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The Operator Theory of the Pseudo-Inverse

I. Bounded Operators*

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I. INTRODUCTION

Every vector-matrix equation $Ax = y$ has a "best approximate" solution $\hat{x} = A^{+}y$, where A^{+} is a unique matrix known as the pseudo-inverse of A. Here "best approximate" means that $\hat{x}$ minimizes the Euclidian norm $\| Ax - y \|$; if $\hat{x}'$ also minimizes this norm and $\hat{x}' \neq \hat{x}$, $\| \hat{x} \| < \| \hat{x}' \|$.

The pseudo-inverse has applications to statistics, prediction theory, and control system synthesis. These are discussed elsewhere [1, 2], and will not be further examined in this paper. The reader is also referred elsewhere for a summary of the properties of the pseudo-inverse, and its computation as a product of more elementary matrices [1, 3, 4].

A predominantly algebraic viewpoint appears to pervade the literature dealing with the pseudo-inverse. Extensive matrix computations and manipulations are generally involved, and the function-analytic interpretation of the pseudo-inverse largely neglected. There is in fact a natural characterization of the pseudo-inverse in terms of Hilbert space projection operators; once this is realized, generalizations to infinite dimensional Hilbert spaces (and, to a limited extent, to Banach spaces) become apparent. The function-analytic approach also puts new tools in the hands of those interested in applications, and yields a structure easier to grasp as a comprehensive entity.[1]

Our program is as follows. A representation theorem applicable to operators on Banach spaces will be proved. This theorem states necessary and sufficient conditions under which a bounded operator A can be written $A = P_R\tilde{A}$, where P_R is the projection on the range of A, and $\tilde{A}$ is invertible. If the range R is closed, such a representation always exists for a suitable extension of an

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[1] This manuscript was essentially completed when [12] appeared, reflecting a viewpoint much like that of the author. While Theorem 5 and several pseudo-inverse identities are in both papers, there is little similarity in the analytic paths pursued.

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operator from one Hilbert space to another. In particular, every (Banach space) operator in spaces of finite dimension can be appropriately extended.

We call $A^x = \tilde{A}^{-1}$ a semi-inverse, and show that (in a Hilbert space but not necessarily a Banach space) $A^x x$ is a norm-minimizing approximate solution of $Ax = y$. If now $N = \{z : Az = 0\}$, M the orthogonal complement of N, and P_M the projection on M, the pseudo-inverse is found to be $A^+ = P_M A^x$. The identities commonly ascribed to the pseudo-inverse are valid in Banach spaces, but the "best approximate solution" property extends only to abstract Hilbert spaces.

The general expression for the pseudo-inverse, when specialized to the finite dimensional case, offers a new method for the explicit computation of the matrix pseudo-inverse. It is believed that this method is more convenient than the one commonly used (see [1, equation 2]). If A is a Hermitian matrix (e. g., a covariance matrix), calculation of the pseudo-inverse is particularly simple.

II. Representation Theorems

In what follows, A is a bounded linear operator which maps a (complex) Banach space B_1 into (another) Banach space B_2. R is taken to be the range of A, i.e., $A(B_1) = R$. If $\bar{R}$ is the closure of R, there may be a complementary subspace S (called the closed complement of R) satisfying $\bar{R} \oplus S = B_2$ and $\bar{R} \cap S = \{0\}$; the existence of such a subspace is discussed in [5]. Note that the term subspace (as used in this paper) will always refer to a closed linear manifold. We define N as the set

$$N = \{x : x \in B_1 , Ax = 0\} \tag{2.1}$$

and see that N is a subspace because A is bounded. A subspace complementary to N is called M whenever N is known to have a closed complement.

The dimension $D[\cdot]$ of specified subsets will play a prominent role in our investigations. The dimension of a subset is, of course, the cardinality of a Hamel basis, which may be taken as a maximal orthonormal set in a Hilbert space. Finally, for any subspace K with closed complement, P_K is the corresponding projection operator (see [6, Definition 2.14.]).

It is now possible to state the principal result of this section, giving necessary and sufficient conditions for the existence of the desired representation. We have

THEOREM 1. *Let A have a representation*

$$A = P\tilde{A} \tag{2.2}$$

where P is a projection, and $\tilde{A}$ is a bounded linear operator from B_1 onto B_2 with bounded inverse $\tilde{A}^{-1}$. Then

(i) *R is closed.*

(ii) *P is the projection on R, i.e., $P = P_R$.*

(iii) *R has a closed complement S, and N has a closed complement M.*

(iv) *$\tilde{A}$ maps N onto S in a* 1-1 *manner.*

Conversely, let (i) *and* (iii) *hold, and assume there exists a closed linear operator whose domain contains N, and which provides a* 1-1 *mapping from N onto S. Then there exists a representation* (2.2) *for A. For any $\delta > 0$, this representation can be chosen so that*

$$\| \tilde{A} \| \leqslant \| A \| + \delta. \tag{2.3}$$

PROOF. (*Necessity*) R is a linear manifold in any case. Since $\tilde{A}$ is invertible, P and $P\tilde{A}$ have the same range. Now the range of a projection P is closed, and by (2.2) and the above argument, coincides with the range of A. This verifies (i) and (ii), as well as the first statement of (iii). Indeed, that there is a closed complement S is implied by the existence of the projection on R (see [5, Lemma 1.1.1]).

To prove (iv), we first note that, because of (2.2), $\tilde{A}x \in S$ whenever $x \in N$, i.e., $\tilde{A}(N) \subset S$. Since $\tilde{A}$ is invertible and thus 1-1, the proof of (iv) can be completed by showing that actually $\tilde{A}(N) = S$. If the statement were false, there would be a nonzero $y \in S$ such that $\tilde{A}x = y$ with $x \in N$. For such x, $P_R\tilde{A}x = 0$; hence $Ax = 0$ from (ii) and (2.2). This means $x \in N$, which is a contradiction. Thus (iv) has been proved.

