

THE PSEUDO-INVERSE OF A MATRIX

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INTRODUCTION

The pseudo-inverse of a matrix is widely used in applied settings, most recently in Data Science. However, the pseudo-inverse is apparently not widely appreciated or presented in the typical undergraduate mathematics curriculum.

This note hopes to remedy this lapse. As the content has been well-understood for the better part of a century, the novelty, if any, is the presentation.

Every (square or non-square) matrix has a pseudo-inverse. The pseudo-inverse, often called the Moore-Penrose inverse [1], [3], [4], is a natural extension of the inverse of a matrix.

The pseudo-inverse of A is sometimes denoted A^+ [5]. However, because the inverse of A is denoted A^{-1} , we find the notation A^- more appropriate.

Let I be the identity matrix. The inverse of A , if it exists, is the unique matrix X satisfying

$$(1) \quad AX = I \quad \text{and} \quad XA = I.$$

If A has d rows and N columns, the *shape* of A is (d, N) . When (1) happens, both X and I have the same shape as A .

The residuals are

$$(2) \quad \|AX - I\|^2 \quad \text{and} \quad \|XA - I\|^2.$$

These are scalar functions of X . For the residuals to be well-defined, the shape of X must equal the shape of A^t . If A is non-square, the identity matrices I in the residuals are not the same shape.

If A is invertible, the unique minimizer of the residuals is $X = A^{-1}$. Given this, one approach to the pseudo-inverse is to seek a matrix X minimizing the residuals.

Let P_c be the projection onto the column space of A , and P_r the projection onto the row space of A . If A is not full-rank, then one of AX or XA can never equal I . Because of this, another approach to the pseudo-inverse is to modify (1) by seeking X satisfying

$$(3) \quad AX = P_c \quad \text{and} \quad XA = P_r.$$

This second approach suggests modifying the residuals to

$$(4) \quad \|AX - P_c\|^2 \quad \text{and} \quad \|XA - P_r\|^2,$$

yielding a third approach. In fact, using $P_c A = A$ and $A P_r = A$, it is easy to check that the residuals (4) differ from the residuals (2) by constants.

If A is not full-rank, the equations (3) may have multiple solutions. A solution X^* of (3) is *least norm* if $\|X^*\| \leq \|X\|$ for all solutions X of (3).

Similarly, a minimizer X^* of $\|AX - I\|^2$ is *least norm* if $\|X^*\| \leq \|X\|$ for all minimizers X of $\|AX - I\|^2$, and a minimizer X^* of $\|XA - I\|^2$ is *least norm* if $\|X^*\| \leq \|X\|$ for all minimizers X of $\|XA - I\|^2$.

Theorem 1. *There is a unique least norm solution of (3), there is a unique least norm minimizer of $\|AX - I\|^2$, and there is a unique least norm minimizer of $\|XA - I\|^2$, and the three matrices agree.*

The *pseudo-inverse* A^- of A is the matrix in Theorem 1. The shape of A^- equals the shape of A^t .

Theorem 2 (Penrose Axioms). *The pseudo-inverse of A is the unique matrix X satisfying*

- A. $AXA = A$,
- B. $XAX = X$,
- C. AX is symmetric,
- D. XA is symmetric.

A projection is a matrix P satisfying $P^t = P$ and $P^2 = P$. The axioms imply $(A^-)^t = (A^t)^-$, and $P^- = P$ if P is a projection.

A matrix U is orthogonal if

$$UU^t = I = U^tU,$$

equivalently if $U^{-1} = U^t$. A matrix U is *pseudo-orthogonal* if $U^- = U^t$.

Theorem 3. *A matrix U is pseudo-orthogonal iff UU^t is a projection iff U^tU is a projection.*

Examples are matrices with orthonormal or zero columns and matrices with orthonormal or zero rows. In particular, a zero matrix is pseudo-orthogonal.

Theorem 4. $P_c = AA^-$ and $P_r = A^-A$.

