San José State University

Math 253: Mathematical Methods for Data Visualization

Lecture 6: Generalized inverse and pseudoinverse

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Outline

- Matrix generalized inverse
- Pseudoinverse
- Application to solving linear systems of equations

Recall

... that a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **invertible** if there exists a square matrix $\mathbf{B}$ of the same size such that

$$\mathbf{AB} = \mathbf{BA} = \mathbf{I}$$

In this case, $\mathbf{B}$ is called the matrix inverse of $\mathbf{A}$ and denoted as $\mathbf{B} = \mathbf{A}^{-1}$.

We already know that two equivalent ways of characterizing a square, invertible matrix $\mathbf{A}$ are

- $\mathbf{A}$ **has full rank**, i.e., $\mathrm{rank}(\mathbf{A}) = n$
- $\mathbf{A}$ **has nonzero determinant**: $\det(\mathbf{A}) \neq 0$

Remark. For any invertible matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ and any vector $\mathbf{b} \in \mathbb{R}^n$, the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ has a unique solution $\mathbf{x}^* = \mathbf{A}^{-1}\mathbf{b}$.

MATLAB command for solving a linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$

$A\backslash b$ % recommended

$inv(A) * b$ % avoid (especially when $\mathbf{A}$ is large)

What about general matrices?

Let $\mathbf{A} \in \mathbb{R}^{m\times n}$. We would like to address the following questions:

- Is there some kind of inverse?
- Given a vector $\mathbf{b} \in \mathbb{R}^m$, how can we solve the linear system $\mathbf{Ax} = \mathbf{b}$?

More motivation

In many practical tasks such as multiple linear regression, the least squares problem arises naturally:

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{A}\mathbf{x}-\mathbf{b}\|^2 \qquad (\text{where } \mathbf{A}\in\mathbb{R}^{m\times n}, \mathbf{b}\in\mathbb{R}^m \text{ are fixed})$$

If $\mathbf{A}$ has full column rank (i.e., $\operatorname{rank}(\mathbf{A}) = n \le m$), then the above problem has a unique solution

$$\mathbf{x}^* = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$$

We want to better understand the matrices:

- $(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$ (pseudoinverse): Optimal solution is $\mathbf{x}^* = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$;
- $\mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$ (projection matrix): Closest approximation of $\mathbf{b}$ is $\mathbf{A}\mathbf{x}^* = \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$

Generalized inverse

Def 0.1. Let $\mathbf{A} \in \mathbb{R}^{m\times n}$ be any matrix. We call the matrix $\mathbf{G} \in \mathbb{R}^{n\times m}$ a **generalized inverse** of $\mathbf{A}$ if it satisfies

$$\mathbf{AGA} = \mathbf{A}$$

Remark. If $\mathbf{A}$ is square and invertible, then it has one and only one generalized inverse which must coincide with the ordinary inverse $\mathbf{A}^{-1}$. To see this, first observe that $\mathbf{A}^{-1}$ apparently satisfies the definition and thus is a generalized inverse. Conversely, if $\mathbf{A}$ has a generalized inverse $\mathbf{G}$, then from the equation $\mathbf{AGA} = \mathbf{A}$ we get

$$\mathbf{G} = \mathbf{A}^{-1}(\mathbf{AGA})\mathbf{A}^{-1} = \mathbf{A}^{-1}(\mathbf{A})\mathbf{A}^{-1} = \mathbf{A}^{-1}$$

This thus justifies the term "generalized inverse".

Remark. For a general matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$, its generalized inverse always exists but might not be unique.