Finally, we deduce the latter part of (iii). From the first part of (iii), the projection P_S exists. Then the projection of N is asserted to be

$$P_N = \tilde{A}^{-1} P_S \tilde{A}. \tag{2.4}$$

It is easily verified that the P_N given by (2.4) is bounded and idempotent, with range N, and so is the desired projection. It follows (again from [5, Lemma 1.1.1]) that N has a closed complement.

To prove sufficiency, we first note the existence of projections P_N and P_R by virtue of (iii). Now take $P = P_R$, and construct an invertible $\tilde{A}$ satisfying (2.2) and (2.3). Let B be the closed operator (mapping N onto S in 1-1 fashion) which exists by hypothesis. Since the restriction of B to N is bounded (see [6, Theorem 2.12.3]), we may assume without loss of generality that $\| BP_N \| = 1$. Let $\delta > 0$ be given. We assert that, for this δ,

$$\tilde{A} = A + \delta BP_N \tag{2.5}$$

has the required properties.

We first show that the range of $\tilde{A}$ is B_2. For any $y \in B_2$, $y = y_1 + y_2$, with $y_1 \in R$ and $y_2 \in S$. There is an $x_1 \in M$ and a $x_2 \in N$ such that $Ax_1 = y_1$ and $\delta B x_2 = y_2$. Letting $x = x_1 + x_2$, we obtain

$$\tilde{A}x = Ax_1 + \delta B x_2 = y, \tag{2.6}$$

so that indeed $\tilde{A}(B_1) = B_2$. To complete the proof of the invertibility of $\tilde{A}$, we demonstrate that $y = 0$ implies $x = 0$. Since $Ax \in R$ and $BP_N x \in S$, $y = 0$ means that both $Ax = 0$ and $BP_N x = 0$. But the former implies that $x \in N$, and the latter that $x \in M$ (if $Bz = 0$ for a nonzero $z \in N$, B cannot be 1-1 from N to S). Hence $x = 0$ as was to be proved.

For (2.3)[2], we merely observe that

$$\| \tilde{A}x \| \leqslant \| Ax \| + \delta \| BP_N x \| \leqslant (\| A \| + \delta) \| x \|. \tag{2.7}$$

Finally, we verify that our construction of $\tilde{A}$ satisfies (2.2). Because the range of BP_N is S, we have $P_R B P_N = 0$. Thus $P_R \tilde{A} = P_R A$ from (2.5). If we combine the latter with the obvious equality $P_R A = A$, we obtain (2.2). This completes the proof of the theorem.

If A has a representation (2.2), $D[N] = D[S]$ as a consequence of (iv). Thus

(v) $D[N] = D[S]$

is a necessary condition for the existence of a representation (2.2). In general, however, (v) cannot be imposed as a sufficiency condition to replace the assumption of a closed operator which is 1-1 from N to S. Although (v) implies the existence of such an operator for many special spaces N and S (e.g., L_p, l_p, c, c_0, $C[0, 1]$ can each be mapped onto each other 1-1; see [7, Sections XI.6 and XI. 7]), it is not always true that there are such operators [8], even for separable spaces B_1 and B_2. One important class of spaces for which (v) does suffice is that of Hilbert spaces, for which there is

COROLLARY 1. *Let A be a linear bounded operator from H_1 into H_2* (both *Hilbert spaces*). *If* (i) and (v) *are satisfied, A has a representation* (2.2). *The operator $\tilde{A}$ appearing in this representation may be chosen such that*

$$\| \tilde{A} \| = \| A \|. \tag{2.8}$$

PROOF. By (v), there is a partial isometry U, which provides a 1-1 norm-preserving mapping from N onto S (see [9, Section 16]). Also, (iii) is automatically satisfied in Hilbert spaces, and we even take S and M orthogonal to R and N, respectively. We define

$$\tilde{A} = A + \| A \| UP_N, \tag{2.9}$$

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[2] It follows from (2.3) that $\tilde{A}$ is bounded. Therefore, its inverse is likewise a bounded operator ([6, Corollary to Theorem 2.12.1]).

and verify the properties of A in precisely the same manner as in the proof of the theorem. It then remains to prove (2.8). From (2.2) we obtain

$$\| A \| \leqslant \| P \| \cdot \| \tilde{A} \| = \| \tilde{A} \|.$$

To reverse this inequality, we make use of the decomposition $x = x_1 + x_2$, $x_1 \in M$, $x_2 \in N$, obtaining

$$\| \tilde{A}x \|^2 = \| Ax_1 \|^2 + \| A \|^2 \| Ux_2 \|^2 \leqslant \| A \|^2(\| x_1 \|^2 + \| x_2 \|^2) = \| A \|^2 \| x \|^2,$$

so that indeed $\| \tilde{A} \| = \| A \|$.

As we shall see later, the case $D[N] \neq D[S]$ presents only apparent difficulties. By enlarging H_1 or H_2 as necessary, we obtain an extension of A which satisfies (v). The same procedure is applicable to operators on Banach spaces, but additional hypotheses are needed. In any case, an operator having a representation (2.2) must satisfy

Corollary 2. *If A has a representation* (2.2), *B_1 and B_2 necessarily have the same dimension.*

Proof. Since $\tilde{A}$ is an invertible operator from B_1 to B_2, the desired conclusion is immediate.

The requirement that the range of A be closed is immutable, and cannot be remedied by "tinkering". It is easy to show that nondegenerate compact (completely continuous) transformations do not have a closed range, and therefore do not possess a representation (2.2). On the other hand, if B_1 and B_2 are Banach spaces of the same finite dimension, there is always a representation (2.2) for A; this settles the problem completely for finite-dimensional vector space. Even if the spaces are of infinite dimension, it is helpful if $D[R]$ is finite. More precisely, we have

Corollary 3. *Let* (1) *B_1 and B_2 have the same finite dimension, or* (2) *$D[R]$ be finite for an operator A taking Hilbert space H_1 into another Hilbert space H_2, both of which have the same* (*arbitrary*) *dimension. Then the representation* (2.2) *exists.*

Proof. For any $y \in R$, there is a $x \in B_1$ such that $y = Ax$. In fact, $y = Ax_1$ for some $x_1 \in M$ from (2.1), assuming only that N has a complementary subspace M (as is the case under the hypotheses of this corollary). Thus A provides a mapping from M onto R. This mapping is even 1-1, because $x \in M$ and $Ax = 0$ implies also $x \in N$ and consequently $x = 0$. Therefore, $D[M] = D[R]$ (whatever the dimensions of B_1 and B_2).

