

# 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  $X$  satisfying either of the equations in (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.

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  $r = 2$ . 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

$$\begin{aligned} 50f &= 1776a + 985b + 194c - 597d - 1388e, \\ 50g &= -28a - 15b - 2c + 11d + 24e. \end{aligned}$$

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

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

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

$$\begin{aligned} 94a &= 11f + 597g, & 47b &= 6f + 347g, & 94c &= 13f + 791g, \\ 47d &= 7f + 444g, & 94e &= 15f + 985g. \end{aligned}$$

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  $\lambda$ .

To find  $\lambda$ , 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  $2 \times 2$  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  $p = (-72, 11, 94, 177, 260)$ ,  $q = (4, 3, 2, 1, 0)$ . Then, as before, one checks  $p, q$  span the row space of  $A$ . Repeating the analysis with

$$Q = A^t A = \begin{pmatrix} 158 & 176 & 194 & 212 & 230 \\ 176 & 197 & 218 & 239 & 260 \\ 194 & 218 & 242 & 266 & 290 \\ 212 & 239 & 266 & 293 & 320 \\ 230 & 260 & 290 & 320 & 350 \end{pmatrix}, \quad B = (p, q) = \begin{pmatrix} -72 & 4 \\ 11 & 3 \\ 94 & 2 \\ 177 & 1 \\ 260 & 0 \end{pmatrix},$$

and  $S = B^{-1}QB$ , 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  $\mathcal{E}$ .  $\square$

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

**Lemma 2.** *There is a unique least norm minimizer of  $\|AX - B\|^2$ , and  $X$  is the least norm minimizer of  $\|AX - B\|^2$  iff  $A^t A X = A^t B$  and  $P_r X = X$ . In particular,  $X$  is the least norm minimizer of  $\|AX - I\|^2$  iff  $AX = P_c$  and  $P_r X = X$ .*

*Proof.* If  $X_1$  and  $X_2$  are minimizers of  $\|AX - B\|^2$ , then  $V = X_1 - X_2$  satisfies  $A^t A V = 0$ . Since the null spaces of  $A$  and  $A^t A$  agree,  $V$  satisfies  $AV = 0$ .

By Lemma 1, a minimizer  $X$  of  $\|AX - B\|^2$  satisfying  $P_r X = X$  exists. If  $AV = 0$ , then  $P_r V = 0$ , so  $X \cdot V = P_r X \cdot V = X \cdot P_r V = 0$ . Hence  $\|X + V\|^2 = \|X\|^2 + \|V\|^2$  for all  $V$  satisfying  $AV = 0$ . Thus  $X$  is a least norm minimizer of  $\|AX - B\|^2$ .

If  $X_1$  and  $X_2$  are least norm minimizers of  $\|AX - B\|^2$ , then, as before,  $V = X_1 - X_2$  satisfies  $AV = 0$ , hence  $P_r V = 0$ . But  $P_r X_1 = X_1$  and  $P_r X_2 = X_2$ , so  $P_r V = V$ . Thus  $V = 0$ , establishing uniqueness.

Since  $\|AX - B\|^2$  is quadratic,  $X$  is a minimizer of  $\|AX - B\|^2$  iff  $(AX - B) \cdot AV = 0$  for all  $V$ , which happens iff  $A^t AX = A^t B$ .

Specializing to  $B = I$ , if  $X$  is a least norm minimizer of  $\|AX - I\|^2$ , then  $A^t AX = A^t$  and  $P_r X = X$ . If  $P = AX$ , this is equivalent to  $A = P^t A$  and  $P_r X = X$ . Multiplying the first equality by  $X$  yields  $P = P^t P$ . It follows  $P$  satisfies  $P^t = P$  and  $P^2 = P$ , hence  $P$  is a projection. From  $PA = A$ , it follows  $P = P_c$ . Conversely, if  $AX = P_c$ , then  $AXA = P_c A = A$ , so  $A^t = (AXA)^t = A^t(AX)$ , so  $X$  is a minimizer of  $\|AX - I\|^2$ .  $\square$

