + LL^T)^{-1}$ either by (5.1.18) or (5.1.20), or evaluate $(I \mid L)^+$ by (5.1.21).

(5.2.8) Example

$$A = \begin{bmatrix} -1 & 0 & 1 & 2 \\ -1 & 1 & 0 & -1 \\ 0 & -1 & 1 & 3 \\ 0 & 1 & -1 & -3 \\ 1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -2 \end{bmatrix}$$

$$(A^T A | A^T) = \left[\begin{array}{cccc|cccccc} 4 & -2 & -2 & \textcircled{-2} & -1 & -1 & 0 & 0 & 1 & 1 \\ -2 & 4 & -2 & -8 & 0 & 1 & -1 & 1 & -1 & 0 \\ -2 & -2 & 4 & 10 & 1 & 0 & 1 & -1 & 0 & -1 \\ -2 & -8 & 10 & 28 & 2 & -1 & 3 & -3 & 1 & -2 \end{array} \right].$$

Pivot on the 4th element of the first row (which means "reduce the 4th element of all the other rows to zero by subtracting an appropriate multiple of the first row from each"):

$$\rightarrow \left[\begin{array}{cccc|cccccc} 4 & -2 & -2 & -2 & -1 & -1 & 0 & 0 & 1 & 1 \\ -18 & 12 & \textcircled{6} & 0 & 4 & 5 & -1 & 1 & -5 & -4 \\ 18 & -12 & -6 & 0 & -4 & -5 & 1 & -1 & 5 & 4 \\ 54 & -36 & -18 & 0 & -12 & -15 & 3 & -3 & 15 & 12 \end{array} \right].$$

Next, pivot on the third element of the second row:

$$\rightarrow \left[\begin{array}{cccc|cccccc} -2 & 2 & 0 & -2 & \frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \frac{1}{3} & -\frac{2}{3} & \frac{1}{3} \\ -18 & 12 & 6 & 0 & 4 & 5 & -1 & 1 & -5 & 4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right].$$

Next, divide the first row by -2 , the second by 6 :

$$\rightarrow \left[\begin{array}{cccc|cccccc} 1 & -1 & 0 & 1 & -\frac{1}{6} & -\frac{2}{6} & \frac{1}{6} & -\frac{1}{6} & \frac{2}{6} & \frac{1}{6} \\ -3 & 2 & 1 & 0 & \frac{4}{6} & \frac{5}{6} & -\frac{1}{6} & \frac{1}{6} & -\frac{5}{6} & -\frac{4}{6} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right]$$

$$= (EA^T A | EA^T).$$

This completes Step 1; EA^T is the right-hand 4×6 block. The left-hand block is reduced to row-echelon form by postmultiplication by

$$P = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

which puts column 4 into column 1, column 3 into column 2, column 1 into column 3, and column 2 into column 4. The result:

$$EA^TAP = \begin{pmatrix} H \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 1 & -1 \\ 0 & 1 & -3 & 2 \\ \hline & & 0 & \end{pmatrix}.$$

The matrix L is the upper right-hand block:

$$L = \begin{pmatrix} 1 & -1 \\ -3 & 2 \end{pmatrix}, \quad I + LL^T = \begin{pmatrix} 3 & -5 \\ -5 & 14 \end{pmatrix}.$$

$$(I + LL^T)^{-1} = \frac{1}{17} \begin{pmatrix} 14 & 5 \\ 5 & 3 \end{pmatrix}.$$

$$H^+ = \begin{bmatrix} (I + LL^T)^{-1} \\ \bar{L}^T(\bar{I} + \bar{L}L^T)^{-1} \end{bmatrix} = \frac{1}{17} \begin{pmatrix} 14 & 5 \\ 5 & 3 \\ -1 & -4 \\ -4 & 1 \end{pmatrix}.$$

$$(H^+ | 0)EA^T = \frac{1}{102} \begin{pmatrix} 6 & -3 & 9 & -9 & 3 & -6 \\ 7 & 5 & 2 & -2 & -5 & -7 \\ -15 & -18 & 3 & -3 & 18 & 15 \\ 8 & 13 & -5 & 5 & -13 & -8 \end{pmatrix}.$$

$$P(H^+ | 0)EAT = \frac{1}{102} \begin{pmatrix} -15 & -18 & 3 & -3 & 18 & 15 \\ 8 & 13 & -5 & 5 & -13 & -8 \\ 7 & 5 & 2 & -2 & -5 & -7 \\ -6 & -3 & 9 & -9 & 3 & -6 \end{pmatrix} = A^+.$$

(5.2.9) **Exercise:** Let E , A , and P be as defined in (5.2.1). Show that the last $m-k$ rows of EA^T are always zero. [*Hint:* $XA^T A = 0$ if and only if $XA^T = 0$. Specialize to matrices of the form

$$X = \begin{matrix} & k & m-k \\ n(0 \mid Y_1) \end{matrix}$$

Comment: A GATE 20 program for this procedure is given in Ben-Israel and Ijiri [1]. Additional refinements are contained in Tewarson [1].

(5.3) Method III (Based on gradient projection method, Pyle [1])

If A is an $n \times m$ matrix and $b \in \mathcal{R}(A)$, the equation

$$(5.3.1) \quad Ax = b$$

has at least one solution and

$$(5.3.2) \quad \hat{x} = A^+ b$$

is the only solution which lies in $\mathcal{R}(A^T)$, (3.1b).

Let the columns of A^T be denoted by a_1, a_2, \dots, a_n and denote by A_k (resp. b_k) the $k \times m$ matrix (resp. k -vector) obtained by deleting the last $n-k$ rows (resp. components) from A (resp. b). Since (5.3.1) has a solution, so does

$$(5.3.3) \quad A_k x_k = b_k \quad k = 1, 2, \dots, n,$$

since the set of simultaneous equations which (5.3.3) represents is a subset of those represented by (5.3.1).

Furthermore,

$$(5.3.4) \quad \hat{x}_k = A_k^+ b_k$$

is the only solution to (5.3.3) which lies in $\mathcal{R}(A_k^T) \equiv \mathcal{L}(a_1, \dots, a_k)$, (3.4, 3.1b). The present procedure develops a simple recursion which relates \hat{x}_{k+1} to \hat{x}_k . Since $\hat{x} = A^+ b$ is the same as \hat{x}_n , the recursion can be carried out n times and the desired solution to (5.3.1) results, provided b is in $\mathcal{R}(A)$. Extensions to the general case follow readily as we will show:

By definition, \hat{x}_1 is the unique vector in $\mathcal{L}(a_1)$ satisfying

$$a_1^T x_1 = \beta_1$$

where β_j is the j th component of b ($j = 1, \dots, n$).

Obviously

$$(5.3.5) \quad \hat{x}_1 = (a_1^T)^+ \beta_1 = \beta_1 a_1 (\|a_1\|^2)^+.$$

If \hat{x}_{k-1} is known, we construct \hat{x}_k as follows:

Let (h_1, h_2, \dots, h_n) be the nonnormalized set of vectors which result from a

Gramm–Schmidt orthogonalization of (a_1, \dots, a_n) :

$$(5.3.6) \quad \begin{aligned} h_1 &= a_1 \\ h_k &= a_k - \sum_{j \in S_k} (a_k^T h_j) h_j / \|h_j\|^2 \end{aligned}$$

where

$$S_k = \{j: j \leq k-1 \text{ and } \|h_j\| \neq 0\} \quad k = 1, \dots, n.$$

We have shown that $h_k \perp \mathcal{L}(a_1, \dots, a_{k-1})$, (2.8), and since \hat{x}_{k-1} satisfies

$$(5.3.7) \quad A_{k-1} \hat{x}_{k-1} = b_{k-1}$$

it follows that

$$(5.3.8) \quad a_j^T (\hat{x}_{k-1} + \alpha_k h_k) = \beta_j \quad j = 1, 2, \dots, k-1$$

for any scalar α_k . [Just write (5.3.7) in componentwise form.]

In particular, if

$$(5.3.9) \quad \hat{\alpha}_k = \begin{cases} 0 & \text{if } h_k = 0 \\ (\beta_k - a_k^T \hat{x}_{k-1}) / (h_k^T a_k) & \text{otherwise} \end{cases}$$

then

$$(5.3.10) \quad \hat{y}_k = \hat{x}_{k-1} + \hat{\alpha}_k h_k$$

satisfies

$$(5.3.11) \quad a_j^T \hat{y}_k = \beta_j \quad j \in S_{k+1}$$

and

$$(5.3.12) \quad \hat{y}_k \in \mathcal{L}(h_1, \dots, h_k).$$

By construction,

$$\begin{aligned} \mathcal{L}(h_j; j \in S_{k+1}) &= \mathcal{L}(h_1, \dots, h_k) \\ &= \mathcal{L}(a_1, \dots, a_k) = \mathcal{L}(a_j; j \in S_{k+1}) \end{aligned}$$

since $h_j = 0$ if and only if a_j is a linear combination of its predecessors, (2.8.6). Therefore, \hat{y}_k is the *unique* vector in $\mathcal{L}(a_j; j \in S_{k+1})$ satisfying (5.3.11). On the other hand,

$$\hat{x}_k = A_k^+ b_k \in \mathcal{L}(a_1, \dots, a_k) = \mathcal{L}(a_j; j \in S_{k+1})$$

satisfies

$$(5.3.13) \quad a_j^T \hat{x}_k = \beta_j \quad j = 1, \dots, k$$

and hence it also satisfies (5.3.11). Since \hat{y}_k is the *unique* vector in $\mathcal{L}(a_j; j \in S_{k+1})$ satisfying (5.3.11), $\hat{y}_k = \hat{x}_k$.

In summary:

(5.3.14) **Theorem:** If

$$A^T = (a_1 | a_2 | \cdots | a_n) \quad \text{and} \quad b = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{pmatrix} \in \mathcal{R}(A)$$

then

$$A^+b = \hat{x}_n$$

where

$$\hat{x}_0 = 0$$

$$\hat{x}_k = \hat{x}_{k-1} + \hat{\alpha}_k h_k \quad k = 1, 2, \dots, n$$

$$\hat{\alpha}_k = \begin{cases} 0 & \text{if } h_k = 0 \\ (\beta_k - a_k^T \hat{x}_{k-1}) / (h_k^T a_k) & \text{otherwise} \end{cases}$$

and $\{h_1, h_2, \dots, h_n\}$ are the nonnormalized vectors resulting from a GSO of $\{a_1, a_2, \dots, a_n\}$.

In general, if $b \notin \mathcal{R}(A)$ [or if you are not able to decide whether $b \in \mathcal{R}(A)$ or not, conveniently] resort to the following trick:

Let

$$d = A^T b$$

and

$$C = A^T A.$$

Then $d \in \mathcal{R}(A^T) = \mathcal{R}(C)$ so that (5.3.14) can be used to compute C^+d . Since $C^+d = (A^T A)^+ A^T b$, this additional step generalizes the procedure to the case of arbitrary b .

If, instead of A^+b , it is desired to compute A^+ , proceed in the following manner:

First, perform a GSO on the columns of A . Denote the *normalized* set of nonzero (orthonormal) vectors by d_1, d_2, \dots, d_r . These vectors span the same linear manifold that the columns of A span, namely $\mathcal{R}(A)$. By (3.7.3), it therefore follows that

$$AA^+ = \sum_{j=1}^r d_j d_j^T.$$

Denote the columns of AA^+ by b_1, b_2, \dots, b_n . Since $\mathcal{R}(A) = \mathcal{R}(AA^+) = \mathcal{L}(b_1, b_2, \dots, b_n)$, it must be that $b_j \in \mathcal{R}(A)$ for each j so that (5.3.14) can be used n times to compute A^+b_j ($j = 1, \dots, n$). Since

$$(A^+b_1 | A^+b_2 | \cdots | A^+b_n) = A^+(b_1 | b_2 | \cdots | b_n) = A^+(AA^+) = A^+,$$

this procedure generates the desired result.

Summary of Method III

1. If it is known that $b \in \mathcal{R}(A)$ then (5.3.14) can be used directly to construct A^+b .

2. If it is not known whether or not $b \in \mathcal{R}(A)$, compute $d = A^T b$, $C = A^T A$ and use (5.3.14) to compute C^+d which coincides with A^+b .

3. To compute A^+ , first perform a GSO on the columns of A . Denote the resulting orthonormal vectors by d_1, d_2, \dots, d_r . Construct the matrix $\sum_{j=1}^r d_j d_j^T$ and denote the columns of this matrix by b_1, b_2, \dots, b_n . Then for each j , $b_j \in \mathcal{R}(A)$ and (5.3.14) can be used to construct A^+b_j , $j = 1, \dots, n$.

$$A^+ = (A^+b_1 | A^+b_2 | \dots | A^+b_n).$$

(5.3.15) **Exercise:** In (5.3.14) we defined

$$\hat{\alpha}_k = \begin{cases} 0 & \text{if } h_k = 0 \\ (\beta_k - a_k^T \hat{x}_{k-1}) / (h_k^T a_k) & \text{otherwise.} \end{cases}$$

Show that $h_k^T a_k \neq 0$ if $h_k \neq 0$.

(5.3.16) **Example:** Compute A^+ where A is given by (5.1.19):

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

The columns of A are

$$c_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad c_2 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \quad c_3 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \quad c_4 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}.$$

The GSO generates the orthonormal set:

$$d_1 = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 1/\sqrt{2} \end{pmatrix} \quad d_2 = \begin{pmatrix} -1/\sqrt{6} \\ 2/\sqrt{6} \\ 1/\sqrt{6} \end{pmatrix}.$$

$$AA^+ = d_1 d_1^T + d_2 d_2^T = \frac{1}{3} \begin{pmatrix} 2 & -1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}.$$

The columns of AA^+ are

$$b_1 = \begin{pmatrix} -\frac{2}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix} \quad b_2 = \begin{pmatrix} -\frac{1}{3} \\ \frac{2}{3} \\ \frac{1}{3} \end{pmatrix} \quad b_3 = \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{2}{3} \end{pmatrix}.$$

To construct A^+b_j , we perform a GSO on the columns of A^T : The columns of A^T are

$$a_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix} \quad a_2 = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \quad a_3 = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix}.$$

The nonnormalized GSO produces

$$h_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix} \quad h_2 = \begin{pmatrix} \frac{1}{3} \\ 1 \\ -\frac{2}{3} \\ \frac{1}{3} \end{pmatrix} \quad h_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

To compute A^+b_1 , use (5.3.14):

$$\hat{\alpha}_1 = \frac{2\sqrt{3}}{9} \quad \hat{x}_1 = \frac{2}{9} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

$$\hat{\alpha}_2 = -\frac{\sqrt{15}}{45} \quad \hat{x}_2 = \frac{1}{15} \begin{pmatrix} 3 \\ -1 \\ 4 \\ 3 \end{pmatrix} = A^+b_1.$$

To compute A^+b_2 :

$$\hat{\alpha}_1 = \frac{\sqrt{3}}{9} \quad \hat{x}_1 = \frac{1}{9} \begin{pmatrix} -1 \\ 0 \\ -1 \\ -1 \end{pmatrix}$$

$$\hat{\alpha}_2 = \frac{\sqrt{15}}{9} \quad \hat{x}_2 = \frac{1}{3} \begin{pmatrix} 0 \\ -1 \\ -1 \\ 0 \end{pmatrix} = A^+ b_2.$$

To compute $A^+ b_3$:

$$\hat{\alpha}_1 = \frac{\sqrt{3}}{9} \quad \hat{x}_1 = \frac{1}{9} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

$$\hat{\alpha}_2 = \frac{4\sqrt{15}}{45} \quad \hat{x}_2 = \frac{1}{15} \begin{pmatrix} 3 \\ 4 \\ -1 \\ 3 \end{pmatrix} = A^+ b_3.$$

Thus

$$A^+ = (A^+ b_1 | A^+ b_2 | A^+ b_3) = \frac{1}{15} \begin{pmatrix} 3 & 0 & 3 \\ -1 & 5 & 4 \\ 4 & -5 & -1 \\ 3 & 0 & 3 \end{pmatrix}$$

which agrees with (5.1.19).

(5.4) Method IV (Based on the Cayley–Hamilton theorem, Decell [2], Ben-Israel and Charnes [1])

The present method is based upon two theorems. The first uses the classical Cayley–Hamilton relation (which says that any square matrix satisfies its own characteristic equation) to deduce an expression for the generalized inverse of a matrix in terms of its characteristic polynomial. The second theorem is a result of Fadeev and Fadeeva [1], which generates the coefficients of said characteristic polynomial in an efficient manner.

(5.4.1) Theorem: (a) Let A be an $n \times n$ symmetric matrix and let $\pi(\lambda) = \det(A - \lambda I)$, which can always be factored as follows:

$$\pi(\lambda) = \alpha \lambda^k (1 - \lambda \varphi(\lambda))$$

where $n - k$ is the rank of A .

Then if A is nonsingular,

$$A^{-1} = \varphi(A)$$

and generally

$$A^+ = \varphi(A) + \varphi(0)[A\varphi(A) - I].$$

(b) If H is an arbitrary $m \times n$ matrix and if the characteristic polynomial of $H^T H$ is given by $\alpha \lambda^k (1 - \lambda \varphi(\lambda))$, then

$$H^+ = \varphi(H^T H) H^T.$$

Comment: The matrix $\varphi(A)$ is obtained by raising A to the appropriate powers and summing these powers using the coefficients of $\varphi(\cdot)$ as weights.

Proof: (a) The Cayley-Hamilton theorem (cf., Bellman [1]) states that A satisfies the matrix equation

$$\pi(A) = 0.$$

Therefore

$$\alpha A^k (I - A\varphi(A)) = 0.$$

If A is nonsingular, $k = 0$ and hence

$$A\varphi(A) = I \quad \text{so that} \quad \varphi(A) = A^{-1}.$$

Generally,

$$A^k = A^{k+1}\varphi(A).$$

Since

$$\begin{aligned} (A^+)^{k+1} A^k &= A^+ (A^{+k} A^k) \\ &= A^+ (A^+ A) \end{aligned} \tag{3.11.3}$$

$$= A^+ (A A^+) \tag{3.11.6}$$

$$= A^+ \tag{3.9.3}$$

it follows that

$$A^+ = (A^+)^{k+1} A^{k+1} \varphi(A).$$

Again, using (3.11.3) and (3.11.6), we see that

$$(5.4.1.1) \quad A^+ = A A^+ \varphi(A).$$

Since $\varphi(A) - \varphi(0)$ involves only positive powers of A and since

$$A A^+ A^\alpha = A^\alpha \quad \text{if} \quad \alpha > 0 \tag{3.11.3}$$

it follows from (5.4.1.1) that

$$\begin{aligned} A^+ &= AA^+ [\varphi(A) - \varphi(0)] + AA^+ \varphi(0) \\ (5.4.1.2) \quad &= \varphi(A) - \varphi(0) + AA^+ \varphi(0) \end{aligned}$$

and so

$$AA^+ = A\varphi(A) + A(I - AA^+)\varphi(0).$$

Since $AA^+ = A^+A$ for symmetric A , (3.11.6), the second term vanishes and

$$(5.4.1.3) \quad AA^+ = A\varphi(A).$$

Since $\varphi(0)$ is a multiple of the identity, it commutes with $A\varphi(A)$ and so, if (5.4.1.3) is inserted into the right side of (5.4.1.2) we find

$$\begin{aligned} A^+ &= \varphi(A) + (A\varphi(A) - I)\varphi(0) \\ &= \varphi(A) + \varphi(0)(A\varphi(A) - I). \end{aligned}$$

(b) From (a),

$$(H^T H)^+ = \varphi(H^T H) + \varphi(0)[H^T H \varphi(H^T H) - I].$$

From (5.4.1.3) and (3.11.7)

$$H^T H \varphi(H^T H) = H^+ H$$

so that

$$\begin{aligned} H^+ &= (H^T H)^+ H^T = \varphi(H^T H) H^T + \varphi(0)[H^T H \varphi(H^T H) - I] H^T \\ &= \varphi(H^T H) H^T + \varphi(0)(H^+ H - I) H^T \\ &= \varphi(H^T H) H^T \quad (\text{since } H^+ H H^T = H^T). \quad \blacksquare \end{aligned}$$

Superficially, the last result appears to be of theoretical interest only, owing to the fact that $\varphi(A)$ is defined in terms of the characteristic polynomial of A which, in turn, is defined in terms of a determinant which requires a prohibitively large amount of computation for large matrices. The following result of Fadeev and Fadeeva [1] reduces that problem to manageable proportions:

(5.4.2) **Theorem:** Let A be an $n \times n$ symmetric matrix and define

$$(5.4.2.1) \quad \left\{ \begin{array}{l} A_1 = A \\ \gamma_k = \text{tr } A_k / k \\ B_k = A_k - \gamma_k I \\ A_{k+1} = AB_k \end{array} \right\} \quad k = 1, 2, \dots, n-1.$$

($\text{tr } A_k$ is the sum of A_k 's diagonal elements.)

Let

$$(5.4.2.2) \quad M = \begin{cases} \text{the first value of } k \leq n \text{ for which } AB_k = 0 \text{ if such exists,} \\ n & \text{otherwise,} \end{cases}$$

and let

$$(5.4.2.3) \quad r \text{ be the largest } k \leq M \text{ for which } \gamma_k \neq 0.$$

Then,

$$(5.4.2.4) \quad \pi(\lambda) \equiv \det(A - \lambda I) = (-1)^n \gamma_r \lambda^{n-r} (1 - \varphi(\lambda))$$

where

$$(5.4.2.5) \quad \varphi(\lambda) = (\gamma_r)^{-1} \left[\lambda^{r-1} - \sum_{j=1}^{r-1} \gamma_j \lambda^{r-1-j} \right].$$

Proof: The proof consists of two parts: First we show that γ_k is the coefficient of

$$(-1)^{n+1} \lambda^{n-k}$$

in the expansion of $\det(A - \lambda I)$ for $k = 1, \dots, n$. Then we use that result to show that $\gamma_k = 0$ for $k \geq r+1$. The desired conclusion follows easily thereafter.

Proof that

$$(5.4.2.6) \quad \det(A - \lambda I) = (-1)^n \left[\lambda^n - \sum_{k=1}^n \gamma_k \lambda^{n-k} \right]:$$

Here, $\gamma_1 = \text{tr } A$ which is the coefficient of $(-1)^{n+1} \lambda^{n-1}$ in the expansion of $\det(A - \lambda I)$. We proceed by induction, supposing that $\gamma_1, \gamma_2, \dots, \gamma_{k-1}$ are, respectively, the coefficients of $(-1)^{n+1} \lambda^{n-1}, (-1)^{n+1} \lambda^{n-2}, \dots, (-1)^{n+1} \lambda^{n-k+1}$ in the expansion of $\det(A - \lambda I)$.

Define

$$(5.4.2.7) \quad \sigma_k \equiv \text{tr}(A^k).$$

From (5.4.2.1),

$$A_{k+1} = AA_k - \gamma_k A$$

which can be iterated backward to obtain

$$(5.4.2.8) \quad A_k = A^k - \sum_{j=1}^{k-1} \gamma_j A^{k-j} \quad k = 1, 2, \dots, n$$

and hence from (5.4.2.7)

$$(5.4.2.9) \quad \text{tr}(A_k) = \sigma_k - \sum_{j=1}^{k-1} \gamma_j \sigma_{k-j}.$$

It is well known that for any A , $\text{tr}(A)$ is the sum of A 's eigenvalues, and if $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of the symmetric matrix A , then $\lambda_1^k, \dots, \lambda_n^k$ are the eigenvalues of A^k , so that

$$\sigma_k = \sum_{j=1}^n \lambda_j^k.$$

Furthermore, Newton's formula states that for any polynomial,

$$\lambda^n - \sum_{j=1}^n \beta_j \lambda^{n-j}$$

having roots at $\lambda_1, \lambda_2, \dots, \lambda_n$, the relations

$$(5.4.2.10) \quad k\beta_k = s_k - \sum_{j=1}^{k-1} \beta_j s_{k-j}$$

hold for $k = 1, 2, \dots, n$, where

$$s_k = \sum_{j=1}^k \lambda_j^k \quad (\text{Bôcher [1]}).$$

Writing

$$\det(A - \lambda I) = (-1)^n \left[\lambda^n - \sum_{j=1}^n \beta_j \lambda^{n-j} \right]$$

we see that under the induction hypothesis, $\beta_j = \gamma_j$, ($j = 1, 2, \dots, k-1$) so by (5.4.2.10),

$$(5.4.2.11) \quad k\beta_k = \sigma_k - \sum_{j=1}^{k-1} \gamma_j \sigma_{k-j}.$$

By (5.4.2.9) and (5.4.2.1)

$$k\beta_k = \text{tr}(A_k) = k\gamma_k$$

which shows that $\gamma_k = \beta_k$ and hence establishes the induction hypothesis for all k .

The recursion (5.4.2.1) guarantees that $A_k = 0$, $B_k = 0$, and $\gamma_k = 0$ for all $k > M$ if $AB_M = 0$ for some $M < n$. The definition of r therefore implies that $\gamma_k = r$ for $k > r$. From this and (5.4.2.6),

$$\begin{aligned} \det(A - \lambda I) &= (-1)^n \left[\lambda^n - \sum_{j=1}^r \gamma_j \lambda^{n-j} \right] \\ &= (-1)^n \gamma_r \lambda^{n-r} \left[1 - (\lambda/\gamma_r) \left(\lambda^{r-1} - \sum_{j=1}^{r-1} \gamma_j \lambda^{r-1-j} \right) \right]. \end{aligned}$$

This proves (5.4.2.4) and (5.4.2.5). ■

The application of (5.4.1) and (5.4.2) to the pseudoinversion of an $n \times m$ matrix is particularly amusing:

(5.4.3) **Theorem:** Let $A = H^T H$ (where H is an arbitrary $m \times n$ matrix), and define A_k, B_k, γ_k, M , and r as in (5.4.2). Then

$$(5.4.3.1) \quad H^+ = (\gamma_r)^{-1} B_{r-1} H^T$$

and the rank of H is r .

Proof: The rank of H is the same as the rank of A . The rank of A is

$$n - (\text{the multiplicity of the characteristic root at } \lambda = 0)$$

since A is symmetric. By (5.4.2.4) this multiplicity is $n - r$, which proves that the rank of H and A is r .

By (5.4.2.5),

$$\varphi(A) = (\gamma_r)^{-1} \left[A^{r-1} - \sum_{j=1}^{r-1} \gamma_j A^{r-1-j} \right]$$

whereas

$$A_{r-1} - \gamma_{r-1} I = A^{r-1} - \sum_{j=1}^{r-1} \gamma_j A^{r-1-j}$$

by (5.4.2.8). Thus

$$\begin{aligned} \varphi(A) &= (\gamma_r)^{-1} (A_{r-1} - \gamma_{r-1} I) \\ &= (\gamma_r)^{-1} B_{r-1}. \end{aligned}$$

The conclusion follows from (5.4.1b). ■

Summary of Method IV

To find H^+ where H is an $m \times n$ matrix:

1. Let $A_1 = H^T H$,
2. $\gamma_k = \text{tr}(A_k/k)$, $B_k = A_k - \gamma_k I$, $A_{k+1} = AB_k$,

$$M = \begin{cases} \text{first value of } k \text{ for which } AB_k = 0 \text{ if such exists and is} \\ \text{less than } n \\ n \quad \text{otherwise,} \end{cases}$$

$$r = \text{largest } k \leq M \text{ for which } \gamma_k \neq 0,$$

3. $H^+ = (\gamma_r)^{-1} B_{r-1} H^T$.

Comment: Although it is true that $A^{-1} = \varphi(A)$ for nonsingular symmetric A , it is not generally true that $A^+ = \varphi(A)$ as evidenced by the example

$$A = \text{diag}(0, 0, \frac{1}{2}, \frac{1}{3}).$$

For this example

$$\varphi(\lambda) = 5 - 6\lambda$$

so that

$$\varphi(A) = \text{diag}(5, 5, 2, 3)$$

whereas

$$A^+ = (0, 0, 2, 3) = \varphi(A) + \varphi(0)[A\varphi(A) - I].$$

(5.4.4) **Example**

$$H = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 2 & 1 & 0 \\ 3 & 1 & -1 \end{pmatrix} \quad A_1 = A = H^T H = \begin{pmatrix} 15 & 6 & -3 \\ 6 & 3 & 0 \\ -3 & 0 & 3 \end{pmatrix}$$

$$\gamma_1 = 21$$

$$B_1 = A_1 - 21I = \begin{pmatrix} -6 & 6 & -3 \\ 6 & -18 & 0 \\ -3 & 0 & -18 \end{pmatrix}$$

$$AB_1 = A_2 = 9 \begin{pmatrix} -5 & -2 & 1 \\ -2 & -2 & -2 \\ 1 & -2 & -5 \end{pmatrix}$$

$$\gamma_2 = -54$$

$$B_2 = A_2 + 54I = 9 \begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix}$$

$$A_3 = AB_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$M = r = 2$$

$$H^+ = \frac{1}{\gamma_2} B_1 H^T = -\frac{1}{18} \begin{pmatrix} -1 & -1 & -2 & -3 \\ -4 & 2 & -4 & 0 \\ -7 & 5 & -2 & 3 \end{pmatrix}.$$

(5.4.5) **Exercise:** Prove the Cayley-Hamilton theorem for symmetric matrices. (*Hint:* Use the diagonalization theorem.)

(5.4.6) **Exercise:** Establish the result analogous to (5.4.3), using the characteristic polynomial for HH^T instead of H^TH .

(5.4.7) *General comments*

In Methods I-IV, the option always exists between working with A or A^T . For example, in Method I, A^+ can be found by performing a GSO on the columns of A or one can compute $(A^T)^+$ by performing a GSO on the columns of A^T . Similarly, $(I + UU^T)^{-1}$ can be evaluated by performing a GSO on the columns of $\begin{pmatrix} U \\ I \end{pmatrix}$ or on the columns of $\begin{pmatrix} U^T \\ I \end{pmatrix}$. The proper choice is governed mainly by the size of the matrices involved.

All four methods depend crucially upon the computational determination of the rank of the matrix being pseudoinverted. In some of these cases, this is done during the course of a GSO, at that point where one decides whether a vector which is numerically close to zero, is *actually* zero. In Method II, a decision must be made as to whether the Gauss-Jordan elimination has reduced a row to zero or not. If an error (usually due to roundoff) is made at such stages, like as not, the error will be propagated through the remainder of the procedure in a discontinuous manner and cause large errors in the final result. A minor modification significantly improves the GSO in this regard. Whereas the "naive" GSO of (2.8) orthogonalizes the h -vectors in the order they are given (so that for each j , $\mathcal{L}(u_1, \dots, u_j) = \mathcal{L}(h_1, \dots, h_j)$, the u 's being the orthogonal set induced by the h 's), the so called "modified GSO" (Osborne [1]) derives each u_{j+1} from that h -vector whose projection on $\mathcal{L}^\perp(u_1, \dots, u_j)$ is longest. Thus, the borderline cases (is the present h -vector linearly independent of the previously used ones?) are put off until last.