If now $D[B_1] = D[B_2] = n$, $D[N]$ and $D[S]$ are respectively of dimension $n - D[M]$ and $n - D[R]$. That is, $D[N]$ and $D[S]$ are equal (by the above result) and finite. Let $\{u_i\}$ and $\{v_i\}$, $i = 1, 2, ..., m$ be maximal independent sets of vectors in N and S, respectively. We define B by the relation $Bu_i = v_i$, and extend B linearly over all of N. It is easy to verify that B is a bounded ([10, p. 216]) linear operator, which is 1-1 from N to S. Thus one of the two sufficiency conditions of Theorem 1 is met. The other condition, that R is closed, is automatically satisfied, for R is a finite-dimensional linear manifold.

Under the second hypothesis, R is again closed. Also, $D[H_1] = D[H_2]$, so that (v) follows from our proof that $D[M] = D[R]$. An application of Corollary 1 then completes the proof.

Another possible representation takes the form

$$A = \hat{A}P_M \tag{2.10}$$

where $\hat{A}$ is again a bounded linear operator with bounded inverse. The sufficiency and necessity conditions for this representation are identical with those of Theorem 1. The same construction (2.5) may be used for $\hat{A}$, so that the sufficiency proof of the theorem is directly applicable. The proof of necessity is more complex, and we shall only sketch it here. First, P must be P_M in order that $Ax = 0$ *iff* $x \in N$. Next, we note from the proof of Corollary 3 that A is *l-l* from M to R; R is a linear manifold dense in $\bar{R}$. Now $\hat{A}(M) = R$ from (2.10). But $\hat{A}$ has a bounded inverse, and M is a closed subspace; hence $\hat{A}(M)$ is closed, proving (i). Again using the invertibility of $\hat{A}$, together with the result $\hat{A}(M) = \bar{R}$, we obtain (iv). These argument have yielded

COROLLARY 4. *The operator A has a representation* (2.2) *iff A also has a representation* (2.10).

We give an alternative proof of the corollary. If there is a representation (2.2), the representation may be reconstructed with an $\tilde{A}$ such as in (2.5). This $\tilde{A}$ maps M onto R and N onto S. Hence $P_R\tilde{A} = P_R\tilde{A}P_M = \tilde{A}P_M$, proving the corollary in one direction. An analogous argument, starting with (2.10), disposes of the converse.

III. Extension of Operators

If B_1 and B_2 are of different finite dimension, the operator A may be represented as a nonsquare matrix. According to Corollary 2, A does not possess a representation (2.2). But A becomes a square matrix by the addition of a suitable number of rows or columns of zeros. In this manner, A may be extended to an operator for which (2.2) exists. Thus the finite-dimensional case is disposed of quite easily.

When at least one of B_1 and B_2 is infinite-dimensional, the extension procedure is less simple. The need for an extension of A appears whenever there is no linear bicontinuous mapping from N onto S; this may occur even when $D[N] = D[S]$. In that event, an effort is made to embed B_1 or B_2 (as appropriate) in a larger space (possibly of the same dimension as the original), and to extend A to the larger space without essential change in its behavior. The purpose of the embedding and extension is to enlarge N or S as needed to obtain the 1-1 map required by Theorem 1.

The desired extension procedure is shown to be feasible if there is a subspace $N' \subset N$ which can be mapped invertibly onto S, or if N can be mapped invertibly onto a subspace $S' \subset S$. Also required is the existence of certain closed complements. There are, however, pathological cases; N and S are both separable, but neither provides a bounded linear invertible operator onto a subspace of the other. Two Banach spaces of this type are L^p and L^q with $1 < p < 2 < q$ (see [7, p. 203]). If N and S are pathological in the manner described, we are unable to show that a proper extension exists, and conjecture that none does. It seems more likely that there be several extensions than none. This happens if there is an invertible operator from N to a subspace S, as well as an invertible operator from S to a subspace of N. Indeed, there may well be a number of operators meeting the conditions cited above, so that there exist a multiplicity of extensions of A which lead to (2.2).

The extension discussed above is more precisely described by

THEOREM 2. *Let A' (a linear bounded operator from B_1' to B_2) satisfy (i). Suppose there exists a linear operator B', bounded on*

$$N' = \{x\colon A'x = 0\} \tag{3.1}$$

which maps N' onto a subspace $S' \subset S$ in a 1-1 *manner. Assume that each of the following subspaces has closed complements: R, S' (in S), N' (in B_1'). Then there exists a Banach space $B_1 \supset B_1'$ and a linear bounded operator A from B_1 to B_2 having the properties*

(a) *$Ax = A'x$ for $x \in B_1'$.*

(b) $Ax = 0$ for $x \in B_1 \ominus B_1'$.

(c) *The ranges of A and A' coincide.*

(*d*) *A has a representation* (2.2).

PROOF. Let $B_3 = S \ominus S'$, and consider the enlarged domain space $B_1 = B_1' \oplus B_3$. Now each $x \in B_1$ may be uniquely decomposed according to $x = x_1 + x_3$ with $x_1 \in B_1'$ and $x_3 \in B_3$. Then B_1 is a Banach space under the norm

$$\| x \| = \| x_1 \| + \| x_3 \|, \tag{3.2}$$

where $\| x_1 \|$ is the B_1-norm of x_1, and $\| x_3 \|$ is the B_2-norm of x_3. We remark that x_1 and x_3 are projections of x; since projections are bounded ([6], Theorem 2.14.2), there exists a finite K such that

$$\| x_1 \| + \| x_3 \| \leqslant K \| x \|. \tag{3.3}$$

A is defined as an operator on B_1 by the equation

$$Ax = A'x_1 . \tag{3.4}$$

This operator is clearly linear. It is also bounded, since from (3.3)

$$\| Ax \| \leqslant K \| A' \| \cdot \| x \|.$$

From (3.4), A satisfies (a) and (b), and so (c) follows at once. In particular, the range of A is closed.

