

Moore–Penrose pseudoinverse

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In mathematics, and in particular linear algebra, a **pseudoinverse** A^+ of a matrix A is a generalization of the inverse matrix.^[1] The most widely known type of matrix pseudoinverse is the **Moore–Penrose pseudoinverse**, which was independently described by E. H. Moore^[2] in 1920, Arne Bjerhammar^[3] in 1951, and Roger Penrose^[4] in 1955. Earlier, Erik Ivar Fredholm had introduced the concept of a pseudoinverse of integral operators in 1903. When referring to a matrix, the term pseudoinverse, without further specification, is often used to indicate the Moore–Penrose pseudoinverse. The term generalized inverse is sometimes used as a synonym for pseudoinverse.

A common use of the pseudoinverse is to compute a 'best fit' (least squares) solution to a system of linear equations that lacks a unique solution (see below under § Applications). Another use is to find the minimum (Euclidean) norm solution to a system of linear equations with multiple solutions. The pseudoinverse facilitates the statement and proof of results in linear algebra.

The pseudoinverse is defined and unique for all matrices whose entries are real or complex numbers. It can be computed using the singular value decomposition.

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Notation

In the following discussion, the following conventions are adopted.

- K will denote one of the fields of real or complex numbers, denoted \mathbb{R} , \mathbb{C} , respectively. The vector space of $m \times n$ matrices over K is denoted by $M(m, n; K)$.
- For $A \in M(m, n; K)$, A^T and A^* denote the transpose and Hermitian transpose (also called conjugate transpose) respectively. If $K = \mathbb{R}$, then $A^* = A^T$.
- For $A \in M(m, n; K)$, then $\text{im}(A)$ denotes the range (image) of A (the space spanned by the column vectors of A) and $\text{ker}(A)$ denotes the kernel (null space) of A .
- Finally, for any positive integer n , $I_n \in M(n, n; K)$ denotes the $n \times n$ identity matrix.

Definition

For $A \in M(m, n; K)$, a pseudoinverse of A is defined as a matrix $A^+ \in M(n, m; K)$ satisfying all of the following four criteria:^{[4][5]}

1. $AA^+A = A$ (AA^+ need not be the general identity matrix, but it maps all column vectors of A to themselves);
2. $A^+AA^+ = A^+$ (A^+ is a weak inverse for the multiplicative semigroup);
3. $(AA^+)^* = AA^+$ (AA^+ is Hermitian); and
4. $(A^+A)^* = A^+A$ (A^+A is also Hermitian).

A^+ exists for any matrix A , but when the latter has full rank, A^+ can be expressed as a simple algebraic formula.

In particular, when A has linearly independent columns (and thus matrix A^*A is invertible), A^+ can be computed as:

$$A^+ = (A^*A)^{-1}A^*.$$

This particular pseudoinverse constitutes a *left inverse*, since, in this case, $A^+A = I$.

When A has linearly independent rows (matrix AA^* is invertible), A^+ can be computed as:

$$A^+ = A^*(AA^*)^{-1}.$$

This is a *right inverse*, as $AA^+ = I$.

Properties

Proofs for some of these facts may be found on a separate page Proofs involving the Moore–Penrose pseudoinverse.

Existence and uniqueness

- The pseudoinverse exists and is unique: for any matrix \mathbf{A} , there is precisely one matrix \mathbf{A}^+ , that satisfies the four properties of the definition.^[5]

A matrix satisfying the first condition of the definition is known as a generalized inverse. If the matrix also satisfies the second definition, it is called a generalized *reflexive* inverse. Generalized inverses always exist but are not in general unique. Uniqueness is a consequence of the last two conditions.