**Lemma 3.** *If  $X$  is the least norm minimizer of  $\|AX - I\|^2$ , then  $XB$  is the least norm minimizer of  $\|AX - B\|^2$ .*

*Proof.* If  $X$  is the least norm minimizer of  $\|AX - I\|^2$ , then  $A^t AX = A^t$  and  $P_r X = X$ . Right-multiplying by  $B$  yields  $A^t A(XB) = A^t B$  and  $P_r(XB) = XB$ , hence  $XB$  is the least norm minimizer of  $\|AX - B\|^2$ .  $\square$

**Lemma 4.**  *$X$  is the least norm minimizer of  $\|AX - I\|^2$  iff  $X$  satisfies the Penrose axioms.*

*Proof.* If  $X$  is the least norm minimizer of  $\|AX - I\|^2$ , by Lemma 2,  $AX = P_c$  and  $P_r X = X$ . Thus  $AXA = P_c A = A$ , yielding **A**. Since  $AX = P_c$  is symmetric, this yields **C**. From Lemma 3,  $XP_c$  is the least norm minimizer of  $\|AX - P_c\|^2$ . Since  $\|AX - I\|^2$  and  $\|AX - P_c\|^2$  differ by a constant, they have the same least norm minimizer, hence  $XP_c = X$ , or  $XAX = X$ , yielding **B**. Let  $P = XA$ . Then  $P_r P = P$ . By **A**,  $A(I - P) = 0$ , so  $P_r(I - P) = 0$ . This shows  $P = P_r$ , hence  $P$  is symmetric, obtaining **D**.

Conversely, assume  $X$  satisfies the Penrose axioms. Then **A** and **C** imply  $A^t AX = (AXA)^t = A^t$ , thus  $X$  is a minimizer of  $\|AX - I\|^2$ . If  $P = XA$ , **B** and **D** imply  $P$  is a projection, hence  $P = A^t X^t$ . 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  $A$ ,  $P = P_r$ , hence  $P_r X = PX = XAX = X$ . This shows  $X$  is the least norm minimizer of  $\|AX - I\|^2$ .  $\square$

**Lemma 5.** *The least norm minimizer of  $\|AX - I\|^2$  is the unique least norm minimizer of  $\|XA - I\|^2$ .*

*Proof.* Let  $X$  be the least norm minimizer of  $\|AX - I\|^2$ . Then  $X^t$  is a least norm minimizer of  $\|XA - I\|^2$ . Conversely, if  $X$  is a least norm minimizer of  $\|XA - I\|^2$ , then  $X^t$  is the least norm minimizer of  $\|A^t X - I\|^2$ . From Lemma 4, it follows  $X^t$  satisfies the Penrose axioms for  $A^t$ ,

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

Since this is equivalent to  $X$  satisfying the Penrose axioms for  $A$ , by Lemma 4 again,  $X$  is the least norm minimizer of  $\|AX - I\|^2$ .  $\square$

**Lemma 6.** *The least norm minimizer of  $\|AX - I\|^2$  equals the least norm solution of (3).*

*Proof.* As before,  $X$  is a least norm solution of (3) iff  $P_r X = X$ ,  $AX = P_c$ ,  $XP_c = X$ ,  $XA = P_r$ . Let  $X$  be the least norm minimizer of  $\|AX - I\|^2$ . From Lemma 2,  $AX = P_c$  and  $P_r X = X$ . Since  $X$  is also the least norm minimizer of  $\|XA - I\|^2$ ,  $X^t$  is the least norm minimizer of  $\|A^t X - I\|^2$ . Since the row and column space projections are interchanged by taking transpose, we have  $A^t X^t = P_r$  and  $P_c X^t = X^t$ . Hence  $XA = P_r$  and  $XP_c = X$ . Thus  $X$  is a least norm solution of (3). The steps are reversible, so the converse holds.  $\square$

This establishes Theorems 1 and 2.

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