Additional algorithms for pseudoinversion are described in the papers by Pereyre and Rosen [1], Golub and Kahan [1], and Golub [1, 2], all of which pay particular attention to the question of numerical stability.

The recursions of (4.3) and (4.6) can be interpreted as computational algorithms for C_m^+ and $(C_m C_m^T)^+$ but the comments above, apply quite strongly in these cases. Extreme care must be exercised in making the decision whether or not a vector c_{m+1} is a linear combination of its predecessors. We will return to these recursions in Chapters VIII and IX.

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Part II

STATISTICAL APPLICATIONS

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THE GENERAL LINEAR HYPOTHESIS

In this chapter, we will apply the results obtained so far to some “classical” statistical problems and thereby produce streamlined derivations (and generalizations) for many of the most important results in linear regression analysis. In particular, we will deal with the Gauss–Markov theorem, the distribution theory for best linear unbiased estimator residuals under the normality hypothesis, confidence ellipsoids for linear regression parameters under the normality assumption, the distribution of the likelihood ratio statistic for testing the general linear hypothesis and its relation to confidence ellipsoids, the relationship between Gauss–Markov estimates and “naive” least squares estimates, and the theory of orthogonal designs.

In fairness to the reader, we admit that this chapter presupposes a familiarity with elementary statistical concepts (as exemplified by the usual introductory, but *post calculus*, course in statistics). Such notions as *independence*, *expectation*, *normal distributions*, *tests of hypotheses*, *variance*, etc. are used freely without much in the way of preliminaries.

If things get too heavy, the reader can skip to Chapters VII and VIII which are essentially nonstatistical. Chapter IX is probabilistic in spirit.

(6.1) Best Linear Unbiased Estimation; The Gauss-Markov Theorem

In many applications, observations are made on a random process, and it is felt that a reasonable "model" for the observations is of the form

$$\zeta(\tau_j) = \sum_{i=1}^p \alpha_i \varphi_i(\tau_j) + \text{a residual}$$

where τ_j is the value of the j th *independent* variable (e.g., the *time* at which the j th observation was made, or the *concentration* of a catalyst in some chemical experiment, or the *amount* of drug injected into the j th laboratory animal in a drug trial experiment); $\zeta(\tau_j)$ is the *observation* (or *datum*, or *dependent variable*) corresponding to the *level* τ_j ; the φ_i 's are a specified family of functions and the α 's are parameters whose value is to be estimated from the data.

(6.1.1) **Example:** The voltage drop across a length of wire is proportional to the current flowing through the wire, the constant of proportionality being the resistance of that wire. It is further known that the resistance of a wire (of uniform thickness) is proportional to its length. The constant of proportionality is the resistance per unit length of the wire and is to be measured as follows. A long length of wire is connected in series to a resistor and a voltage source. See Figure 1. A voltmeter is used to measure the difference

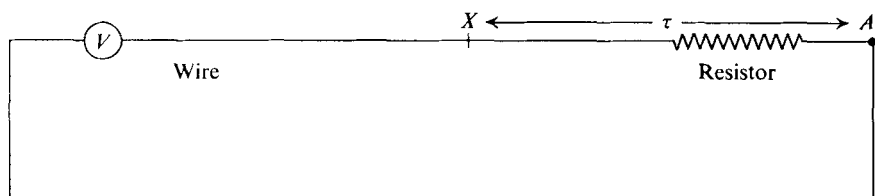


Figure 1.

in voltage between the fixed point A and the variable point X . As X moves, the distance, τ , between X and A changes. The voltage drop, $\zeta(\tau)$, is recorded at various values of τ (say $\tau_1, \tau_2, \dots, \tau_n$). Since the resistance between A and X is a linear function of τ , a sensible model for this data is

$$\zeta(\tau_j) = \rho\tau_j + R + \text{residual error}$$

so long as X is to the left of the resistor (which is used to prevent "short circuiting" the voltage source). Here, ρ is the resistance per unit length, R is the resistance between A and the left end of the resistor. For this model, $\varphi_1(\tau) = \tau$, $\varphi_2(\tau) = 1$, $\alpha_1 = \rho$, and $\alpha_2 = R$. The residual errors are due to inaccuracy in measurement and in the physical model for the phenomenon being studied.

(6.1.2) **Example:** The mean daily temperature at a given location fluctuates in a quasi-periodic manner with the period of the fluctuation corresponding to the change of seasons. If mean temperatures are recorded daily, then a reasonable model for the temperature $\zeta(\tau_j)$ on the τ_j th day is

$$\zeta(\tau_j) = \alpha_0 + \sum_{i=1}^k \alpha_i \cos \frac{2\pi i \tau_j}{365.25} + \beta_i \sin \frac{2\pi i \tau_j}{365.25} + \text{residual}$$

where the period 365.25 takes into account that a calendar year is slightly out of phase with a solar year. The number of harmonics (k) should be chosen reasonably small to keep the model simple. The α 's and β 's are not known and must be estimated from the data. The residual error now is attributable mainly to the nondeterministic nature of temperature variation rather than errors in measurement.

Both examples are special cases of a so-called *general linear model* in which the vector of observations

$$(6.1.3) \quad \mathbf{z} = \begin{pmatrix} \zeta(\tau_1) \\ \zeta(\tau_2) \\ \vdots \\ \zeta(\tau_n) \end{pmatrix}$$

is assumed to take the form

$$(6.1.4) \quad \mathbf{z} = H\mathbf{x} + \mathbf{v}$$

where H is an $n \times p$ matrix whose j th row is

$$(6.1.5) \quad h_j^T = (\varphi_1(\tau_j), \varphi_2(\tau_j), \dots, \varphi_p(\tau_j))$$

\mathbf{x} is the p -dimensional vector of unknown coefficients which is to be estimated from the data:

$$(6.1.6) \quad \mathbf{x} = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_p \end{pmatrix}$$

and \mathbf{v} is a vector of residuals which is assumed to be a vector random variable with mean value 0:

$$(6.1.7) \quad \mathcal{E}\mathbf{v} = 0.$$

Following Scheffé [1] we define a *parametric function* ψ to be a scalar-valued linear function of the unknown vector parameter \mathbf{x} :

$$\psi = c^T \mathbf{x}$$

where c is a specified p -dimensional vector. (For instance, each component of \mathbf{x} is a *parametric function*.)

A parametric function ψ is said to be *estimable* if it has an *unbiased* linear estimate. (This means that there exists a vector of constant coefficients a , such that

$$\mathcal{E}a^T\mathbf{z} = \psi$$

no matter what the true value of x .) The question of estimability for parametric functions is easily decided:

(6.1.8) **Theorem:** The parametric function $\psi = c^T x$ is estimable if and only if $H^+ Hc = c$ [i.e., if and only if $c \in \mathcal{R}(H^T)$].

Proof: Since $\mathcal{E}a^T\mathbf{z} = a^T \mathcal{E}\mathbf{z} = a^T [\mathcal{E}Hx + \mathcal{E}\mathbf{v}]$ and since $\mathcal{E}\mathbf{v} = 0$ and Hx is nonrandom, we see that $\psi = c^T x$ is estimable if and only if there exists a vector a such that

$$(6.1.8.1) \quad a^T Hx = c^T x \quad \text{for all } x.$$

But (6.1.8.1) holds for all x if and only if there exists an a such that $H^T a - c$ is orthogonal to all x and the last is true if and only if there is a vector a such that

$$(6.1.8.2) \quad H^T a = c. \quad (2.9.4)$$

The conclusion now follows from (3.12c). ■

The *variance* of an unbiased estimator for ψ is a hallowed measure of its efficacy. Suppose that the residual covariance matrix is denoted by V^2 :

$$(6.1.9) \quad \mathcal{E}\mathbf{v}\mathbf{v}^T = V^2$$

where V^2 is an $n \times n$ nonnegative definite matrix. [Since $u^T V^2 u = u^T (\mathcal{E}\mathbf{v}\mathbf{v}^T) u = \mathcal{E}(\mathbf{v}^T u)^2$, it follows that $u^T V^2 u \geq 0$ for all u and is therefore nonnegative as asserted.]

If $\hat{\psi} = a^T \mathbf{z}$ is an unbiased estimator for ψ , its variance is

$$(6.1.10) \quad \mathcal{E}(\hat{\psi} - \psi)^2 = \mathcal{E}(a^T \mathbf{v})(\mathbf{v}^T a) = a^T V^2 a.$$

The *best* linear unbiased estimator (BLUE) for ψ is (defined to be) the one with minimum variance. It is a quick matter to exhibit a formula for the BLUE of a parametric function:

(6.1.11) **Theorem:** Let $\psi = c^T x$ be an estimable parametric function and let

$$(6.1.11.1) \quad \hat{a} = (I - \bar{V}^+ V)(H^+)^T c$$

where

$$(6.1.11.2) \quad \bar{V} = V(I - HH^+).$$

Then

- (a) $\hat{\Psi} = \hat{a}^T \mathbf{z}$ is a BLUE for ψ and
- (b) if Ψ^* is any other linear unbiased estimator for ψ

$$\mathcal{E}(\Psi^* - \psi)^2 > \mathcal{E}(\hat{\Psi} - \psi)^2$$

unless $\hat{\Psi} = \Psi^*$ with probability 1.

Proof: If ψ is estimable, then $a^T \mathbf{z}$ is unbiased if and only if a satisfies (6.1.8.2). By (3.12c), all such a 's are of the form

$$(6.1.11.3) \quad a_u = H^T c - (I - HH^+)u \quad \text{for some } u.$$

(We used the identity $HH^+ = H^T H^T$.) The variance of the estimator $\Psi_u = a_u^T \mathbf{z}$ is

$$\mathcal{E}(\Psi_u - \psi)^2 = \mathcal{E}(a_u^T \mathbf{z} - c^T x)^2 = \mathcal{E}a_u^T (\mathbf{z} - Hx)^2$$

[since a satisfies (6.1.8.2)]

$$\begin{aligned} &= \mathcal{E}(a_u^T \mathbf{v})^2 \\ &= a_u^T V^2 a_u = \|Va_u\|^2 \end{aligned}$$

(V is the symmetric square root of V^2 .) Since

$$\|Va_u\|^2 = \|VH^T c - \bar{V}u\|^2$$

we see that the variance of the linear unbiased estimator Ψ_u is minimized if u is of the form

$$\hat{u} = \bar{V}^+ VH^T c + (I - \bar{V}^+ \bar{V})w$$

where w is free to vary. Thus by (6.1.11.3) and (3.13.10),

$$\begin{aligned} a_{\hat{u}} &= (I - \bar{V}^+ V)(H^T)^T c - (I - HH^+)(I - \bar{V}^+ \bar{V})w \\ &= \hat{a} - (I - HH^+)(I - \bar{V}^+ \bar{V})w \end{aligned}$$

where w is free to vary. But for such an $a_{\hat{u}}$

$$\begin{aligned} \mathcal{E}[(a_{\hat{u}} - \hat{a})^T \mathbf{z}]^2 &= w^T (I - \bar{V}^+ \bar{V})(I - HH^+)V^2(I - HH^+)(I - \bar{V}^+ V)w \\ &= \|\bar{V}(I - \bar{V}^+ \bar{V})w\|^2 \\ &= 0 \end{aligned} \tag{3.9.1}$$

so that

$$(a_{\hat{u}} - \hat{a})^T \mathbf{z} = 0 \quad \text{with probability 1.}$$

Thus, *all* BLUE's for ψ are of the form $\hat{a}^T \mathbf{z}$ with probability 1. ■

Comment: The results of (6.1.11) hold whether the residual covariance is singular or not. This result generalizes the Gauss–Markov theorem, which restricts its attention to nonsingular residual covariances (cf. Zyskind and Martin [1], Zyskind [1]).

Theorem (6.1.11) yields the classical result as a special case:

(6.1.12) **Theorem** (Gauss–Markov): Let

$$\bar{V} = V(I - HH^+),$$

$$(6.1.12.1) \quad G = H^+[I - (\bar{V}^+V)^T]$$

and

$$(6.1.12.2) \quad \hat{\mathbf{x}} = G\mathbf{z}.$$

Then

(a) $\mathcal{E}\hat{\mathbf{x}} = H^+H\mathbf{x}$ for all \mathbf{x} .

(b) If $\psi = c^T\mathbf{x}$ is an estimable parametric function, there is a unique BLUE for ψ , namely $c^T\hat{\mathbf{x}}$.

(c) If V^2 is nonsingular

$$\hat{\mathbf{x}} = (H^TV^{-2}H)^+H^TV^{-2}\mathbf{z}.$$

Proof: (a) $\mathcal{E}\hat{\mathbf{x}} = GH\mathbf{x} = H^+H\mathbf{x} - H^+V^T(\bar{V}^+)^TH\mathbf{x}$.

But

$$(\bar{V}^+)^TH = (\bar{V}\bar{V}^T)^+ \bar{V}H \quad (3.8.1)$$

and

$$\bar{V}H = 0. \quad (6.11.2)$$

(b) The BLUE for ψ is unique by (6.1.11), and is expressible in the form

$$\hat{\psi} = \hat{a}^T\mathbf{z}$$

where

$$\hat{a} = [H^+(I - (\bar{V}^+V)^T)]^T c = G^T c.$$

Thus

$$\hat{\psi} = c^T\hat{\mathbf{x}} \quad \text{as asserted.}$$

(c) By (6.1.12.1),

$$G = H^+V[I - (\bar{V}^+V)^T]V^{-1}$$

if V is nonsingular.

By (3.13.10)

$$\bar{V}^{+\mathbf{T}} = [(I - HH^+) \bar{V}^+]^{\mathbf{T}}$$

so

$$\bar{V}^{+\mathbf{T}} V = \bar{V}^{+\mathbf{T}} \bar{V}^{\mathbf{T}}$$

hence

$$G = H^+ V [I - \bar{V}^{\mathbf{T}} + \bar{V}^{\mathbf{T}}] V^{-1}.$$

By (4.15) the last is exactly

$$(V^{-1}H)^+ V^{-1}$$

since

$$\bar{V}^{\mathbf{T}} = QV \quad \text{where} \quad Q = I - HH^+$$

so that

$$G = (V^{-1}H)^+ V^{-1} = (H^{\mathbf{T}} V^{-2} H)^+ H^{\mathbf{T}} V^{-2} \quad (3.8.1)$$

and

$$\hat{\mathbf{x}} = G\mathbf{z} = (H^{\mathbf{T}} V^{-2} H)^+ H^{\mathbf{T}} V^{-2} \mathbf{z}. \quad \blacksquare$$

Comment: When V^2 is nonsingular, then $\hat{\mathbf{x}} = (V^{-1}H)^+ V^{-1} \mathbf{z}$ minimizes

$$\|V^{-1} \mathbf{z} - V^{-1} H\mathbf{x}\|^2 = (\mathbf{z} - H\mathbf{x})^{\mathbf{T}} V^{-2} (\mathbf{z} - H\mathbf{x})$$

which is a weighted sum of squares. In the special case where

$$V = \text{diag}(v_1, v_2, \dots, v_n)$$

$$\mathbf{z} = \begin{pmatrix} \zeta_1 \\ \vdots \\ \zeta_n \end{pmatrix} \quad \text{and} \quad H = \begin{pmatrix} h_1^{\mathbf{T}} \\ -\frac{h_1^{\mathbf{T}}}{v_1} \\ h_2^{\mathbf{T}} \\ -\frac{h_2^{\mathbf{T}}}{v_2} \\ \vdots \\ -\frac{h_n^{\mathbf{T}}}{v_n} \end{pmatrix}$$

$\hat{\mathbf{x}}$ minimizes

$$\sum_{j=1}^n (\zeta_j - h_j^{\mathbf{T}} \mathbf{x}) / v_j^2$$

which is the sum of squares of the deviations between each observation, ζ_j , and its expectation, each term being weighted according to that observation's accuracy ($v_j^2 = \text{variance of } \zeta_j$). Accurate observations (small v_j) are weighted more heavily than inaccurate ones. This interpretation is explored in greater depth in Chapter VII, where we examine the relationship between constrained least squares estimators and weighted least squares.

(6.1.13) **Counterexample:** If V^2 is singular, the BLUE for $c^T x$ is not $c^T(H^T V^{+2} H)^+ H^T V^{+2} z$: Take

$$V = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad H = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad x = \xi \quad (\text{scalar}) \quad z = \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix}.$$

Componentwise,

$$\zeta_1 = \xi + v_1 \quad \text{where } v_1 \text{ has unit variance}$$

$$\zeta_2 = \xi.$$

The second observation gives an error-free look at the unknown parameter and the best estimator would be ζ_2 .

On the other hand,

$$(H^T V^{+2} H)^+ = 1 \quad H^T V^{+2} = (1 \ 0)$$

so if $c = 1$,

$$c^T(H^T V^{+2} H)^+ H^T V^{+2} z = \zeta_1$$

which is not correct.

The correct result is obtained if (6.1.12.2) is used:

$$H^+ = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad I - HH^+ = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \quad \bar{V} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ 0 & 0 \end{pmatrix}$$

$$\bar{V}^+ = \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix} \quad \bar{V}^+ V = \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix};$$

$$I - (\bar{V}^+ V)^T = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \quad G = H^+ [I - (\bar{V}^+ V)^T] = (0 \ 1) \quad Gz = \zeta_2.$$

(6.1.14) **Exercise:** When do least squares estimators coincide with Gauss-Markov estimators?

If $z = Hx + v$ where $\mathcal{E}vv^T = V^2$, the *naive least squares* estimate is defined to be

$$\hat{\mathbf{x}} = H^+ z.$$

If $\psi = c^T x$ is an estimable parametric function, the naive least squares estimate for ψ is defined to be $c^T \hat{\mathbf{x}}$.

(6.1.14.1) Show that the naive least squares estimate for every estimable parametric function is a BLUE if and only if

$$\bar{V}^+ \bar{V} = (\bar{V}^+ V)$$

where

$$\bar{V} = V(I - HH^+).$$

(6.1.14.2) If V is nonsingular, the condition in (6.1.14.1) reduces to

$$(\bar{V})^+ = (I - HH^+)V^{-1}.$$

(6.1.14.3) In general, the condition (6.1.14.1) is equivalent to

$$\mathcal{R}(V^2H) \subseteq \mathcal{R}(H)$$

(i.e., the range of H is invariant under V^2).

Comment (Jocular): Naive least squares estimates $\hat{\mathbf{x}}$ are chosen so that $\|\mathbf{z} - H\mathbf{x}\|^2$ has “tiniest residual.” If $c^T\mathbf{x}$ is estimable, $c^T\hat{\mathbf{x}}$ is unbiased. Therefore, $c^T\hat{\mathbf{x}}$ is a TRUE (tiniest residual unbiased estimator) for $c^T\mathbf{x}$. (6.7.3) says that $\hat{\mathbf{x}}$ is TRUE-BLUE if and only if $\mathcal{R}(V^2H) \subseteq \mathcal{R}(H)$.

Other conditions equivalent to (6.7) are given in Zyskind [1], Krusbal [1], Mitra *et al.* [1], and Watson [1]. For instance, it is shown by Zyskind that (6.7.1) is equivalent to $\mathcal{R}(H) = \mathcal{L}(y_1, \dots, y_r)$ where the y_j 's are a subset of V 's eigenvectors. Mitra *et al.* show that another necessary and sufficient condition is that V^2 should be of the form

$$V^2 = HSH^T + (I - HH^+)T(I - HH^+) + k^2I$$

where S, T are nonnegative definite and k is a scalar.

(6.1.15) **Exercise** *Generalized least squares* (Price [1])

It has been shown that $\hat{\mathbf{x}} = H^+\mathbf{z}$ is the unique vector which minimizes $\|\mathbf{x}\|^2 \equiv \mathbf{x}^T\mathbf{x}$, among those which also minimize $(\mathbf{z} - H\mathbf{x})^T(\mathbf{z} - H\mathbf{x})$. Let V^2 and W^2 be nonnegative-definite matrices.

Show that among those \mathbf{x} 's which minimize $(\mathbf{z} - H\mathbf{x})^TV^2(\mathbf{z} - H\mathbf{x})$, one which minimizes $\|\mathbf{x}\|_{W^2}^2 \equiv \mathbf{x}^TW^2\mathbf{x}$ is

$$\bar{\mathbf{x}} = [I - (PW^2P)^+PW^2](H^TV^2H)^+H^TV^2\mathbf{z}$$

where

$$P = I - (VH)^+(VH).$$

Are there others?

(6.2) Distribution for Quadratic Forms in Normal Random Variables

In this section, we will investigate the distribution theory for certain types of quadratic forms in random variables which have normal distributions and

apply these results to regression analysis (tests of the general linear hypothesis and construction of confidence ellipsoids).

We first review some well-known facts about normal random variables (Scheffé [1]; Anderson [1]).

(6.2.1) If $\xi_1, \xi_2, \dots, \xi_n$ have a joint normal distribution, they are mutually independent if and only if their covariance matrix is diagonal.

(6.2.2) If $\xi_1, \xi_2, \dots, \xi_n$ are independent and normally distributed with means $\mu_1, \mu_2, \dots, \mu_n$ and unit variances, then the distribution of

$$\sum_{j=1}^n \xi_j^2$$

depends on the μ_j 's only through

$$\delta = \left(\sum_{j=1}^n \mu_j^2 \right)^{1/2}$$

and this distribution is a *noncentral chi-squared* distribution with n degrees of freedom and noncentrality parameter δ . If $\delta = 0$, the distribution is a chi-square distribution (central), with reference to centrality usually omitted.

(6.2.3) If χ_n^2 has a noncentral chi-square distribution with n degrees of freedom and noncentrality parameter δ and if χ_m^2 is independent of χ_n^2 and has a (central) chi-square distribution with m degrees of freedom, then

$$n^{-1} \chi_n^2 / m^{-1} \chi_m^2$$

has a *noncentral F* distribution with n and m degrees of freedom and noncentrality parameter δ . Reference to centrality is usually omitted when $\delta = 0$.

(6.2.4) The random vector \mathbf{z} has a multivariate normal distribution with mean \mathbf{m} and covariance R if and only if there exists a matrix H such that

(a) $\mathbf{z} = H\mathbf{x} + \mathbf{m}$, where the components of \mathbf{x} are independent normal random variables with mean zero and unit variance, and

(b) $R = HH^T$.

If $(\frac{\mathbf{u}}{\sqrt{\mathbf{v}}})$ has a zero mean multivariate normal distribution, then \mathbf{u} is independent of \mathbf{v} if and only if

$$\mathcal{C}\mathbf{u}\mathbf{v}^T = 0.$$

If \mathbf{z} is a vector random variable which has a multivariate normal distribution with mean \mathbf{m} and nonsingular covariance R , the density function of \mathbf{z} has the form

$$\text{const} \times \exp - \frac{1}{2}(\mathbf{z} - \mathbf{m})^T R^{-1}(\mathbf{z} - \mathbf{m}).$$

There is a well known proverb in statistical lore that asserts "the exponent of a normal distribution with nonsingular covariance has a chi-square distribution." We will now prove a generalized version of this statement.

(6.2.5) **Theorem:** If \mathbf{z} is a vector random variable having a normal distribution with mean \mathbf{m} and covariance R and if the rank of R is ρ , then

(a) $\mathbf{z}^T R^+ \mathbf{z}$ has a noncentral chi-square distribution with ρ degrees of freedom (df) and noncentrality parameter

$$\delta = (\mathbf{m}^T R^+ \mathbf{m})^{1/2}.$$

(b) $(\mathbf{z} - \mathbf{m})^T R^+ (\mathbf{z} - \mathbf{m})$ has a chi-square distribution with ρ df.

Proof: R is nonnegative definite since

$$\mathbf{u}^T R \mathbf{u} = \mathcal{E}(\mathbf{u}^T \mathbf{x})^2 \geq 0 \quad \text{where } \mathbf{x} = \mathbf{z} - \mathbf{m},$$

so R has a symmetric square root $R^{1/2}$. Let $\mathbf{m}_1 = (R^{1/2})^+ \mathbf{m}$ and $\mathbf{m}_2 = (I - R^{1/2} R^{1/2+}) \mathbf{m}$. Then

$$\mathbf{m} = R^{1/2} \mathbf{m}_1 + \mathbf{m}_2.$$

If \mathbf{y} is a normally distributed random vector with mean zero and covariance I , then

$$\bar{\mathbf{z}} \equiv R^{1/2}(\mathbf{y} + \mathbf{m}_1) + \mathbf{m}_2$$

has the same distribution as \mathbf{z} , hence $\bar{\mathbf{z}}^T R^+ \bar{\mathbf{z}}$ has the same distribution as $\mathbf{z}^T R^+ \mathbf{z}$ and it will suffice to establish (a) for $\bar{\mathbf{z}}^T R^+ \bar{\mathbf{z}}$:

$$\begin{aligned} \bar{\mathbf{z}}^T R^+ \bar{\mathbf{z}} &= (\mathbf{y} + \mathbf{m}_1)^T R^{1/2} R^+ R^{1/2} (\mathbf{y} + \mathbf{m}_1) \\ &\quad + 2(\mathbf{y} + \mathbf{m}_1)^T R^{1/2} R^+ \mathbf{m}_2 \\ &\quad + \mathbf{m}_2^T R^+ \mathbf{m}_2. \end{aligned}$$

Since $R^{1/2} R^{1/2+} = R R^+ = R^+ R$, it is easy to see that $R^+ \mathbf{m}_2 = 0$. Using the diagonalization theorem, it is easy to see that

$$R^{1/2} R^+ R^{1/2} = R R^+ = \sum_{i=1}^{\rho} \mathbf{r}_i \mathbf{r}_i^T$$

where the \mathbf{r}_i 's are the orthonormal eigenvectors associated with the nonzero eigenvalues of R :

$$\begin{aligned} R &= \sum_{j=1}^{\rho} \lambda_j \mathbf{r}_j \mathbf{r}_j^T & R^{1/2} &= \sum_{j=1}^{\rho} \lambda_j^{1/2} \mathbf{r}_j \mathbf{r}_j^T \\ R^+ &= \sum_{j=1}^{\rho} \lambda_j^{-1} \mathbf{r}_j \mathbf{r}_j^T. \end{aligned} \quad [\text{cf. (3.6)}]$$

$$R R^+ = R^+ R = \sum_{j=1}^{\rho} \mathbf{r}_j \mathbf{r}_j^T.$$

Thus

$$\begin{aligned}\bar{\mathbf{z}}^T R^+ \bar{\mathbf{z}} &= (\mathbf{y} + m_1)^T R R^+ (\mathbf{y} + m_1) \\ &= \sum_{j=1}^{\rho} [r_j^T (\mathbf{y} + m_1)]^2.\end{aligned}$$

The vector random variable

$$P(\mathbf{y} + m_1)$$

where

$$P = \begin{pmatrix} r_1^T \\ \vdots \\ r_\rho^T \end{pmatrix}$$

has a multivariate normal distribution with mean Pm_1 and covariance

$$P(\mathcal{E} \mathbf{y} \mathbf{y}^T) P^T = P P^T \quad \text{since } \mathcal{E} \mathbf{y} \mathbf{y}^T = I.$$

The rows of P are orthonormal, so $P P^T = I$ (of order $\rho \times \rho$), hence by (6.2.1), the components of $P(\mathbf{y} + m_1)$ are *independent* normal with mean zero and unit variance, so by (6.2.2)

$$\|P(\mathbf{y} + m_1)\|^2$$

has a noncentral chi-square distribution with ρ degrees of freedom and noncentrality parameter $\|Pm_1\|$. But

$$\|P(\mathbf{y} + m_1)\|^2 = (\mathbf{y} + m)^T P^T P (\mathbf{y} + m)$$

and

$$P^T P = \sum_{j=1}^{\rho} r_j r_j^T = R^+ R.$$

Therefore

$$\|P(\mathbf{y} + m_1)\|^2 = \bar{\mathbf{z}}^T R^+ \bar{\mathbf{z}}^T$$

and

$$\|Pm_1\|^2 = m_1^T R R^+ m_1 = m^T R^+ m = \delta^2$$

since

$$m_1^T R R^+ m_1 = \|R R^+ m_1\|^2$$

and

$$R R^+ m_1 = R R^+ (R^{1/2})^+ m = R^+{}^{1/2} m.$$

Part (b) follows as a special case of part (a) when $m = 0$, since $\bar{\mathbf{z}} - m$ has mean zero. ■ (See Rao [1], for related results.)

(6.2.6) **Exercise:** If \mathbf{z} has a multivariate distribution with mean m and covariance $\sigma^2 I$, and if R is a projection matrix with rank ρ , then

$$\sigma^{-2} \|\mathbf{Rz}\|^2$$

has a noncentral chi-square distribution with noncentrality parameter

$$\sigma^{-1} (m^T R m)^{1/2} \quad \text{and} \quad \rho \text{ df.}$$

(6.3) Estimable Vector Parametric Functions and Confidence Ellipsoids in the Case of Normal Residuals

In (6.1) we introduced the notion of an estimable parametric function (a real-valued linear function of the unknown vector parameter). We now extend this notion to vector-valued linear functions:

If

$$\mathbf{z} = H\mathbf{x} + \mathbf{v}$$

where \mathbf{v} is a zero mean vector random variable, H is a known matrix and \mathbf{x} is an unknown vector parameter, we define an *estimable vector parametric function* (evpf) to be any vector-valued linear function of \mathbf{x} whose components are estimable parametric functions. Thus, an evpf is any vector of the form $y = G\mathbf{x}$ where G is a matrix whose rows are $g_1^T, g_2^T, \dots, g_k^T$, where, for each j , $g_j^T \mathbf{x}$ is an estimable parametric function.

It is a trivial consequence of (6.1.8) that

$$(6.3.1) \quad G\mathbf{x} \text{ is an evpf if and only if } \mathcal{R}(G^T) \subseteq \mathcal{R}(H^T).$$

By (3.13.1), the last statement is equivalent to

$$(6.3.2) \quad G\mathbf{x} \text{ is an evpf if and only if } GH^+H = G.$$

If

$$G = \begin{pmatrix} g_1^T \\ \vdots \\ g_k^T \end{pmatrix}$$

is an evpf, then each component of $G\mathbf{x}$ has a BLUE, namely $g_j^T \hat{\mathbf{x}}$ where $\hat{\mathbf{x}}$ is the Gauss-Markov estimator defined in (6.1.12). Henceforth, we will call $G\hat{\mathbf{x}}$ the BLUE for the evpf $G\mathbf{x}$.