Basic properties

- If \mathbf{A} has real entries, then so does \mathbf{A}^+ .
- If \mathbf{A} is invertible, its pseudoinverse is its inverse. That is: $\mathbf{A}^+ = \mathbf{A}^{-1}$.^{[6]:243}
- The pseudoinverse of a zero matrix is its transpose.
- The pseudoinverse of the pseudoinverse is the original matrix: $(\mathbf{A}^+)^+ = \mathbf{A}$.^{[6]:245}
- Pseudoinversion commutes with transposition, conjugation, and taking the conjugate transpose:^{[6]:245}

$$(\mathbf{A}^T)^+ = (\mathbf{A}^+)^T, \quad (\overline{\mathbf{A}})^+ = \overline{\mathbf{A}^+}, \quad (\mathbf{A}^*)^+ = (\mathbf{A}^+)^*.$$

- The pseudoinverse of a scalar multiple of \mathbf{A} is the reciprocal multiple of \mathbf{A}^+ :

$$(\alpha \mathbf{A})^+ = \alpha^{-1} \mathbf{A}^+ \text{ for } \alpha \neq 0.$$

Identities

The following identities can be used to cancel certain subexpressions or expand expressions involving pseudoinverses. Proofs for these properties can be found in the proofs subpage.

$$\begin{array}{lcl} \mathbf{A}^+ & = & \mathbf{A}^+ \mathbf{A}^+ \mathbf{A}^* \mathbf{A}^* \\ \mathbf{A}^+ & = & \mathbf{A}^* \mathbf{A}^+ \mathbf{A}^* \mathbf{A}^+ \\ \mathbf{A} & = & \mathbf{A}^+ \mathbf{A}^* \mathbf{A} \\ \mathbf{A} & = & \mathbf{A} \mathbf{A}^* \mathbf{A}^+ \\ \mathbf{A}^* & = & \mathbf{A}^* \mathbf{A} \mathbf{A}^+ \\ \mathbf{A}^* & = & \mathbf{A}^+ \mathbf{A} \mathbf{A}^* \end{array}$$

Reduction to Hermitian case

The computation of the pseudoinverse is reducible to its construction in the Hermitian case. This is possible through the equivalences:

- $\mathbf{A}^+ = (\mathbf{A}^* \mathbf{A})^+ \mathbf{A}^*$
- $\mathbf{A}^+ = \mathbf{A}^* (\mathbf{A} \mathbf{A}^*)^+$

as $\mathbf{A}^* \mathbf{A}$ and $\mathbf{A} \mathbf{A}^*$ are Hermitian.

Products

If $A \in M(m, n; K)$, $B \in M(n, p; K)$ and either,

- A has orthonormal columns (i.e., $A^* A = I_n$) or,
- B has orthonormal rows (i.e., $BB^* = I_n$) or,
- A has all columns linearly independent (full column rank) and B has all rows linearly independent (full row rank) or,
- $B = A^*$ (i.e., B is the conjugate transpose of A),

then

$$(AB)^+ \equiv B^+ A^+.$$

The last property yields the equivalences:

$$\begin{aligned} (AA^*)^+ &\equiv A^{+*} A^+ \\ (A^* A)^+ &\equiv A^+ A^{+*} \end{aligned}$$

Projectors

$P = AA^+$ and $Q = A^+ A$ are orthogonal projection operators – that is, they are Hermitian ($P = P^*$, $Q = Q^*$) and idempotent ($P^2 = P$ and $Q^2 = Q$). The following hold:

- $PA = AQ = A$ and $A^+ P = QA^+ = A^+$
- P is the orthogonal projector onto the range of A (which equals the orthogonal complement of the kernel of A^*).
- Q is the orthogonal projector onto the range of A^* (which equals the orthogonal complement of the kernel of A).
- $(I - Q) = (I - A^+ A)$ is the orthogonal projector onto the kernel of A .
- $(I - P) = (I - AA^+)$ is the orthogonal projector onto the kernel of A^* .^[5]

The last two properties imply the following identities:

- $A(I - A^+ A) = (I - AA^+)A = 0$
- $A^*(I - AA^+) = (I - A^+ A)A^* = 0$

Another property is the following: if $A \in R^{n \times n}$ is Hermitian and idempotent (true if and only if it represents an orthogonal projection), then, for any matrix $B \in R^{m \times n}$ the following equation holds:^[7]

$$A(BA)^+ = (BA)^+$$

This can be proven by defining matrices $C = BA$, $D = A(BA)^+$, and checking that D is indeed a pseudoinverse for C by verifying that the defining properties of the pseudoinverse hold, when A is Hermitian and idempotent.