For example, let $\mathbf{A} = [1, 2] \in \mathbb{R}^{1\times 2}$. Its generalized inverse is a matrix $\mathbf{G} = \begin{bmatrix} x \\ y \end{bmatrix} \in \mathbb{R}^{2\times 1}$ satisfying

$$[1, 2] = \mathbf{A} = \mathbf{AGA} = [1, 2] \begin{bmatrix} x \\ y \end{bmatrix} [1, 2] = (x + 2y) \cdot [1, 2].$$

This shows that any $\mathbf{G} = \begin{bmatrix} x \\ y \end{bmatrix} \in \mathbb{R}^{2\times 1}$ with $x + 2y = 1$ is a generalized inverse of $\mathbf{A}$, e.g., $\mathbf{G} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ or $\mathbf{G} = \begin{bmatrix} 3 \\ -1 \end{bmatrix}$.

The following theorem indicates a way to find the generalized inverse of any matrix.

Theorem 0.1. Let $\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \in \mathbb{R}^{m\times n}$ be a matrix of rank r, and $A_{11} \in \mathbb{R}^{r\times r}$. If A_{11} is invertible, then $\mathbf{G} = \begin{bmatrix} A_{11}^{-1} & O \\ O & O \end{bmatrix} \in \mathbb{R}^{n\times m}$ is a generalized inverse of $\mathbf{A}$.

Remark. Any matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$ with rank r can be rearranged through row and column permutations to have the above partitioned form with an invertible $r \times r$ submatrix in the top-left corner. This theorem essentially establishes the existence of a generalized inverse for any matrix.

Remark. We skip the proof but illustrate the theorem with an example:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

Since $\mathrm{rank}(\mathbf{A}) = 2$ and the top-left 2×2 block is invertible, we can easily find a generalized inverse

$$\mathbf{G} = \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

To verify:

$$\mathbf{AGA} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} = \mathbf{A}$$

The generalized inverse can also be used to find a solution to a consistent linear system (i.e., there exists at least a solution).

Theorem 0.2. Consider the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$. Suppose $\mathbf{b} \in \mathrm{Col}(\mathbf{A})$ such that the system is consistent. Let $\mathbf{G}$ be a generalized inverse of $\mathbf{A}$, i.e., $\mathbf{A}\mathbf{G}\mathbf{A} = \mathbf{A}$. Then $\mathbf{x}^* = \mathbf{G}\mathbf{b}$ is a particular solution to the system.

Proof. Multiplying both sides of $\mathbf{A}\mathbf{x} = \mathbf{b}$ by $\mathbf{A}\mathbf{G}$ gives that

$$(\mathbf{A}\mathbf{G})\mathbf{b} = (\mathbf{A}\mathbf{G})\mathbf{A}\mathbf{x} = (\mathbf{A}\mathbf{G}\mathbf{A})\mathbf{x} = \mathbf{A}\mathbf{x} = \mathbf{b}.$$

This shows that $\mathbf{x}^* = \mathbf{G}\mathbf{b}$ is a particular solution to the linear system. □

Example 0.1. Consider the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$, where

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 6 \\ 15 \\ 24 \end{bmatrix}.$$

According to the system, a particular solution to the system is

$$\mathbf{x}^* = \mathbf{G}\mathbf{b} = \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 6 \\ 15 \\ 24 \end{bmatrix} = \begin{bmatrix} 0 \\ 3 \\ 0 \end{bmatrix}$$

Projection matrices

Def 0.2. A square matrix $\mathbf{P}$ is called a **projection matrix** if $\mathbf{P} = \mathbf{P}^2$.

Example 0.2. The following are some projection matrices (but not all):

$$\mathbf{I}, \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{O}$$

Remark. Projection matrices must have a determinant of 0 or 1, because

$$\det(\mathbf{P}) = \det(\mathbf{P}^2) = [\det(\mathbf{P})]^2.$$

Remark. The following statements explain what a projection matrix does:

- A projection matrix $\mathbf{P} \in \mathbb{R}^{n\times n}$ projects any vector in $\mathbb{R}^n$ onto its range (column space). To see this, let $\mathbf{x} \in \mathbb{R}^n$. Then

$$\mathbf{P}\mathbf{x} = [\mathbf{p}_1 \ldots \mathbf{p}_n] \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \sum x_i \mathbf{p}_i \in \mathrm{Col}(\mathbf{P}) \equiv \mathrm{Range}(\mathbf{P})$$

