THE PSEUDOINVERSE OF A MATRIX

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Introduction

The pseudoinverse of a matrix is widely used, and its numerical evaluation has been thoroughly studied over the years.

What is apparently lacking, in the typical undergraduate mathematics curriculum, is a clear and short presentation of its *conceptual inevitability*.

This note hopes to remedy this lapse. As the pseudoinverse has been studied for the better part of a century, the note's novelty, if any, is in the presentation.

Every (square or non-square) matrix has a pseudoinverse. The pseudoinverse, sometimes called a generalized inverse or Moore-Penrose inverse, is a natural extension of the inverse of a matrix.

The pseudoinverse of A is sometimes denoted A^+. 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

$$AX = I = XA. \tag{1}$$

Matrices are the same shape if they have the same number of rows and columns. When (1) happens, A, X, and I are the same shape.

The residuals are

$$\|AX - I\|^2 \qquad \text{and} \qquad \|XA - I\|^2. \tag{2}$$

These are scalar functions of X. The residuals are well-defined only if X and A^t are the same shape. 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 pseudoinverse is to seek a matrix X minimizing the residuals.

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

$$AX = P_c \qquad \text{and} \qquad XA = P_r.$$

This second approach suggests modifying the residuals to

$$\|AX - P_c\|^2 \qquad \text{and} \qquad \|XA - P_r\|^2, \tag{3}$$

yielding a third approach. In fact, using $P_cA = A$ and $AP_r = A$, it is easy to check that the residuals (3) differ from the residuals (2) by constants.

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A solution X_0 of $f(X) = 0$ is *least norm* if $\|X_0\| \le \|X\|$ for all solutions X of $f(X) = 0$. A minimizer X_0 of $f(X)$ is *least norm* if $\|X_0\| \le \|X\|$ for all minimizers X of $f(X)$.

The *pseudoinverse* A^- of A is the matrix X in the following Theorem. In particular, A^- and A^t are the same shape.

Theorem. *There is a unique least norm solution of $AX = P_c$, a unique least norm solution of $XA = P_r$, a unique least norm minimizer of $\|AX - I\|^2$, a unique least norm minimizer of $\|XA - I\|^2$, a unique solution of the Penrose axioms*

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

and the five matrices are equal.

Immediate consequences are $(A^-)^t = (A^t)^-$, 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 $U^- = U^t$.

Corollary. *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.

Corollary. *$P_c = AA^-$ and $P_r = A^-A$.*

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

Let u, v, w be vectors. The dot product is denoted $v \cdot w$, and 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 $v_1, v_2, \ldots, v_r$ are orthonormal vectors and $\lambda_1, \lambda_2, \ldots, \lambda_r$ are nonzero.

Corollary. *The pseudoinverse 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 $u_1, u_2, \ldots, u_r$ and $v_1, v_2, \ldots, v_r$ are orthonormal vectors, and $\sigma_1, \sigma_2, \ldots, \sigma_r$ are positive.

Corollary. *The pseudoinverse of A is*

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

This result is the basis for a common numerical evaluation of A^-.

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

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

All computations are done using the Python library `numpy`.

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

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

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

$$f = t_1 a + t_2 b + t_3 c + t_4 d + t_5 e.$$

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

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

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 λ.

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

$$Q(sf + tg) = \lambda(sf + tg). \tag{4}$$

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

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

To solve for (s,t), let

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

Let $b = QB\begin{pmatrix} s \\ t \end{pmatrix}$ and $x = \lambda\begin{pmatrix} s \\ t \end{pmatrix}$. Then (4) may be written $Bx = b$, which is solved by $x = B^- b = S\begin{pmatrix} s \\ t \end{pmatrix}$. It follows (4) 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, using A^t instead of A, one checks p, q span the row space of A. Repeating the analysis with

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

and $S = B^- QB$, leads to the same S, 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

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

Proof of the Theorem

The proof is presented as a series of Lemmas, some of whose proofs are left to the reader. The euclidean space $\mathbf{R}^{N\times d}$ is the set of real matrices X with N rows and d columns. The dot product and norm squared in $\mathbf{R}^{N\times d}$ are

$$X \cdot Y = \operatorname{trace}(X^t Y), \qquad \|X\|^2 = X \cdot X.$$

If X is in $\mathbf{R}^{N\times d}$, then X^t is in $\mathbf{R}^{d\times N}$, and $\|X\|^2 = \|X^t\|^2$. Let A be in $\mathbf{R}^{d\times N}$ and let B be in $\mathbf{R}^{d\times d}$. Then $AX - B$ is in $\mathbf{R}^{d\times d}$.

Since the row and null spaces of A are orthogonal, $AV = 0$ iff $P_r V = 0$. Since $V \cdot A^t AV = AV \cdot AV = \|AV\|^2$, $AV = 0$ iff $A^t AV = 0$.