From the last property it follows that, if $A \in R^{n \times n}$ is Hermitian and idempotent, for any matrix $B \in R^{n \times m}$

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

Finally, it should be noted that if A is an orthogonal projection matrix, then its pseudoinverse trivially coincides with the matrix itself, i.e. $A^+ = A$.

Geometric construction

If we view the matrix as a linear map $A : K^n \rightarrow K^m$ over a field K then $A^+ : K^m \rightarrow K^n$ can be decomposed as follows. We write \oplus for the direct sum, \perp for the orthogonal complement, \ker for the kernel of a map, and ran for the image of a map. Notice that $K^n = (\ker A)^\perp \oplus \ker A$ and $K^m = \text{ran } A \oplus (\text{ran } A)^\perp$. The restriction $A : (\ker A)^\perp \rightarrow \text{ran } A$ is then an isomorphism. These imply that A^+ is defined on $\text{ran } A$ to be the inverse of this isomorphism, and on $(\text{ran } A)^\perp$ to be zero.

In other words: To find A^+b for given b in K^m , first project b orthogonally onto the range of A , finding a point $p(b)$ in the range. Then form $A^{-1}(\{p(b)\})$, i.e. find those vectors in K^n that A sends to $p(b)$. This will be an affine subspace of K^n parallel to the kernel of A . The element of this subspace that has the smallest length (i.e. is closest to the origin) is the answer A^+b we are looking for. It can be found by taking an arbitrary member of $A^{-1}(\{p(b)\})$ and projecting it orthogonally onto the orthogonal complement of the kernel of A .

This description is closely related to the Minimum norm solution to a linear system.

Subspaces

$$\ker(A^+) = \ker(A^*)$$

$$\text{ran}(A^+) = \text{ran}(A^*)$$

Limit relations

- The pseudoinverse are limits:

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

(see Tikhonov regularization). These limits exist even if $(A A^*)^{-1}$ or $(A^* A)^{-1}$ do not exist.^{[5]:263}

Continuity

- In contrast to ordinary matrix inversion, the process of taking pseudoinverses is not continuous: if the sequence (A_n) converges to the matrix A (in the maximum norm or Frobenius norm, say), then $(A_n)^+$ need not converge to A^+ . However, if all the matrices have the same rank, $(A_n)^+$ will converge to A^+ .^[8]

Derivative

The derivative of a real valued pseudoinverse matrix which has constant rank at a point x may be calculated in terms of the derivative of the original matrix:^[9]

$$\frac{d}{dx} A^+(x) = -A^+ \left(\frac{d}{dx} A \right) A^+ + A^+ A^{+T} \left(\frac{d}{dx} A^T \right) (I - A A^+) + (I - A^+ A) \left(\frac{d}{dx} A^T \right) A^{+T} A^+$$

Special cases

Scalars

It is also possible to define a pseudoinverse for scalars and vectors. This amounts to treating these as matrices. The pseudoinverse of a scalar x is zero if x is zero and the reciprocal of x otherwise:

$$x^+ = \begin{cases} 0, & \text{if } x = 0; \\ x^{-1}, & \text{otherwise.} \end{cases}$$

Vectors

The pseudoinverse of the null (all zero) vector is the transposed null vector. The pseudoinverse of a non-null vector is the conjugate transposed vector divided by its squared magnitude:

$$x^+ = \begin{cases} 0^T, & \text{if } x = 0; \\ \frac{x^*}{x^*x}, & \text{otherwise.} \end{cases}$$

Linearly independent columns

If the **columns** of \mathbf{A} are linearly independent (so that $m \geq n$), then $\mathbf{A}^* \mathbf{A}$ is invertible. In this case, an explicit formula is:^[1]

$$\mathbf{A}^+ = (\mathbf{A}^* \mathbf{A})^{-1} \mathbf{A}^*.$$

It follows that \mathbf{A}^+ is then a left inverse of \mathbf{A} : $\mathbf{A}^+ \mathbf{A} = \mathbf{I}_n$.