Recall a linear system $Ax = b$ is solvable if b is in the column space of A . By Theorem 4, this happens iff $AA^-b = b$, exhibiting a solution $x = A^-b$ of $Ax = b$.

Let $u \cdot v$ be the dot product of vectors u, v . The tensor product of u, v is the matrix $u \otimes v$ satisfying $(u \otimes v)w = (v \cdot w)u$.

Let Q be a symmetric matrix of rank r and with eigenvalue decomposition

$$Q = \lambda_1 v_1 \otimes v_1 + \lambda_2 v_2 \otimes v_2 + \cdots + \lambda_r v_r \otimes v_r.$$

Here v_1, v_2, \dots, v_r are orthonormal vectors and $\lambda_1, \lambda_2, \dots, \lambda_r$ are nonzero.

Theorem 5. *The pseudo-inverse of Q is*

$$Q^- = \frac{1}{\lambda_1} v_1 \otimes v_1 + \frac{1}{\lambda_2} v_2 \otimes v_2 + \cdots + \frac{1}{\lambda_r} v_r \otimes v_r.$$

Let A be a matrix of rank r and with singular value decomposition

$$A = \sigma_1 u_1 \otimes v_1 + \sigma_2 u_2 \otimes v_2 + \cdots + \sigma_r u_r \otimes v_r.$$

Here u_1, u_2, \dots, u_r and v_1, v_2, \dots, v_r are orthonormal vectors, and $\sigma_1, \sigma_2, \dots, \sigma_r$ are positive.

Theorem 6. *The pseudo-inverse of A is*

$$A^- = \frac{1}{\sigma_1} v_1 \otimes u_1 + \frac{1}{\sigma_2} v_2 \otimes u_2 + \cdots + \frac{1}{\sigma_r} v_r \otimes u_r.$$

Because Theorems 3, 4, 5, 6 are consequences of Theorem 2, it is enough to establish the first two theorems.

AN EXAMPLE

Let

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 6 & 7 & 8 & 9 & 10 \\ 11 & 12 & 13 & 14 & 15 \end{pmatrix}.$$

Using the Penrose axioms, one verifies

$$A^- = \frac{1}{150} \begin{pmatrix} -37 & -10 & 17 \\ -20 & -5 & 10 \\ -3 & 0 & 3 \\ 14 & 5 & -4 \\ 31 & 10 & -11 \end{pmatrix}.$$

If the rows of A are u, v, w , then $w = 2v - u$, so the rank of A is 2. Let a, b, c, d, e be the columns of A . We show

$$f = (-100, -3, 94), \quad g = (2, 1, 0)$$

span the column space of A .

To this end, recall $x = (t_1, t_2, t_3, t_4, t_5)$ solves $Ax = f$ iff

$$f = t_1a + t_2b + t_3c + t_4d + t_5e.$$

Using $x = A^-f$ and $x = A^-g$ to solve $Ax = f$ and $Ax = g$ and writing out the components of x , we obtain

$$50f = 1776a + 985b + 194c - 597d - 1388e,$$

$$50g = -28a - 15b - 2c + 11d + 24e.$$

Similarly, let B be the matrix with columns f and g ,

$$B = \begin{pmatrix} -100 & 2 \\ -3 & 1 \\ 94 & 0 \end{pmatrix},$$

and solve $Bx = a, Bx = b, Bx = c, Bx = d, Bx = e$ using

$$B^- = \frac{1}{564} \begin{pmatrix} -1 & 2 & 5 \\ 185 & 194 & 203 \end{pmatrix}.$$

Writing out the components of x , we obtain

$$94a = 11f + 597g, \quad 47b = 6f + 347g, \quad 94c = 13f + 791g,$$

$$47d = 7f + 444g, \quad 94e = 15f + 985g.$$

This shows f, g span the column space of A .

Let

$$Q = AA^t = \begin{pmatrix} 55 & 130 & 205 \\ 130 & 330 & 530 \\ 205 & 530 & 855 \end{pmatrix}.$$

Since the column spaces of A and Q agree, Q has two nonzero eigenvalues λ .