The proof is completed by defining an operator B satisfying the conditions of Theorem 1. B must be bounded on $N = N' \oplus B_3$, and provide a 1-1 mapping from N onto $S = S' \oplus B_3$. By hypothesis, B' is bounded on N', and is 1-1 from N' onto S'. We take $B(M) = 0$ (note that $M' = M$ under the embedding of B_1' in B_1). For $x \in N$, we use the decomposition $x = x_2 + x_3$ with $x_2 \in N'$ and $x_3 \in B_3$. In terms of this decomposition, B is now given by

$$Bx = B'x_2 + x_3 \quad \text{for} \quad x \in N. \tag{3.5}$$

Then B is easily seen to be linear. B is also bounded by a repetition of the argument for the boundedness of A. Since the range of B' is S', B has range $S' \oplus B_3 = S$. Finally, if $x \in N$ and $Bx = 0$, $x_3 = 0$ and $B'x_2 = 0$ (since S' and B_3 have only $\{0\}$ in common). But $B'x_2 = 0$ implies $x_2 = 0$; hence $Bx = 0$ implies $x = 0$ (for $x \in N$), and so B is 1-1 from N to S.

THEOREM 3. *Let A' (a linear bounded operator from B_1 into B_2') satisfy (i). Suppose there exists a linear operator B', bounded on a subspace*

$$N' \subset N = \{x \colon A'x = 0\},$$

and mapping N' onto S' in 1-1 fashion. Assume that each of the following subspaces have closed complements: N, N' (in N), R (in B_2'). Then there exists a Banach space $B_2 \supset B_2'$ and a linear bounded operator A from B_1 to B_2 having the properties

(a′) $Ax = A'x$ for $x \in B_1$

(c) *The ranges of A and A' coincide.*

(d) *A has a representation* (2.2).

PROOF. Let $B_3 = N \ominus N'$, and take $B_2 = B_2' \oplus B_3$. We may then define the operator A by (a'); since A and A' have the same domain space B_1, and assume the same values for each $x \in B_1$, their ranges coincide. Of course,

$B_2 = B_2' \oplus B_3$ means that B_2' is embedded in B_2 as a subspace. For this purpose, we equip B_2 with norm

$$\| y \| = \| y_2 \| + \| y_3 \| \tag{3.6}$$

where $y = y_2 + y_3$ with $y_2 \in B_2'$ and $y_3 \in B_3$, and the respective norms on the right side of (3.6) are the B_2' and B_1 norms. It follows from (3.6) that the operator norms of A and A' are equal, and that R is a closed subspace in B_2.

The construction of an operator B invertible from N onto $S = S' \oplus B_3$ proceeds as in the proof of Theorem 2. We take, for $x \in N$, $x = x_2 + x_3$ with $x_2 \in N'$ and $x_3 \in B_3$, the definition of B to be $Bx = B'x_2 + x_3$. Repeating the arguments of Theorem 2, we may show that B is an invertible operator from N to S. That B is bounded on N follows from $\| Bx \| \leqslant \max [\| B' \|, 1] \{\| x_2 \| + \| x_3 \|\}$, and $\| x_2 \| + \| x_3 \| \leqslant K \| x \|$ for some $K < \infty$. The proof of Theorem 3 is then complete.

The two theorems just proved apply in particular when $D[N]$ and/or $D[S]$ is finite, e.g., if B_1 and/or B_2 is of finite dimension. The necessary extensions can also be constructed for Hilbert spaces H_1 and H_2 of arbitrary dimension, assuming only that the original operator has closed range.

THEOREM 4. *Let A' be a linear bounded operator from one Hilbert space to another, and let (i) hold for A'. Then there exists an operator A having the properties stated in Theorem 2 or Theorem 3, according as $D[H_1] < D[H_2]$ or $D[H_1] > D[H_2]$. The operator A is again an operator from one Hilbert space to another.*

PROOF. For $D[H_1] < D[H_2]$, the equality $D[M] = D[R]$ implies $D[N] < D[S]$. Hence there is a partial isometry, mapping N onto some subspace $S' \subset S$ in 1-1 fashion. One now proceeds as in the proof of Theorem 2, embedding H_1 in $H_1 \oplus [S \ominus S']$. In order that $H_1 \oplus [S \ominus S']$ be a Hilbert space, (3.2) must be modified to $\| x \|^2 = \| x_1 \|^2 + \| x_2 \|^2$; otherwise, the proof is precisely the same.

If $D[H_1] > D[H_2]$, the proof of Theorem 3, together with the above remarks, may be applied to yield the proof.

IV. SEMI- AND PSEUDO-INVERSES

If A has a representation (2.2), its *semi-inverse* A^x is defined by

$$A^x = \tilde{A}^{-1}. \tag{4.1}$$

There is a (nondenumerable) infinity of semi-inverses for a given operator A, unless A is itself invertible. This is shown by the construction (2.5) for $\tilde{A}$ when A is not invertible. If A does have an inverse, $P_R = I$ (the identity operator) in (2.2), so that $\tilde{A} = A$. It is easily verified that the semi-inverse satisfies the identity $AA^xA = A$, as well as many other equalities which also hold for pseudo-inverses. As we shall show, the pseudo-inverse A^+ can be written in terms of A^x as

$$A^+ = P_M A^x, \tag{4.2}$$

even in Hilbert spaces of arbitrary dimension. Of course, this A^+ also exists in Banach spaces, but lacks the "best approximate solution" property.