For the sake of the following discussion, let us focus our attention on the case where the residuals \mathbf{v} are normally distributed and have covariance V^2 proportional to the identity matrix:

$$(6.3.3) \quad V^2 = \mathcal{E}\mathbf{v}\mathbf{v}^T = \sigma^2 I.$$

According to (6.1.12), the BLUE for an evpf, $y = Gx$, is $\hat{y} = G\hat{x}$, where

$$\hat{x} = H^+ z$$

happens to be the least squares estimate for x .

The vector random variable $\hat{y} - y$ has zero mean (since $G\hat{x}$ is unbiased), and the covariance of $\hat{y} - y$ is

$$\mathcal{E}(\hat{y} - y)(\hat{y} - y)^T.$$

But

$$y = Gx = GH^+ Hx \quad (6.3.2)$$

and

$$\hat{y} = G\hat{x} = GH^+ z = GH^+ Hx + GH^+ v$$

so that

$$\hat{y} - y = GH^+ v$$

and

$$\begin{aligned} (6.3.4) \quad \text{Cov}(\hat{y} - y) &\equiv \mathcal{E}(\hat{y} - y)(\hat{y} - y)^T = \mathcal{E}[(GH^+)vv^T(GH^+)^T] \\ &= \sigma^2 G(H^T H)^+ G^T. \end{aligned}$$

Therefore, $\hat{y} - y$ has a multivariate normal distribution with mean zero and covariance $\sigma^2 G(H^T H)^+ G^T$ so, by virtue of (6.2.5),

$$(6.3.5) \quad \sigma^{-2}(y - \hat{y})^T [G(H^T H)^+ G^T]^+ (y - \hat{y})$$

has a (central) chi-square distribution with k_1 ($= \text{rank } GH^+$) degrees of freedom, since

$$\text{rk}(A) = \text{rk}(AA^T) \quad \text{for any matrix } A. \quad (4.10.2)$$

It is always true that

$$(6.3.6) \quad \mathcal{R}(GH^+ H) \subseteq \mathcal{R}(GH^+) \subseteq \mathcal{R}(G)$$

and if G is an evpf

$$\mathcal{R}(G) = \mathcal{R}(GH^+ H) \quad \text{as well} \quad (6.3.2)$$

so in this case,

$$(6.3.6.1) \quad \mathcal{R}(GH^+) = \mathcal{R}(G).$$

Therefore

$$k_1 = \text{rk}(G).$$

The last result [concerning the distribution of (6.3.5)] can be used to construct a confidence set for y provided σ^2 is *known*. For if $\omega_{1-\alpha}$ is the upper

100(1- α) percentile of said chi-square distribution, then

$$\Pr \{ (y - \hat{y})^T [G(H^T H)^+ G^T]^+ (y - \hat{y}) \leq \sigma^2 \omega_{1-\alpha} \} = 1 - \alpha$$

which means that the ellipsoid

$$\mathcal{S}(\sigma^2 \omega_{1-\alpha}) = \{u: (u - \hat{y})^T [G(H^T H)^+ G^T]^+ (u - \hat{y}) \leq \sigma^2 \omega_{1-\alpha}\}$$

covers the true value of y with probability $1 - \alpha$.

If σ^2 is *not known*, its maximum likelihood estimate is proportional to

$$(6.3.7) \quad \hat{\sigma}^2 = (n - k_2)^{-1} \|\mathbf{z} - H\hat{\mathbf{x}}\|^2$$

where n is the number of observations (= number of rows in H) and k_2 is the rank of H .

We will now show that

$$(6.3.8) \quad \begin{cases} \sigma^{-2} \|\mathbf{z} - H\hat{\mathbf{x}}\|^2 \text{ has a chi-square distribution} \\ \text{with } n - k_2 \text{ df and is independent of } y - \hat{y}. \end{cases}$$

Once (6.3.8) is established, then from (6.2.3)

$$(6.3.9) \quad \frac{(k_1 \sigma^2)^{-1} (y - \hat{y})^T [G(H^T H)^+ G^T]^+ (y - \hat{y})}{\sigma^{-2} \hat{\sigma}^2} \\ = (k_1 \hat{\sigma}^2)^{-1} (y - \hat{y})^T [G(H^T H)^+ G^T]^+ (y - \hat{y})$$

has an F distribution with k_1 and $n - k_2$ df. Because of this, the ellipsoid $\mathcal{S}(k_1 \hat{\sigma}^2 \tilde{\omega}_{1-\alpha})$ covers the true value of y with probability $1 - \alpha$ if $\tilde{\omega}_{1-\alpha}$ is the upper 100(1- α) percentile of said F distribution, since

$$\Pr \{ y \in \mathcal{S}(k_1 \hat{\sigma}^2 \tilde{\omega}_{1-\alpha}) \} \\ = \Pr \{ (k_1 \hat{\sigma}^2)^{-1} (y - \hat{y})^T [G(H^T H)^+ G^T]^+ (y - \hat{y}) \leq \tilde{\omega}_{1-\alpha} \} = 1 - \alpha.$$

To prove (6.3.8), we notice that

$$(6.3.10) \quad \begin{aligned} \sigma^{-1} (\mathbf{z} - H\hat{\mathbf{x}}) &= \sigma^{-1} (I - HH^+) \mathbf{z} \\ &= \sigma^{-1} (I - HH^+) (H\mathbf{x} + \mathbf{v}) \\ &= \sigma^{-1} (I - HH^+) \mathbf{v} \end{aligned}$$

where $\sigma^{-1} \mathbf{v}$ has a multivariate normal distribution with mean zero and covariance I . Furthermore,

$$\hat{\mathbf{y}} - y = GH^+ \mathbf{v} \quad (6.3.4)$$

hence

$$\sigma^{-2} \mathcal{E}(\hat{\mathbf{y}} - y)(\mathbf{z} - H\hat{\mathbf{x}})^T = GH^+(I - HH^+) = 0$$

so that $(\hat{y} - y)$ and $\mathbf{z} - H\hat{\mathbf{x}}$ are jointly normally distributed (both are linear functions of \mathbf{v}) and are uncorrelated. By (6.2.4) they must be independent. So, then, are

$$\hat{\sigma}^2 = (n - k_2)^{-1} \|\mathbf{z} - H\hat{\mathbf{x}}\|^2 \quad \text{and} \quad (y - \hat{y}).$$

(6.3.10) shows that $\sigma^{-1}(\mathbf{z} - H\hat{\mathbf{x}})$ is of the form $\sigma^{-1}P\mathbf{v}$ where P is a projection, so by (6.2.6) $(\sigma^2)^{-1} \|\mathbf{z} - H\hat{\mathbf{x}}\|^2$ has a chi-square distribution with as many degrees of freedom as the rank of $I - HH^+$.

(6.3.11) **Exercise**

$$\text{rk}(I - HH^+) = \text{rk}(I) - \text{rk}(H).$$

[Hint: I is a projection and so is HH^+ . Use (4.10.1)–(4.10.3).]

(6.3.12) **Exercise:** Generalize the results of (6.3) to the case where the residuals have a normal distribution with zero mean and covariance $\sigma^2 V^2$ where σ^2 is unknown and V^2 is a known nonnegative-definite matrix.

(6.4) Tests of the General Linear Hypothesis

Consider the observation model described in the previous section. Instead of a confidence ellipsoid for $y = Gx$, we seek a test of the hypothesis

$$\mathcal{H}_0: Gx = 0.$$

In the case where σ^2 is known, it turns out that the appropriate likelihood ratio test is to reject \mathcal{H}_0 for large values of

$$(6.4.1) \quad \rho_1 = \sigma^{-2} \{ \|\mathbf{z} - H\bar{\mathbf{x}}\|^2 - \|\mathbf{z} - H\hat{\mathbf{x}}\|^2 \}$$

where $\hat{\mathbf{x}}$ is the least squares estimator for x :

$$(6.4.2) \quad \hat{\mathbf{x}} = H^+ \mathbf{z}$$

and $\bar{\mathbf{x}}$ is the least squares estimator for x , computed subject to the constraint that $Gx = 0$:

$$(6.4.3) \quad \bar{\mathbf{x}} = \bar{H}^+ \mathbf{z}$$

where

$$\bar{H} = H(I - G^+G). \quad (3.12.4)$$

If σ^2 is not known, the likelihood ratio test rejects \mathcal{H}_0 for large values of

$$(6.4.4) \quad \rho_2 = \|\mathbf{z} - H\bar{\mathbf{x}}\|^2 / \|\mathbf{z} - H\hat{\mathbf{x}}\|^2.$$

(6.4.5) **Exercise:** If $\hat{\mathbf{x}}^*$ and $\bar{\mathbf{x}}^*$ are any other least squares estimate and constrained least squares estimate (computed subject to $G\mathbf{x} = 0$), show that

$$H\hat{\mathbf{x}}^* = H\hat{\mathbf{x}} \quad \text{and} \quad H\bar{\mathbf{x}}^* = H\bar{\mathbf{x}}$$

so that the same test statistics, ρ_1 and ρ_2 , result. [*Hint:* Use (3.12.2) and (3.12.4).]

We will now prove that

(6.4.6) ρ_1 has a noncentral chi-square distribution with $\tau [= \text{rk}(HH^+ - \bar{H}\bar{H}^+)]$ degrees of freedom and noncentrality parameter δ where

$$(6.4.7) \quad \delta = \sigma^{-1} \|(HH^+ - \bar{H}\bar{H}^+)H\mathbf{x}\|$$

and

$$(6.4.8) \quad \frac{n-k_2}{\tau}(\rho_2 - 1) \equiv \frac{n-k_2}{\tau} \left[\frac{\|\mathbf{z} - H\bar{\mathbf{x}}\|^2 - \|\mathbf{z} - H\hat{\mathbf{x}}\|^2}{\|\mathbf{z} - H\hat{\mathbf{x}}\|^2} \right]$$

has a noncentral F distribution with τ and $n-k_2$ degrees of freedom [$k_2 = \text{rk}(H)$] and noncentrality parameter δ .

Furthermore,

$$(6.4.9) \quad \delta = 0 \quad \text{if} \quad G\mathbf{x} = 0$$

so that the distributions of ρ_1 and ρ_2 are central chi-square and F when the null hypothesis is true.

To prove (6.4.7), we note that

$$(6.4.10) \quad \mathcal{R}(\bar{H}) \subseteq \mathcal{R}(H)$$

so that $(HH^+)(\bar{H}\bar{H}^+) = \bar{H}\bar{H}^+$. After a slight amount of algebra, it follows that

$$\begin{aligned} (6.4.11) \quad \|(HH^+ - \bar{H}\bar{H}^+)\mathbf{z}\|^2 &= \|(\mathbf{z} - \bar{H}\bar{H}^+\mathbf{z}) - (\mathbf{z} - HH^+\mathbf{z})\|^2 \\ &= \|(\mathbf{z} - \bar{H}\bar{\mathbf{x}}) - (\mathbf{z} - H\hat{\mathbf{x}})\|^2 \\ &= \|\mathbf{z} - \bar{H}\bar{\mathbf{x}}\|^2 - \|\mathbf{z} - H\hat{\mathbf{x}}\|^2. \end{aligned}$$

Thus

$$\rho_1 = \|\sigma^{-1}(HH^+ - \bar{H}\bar{H}^+)\mathbf{z}\|^2.$$

The random variable $\sigma^{-1}\mathbf{z}$ is normally distributed with mean $\sigma^{-1}H\mathbf{x}$ and covariance I . Since $\mathcal{R}(\bar{H}) \subseteq \mathcal{R}(H)$, $HH^+ - \bar{H}\bar{H}^+$ is the projection on $\mathcal{R}(H) - \mathcal{R}(\bar{H})$, (2.7.4b), and so (6.2.6) guarantees that

$$\|\sigma^{-1}(HH^+ - \bar{H}\bar{H}^+)\mathbf{z}\|^2$$

has a noncentral chi-square distribution with noncentrality parameter δ and τ df. This establishes (6.4.7).

To prove (6.4.8), it suffices to point out that $\mathbf{z} - H\hat{\mathbf{x}} = (I - HH^+)\mathbf{z}$ is uncorrelated with $(HH^+ - \bar{H}\bar{H}^+)\mathbf{z}$ because

$$\begin{aligned} \mathcal{E}(\mathbf{z} - H\hat{\mathbf{x}})[(HH^+ - \bar{H}\bar{H}^+)(\mathbf{z} - H\mathbf{x})]^T \\ = (I - HH^+)\mathcal{E}\mathbf{v}\mathbf{v}^T(HH^+ - \bar{H}\bar{H}^+) \\ = 0 \end{aligned}$$

because $\mathcal{E}\mathbf{v}\mathbf{v}^T = \sigma^2 I$ and $HH^+(\bar{H}\bar{H}^+) = \bar{H}\bar{H}^+$, (6.4.10). Therefore $\|\mathbf{z} - H\hat{\mathbf{x}}\|^2$ is independent of $\|(HH^+ - \bar{H}\bar{H}^+)\mathbf{z}\|^2 = \|\mathbf{z} - \bar{H}\bar{\mathbf{x}}\|^2 - \|\mathbf{z} - H\hat{\mathbf{x}}\|^2$, (6.4.11), and we showed in (6.3) that $(\sigma^2)^{-1}\|\mathbf{z} - H\hat{\mathbf{x}}\|^2$ has a central chi-square distribution with $n - k_2$ df, where $k_2 = \text{rk}(H)$. The result now follows from (6.2.3).

To prove (6.4.9), we note that $\mathbf{x} = (I - G^+G)\mathbf{x}$ if $G\mathbf{x} = 0$ so that

$$\begin{aligned} (HH^+ - \bar{H}\bar{H}^+)H\mathbf{x} &= HH^+H\mathbf{x} - \bar{H}\bar{H}^+H\mathbf{x} \\ &= H\mathbf{x} - \bar{H}\bar{H}^+H(I - G^+G)\mathbf{x} \\ &= H(I - G^+G)\mathbf{x} - \bar{H}\bar{H}^+\bar{H}\mathbf{x} \\ &= 0 \end{aligned}$$

which implies

$$\delta = 0.$$

If $\delta > 0$, the values of \mathbf{p}_1 and \mathbf{p}_2 tend to be larger than if $\delta = 0$. To test \mathcal{H}_0 at the significance level α , reject \mathcal{H}_0 if $\mathbf{p}_1 > \omega_{1-\alpha}$ [the upper 100 $(1-\alpha)$ percentile of the central chi-square distribution with τ df] provided σ is known. Otherwise, reject \mathcal{H}_0 if $\tau^{-1}(m - k_2)(\mathbf{p}_2 - 1) > \tilde{\omega}_{1-\alpha}$, the upper 100 $(1-\alpha)$ percentile of the central F distribution with τ and $n - k_2$ df. The power of both tests against various alternatives is a function of δ only, and may be computed using the appropriate noncentral F and chi-square tables.

(6.5) The Relationship between Confidence Ellipsoids for $G\mathbf{x}$ and Tests of the General Linear Hypothesis

We will now show that the likelihood ratio tests which we developed in (6.4) (σ known and σ unknown) are equivalent to the test procedures which reject the hypothesis $G\mathbf{x} = 0$ whenever the $1-\alpha$ -level confidence ellipsoid (σ known, σ unknown) for $G\mathbf{x}$ fails to cover the point 0. (Recall, we developed two ellipsoids; one for known sigma, one for unknown sigma.) This result, plus an alternate representation for δ , the noncentrality parameter, and τ , the rank of $HH^+ - \bar{H}\bar{H}^+$ follow easily from

(6.5.1) **Theorem:** If $\mathcal{R}(G^T) \subseteq \mathcal{R}(H^T)$ and $\bar{H} = H(I - G^+G)$ then

$$(a) \quad \text{rk}[H(I - G^+G)] = \text{rk}(H) - \text{rk}(G)$$

and

$$(b) \quad (GH^+)^+(GH^+) = HH^+ - \bar{H}\bar{H}^+$$

$$\begin{aligned} \text{Proof: } (a) \quad \text{rk}[H(I - G^+G)] &= \text{rk}[H^+H(I - G^+G)] & (4.10.2b) \\ &= \text{rk}[H^+H - G^+G] \end{aligned}$$

since $H^+HG^+G = G^+G$ whenever $\mathcal{R}(G^T) \subseteq \mathcal{R}(H^T)$, (3.5), so that

$$\begin{aligned} \text{rk}[H(I - G^+G)] &= \text{rk}(H^+H - G^+G) \\ &= \text{rk}(H^+H) - \text{rk}(G^+G) & (4.10.3) \end{aligned}$$

$$= \text{rk}(H) - \text{rk}(G). \quad (4.10.2)$$

(b) Let

$$P_1 = (GH^+)^+(GH^+)$$

and

$$P_2 = \bar{H}\bar{H}^+.$$

$$\mathcal{R}(P_1) = \mathcal{R}(H^{+T}G^T) \subseteq \mathcal{R}(H^{+T}) = \mathcal{R}(H) = \mathcal{R}(HH^+) \quad (3.5) \text{ and } (3.11.5)$$

and

$$\mathcal{R}(P_2) = \mathcal{R}(\bar{H}) \subseteq \mathcal{R}(H) = \mathcal{R}(HH^+).$$

By virtue of the fact that $\mathcal{R}(G^T) \subseteq \mathcal{R}(H^T)$, it follows that

$$(6.5.1.1) \quad G = GH^+H. \quad (6.3.1) \text{ and } (6.3.2)$$

Hence

$$GH^+\bar{H} = GH^+H(I - G^+G) = 0.$$

Therefore $P_1P_2 = 0$ and by (4.10.3), it suffices to show that $\text{rk}(P_1) + \text{rk}(P_2) = \text{rk}(HH^+)$. It will then follow immediately that $HH^+ = P_1 + P_2$.

But

$$\text{rk}(P_1) = \text{rk}(GH^+) = \text{rk}(GH^+H) = \text{rk}(G) \quad (6.5.1.1) \text{ and } (4.10.2)$$

and

$$\begin{aligned} \text{rk}(P_2) &= \text{rk}(\bar{H}) = \text{rk}[H(I - G^+G)] \\ &= \text{rk}(H) - \text{rk}(G) \quad [\text{part (a)}]. \end{aligned}$$

Thus,

$$\text{rk}(P_1) + \text{rk}(P_2) = \text{rk}(H) = \text{rk}(HH^+) \quad (4.10.2)$$

and this proves (b), (4.10.3b). ■

(6.5.2) **Corollary:** Let δ and τ be as defined in (6.4.6) and (6.4.7). If Gx is an evpf, then $\tau = \text{rk}(G)$ and $\delta = \sigma^{-1} \|(GH^+)^+ Gx\|$.

Proof

$$\tau = \text{rk}(HH^+ - \bar{H}\bar{H}^+).$$

If G is an evpf, then $\mathcal{R}(G^T) \subseteq \mathcal{R}(H^T)$, (6.3.1), and by (6.5.1b) and (6.3.6.1),

$$\tau = \text{rk}[(GH^+)^+(GH^+)] = \text{rk}(GH^+) = \text{rk}(G).$$

By the same token,

$$\begin{aligned} \delta &= \sigma^{-1} \|(HH^+ - \bar{H}\bar{H}^+)Hx\| \\ &= \sigma^{-1} \|(GH^+)^+(GH^+Hx)\| \\ &= \sigma^{-1} \|(GH^+)^+Gx\| \quad \text{if } G \text{ is an evpf.} \quad \blacksquare \end{aligned} \quad (6.3.2)$$

Referring to section (6.3), we now see that the confidence ellipsoid $\mathcal{S}(\sigma^2\omega_{1-\alpha})$ covers the point $y = 0$ if and only if

$$(6.5.3) \quad \hat{y}^T [G(H^T H)^+ G^T]^+ \hat{y} \leq \sigma^2 \omega_{1-\alpha}$$

where $\omega_{1-\alpha}$ is the upper $100(1-\alpha)$ percentile of the chi-square distribution with τ df. Since $\hat{y} = GH^+z$, we can write (6.5.3) as

$$(6.5.4) \quad \|(GH^+)^+ GH^+ z\|^2 \leq \sigma^2 \omega_{1-\alpha}$$

which, by virtue of (6.5.1b), is the same as

$$(6.5.5) \quad (\sigma^2)^{-1} \|(HH^+ - \bar{H}\bar{H}^+)z\|^2 \leq \omega_{1-\alpha}.$$

Thus, the likelihood ratio test for the case of known σ , rejects \mathcal{H}_0 at the level α if and only if the $(1-\alpha)$ level confidence ellipsoid for Gx fails to cover the point $y = 0$.

(6.5.6) **Exercise:** Show that the likelihood ration test (for unknown σ) at the level α rejects \mathcal{H}_0 if and only if

$$\mathcal{S}(k_1 \hat{\sigma}^2 \tilde{\omega}_{1-\alpha}) \quad [\text{defined in (6.3)}]$$

fails to cover $y = 0$.

(6.5.7) **Exercise:** If G is an evpf then $\delta = 0$ if and only if $Gx = 0$.

(6.6) Orthogonal Designs

In statistical investigations, it is often desired to obtain information about the value of one or more parameters and in an effort to do so, the researcher designs an experiment which will yield data of the form

$$z = Hx + v$$

where \mathbf{z} is the “observation vector,” \mathbf{x} is an unknown vector whose components include the parameters of interest (and possibly other so-called “nuisance parameters”) \mathbf{v} is the vector of residuals (or “observation errors”). H is a known matrix, often referred to as the “experimental design.” The art of experimental design occupies an important niche in the lore of applied statistics and one of its basic concepts is the notion of “orthogonal design.”

Suppose $y_j = G_j \mathbf{x}$ are evpf's for $j = 1, 2, \dots, p$ (i.e., each component of each y_j is an estimable parametric function).

The design H is said to be *orthogonal with respect to the evpf's* $G_1 \mathbf{x}, G_2 \mathbf{x}, \dots, G_p \mathbf{x}$ if and only if the BLUE's for y_i and y_j are uncorrelated when $i \neq j$.

One reason that orthogonal designs are desirable is to be explained in Theorem (6.6.9). The BLUE for each y_j can be computed as though all the other y_i 's are known to be zero. This fact often reduces the computational complexity of a least squares problem by several orders of magnitude.

For the sake of clarity, we will confine our attention to the case where the residual vector \mathbf{v} has covariance proportional to the identity matrix. In that case, the BLUE for y_j is

$$(6.6.1) \quad \hat{y}_j = G_j H^+ \mathbf{z} \quad (j = 1, \dots, p) \quad (6.1.12)$$

and

$$\begin{aligned} \text{Cov}(\hat{y}_i, \hat{y}_j) &\equiv \mathcal{E}(\hat{y}_i - y_i)(\hat{y}_j - y_j)^T \\ &= \mathcal{E}G_i H^+ (\mathbf{z} - H\mathbf{x})(\mathbf{z} - H\mathbf{x})^T (G_j H^+)^T \\ &= G_i H^+ \mathcal{E}\mathbf{v}\mathbf{v}^T H^{+T} G_j^T \\ &= \sigma^2 G_i H^+ H^{+T} G_j^T \\ &= \sigma^2 G_i (H^T H)^+ G_j^T. \end{aligned}$$

Thus, \hat{y}_i is uncorrelated with \hat{y}_j if and only if

$$(6.6.2) \quad G_i (H^T H)^+ G_j^T = 0$$

which is the same as saying the row vectors of G_i must be “orthogonal” to the row vectors of G_j with respect to the inner product induced by $(H^T H)^+$ (which, by the way, is proportional to the covariance of $\hat{\mathbf{x}} = H^+ \mathbf{z}$, the BLUE for \mathbf{x}). Equation (6.6.2) can be written in the alternate form

$$(6.6.3) \quad (G_i H^+)(G_j H^+)^T = 0 \quad i \neq j$$

so that H is orthogonal with respect to $G_1 \mathbf{x}, G_2 \mathbf{x}, \dots, G_p \mathbf{x}$ if and only if

$$\mathcal{R}[(G_j H^+)^T] \subseteq \mathcal{N}(G_i H^+) \quad \text{when } i \neq j.$$

Since

$$\mathcal{R}[(G_j H^+)^T] = \mathcal{R}[(G_j H^+)^+ (G_j H^+)]$$

and

$$\mathcal{N}(G_i H^+) = \mathcal{N}[(G_i H^+)^+ (G_i H^+)] \quad (3.11.5)$$

we see that H is orthogonal with respect to $G_1 x, \dots, G_p x$ if and only if

$$(6.6.4) \quad P_i P_j = 0 \quad \text{when } i \neq j$$

where

$$(6.6.5) \quad P_j = (G_j H^+)^+ (G_j H^+) \quad j = 1, 2, \dots, p.$$

In the proof of (6.5.1b) we showed that

$$\mathcal{R}[(GH^+)^+ (GH^+)] \subseteq \mathcal{R}(HH^+)$$

if Gx is an evpf, so it follows that

$$(6.6.6) \quad \mathcal{R}\left[\sum_{j=1}^p (G_j H^+)^+ (G_j H^+)\right] \subseteq \mathcal{R}(HH^+).$$

If equality holds in (6.6.6), then by (3.7.7), HH^+ is expressible as the sum of *orthogonal projections*, a fact which we will see to be of more than passing interest. [Two projections P_1 and P_2 are said to be *orthogonal* if $P_1 P_2 = 0$. Clearly $P_1 P_2 = 0$ if and only if $P_2 P_1 = 0$ and the last is true if and only if $\mathcal{R}(P_1) \subseteq \mathcal{N}(P_2)$.]

If strict inclusion holds in (6.6.6) (as it may) we can, by suitably defining one more evpf (which we call $y_0 = G_0 x$), decompose HH^+ into a sum of orthogonal projections:

$$HH^+ = \sum_{j=0}^p (G_j H^+)^+ (G_j H^+).$$

In the next theorem, we show how to define G_0 :

(6.6.7) **Theorem:** If H is an orthogonal design with respect to $G_1 x, \dots, G_p x$ and if

$$(6.6.7.1) \quad T = HH^+ - \sum_{j=1}^p (G_j H^+)^+ (G_j H^+) \neq 0$$

then H is also an orthogonal design with respect to $G_0 x, G_1 x, \dots, G_p x$ where

$$G_0 = TH.$$

Furthermore,

$$(6.6.7.2) \quad HH^+ = \sum_{j=0}^p (G_j H^+)^+ (G_j H^+)$$

and the projections in the sum are mutually orthogonal.

Proof

$$G_0 H^+ H = THH^+ H = TH = G_0$$

so G_0 is an evpf, (6.3.2).

To show that H is orthogonal with respect to $G_0 x, G_1 x, \dots, G_p x$, we must show that

$$(G_k H^+)(G_0 H^+)^T = 0 \quad k = 1, \dots, p.$$

The left side is

$$(G_k H^+)(THH^+)^T = G_k H^+ T$$

(since $H^+ HH^+ = H^+$ and T is symmetric). If $G_k H^+$ is applied to each term on the right side of (6.6.7.1), we see that

$$\begin{aligned} G_k H^+ T &= G_k H^+ [HH^+ - (G_k H^+)^+ (G_k H^+)] \\ &= G_k H^+ - G_k H^+ = 0. \end{aligned}$$

This shows that H is orthogonal with respect to $G_0 x, \dots, G_p x$. Since $G_0 = TH$,

$$[G_0 H^+]^T = [THH^+]^T = HH^+ T$$

and since $\mathcal{R}(T) \subseteq \mathcal{R}(HH^+)$, (6.6.6),

$$HH^+ T = T. \quad (3.13.1)$$

Thus,

$$T = T^T = (G_0 H^+)^T$$

and since T is the projection on $\mathcal{R}(HH^+) - \mathcal{R}(P_1 + P_2 + \dots + P_p)$,

$$(G_0 H^+)^+ = T^+ = T$$

so that

$$T = T^2 = (G_0 H^+)^+ (G_0 H^+)$$

which is another way of expressing (6.6.7.2). ■

Comment: The zeroth term of the sum (6.6.7.2) has an interpretation: Recall that the set of all estimable parametric functions consists of all parameters of the form $g^T x$ where g is free to range over $\mathcal{R}(H^+ H)$. The

components of the evpf's G_1x, G_2x, \dots, G_px collectively correspond to the class of estimable parametric functions of the form g^Tx where g is free to range over $\mathcal{R}[(G_1^T | G_2^T | \dots | G_p^T)]$. Since $H^+HG_j^T = G_j^T$, this manifold is a subspace of $\mathcal{R}(H^+H)$. Now, G_0 is defined in such a way that

$$\mathcal{R}[(G_0^T | G_1^T | \dots | G_p^T)] = \mathcal{R}(H^+H)$$

and so that H remains an orthogonal design.

(6.6.8) **Exercise:** Show that $\mathcal{R}[(G_0^T | G_1^T | \dots | G_p^T)] = \mathcal{R}[H^+H]$.

The concept of "orthogonal design" was of great importance in the days before the widespread availability of digital computers. The task of solving the least squares "normal equations" and evaluating the residual sum of squares on a desk calculator, was tedious at best and overwhelming if the dimensionality of the unknown vector x was greater than 6 or 7 *unless* the design was orthogonal. In that case, as we will see in the next theorem, each evpf could be estimated separately as though the rest were known to be zero.

The general effect was to reduce the estimation of a k -dimensional parameter (with associated computations equivalent in complexity to that of inverting a $k \times k$ matrix) to the estimation of $p+1$ parameters, each of dimension ρ_i (each requiring the equivalent of a $\rho_i \times \rho_i$ matrix inversion) where $\sum_i \rho_i = k$. Generally speaking, the inversion of a $k \times k$ matrix requires on the order of k^3 arithmetic operations. Therefore

$$k^3 = \left(\sum_i \rho_i \right)^3 > \sum_i \rho_i^3$$

so that considerable computational savings would be realized were one to capitalize on the orthogonality of the design.

Finally, an intuitively informative decomposition for the residual sum of squares, $\|z - Hx\|^2$ is another dividend associated with orthogonal designs. To be precise:

(6.6.9) **Theorem** (*Orthogonal decomposition for analysis of variance*)

(a) If $z = Hx + v$ where v is a zero-mean vector random variable with covariance $\sigma^2 I$, if $y_i = G_i x$ ($i = 1, \dots, p$) are evpf's, and if H is an orthogonal design with respect to these evpf's, then

$$(6.6.9.1) \quad \|z - Hx\|^2 = \|z - H\hat{x}\|^2 + \sum_{j=0}^p (\hat{y}_j - y_j)^T [G_j(H^TH)^+ G_j^T]^+ (\hat{y}_j - y_j)$$

where G_0 is the (possibly zero) matrix defined in (6.6.7), $\hat{x} = H^+z$ is the least squares estimate for x and $\hat{y}_j = G_j \hat{x}$ is the BLUE for y_j ($j = 0, 1, \dots, p$).