To find λ , we restrict Q to its column space by inserting $u = sf + tg$ into $Qu = \lambda u$, leading to

$$(5) \quad Q(sf + tg) = \lambda(sf + tg).$$

Taking the dot product with f then with g leads to the 2×2 homogeneous linear system $(M - \lambda N) \begin{pmatrix} s \\ t \end{pmatrix} = 0$, where

$$M = \begin{pmatrix} f \cdot Qf & f \cdot Qg \\ g \cdot Qf & g \cdot Qg \end{pmatrix} = \begin{pmatrix} 4032830 & 62590 \\ 62590 & 1070 \end{pmatrix},$$

and

$$N = \begin{pmatrix} f \cdot f & f \cdot g \\ g \cdot f & g \cdot g \end{pmatrix} = \begin{pmatrix} 18845 & -203 \\ -203 & 5 \end{pmatrix}.$$

Setting the determinant of $M - \lambda N$ to zero yields

$$\lambda^2 - 1240\lambda + 7500 = 0,$$

which is solved by

$$\lambda_{\pm} = 620 \pm 10\delta, \quad \delta = \sqrt{3769}.$$

To solve for (s, t) , let

$$S = B^{-1}QB = \begin{pmatrix} 620 & 10 \\ 10\delta^2 & 620 \end{pmatrix}.$$

Let $b = QB \begin{pmatrix} s \\ t \end{pmatrix}$ and $x = \lambda \begin{pmatrix} s \\ t \end{pmatrix}$. Then (5) may be written $Bx = b$, which is solved by $x = B^{-1}b = S \begin{pmatrix} s \\ t \end{pmatrix}$. It follows (5) is implied by

$$S \begin{pmatrix} s \\ t \end{pmatrix} = \lambda \begin{pmatrix} s \\ t \end{pmatrix},$$

which is solved by

$$(s, t) = (1, \pm\delta).$$

Thus the corresponding eigenvectors of Q are $f \pm \delta g$. Let u_{\pm} be the unit vectors proportional to $f \pm \delta g$.

Since u_{\pm} correspond to distinct eigenvalues, they are orthogonal. Hence u_{\pm} form an orthonormal basis for the column space of A . From this, the eigenvalue decomposition of AA^t is

$$AA^t = \lambda_+ u_+ \otimes u_+ + \lambda_- u_- \otimes u_-.$$

Let

$$p = (-72, 11, 94, 177, 260), \quad q = (4, 3, 2, 1, 0).$$

Then, as before, one checks p, q span the row space of A .

Repeating the analysis with

$$Q = A^t A = \begin{pmatrix} 158 & 176 & 194 & 212 & 230 \\ 176 & 197 & 218 & 239 & 260 \\ 194 & 218 & 242 & 266 & 290 \\ 212 & 239 & 266 & 293 & 320 \\ 230 & 260 & 290 & 320 & 350 \end{pmatrix},$$

p, q replacing f, g , $C = (p, q)$, and $S = C^{-1}QC$, leads to the same nonzero eigenvalues and the two eigenvectors $p \pm \delta q$ of Q . Let v_{\pm} be the unit vectors proportional to $p \pm \delta q$. Then v_{\pm} form an orthonormal basis for the row space of A , and

$$A^t A = \lambda_+ v_+ \otimes v_+ + \lambda_- v_- \otimes v_-.$$

Let $\sigma_{\pm} = \sqrt{\lambda_{\pm}}$. From this, it follows the singular value decomposition of A is

$$A = \sigma_+ u_+ \otimes v_+ + \sigma_- u_- \otimes v_-.$$

PROOFS

The set of matrices with fixed shape is a euclidean vector space with dot product and norm squared

$$A \cdot B = \text{trace}(A^t B), \quad \|A\|^2 = A \cdot A.$$

Although everything works just as well for complex matrices, we assume throughout our matrices are real.