- A projection matrix keeps all points from its range (when applied to them) in their original places. To see this, let $\mathbf{v} \in \mathrm{Range}(\mathbf{P})$. Then there exists some $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{v} = \mathbf{P}\mathbf{x}$. It follows that

$$\mathbf{P}\mathbf{v} = \mathbf{P}(\mathbf{P}\mathbf{x}) = \mathbf{P}^2\mathbf{x} = \mathbf{P}\mathbf{x} = \mathbf{v}.$$

Theorem 0.3. **Let $\mathbf{A} \in \mathbb{R}^{m\times n}$ with a generalized inverse $\mathbf{G} \in \mathbb{R}^{n\times m}$. Then $\mathbf{AG} \in \mathbb{R}^{m\times m}$ is a projection matrix.**

Proof. From $\mathbf{AGA} = \mathbf{A}$, we obtain

$$(\mathbf{AG})(\mathbf{AG}) = (\mathbf{AGA})\mathbf{G} = \mathbf{AG}.$$

This shows that $\mathbf{AG}$ is a projection matrix. □

Remark. Similarly, we can show that $\mathbf{GA} \in \mathbb{R}^{n\times n}$ is also a projection matrix

$$(\mathbf{GA})(\mathbf{GA}) = \mathbf{GA}$$

We'll focus on $\mathbf{AG}$ below.

Remark. $\mathbf{AG}$ and $\mathbf{A}$ must have the same column space. To see this,

(1) For any $\mathbf{y} \in \mathrm{Col}(\mathbf{AG})$, there exists some $\mathbf{x} \in \mathbb{R}^m$ such that $\mathbf{y} = (\mathbf{AG})\mathbf{x}$. It follows that $\mathbf{y} = \mathbf{A}(\mathbf{Gx}) \in \mathrm{Col}(\mathbf{A})$. This shows that $\mathrm{Col}(\mathbf{AG}) \subseteq \mathrm{Col}(\mathbf{A})$.

(2) For any $\mathbf{y} \in \mathrm{Col}(\mathbf{A})$, there exists some $\mathbf{x} \in \mathbb{R}^n$ such that $\mathbf{y} = \mathbf{Ax}$. Write $\mathbf{y} = (\mathbf{AGA})\mathbf{x} = (\mathbf{AG})(\mathbf{Ax})$. This shows that $\mathbf{y} \in \mathrm{Col}(\mathbf{AG})$. Thus, $\mathrm{Col}(\mathbf{A}) \subseteq \mathrm{Col}(\mathbf{AG})$.

Therefore, **$\mathbf{AG}$ is a projection matrix onto the column space of $\mathbf{A}$**.

Similarly, we can show that $\mathbf{GA}$ is a projection matrix onto the row space of $\mathbf{A}$.

Example 0.3. Consider the matrix $\mathbf{A}$ and its generalized inverse $\mathbf{G}$:

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}, \qquad \mathbf{G} = \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

We have

$$\mathbf{AG} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 2 & 0 \end{bmatrix}$$

According to the previous slide,

- $\mathbf{AG}$ and $\mathbf{A}$ have the same column space.
- $\mathbf{AG}$ is a projection matrix onto the column space of $\mathbf{A}$.

Pseudoinverse

Briefly speaking, the matrix pseudoinverse is a generalized inverse with more constraints.

Def 0.3. Let $\mathbf{A} \in \mathbb{R}^{m\times n}$. We call the matrix $\mathbf{B} \in \mathbb{R}^{n\times m}$ the **pseudoinverse** of $\mathbf{A}$ if it satisfies all four conditions below:

(1) $\mathbf{ABA} = \mathbf{A}$ $\longleftarrow$ $\mathbf{B}$ is a generalized inverse of $\mathbf{A}$

(2) $\mathbf{BAB} = \mathbf{B}$ $\longleftarrow$ $\mathbf{A}$ is a generalized inverse of $\mathbf{B}$

(3) $(\mathbf{AB})^T = \mathbf{AB}$ $\longleftarrow$ $\mathbf{AB}$ is symmetric

(4) $(\mathbf{BA})^T = \mathbf{BA}$ $\longleftarrow$ $\mathbf{BA}$ is symmetric

Remark.