Lemma 1. *$\|X\|^2 \le \|X + V\|^2$ for all V in $\mathbf{R}^{N\times d}$ satisfying $AV = 0$ iff $P_r X = X$.*

Let $f(X)$ be a scalar function defined on a euclidean space $\mathcal{E}$ of matrices. If X_0 in $\mathcal{E}$ satisfies $f(X_0) \le f(X)$ for all X in $\mathcal{E}$, then X_0 is a *minimizer of $f(X)$ on $\mathcal{E}$.*

A function $f(X)$ is *proper on $\mathcal{E}$* if for every sequence X_n in $\mathcal{E}$,

$$\|X_n\| \to \infty \qquad \Longrightarrow \qquad f(X_n) \to +\infty.$$

If $f(X)$ is continuous and proper on $\mathcal{E}$, a basic calculus result [1] guarantees the existence of a minimizer of $f(X)$ on $\mathcal{E}$. When $\mathcal{E}$ is not specified, $\mathcal{E} = \mathbf{R}^{N\times d}$.

Lemma 2. *There is a minimizer X_0 of $\|AX - B\|^2$ satisfying $P_r X_0 = X_0$.*

Proof. Let $\mathcal{E}$ be the subspace of $\mathbf{R}^{N\times d}$ of matrices X satisfying $P_r X = X$. We show $f(X) = \|AX - B\|^2$ is proper on $\mathcal{E}$, arguing by contradiction.

If $f(X)$ is not proper on $\mathcal{E}$, there is a sequence of matrices X_n in $\mathcal{E}$ with $f(X_n)$ bounded and $X_n \to \infty$, hence with $\|AX_n\| \le c$ 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

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

$AX' = 0$, hence $P_r X' = 0$, hence $X' = 0$, which contradicts $\|X'\| = 1$.

Thus there is a minimizer X_0 of $f(X)$ on $\mathcal{E}$. For X in $\mathbf{R}^{N\times d}$, $P_r X$ is in $\mathcal{E}$, and $f(X) = f(P_r X)$, hence X_0 is a minimizer of $f(X)$. □

Lemma 3. *There is a unique least norm minimizer X of $\|AX - B\|^2$, and the least norm minimizer X of $\|AX - B\|^2$ equals the unique solution of the pair $A^t AX = A^t B$, $P_r X = X$.*

Proof. Since $f(X) = \|AX - B\|^2$ is convex, X is a minimizer of $f(X)$ iff the derivative of $f(X + tV)$ at $t = 0$ vanishes for all V. Writing this out, $(AX - B) \cdot AV = 0$ for all V, which happens iff $A^t AX = A^t B$.

By Lemma 2, there is a minimizer X satisfying $P_r X = X$. By Lemma 1, a minimizer X is least norm iff $P_r X = X$, hence there is a least norm minimizer.

If X and X_0 are minimizers, then $V = X - X_0$ satisfies $A^t AV = 0$, hence $P_r V = 0$. If X and X_0 are least norm minimizers, then $P_r V = V$, so $V = 0$. This establishes the uniqueness of the least norm minimizer.

Since the steps are reversible, the solution of the pair $A^t AX = A^t B$, $P_r X = X$ is unique. □

Lemma 4. *If X_0 is the least norm minimizer of $\|AX - I\|^2$, then $X_0 B$ is the least norm minimizer of $\|AX - B\|^2$.*

Lemma 5. *The least norm minimizer X of $\|AX - I\|^2$ equals the unique least norm solution of $AX = P_c$.*

Proof. X is a least norm solution of $AX = P_c$ iff X is a solution of the pair $AX = P_c$, $P_r X = X$, so it is enough to show $A^t AX = A^t$ iff $AX = P_c$.

If $P = AX$ and $A^t AX = A^t$, then $A = P^t A$. Right-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 $A = PA$ and $P = AX$, $P = P_c$, hence $AX = P_c$. Conversely, if $AX = P_c$, then $AXA = P_c A = A$, so $A^t(AX) = (AXA)^t = A^t$. □

Lemma 6. *There is a unique least norm minimizer X of $\|XA - I\|^2$, and the least norm minimizer X of $\|XA - I\|^2$ equals the unique least norm solution of $XA = P_r$.*

Proof. Use Lemma 5 with $\|XA - I\|^2 = \|A^t X^t - I\|^2$. □

Lemma 7. *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 $\|AX - I\|^2$, then $AX = P_c$. Thus $AXA = P_c A = A$, yielding **A**. Since P_c is symmetric, we also have **C**. From Lemma 4, 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, their minimizers agree, hence they have the same least norm minimizer. This shows $XP_c = X$, or $XAX = X$, yielding **B**. Let $P = XA$. Since $P_r X = X$, $P_r P = P$. 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 $A^t AX = (AXA)^t = A^t$, hence X is a minimizer of $\|AX - I\|^2$. If $P = XA$, **B** and **D** imply P is a projection, hence $P = A^t X^t$. By **A**, $A^t = (AXA)^t = PA^t$. Since $P = A^t X^t$ and $A^t = PA^t$, the column spaces of P and A^t agree, hence the column space of P equals the row space of A. Thus $P = P_r$, hence $P_r X = PX = XAX = X$. Hence X is the least norm minimizer of $\|AX - I\|^2$. □

Lemma 8. *The least norm minimizer of $\|XA - I\|^2$ equals the least norm minimizer of $\|AX - I\|^2$.*

Proof. Note X^t satisfies the Penrose axioms for A^t iff X satisfies the Penrose axioms for A. Now use $\|XA - I\|^2 = \|A^t X^t - I\|^2$ and Lemma 7. □

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