Linearly independent rows

If the **rows** of \mathbf{A} are linearly independent (so that $m \leq n$), then $\mathbf{A} \mathbf{A}^*$ is invertible. In this case, an explicit formula is:

$$\mathbf{A}^+ = \mathbf{A}^* (\mathbf{A} \mathbf{A}^*)^{-1}.$$

It follows that \mathbf{A}^+ is a right inverse of \mathbf{A} : $\mathbf{A} \mathbf{A}^+ = \mathbf{I}_m$.

Orthonormal columns or rows

This is a special case of either full column rank or full row rank (treated above). If \mathbf{A} has orthonormal columns ($\mathbf{A}^* \mathbf{A} = \mathbf{I}_n$) or orthonormal rows ($\mathbf{A} \mathbf{A}^* = \mathbf{I}_m$), then:

$$\mathbf{A}^+ = \mathbf{A}^*.$$

Orthogonal projection matrices

If \mathbf{A} is an orthogonal projection matrix, i.e. $\mathbf{A} = \mathbf{A}^*$ and $\mathbf{A}^2 = \mathbf{A}$, then the pseudoinverse trivially coincides with the matrix itself:

$$\mathbf{A}^+ = \mathbf{A}.$$

Circulant matrices

For a circulant matrix \mathbf{C} , the singular value decomposition is given by the Fourier transform, that is the singular values are the Fourier coefficients. Let \mathcal{F} be the Discrete Fourier Transform (DFT) matrix, then^[10]

$$\begin{aligned} \mathbf{C} &= \mathcal{F} \cdot \Sigma \cdot \mathcal{F}^* \\ \mathbf{C}^+ &= \mathcal{F} \cdot \Sigma^+ \cdot \mathcal{F}^* \end{aligned}$$

Construction

Rank decomposition

Let $r \leq \min(m, n)$ denote the rank of $A \in M(m, n; K)$. Then A can be (rank) decomposed as $A = BC$ where $B \in M(m, r; K)$ and $C \in M(r, n; K)$ are of rank r . Then $A^+ = C^+ B^+ = C^*(CC^*)^{-1}(B^*B)^{-1}B^*$.

The QR method

For $K = \mathbb{R}$ or $K = \mathbb{C}$ computing the product AA^* or A^*A and their inverses explicitly is often a source of numerical rounding errors and computational cost in practice. An alternative approach using the QR decomposition of A may be used instead.

Consider the case when A is of full column rank, so that $A^+ = (A^*A)^{-1}A^*$. Then the Cholesky decomposition $A^*A = R^*R$, where R is an upper triangular matrix, may be used. Multiplication by the inverse is then done easily by solving a system with multiple right-hand sides,

$$A^+ = (A^*A)^{-1}A^* \Leftrightarrow (A^*A)A^+ = A^* \Leftrightarrow R^*RA^+ = A^*$$

which may be solved by forward substitution followed by back substitution.

The Cholesky decomposition may be computed without forming A^*A explicitly, by alternatively using the QR decomposition of $A = QR$, where Q has orthonormal columns, $Q^*Q = I$, and R is upper triangular. Then

$$A^*A = (QR)^*(QR) = R^*Q^*QR = R^*R,$$

so R is the Cholesky factor of A^*A .

The case of full row rank is treated similarly by using the formula $A^+ = A^*(AA^*)^{-1}$ and using a similar argument, swapping the roles of A and A^* .

Singular value decomposition (SVD)

A computationally simple and accurate way to compute the pseudo inverse is by using the singular value decomposition.^{[1][5][11]} If $A = U\Sigma V^*$ is the singular value decomposition of A , then $A^+ = V\Sigma^+U^*$. For a rectangular diagonal matrix such as Σ , we get the pseudo inverse by taking the reciprocal of each non-zero element on the diagonal, leaving the zeros in place, and then transposing the matrix. In numerical computation, only elements larger than some small tolerance are taken to be nonzero, and the others are replaced by zeros. For example, in the MATLAB, GNU Octave, or NumPy function `pinv`, the tolerance is taken to be $t = \varepsilon \cdot \max(m, n) \cdot \max(\Sigma)$, where ε is the machine epsilon.

The computational cost of this method is dominated by the cost of computing the SVD, which is several times higher than matrix–matrix multiplication, even if a state-of-the art implementation (such as that of LAPACK) is used.