It may be directly verified that the A^+ defined by (4.2) satisfies the relations usually imputed to the pseudo-inverse, e.g., even in Banach spaces

$$A^+AA^+ = A^+ \quad \text{and} \quad AA^+A = A; \tag{4.3}$$

these are obtained from the equalities $P_R A = AP_M = A$ and the fact

$$AA^x = P_R \tag{4.4}$$

which follows from (2.2). One also obtains $AA^+ = AP_M A^x = AA^x = P_R$ so that, if B_2 is a Hilbert space H_2,

$$(AA^+)^* = AA^+, \tag{4.5}$$

where $*$ denotes adjoint. Moreover,

$$(A^+A)^* = A^+A. \tag{4.6}$$

To show this, we observe that $\tilde{A}x = Ax + y_2$, $y_2 \in S$, for all $x \in B_1$. Then $x = A^xAx + x_2$, where $x_2 \in N$ because of condition (iv) of Theorem 1. There follows $P_M = P_M A^x A = A^+A$. In Banach spaces, the representation (2.2) also leads to a proof that

$$(A^+)^+ = A. \tag{4.7}$$

Now, from (4.2), A^+ already has a representation (2.2) in which $\tilde{A}^+ = A^x = \tilde{A}^{-1}$, so that $(A^+)^x = \tilde{A}$. A second consequence of (4.2) is that (since A^x is invertible, mapping S onto N) $A^+x = 0$ *iff* $x \in S$. Then $(A^+)^+ = P_R\tilde{A} = A$, as was to be shown. Other identities for the pseudo- and semi-inverses can be obtained by the techniques employed above, but this will not be done here.

As we have seen, the A^+ given by (4.2) and alleged to be the pseudo-inverse possesses (for abstract Banach and Hilbert spaces) the properties usually associated with the finite dimensional (matrix) pseudo-inverse. If A^+ is to be viewed as a generalization of the matrix pseudo-inverse, however, we must show that A^+ is a "best approximate solution" of the equation $Ax = y$. To this end, we formally define the pseudo-inverse as any linear operator having the "best approximate solution" property. That is, A^0 is a pseudo-inverse for A whenever $\inf_{x \in B_1} \| Ax - y \| = \| A(A^0y) - y \|$ for each $y \in B_2$, with $\| A^0 y \| < \| x_0 \|$ for any other vector x_0 which also attains the above infimum. That A^+ is the unique operator that does give such a solution, but only when B_1 and B_2 are Hilbert spaces, is shown in the remainder of this section.

THEOREM 5. *Let H_1, H_2 be Hilbert spaces, A a bounded linear operator from H_1 to H_2. If A has a representation* (2.2), *then for any $y \in H_2$,*

$$\inf_{x \in H_1} \| Ax - y \| = \| Ax_0 - y \| \tag{4.8}$$

in which

$$x_0 = A^x y \tag{4.9}$$

The infimum is also attained by any $x \in H_1$ satisfying

$$Ax = Ax_0, \tag{4.10}$$

and only by such x. Let $\chi_0 = \{x\colon Ax = Ax_0\}$ (the space of all x attaining the infimum). Then $\inf_{x \in \chi_0} \| x \| = \| \hat{x} \|$, where $\hat{x}$ is specified by

$$\hat{x} = P_M A^x y = A^+ y. \tag{4.11}$$

For any other $x \in \chi_0$,

$$\| x \| > \| \hat{x} \|. \tag{4.12}$$

PROOF. We may write

$$\| Ax - y \|^2 = \| (Ax_0 - y) + (Ax - Ax_0) \|^2 = \| Ax_0 - y \|^2 + \| A(x - x_0) \|^2 \tag{4.13}$$

provided that $Ax_0 - y$ and $A(x - x_0)$ are orthogonal. Now from (4.9) and (4.4)

$$Ax_0 - y = (P_R - I)y = -P_S y. \tag{4.14}$$

On the other hand, $[A(x - x_0)] \in R$, which is orthogonal to S. This shows the infimum to be attained *iff* x is such that $Ax = Ax_0$.

Consider now the quotient space H_1/N, whose elements are the residue classes of vectors in H_1 modulo N. Thus, x' and x'' belong to the same residue class *iff* $(x' - x'') \in N$, that is, *iff* $Ax' = Ax''$. If χ_0 is the residue class containing x_0, we see that $\| Ax - y \|$ is minimized by any $x \in \chi_0$, and only by x belonging to this class. Since $AP_M = A$, the $\hat{x}$ defined by (4.11) is in χ_0. Then $\hat{x}$ may be taken as the representant element of χ_0; for any $x \in \chi_0$,

$$x = \hat{x} + z, \quad z \in N. \tag{4.15}$$

Because $\hat{x} \in M$ from (4.11), $\hat{x}$ and z are orthogonal. Hence

$$\| x \|^2 = \| \hat{x} \|^2 + \| z \|^2 \tag{4.16}$$

for any x satisfying (4.10), i.e., any $x \in \chi_0$. Clearly, $\| x \| > \| \hat{x} \|$ unless $z = 0$, n which case $x = \hat{x}$.

The question of the uniqueness of A^+ is settled by

COROLLARY 1. *A^+ is the unique operator from H_2 to H_1 which yields for every $y \in H_2$ an element of H_1 with the minimum properties of $\hat{x}$ mentioned in the theorem.*

PROOF. If A' is another such operator, we must have $A'y = \hat{x}$, since $\hat{x}$ is the only element with the required properties. Since this statement is true for every $y \in H_2$, we have $(A^+ - A')y = 0$ for all $y \in H_2$, and so $A^+ = A'$.

Theorem 5 can be generalized somewhat by minimizing $\| C(Ax - y) \|$, where C is another operator. The following result gives the conditions under which the pseudo-inverse retains the "best approximate solution" property.

COROLLARY 2. *Let C be a linear bounded operator from H_2 to H_3. Then*

$$\inf_{x \in H_1} \| C(Ax - y) \| = \| C(Ax_0 - y) \| \tag{4.17}$$

iff C^*C reduces R. When (4.17) *is valid, any x satisfying $Ax = Ax_0$ also attains the infimum.*

PROOF. The last statement is obvious. To prove the first part of the corollary, note the equivalence of the following:

(1) The specified infimum is attained by x_0.
(2) $(C[Ax_0 - y], CAz) = 0$ for all $z \in H_1$.
(3) $(C^*C[Ax_0 - y])$ is orthogonal to R.
(4) $P_R C^*CP_S = 0$.
(5) $C^*C(S) \subset S$.
(6) R is reduced by C^*C.

Note that C^*C is a Hermitian operator from H_2 to H_2. If such an operator has an invariant subspace, that subspace (as well as its orthogonal complement) is actually reduced (see [9, Section 23]).