- If $\mathbf{B}$ satisfies Condition (1), it is known as a generalized inverse of $\mathbf{A}$; if $\mathbf{B}$ satisfies Conditions (1) and (2), it is called a **reflexive generalized inverse**. Only when $\mathbf{B}$ satisfies all 4 conditions, it is called the pseudoinverse of $\mathbf{A}$.
- It can be shown that for any matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$, the pseudoinverse always exists and is unique. We denote the pseudoinverse of $\mathbf{A}$ as $\mathbf{A}^\dagger$.
- A pseudoinverse is sometimes called the **Moore–Penrose inverse**, after the pioneering works by E. H. Moore and Roger Penrose.
- The symmetric form of the definition implies $\mathbf{B} = \mathbf{A}^\dagger$ and $\mathbf{A} = \mathbf{B}^\dagger$, and thus, $\mathbf{A} = (\mathbf{A}^\dagger)^\dagger$.

Example 0.4. Consider $\mathbf{A} = [1,2] \in \mathbb{R}^{1\times 2}$ again. We showed that any matrix $\mathbf{G} = (x,y)^T \in \mathbb{R}^{2\times 1}$ with $x + 2y = 1$ is a generalized inverse of $\mathbf{A}$:

$$[1,2] = \mathbf{A} = \mathbf{AGA} = [1,2]\begin{bmatrix} x \\ y \end{bmatrix}[1,2] = (x+2y)\cdot[1,2].$$

To find its pseudoinverse, we need to write down three more equations:

$$\begin{bmatrix} x \\ y \end{bmatrix} = \mathbf{G} = \mathbf{GAG} = \begin{bmatrix} x \\ y \end{bmatrix}[1,2]\begin{bmatrix} x \\ y \end{bmatrix} = (x+2y)\cdot\begin{bmatrix} x \\ y \end{bmatrix}$$

$$x + 2y = (\mathbf{AG})^T = \mathbf{AG} = [1,2]\begin{bmatrix} x \\ y \end{bmatrix} = x + 2y$$

$$\begin{bmatrix} x & y \\ 2x & 2y \end{bmatrix} = (\mathbf{GA})^T = \mathbf{GA} = \begin{bmatrix} x \\ y \end{bmatrix}[1,2] = \begin{bmatrix} x & 2x \\ y & 2y \end{bmatrix} \longrightarrow 2x = y$$

Solving the two equations together gives that $x = \frac{1}{5}, y = \frac{2}{5}$. Thus, the pseudoinverse of $\mathbf{A}$ is

$$\mathbf{A}^\dagger = \begin{bmatrix} \frac{1}{5} & \frac{2}{5} \end{bmatrix}^T.$$

Example 0.5. Let

$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}.$$

Verify that

$$\mathbf{A}^\dagger = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ 0 & 0 \end{bmatrix}$$

Example 0.6 (Cont'd)**.** Consider the matrix again

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

which has the following generalized inverse

$$\mathbf{G} = \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

That is, $\mathbf{AGA} = \mathbf{A}$. It can be verified that $\mathbf{A}$ is also a generalized inverse of $\mathbf{G}$:

$$\mathbf{GAG} = \mathbf{G}$$

Thus, $\mathbf{G}$ must be at least a reflexive generalized inverse of $\mathbf{A}$.

However, neither $\mathbf{AG}$ nor $\mathbf{GA}$ is symmetric:

$$\mathbf{AG} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 2 & 0 \end{bmatrix}$$

$$\mathbf{GA} = \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} & 0 \\ \frac{4}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{bmatrix}$$

Therefore, $\mathbf{G}$ is not the pseudoinverse of $\mathbf{A}$.