The above procedure shows why taking the pseudo inverse is not a continuous operation: if the original matrix A has a singular value 0 (a diagonal entry of the matrix Σ above), then modifying A slightly may turn this zero into a tiny positive number, thereby affecting the pseudo inverse dramatically as we now have to take the reciprocal of a tiny number.

Block matrices

Optimized approaches exist for calculating the pseudoinverse of block structured matrices.

The iterative method of Ben-Israel and Cohen

Another method for computing the pseudoinverse (cf. Drazin inverse) uses the recursion

$$\mathbf{A}_{i+1} = 2\mathbf{A}_i - \mathbf{A}_i \mathbf{A} \mathbf{A}_i,$$

which is sometimes referred to as hyper-power sequence. This recursion produces a sequence converging quadratically to the pseudoinverse of \mathbf{A} if it is started with an appropriate \mathbf{A}_0 satisfying $\mathbf{A}_0 \mathbf{A} = (\mathbf{A}_0 \mathbf{A})^*$. The choice $\mathbf{A}_0 = \alpha \mathbf{A}^*$ (where $0 < \alpha < 2/\sigma_1^2(\mathbf{A})$, with $\sigma_1(\mathbf{A})$ denoting the largest singular value of \mathbf{A})^[12] has been argued not to be competitive to the method using the SVD mentioned above, because even for moderately ill-conditioned matrices it takes a long time before \mathbf{A}_i enters the region of quadratic convergence.^[13] However, if started with \mathbf{A}_0 already close to the Moore–Penrose pseudoinverse and $\mathbf{A}_0 \mathbf{A} = (\mathbf{A}_0 \mathbf{A})^*$, for example $\mathbf{A}_0 := (\mathbf{A}^* \mathbf{A} + \delta \mathbf{I})^{-1} \mathbf{A}^*$, convergence is fast (quadratic).

Updating the pseudoinverse

For the cases where \mathbf{A} has full row or column rank, and the inverse of the correlation matrix ($\mathbf{A} \mathbf{A}^*$ for \mathbf{A} with full row rank or $\mathbf{A}^* \mathbf{A}$ for full column rank) is already known, the pseudoinverse for matrices related to \mathbf{A} can be computed by applying the Sherman–Morrison–Woodbury formula to update the inverse of the correlation matrix, which may need less work. In particular, if the related matrix differs from the original one by only a changed, added or deleted row or column, incremental algorithms^{[14][15]} exist that exploit the relationship.

Similarly, it is possible to update the Cholesky factor when a row or column is added, without creating the inverse of the correlation matrix explicitly. However, updating the pseudoinverse in the general rank-deficient case is much more complicated.^{[16][17]}

Software libraries

The Python package NumPy provides a pseudoinverse calculation through its functions `matrix.I` and `linalg.pinv`; its `pinv` uses the SVD-based algorithm. SciPy adds a function `scipy.linalg.pinv` that uses a least-squares solver. High quality implementations of SVD, QR, and back substitution are available in standard libraries, such as LAPACK. Writing one's own implementation of SVD is a major programming project that requires a significant numerical expertise. In special circumstances, such as parallel computing or embedded computing, however, alternative implementations by QR or even the use of an explicit inverse might be preferable, and custom implementations may be unavoidable.

The MASS package for R provides a calculation of the Moore–Penrose pseudoinverse through the `ginv` function.^[18] The `ginv` function calculates a pseudoinverse using the singular value decomposition provided by the `svd` function in the base R package.

The Octave programming language provides a pseudo inverse through the standard package function `pinv` as well as the `pseudo_inverse()` method.