Under the conditions of Corollary 2, $\hat{x}$ may or may not retain the minimum property (4.12); that x be such that $Ax = Ax_0$ is only a sufficient condition for x to attain the infimum. For example, if $C = 0$, the infimum is attained by $x = 0$, which is also the element of minimum norm attaining the infimum. On the other hand, should C be any unitary operator, $\hat{x}$ is the unique element of minimum norm of all those attaining the infimum (4.17).

Suppose now that A is a bounded linear operator from B_1 to H_2, the domain space no longer being a Hilbert space. How much of Theorem 5 remains true? Upon examination of the proof we conclude that only (4.16) fails to hold. Therefore, Theorem 5 is valid except for the assertion that $\hat{x}$ has minimum norm of all those elements attaining the infimum (4.8).

Finally, if both B_1 and B_2 are merely Banach spaces the pseudo-inverse of A (if it exists) continues to satisfy identities such as (4.3) and (4.7), but lacks any minimizing properties whatsoever. Consider the simple example of any space having projections of norm greater than unity; even two-dimensional spaces may have such projections. Now take a subspace S with $\| P_S \| > 1$, and let A be any operator with representation (2.2) of the form $A = P_R \tilde{A}$, $\tilde{A}$ being arbitrary. There is a $y \in B_2$ such that $\|P_S y\| > \| y \|$. For this y

$$\| Ax_0 - y \| = \| A\hat{x} - y \| = \| -P_S y \| > \| y \| \tag{4.18}$$

so that $x = 0$ actually yields a smaller norm that $x_0 = A^x y$ or $\hat{x} = A^+ y$. One can even exhibit linear Banach space operators A for which $Ax = y$ has a unique "best approximate solution" $\hat{x} = F(y)$, where $F(\cdot)$ is a nonlinear operator on B_2; indeed, the simplest such example applies to a linear operator A mapping a two dimensional Banach space into itself.

There is no general result giving the "best approximate solution" for general Banach spaces. Indeed, one should ask whether the "best approximate solution" even exists. The following theorem states sufficiency conditions for its existence:

THEOREM 6. *Let B_1 and B_2 be uniformly convex Banach spaces, and let A be a bounded linear operator from B_1 to B_2 with closed range in B_2. For any $y \in B_2$, there exists an $x_0 \in B_1$ satisfying*

$$\inf_{x \in B_1} \| Ax - y \| = \| Ax_0 - y \|. \tag{4.19}$$

The infimum is also attained by any $x \in B_1$ such that

$$Ax = Ax_0 \tag{4.20}$$

and only by such x. Let $\chi_0 = \{x: Ax = Ax_0\}$ (the space of all x attaining the infimum). Then there exists a unique $\hat{x}$ such that

$$\inf_{x \in \chi_0} \| x \| = \| \hat{x} \| \tag{4.21}$$

Remark. Uniformly convex spaces are discussed in [11]. L_p spaces, $1 < p < \infty$, are uniformly convex, as are all Hilbert spaces.

PROOF. Our demonstration is based on the following result [6, *p.* 19]: if C is a closed convex subset of a uniformly convex Banach space, there exists a unique $x_0 \in C$ such that $\inf_{x \in C} \| x - y \| = \| x_0 - y \|$. We apply the result just quoted. Since

$$\inf_{x \in B_1} \| Ax - y \| = \inf_{z \in R} \| z - y \| \tag{4.22}$$

there is a unique $z_0 \in R$ which attains the infimum (4.22); this is true because B_2 is uniformly convex, and R, being a closed subspace in B_2, is convex. Now $z_0 \in R$ implies that there is at least one $x \in B_1$, say x_0, for which $Ax_0 = z_0$. In fact, it follows from the uniqueness of z_0 that a specified x attains the infimum (4.19) *iff* $Ax = z_0$, i.e., *iff* $Ax = Ax_0$.

It remains to show that there is a unique $x \in B_1$ which minimizes the norm over all x satisfying (4.20). To this end, consider the residue class B_1/N. As in the proof of Theorem 5, the minimum is attained *iff* $x \in \chi_0$. We again write, for each $x \in \chi_0$,

$$x = x_0 + u \qquad u \in N, \tag{4.23}$$

where x_0 is the representant of χ_0. Now

$$\inf_{x \in \chi_0} \| x \| = \inf_{u \in N} \| x_0 + u \|. \tag{4.24}$$

Since N is a closed subspace, and hence a closed convex set in the uniformly convex space B_1, there exists a unique $u_0 \in N$ such that

$$\inf_{x \in \chi_0} \| x \| = \| x_0 + u_0 \|. \tag{4.25}$$

We call $\hat{x} = x_0 + u_0$, and note that the uniqueness of u_0 makes $\hat{x}$ unique. Indeed, any other $x' \in \chi_0$ can also be written in terms of the representant x_0, i.e., $x' = x_0 + u'$ with $u' \neq u_0$. Then

$$\| x' \| = \| x_0 + u' \| > \| x_0 + u_0 \| = \| \hat{x} \|.$$

COROLLARY. *There exists a unique $x_1 \in M$ satisfying*

$$\inf_{x \in B_1} \| Ax - y \| = \| Ax_1 - y \|. \tag{4.26}$$

PROOF. Let $x \in B_1$ be any element attaining the infimum. Writing $x = x_1 + x_2$, $x_1 \in M$, $x_2 \in N$ we have $Ax_1 = Ax$, so that $x_1 \in M$ also attains the infimum (4.26). Let $x_1' \in M$ be any other vector which attains the infimum (4.26). Then, from the theorem, $A(x_1 - x_1') = 0$, so $(x_1 - x_1') \in N$. But $(x_1 - x_1') \in M$ from the definitions of x_1 and x_1'. Therefore, $x_1 - x_1' = 0$, thus proving the corollary.

V. Computation of the Pseudo-Inverse Matrix

In this (final) section we shall propose a new method for computing the pseudo-inverse matrix. This method, based on (4.2), is believed to be simpler and intuitively more appealing than the standard formula [1, eq. 2]. The calculation becomes particularly simple for Hermitian matrices.