(b) \hat{y}_j can be computed in the following (alternative) fashion: Let $\hat{\mathbf{x}}_j$ be any vector minimizing $\|\mathbf{z} - H\mathbf{x}\|^2$ subject to the constraints

$$G_i \mathbf{x} = 0 \quad \text{for } i = 1, 2, \dots, j-1, j+1, \dots, p.$$

Then

$$(6.6.9.2) \quad \hat{y}_j = G_j \hat{\mathbf{x}}_j.$$

(c) If it is assumed, in addition, that the residual vector \mathbf{v} is normally distributed, then the first term on the right side of (6.6.9.1) (when divided by σ^2) has a chi-square distribution with $n-k$ df, where n is the dimension of \mathbf{z} and k is the rank of H . The j th term of the sum (when divided by σ^2) has a chi-square distribution with ρ_j df, where ρ_j is the rank of G_j . All $p+2$ terms are mutually independent and $\sum_{i=0}^p \rho_i = k$.

Comment: The sum of squares decomposition (6.6.9.1), “explains” the “total” sum of squares $\|\mathbf{z} - H\mathbf{x}\|^2$ in terms of the sum of squares associated with each of the evpf’s y_j and the so-called residual sum of squares $\|\mathbf{z} - H\hat{\mathbf{x}}\|^2$. These quantities are traditionally computed with the y_j ’s set equal to zero and they are exhibited under the title “analysis of variance table” (Scheffé [1, Chap. 4]).

Proof: (a) Since

$$(6.6.9.3) \quad \begin{aligned} \mathbf{z} - H\mathbf{x} &= \mathbf{z} - HH^+ \mathbf{z} + HH^+ (\mathbf{z} - H\mathbf{x}) \\ &= (I - HH^+) \mathbf{z} + HH^+ (\mathbf{z} - H\mathbf{x}) \end{aligned}$$

we deduce from (6.6.7.2) that

$$(6.6.9.4) \quad \mathbf{z} - H\mathbf{x} = (I - HH^+) \mathbf{z} + \sum_{j=0}^p (G_j H^+)^+ (G_j H^+) (\mathbf{z} - H\mathbf{x}).$$

The G_j ’s are associated with evpf’s, hence

$$G_j H^+ H\mathbf{x} = G_j \mathbf{x} = y_j \quad (6.3.2)$$

and since $H^+ \mathbf{z} = \hat{\mathbf{x}}$ is the BLUE for $H^+ H\mathbf{x}$ and $G_j \hat{\mathbf{x}} = \hat{y}_j$ is the BLUE for y_j , we see that

$$(6.6.9.5) \quad \mathbf{z} - H\mathbf{x} = (\mathbf{z} - H\hat{\mathbf{x}}) + \sum_{j=0}^p (G_j H^+)^+ (\hat{y}_j - y_j).$$

The first term on the right side of (6.6.9.4) is uncorrelated with and orthogonal to each term in the sum since (a) $I - HH^+$ projects onto $\mathcal{R}(H)^\perp [= \mathcal{N}(H^T)]$, whereas each term of the sum projects onto a subspace of $\mathcal{R}(H)$, (6.6.6), and (b) the covariance of $\mathbf{z} - H\mathbf{x}$ is proportional to the identity. Since H is an orthogonal design with respect to the $G_j \mathbf{x}$ ’s, the

projections in the sum are mutually orthogonal, (6.6.4). So then are each of the *vectors* in the sum, and since the covariance of $\mathbf{z} - H\mathbf{x}$ is proportional to the identity, the terms are also mutually uncorrelated.

The mutual orthogonality of all terms allows for the sum of squares decomposition for (6.6.9.5):

$$\begin{aligned}\|\mathbf{z} - H\mathbf{x}\|^2 &= \|\mathbf{z} - H\hat{\mathbf{x}}\|^2 + \sum_{j=0}^p \|(G_j H^+)^+ (\hat{\mathbf{y}}_j - y_j)\|^2 \\ &= \|\mathbf{z} - H\hat{\mathbf{x}}\|^2 + \sum_{j=0}^p (\hat{\mathbf{y}}_j - y_j)^T [G_j (H^T H)^+ G_j^T]^+ (\hat{\mathbf{y}}_j - y_j),\end{aligned}$$

which establishes (a).

(b) If $\hat{\mathbf{x}}_j$ minimizes $\|\mathbf{z} - H\mathbf{x}\|^2$ subject to $G_i \mathbf{x} = 0$ for all $i \neq j$, then

$$\hat{\mathbf{m}}_j = H\hat{\mathbf{x}}_j$$

minimizes $\|\mathbf{z} - m\|^2$ subject to $G_i H^+ m = 0$ for all $i \neq j$ and $m \in \mathcal{R}(H)$, since $G_i H^+ m = G_i H^+ H\mathbf{x}$ and $G_i H^+ H\mathbf{x} = G_i \mathbf{x}$ when G_i is an evpf, (6.3.2).

Therefore, $\hat{\mathbf{m}}_j$ minimizes $\|\mathbf{z} - m\|^2$ subject to the constraint

$$(6.6.9.6) \quad (I - HH^+)m + \sum_{\substack{i=0 \\ i \neq j}}^p (G_i H^+)^+ (G_i H^+)m = 0,$$

since

$$G_i H^+ m = 0$$

if and only if

$$(G_i H^+)^+ (G_i H^+)m = 0$$

and since the terms in (6.6.9.6) are mutually orthogonal.

By (6.6.7.2),

$$(6.6.9.7) \quad (I - HH^+) + \sum_{\substack{i=0 \\ i \neq j}}^p (G_i H^+)^+ (G_i H^+) = I - (G_j H^+)^+ (G_j H^+) \equiv Q_j$$

which is a projection, so that

$$\|\mathbf{z} - m\|^2 = \|\mathbf{z} - Q_j m - (I - Q_j)m\|^2$$

is minimized subject to the constraint $Q_j m = 0$ if and only if

$$(6.6.9.8) \quad \hat{\mathbf{m}}_j = (I - Q_j)\mathbf{z}. \quad (3.12.4)$$

Since $\hat{\mathbf{m}}_j = H\hat{\mathbf{x}}_j$, we see that

$$G_j H^+ \hat{\mathbf{m}}_j = G_j H^+ H\hat{\mathbf{x}}_j = G_j \hat{\mathbf{x}}_j \quad (6.3.2)$$

whereas (6.6.9.8) implies that

$$\begin{aligned} G_j H^+ \hat{\mathbf{m}}_j &= G_j H^+ [(G_j H^+)^+ (G_j H^+)] \mathbf{z} \\ &= G_j H^+ \mathbf{z} = G_j \hat{\mathbf{x}}. \end{aligned}$$

Hence

$$G_j \hat{\mathbf{x}} = G_j \hat{\mathbf{x}}_j = \hat{\mathbf{y}}_j$$

which proves (6.6.9.2).

(c) In part (a), we showed that all terms on the right side of (6.6.9.5) are uncorrelated. If a normality assumption is added, they are independent as well, (6.2.4), which implies that all terms on the right side of (6.6.9.1) are mutually independent. The distribution of $\sigma^{-2} \|\mathbf{z} - H\hat{\mathbf{x}}\|^2$ has been shown to be chi-square with $n-k$ df [(6.3.10), (6.3.11)]. The distribution of $\sigma^{-2} (\hat{\mathbf{y}}_j - y_j)^T [G_j (H^T H)^+ G_j^T] (\hat{\mathbf{y}}_j - y_j)$ was shown to be chi-square with ρ_j df in (6.3.5).

The left side of (6.6.9.1), when divided by σ^2 , is of the form

$$\sum_{j=1}^n (\mathbf{v}_j / \sigma)^2$$

where the \mathbf{v}_j 's are independent with mean zero and variance σ^2 , so that the left side of (6.6.9.1), when divided by σ^2 is chi-square with n df. Thus,

$$n = n - k + \sum_{j=0}^p \rho_j$$

so that

$$\sum_{j=0}^p \rho_j = k.$$

Comment: By definition, H is always orthogonal with respect to a single evpf $G_1 x$. This means that a decomposition of the form (6.6.9.1) can be exhibited for the case $p = 1$, provided G_0 is properly defined [according to (6.6.7)].

(6.6.10) **Exercise:** (a) H is orthogonal with respect to $G_i x$ ($i = 1, 2, \dots, p$) if and only if

$$(HH^+ - \bar{H}_i \bar{H}_i^+)(HH^+ - \bar{H}_j \bar{H}_j^+) = 0$$

when $i \neq j$, where $\bar{H}_j = H(I - G_j G_j^+)$. [Hint: Use (6.5.1b).]

(b) Let x_j^* be any x which minimizes $\|\mathbf{z} - Hx\|^2$ subject to

$$x \in \mathcal{N}(G_1) \cap \dots \cap \mathcal{N}(G_{j-1}) \cap \mathcal{N}(G_{j+1}) \cap \dots \cap \mathcal{N}(G_p).$$

Let $y_j^* = G_j x_j^*$ and let $\hat{y}_j = G_j \hat{x}$, the BLUE for $y_j = G_j x$. H is orthogonal with respect to $G_i x$ ($i = 1, 2, \dots, p$) if and only if

$$y_j^* = \hat{y}_j \quad \text{for } j = 1, 2, \dots, p.$$

(6.6.11) **Example** (*Straight line regression*): Observations are taken, of the form

$$\zeta_i = \alpha + \beta \tau_i + \mathbf{v}_i \quad i = 1, \dots, n.$$

In the vector-matrix notation,

$$\mathbf{z} = H\mathbf{x} + \mathbf{v}$$

where

$$\mathbf{z} = \begin{pmatrix} \zeta_1 \\ \vdots \\ \zeta_n \end{pmatrix} \quad H = (e \vdots t) \quad x = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$e = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \quad t = \begin{pmatrix} \tau_1 \\ \vdots \\ \tau_n \end{pmatrix} \quad \text{and} \quad \mathbf{v} = \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_n \end{pmatrix}.$$

If we let $G_1 = (1 \ 0)$ and $G_2 = (0 \ 1)$, then $y_1 = G_1 x = \alpha$ and $y_2 = G_2 x = \beta$. H has rank $k = 2$ if the τ 's are not all the same, in which case $H^+ H = I$ so y_1 and y_2 are evpf's.

$$\bar{H}_j \equiv H(I - G_j G_j^+) = \begin{cases} (0 \vdots t) & j = 1 \\ (e \vdots 0) & j = 2 \end{cases}$$

so that

$$\bar{H}_j \bar{H}_j^+ = \begin{cases} tt^T / \|t\|^2 & j = 1 \\ ee^T / \|e\|^2 & j = 2. \end{cases}$$

The quickest way to find HH^+ is to perform a Gramm-Schmidt orthogonalization on the columns of H and then apply (3.7.3):

$$HH^+ = \frac{ee^T}{\|e\|^2} + \frac{uu^T}{\|u\|^2} \quad \text{where } u = t - \frac{(e^T t)}{\|e\|^2} e$$

$$= \frac{tt^T}{\|t\|^2} + \frac{ww^T}{\|w\|^2} \quad \text{where } w = e - \frac{(t^T e)}{\|t\|^2} t.$$

Thus

$$HH^+ - \bar{H}_1 \bar{H}_1^+ = ww^T / \|w\|^2$$

$$HH^+ - \bar{H}_2 \bar{H}_2^+ = uu^T / \|u\|^2$$

and so

$$(HH^+ - \bar{H}_1 \bar{H}_1^+)(HH^+ - \bar{H}_2 \bar{H}_2^+) = \frac{w^T u}{\|u\|^2 \|w\|^2} (wu^T).$$

By virtue of (6.6.10) H is an orthogonal design with respect to $G_1 x, G_2 x$ if and only if the last expression vanishes. Since

$$w^T u = (e^T t) \left[\frac{(e^T t)^2 - \|e\|^2 \|t\|^2}{\|e\|^2 \|t\|^2} \right]$$

and since t is not a multiple of e if the τ 's are not all the same, Schwarz's inequality tells us that the term in square brackets is strictly negative so $w^T u = 0$ if and only if $(e^T t) = 0$. In summary, H is orthogonal with respect to α and β if and only if $n^{-1} \sum_{j=1}^n \tau_j \equiv \bar{\tau} = 0$. So, H is an orthogonal design if and only if the observations are chosen at values of τ_j whose average value is zero. In that case, we can compute the BLUE for α as though $\beta = 0$:

"Pretend" that

$$\zeta_i = \alpha + v_i \quad i = 1, \dots, n.$$

Then the BLUE for α is

$$\hat{\alpha} = n^{-1} \sum_{i=1}^n \zeta_i.$$

Similarly, we can compute the BLUE for β as though $\alpha = 0$:

"Pretend" that

$$\zeta_i = \beta \tau_i + v_i \quad i = 1, \dots, n.$$

The BLUE for β is

$$\hat{\beta} = t^+ z = \sum_{j=1}^n \zeta_j \tau_j / \sum_{j=1}^n \tau_j^2.$$

In this special two-dimensional problem, the BLUE for x can be exhibited explicitly in the general (nonorthogonal) case:

$$\hat{x} = \begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix}$$

where

$$\hat{\beta} = \sum_{j=1}^n (\zeta_j - \bar{\zeta})(\tau_j - \bar{\tau}) / \sum_{j=1}^n (\tau_j - \bar{\tau})^2$$

$$\bar{\zeta} = n^{-1} \sum_{j=1}^n \zeta_j \quad \bar{\tau} = n^{-1} \sum_{j=1}^n \tau_j$$

and

$$\hat{\alpha} = \bar{\zeta} - \hat{\beta} \bar{\tau}.$$

It is apparent that the orthogonality condition $\bar{\tau} = 0$, reduces these formulas to the estimates for α and β given previously.

The sum of squares decomposition for the *orthogonal case* is

$$\sigma^{-2} \sum_{j=1}^n (\zeta_j - \alpha - \beta \tau_j)^2 = \sigma^{-2} \sum_{j=1}^n (\zeta_j - \hat{\alpha} - \hat{\beta} \tau_j)^2 + (\hat{\beta} - \beta)^2 / \sigma_{\beta}^2 + (\hat{\alpha} - \alpha)^2 / \sigma_{\hat{\alpha}}^2$$

where

$$\begin{aligned} \hat{\alpha} &= n^{-1} \sum_{i=1}^n \zeta_i & \sigma_{\hat{\alpha}}^2 &= \sigma^2 / n \\ \hat{\beta} &= \sum_{i=1}^n \zeta_i \tau_i / \sum_{i=1}^n \tau_i^2 & \sigma_{\hat{\beta}}^2 &= \sigma^2 / \sum_{i=1}^n \tau_i^2. \end{aligned}$$

If the design were not orthogonal with respect to α and β , it would still be orthogonal to either one, taken separately. Suppose β were the parameter of interest. Let us redefine

$$G_1 = (0 \quad 1)$$

so that

$$G_1 x = \beta.$$

Using (6.6.7), we define

$$G_0 = [HH^+ - (G_1 H^+)^+ (G_1 H^+)] H = e(n! n\bar{\tau}).$$

Thus,

$$G_0 x = n(\alpha + \bar{\tau}\beta)e$$

and H is orthogonal with respect to $G_0 x$, $G_1 x$. We can compute $\hat{\beta}$ by minimizing $\|z - Hx\|^2$ subject to $G_0 x = 0$ (i.e., $\alpha = -\bar{\tau}\beta$). In this case, the sum of squares

$$\sum_{j=1}^n (\zeta_j - \alpha - \beta \tau_j)^2$$

becomes

$$\sum_{j=1}^n (\zeta_j + \bar{\tau}\beta - \tau_j \beta)^2 = \sum_{j=1}^n [\zeta_j - \beta(\tau_j - \bar{\tau})]^2$$

which is minimized when

$$\begin{aligned} \hat{\beta} &= \sum_{j=1}^n \zeta_j (\tau_j - \bar{\tau}) / \sum_{j=1}^n (\tau_j - \bar{\tau})^2 \\ &= \sum_{j=1}^n (\zeta_j - \bar{\zeta}) (\tau_j - \bar{\tau}) / \sum_{j=1}^n (\tau_j - \bar{\tau})^2 \end{aligned}$$

as it should.

(6.6.12) **Exercise** (*Two-way layout*): Suppose observations are made of the form

$$\zeta_{ij} = \alpha_i + \beta_j + v_{ij} \quad i = 1, \dots, I \quad j = 1, \dots, J$$

where the α 's and β 's are not known and the residuals, v_{ij} , have zero mean and are uncorrelated with common variance, σ^2 .

$$\mathbf{z} = \begin{bmatrix} \zeta_{11} \\ \zeta_{12} \\ \vdots \\ \zeta_{1J} \\ \zeta_{21} \\ \vdots \\ \zeta_{2J} \\ \vdots \\ \zeta_{I1} \\ \vdots \\ \zeta_{IJ} \end{bmatrix} \quad \mathbf{x} = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_I \\ \beta_1 \\ \vdots \\ \beta_J \end{bmatrix} \quad \mathbf{v} = \begin{bmatrix} v_{11} \\ v_{12} \\ \vdots \\ v_{1J} \\ v_{21} \\ \vdots \\ v_{2J} \\ \vdots \\ v_{I1} \\ \vdots \\ v_{IJ} \end{bmatrix}$$

and

$$H = \begin{array}{c} J \\ \left[\begin{array}{cc|cc} I & & & \\ 1 & 0 \dots 0 & 1 & 0 \dots 0 \\ 1 & 0 \dots 0 & 0 & 1 \dots 0 \\ \hline 1 & 0 \dots 0 & 0 & 0 \dots 1 \\ 0 & 1 \dots 0 & 1 & 0 \dots 0 \\ 0 & 1 \dots 0 & 0 & 1 \dots 0 \end{array} \right] \end{array} \begin{array}{c} \uparrow \\ I \text{ blocks of} \\ J \text{ each} \\ \downarrow \end{array}$$

$$\begin{array}{c} J \\ \left[\begin{array}{cc|cc} 0 & 1 \dots 0 & 0 & 0 \dots 1 \\ 0 & 0 \dots 1 & 1 & 0 \dots 0 \\ \hline 0 & 0 \dots 1 & 0 & 1 \dots 0 \\ 0 & 0 \dots 1 & 0 & 0 \dots 1 \end{array} \right] \end{array} \begin{array}{c} \downarrow \end{array}$$

Let

$$G_1 x = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_I \end{bmatrix} \quad \text{and} \quad G_2 x = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_J \end{bmatrix}.$$

Show that the design is not orthogonal with respect to $G_1 x$ and $G_2 x$. (*Hint*: Show that the l.s.e. for $G_1 x$ is correlated with the l.s.e. for $G_2 x$.)

(6.6.13) (Continued): Let

$$\begin{aligned}\varepsilon &= I^{-1} \sum_{i=1}^I \alpha_i + J^{-1} \sum_{j=1}^J \beta_j \\ \delta_i &= \alpha_i - I^{-1} \sum_{j=1}^I \alpha_j \quad i = 1, \dots, I \\ \gamma_j &= \beta_j - J^{-1} \sum_{k=1}^J \beta_k \quad j = 1, \dots, J \\ x &= \begin{bmatrix} \varepsilon \\ \delta_1 \\ \vdots \\ \delta_{I-1} \\ \gamma_1 \\ \vdots \\ \gamma_{J-1} \end{bmatrix}\end{aligned}$$

and let \mathbf{z} and \mathbf{v} be as in (6.6.12).

(a) Find H so that

$$\mathbf{z} = H\mathbf{x} + \mathbf{v}$$

(Hint: $\zeta_{ij} = \varepsilon + \delta_i + \gamma_j + v_{ij}$, $i = 1, \dots, I$, $j = 1, \dots, J$.)

(b) Let

$$G_1 \mathbf{x} = \varepsilon \quad G_2 \mathbf{x} = \begin{bmatrix} \delta_1 \\ \vdots \\ \delta_{I-1} \end{bmatrix} \quad \text{and} \quad G_3 \mathbf{x} = \begin{bmatrix} \gamma_1 \\ \vdots \\ \gamma_{J-1} \end{bmatrix}.$$

Show that H is orthogonal with respect to $G_1 \mathbf{x}$, $G_2 \mathbf{x}$, and $G_3 \mathbf{x}$.

(c) Define $\hat{\delta}_I = -\sum_{j=1}^{I-1} \hat{\delta}_j$, $\hat{\gamma}_J = -\sum_{j=1}^{J-1} \hat{\gamma}_j$. Then the orthogonal decomposition for the sum of squares for an orthogonal two-way layout is

$$\begin{aligned}\sum_{ij} (\zeta_{ij} - \varepsilon - \delta_i - \gamma_j)^2 &= \sum_{ij} (\zeta_{ij} - \hat{\varepsilon} - \hat{\delta}_i - \hat{\gamma}_j)^2 \\ &\quad + J \sum_i (\hat{\delta}_i - \delta_i)^2 + I \sum_j (\hat{\gamma}_j - \gamma_j)^2 \\ &\quad + IJ(\hat{\varepsilon} - \varepsilon)^2.\end{aligned}$$

If the residuals v_{ij} are independent and normally distributed with mean 0 and variance 1, the terms on the right have independent chi-square distributions with $IJ - (I + J - 1)$, $I - 1$, $J - 1$ and 1 df, respectively.

(6.6.14) **Exercise:** Let

$$H = {}_n(H_1 \mid H_2)$$

be an $n \times (p+q)$ matrix of rank $p+q$, and suppose

$$\mathbf{z} = H\mathbf{x} + \mathbf{v}$$

where the residual \mathbf{v} has covariance I .

The least squares estimate (=BLUE) for \mathbf{x} is unique and can be obtained via the pseudoinversion of the $n \times (p+q)$ matrix H :

$$\hat{\mathbf{x}} = H^+ \mathbf{z}.$$

An alternative method which may involve less work (and which has applications to stepwise regression in Chapter VIII) goes like this:

Let

$$\mathbf{x} = \begin{matrix} p \\ q \end{matrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \quad G_0 = H_1 H_1^+ H$$

and

$$G = \begin{matrix} p & q \\ q & 0 \end{matrix} \begin{pmatrix} 0 & I \end{pmatrix}.$$

Then

(a) H is an orthogonal design with respect to $G_0 \mathbf{x}$ and $G\mathbf{x}$.

(b) The BLUE for x_2 is unique and is given by

$$\hat{\mathbf{x}}_2 = G\mathbf{x}^*$$

where \mathbf{x}^* minimizes $\|\mathbf{z} - H\mathbf{x}\|^2$ subject to $G_0 \mathbf{x} = 0$.

(c) $\hat{\mathbf{x}}_2 = (Q_1 H_2)^+ \mathbf{z} \equiv (H_2^T Q_1 H_2)^+ H_2^T Q_1 \mathbf{z}$, where

$$Q_1 = I - H_1 H_1^+ \equiv I - H_1 (H_1^T H_1)^{-1} H_1^T.$$

(d) The BLUE for x_1 is unique and is given by

$$\hat{\mathbf{x}}_1 = H_1^+ (\mathbf{z} - H_2 \hat{\mathbf{x}}_2) \equiv (H_1^T H_1)^{-1} H_1^T (\mathbf{z} - H_2 \hat{\mathbf{x}}_2).$$

[Comment: $\hat{\mathbf{x}}_1$ and $\hat{\mathbf{x}}_2$ and hence,

$$\hat{\mathbf{x}} = \begin{pmatrix} \hat{\mathbf{x}}_1 \\ \hat{\mathbf{x}}_2 \end{pmatrix}$$

can be obtained by way of a $q \times q$ inversion and a $p \times p$ inversion. If $p \approx q$ and both are large, a sizable computational saving can result.]

(e) Let $\mathbf{x}_1^* = H_1^+ \mathbf{z}$.

Then

$$\|\mathbf{z} - H\hat{\mathbf{x}}\|^2 = \|\mathbf{z} - H_1 \mathbf{x}_1^*\|^2 - \hat{\mathbf{x}}_2^T (H_2^T Q_1 H_2) \hat{\mathbf{x}}_2.$$

(Thus, the residual sum of squares associated with the BLUE for x under the “full” model

$$\mathbf{z} = H_1 x_1 + H_2 x_2 + \mathbf{v}$$

differs from the residual sum of squares associated with the BLUE for x_1 in the restricted model

$$\mathbf{z} = H_1 x_1 + \mathbf{v}$$

by the “correction factor”

$$\hat{\mathbf{x}}_2 H_2^T Q_1 H_2 \hat{\mathbf{x}}_2 \equiv \|Q_1 H_2 \hat{\mathbf{x}}_2\|^2.)$$

CONSTRAINED LEAST SQUARES, PENALTY FUNCTIONS, AND BLUE'S

(7.1) Penalty Functions

In many applications, we have seen that it is necessary to compute a weighted least squares estimator subject to linear equality constraints. That is, it is necessary to find a value of x which minimizes

$$(7.1.1) \quad (z - Hx)^T V^{-2} (z - Hx)$$

subject to the constraints

$$(7.1.2) \quad Gx = u$$

where V is a known positive-definite matrix, z and u are given vectors, and H and G are given rectangular matrices.

A very general result in the theory of minimization which is associated with the "penalty function method," asserts that the value of x which minimizes

$$(7.1.3) \quad h(x) + \lambda^{-2} g^2(x)$$

[call it $x(\lambda)$], converges (as $\lambda \rightarrow 0$) to

$$(7.1.4) \quad x^0 = \lim_{\lambda \rightarrow 0} x(\lambda)$$

if certain mild continuity restrictions are met, and that x^0 minimizes $h(x)$ subject to the constraint $g(x) = 0$ (Butler and Martin [1]). Furthermore,

$$(7.1.5) \quad \lim_{\lambda \rightarrow 0} [h(x(\lambda)) + \lambda^{-2} g^2(x(\lambda))] = h(x^0)$$

so that the minimal value of (7.1.3) converges to the minimal value of h on the constraint set.

The term $(\lambda^{-2})g^2(x)$ is called a "penalty function" because the minimization of $h(x) + \lambda^{-2}g^2(x)$ suffers when x lies outside the constraint set $[g(x) = 0]$ if λ is small.

In the case at hand, if we let

$$(7.1.6) \quad h(x) = (z - Hx)^T V^{-2} (z - Hx)$$

and

$$(7.1.7) \quad g^2(x) = (u - Gx)^T (u - Gx)$$

and if $x(\lambda)$ is a value of x which minimizes

$$(7.1.8) \quad (z - Hx)^T V^{-2} (z - Hx) + \lambda^{-2} (u - Gx)^T (u - Gx)$$

then it is reasonable to expect that

$$(7.1.9) \quad x^0 = \lim_{\lambda \rightarrow 0} x(\lambda)$$

exists and minimizes (7.1.6) subject to $g^2(x) = 0$ (i.e., $Gx = u$). Instead of invoking the general theorem, we will produce a self-contained proof based upon the material developed so far:

(7.1.10) **Theorem:** Let H be an $n \times m$ matrix, G be a $k \times m$ matrix and V be an $n \times n$ positive-definite matrix. Let

$$\tilde{H} = \begin{pmatrix} H \\ \bar{G} \end{pmatrix} \quad \tilde{V}(\lambda) = \begin{pmatrix} V & 0 \\ 0 & \lambda I \end{pmatrix} \quad [\text{order } (n+k) \times (n+k)]$$

and

$$\tilde{z} = \begin{pmatrix} z \\ u \end{pmatrix}$$

where z is a given n -vector and u is a given k -vector.

Let

$$\tilde{x}(\lambda) = [\tilde{V}^{-1}(\lambda) \tilde{H}]^+ \tilde{V}^{-1}(\lambda) \tilde{z}.$$

Then

(a) $\tilde{x}(\lambda)$ is the vector of minimum norm among those which minimize $(\tilde{z} - \tilde{H}x)^T \tilde{V}^{-2}(\lambda) (\tilde{z} - \tilde{H}x) \equiv (z - Hx)^T V^{-2} (z - Hx) + \lambda^{-2} (u - Gx)^T (u - Gx).$

(b) $\lim_{\lambda \rightarrow 0} \tilde{x}(\lambda) = x^0$ always exists.

(c) Among all vectors which minimize $\|u - Gx\|^2$, x^0 is the one of minimum norm among those which minimize $(z - Hx)^T V^{-2} (z - Hx)$.

(d) If $u \in \mathcal{R}(G)$, then the set of x 's which minimize $\|u - Gx\|^2$ is identical with the set of x 's which satisfy the constraint $Gx = u$. In this case, x^0 minimizes $(z - Hx)^T V^{-2} (z - Hx)$ subject to the constraint $Gx = u$.

Furthermore,

$$\lim_{\lambda \rightarrow 0} [\tilde{z} - \tilde{H}\tilde{x}(\lambda)]^T V^{-2}(\lambda) [\tilde{z} - \tilde{H}\tilde{x}(\lambda)] = (z - Hx^0)^T V^{-2} (z - Hx^0).$$

Proof of theorem: (a) $(\tilde{z} - \tilde{H}x)^T \tilde{V}^{-2}(\lambda) (\tilde{z} - \tilde{H}x) = \|\tilde{V}^{-1}\tilde{z} - \tilde{V}^{-1}\tilde{H}x\|^2$ and part (a) follows from (3.4).