Applications

Linear least-squares

The pseudoinverse provides a least squares solution to a system of linear equations.^[19] For $A \in \mathbf{M}(m, n; K)$, given a system of linear equations

$$Ax = b,$$

in general, a vector x that solves the system may not exist, or if one does exist, it may not be unique. The pseudoinverse solves the "least-squares" problem as follows:

- $\forall x \in K^n$, we have $\|Ax - b\|_2 \geq \|Az - b\|_2$ where $z = A^+b$ and $\|\cdot\|_2$ denotes the Euclidean norm. This weak inequality holds with equality if and only if $x = A^+b + (I - A^+A)w$ for any vector w ; this provides an infinitude of minimizing solutions unless A has full column rank, in which case $(I - A^+A)$ is a zero matrix.^[20] The solution with minimum Euclidean norm is z .^[20]

This result is easily extended to systems with multiple right-hand sides, when the Euclidean norm is replaced by the Frobenius norm. Let $B \in \mathbf{M}(m, p; K)$.

- $\forall X \in \mathbf{M}(n, p; K)$, we have $\|AX - B\|_F \geq \|AZ - B\|_F$ where $Z = A^+B$ and $\|\cdot\|_F$ denotes the Frobenius norm.

Obtaining all solutions of a linear system

If the linear system

$$Ax = b$$

has any solutions, they are all given by^[21]

$$x = A^+b + [I - A^+A]w$$

for arbitrary vector w . Solution(s) exist if and only if $AA^+b = b$.^[21] If the latter holds, then the solution is unique if and only if A has full column rank, in which case $[I - A^+A]$ is a zero matrix. If solutions exist but A does not have full column rank, then we have an indeterminate system, all of whose infinitude of solutions are given by this last equation. This solution is deeply connected to the Udwadia–Kalaba equation of classical mechanics to forces of constraint that do not obey D'Alembert's principle.

Minimum norm solution to a linear system

For linear systems $Ax = b$, with non-unique solutions (such as under-determined systems), the pseudoinverse may be used to construct the solution of minimum Euclidean norm $\|x\|_2$ among all solutions.

- If $Ax = b$ is satisfiable, the vector $z = A^+b$ is a solution, and satisfies $\|z\|_2 \leq \|x\|_2$ for all solutions.

This result is easily extended to systems with multiple right-hand sides, when the Euclidean norm is replaced by the Frobenius norm. Let $B \in \mathbf{M}(m, p; K)$.

- If $AX = B$ is satisfiable, the matrix $Z = A^+B$ is a solution, and satisfies $\|Z\|_F \leq \|X\|_F$ for all solutions.

Condition number

Using the pseudoinverse and a matrix norm, one can define a condition number for any matrix:

$$\text{cond}(A) = \|A\| \|A^+\|.$$

A large condition number implies that the problem of finding least-squares solutions to the corresponding system of linear equations is ill-conditioned in the sense that small errors in the entries of A can lead to huge errors in the entries of the solution.^[22]

Generalizations

In order to solve more general least-squares problems, one can define Moore–Penrose pseudoinverses for all continuous linear operators $A : H_1 \rightarrow H_2$ between two Hilbert spaces H_1 and H_2 , using the same four conditions as in our definition above. It turns out that not every continuous linear operator has a continuous linear pseudoinverse in this sense.^[22] Those that do are precisely the ones whose range is closed in H_2 .

In abstract algebra, a Moore–Penrose pseudoinverse may be defined on a *-regular semigroup. This abstract definition coincides with the one in linear algebra.

See also

- Proofs involving the Moore–Penrose pseudoinverse
- Drazin inverse
- Hat matrix
- Inverse element
- Linear least squares (mathematics)
- Pseudo-determinant
- Von Neumann regular ring

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External links

- Pseudoinverse on PlanetMath (<http://planetmath.org/Pseudoinverse>)
- Interactive program & tutorial of Moore–Penrose Pseudoinverse (<http://people.revoledu.com/kardi/tutorial/LinearAlgebra/MatrixGeneralizedInverse.html>)
- "Moore–Penrose inverse" (<http://planetmath.org/?op=getobj&from=objects&id=6067>). *PlanetMath*.
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- Weisstein, Eric W. "Moore–Penrose Inverse" (<http://mathworld.wolfram.com/Moore-PenroseMatrixInverse.html>). *MathWorld*.
- The Moore–Penrose Pseudoinverse. A Tutorial Review of the Theory (<http://arxiv.org/abs/1110.6882>)
- Online Moore-Penrose Inverse calculator (http://engineerjs.com/doc/ejs/engine/linalg-1/_pinv.html)

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