Orthogonal projection matrices

Since the matrix pseudoinverse is still a generalized inverse, it will automatically inherit the properties of the matrix generalized inverse. Nevertheless, in many cases, stronger results can be obtained for a matrix pseudoinverse.

Def 0.4. A square matrix $\mathbf{P}$ is called a **orthogonal projection matrix** if $\mathbf{P} = \mathbf{P}^T$ and $\mathbf{P} = \mathbf{P}^2$.

Example 0.7. $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, $\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$ are both orthogonal projection matrices, but $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 2 & 0 \end{bmatrix}$ is not (it is just a projection matrix).

Theorem 0.4. For any matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$, $\mathbf{A}\mathbf{A}^\dagger$ is an orthogonal projection matrix (onto the column space of $\mathbf{A}$).

Proof. First, $\mathbf{A}^\dagger$ is still a generalized inverse. Thus, $\mathbf{A}\mathbf{A}^\dagger$ is a projection matrix (onto the column space of $\mathbf{A}$).

Secondly, since $\mathbf{A}^\dagger$ is the pseudoinverse of $\mathbf{A}$, $\mathbf{A}\mathbf{A}^\dagger$ must be symmetric.

Therefore, by definition, $\mathbf{A}\mathbf{A}^\dagger$ is an orthogonal projection matrix. □

Remark. Similarly, $\mathbf{A}^\dagger\mathbf{A}$ is also an orthogonal projection matrix (onto the row space of $\mathbf{A}$).

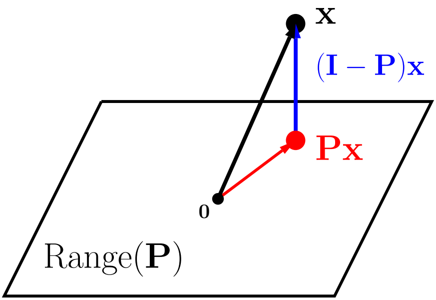
Remark. For any projection matrix $\mathbf{P} \in \mathbb{R}^{n\times n}$ and vector $\mathbf{x} \in \mathbb{R}^n$, we have

$$\mathbf{x} = \mathbf{P}\mathbf{x} + (\mathbf{I} - \mathbf{P})\mathbf{x}$$

If $\mathbf{P}$ is an orthogonal projection (i.e., $\mathbf{P} = \mathbf{P}^T$), then the two components are orthogonal to each other:

$$\begin{aligned}(\mathbf{P}\mathbf{x})^T(\mathbf{I} - \mathbf{P})\mathbf{x} &= \mathbf{x}^T\mathbf{P}(\mathbf{I} - \mathbf{P})\mathbf{x} \\ &= \mathbf{x}^T(\mathbf{P} - \mathbf{P}^2)\mathbf{x} \\ &= 0.\end{aligned}$$

This implies that orthogonal projections produce orthogonal decompositions of vectors.



Finding matrix pseudoinverse

Let $\mathbf{A} \in \mathbb{R}^{m\times n}$. Our goal is to find $\mathbf{A}^\dagger$ (which exists and is unique).

We first consider the following two special settings:

- **$\mathbf{A}$ is a tall matrix with full column rank** (i.e., $\operatorname{rank}(\mathbf{A}) = n \leq m$). Note that in this case, $\mathbf{A}^T\mathbf{A} \in \mathbb{R}^{n\times n}$ is invertible.

- **$\mathbf{A}$ is a "diagonal" matrix** (i.e., $a_{ij} = 0$ whenever $i \neq j$).

Afterwards, we present a theorem to show how to find the pseudoinverse of a general matrix via its SVD.