(b) and (c): Let

$$(7.1.10.1) \quad F = V^{-1}H$$

$$(7.1.10.2) \quad w = V^{-1}z.$$

Then by (3.8.1)

$$\begin{aligned} \tilde{x}(\lambda) &= [\tilde{V}^{-1}(\lambda)\tilde{H}]^+ \tilde{V}^{-1}\tilde{z} \\ &= [F^T F + \lambda^{-2}G^T G]^+ [F^T w + \lambda^{-2}G^T u]. \end{aligned}$$

By (4.9),

$$[F^T F + \lambda^{-2}G^T G]^+ = (\bar{F}^T \bar{F})^+ + \lambda^2(I - \bar{F}^+ F)[(G^+ G)^+ + J(\lambda)](I - \bar{F}^+ F)^T,$$

where

$$\bar{F} = F(I - G^+ G) \quad \text{and} \quad J(\lambda) = O(\lambda^2) \quad \text{as } \lambda \rightarrow 0.$$

Thus

$$\begin{aligned} (7.1.10.3) \quad \tilde{x}(\lambda) &= (\bar{F}^T \bar{F})^+ F^T w + \lambda^{-2}(\bar{F}^T \bar{F})^+ G^T u \\ &\quad + (I - \bar{F}^+ F)[(G^T G)^+ + O(\lambda^2)](I - \bar{F}^+ F)^T G^T u \quad \text{as } \lambda \rightarrow 0. \end{aligned}$$

But

$$(7.1.10.4) \quad \bar{F}G^T = F(I - G^+ G)G^T = F[G(I - G^+ G)]^T = 0$$

so

$$\mathcal{R}[G^T] \subseteq \mathcal{N}(\bar{F}) = \mathcal{N}(\bar{F}^{+T}) = \mathcal{N}(\bar{F}^+ \bar{F}) = \mathcal{N}[(\bar{F}^T \bar{F})^+] \quad (3.11.5)$$

and so

$$(7.1.10.5) \quad (\bar{F}^T \bar{F})^+ G^T = 0 \quad \text{and} \quad \bar{F}^{+T} G^T = 0.$$

Therefore

$$\begin{aligned} (7.1.10.6) \quad (I - \bar{F}^+ F)(G^T G)^+ (I - \bar{F}^+ F)^T G^T &= (I - \bar{F}^+ F)(G^T G)^+ G^T \\ &= (I - \bar{F}^+ F)G^+ \end{aligned} \quad (3.8.1)$$

and by (3.13.10)

$$(7.1.10.7) \quad (\bar{F}^T \bar{F})^+ F^T = F^+.$$

Combining (7.1.10.3)–(7.1.10.6),

$$(7.1.10.8) \quad \tilde{x}(\lambda) = \bar{F}^+ w + (I - \bar{F}^+ F)[G^+ u + O(\lambda^2)] \quad \text{as } \lambda \rightarrow 0$$

so

$$(7.1.10.9) \quad \tilde{x}(\lambda) = x^0 + O(\lambda^2) \quad \text{as } \lambda \rightarrow 0$$

where

$$(7.1.10.10) \quad \begin{aligned} x^0 &= \bar{F}^+ w + (I - \bar{F}^+ F)G^+ u \\ &= \bar{F}^+(w - FG^+ u) + G^+ u. \end{aligned}$$

By (3.12.7), the latter is exactly the vector of minimum norm which minimizes $\|w - Fx\|^2$ among those vectors which also minimize $\|u - Gx\|^2$. This proves (b) and (c), since

$$\|w - Fx\|^2 = (z - Hx)^T V^{-2} (z - Hx).$$

$$\begin{aligned} (d) \quad & \lim_{\lambda \rightarrow 0} [\tilde{z} - \tilde{H}\tilde{x}(\lambda)]^T \tilde{V}^{-2}(\lambda) [\tilde{z} - \tilde{H}\tilde{x}(\lambda)] \\ &= \lim_{\lambda \rightarrow 0} \{ \|w - F\tilde{x}(\lambda)\|^2 + \lambda^{-2} \|u - G\tilde{x}(\lambda)\|^2 \} \\ &= \lim_{\lambda \rightarrow 0} \{ \|w - Fx^0 + O(\lambda^2)\|^2 + \lambda^{-2} \|u - Gx^0 + O(\lambda^2)\|^2 \}. \end{aligned}$$

If $u \in \mathcal{R}(G)$, then x^0 must satisfy the equation $Gx = u$ if it minimizes $\|Gx - u\|^2$, so that the last term tends to zero as $\lambda \rightarrow 0$ while the first tends to $\|w - Fx^0\|^2$. ■

(7.2) Constrained Least Squares Estimators as Limiting Cases of BLUE's

By (6.1.12c), $\tilde{x}(\lambda)$, defined in (7.1.10), coincides with the BLUE for x when observations of the form

$$(7.2.1) \quad \tilde{z} = \tilde{H}x + \tilde{v}$$

are used to estimate x , where \tilde{v} is a vector random variable with mean zero and covariance $\tilde{V}^2(\lambda)$, where $\tilde{V}(\lambda)$ is defined in (7.1.10). Thus, (7.1.10) shows that any constrained weighted least squares estimator can be viewed as the limiting case of a BLUE, some of whose observations are extremely reliable (i.e., have extremely low residual variances). To put it another way, constrained, weighted least squares estimators can be approximated arbitrarily well, by treating the constraints as fictitious “observations” which are

extremely accurate, and computing the BLUE for x using both the "real" observations (pretending they have covariance V) and the "fictitious" ones (pretending they have covariance $\lambda^2 I$, with λ^2 small).

(7.2.2) **Exercise:** If \tilde{v} has covariance

$$\tilde{V}(0) = \begin{pmatrix} V & 0 \\ 0 & 0 \end{pmatrix}$$

the BLUE for x is given by

$$(7.2.2.1) \quad \tilde{x}(0) = \tilde{H}^+ [I - \tilde{V}(0)(\tilde{Q}\tilde{V}(0))^+] \tilde{z}$$

where $\tilde{Q} = (I - \tilde{H}\tilde{H}^+)$, (6.1.12). Is it true that $\tilde{x}(0)$ coincides with $x^0 = \lim_{\lambda \rightarrow 0} \tilde{x}(\lambda)$? (This would mean that constrained least squares estimates are obtainable as BLUE'S by treating the constraints as "perfectly noiseless" observations. See Zyskind and Martin [1]; Goldman and Zelen [1].)

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RECURSIVE COMPUTATION OF LEAST SQUARES ESTIMATORS

(8.1) Unconstrained Least Squares

In many contemporary applications of the least squares technique, the data arrives in a stream (i.e., in temporal succession) and in such cases it is desirable to carry out the computation of the least squares estimate so that at each instant of time it fully reflects all the data that have been collected so far (cf. American Statistical Association [1] for notable applications of this philosophy).

In Chapter V, several algorithms were described for computing H^+z , but none of these were ideally suited for a situation where the least squares estimate is to be updated every time a new datum is obtained.

For the sake of concreteness, we will initially view this question in the framework of linear regression analysis, but this interpretation is not essential. We are really just relating the least squares estimate for x , based on n data points, to the least squares estimate for x based on $n+1$ data points.

Imagine a stream of scalar observations, ζ_1, ζ_2, \dots arriving in temporal succession, and assume that the j th observation is of the form

$$(8.1.1) \quad \zeta_j = h_j^T x + v_j$$

where each h_j is a known p -dimensional vector, the \mathbf{v}_j 's are uncorrelated zero mean residuals with common variance and x is an unknown p -dimensional vector.

In (6.1.12), we showed that the BLUE for x based on the data

$$\tilde{\mathbf{z}}_n = \begin{pmatrix} \zeta_1 \\ \vdots \\ \zeta_n \end{pmatrix}$$

is

$$(8.1.2) \quad \hat{\mathbf{x}}_n = H_n^+ \mathbf{z}_n$$

where

$$H_n = \begin{bmatrix} h_1^T \\ -h_2^T \\ \vdots \\ -h_n^T \end{bmatrix}.$$

If a new observation of the form

$$\zeta_{n+1} = h_{n+1}^T x + \mathbf{v}_{n+1}$$

is taken, then the BLUE for x is

$$(8.1.3) \quad \hat{\mathbf{x}}_{n+1} = H_{n+1}^+ \mathbf{z}_{n+1}$$

where

$$H_{n+1} = \begin{bmatrix} -H_n \\ h_{n+1}^T \end{bmatrix}$$

and

$$\mathbf{z}_{n+1} = \begin{bmatrix} -\mathbf{z}_n \\ \zeta_{n+1} \end{bmatrix}.$$

It turns out that $\hat{\mathbf{x}}_{n+1}$ is nicely related to $\hat{\mathbf{x}}_n$: By (4.3.2)

$$(8.1.4) \quad H_{n+1}^+ = [(I - K_{n+1} h_{n+1}^T) H_n^+ \mid K_{n+1}]$$

where

$$(8.1.5) \quad K_{n+1} = \begin{cases} \frac{(I - H_n^+ H_n) h_{n+1}}{h_{n+1}^T (I - H_n^+ H_n) h_{n+1}} & \text{if } (I - H_n^+ H_n) h_{n+1} \neq 0 \\ \frac{H_n^+ H_n^T h_{n+1}}{1 + h_{n+1}^T H_n^+ H_n^T h_{n+1}} & \text{otherwise.} \end{cases}$$

Thus,

$$\begin{aligned}
 (8.1.6) \quad \hat{\mathbf{x}}_{n+1} &\equiv H_{n+1}^+ \mathbf{z}_{n+1} \\
 &= (I - K_{n+1} h_{n+1}^T) H_n^+ \mathbf{z}_n + K_{n+1} \zeta_{n+1} \\
 &= \hat{\mathbf{x}}_n + K_{n+1} [\zeta_{n+1} - h_{n+1}^T \hat{\mathbf{x}}_n]
 \end{aligned}$$

where

$$\hat{\mathbf{x}}_0 = 0.$$

Notice that the recursion (8.1.6) takes the so-called “differential-correction” form: If $\hat{\mathbf{x}}_n$ is used as an estimate for x , a “predictor” for ζ_{n+1} (the next datum) is $h_{n+1}^T \hat{\mathbf{x}}_n$. The prediction error is $\zeta_{n+1} - h_{n+1}^T \hat{\mathbf{x}}_n$. From (8.1.6) the new estimate $\hat{\mathbf{x}}_{n+1}$ is obtained from $\hat{\mathbf{x}}_n$ by adding on a term proportional to the prediction error. The “vector of proportionality” K_{n+1} is sometimes referred to as the “smoothing vector.” It does not depend on the data, (8.1.5).

The recursion need not be restricted in its interpretation to the present statistical domain of discourse. It is a fully general result which relates $H^+ z$ to

$$\begin{pmatrix} H \\ \bar{h}^T \end{pmatrix}^+ \begin{pmatrix} z \\ \bar{\zeta} \end{pmatrix},$$

where h^T is an arbitrary row vector (of the correct size) and ζ is an arbitrary scalar.

(8.1.7) *Special case:* Suppose H_n is of full rank (= the number of columns of H_n). This means that H_n 's columns are linearly independent. So then are H_{n+1} 's. Consequently, $H_m^T H_m$ has an inverse for all $m \geq n$.

This allows an alternative derivation: Let

$$B_m = (H_m^T H_m)^{-1} \quad \text{for } m \geq n.$$

We have already shown, (4.6.1), that

$$(8.1.7.1) \quad B_{m+1} = B_m - \frac{(B_m h_{m+1})(B_m h_{m+1})^T}{1 + h_{m+1}^T B_m h_{m+1}}$$

where h_{m+1}^T is the row vector that is adjoined to H_m to produce H_{m+1} .

Since

$$\begin{aligned}
 \hat{\mathbf{x}}_{m+1} &= H_{m+1}^+ \mathbf{z}_{m+1} = B_{m+1} H_{m+1}^T \mathbf{z}_{m+1} \\
 &= B_{m+1} (H_m^T : h_{m+1}) \begin{pmatrix} \mathbf{z}_m \\ \zeta_{m+1} \end{pmatrix}
 \end{aligned}$$

we can apply (8.1.7.1) and obtain (using the symmetry of B_m)

$$\hat{\mathbf{x}}_{m+1} = J_{m+1} B_m [H_m^T \mathbf{z}_m + h_{m+1} \zeta_{m+1}]$$

where

$$J_{m+1} = I - \frac{(B_m h_{m+1}) h_{m+1}^T}{1 + h_{m+1}^T B_m h_{m+1}}.$$

Since $B_m H_m^T \mathbf{z}_m = H_m^+ \mathbf{z}_m = \hat{\mathbf{x}}_m$ and

$$J_{m+1} B_m h_{m+1} = \frac{B_m h_{m+1}}{1 + h_{m+1}^T B_m h_{m+1}}$$

we find that

$$(8.1.7.2) \quad \hat{\mathbf{x}}_{m+1} = \hat{\mathbf{x}}_m + \frac{B_m h_{m+1}}{1 + h_{m+1}^T B_m h_{m+1}} [\zeta_{m+1} - h_{m+1}^T \hat{\mathbf{x}}_m].$$

Since the columns of H_m are linearly independent by assumption, $\mathcal{N}(H_m) = \{0\}$, hence the projection on $\mathcal{N}(H_m)$ is zero: $I - H_m^+ H_m = 0$. It follows that $(I - H_m^+ H_m) h_{m+1} = 0$, so that K_{m+1} , defined in (8.1.5), is given by the second half of the right side which coincides with $B_m h_{m+1} / (1 + h_{m+1}^T B_m h_{m+1})$ as it should.

(8.1.8) Exercise

(a) h_{n+1} is a linear combination (l.c.) of h_1, \dots, h_n if and only if $(I - H_n^+ H_n) h_{n+1} = 0$.

(b) Let $A_n = I - H_n^+ H_n$ and $B_n = (H_n^T H_n)^+$. Then

$$(8.1.8.1) \quad K_{n+1} = \begin{cases} \frac{A_n h_{n+1}}{h_{n+1}^T A_n h_{n+1}} & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ \frac{B_n h_{n+1}}{1 + h_{n+1}^T B_n h_{n+1}} & \text{otherwise} \end{cases}$$

where

$$(8.1.8.2) \quad A_{n+1} = \begin{cases} A_n - \frac{(A_n h_{n+1})(A_n h_{n+1})^T}{h_{n+1}^T A_n h_{n+1}} & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ A_n & \text{otherwise} \end{cases}$$

$$A_0 = I \quad B_0 = 0$$

and

$$(8.1.8.3) \quad B_{n+1} = \begin{cases} B_n - \frac{(B_n h_{n+1})(A_n h_{n+1})^T + (A_n h_{n+1})(B_n h_{n+1})^T}{h_{n+1}^T A_n h_{n+1}} \\ \quad + \frac{1 + h_{n+1}^T B_n h_{n+1}}{(h_{n+1}^T A_n h_{n+1})^2} (A_n h_{n+1})(A_n h_{n+1})^T \\ \quad \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ B_n - \frac{(B_n h_{n+1})(B_n h_{n+1})^T}{1 + h_{n+1}^T B_n h_{n+1}} \quad \text{otherwise.} \end{cases}$$

[Hint: Use (4.6) and (3.14.1) and/or (4.6.4d).]

(8.2) Recursive Computation of Residual Errors

Denote the residual error associated with $\hat{x}_n = H_n^+ z_n$, by ε_n :

$$(8.2.1) \quad \varepsilon_n = \|z_n - H_n \hat{x}_n\|^2.$$

The results of (8.1) can be used to relate ε_{n+1} and ε_n :

(8.2.2) **Theorem:** $\varepsilon_0 = 0$

$$\varepsilon_{n+1} = \begin{cases} \varepsilon_n & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ \varepsilon_n + \frac{(\zeta_{n+1} - h_{n+1}^T \hat{x}_n)^2}{1 + h_{n+1}^T B_n h_{n+1}} & \text{otherwise} \end{cases}$$

where $B_n = (H_n^T H_n)^+$ satisfies (8.1.8.3).

Comment: (8.2.1) is the same as $\sum_{j=1}^n (\zeta_j - h_j^T \hat{x}_n)^2$, so (8.2.2) asserts the truth of the following identity:

$$\sum_{j=1}^n (\zeta_j - h_j^T \hat{x}_n)^2 = \sum_{j \in J_n} (\zeta_j - h_j^T \hat{x}_{j-1})^2 / (1 + h_j^T B_{j-1} h_j)$$

where

$$J_n = \{j: j \leq n \text{ and } h_j \text{ is a l.c. of } h_1, \dots, h_{j-1}\}.$$

The identity holds for all scalars ζ_1, \dots, ζ_n , all vectors, h_1, h_2, \dots, h_n , and all n .

Proof: Since

$$H_{n+1} = \begin{bmatrix} H_n \\ h_{n+1}^T \end{bmatrix} \quad \text{and} \quad z_{n+1} = \begin{bmatrix} z_n \\ \zeta_{n+1} \end{bmatrix}$$

we see from (8.1.6) that

(8.2.2.1)

$$z_{n+1} - H_{n+1} \hat{x}_{n+1} = \begin{pmatrix} z_n - H_n \hat{x}_n \\ \zeta_{n+1} - h_{n+1}^T \hat{x}_n \end{pmatrix} - \begin{pmatrix} H_n K_{n+1} \\ h_{n+1}^T K_{n+1} \end{pmatrix} (\zeta_{n+1} - h_{n+1}^T \hat{x}_n).$$

Case 1: h_{n+1} is not a l.c. of h_1, \dots, h_n :

Then $(I - H_n^+ H_n) h_{n+1} \neq 0$, and K_{n+1} is defined by the first part of (8.1.8.1). Therefore

$$H_n K_{n+1} = H_n A_n h_{n+1} / (h_{n+1}^T A_n h_{n+1}).$$

Since

$$A_n = I - H_n^+ H_n$$

it follows that

$$H_n A_n = 0$$

so

$$H_n K_{n+1} = 0 \quad \text{and} \quad h_{n+1}^T K_{n+1} = 1.$$

Hence by (8.2.2.1),

$$\begin{aligned} \varepsilon_{n+1} &= \|z_{n+1} - H_{n+1} \hat{x}_{n+1}\|^2 \\ &= \|z_n - H_n \hat{x}_n\|^2 = \varepsilon_n. \end{aligned}$$

Case 2: h_{n+1} is a l.c. of h_1, \dots, h_n : In this case, K_n is defined by the second half of (8.1.8.1). Then by (8.2.2.1),

$$\begin{aligned} (8.2.2.2) \quad & \|z_{n+1} - H_{n+1} \hat{x}_{n+1}\|^2 \\ &= \|z_n - H_n \hat{x}_n\|^2 + (\zeta_{n+1} - h_{n+1}^T \hat{x}_n)^2 \\ &\quad - 2\{(z_n - H_n \hat{x}_n)^T H_n K_{n+1} + (\zeta_{n+1} - h_{n+1}^T \hat{x}_n) h_{n+1}^T K_{n+1}\} \\ &\quad \times (\zeta_{n+1} - h_{n+1}^T \hat{x}_n) \\ &\quad + \{K_{n+1}^T H_n^T H_n K_{n+1} + (h_{n+1}^T K_{n+1})^2\} (\zeta_{n+1} - h_{n+1}^T \hat{x}_n)^2 \\ &= \|z_n - H_n \hat{x}_n\|^2 - 2z_n^T (I - H_n H_n^+) H_n K_{n+1} (\zeta_{n+1} - h_{n+1}^T \hat{x}_n) \\ &\quad + [(K_{n+1}^T H_n^T H_n K_{n+1}) + (1 - h_{n+1}^T K_{n+1})^2] (\zeta_{n+1} - h_{n+1}^T \hat{x}_n)^2. \end{aligned}$$

[We have used the fact that $(z_n - H_n \hat{x}_n)^T = z_n^T (I - H_n H_n^+)$ to generate the second term in (8.2.2.2.).]

Since $(I - H_n H_n^+) H_n = 0$, the second term vanishes. Since K_{n+1} is defined by the second half of (8.1.8.1) and since

$$B_n^T (H_n^T H_n) B_n = B_n$$

[because $B_n = (H_n^T H_n)^+$, which is symmetric]

it follows that

$$K_{n+1}^T (H_n^T H_n) K_{n+1} = \frac{h_{n+1}^T B_n h_{n+1}}{(1 + h_{n+1}^T B_n h_{n+1})^2}$$

and

$$(1 - h_{n+1}^T K_{n+1})^2 = \frac{1}{(1 + h_{n+1}^T B_n h_{n+1})^2}.$$

The third term in (8.2.2.2), reduces to $(\zeta_{n+1} - h_{n+1}^T \hat{x}_n)^2 / (1 + h_{n+1}^T B_n h_{n+1})$ and this proves the theorem. ■

(8.3) Weighted Least Squares

The recursion (8.1.6) and (8.1.8) can be viewed as a relationship between the value of x which minimizes

$$\sum_{j=1}^n (\zeta_j - h_j^T x)^2$$

and the value of x which minimizes

$$\sum_{j=1}^{n+1} (\zeta_j - h_j^T x)^2.$$

Not surprisingly, a similar relationship holds between the values of x which respectively minimize

$$\sum_{j=1}^n (\zeta_j - h_j^T x)^2 / \sigma_j^2 \quad \text{and} \quad \sum_{j=1}^{n+1} (\zeta_j - h_j^T x)^2 / \sigma_j^2.$$

(8.3.1) **Exercise:** Let $\sigma_1^2, \sigma_2^2, \dots$ be a sequence of positive scalars and let \tilde{x}_n be the vector of minimum norm among those which minimize $\sum_{j=1}^n (\zeta_j - h_j^T x)^2 / \sigma_j^2$. Then $\tilde{x}_0 = 0$,

$$(8.3.1.1) \quad \tilde{x}_{n+1} = \tilde{x}_n + \tilde{K}_{n+1} (\zeta_{n+1} - h_{n+1}^T \tilde{x}_n)$$

where

$$(8.3.1.2) \quad \tilde{K}_{n+1} = \begin{cases} A_n h_{n+1} / h_{n+1}^T A_n h_{n+1} & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ \tilde{B}_n h_{n+1} / (\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1}) & \text{otherwise,} \end{cases}$$

$$A_0 = I,$$

$$(8.3.1.3) \quad A_{n+1} = \begin{cases} A_n - \frac{(A_n h_{n+1})(A_n h_{n+1})^T}{h_{n+1}^T A_n h_{n+1}} & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ A_n & \text{otherwise,} \end{cases}$$

$$\tilde{B}_0 = 0,$$

$$(8.3.1.4) \quad \tilde{B}_{n+1} = \begin{cases} \tilde{B}_n - \frac{(\tilde{B}_n h_{n+1})(A_n h_{n+1})^T + (A_n h_{n+1})(\tilde{B}_n h_{n+1})^T}{h_{n+1}^T A_n h_{n+1}} \\ \quad + \frac{\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1}}{(h_{n+1}^T A_n h_{n+1})^2} (A_n h_{n+1})(A_n h_{n+1})^T & \text{if } h_{n+1} \text{ is not a l.c. of} \\ & h_1, \dots, h_n \\ \tilde{B}_n - \frac{(\tilde{B}_n h_{n+1})(\tilde{B}_n h_{n+1})^T}{\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1}} & \text{otherwise.} \end{cases}$$

Denoting the associated residual error by $\tilde{\epsilon}_n (= \sum_{j=1}^n (\zeta_j - h_j^T \tilde{x}_n)^2 / \sigma_j^2)$, we have

$$\tilde{\epsilon}_0 = 0,$$

$$(8.3.1.5) \quad \tilde{\epsilon}_{n+1} = \begin{cases} \tilde{\epsilon}_n & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ \tilde{\epsilon}_n + \frac{(\zeta_{n+1} - h_{n+1}^T \tilde{x}_n)^2}{(\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1})} & \text{otherwise.} \end{cases}$$

For each n ,

$$(8.3.1.6) \quad A_n = I - H_n^+ H_n$$

and

$$(8.3.1.7) \quad \begin{aligned} \tilde{B}_n &= \left(\sum_{j=1}^n h_j h_j^T / \sigma_j^2 \right)^+ \\ &= (H_n^T V_n^{-2} H_n)^+ \end{aligned}$$

where

$$(8.3.1.8) \quad H_n = \begin{pmatrix} h_1^T \\ \vdots \\ h_n^T \end{pmatrix} \quad \text{and} \quad V_n^2 = \text{diag}(\sigma_1^2, \dots, \sigma_n^2).$$

[Hint: Let $\tilde{\zeta}_j = \zeta_j / \sigma_j$, $\tilde{h}_j = h_j / \sigma_j$ and notice that

$$\mathcal{L}(h_1, h_2, \dots, h_n) = \mathcal{L}(\tilde{h}_1, \tilde{h}_2, \dots, \tilde{h}_n)$$

and

$$\sum_{j=1}^n (\zeta_j - h_j^T x)^2 / \sigma_j^2 = \sum_{j=1}^n (\tilde{\zeta}_j - \tilde{h}_j^T x)^2.$$

Apply (8.1.6)–(8.1.8) to the $\tilde{\zeta}_j$ and \tilde{h}_j 's and then translate back to ζ_j 's and h_j 's.]

(8.4) Recursive Constrained Least Squares, I

In (3.12.4b) we showed that

$$(8.4.1) \quad x^0 = G^+u + [H(I - G^+G)]^+(z - HG^+u)$$

is the vector of minimum norm among those which minimize

$$(8.4.2) \quad \|z - Hx\|^2$$

subject to the constraints

$$(8.4.3) \quad Gx = u$$

provided the constraint set is nonempty.

Imagine a "stream" of data, $\zeta_1, \zeta_2, \dots, \zeta_n, \dots$, and denote the vector of n observations by z_n and let x_n^0 be the minimum norm vector among those which minimize $\|z_n - H_n x\|^2 = \sum_{j=1}^n (\zeta_j - h_j^T x)^2$, subject to $Gx = 0$:

$$(8.4.4) \quad x_n^0 = G^+u + \bar{H}_n^+ \bar{z}_n$$

where $\bar{H}_n = H_n(I - G^+G)$ is the matrix whose j th row is

$$\bar{h}_j^T = [(I - G^+G)h_j]^T \quad (j = 1, 2, \dots, n)$$

and $\bar{z}_n = z_n - H_n G^+u$ is the n vector whose j th component is

$$\bar{\zeta}_j = \zeta_j - h_j^T G^+u \quad (j = 1, 2, \dots, n).$$

The recursion for $\hat{x}_n = H_n^+ z_n$ can be applied almost verbatim to the computation of

$$x_n^0 = G^+u + \bar{H}^+ \bar{z}_n.$$

(8.4.5) **Theorem:** Let $x_0^0 = G^+u$, $x_{n+1}^0 = x_n^0 + \bar{K}_{n+1}(\bar{\zeta}_{n+1} - \bar{h}_{n+1}^T x_n^0)$ where

$$\bar{K}_{n+1} = \begin{cases} \frac{\bar{A}_n \bar{h}_{n+1}}{\bar{h}_{n+1}^T \bar{A}_n \bar{h}_{n+1}} & \text{if } \bar{h}_{n+1} \text{ is not a l.c. of } \bar{h}_1, \bar{h}_2, \dots, \bar{h}_n \\ \frac{\bar{B}_n \bar{h}_{n+1}}{(1 + \bar{h}_{n+1}^T \bar{B}_n \bar{h}_{n+1})} & \text{otherwise} \end{cases}$$

where

$$\bar{A}_n = I - \bar{H}_n^+ \bar{H}_n \quad \text{and} \quad \bar{B}_n = (\bar{H}_n^T \bar{H}_n)^+$$

can be computed recursively by (8.1.8.2) and (8.1.8.3) with h 's replaced by \bar{h} 's throughout.

Proof: Let y_n^0 satisfy the same recursion as above except that $y_0^0 = 0$. Then by (8.1.6), $y_n^0 = \bar{H}_n^+ \bar{z}_n$ for every n . If we set $d_n = x_n^0 - y_n^0$, then d_n satisfies

$$d_{n+1} = (I - \bar{K}_{n+1} \bar{h}_{n+1}^T) d_n = \left[\prod_{j=1}^{n+1} (I - \bar{K}_j \bar{h}_j^T) \right] d_0.$$

But $d_0 = x_0^0 = G^+ u$ and $\bar{h}_j^T d_0 = h_j^T (I - G^+ G) G^+ u = 0$ so that

$$d_{n+1} = d_0 \quad \text{for all } n$$

which proves that $x_{n+1}^0 = y_{n+1}^0 + d_0$: Thus,

$$x_{n+1}^0 = G^+ u + \bar{H}_n^+ \bar{z}_n. \quad \blacksquare$$

If the previously mentioned recursion is used to process data in "real time," one precomputes $G^+ u$ and $I - G^+ G$. As each datum ζ_j is obtained, it is transformed to $\bar{\zeta}_j = \zeta_j - h_j^T G^+ u$ and the corresponding regression vector is transformed to $\bar{h}_j = (I - G^+ G) h_j$. The \bar{A}_n 's and \bar{B}_n 's are computed by the ancillary recursions (8.1.8.2) and (8.1.8.3).

The vector $G^+ u$ can be computed by any of the methods of Chapter V or recursively: Let the rows of G be denoted by g_1^T, \dots, g_k^T . Define

$$G_m = \begin{pmatrix} g_1^T \\ \vdots \\ g_m^T \end{pmatrix} \quad m = 1, 2, \dots, k.$$

Use (8.1.6), (8.1.8.2), and (8.1.8.3) to compute $G_m^+ u_m$ where u_m is the vector consisting of u 's first m component, for $m = 1, 2, \dots, k$. As a by-product, the A recursion will generate $I - G^+ G$.

(8.4.6) **Exercise:** Let

$$G = \begin{pmatrix} g_1^T \\ \vdots \\ g_k^T \end{pmatrix}$$

and let h_1, \dots, h_n, \dots be a sequence of vectors having the same dimensionality as the g 's. Let

$$\bar{h}_j = (I - G^+ G) h_j \quad (j = 1, 2, \dots).$$

Show that for any n , \bar{h}_n is a linear combination of $\bar{h}_1, \bar{h}_2, \dots, \bar{h}_{n-1}$ if and only if

$$h_n \in \mathcal{L}(g_1, \dots, g_k, h_1, \dots, h_{n-1})$$

(i.e., h_n is a linear combination of h_1, \dots, h_{n-1} and the g 's).

(8.4.7) **Exercise:** Suppose $f \in \mathcal{L}(g_1, \dots, g_k, h_1, \dots, h_n)$: Then

$$\lim_{\lambda \rightarrow 0} \left(\sum_{j=1}^n h_j h_j^T + \lambda^{-2} \sum_{j=1}^k g_j g_j^T \right)^+ f = 0$$

if and only if $f \in \mathcal{L}(g_1, \dots, g_k)$.

(8.4.8) **Exercise:** Extend the results of (8.4.5) and develop a recursion for \tilde{x}_n^0 , the value of x which minimizes

$$\sum_{j=1}^n (\zeta_j - h_j^T x) / \sigma_j^2$$

subject to $Gx = u$.

(8.5) Recursive Constrained Least Squares, II

In (8.4) we showed how constraints can be incorporated into a least squares recursion by altering the h -vectors and the observations, and by suitably initializing the x -vector.

An essential feature of the technique is the necessity to specify the constraints in *advance* of the data acquisition. Under certain circumstances, this is a drawback. Often, one wishes to collect all the data and afterward compute the least squares estimate subject to a succession of progressively more restrictive linear side conditions. By examining the residual errors [cf. (6.4)] one can judge the reasonableness of the constraints in the light of the available data. Or, one may wish to incorporate a few side conditions into the computation at the outset and then, after the data acquisition (or perhaps, even *during*) experiment with constraints.

In this section we shall show that constraints can be incorporated into the recursion (8.3.1) by treating them as fictitious observations with zero variance.

(8.5.1) **Theorem:** Let h_1, h_2, \dots be a sequence of vectors, let ζ_1, ζ_2, \dots be a sequence of scalars, and let $\sigma_1^2, \sigma_2^2, \dots$ be another sequence of nonnegative (but not necessarily positive) scalars. Let $\tilde{x}_n, \tilde{K}_n, \tilde{B}_n, A_n$, and \tilde{e}_n be defined recursively as in (8.3.1).