We restrict ourselves to finite dimensional vector spaces equipped with the dot product as inner product $(\cdot, \cdot)$, and Euclidian length as norm. The vector spaces are then Hilbert spaces H_1' and H_2 of dimension k and n, respectively. The operator A' from H_1' to H_2 can be regarded as an nxk matrix. For the sake of fixing ideas, we shall take $n \geqslant k$, and assume the matrix to be of rank $r(\leqslant k)$.

As a first step, the extension procedure of Theorem 2 is applied to A' and the two vector spaces. One simply adds $n - k$ columns of zeros to A' to enlarge it to the nxn matrix A. Now A operates on the n dimensional vectors of B_1, and it can be directly verified that A has the properties (a), (b), and (c) of Theorem 2.

Evidently, A^+ can be obtained from P_M and $\tilde{A}$ (see (4.1) and (4.2)). Therefore, our procedure consists of a set of instructions for obtaining these two matrices. We shall prove later that the suggested procedures do indeed provide the correct result.

Let the columns of A be denoted by $a_1, a_2, ..., a_n$. Since A is of rank r, a set of r independent column vectors can be obtained by applying the Gram-Schmidt procedure [19, Section 14] to $a_1, a_2, ..., a_k$, and throwing out any a_i which appears as a linear combination of the orthonormal vector set generated by $a_1, a_2, ..., a_{i-1}$. We may assume for convenience that a_1, $a_2, ..., a_r$ is such an independent set of vectors We will be able to show that

$$R = V\{a_j, j = 1, 2, .., r\} = V\{e_j, j = 1, 2, ..., r\}, \tag{5.1}$$

Where "V" means "span of", and $\{e_j\}, j = 1, 2, ..., r$ is a maximal orthonormal set generated by the a's.

Next, one obtains $e_{r+1}, ..., e_n$, the $n - r$ orthonormal vectors orthogonal to R; then $\{e_j\}$, $j = 1, 2, ..., n$ is a complete orthonormal set. Then $\tilde{A}$ is defined as the $n \times n$ matrix whose columns are respectively

$$a_1, a_2 ..., a_r, a_{r+1} + e_{r+1}, ..., a_k + e_k, e_{k+1}, ..., e_n. \tag{5.2}$$

It remains to find P_M. Let A^* be the adjoint (conjugate transpose) of A, and let its columns be $b_1, b_2, ..., b_n$. There is again a maximally independent set of column vectors, say $b_{i_1}, b_{i_2}, ..., b_{i_r}$ and a corresponding orthonormal set $u_{i_1}, u_{i_2}, ..., u_{i_r}$. We assert that

$$M = V\{b_{i_j}, j = 1, 2, ..., r\} = V\{u_{i_j}, j = 1, 2, ..., r\}. \tag{5.3}$$

The complete orthonormal set $\{u_i\}$, $i = 1, 2, ..., n$, is now obtained by calculating the other u_i, $i \neq i_j$; the order or choice of these is immaterial. Denote by C^* the matrix whose columns are respectively $u_1, u_2, ..., u_n$, and take D to be a diagonal matirix with all off-diagonal elements zero and diagonal entries

$$d_{ii} = \begin{cases} 1 & \text{if } i = i_j, \ j = 1, 2, ..., r \\ 0 & \text{otherwise} \end{cases} \tag{5.4}$$

Now our work is complete, for we have

$$P_M = C^*DC. \tag{5.5}$$

To prove the above statements, we introduce M^*, N^*, R^*, and S^* as the subspaces which bear the same relation to A^* as M, N, R, and S respectively to A. Our first assertion holds more generally than is required for present considerations.

LEMMA. *Let A be a linear bounded operator with closed range, mapping H into itself. Then*

$$M = R^*, N = S^*, R = M^*, S = N^*. \tag{5.6}$$

PROOF. Because of the complementarity of the above subspaces, it is necessary only to demonstrate that $N = S^*$ and $S = N^*$. Now if $x \in N$, $(x, A^*y) = (Ax, y) = 0$ for every y, and so $x \perp R^*$, i.e., $x \in S^*$. This shows $N \subset S^*$, and we have yet to prove equality. If $N \neq S^*$, there exists a nonzero $x \in S^*$ which also is in M. Hence $Ax \neq 0$, and there is a $y \in H$ such that $(Ax, y) \neq 0$. Therefore $(x, A^*y) \neq 0$, and we reach the contradiction that $x \notin S^*$. To show $S = N^*$, let $y \in S$, which gives

$$(x, A^*y) = (Ax, y) = 0$$

for every $x \in H$. Proceeding as before, we conclude that $y \in N^*$, or $S \subset N^*$. The remainder of the proof mirrors the earlier part.

According to the above Lemma, the validity of (5.1) can be shown by demonstrating that $M' = M^*$, where

$$M' = V\{e_j, j = 1, 2, ..., r\}. \tag{5.7}$$

Since $A^*e_j = 0$ for $j = r + 1, r + 2, ..., n$, we have $(M')^{\perp} \subset N^*$, or equivalently, $M^* \subset M'$. Now let v be an arbitrary nonzero vector in M', i.e.,

$$v = \sum_1^r \alpha_i e_i . \tag{5.8}$$

That $A^*c \neq 0$ follows; since $(a_j, e_k) = 0$ for $k \neq j$ and $(a_j, e_j) \neq 0$, the first nonzero α_m gives the m'th vector component of A^*v the value

$$\alpha_m(a_m, e_j) \neq 0.$$

Therefore, $M^* = M'$.

The same argument shows that the span (5.3) is R^*. But by the Lemma, $R^* = M$, so the span is M, as claimed.

We turn now to a verification of the fact that the matrix whose columns are specified by (5.2) is indeed $\tilde{A}$. In the first place, the columns (5.2) are easily seen to be linearly independent, so that the asserted $\tilde{A}$ is invertible, as it should be. To prove that it also satisfies (2.2), we decompose $\tilde{A}$ as follows:

$$\tilde{A} = A + B \tag{5.9}$$

where B is a matrix whose first r columns are zero, the last $n - r$ being respectively $e_{r+1}, e_{r+1}, \ldots, e_n$. Our characterization of the range of a matrix, together with (5.1), proves that $P_R B = 0$, since B has range S. Since A has range R, $P_R A = A$, and so $A = P_R \tilde{A}$, as was to be shown.