Let X_n be a sequence of matrices with fixed shape. We say $X_n \rightarrow \infty$ if $\|X_n\| \rightarrow \infty$. A scalar-valued function $f(X)$ is *proper* if

$$X_n \rightarrow \infty \implies f(X_n) \rightarrow +\infty.$$

If $f(X)$ is continuous and proper, a basic calculus result [2] guarantees the existence of an X^* satisfying $f(X^*) \leq f(X)$ for all X . Such an X^* is a *minimizer*.

Lemma 1. *Let A and B and X be matrices with compatible shapes, in the sense*

$$f(X) = \|AX - B\|^2$$

is well-defined. Then a minimizer X^ of $f(X)$ exists, and can be chosen to satisfy $P_r X^* = X^*$.*

Proof. We show $f(X) = \|AX - B\|^2$ is proper on the euclidean space \mathcal{E} of matrices X satisfying $P_r X = X$. Argue by contradiction. If $f(X)$ is not proper, there is a sequence of matrices X_n in \mathcal{E} , and $X_n \rightarrow \infty$ with $f(X_n)$ bounded, hence with $\|AX_n\| \leq c$ for some finite c . Let $r_n = \|X_n\|$ and $X'_n = X_n/r_n$. Since $\|X'_n\| = 1$, X'_n is a bounded sequence, hence a subsequence X'_n converges to some X' . By continuity, $\|X'\| = 1$ and $P_r X' = X'$. Since

$$\|AX'\| = \lim_{n \rightarrow \infty} \|AX'_n\| = \lim_{n \rightarrow \infty} \frac{\|AX_n\|}{r_n} \leq \lim_{n \rightarrow \infty} \frac{c}{r_n} = 0,$$

$AX' = 0$. Since the row and null spaces of A are orthogonal, $P_r X' = 0$, hence $X' = 0$, which contradicts $\|X'\| = 1$. Thus $f(X)$ has a minimizer X^* on \mathcal{E} . Since any X may be written as $X = P_r X + (I - P_r)X$, and $A(I - P_r)X = 0$, X^* is a minimizer on all matrices X with fixed shape, not just X in \mathcal{E} . \square

Lemma 2. *Let A be a matrix. A matrix X is a minimizer of $f(X) = \|AX - B\|^2$ iff $A^t AX = A^t B$. In particular, X is a minimizer of $f(X) = \|AX - I\|^2$ iff $AX = P_c$.*

Proof. Since $f(X)$ is quadratic, or by calculus, X is a minimizer iff $(AX - B) \cdot AV = 0$ for all V , which happens iff $A^t AX = A^t B$. Let $P = AX$. When $B = I$, this happens iff $A = P^t A$. Multiplying by X yields $P = P^t P$. It follows P satisfies $P^t = P$ and $P^2 = P$, hence P is a projection. Since $PA = A$, it follows $P = P_c$. \square

A minimizer X^* of $f(X) = \|AX - B\|^2$ is *least norm* if $\|X^*\| \leq \|X\|$ for all minimizers X of $f(X) = \|AX - B\|^2$.

Lemma 3. *A minimizer X^* for $\|AX - B\|^2$ is least norm iff $P_r X^* = X^*$, and there is at most one least norm minimizer of $\|AX - B\|^2$.*

Proof. From Lemma 2, if X_1 and X_2 are minimizers, then $A^tAX_1 = A^tAX_2$, hence $V = X_1 - X_2$ satisfies $A^tAV = 0$. Since the null spaces of A and A^tA agree, this happens iff $AV = 0$. Since the row and null spaces of A are orthogonal, this happens iff $P_rV = 0$. Thus X^* is a least norm minimizer iff $\|X^*\|^2 \leq \|X^* + V\|^2$ for all V satisfying $P_rV = 0$. Since $\|X^* + V\|^2$ is quadratic in V , or by calculus, X^* is least norm iff $X^* \cdot V = 0$ for all V satisfying $P_rV = 0$. Since the row and null spaces of A are orthogonal, this happens iff $P_rX^* = X^*$. If X_1 and X_2 are least norm minimizers, then $V = X_1 - X_2$ satisfies $P_rV = V$ and $P_rV = 0$, hence $V = 0$. This establishes uniqueness of the least norm minimizer for $\|AX - B\|^2$. \square

We conclude there is a unique least norm minimizer $X^-(B)$ of $\|AX - B\|^2$ corresponding to each B . Let $A_c = X^-(I)$ be the least norm minimizer of $\|AX - I\|^2$.