(a) If the σ_j^2 are all positive, then for each n , \tilde{x}_n minimizes the weighted sum of squares

$$\sum_{j=1}^n (\zeta_j - h_j^T x)^2 / \sigma_j^2$$

$$\tilde{B}_n = \left(\sum_{j=1}^n h_j h_j^T / \sigma_j^2 \right)^+$$

and

$$\tilde{\varepsilon}_n = \sum_{j=1}^n (\zeta_j - h_j^T \tilde{x}_n)^2 / \sigma_j^2.$$

(b) If some of the σ_j^2 are zero, say

$$\sigma_j^2 \begin{cases} = 0 & \text{if } j \in S \\ > 0 & \text{if } j \notin S \end{cases}$$

where S is a finite set of integers, then for each n , \tilde{x}_n minimizes

$$\sum_{j \in T_n} (\zeta_j - h_j^T x)^2 / \sigma_j^2$$

subject to the constraints

$$h_j^T x = \zeta_j \quad j \in S_n$$

and

$$\tilde{\varepsilon}_n = \sum_{j \in T_n} (\zeta_j - h_j^T \tilde{x}_n)^2 / \sigma_j^2$$

provided $\{h_j; j \in S\}$ is a linearly independent set. (Here we define $S_n = \{1, 2, \dots, n\} \cap S$ and $T_n = S - S_n$.)

Proof: (a) We have merely restated the results of (8.3.1) for easy reference.

(b) If some of the σ_j 's are zero, (8.3.1) does not apply directly, since those results were derived, under the assumption of positive σ_j 's. For this reason, we define

$$\tau_j^2(\lambda) = \begin{cases} \sigma_j^2 & \text{if } j \notin S \\ \lambda^2 & \text{if } j \in S \end{cases}$$

and consider the recursions of (8.3.1) with σ_j^2 replaced throughout by $\tau_j^2(\lambda)$. The A recursion does not depend on λ , but the x , B , K , and ε recursions do, so we display the relationship by denoting the outputs of these recursions by $\tilde{x}_n(\lambda)$, $\tilde{B}_n(\lambda)$, $\tilde{K}_n(\lambda)$, and $\tilde{\varepsilon}_n(\lambda)$. We will show that $\tilde{x}_n(\lambda)$ and $\tilde{\varepsilon}_n(\lambda)$ converge to the desired quantities¹ as $\lambda \rightarrow 0$ and that $\lim_{\lambda \rightarrow 0} \tilde{x}_n(\lambda)$ and $\lim_{\lambda \rightarrow 0} \tilde{\varepsilon}_n(\lambda)$ satisfy the stated recursions with $\tilde{B}_n(\lambda)$ replaced by $\tilde{B}_n = \lim_{\lambda \rightarrow 0} \tilde{B}_n(\lambda)$, $\tilde{K}_n(\lambda)$ replaced by $\lim_{\lambda \rightarrow 0} \tilde{K}_n(\lambda)$ and $\tau_j^2(\lambda)$ replaced throughout by σ_j^2 or 0 depending on whether $j \in T_j$ or $j \in S_j$.

(1) *Convergence of $\tilde{x}_n(\lambda)$ and $\tilde{\varepsilon}_n(\lambda)$*

By (8.3.1), $\tilde{x}_n(\lambda)$ is the vector of minimum norm among those which minimize

$$\sum_{j=1}^n (\zeta_j - h_j^T x)^2 / \tau_j^2(\lambda).$$

¹ The constrained least squares estimate and the associated residual error.

Therefore

$$(8.5.1.1) \quad \tilde{x}_n(\lambda) = \tilde{H}_n^+(\lambda) \tilde{z}_n(\lambda) = [\tilde{H}_n^T(\lambda) \tilde{H}_n(\lambda)]^+ \tilde{H}_n^T(\lambda) \tilde{z}_n(\lambda)$$

where

$$\tilde{H}_n(\lambda) = \begin{bmatrix} h_1^T/\tau_1(\lambda) \\ \vdots \\ h_n^T/\tau_n(\lambda) \end{bmatrix} \quad \text{and} \quad \tilde{z}_n(\lambda) = \begin{bmatrix} \zeta_1/\tau_1(\lambda) \\ \vdots \\ \zeta_n/\tau_n(\lambda) \end{bmatrix}.$$

Consequently we can rewrite (8.5.1.1) as

$$(8.5.1.2) \quad \tilde{x}_n(\lambda) = \left[\sum_{j \in T_n} h_j h_j^T / \sigma_j^2 + \sum_{j \in S_n} h_j h_j^T / \lambda^2 \right]^+ \times \left(\sum_{j \in T_n} h_j^T \zeta_j / \sigma_j^2 + \lambda^{-2} \sum_{j \in S_n} h_j^T \zeta_j \right).$$

In (7.1.10.2)–(7.1.10.10) we showed that if the equation $Gx = u$ has a solution, and

$$\tilde{x}(\lambda) = (F^T F + \lambda^{-2} G^T G)^+ (F^T w + \lambda^{-2} G^T u)$$

then

$$\lim_{\lambda \rightarrow 0} \tilde{x}(\lambda) = x^0$$

the vector of minimum norm among those which minimize $\|w - Fx\|^2$ subject to $Gx = u$, and that

$$\lim_{\lambda \rightarrow 0} [\|w - F\tilde{x}(\lambda)\|^2 + \lambda^{-2} \|u - G\tilde{x}(\lambda)\|^2] = \|w - Fx^0\|^2.$$

In the case at hand we let

$$(8.5.1.3) \quad F \text{ be the matrix whose rows are } \{h_j^T / \sigma_j; j \in T_n\}$$

and

$$(8.5.1.4) \quad G \text{ be the matrix whose rows are } \{h_j^T; j \in S_n\}.$$

$$(8.5.1.5) \quad w \text{ and } u \text{ are the vectors whose respective components are}$$

$$\{\zeta_j / \sigma_j; j \in T_n\} \quad \text{and} \quad \{\zeta_j; j \in S_n\}.$$

Then (8.5.1.2) takes the form

$$\tilde{x}_n(\lambda) = [F^T F + \lambda^{-2} G^T G]^+ [F^T w + \lambda^{-2} G^T u].$$

The rows of G are linearly independent by assumption, hence the equation $Gx = u$ has a solution, (3.12.5), hence

$$\lim_{\lambda \rightarrow 0} \tilde{x}_n(\lambda) = \tilde{x}_n$$

which minimizes $\sum_{j \in T_n} (\zeta_j - h_j^T x)^2 / \sigma_j^2$ subject to the constraints $h_j^T x = \zeta_j$; $j \in S_n$. Furthermore

$$\lim_{\lambda \rightarrow 0} \tilde{e}_n(\lambda) = \tilde{e}_n = \sum_{j \in T_n} (\zeta_j - h_j^T \tilde{x}_n)^2 / \sigma_j^2.$$

(2) *Convergence of $\tilde{B}_n(\lambda)$*

$\tilde{B}_n(\lambda) = [\tilde{H}_n^T(\lambda) \tilde{H}_n(\lambda)]^+$, (8.3.1.7), which is of the form $[F^T F + \lambda^{-2} G^T G]^+$ where F and G were defined earlier. By (4.9), $\lim_{\lambda \rightarrow 0} (F^T F + \lambda^{-2} G^T G)^+$ always exists. So then does

$$(8.5.1.6) \quad \tilde{B}_n = \lim_{\lambda \rightarrow 0} \tilde{B}_n(\lambda).$$

$\tilde{B}_{n+1}(\lambda)$ is related to $\tilde{B}_n(\lambda)$ through the recursion (8.3.1.4) with σ_{n+1}^2 replaced by $\tau_{n+1}^2(\lambda)$. If $n+1 \in T_{n+1}$, then $\lim_{\lambda \rightarrow 0} \tau_{n+1}^2(\lambda) = \sigma_{n+1}^2$ and so \tilde{B}_{n+1} is related to \tilde{B}_n through (8.3.1.4). If $(n+1) \in S_{n+1}$, then $\lim_{\lambda \rightarrow 0} \tau_{n+1}^2(\lambda) = 0$. \tilde{B}_{n+1} will be related to \tilde{B}_n through (8.3.1.4) with σ_{n+1}^2 set equal to zero if we can rule out the possibility that $h_{n+1}^T \tilde{B}_{n+1} h_{n+1} = 0$ when h_{n+1} is a l.c. of h_1, \dots, h_n . But if $n+1 \in S_{n+1}$ and h_{n+1} is a l.c. of h_1, \dots, h_n , then $h_{n+1}^T \tilde{B}_{n+1} h_{n+1} = 0$ if and only if

$$\tilde{B}_{n+1} h_{n+1} = \lim_{\lambda \rightarrow 0} \left[\sum_{j \in T_n} h_j h_j^T / \sigma_j^2 + \lambda^{-2} \sum_{j \in S_n} h_j h_j^T \right]^+ h_{n+1} = 0$$

and by (8.4.7) this can only happen if h_{n+1} is a l.c. of $\{h_j; j \in S_n\}$. The last possibility is excluded because $\{h_j; j \in S\}$ is required to be a linearly independent set by assumption. Thus

$$\tilde{B}_n = \lim_{\lambda \rightarrow 0} \tilde{B}_n(\lambda)$$

exists for each n and satisfies (8.3.1.4).

(3) *Recursions for \tilde{x}_n and \tilde{e}_n*

Since

$$(8.5.1.7) \quad \tilde{x}_{n+1}(\lambda) = \tilde{x}_n(\lambda) + \tilde{K}_{n+1}(\lambda) [\zeta_{n+1} - h_{n+1}^T \tilde{x}_n(\lambda)]$$

and since

$$\tilde{K}_{n+1} = \lim_{\lambda \rightarrow 0} \tilde{K}_{n+1}(\lambda) = \begin{cases} \frac{A_n h_{n+1}}{h_{n+1}^T A_n h_{n+1}} & \text{if } h_{n+1} \text{ is not a l.c.} \\ & \text{of } h_1, \dots, h_n \\ \frac{\tilde{B}_n h_{n+1}}{(\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1})} & \text{otherwise} \end{cases}$$

(where $\sigma_{n+1}^2 = 0$ if $n+1 \in S$), we see that

$$\tilde{x}_{n+1} = \tilde{x}_n + \tilde{K}_{n+1} [\zeta_{n+1} - h_{n+1}^T \tilde{x}_n]$$

since all terms on the right side of (8.5.1.7) have limits.

Similarly

$$\tilde{\varepsilon}_{n+1}(\lambda) = \tilde{\varepsilon}_n(\lambda) + \begin{cases} 0 & \text{if } h_{n+1} \text{ is not a l.c.} \\ & \text{of } h_1, \dots, h_n \\ \frac{[\zeta_{n+1} - h_{n+1}^T \tilde{x}_n(\lambda)]^2}{[\tau_{n+1}^2(\lambda) + h_{n+1}^T \tilde{B}_n(\lambda) h_{n+1}]} & \text{otherwise} \end{cases}$$

and since both sides tend to limits,

$$\tilde{\varepsilon}_{n+1} = \tilde{\varepsilon}_n + \begin{cases} 0 & \text{if } h_{n+1} \text{ is not a l.c. of} \\ & h_1, \dots, h_n \\ \frac{(\zeta_{n+1} - h_{n+1}^T \tilde{x}_n)^2}{(\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1})} & \text{otherwise.} \end{cases}$$

Notice that $h_{n+1}^T \tilde{B}_n h_{n+1} > 0$ if h_{n+1} is a l.c. of h_1, \dots, h_n and $n+1 \in S_{n+1}$ (by previous argument).

(8.5.2) **Exercise:** Let \tilde{B}_n be as defined earlier, and let P_n be the projection on the linear manifold spanned by $\{h_j; j \in S_n\}$. Assuming the last to be a linearly independent set, show that

$$\tilde{B}_n = \left[(I - P_n) \left(\sum_{j \in T_n} h_j h_j^T / \sigma_j^2 \right) (I - P_n) \right]^+.$$

(8.5.3) **Exercise:** If the rows of H are linearly independent of the rows of G , then

$$\min_x \|z - Hx\|^2 = \min_{Gx=u} \|z - Hx\|^2$$

(i.e., the minimal residual error for the unconstrained l.s.e. is the same as the residual error for the constrained l.s.e. in this case.)

(8.5.4) **Exercise:** Suppose the set $\{h_j; j \in S\}$ is not linearly independent. Show that

$$\tilde{B}_{n+1} = \lim_{\lambda \rightarrow 0} \tilde{B}_{n+1}(\lambda) = \tilde{B}_n$$

if h_{n+1} is a l.c. of $\{h_j; j \in S_n\}$ and $\sigma_{n+1}^2 = 0$.

(8.5.5) (Continued): Let $\mathcal{C}_n = \{x: h_j^T x = \zeta_j; j \in S_n\}$.

(a) Show that

$$\lim_{\lambda \rightarrow 0} [\zeta_{n+1} - h_{n+1}^T \tilde{x}_n(\lambda)]^2 / [\tau_{n+1}^2(\lambda) + h_{n+1}^T \tilde{B}_n(\lambda) h_{n+1}] = 0$$

if $n+1 \in S_{n+1}$, h_{n+1} is a l.c. of $\{h_j; j \in S_n\}$, and \mathcal{C}_{n+1} is not empty.

Hence, if the restriction in (8.5.1) that $\{h_j; j \in S\}$ be a linearly independent set is dropped, and if we define

$$\tilde{x}_{n+1} = \tilde{x}_n + \tilde{K}_{n+1}(\zeta_{n+1} - h_{n+1}^T \tilde{x}_n)$$

where

$$\begin{aligned} \tilde{K}_{n+1} &= \begin{cases} \frac{A_n h_{n+1}}{h_{n+1}^T A_n h_{n+1}} & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ \frac{\tilde{B}_n h_{n+1}}{\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1}} & \text{otherwise} \end{cases} \\ \tilde{e}_{n+1} &= \tilde{e}_n + \begin{cases} 0 & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \text{ or if } n+1 \in S_{n+1} \text{ and } h_{n+1} \text{ is a l.c. of } \{h_j; j \in S_n\} \\ \frac{[\zeta_{n+1} - h_{n+1}^T \tilde{x}_n]^2}{(\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1})} & \text{otherwise,} \end{cases} \\ A_{n+1} &= A_n - \begin{cases} \frac{(A_n h_{n+1})(A_n h_{n+1})^T}{h_{n+1}^T A_n h_{n+1}} & \text{if } h_{n+1} \text{ is a l.c. of } h_1, \dots, h_n \\ 0 & \text{otherwise} \end{cases} \\ \tilde{B}_{n+1} &= \begin{cases} \tilde{B}_n - \frac{(\tilde{B}_n h_{n+1})(A_n h_{n+1})^T + (A_n h_{n+1})(\tilde{B}_n h_{n+1})^T}{h_{n+1}^T A_n h_{n+1}} \\ \quad + \frac{\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1}}{(h_{n+1}^T A_n h_{n+1})^2} (A_n h_{n+1})(A_n h_{n+1})^T & \text{if } h_{n+1} \text{ is not a l.c. of } h_1, \dots, h_n \\ \tilde{B}_n & \text{if } n+1 \in S_{n+1} \text{ and } h_{n+1} \text{ is a l.c. of } \{h_j; j \in S_n\} \\ \tilde{B}_n - \frac{(\tilde{B}_n h_{n+1})(\tilde{B}_n h_{n+1})^T}{\sigma_{n+1}^2 + h_{n+1}^T \tilde{B}_n h_{n+1}} & \text{otherwise} \end{cases} \end{aligned}$$

then for each n ,

(b) \tilde{x}_n is the vector of minimum norm among those which minimize $\sum_{j \in T_n} (\zeta_j - h_j^T x)^2 / \sigma_j^2$ subject to $x \in \mathcal{C}_n$, provided \mathcal{C}_n is nonempty. Furthermore, \tilde{e}_n is the associated residual error.

(8.5.6) **Example:** In (4.3) we showed how to relate $(H^T; h)^+$ to H^{T+} . Using the results of (8.5), we can go in the opposite direction: Given $(H^T; h)^+$, we can compute H^{T+} without having to “start from scratch.” The key to this procedure resides in the fact that the vector of minimum norm among those which minimize $\|y - Cv\|^2$ subject to the constraint $g^T v = 0$ (where $C = (H^T; h)$ [an $m \times (n+1)$ matrix] and $g^T = (0, 0, \dots, 0, 1)$ [a $1 \times (n+1)$])

row vector] is

$$(8.5.6.1) \quad \hat{v} = \begin{pmatrix} H^{T+} \\ -\bar{0} \end{pmatrix} y.$$

This is a direct consequence of (3.12.4):

$$\hat{v} = \bar{C}^+ y \quad \text{where} \quad \bar{C} = C(I - gg^+).$$

Since

$$I - gg^+ = \begin{matrix} n & 1 \\ \left(\begin{array}{c|c} I & 0 \\ \hline 0 & 0 \end{array} \right) \end{matrix} \hat{v}$$

$\bar{C} = (H^T; 0)$ and so

$$\bar{C}^+ = \begin{pmatrix} H^{T+} \\ -\bar{0} \end{pmatrix}.$$

But the results of (8.5) tell us that the constraint

$$g^T v = 0$$

can be thought of as a “new” observation $\zeta_{m+1} = 0$ with zero variance, and that

$$\hat{v} = C^+ y$$

can be updated in the light of the new observation according to (8.3.1.1)–(8.3.1.4):

$$\hat{v} = \hat{v} + K_C(\zeta_{m+1} - g^T \hat{v}) = \hat{v} - K_C(g^T \hat{v})$$

where

$$K_C = \begin{cases} \frac{(I - C^+ C)g}{g^T(I - C^+ C)g} & \text{if } g \text{ is not a l.c. of the rows of } C \\ \frac{(C^T C)^+ g}{g^T(C^T C)^+ g} & \text{otherwise.} \end{cases}$$

But g is a l.c. of the rows of C if and only if g is a l.c. of the columns of C^T which is the same as $g \in \mathcal{R}(C^T)$ so that g is a l.c. of the rows of C if and only if

$$C^+ C g = g. \quad (3.7.10)$$

Since

$$C = (H^T; h) \quad \text{and} \quad g = (0, \dots, 0, 1)$$

it follows that

$$Cg = h$$

so that

$$C^+ Cg = C^+ h.$$

Thus,

$$\begin{pmatrix} H^T \\ \vdots \\ 0 \end{pmatrix} y = \hat{v} = (I - K_C g^T) \hat{v} = (I - K_C g^T)(H^T; h)^+ y \quad \text{for all } y$$

so that

$$(8.5.6.2) \quad \begin{pmatrix} H^T \\ \vdots \\ 0 \end{pmatrix} = (I - K_C g^T)(H^T; h)^+$$

where

$$K_C = \begin{cases} \frac{(I - C^+ C)g}{g^T(I - C^+ C)g} & \text{if } C^+ h \neq g \\ \frac{(C^T C)^+ g}{g^T(C^T C)^+ g} & \text{otherwise} \end{cases}$$

where $C = (H^T; h)$ and $g = (0, 0, \dots, 0, 1)$. (8.5.6.2) is the desired result which relates H^{T+} to $(H^T; h)^+$.

(8.5.7) **Exercise** [Continuation of (8.5.6)]

(a) $C^+ h = g$ if and only if $(I - H^+ H)h \neq 0$.

(b) $K_C = \begin{cases} (g - C^+ h)/(1 - h^T(CC^T)^+ h) & \text{if } (I - H^+ H)h = 0 \\ C^+(CC^T)^+ h / \|(CC^T)^+ h\|^2 & \text{otherwise.} \end{cases}$

(8.5.8) **Example** *Straight line regression performed recursively*

Suppose observations are collected which are of the form

$$(8.5.8.1) \quad \zeta_n = \alpha + \beta n + v_n \quad n = 1, 2, 3$$

where the v 's are uncorrelated, zero mean random variables with common variance. α and β are not known and are to be estimated.

Denote the least squares estimate (=BLUE) for $x = \begin{pmatrix} 1 \\ \beta \end{pmatrix}$, based on the first k observations by

$$\hat{x}_k = \begin{pmatrix} \hat{\alpha}_k \\ \hat{\beta}_k \end{pmatrix} \quad k = 1, 2, 3.$$

If we let

$$h_k = \begin{pmatrix} 1 \\ k \end{pmatrix} \quad k = 1, 2, 3$$

then \hat{x}_k can be computed recursively via (8.3.1):

$$A_0 = I \quad B_0 = 0 \quad \hat{x}_0 = 0$$

$$K_1 = \frac{A_0 h_1}{h_1^T A_0 h_1} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

$$\hat{x}_1 = K_1 (\zeta_1 - h_1^T \hat{x}_0) = \begin{pmatrix} \zeta_1/2 \\ \zeta_1/2 \end{pmatrix}.$$

$$\begin{aligned} A_1 &= A_0 - h_1 h_1^T / \|h_1\|^2 \\ &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \end{aligned}$$

$$B_1 = (A_0 h_1) \frac{(A_0 h_1)^T}{(h_1^T A_0 h_1)^2} = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

$$A_1 h_2 = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix} \quad B_1 h_2 = \begin{pmatrix} \frac{3}{4} \\ \frac{3}{4} \end{pmatrix}.$$

Since h_2 is not a multiple of h_1 ,

$$K_2 = \frac{A_1 h_2}{h_2^T A_1 h_2} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

$$\begin{aligned} \hat{x}_2 &= \hat{x}_1 + K_2 (\zeta_2 - h_2^T \hat{x}_1) \\ &= \begin{pmatrix} \zeta_1/2 \\ \zeta_1/2 \end{pmatrix} + \begin{pmatrix} -1 \\ 1 \end{pmatrix} (\zeta_2 - \frac{3}{2}\zeta_1) \\ &= \begin{pmatrix} 2\zeta_1 - \zeta_2 \\ \zeta_2 - \zeta_1 \end{pmatrix} \end{aligned}$$

$$A_2 = A_1 - (A_1 h_2)(A_1 h_2)^T / (h_2^T A_1 h_2) = 0$$

$$\begin{aligned} B_2 &= B_1 - [(B_1 h_2)(A_1 h_2)^T + (A_1 h_2)(B_1 h_2)^T] / h_2^T A_1 h_2 \\ &\quad + (1 + h_2^T B_1 h_2)(A_1 h_2)(A_1 h_2)^T / (h_2^T A_1 h_2)^2 \\ &= \begin{pmatrix} \frac{1}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix} - \begin{pmatrix} -\frac{3}{2} & 0 \\ 0 & \frac{3}{2} \end{pmatrix} + \begin{pmatrix} \frac{13}{4} & -\frac{13}{4} \\ -\frac{13}{4} & \frac{13}{4} \end{pmatrix} \\ &= \begin{pmatrix} 5 & -3 \\ -3 & 2 \end{pmatrix}. \end{aligned}$$

$$B_2 h_3 = \begin{pmatrix} -4 \\ 3 \end{pmatrix}$$

and since h_3 is a linear combination of h_1 and h_2 ($h_3 = 2h_2 - h_1$),

$$(8.5.8.2) \quad \begin{aligned} K_3 &= \frac{B_2 h_3}{(1 + h_3^T B_2 h_3)} = \begin{pmatrix} -\frac{2}{3} \\ \frac{1}{2} \end{pmatrix} \\ \hat{x}_3 &= \hat{x}_2 + K_3(\zeta_3 - h_3^T \hat{x}_2) \\ &= \begin{pmatrix} 4\zeta_1/3 + \zeta_2/3 - 2\zeta_3/3 \\ \zeta_3/2 - \zeta_1/2 \end{pmatrix}. \end{aligned}$$

In Exercise (6.6.11), $\hat{\alpha}_3$ and $\hat{\beta}_3$ are given in closed form:

$$\hat{\beta}_3 = \left[\sum_{j=1}^3 (\zeta_j - \bar{\zeta})(\tau_j - \bar{\tau}) \right] \left[\sum_{j=1}^3 (\tau_j - \bar{\tau})^2 \right]^{-1}$$

and

$$\hat{\alpha}_3 = \bar{\zeta} - \hat{\beta}_3 \bar{\tau}$$

where

$$\bar{\zeta} = \frac{1}{3} \sum_{j=1}^3 \zeta_j \quad \text{and} \quad \bar{\tau} = \frac{1}{3} \sum_{j=1}^3 \tau_j.$$

In the present case, $\tau_j = j$ so $\bar{\tau} = 2$. Thus

$$\hat{\beta}_3 = \frac{-(\zeta_1 - \bar{\zeta}) + (\zeta_3 - \bar{\zeta})}{2} = \frac{\zeta_3 - \zeta_1}{2}$$

and

$$\begin{aligned} \hat{\alpha}_3 &= \bar{\zeta} - 2 \left(\frac{\zeta_3 - \zeta_1}{2} \right) = \frac{\zeta_1 + \zeta_2 + \zeta_3}{3} - \zeta_3 + \zeta_1 \\ &= \frac{4\zeta_1}{3} + \frac{\zeta_2}{3} - \frac{2\zeta_3}{3} \end{aligned}$$

which agrees with (8.5.8.2).

The covariance for \hat{x}_3 is given by $\sigma^2 B_3$ where σ^2 is the variance of the v 's and

$$(8.5.8.3) \quad \begin{aligned} B_3 &= B_2 - (B_2 h_3)(B_2 h_3)^T / (1 + h_3^T B_2 h_3) \\ &= \begin{pmatrix} \frac{7}{3} & -1 \\ -1 & \frac{1}{2} \end{pmatrix}. \end{aligned}$$

($A_3 = 0$ since h_1 and h_2 span two-dimensional space.)

(8.5.9) Adding a Constraint

Suppose we now wish to compute the least squares estimate for $x = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ based on the first three observations, subject to the constraint $\beta = 0$.

According to (8.5.1), this may be achieved by adding the fictitious observation $\zeta_4 = 0$ "pretending" at the same time that

$$\zeta_4 = h_4^T x + v_4$$

where v_4 has zero variance and

$$h_4 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We apply (8.3.1) with $\sigma_4^2 = 0$ and find that

$$K_4 = \frac{B_3 h_4}{h_4^T B_3 h_4} = \begin{pmatrix} -2 \\ 1 \end{pmatrix}$$

$$\begin{aligned} (8.5.9.1) \quad \hat{x}_4 &= \hat{x}_3 + K_4(0 - h_4^T \hat{x}_3) \\ &= (I - K_4 h_4^T) \hat{x}_3 = \begin{pmatrix} \frac{1}{3}(\zeta_1 + \zeta_2 + \zeta_3) \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} \bar{\zeta} \\ 0 \end{pmatrix} \end{aligned}$$

which is what we should get if there is any justice.

(8.5.10) Incorporating the Constraint

Using (8.4), we could carry the constraint right along and compute the least squares estimate for x based on one, two, and three observations, all subject to $\beta = 0$.

The constraint $\beta = 0$ is the same as $Gx = 0$ where $G = (0 \ 1)$. Then

$$G^+ = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad I - G^+ G = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\bar{h}_k = (I - G^+ G) h_k = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad k = 1, 2, 3.$$

Therefore, \bar{h}_2 is a l.c. of \bar{h}_1 as is \bar{h}_3 and

$$\bar{K}_1 = \frac{\bar{A}_0 \bar{h}_1}{\bar{h}_1^T \bar{A}_0 \bar{h}_1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\bar{x}_1 = \bar{K}_1(\zeta_1) = \begin{pmatrix} \zeta_1 \\ 0 \end{pmatrix}$$

$$\bar{A}_1 = \frac{\bar{A}_0 - \bar{h}_1 \bar{h}_1^T}{\|\bar{h}_1\|^2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\bar{B}_1 = \frac{(\bar{A}_0 \bar{h}_1)(\bar{A}_0 \bar{h}_1)^T}{(\bar{h}_1^T \bar{A}_0 \bar{h}_1)^2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\bar{K}_2 = \frac{\bar{B}_1 \bar{h}_2}{(1 + \bar{h}_2^T \bar{B}_1 \bar{h}_2)} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$$

$$\bar{x}_2 = \bar{x}_1 + \bar{K}_2(\zeta_2 - \bar{h}_2^T \bar{x}_1) = \begin{pmatrix} \frac{1}{2}(\zeta_1 + \zeta_2) \\ 0 \end{pmatrix}$$

$$\bar{A}_2 = \bar{A}_1$$

$$\bar{B}_2 = \bar{B}_1 - \frac{(\bar{B}_1 \bar{h}_1)(\bar{B}_1 \bar{h}_1)^T}{(1 + \bar{h}_1^T \bar{B}_1 \bar{h}_1)} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix}$$

$$\bar{K}_3 = \frac{\bar{B}_2 \bar{h}_3}{(1 + \bar{h}_3^T \bar{B}_2 \bar{h}_3)} = \begin{pmatrix} \frac{1}{3} \\ 0 \end{pmatrix}$$

$$\bar{x}_3 = \bar{x}_2 + \bar{K}_3(\zeta_3 - \bar{h}_3^T \bar{x}_2) = \begin{pmatrix} \frac{1}{3}(\zeta_1 + \zeta_2 + \zeta_3) \\ 0 \end{pmatrix} = \begin{pmatrix} \bar{\zeta} \\ 0 \end{pmatrix}$$

which agrees with (8.5.9.1).

(8.6) Additional Regressors, II (Stepwise Regression)

In (4.4) we discussed the problem of enriching a linear model by adding additional regressors and we derived a recursive relationship between the best m -dimensional regression and the best $(m+1)$ -dimensional regression in (4.4.4). That result is limited to the situation where regressors are added one at a time. This restriction is not essential. Indeed, the results of (6.6.14) can be applied to yield immediate results for the general case:

Suppose then, that a "preliminary" model of the form

$$(8.6.1) \quad \mathbf{z} = H_1 \mathbf{x}_1 + \mathbf{v}$$

is analyzed, where H_1 is an $n \times p$ matrix, and \mathbf{v} 's covariance is proportional to the identity matrix. The BLUE for \mathbf{x}_1 would then be

$$(8.6.2) \quad \mathbf{x}_1^* = H_1^+ \mathbf{z}$$

with the associated residual error

$$(8.6.3) \quad \boldsymbol{\varepsilon}_1 = \|\mathbf{z} - H_1 \mathbf{x}_1^*\|^2.$$

If $\boldsymbol{\varepsilon}_1$ were judged to be too large, an enriched model of the form

$$(8.6.4) \quad \mathbf{z} = (H_1 : H_2) \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} + \mathbf{v}$$

might be investigated, where H_2 is some suitably chosen $n \times q$ matrix.