To prove that the projection on M is given by (5.5), we proceed somewhat more generally to describe projections on any subspace of our finite dimensional vector space.

THEOREM 7. *A matrix P is a projection operator* iff *it has a representation*

$$P = C^*DC \tag{5.10}$$

where C^* is a unitary matrix whose columns we designate $e_1, e_2, \ldots, e_n$, and D is a diagonal matrix whose diagonal elements d_{ii} are each either unity or zero, and whose off-diagonal elements are zero. The range Q of the projection is

$$Q = V\{e_{i_1}, e_{i_2}, \ldots, e_{i_k}\} \tag{5.11}$$

where $d_{i_j i_j} = 1, j = 1, 2, \ldots, k$, and the other d_{ii}'s are zero.

PROOF. Since $C^*C = I$ and D is idempotent, any operator with the representation (5.10) is idempotent. Such an operator is also Hermitian, and any idempotent Hermitian operator is known to be a projection [9, Section 26].

The range of $P = C^*DC$ can be determined by computing Pe_i, $i = 1, 2, \ldots, n$, and recalling that $\{e_i\}$ is a complete orthonormal set. It is evident that Ce_i is the vector all of whose components are zero except the ith, which is unity. If $i \neq i_j$ for any $j = 1, 2, \ldots, k$, $DCe_i = 0$, so $Pe_i = 0$ and e_i (which is orthogonal to Q) is orthogonal to the range of P. On the other hand, if

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$i = i_j$ for some j, $DCe_i = Ce_i$, and $Pe_i = C^*Ce_i = e_i$. Thus Q is the range of P.

If P is a projection, there exists an orthonormal set $e_1, e_2, \ldots, e_k$ such that P is the projection on $V\{e_i, i = 1, 2, \ldots, k\}$. The set of orthonormal vectors can then be completed by adding orthonormal $e_{k+1}, e_{k+2}, \ldots, e_n$. Define C^* as the unitary matrix whose columns are respectively the e_1, $e_2, \ldots, e_n$ just defined. Let D be the diagonal matrix with zero off-diagonal entries and

$$d_{ii} = \begin{cases} 1 & i = 1, 2, \ldots, k \\ 0 & \text{otherwise.} \end{cases} \tag{5.12}$$

By the first paragraph of the proof of this theorem,

$$P = C^*DC \tag{5.13}$$

is a projection. The second paragraph shows that the projection has range $V\{e_i, i = 1, 2, \ldots, k\}$. Our construction is complete, thereby proving the necessity part of the theorem.

For a Hermitian operator with closed range in arbitrary Hilbert space (mapping the space into itself), there are certain special properties related to the semi- and pseudo- inverse. Since $A = A^*$, we have $M = M^*$ and hence (by the Lemma of this section)

$$M = R. \tag{5.14}$$

It follows from the first proof of Corollary 4 to Theorem 1 that the same $\tilde{A}$ may appear in both representations (2.2) and (2.10). Combining this fact with (5.14) yields

$$P_R = A^x A \quad \text{and} \quad P_R = AA^x. \tag{5.15}$$

Thus A commutes with A^x, and in fact

$$A^+A = AA^+ \tag{5.16}$$

from $A = AP_M$ and $P_R = P_R{}^2$.

The special properties of Hermitian matrices lead to an especially easy method of computing the pseudo-inverse. Any such matrix A can be written in its canonical form,

$$A = C^*FC, \tag{5.17}$$

in which C^* is a unitary matrix whose columns $e_1, e_2, \ldots, e_n$ constitute a complete orthonormal set, and F is a diagonal matrix of eigenvalues of A, i.e.

$f_{ii} = \lambda_i$. It may be supposed that the λ_i are arranged in order of decreasing modulus, with only $\lambda_1, \lambda_2, ..., \lambda_k$ nonzero. Since $Ae_i = \lambda_i e_i$, we have

$$R = V\{e_i, i = 1, 2, ..., k\}. \tag{5.18}$$

From Theorem 7, the projection on R is seen to be

$$P_R = P_M = C^*GC \tag{5.19}$$

in which G is a diagonal matrix with zero off-diagonal elements and

$$g_{ii} = \begin{cases} 1 & i = 1, 2, ..., k \\ 0 & \text{otherwise.} \end{cases} \tag{5.20}$$

Since $\tilde{A}$ is not unique (unless A is invertible), we are free to choose its most convenient form. In this case, $\tilde{A}$ may be taken as

$$\tilde{A} = C^*VC, \tag{5.21}$$

where V is diagonal with zero off-diagonal terms and

$$v_{ii} = \begin{cases} \lambda_i & i = 1, 2, ..., k \\ 1 & \text{otherwise.} \end{cases} \tag{5.22}$$

Since $GV = F$ and $C^*C = I$, a direct calculation yields $P_R\tilde{A} = C^*FC = A$. Moreover, $\tilde{A}$ has an inverse

$$A^x = C^*(V^{-1})C. \tag{5.23}$$

If we call $V^{-1} = W$, we see that W is again a diagonal matrix with zero off-diagonal terms and diagonal entries

$$w_{ii} = \begin{cases} \lambda_i^{-1} & i = 1, 2, ..., k \\ 1 & \text{otherwise.} \end{cases} \tag{5.24}$$

As the final step, A^+ is computed as $P_M A^x$. Thus,

$$A^+ = (C^*GC)(C(WC) = C^*GWC, \tag{5.25}$$

which can be further simplified. Indeed, if we let $Z = GW$, we note that Z is once more a diagonal matrix with zero off-diagonal elements and diagonal entries

$$z_{ii} = \begin{cases} \lambda_i^{-1} & i = 1, 2, ..., k \\ 0 & \text{otherwise.} \end{cases}$$

It should be clear from this form that

$$A^+ = C^*ZC \tag{5.26}$$

can be written by inspection once the eigenvalues and eigenvectors (the e_i) are known, or what is equivalent, once the canonical form (5.17) is obtained.

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