Lemma 4. *With A fixed, $X^-(B) = A_cB$ for all B .*

Proof. $X = A_c$ satisfies $A^tAX = A^t$ and the column space of X lies in the row space of A . Right-multiplying by B , $X = A_cB$ satisfies $A^tAX = A^tB$ and the column space of X lies in the row space of A . By uniqueness, $A_cB = X^-(B)$. \square

Lemma 5. *If X satisfies the Penrose axioms, then X satisfies (3).*

Proof. Assume X satisfies the Penrose axioms and let $P = AX$. Then **A** and **C** imply P is a projection. By definition, the column space of P lies in the column space of A . Conversely, since $A = AXA = PA$, the column space of A lies in the column space of P . Hence the column spaces agree, or $P = P_c$. This shows $AX = P_c$.

Similarly, **B** and **D** imply $P = XA$ is a projection, hence $P = A^tX^t$. Thus the column space of P lies in the column space of A^t . By **A**, $A^t = (AXA)^t = PA^t$, so the column space of A^t lies in the column space of P . Hence the column spaces agree. Since the column space of A^t equals the row space of A , $P = P_r$. This shows $XA = P_r$. \square

Lemma 6. *The matrix $X = A_c$ is the unique solution of the Penrose axioms. In particular, $X = A_c$ satisfies (3).*

Proof. We have to show A_c satisfies the axioms **A**, **B**, **C**, and **D**, and conversely. By Lemma 2, $AA_c = P_c$. Thus AA_c is symmetric and $AA_cA = P_cA = A$, yielding **A** and **C**.

For **B**, choose $B = AA_c$. Then $A_cB = A_cAA_c$ is the least norm minimizer of $f(X) = \|AX - B\|^2$, and A_c is trivially a minimizer, hence $V = A_c - A_cAA_c$ satisfies $P_rV = 0$. Since $P_rA_c = A_c$, we also have $P_rV = V$. Thus $V = 0$, yielding **B**.

Let $P = A_cA$. Then $P_rP = P$. By **A**, $A(I - P) = 0$, so $P_r(I - P) = 0$. This shows $P = P_r$, hence P is symmetric, obtaining **D**.

For the converse, suppose X satisfies **A**, **B**, **C**, and **D**. Then **A** and **C** imply $A^t(AX - I) = 0$, thus X is a minimizer of $f(X) = \|AX - I\|^2$. From Lemma 5, $X = XAX = P_rX$, so $P_rX = X$. This shows X is the least norm minimizer $X^-(I) = A_c$. \square

Lemma 7. *The least norm minimizer A_c of $\|AX - I\|^2$ equals the least norm minimizer of $\|XA - I\|^2$.*

Proof. By transposing, X is a minimizer of $\|XA - I\|^2$ iff X^t is a minimizer of $\|A^tX - I\|^2$. It follows X is a least norm minimizer of $\|XA - I\|^2$ iff X^t is a least norm minimizer of $\|A^tX - I\|^2$. From Lemma 6, it follows X is a least norm minimizer of $\|XA - I\|^2$ iff

- A. $A^tX^tA^t = A^t$,
- B. $X^tA^tX^t = X^t$,
- C. A^tX^t is symmetric,
- D. X^tA^t is symmetric.

But these are the Penrose axioms. By uniqueness, a least norm minimizer of $\|XA - I\|^2$ must equal A_c . \square

This establishes Theorems 1 and 2.

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