The BLUE for

$$\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}$$

would now be

$$(8.6.5) \quad \begin{pmatrix} \hat{\mathbf{x}}_1 \\ \hat{\mathbf{x}}_2 \end{pmatrix} = (H_1 : H_2)^+ \mathbf{z}$$

and the residual error would be

$$(8.6.6) \quad \boldsymbol{\varepsilon}_{12} = \|\mathbf{z} - H_1 \hat{\mathbf{x}}_1 - H_2 \hat{\mathbf{x}}_2\|^2.$$

If $(H_1 : H_2)$ has rank $p+q$, we can apply the results of (6.6.14) to these computations: Letting $Q_1 = I - H_1 H_1^+$ we find that

$$(8.6.7) \quad \hat{\mathbf{x}}_2 = (Q_1 H_2)^+ \mathbf{z}$$

$$(8.6.8) \quad \hat{\mathbf{x}}_1 = H_1^+ (\mathbf{z} - H_2 \hat{\mathbf{x}}_2)$$

$$(8.6.9) \quad \boldsymbol{\varepsilon}_{12} = \boldsymbol{\varepsilon}_1 - \|Q_1 H_2 \hat{\mathbf{x}}_2\|^2.$$

(8.6.10) Exercise

(a) If $(H_1 : H_2)$ has full column rank then $H_2^T Q_1 H_2$ is nonsingular.

(b) In this case

$$H_2^T Q_1 H_2 \hat{\mathbf{x}}_2 = H_2^T Q_1 \mathbf{z}$$

and

(c) $\boldsymbol{\varepsilon}_{12} = \boldsymbol{\varepsilon}_1 - (H_2 \hat{\mathbf{x}}_2)^T (Q_1 \mathbf{z}).$

(8.7) **Example** *Relationship between analysis of variance and analysis of covariance* (Scheffé [1, Section 6.3]): Let

$$(8.7.1) \quad \mathbf{z} = \begin{bmatrix} \zeta_{11} \\ \zeta_{12} \\ \zeta_{1J_1} \\ \zeta_{21} \\ \vdots \\ \zeta_{kJ_k} \end{bmatrix}$$

and suppose a model for the observations of the form

$$(8.7.2) \quad \zeta_{ij} = \beta_i + \mathbf{v}_{ij} \quad j = 1, \dots, J_i; \quad i = 1, \dots, k,$$

were assumed (one-way layout), where the J_i 's were uncorrelated zero mean random variables with common variance.

The BLUE (=least squares estimate) for the vector of β_i 's is unique and easily seen to be given by

$$(8.7.3) \quad \beta_i^* = (J_i)^{-1} \sum_j \zeta_{ij} \equiv \bar{\zeta}_i.$$

which may be verified by differentiating

$$\sum_{ij} (\zeta_{ij} - \beta_i)^2$$

with respect to the β_i 's, setting the results equal to zero and solving the resulting normal equations.

The associated residual sum of squares is

$$(8.7.4) \quad \epsilon_1 = \sum_{ij} (\zeta_{ij} - \bar{\zeta}_i)^2.$$

In vector notation, we write

$$\mathbf{z} = H_1 \mathbf{x}_1 + \mathbf{v}$$

where

$$\mathbf{x}_1 = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}.$$

The BLUE for \mathbf{x}_1 is

$$(8.7.5) \quad \mathbf{x}_1^* = \begin{pmatrix} \beta_1^* \\ \vdots \\ \beta_k^* \end{pmatrix} = H_1^+ \mathbf{z} = \begin{pmatrix} \bar{\zeta}_1 \\ \vdots \\ \bar{\zeta}_k \end{pmatrix}$$

and

$$(8.7.6) \quad \begin{aligned} \epsilon_1 &= \|z - H_1 x_1^*\|^2 = \|(I - H_1 H_1^+) z\|^2 \\ &= \|Q_1 z\|^2 = \sum_{ij} (\zeta_{ij} - \bar{\zeta}_{i.})^2. \end{aligned}$$

Equation (8.7.5) tells us that the operator H_1^+ transforms any vector z which is written in the double subscript form (8.7.1), into the vector $H_1^+ z$ whose components are obtained by averaging the components of z having the same initial subscript.

Symbolically,

$$(8.7.7) \quad H_1^+ \begin{bmatrix} \zeta_{11} \\ \zeta_{12} \\ \vdots \\ \zeta_{kJ_k} \end{bmatrix} = \begin{bmatrix} \bar{\zeta}_{1.} \\ \vdots \\ \bar{\zeta}_{k.} \end{bmatrix}.$$

By the same token, (8.7.6) tells us that Q_1 transforms any vector z of the form (8.7.1) into a vector

$$(8.7.8) \quad \bar{z} = Q_1 z = \begin{bmatrix} \bar{\zeta}_{11} \\ \bar{\zeta}_{12} \\ \vdots \\ \bar{\zeta}_{kJ_k} \end{bmatrix}$$

where

$$(8.7.9) \quad \bar{\zeta}_{ij} = \zeta_{ij} - \bar{\zeta}_{i.}.$$

If ϵ_1 is judged to be too large and the model is enriched by the addition of a regression term of the form $\gamma\eta_{ij}$ (where γ is unknown and the η_{ij} 's are known), the model takes the form

$$(8.7.10) \quad \zeta_{ij} = \beta_i + \gamma\eta_{ij} + v_{ij}.$$

In the vector notation

$$(8.7.11) \quad z = H_1 x_1 + H_2 x_2 + v$$

where H_2 is a matrix with one column (i.e., a vector) and x_2 has one component:

$$(8.7.12) \quad x_2 = [\gamma]$$

$$(8.7.13) \quad H_2 = \begin{bmatrix} \eta_{11} \\ \eta_{12} \\ \vdots \\ \eta_{kJ_k} \end{bmatrix}.$$

Applying (8.6.7), we see that the BLUE for x_2 is

$$(8.7.14) \quad \hat{\mathbf{x}}_2 = (Q_1 H_2)^+ \mathbf{z}.$$

By virtue of (8.7.8),

$$(8.7.15) \quad Q_1 H_2 = \bar{H}_2 = \begin{bmatrix} \bar{\eta}_{11} \\ \vdots \\ \bar{\eta}_{kJ_k} \end{bmatrix}$$

where

$$(8.7.16) \quad \bar{\eta}_{ij} = \eta_{ij} - \eta_i.$$

We know that for any matrix with one column,

$$(8.7.17) \quad \bar{H}_2^+ = (\bar{H}_2^T \bar{H}_2)^{-1} \bar{H}_2^T = \bar{H}_2^T / \|\bar{H}_2\|^2,$$

and so

$$\hat{\mathbf{x}}_2 = (\bar{H}_2^T \mathbf{z}) / \|\bar{H}_2\|^2$$

or equivalently

$$(8.7.18) \quad \hat{\gamma} = \sum_{ij} \bar{\eta}_{ij} \zeta_{ij} / \sum_{ij} \bar{\eta}_{ij}^2.$$

The BLUE for the β 's in the enriched model are found using (8.6.8):

$$(8.7.19) \quad \hat{\mathbf{x}}_1 = H_1^+ (\mathbf{z} - H_2 \hat{\mathbf{x}}_2).$$

But

$$(8.7.20) \quad \mathbf{z} - H_2 \hat{\mathbf{x}}_2 \equiv \mathbf{z}^* = \begin{bmatrix} \zeta_{11}^* \\ \vdots \\ \zeta_{kJ_k}^* \end{bmatrix}$$

where

$$(8.7.21) \quad \zeta_{ij}^* = \zeta_{ij} - \hat{\gamma} \eta_{ij}.$$

By virtue of (8.7.7), the i th component of $H_1^+ \mathbf{z}^*$ is ζ_i^* , so

$$(8.7.22) \quad \hat{\mathbf{x}}_1 = \begin{pmatrix} \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_k \end{pmatrix} = \begin{pmatrix} \zeta_1^* \\ \vdots \\ \zeta_k^* \end{pmatrix}.$$

Finally, the residual sum of squares ϵ_{12} , is obtained via (8.6.9):

$$\epsilon_{12} \equiv \|\mathbf{z} - H_1 \hat{\mathbf{x}}_1 - H_2 \hat{\mathbf{x}}_2\|^2 = \epsilon_1 - \hat{\gamma}^2 \|Q_1 H_2\|^2.$$

By virtue of (8.7.15), the last is equal to

$$(8.7.23) \quad \epsilon_{12} = \epsilon_1 - \hat{\gamma}^2 \sum_{ij} \bar{\eta}_{ij}^2 = \sum_{ij} (\zeta_{ij}^2 - \hat{\gamma}^2 \bar{\eta}_{ij}^2).$$

(8.8) Missing Observations

In (6.6) we discussed the computational advantages of orthogonal designs when computations are carried out on a desk calculator. But the best laid plans of men for mice often go haywire and it is painfully common for something to foul up the experimental design during the course of the experiment (e.g., an experimental animal dies) thereby causing an experimental observation to be ruined, and destroying the orthogonality of the design. For example, suppose the experiment were planned in such a way that the observation vector z is of the form

$$z = Hx + v$$

where x is the (k -dimensional vector) parameter of interest. Suppose further, that the experiment had been carefully designed so that the columns of H would be mutually orthogonal and have unit lengths. Then the least squares estimate would be marvelously easy to compute:

$$\hat{x} = H^+ z = (H^T H)^{-1} H^T z = H^T z$$

(since $H^T H = I$ if the columns of H are orthonormal).

If a rat dies before the experiment is over, an observation is ruined. The actual vector of observation is now

$$z^* = H^* x + v$$

where H^* is a maimed version of H : One row is missing so that H^* 's columns are no longer orthogonal. It looks as though we are stuck with the job of psuedoinverting H^* or something equally messy, right?

Wrong! For the sake of concreteness, assume that the missing observation corresponds to the last one, so that if H is an $n \times k$ matrix, H^* is an $(n-1) \times k$ matrix and

$$H = \begin{pmatrix} H^* \\ \bar{h}^T \end{pmatrix}$$

(where \bar{h}^T is the last row vector of H , the one that is missing from H^*).

By (8.5.6.2)

$$[(H^*)^+ | 0] = H^T (I - gK^T)$$

where

$$g = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix} \quad (n \text{ components})$$

and

$$K = \begin{cases} \frac{(I - HH^+)g}{g^T(I - HH^+)g} & \text{if } g \text{ is not a l.c. of the columns of } H \\ \frac{(HH^T)^+g}{g^T(HH^T)^+g} & \text{otherwise.} \end{cases}$$

Since the columns of H (call them g_1, g_2, \dots, g_k) are orthonormal, the question of whether g is a l.c. of g_1, \dots, g_k is easily settled:

$$HH^+g = HH^Tg = \sum_{j=1}^k (g_j^Tg)g_j$$

so that one need only compare g to the right side of the last equation to see whether or not $(I - HH^+)g = 0$. Notice also that $(HH^T)^+ = HH^T$, (3.7.3).

Thus

$$[(H^*)^+; 0] = H^T(I - gK^T)$$

where

$$\begin{aligned} K &= \begin{cases} (I - HH^T)g/(1 - \|H^Tg\|^2) & \text{if } HH^Tg \neq g \\ HH^Tg/\|HH^Tg\|^2 & \text{if } HH^Tg = g \end{cases} \\ &= \begin{cases} (I - HH^T)g/(1 - \|H^Tg\|^2) & \text{if } HH^Tg \neq g \\ g & \text{otherwise.} \end{cases} \end{aligned}$$

In this case, a very simple relationship exists between the pseudoinverse of the matrix H (whose columns are orthonormal) and the pseudoinverse of H^* , the matrix obtained by deleting H 's last row.

The least squares estimate for x and the corresponding residual sum of squares for the "censored" data, z^* , is thereby simply related to that which would have been obtained if the rat had not died:

$$\hat{x}^* = H^{*+}z^* = [(H^*)^+; 0]z$$

(since

$$z = \begin{pmatrix} z^* \\ \zeta \end{pmatrix}$$

where ζ is the missing observation) so

$$\hat{x}^* = H^T(I - gK^T)z = H^T\bar{z}$$

where

$$\bar{z} = z - g(K^Tz)$$

is a modified observation vector which agrees with the uncensored sample z , in the first n components, but “pretends” that the missing observation was actually observed and had the value $\zeta - K^T z$.

Since $K^T g = 1$, it follows that

$$(I - gK^T)g = g(I - K^T g) = 0$$

so that

$$(I - gK^T)(z_1 - z_2) = 0$$

if z_1 and z_2 agree in their first $n-1$ components. Therefore, \bar{z} does not depend explicitly on the choice of z 's last component, ζ , and we can choose $\zeta = 0$.

This analysis can be generalized to the case of a missing observation for an arbitrary design.

(8.8.1) **Theorem:** Let

$$H = \begin{pmatrix} \tilde{H} \\ \tilde{h}^T \end{pmatrix} \quad z = \begin{pmatrix} \tilde{z} \\ 0 \end{pmatrix} \quad B = (H^T H)^+$$

$$\hat{x} = H^+ z \quad \varepsilon = \|z - H\hat{x}\|^2 \quad \tilde{x} = \tilde{H}^+ \tilde{z} \quad \text{and} \quad \tilde{\varepsilon} = \|\tilde{z} - \tilde{H}\tilde{x}\|^2.$$

Then

$$(8.8.1.1) \quad \tilde{x} = (I - Bh h^T M) \hat{x}$$

where

$$M = \begin{cases} -I/(1 - h^T B h) & \text{if } h \text{ is a l.c. of the rows of } \tilde{H} \\ B/\|Bh\|^2 & \text{otherwise} \end{cases}$$

$$(8.8.1.2) \quad \tilde{\varepsilon} = \begin{cases} \varepsilon - (h^T \hat{x})^2/(1 - h^T B h) & \text{if } h \text{ is a l.c. of the rows of } \tilde{H} \\ \varepsilon & \text{otherwise} \end{cases}$$

Comment: \hat{x} is the least squares estimate for x based on the full data model

$$z = Hx + v,$$

and ε is the associated residual sum of squares.

If an observation is missing (say the last), then the observations are of the form

$$\tilde{z} = \tilde{H}x + \tilde{v}$$

where \tilde{H} is obtained from H by deleting its last row. The new least squares estimate is

$$\tilde{x} = \tilde{H}^+ \tilde{z}$$

and its residual sum of squares is $\tilde{\varepsilon} = \|\tilde{z} - \tilde{H}\tilde{x}\|^2$.

If more than one observation is missing, the recursion (8.8.1) can be iterated as many times as necessary. However, care must be exercised in defining $\tilde{B} = (\tilde{H}^T \tilde{H})^+$ for all cases [cf. (8.8.2)], not just in the case where h is a l.c. of \tilde{H} 's rows.

Proof of theorem: $\tilde{x} = (\tilde{H}^+; 0)z = H^+(I - gk^T)z$ where

$$k = \begin{cases} (g - H^T h)/1 - h^T(H^T H)^+ h & \text{if } h \text{ is a l.c. of the rows of } \tilde{H} \\ H^T + (H^T H)^+ h / \|(H^T H)^+ h\|^2 & \text{otherwise.} \end{cases} \quad (8.5.6.2) \text{ and } (8.5.7)$$

Since z 's last component is zero, $g^T z = 0$ so that

$$k^T z = \begin{cases} -h^T \hat{x} / 1 - h^T B h & \text{if } h \text{ is a l.c. of } \tilde{H}'\text{'s rows} \\ h^T B \hat{x} / \|B h\|^2 & \text{otherwise.} \end{cases}$$

(8.8.1.1) follows once we observe that

$$H^+ g = B H^T g = B(\tilde{H}^T; h)g = B h$$

since g has all zero components except the last.

The formula for $\tilde{\varepsilon}$ follows from (8.2.2).

(8.8.2) **Exercise:** Let $\tilde{B} = (\tilde{H}^T \tilde{H})^+$. Then

$$(a) \quad \tilde{B} = \begin{cases} B - \frac{(Bh)(B^2 h)^T + (B^2 h)(Bh)^T}{\|Bh\|^2} \\ \quad + \frac{h^T B^3 h}{\|Bh\|^4} (Bh)(Bh)^T & \text{if } h \text{ is not a l.c. of } \tilde{H}'\text{'s rows} \\ B + \frac{(Bh)(Bh)^T}{1 - h^T B h} & \text{otherwise.} \end{cases}$$

(b) $h^T B h < 1$ if h is a l.c. of \tilde{H} 's rows.

(8.8.3) **Example:** Suppose

$$H = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} (n \times 1) \quad \text{and} \quad \tilde{H} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} (n-1) \times 1.$$

Let

$$\tilde{z} = \begin{pmatrix} \zeta_1 \\ \vdots \\ \zeta_{n-1} \end{pmatrix} \quad \text{and} \quad z = \begin{pmatrix} \tilde{z} \\ 0 \end{pmatrix}.$$

Then $h = (1)$, $B = (H^T H)^{-1} = n^{-1}$,

$$\hat{x} = H^+ z = n^{-1} \sum_{j=1}^n \zeta_j = n^{-1} \sum_{j=1}^{n-1} \zeta_j$$

$$\varepsilon = \sum_{j=1}^n (\zeta_j - \hat{x})^2 = \sum_{j=1}^{n-1} \zeta_j^2 - n\hat{x}^2.$$

From (8.8.1)

$$M = -1/(1 - n^{-1}) = -n/(n-1)$$

$$\begin{aligned} \tilde{x} &= \left[1 - (n^{-1}) \left(\frac{-n}{n-1} \right) \right] \hat{x} = \left(1 + \frac{1}{n-1} \right) \hat{x} \\ &= \left(\frac{n}{n-1} \right) \left(n^{-1} \sum_{j=1}^{n-1} \zeta_j \right) = \frac{1}{n-1} \sum_{j=1}^{n-1} \zeta_j \end{aligned}$$

and

$$\begin{aligned} \tilde{\varepsilon} &= \varepsilon - \hat{x}^2 / \left(1 - \frac{1}{n} \right) \\ &= \sum_{j=1}^{n-1} \zeta_j^2 - \frac{n^2 \hat{x}^2}{n-1}. \end{aligned}$$

But $\tilde{x} = [n/(n-1)] \hat{x}$, so

$$\frac{n^2 \hat{x}^2}{n-1} = (n-1) \tilde{x}^2$$

hence

$$\tilde{\varepsilon} = \sum_{j=1}^{n-1} \zeta_j^2 - (n-1) \tilde{x}^2$$

as it should.

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NONNEGATIVE DEFINITE MATRICES, CONDITIONAL EXPECTATION, AND KALMAN FILTERING

(9.1) Nonnegative Definiteness

It is well known that the following conditions are equivalent definitions for nonnegative definiteness of a symmetric matrix S , (Bellman [1]):

(9.1.1) $S = HH^T$ for some matrix H ;

(9.1.2) $x^T S x \geq 0$ for all vectors x ;

(9.1.3) The eigenvalues of S are nonnegative;

(9.1.4) There is a symmetric matrix R such that $R^2 = S$. (R is called the square root of S , and is denoted by the symbol, $S^{1/2}$.)

If S is nonnegative definite *and* nonsingular, it is said to be *positive definite*. In this case, $S^{1/2}$ is also positive definite and the inequality in (9.1.2) is strong for all nonzero x .

The statement “ S is nonnegative definite” is abbreviated “ $S \geq 0$.” Similarly, “ $S > 0$ ” means “ S is positive definite.”

(9.1.5) **Exercise:** If $S \geq 0$ and $T \geq 0$ then $S + T \geq 0$ with strict inequality holding if and only if $\mathcal{N}(S) \cap \mathcal{N}(T) = \{0\}$.

One of the classical results concerning nonnegative definiteness, states that

S is nonnegative definite (positive definite) if and only if the principal sub-determinants of S are all nonnegative (positive), (Bellman [1]). This result reduces the decision about S 's nonnegativeness to the evaluation of a number of determinants.

The material which we have developed in earlier chapters concerning pseudoinverses, can be used to prove some new results about nonnegative (positive) definiteness.

(9.1.6) **Theorem** (Albert [1]): Let S be a square matrix:

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{12}^T & S_{22} \end{pmatrix}$$

where S_{11} is a symmetric $n \times n$ matrix and S_{22} is a symmetric $m \times m$ matrix. Then

(a) $S \geq 0$ if and only if $S_{11} \geq 0$, $S_{11} S_{11}^+ S_{12} = S_{12}$ and

$$S_{22} - S_{12}^T S_{11}^+ S_{12} \geq 0.$$

(b) $S > 0$ if and only if $S_{11} > 0$, $S_{22} > 0$, $S_{11} - S_{12} S_{22}^{-1} S_{12}^T > 0$ and

$$S_{22} - S_{12}^T S_{11}^{-1} S_{12} > 0.$$

Proof: (a) (Sufficiency): If $S \geq 0$ then $S = HH^T$, (9.1.1), where H has $n+m$ rows. Write H as a partitioned matrix:

$$H = \begin{pmatrix} X \\ Y \end{pmatrix}.$$

Then,

$$S = HH^T = \begin{pmatrix} XX^T & XY^T \\ YX^T & YY^T \end{pmatrix},$$

so that

$$S_{11} = XX^T \geq 0 \quad \text{and} \quad S_{12} = XY^T.$$

By (3.11.9),

$$S_{11} S_{11}^+ = (XX^T)(XX^T)^+ = XX^+$$

so that

$$(S_{11} S_{11}^+) S_{12} = (XX^+) XY^T = XY^T = S_{12}.$$

Finally, if we let

$$U = Y - S_{12}^T S_{11}^+ X$$

then

$$0 \leq UU^T = S_{22} - S_{12}^T S_{11}^+ S_{12}.$$

(Necessity): Let

$$U = {}_n(I; 0) \quad V = {}_m(0; I) \quad X = S_{11}^{1/2} U \\ Y = S_{12}^T S_{11}^+ S_{11}^{1/2} U + (S_{22} - S_{12}^T S_{11}^+ S_{12})^{1/2} V.$$

Since $UV^T = {}_n 0$, we see that

$$0 \leq \begin{pmatrix} X \\ \bar{Y} \end{pmatrix} \begin{pmatrix} X \\ \bar{Y} \end{pmatrix}^T = \begin{pmatrix} S_{11} & S_{12} \\ S_{12}^T & S_{22} \end{pmatrix} = S.$$

(b) (Sufficiency): If $S > 0$ then by part (a), $S_{11} \geq 0$. Furthermore, $\det S_{11} > 0$ since all principal subdeterminants of S are positive. Hence S_{11} is nonsingular and therefore $S_{11} > 0$. Similarly, $S_{22} - S_{12}^T S_{11}^{-1} S_{12} \geq 0$ so that $S_{22} \geq 0$ and by the same argument $S_{22} > 0$.

The eigenvalues of S^{-1} are the reciprocals of S 's and so, $S^{-1} > 0$ if $S > 0$, (9.1.3). We can therefore write

$$S^{-1} = {}_n \begin{pmatrix} A & B \\ \bar{B}^T & \bar{C} \end{pmatrix} > 0$$

where the condition

$$SS^{-1} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$$

dictates that

$$(S_{11} - S_{12} S_{22}^{-1} S_{12}^T) A = I$$

and

$$(S_{22} - S_{12}^T S_{11}^{-1} S_{12}) C = I.$$

$A > 0$ and $C > 0$ since $S^{-1} > 0$. Hence $A^{-1} > 0$ and $C^{-1} > 0$ by the same argument as above. This proves sufficiency.

(Necessity): From part (a), $S \geq 0$. Let

$$A = (S_{11} - S_{12} S_{22}^{-1} S_{12}^T)^{-1} \\ B = -S_{11}^{-1} S_{12} (S_{22} - S_{12}^T S_{11}^{-1} S_{12})^{-1}$$

and

$$C = (S_{22} - S_{12}^T S_{11}^{-1} S_{12})^{-1}.$$

It is easy to show that

$$A^{-1} B C^{-1} = A^{-1} [-(S_{11} - S_{12} S_{22}^{-1} S_{12})^{-1} S_{12} S_{22}^{-1}] C^{-1}$$

so that

$$B = -(S_{11} - S_{12} S_{22}^{-1} S_{12})^{-1} S_{12} S_{22}^{-1}.$$

Routine calculations then verify that

$$S \begin{pmatrix} A & B \\ B^T & C \end{pmatrix} = I$$

so S is nonsingular. ■

Comment: In earlier chapters we pointed out that the class of covariance matrices coincides with the class of nonnegative-definite matrices. The preceding theorem tells us that the partitioned submatrices of covariance matrices have particular properties. This has a statistical interpretation which we will exploit in the section on conditional expectations.

(9.1.7) **Exercise:** Let S_N be an $N \times N$ symmetric matrix whose (i, j) th element is $\sigma(i, j)$. Let S_k be the $k \times k$ submatrix occupying the upper left corner of S_N , and let s_k be the k -dimensional column vector (just to the right of S_k) with components $\sigma(k+1, 1), \sigma(k+1, 2), \dots, \sigma(k+1, k)$. Define $S_0 = 0$ and $s_0 = 0$. Then

$$(a) \quad S_N \geq 0 \text{ if and only if } S_{k-1} S_{k-1}^+ s_{k-1} = s_{k-1}$$

and

$$\sigma(k, k) \geq s_{k-1}^T S_{k-1}^+ s_{k-1} \quad \text{for } k = 1, 2, \dots, N.$$

$$(b) \quad S_N > 0 \text{ if and only if } \sigma(k, k) > s_{k-1}^T S_{k-1}^+ s_{k-1} \text{ for } k = 1, 2, \dots, N.$$

[Hint: Use (9.1.6) and proceed by induction. Notice that if $S_k > 0$, then $[S_k^{1/2}(I - xx^T)S_k^{1/2}] > 0$ if and only if $I - xx^T > 0$ which is true if and only if $x^T x < 1$. Apply to

$$x = [\sigma(k+1, k+1) S_k]^{-1/2} s_k.$$

See Albert [1] for details.]

(9.1.8) **Exercise** (*Recursions for S_k^+*): Suppose $S_k \geq 0$ and

$$S_{k+1} = \begin{pmatrix} k & 1 \\ \frac{S_k}{s_k^T} & \frac{s_k}{\sigma(k+1, k+1)} \end{pmatrix}$$

Let

$$t_k = S_k^+ s_k \quad \alpha_k = \sigma(k+1, k+1) - s_k^T S_k^+ s_k$$

$$\beta_k = 1 + \|t_k\|^2 \quad T_k = I - t_k t_k^T / \beta_k.$$

Then

(a) $S_{k+1} \geq 0$ if and only if $S_k t_k = s_k$ and $\alpha_k \geq 0$.

(b) In this case

$$S_{k+1}^+ = \begin{cases} \begin{bmatrix} S_k^+ + t_k t_k^T / \alpha_k & -t_k / \alpha_k \\ -t_k^T / \alpha_k & 1 / \alpha_k \end{bmatrix} & \text{if } \alpha_k > 0 \\ \begin{bmatrix} T_k S_k^+ T_k & T_k S_k^+ t_k / \beta_k \\ (T_k S_k^+ t_k / \beta_k)^T & t_k^T S_k^+ t_k / \beta_k^2 \end{bmatrix} & \text{if } \alpha_k = 0 \end{cases}$$

(see Albert [1]).

(9.2) Conditional Expectations for Normal Random Variables

A vector valued, normally distributed random variable \mathbf{x} has a distribution which is completely specified by its mean,

$$m_{\mathbf{x}} \equiv \mathcal{E} \mathbf{x}$$

and its covariance

$$S_{\mathbf{x}\mathbf{x}} = \mathcal{E}(\mathbf{x} - m_{\mathbf{x}})(\mathbf{x} - m_{\mathbf{x}})^T \quad \text{Anderson [1].}$$

It is known, Anderson [1], that if $\mathbf{y} = G\mathbf{x}$ and $\mathbf{z} = H\mathbf{x}$, then the conditional distribution of \mathbf{y} , given that $\mathbf{z} = z$ is, for each possible value of z [i.e., each $z \in \mathcal{R}(H)$] normal, and therefore specified completely by its conditional mean and covariance. We shall use the results of the last section to derive the key properties of conditional means and covariances in a streamlined fashion.

(9.2.1) **Theorem:** Suppose

$$\mathbf{x} = \begin{pmatrix} p(\mathbf{x}_1) \\ q(\mathbf{x}_2) \end{pmatrix}$$

has a multivariate normal distribution with mean zero and covariance

$$S = \begin{pmatrix} p(S_{11} | S_{12}) \\ q(S_{12}^T | S_{22}) \end{pmatrix}.$$

Then

(a) \mathbf{x} has the same distribution as

$$\mathbf{x}^* = \begin{pmatrix} p(\mathbf{x}_1^*) \\ q(\mathbf{x}_2^*) \end{pmatrix}$$

where

$$\mathbf{x}_1^* = S_{11}^{1/2} \mathbf{w}_1$$

$$\mathbf{x}_2^* = S_{12}^T S_{11}^+ \mathbf{x}_1^* + (S_{22} - S_{12}^T S_{11}^+ S_{12})^{1/2} \mathbf{w}_2$$

and

$$\begin{pmatrix} p \\ q \end{pmatrix} \begin{pmatrix} \mathbf{w}_1 \\ \mathbf{w}_2 \end{pmatrix}$$

has a normal distribution with mean zero and covariance I .

(b) The conditional distribution of \mathbf{x}_2 given that $\mathbf{x}_1 = x$ is normal with conditional mean

$$m_{2|1}(x) \equiv \mathcal{E}(\mathbf{x}_2 | \mathbf{x}_1 = x) = S_{12}^T S_{11}^+ x,$$

provided $x \in \mathcal{R}(S_{11})$.

The conditional covariance of \mathbf{x}_2 given that $\mathbf{x}_1 = x$ is

$$\begin{aligned} S_{22|1} &\equiv \mathcal{E}[(\mathbf{x}_2 - m_{2|1}(x))(\mathbf{x}_2 - m_{2|1}(x))^T | \mathbf{x}_1 = x] \\ &= S_{22} - S_{12}^T S_{11}^+ S_{12} \end{aligned}$$

provided $x \in \mathcal{R}(S_{11})$. (Notice that $S_{22|1}$ does not depend explicitly on x .)

(c) If

$$\mathbf{x} = \begin{pmatrix} p \\ q \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}$$

has mean value

$$m = \begin{pmatrix} p \\ q \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \end{pmatrix}$$

which is different from zero, then the conditional covariance of \mathbf{x}_2 given that $\mathbf{x}_1 = x$ is the same as in (b) and

$$m_{2|1}(x) \equiv \mathcal{E}(\mathbf{x}_2 | \mathbf{x}_1 = x) = m_2 + S_{12}^T S_{11}^+ (x - m_1),$$

provided

$$x - m_1 \in \mathcal{R}(S_{11}).$$

Proof: (a) Since S is a covariance, it is nonnegative definite; so from (9.1.6), $S_{11} \geq 0$, $S_{22} - S_{12}^T S_{11}^+ S_{12} \geq 0$, hence both of the aforementioned matrices have square roots. Part (a) follows since \mathbf{x}^* has a multivariate normal distribution with mean zero and (after a little algebra), covariance S . Notice that \mathbf{x}_1^* (hence \mathbf{x}_1) must lie in $\mathcal{R}(S_{11}^{1/2}) = \mathcal{R}(S_{11})$ with probability 1.

(b) Without loss of generality, part (a) permits us to assume that $\mathbf{x}_1 = \mathbf{x}_1^*$ and $\mathbf{x}_2 = \mathbf{x}_2^*$ when we are exploring any properties of \mathbf{x} 's distribution.

Since \mathbf{w}_1 and \mathbf{w}_2 are independent, so then are \mathbf{x}_1 and \mathbf{w}_2 so that $\mathcal{E}(\mathbf{w}_2 | \mathbf{x}_1 = x) = \mathcal{E}(\mathbf{w}_2) = 0$. Thus, from part (a), if

$$x \in \mathcal{R}(S_{11}^{1/2}) = \mathcal{R}(S_{11})$$

$$m_{2|1}(x) = \mathcal{E}(\mathbf{x}_2 | \mathbf{x}_1 = x) = S_{12}^T S_{11}^+ \mathcal{E}(\mathbf{x}_1 | \mathbf{x}_1 = x) = S_{12}^T S_{11}^+ x$$

and

$$\begin{aligned} S_{22|1} &= \mathcal{E}[(\mathbf{x}_2 - m_{2|1}(x))(\mathbf{x}_2 - m_{2|1}(x))^T | \mathbf{x}_1 = x] \\ &= \mathcal{E}[(T\mathbf{w}_2)(T\mathbf{w}_2)^T | \mathbf{x}_1 = x] \end{aligned}$$

where

$$T = (S_{22} - S_{12}^T S_{11}^+ S_{12})^{1/2}.$$

Again, using the independence of \mathbf{w}_2 and \mathbf{x}_1 , we see that

$$\begin{aligned} \mathcal{E}[(T\mathbf{w}_2)(T\mathbf{w}_2)^T | \mathbf{x}_1 = x] &= \mathcal{E}(T\mathbf{w}_2 \mathbf{w}_2^T T^T) \\ &= TT^T = (S_{22} - S_{12}^T S_{11}^+ S_{12}) \end{aligned}$$

since

$$\mathcal{E}(\mathbf{w}_2 \mathbf{w}_2^T) = I.$$

(c) Apply (b) to $\mathbf{x}_2 - m_2$ and $\mathbf{x}_1 - m_1$:

$$\mathcal{E}(\mathbf{x}_2 - m_2 | \mathbf{x}_1 - m_1 = x - m_1) = S_{12}^T S_{11}^+ (x - m_1)$$

so

$$\mathcal{E}(\mathbf{x}_2 | \mathbf{x} = x) - m_2 = S_{12}^T S_{11}^+ (x - m_1).$$

The formula for the conditional covariance is unchanged if a constant vector is added to $\mathbf{x}_2 - m_2$. Again, we must tack on the restriction that $x - m_1$ be in $\mathcal{R}(S_{11})$ in order that the formulas hold. (See Marsaglia [1].) ■

The results of (9.2.1c) establish a relationship between the conditional mean and covariance of \mathbf{u} given $\mathbf{v} = v$ and the unconditional mean and covariance of \mathbf{u} for jointly normally distributed \mathbf{u} and \mathbf{v} . The same argument can be applied to establish a similar relationship between the conditional mean (and covariance) of \mathbf{u} given $\mathbf{v} = v$ and $\mathbf{y} = y$, and the conditional mean (and covariance) of \mathbf{u} given $\mathbf{v} = v$, for any jointly normally distributed vector random variables, \mathbf{v} , \mathbf{y} , and \mathbf{u} :

(9.2.2) **Theorem:** Suppose

$$\begin{pmatrix} p+q \\ r \end{pmatrix} \begin{pmatrix} \mathbf{z} \\ \mathbf{u} \end{pmatrix}$$

has a multivariate normal distribution with mean m and covariance

$$S = \begin{pmatrix} S_{zz} & S_{zu} \\ S_{zu}^T & S_{uu} \end{pmatrix}$$

and suppose

$$\mathbf{z} = \begin{pmatrix} p \\ q \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{y} \end{pmatrix}.$$

Let

$$(9.2.2.1) \quad m_{\mathbf{u}} = \mathcal{E} \mathbf{u} \quad m_{\mathbf{v}} = \mathcal{E} \mathbf{v} \quad m_{\mathbf{y}} = \mathcal{E} \mathbf{y}$$

$$m_{\mathbf{z}|\mathbf{u}}(u) = \mathcal{E}(\mathbf{z} | \mathbf{u} = u)$$

$$(9.2.2.2) \quad m_{\mathbf{v}|\mathbf{u}}(u) = \mathcal{E}(\mathbf{v} | \mathbf{u} = u)$$

$$m_{\mathbf{y}|\mathbf{u}}(u) = \mathcal{E}(\mathbf{y} | \mathbf{u} = u)$$

and

$$(9.2.2.3) \quad S_{zz|\mathbf{u}} \quad S_{vv|\mathbf{u}} \quad \text{and} \quad S_{yy|\mathbf{u}}$$

be the respective conditional covariances of \mathbf{z} , \mathbf{v} , and \mathbf{y} given $\mathbf{u} = u$.

Then

(a) If $u - m_{\mathbf{u}} \in \mathcal{R}(S_{\mathbf{u}\mathbf{u}})$, the conditional distribution of \mathbf{z} , given that $\mathbf{u} = u$, is normal with mean

$$(9.2.2.4) \quad m_{\mathbf{z}|\mathbf{u}}(u) \equiv \begin{pmatrix} p \\ q \end{pmatrix} \begin{bmatrix} m_{\mathbf{v}|\mathbf{u}}(u) \\ m_{\mathbf{y}|\mathbf{u}}(u) \end{bmatrix} = m_{\mathbf{z}} + S_{\mathbf{zu}} S_{\mathbf{uu}}^+ (u - m_{\mathbf{u}})$$

and covariance

$$(9.2.2.5) \quad S_{zz|\mathbf{u}} = \begin{pmatrix} p \\ q \end{pmatrix} \begin{pmatrix} S_{vv|\mathbf{u}} & S_{vy|\mathbf{u}} \\ S_{vy|\mathbf{u}}^T & S_{yy|\mathbf{u}} \end{pmatrix} = S_{zz} - S_{\mathbf{zu}} S_{\mathbf{uu}}^+ S_{\mathbf{zu}}^T.$$

(b) If $u - m_{\mathbf{u}} \in \mathcal{R}(S_{\mathbf{u}\mathbf{u}})$ and

$$y - m_{\mathbf{y}|\mathbf{u}}(u) \in \mathcal{R}(S_{\mathbf{y}\mathbf{y}|\mathbf{u}})$$

then the conditional distribution of \mathbf{v} given that $\mathbf{u} = u$ and $\mathbf{y} = y$, is normal with mean

$$(9.2.2.6) \quad m_{\mathbf{v}|\mathbf{u},\mathbf{y}}(u, y) = m_{\mathbf{v}|\mathbf{u}}(u) + S_{\mathbf{vy}|\mathbf{u}} S_{\mathbf{yy}|\mathbf{u}}^+ (y - m_{\mathbf{y}|\mathbf{u}}(u))$$

and covariance

$$(9.2.2.7) \quad S_{vv|\mathbf{u},\mathbf{y}} = S_{vv|\mathbf{u}} - S_{\mathbf{vy}|\mathbf{u}} S_{\mathbf{yy}|\mathbf{u}}^+ S_{\mathbf{vy}|\mathbf{u}}^T$$

which does not depend explicitly on u and y .

Comment: Notice the formal similarity between (9.2.2.6) and (9.2.2.4) on the one hand and between (9.2.2.7) and (9.2.2.5), on the other.

Proof: Part (a) follows from (9.2.1) and from the fact that \mathbf{z} can be partitioned in the form

$$\mathbf{z} = \begin{pmatrix} p \\ q \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{y} \end{pmatrix}.$$

(b) Let u be fixed and a possible value for the random variable \mathbf{u} [i.e., $u - m_{\mathbf{u}} \in \mathcal{R}(S_{\mathbf{u}\mathbf{u}})$]. The conditional joint distribution of \mathbf{v} and \mathbf{y} given that $\mathbf{u} = u$ is normal with mean

$$(9.2.2.8) \quad \begin{pmatrix} m_{\mathbf{v}|\mathbf{u}}(u) \\ m_{\mathbf{y}|\mathbf{u}}(u) \end{pmatrix} \equiv m_{\mathbf{z}|\mathbf{u}}(u)$$

and covariance

$$(9.2.2.9) \quad \begin{pmatrix} S_{\mathbf{v}\mathbf{v}|\mathbf{u}} & S_{\mathbf{v}\mathbf{y}|\mathbf{u}} \\ S_{\mathbf{y}\mathbf{v}|\mathbf{u}} & S_{\mathbf{y}\mathbf{y}|\mathbf{u}} \end{pmatrix} \equiv S_{\mathbf{z}\mathbf{z}|\mathbf{u}}$$

where the elements of $m_{\mathbf{z}|\mathbf{u}}(u)$ and $S_{\mathbf{z}\mathbf{z}|\mathbf{u}}$ are given in part (a). For fixed u , let

$$(9.2.2.10) \quad \mathbf{z}^* = \begin{pmatrix} \mathbf{v}^* \\ \mathbf{y}^* \end{pmatrix}$$

be a random variable which has a normal distribution with (unconditional) mean

$$(9.2.2.11) \quad m_{\mathbf{z}^*} = m_{\mathbf{z}|\mathbf{u}}(u)$$

and (unconditional) covariance

$$(9.2.2.12) \quad S_{\mathbf{z}^*\mathbf{z}^*} = S_{\mathbf{z}\mathbf{z}|\mathbf{u}}.$$

Then for fixed u , the joint (unconditional) distribution of \mathbf{v}^* and \mathbf{y}^* is the same as the joint (conditional) distribution of \mathbf{v} and \mathbf{y} , given that $\mathbf{u} = u$. Therefore, the conditional distribution of \mathbf{v}^* , given that $\mathbf{y}^* = y$ is the same as the conditional distribution of \mathbf{v} given that $\mathbf{y} = y$ and $\mathbf{u} = u$ provided that y is an allowable realization of \mathbf{y}^* [i.e., $y - m_{\mathbf{y}^*} \in \mathcal{R}(S_{\mathbf{y}^*\mathbf{y}^*})$].

So, for each y with $y - m_{\mathbf{y}^*} \in \mathcal{R}(S_{\mathbf{y}^*\mathbf{y}^*})$, the means and covariances of the two conditional distributions must coincide:

$$(9.2.2.13) \quad m_{\mathbf{v}|\mathbf{u},\mathbf{y}}(u, y) = m_{\mathbf{v}^*|\mathbf{y}^*}(y)$$

$$(9.2.2.14) \quad S_{\mathbf{v}\mathbf{v}|\mathbf{u},\mathbf{y}} = S_{\mathbf{v}^*\mathbf{v}^*|\mathbf{y}^*}.$$

From part (a)

$$(9.2.2.15) \quad m_{\mathbf{v}^*|\mathbf{y}^*}(y) = m_{\mathbf{v}^*} + S_{\mathbf{y}^*\mathbf{v}^*}^T S_{\mathbf{y}^*\mathbf{y}^*}^+(y - m_{\mathbf{y}^*})$$

and

$$(9.2.2.16) \quad S_{v^*v^*|y^*} = S_{v^*v^*} - S_{v^*y^*} S_{y^*y^*}^+ S_{v^*y^*}^T.$$

Since

$$(9.2.2.17) \quad m_{z^*} = \begin{pmatrix} m_{v^*} \\ m_{y^*} \end{pmatrix} = \begin{pmatrix} m_{v|u} \\ m_{y|u} \end{pmatrix} \quad (9.2.2.11)$$

and

$$(9.2.2.18) \quad S_{z^*z^*} = \begin{pmatrix} S_{v^*v^*} & S_{v^*y^*} \\ S_{y^*v^*}^T & S_{y^*y^*} \end{pmatrix} = \begin{pmatrix} S_{vv|u} & S_{vy|u} \\ S_{yv|u}^T & S_{yy|u} \end{pmatrix} \quad (9.2.2.12)$$

(9.2.2.6) follows from (9.2.2.13), (9.2.2.15), and (9.2.2.17) while (9.2.2.7) follows from (9.2.2.14), (9.2.2.16), and (9.2.2.18). ■

(9.2.2.19) **Exercise:** If

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \\ \mathbf{z} \end{pmatrix}$$

have a joint normal distribution and \mathbf{z} is independent of

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}$$

then $S_{\mathbf{zx}|\mathbf{y}} = 0$.

(9.2.3) **Exercise:** (a) For any matrices of the right size,

$$\text{tr}(AB) = \text{tr}(BA).$$

(b) If \mathbf{x} is a random variable with covariance $S_{\mathbf{xx}}$, then $\mathcal{E}\|\mathbf{x}\|^2 = \text{tr}(S_{\mathbf{xx}})$.

(9.2.4.1) **Exercise** (*Optimum properties of conditional expectation and wide-sense conditional expectation*): If

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}$$

is a vector random variable with covariance matrix

$$\begin{pmatrix} S_{\mathbf{xx}} & S_{\mathbf{xy}} \\ S_{\mathbf{yx}}^T & S_{\mathbf{yy}} \end{pmatrix}$$

we say that $m_{\mathbf{x}} + S_{\mathbf{xy}} S_{\mathbf{yy}}^+ (\mathbf{y} - m_{\mathbf{y}})$ is the *wide-sense conditional expectation* of \mathbf{x} given $\mathbf{y} = y$. (If \mathbf{x} and \mathbf{y} have a joint normal distribution, the wide-sense conditional expectation coincides with the usual conditional expectation.)

(a) Assume that $m_{\mathbf{x}}$ and $m_{\mathbf{y}}$ are both zero. Show that $\mathcal{E}\|\mathbf{x} - A\mathbf{y}\|^2 \geq \mathcal{E}\|\mathbf{x} - S_{\mathbf{xy}} S_{\mathbf{yy}}^+ \mathbf{y}\|^2$ for any matrix A of the right size, with strict inequality holding unless $AS_{\mathbf{yy}} = S_{\mathbf{xy}}$.

(b) If

$$\begin{pmatrix} \mathbf{x} \\ - \\ \mathbf{y} \end{pmatrix}$$

has a joint normal distribution and $g(\cdot)$ is a measurable mapping from q -dimensional Euclidean space to p -dimensional Euclidean space, then

$$\mathcal{E}\|\mathbf{x} - g(\mathbf{y})\|^2 \geq \mathcal{E}\|\mathbf{x} - S_{\mathbf{xy}} S_{\mathbf{yy}}^+ \mathbf{y}\|^2$$

with strict inequality holding unless $g(\mathbf{y}) = S_{\mathbf{xy}} S_{\mathbf{yy}}^+ \mathbf{y}$ for almost all \mathbf{y} .

Comment: (a) Shows that the wide sense conditional expectation is the best linear predictor for \mathbf{x} , based on \mathbf{y} when mean square error is to be minimized.

(b) Shows that the wide sense conditional expectation is the best predictor of all (linear or not), in the normal case.

(9.2.4.2) **Exercise:** Suppose

$$S_{\mathbf{zz}} = \begin{pmatrix} S_{\mathbf{uu}} & S_{\mathbf{uy}} \\ S_{\mathbf{uy}}^T & S_{\mathbf{yy}} \end{pmatrix} \geq 0.$$

Then $u \in S_{\mathbf{uu}}$ and $y - S_{\mathbf{uy}}^T S_{\mathbf{uu}}^+ u \in \mathcal{R}(S_{\mathbf{yy}|\mathbf{u}})$ if and only if

$$z = \begin{pmatrix} u \\ - \\ y \end{pmatrix} \in \mathcal{R}(S_{\mathbf{zz}}).$$

Comment: The last result explains away the apparently asymmetric conditions on $u - m_{\mathbf{u}}$ and $y - m_{\mathbf{y}|\mathbf{u}}(u)$ which are necessary in order that (9.2.2b) should hold. In short, (9.2.2.6) and (9.2.2.7) hold provided

$$\begin{pmatrix} u - m_{\mathbf{u}} \\ - \\ y - m_{\mathbf{y}} \end{pmatrix} \in \mathcal{R}(S_{\mathbf{zz}}).$$

(9.2.5) **Exercise:** Suppose

$$\begin{pmatrix} \mathbf{x}^* \\ - \\ \mathbf{w} \\ - \\ \mathbf{y} \end{pmatrix}$$

has a multivariate normal distribution. Let

$$m_{\mathbf{x}^*|\mathbf{y}}(y) = \mathcal{E}(\mathbf{x}^*|\mathbf{y} = y)$$

$$m_{\mathbf{w}} = \mathcal{E}(\mathbf{w})$$

$$S_{\mathbf{x}^*\mathbf{x}^*|\mathbf{y}} = \mathcal{E}[(\mathbf{x}^* - m_{\mathbf{x}^*|\mathbf{y}}(y))(\mathbf{x}^* - m_{\mathbf{x}^*|\mathbf{y}}(y))^T | \mathbf{y} = y]$$

and

$$S_{\mathbf{w}\mathbf{w}} = \mathcal{E}(\mathbf{w} - m_{\mathbf{w}})(\mathbf{w} - m_{\mathbf{w}})^T.$$

If

$$(9.2.5.1) \quad \mathbf{x} = \Phi \mathbf{x}^* + \mathbf{w} \quad (\text{where } \Phi \text{ is a deterministic square matrix})$$

and if \mathbf{w} is independent of

$$\begin{pmatrix} \mathbf{x}^* \\ \vdots \\ \mathbf{y} \end{pmatrix}$$

then

$$(9.2.5.2) \quad m_{\mathbf{x}|\mathbf{y}}(y) = \Phi m_{\mathbf{x}^*|\mathbf{y}}(y) + m_{\mathbf{w}}$$

$$(9.2.5.3) \quad S_{\mathbf{xx}|\mathbf{y}} = \Phi S_{\mathbf{x}^*\mathbf{x}^*|\mathbf{y}} \Phi^T + S_{\mathbf{w}\mathbf{w}}.$$

(9.2.6) **Exercise:** If \mathbf{v} has a normal distribution with mean 0 and covariances $S_{\mathbf{vv}}$ and is independent of

$$\begin{pmatrix} \mathbf{x} \\ \vdots \\ \mathbf{y} \end{pmatrix}$$

which has a normal distribution, and if

$$(9.2.6.1) \quad \mathbf{z} = H\mathbf{x} + \mathbf{v}$$

where H is a deterministic matrix, then

$$(9.2.6.2) \quad m_{\mathbf{x}|\mathbf{y}\mathbf{z}}(y, z) = m_{\mathbf{x}|\mathbf{y}}(y) + S_{\mathbf{xx}|\mathbf{y}} H^T (H S_{\mathbf{xx}|\mathbf{y}} H^T + S_{\mathbf{vv}})^+ (z - H m_{\mathbf{x}|\mathbf{y}}(y))$$

and

$$(9.2.6.3) \quad S_{\mathbf{xx}|\mathbf{y}\mathbf{z}} = S_{\mathbf{xx}|\mathbf{y}} - S_{\mathbf{xx}|\mathbf{y}} H^T (H S_{\mathbf{xx}|\mathbf{y}} H^T + S_{\mathbf{vv}})^+ H S_{\mathbf{xx}|\mathbf{y}}$$

where $m_{\mathbf{x}|\mathbf{y},\mathbf{z}}(y, z)$ is the conditional expectation of \mathbf{x} given that $\mathbf{y} = y$ and $\mathbf{z} = z$, $S_{\mathbf{xx}|\mathbf{y},\mathbf{z}}$ is the conditional covariance of \mathbf{x} given $\mathbf{y} = y$ and $\mathbf{z} = z$, etc.

Comment: (9.2.6) shows how the acquisition of new data changes the *posterior* distribution. If \mathbf{y} represents all the data up to the last sampling period, then the *posterior* distribution of \mathbf{x} (i.e., conditional distribution) given the data $\mathbf{y} = y$, contains all of the available information about \mathbf{x} that can be learned from analyzing \mathbf{z} . This distribution, in the normal case, is characterized

by its mean and covariance. If a new datum of the form (9.2.6.1) is observed, then the posterior distribution of \mathbf{x} changes and is now characterized by its conditional mean and covariance given \mathbf{y} and \mathbf{z} . (9.2.6.2) and (9.2.6.3) show how the new mean and covariance are related to the old.

(9.3) Kalman Filtering

Suppose $\{\mathbf{x}_n; n = 0, 1, 2, \dots\}$ is a vector valued stochastic process whose evolution is governed by a so-called “state equation” of the form

$$(9.3.1) \quad \mathbf{x}_{n+1} = \Phi_n \mathbf{x}_n + \mathbf{w}_n$$

where $\{\mathbf{w}_n; n = 0, 1, 2, \dots\}$ is a sequence of independent vector valued normal random variables with means 0 and covariances

$$(9.3.2) \quad T_n = \mathcal{E} \mathbf{w}_n \mathbf{w}_n^T.$$

The so-called “state variable” can be partially observed in the presence of noise, the observations being of the form

$$(9.3.3) \quad \mathbf{z}_n = H_n \mathbf{x}_n + \mathbf{v}_n \quad n = 1, 2, \dots$$

where $\{\mathbf{v}_n; n = 1, 2, \dots\}$ is a sequence of independent vector valued normal random variables with zero means and covariances

$$(9.3.4) \quad R_n = \mathcal{E} \mathbf{v}_n \mathbf{v}_n^T.$$

The $\{\mathbf{v}_n\}$ and $\{\mathbf{w}_n\}$ processes are assumed to be independent,¹ and the initial state \mathbf{x}_0 is assumed to be a normally distributed zero mean random vector which is independent of the \mathbf{v}_n 's and \mathbf{w}_n 's. Under these assumptions, it is not hard to show that the joint distribution of $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_{n+1}, \mathbf{z}_1, \dots, \mathbf{z}_n$ is normal.

In (9.2.4.1), it was established that the best mean square predictor for \mathbf{x}_n , based upon the observations

$$\mathbf{z}_1 = z_1, \mathbf{z}_2 = z_2, \dots, \mathbf{z}_n = z_n$$

is

$$(9.3.5) \quad x_{n|n} \equiv \mathcal{E}(\mathbf{x}_n | \mathbf{z}_1 = z_1, \dots, \mathbf{z}_n = z_n)$$

where we adopt the convention that

$$x_{0|0} = 0.$$

¹ This assumption can be dispensed with at the expense of slightly more complicated formulas.

Similarly the best predictor for \mathbf{x}_{n+1} given the first n observations, is

$$(9.3.6) \quad x_{n+1|n} = \mathcal{E}(\mathbf{x}_{n+1} | \mathbf{z}_1 = z_1, \dots, \mathbf{z}_n = z_n).$$

If we denote the conditional covariances of \mathbf{x}_n and \mathbf{x}_{n+1} , given $\mathbf{z}_1 = z_1, \dots, \mathbf{z}_n = z_n$ by $S_{n|n}$ and $S_{n+1|n}$ respectively, then by virtue of (9.2.5) and (9.2.6)

$$(9.3.7) \quad x_{n+1|n} = \Phi_n x_{n|n} \quad n = 0, 1, 2, \dots$$

$$(9.3.8) \quad x_{n+1|n+1} = x_{n+1|n} + K_{n+1}(z_{n+1} - H_{n+1} x_{n+1|n})$$

where

$$(9.3.9) \quad K_{n+1} = S_{n+1|n} H_{n+1}^T (H_{n+1} S_{n+1|n} H_{n+1}^T + R_{n+1})^+$$

$$(9.3.10) \quad S_{n+1|n} = \Phi_n S_{n|n} \Phi_n^T + T_n$$

and

$$(9.3.11) \quad S_{n+1|n+1} = S_{n+1|n} - S_{n+1|n} H_{n+1}^T \\ \times (H_{n+1} S_{n+1|n} H_{n+1}^T + R_{n+1})^+ H_{n+1} S_{n+1|n}.$$

These relations are initialized by

$$(9.3.12) \quad x_{0|0} = 0 \\ S_{0|0} = \mathcal{E} \mathbf{x}_0 \mathbf{x}_0^T.$$

[These recursions follow instantly from (9.2.5) and (9.2.6) if we identify

$$\mathbf{y} \text{ with the "super vector"} \quad \begin{bmatrix} \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_2 \\ \vdots \\ \mathbf{z}_n \\ \vdots \end{bmatrix}$$

\mathbf{z} with \mathbf{z}_{n+1} , \mathbf{x}^* with \mathbf{x}_n , and \mathbf{x} with \mathbf{x}_{n+1} .]

The relations (9.3.7)–(9.3.12) are the famous Kalman “filtering equations,” Kalman [1], about which an enormous literature has grown up in the systems engineering journals. The practical importance of these recursions is best exemplified by Battin [1], Battin and Levine [1], and American Statistical Association [1].

Comments: The restrictions that \mathbf{x}_0 and the state equation noise have zero means is not essential. If \mathbf{x}_0 has mean m_0 , then the recursion (9.3.7) is reinitialized by $x_{0|0} = m_0$. If the state equation noise, \mathbf{w}_n , has mean m_n , then (9.3.7) becomes

$$(9.3.7') \quad x_{n+1|n} = \Phi_n x_{n|n} + m_n.$$

The key feature of the Kalman equations are their recursive nature. The stream of data $\mathbf{z}_1, \mathbf{z}_2, \dots$ is incorporated "in real time" to produce a stream of estimates for the current values of the state variable.

The normality assumption can be dropped, in which case, the recursions generate wide-sense conditional expectations.

(9.4) The Relationship between Least Squares Estimates and Conditional Expectations

Suppose

$$(9.4.1) \quad \mathbf{z} = H\mathbf{x} + \mathbf{v}$$

where

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix}$$

has a normal distribution with mean 0 and covariance

$$S = \begin{pmatrix} (\lambda^{-2})^{-1} C^2 & 0 \\ 0 & I \end{pmatrix}.$$

The conditional expectation of \mathbf{x} given $\mathbf{z} = \mathbf{z}$ is

$$(9.4.2) \quad m_{\mathbf{x}|\mathbf{z}}(\mathbf{z}) = \lambda^{-2} C^2 H^T (\lambda^{-2} H C^2 H^T + I)^{-1} \mathbf{z}.$$

By (4.9.5),

$$\begin{aligned} (9.4.3) \quad \left(\frac{H C^2 H^T}{\lambda^2} + I \right)^+ &= I - (H C^2 H^T)(H C^2 H^T)^+ + \lambda^2 (H C^2 H^T)^+ \\ &\quad + O(\lambda^4) \quad \text{as } \lambda \rightarrow 0 \\ &= I - (H C)(H C)^+ + \lambda^2 (H C^2 H^T)^+ + O(\lambda^4) \end{aligned} \quad (3.11.7)$$

so that

$$\begin{aligned} m_{\mathbf{x}|\mathbf{z}}(\mathbf{z}) &= (C/\lambda^2) [(I - (H C)(H C)^+)(H C)]^T \mathbf{z} + C(H C)^T (H C^2 H^T)^+ \mathbf{z} + O(\lambda^2) \\ &= C(H C)^+ \mathbf{z} + O(\lambda^2) \quad \text{as } \lambda \rightarrow 0. \end{aligned}$$

But $C(H C)^+ \mathbf{z}$ minimizes $\|\mathbf{z} - H\mathbf{x}\|^2$ subject to the constraint $\mathbf{x} \in \mathcal{R}(C)$ since

$$\min_{\mathbf{x} \in \mathcal{R}(C)} \|\mathbf{z} - H\mathbf{x}\|^2 = \min_{\mathbf{y}} \|\mathbf{z} - H C \mathbf{y}\|^2$$

occurs when $\mathbf{x} = C\hat{\mathbf{y}}$ and $\hat{\mathbf{y}} = (H C)^+ \mathbf{z}$. Thus, for small values of λ , $\mathcal{E}(\mathbf{x} | \mathbf{z} = \mathbf{z})$ is close to the constrained least squares estimator for \mathbf{x} [subject to the constraint $(I - C C^+) \mathbf{x} = 0$].

If C is nonsingular, $I - CC^+ = 0$ and so in this case, $\mathcal{E}(\mathbf{x} | \mathbf{z} = \mathbf{z})$ is close to the naive least squares estimate for \mathbf{x} .

(9.4.4) **Example:** Suppose $\{\mathbf{v}_n; n = 1, 2, \dots\}$ is a sequence of independent normally distributed random variables with mean zero and variances σ_n^2 . Suppose, \mathbf{x} is a zero mean p -dimensional vector random variable having a normal distribution with mean 0 and covariance $(1/\lambda^2)C$. Assume that \mathbf{x} is independent of the \mathbf{v}_n 's.

Suppose observations of the form

$$\zeta_n = h_n^T \mathbf{x} + \mathbf{v}_n \quad n = 1, 2, \dots$$

are made in order to estimate x . Let $\hat{x}_n(\lambda)$ be the conditional expectation of \mathbf{x} given $\zeta_1 = \zeta_1, \dots, \zeta_n = \zeta_n$, and let $S_n(\lambda)$ be the conditional covariance of \mathbf{x}_n given the data up through the n th.

Then the Kalman recursions reduce to

$$\hat{x}_0(\lambda) = 0 \quad S_0(\lambda) = \lambda^{-2}C,$$

$$\hat{x}_{n+1}(\lambda) = \hat{x}_n(\lambda) + \frac{S_n(\lambda) h_{n+1}}{\sigma_{n+1}^2 + h_{n+1}^T S_n(\lambda) h_{n+1}} (\zeta_{n+1} - h_{n+1}^T \hat{x}_n(\lambda))$$

$$S_{n+1}(\lambda) = S_n(\lambda) - \frac{(S_n(\lambda) h_{n+1})(S_n(\lambda) h_{n+1})^T}{\sigma_{n+1}^2 + h_{n+1}^T S_n(\lambda) h_{n+1}}.$$

Compare this with the recursions (8.3.1) and (8.4.5). [Read B_n for $S_n(\lambda)$.] When λ is close to zero, the present recursions generate a sequence which is close to \bar{x}_n , the least squares estimate for x based on ζ_1, \dots, ζ_n computed subject to the constraints $(I - CC^+)x = 0$. (See Albert and Sittler [1].)

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