Theorem 0.5. Let $\mathbf{A} \in \mathbb{R}^{m\times n}$ be any tall matrix with full column rank (i.e., $\mathrm{rank}(\mathbf{A}) = n \leq m$). Then the pseudoinverse of $\mathbf{A}$ is

$$\mathbf{A}^\dagger = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T.$$

Proof. It suffices to verify the four conditions for being a pseudoinverse:

$$\begin{aligned}
\mathbf{A}\mathbf{A}^\dagger\mathbf{A} &= \mathbf{A}\cdot(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\cdot\mathbf{A} = \mathbf{A} \\
\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger &= (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\cdot\mathbf{A}\cdot(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T = \mathbf{A}^\dagger \\
\mathbf{A}\mathbf{A}^\dagger &= \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T \qquad \text{(symmetric)} \\
\mathbf{A}^\dagger\mathbf{A} &= (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\cdot\mathbf{A} = \mathbf{I}_n \qquad \text{(symmetric)}
\end{aligned}$$

Therefore, $\mathbf{A}^\dagger = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$ is the pseudoinverse of $\mathbf{A}$. □

Remark. The theorem implies that for any tall matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$ with full column rank (i.e., $\mathrm{rank}(\mathbf{A}) = n \le m$), the following is an **orthogonal projection** matrix (onto the column space of $\mathbf{A}$):

$$\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T.$$

Remark. Let $\mathbf{U} \in \mathbb{R}^{m\times n}$ be a tall matrix with orthonormal columns (e.g., an orthonormal basis matrix). Then it has full column rank, and

$$\mathbf{U}^T\mathbf{U} = \begin{bmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_n^T \end{bmatrix} [\mathbf{u}_1 \ldots \mathbf{u}_n] = \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} = \mathbf{I}_n$$

It follows that

$$\mathbf{U}^\dagger = \mathbf{U}^T \text{ (pseudoinverse)}, \quad \text{and } \mathbf{U}\mathbf{U}^\dagger = \mathbf{U}\mathbf{U}^T \text{(orthogonal projection matrix)}$$

Example 0.8. Find the pseudoinverse of

$$\mathbf{X} = \begin{pmatrix} 1 & -1 \\ 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Solution: Observe that this matrix has full column rank (i.e., 2). We first compute

$$\mathbf{X}^T\mathbf{X} = \begin{pmatrix} 1 & 0 & 1 \\ -1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

It follows that

$$\mathbf{X}^\dagger = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 \\ -1 & 1 & 0 \end{pmatrix} = \frac{1}{3}\begin{pmatrix} 1 & 1 & 2 \\ -1 & 2 & 1 \end{pmatrix}$$

Theorem 0.6. Let $\mathbf{A} \in \mathbb{R}^{m\times n}$ be a diagonal matrix, i.e., all of its entries are zero except some of those along its diagonal. Then the pseudoinverse of $\mathbf{A}$ is another diagonal matrix $\mathbf{B} \in \mathbb{R}^{n\times m}$ such that

$$b_{ii} = \begin{cases} \frac{1}{a_{ii}}, & \text{if } a_{ii} \neq 0 \\ 0, & \text{if } a_{ii} = 0 \end{cases}$$

Proof. We verify this result using an example. Let

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{3} \\ 0 & 0 \end{bmatrix}.$$

Then

$$\mathbf{AB} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{BA} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

both of which are symmetric. Furthermore,

$$\mathbf{ABA} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix} = \mathbf{A}$$

$$\mathbf{BAB} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{3} \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & \frac{1}{3} \\ 0 & 0 \end{bmatrix} = \mathbf{B}.$$

Thus, $\mathbf{B}$ is the pseudoinverse of $\mathbf{A}$. □

Theorem 0.7. Let $\mathbf{A} \in \mathbb{R}^{m\times n}$ be any matrix. Suppose its full SVD is $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$. Then the pseudoinverse of $\mathbf{A}$ is

$$\mathbf{A}^\dagger = \mathbf{V}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T$$

Proof. We verify the four conditions directly:

$$\begin{aligned}
\mathbf{A}\mathbf{A}^\dagger\mathbf{A} &= \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T \cdot \mathbf{V}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T \cdot \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^\dagger\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{A}\\
\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger &= \mathbf{V}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T \cdot \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T \cdot \mathbf{V}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T = \mathbf{V}\boldsymbol{\Sigma}^\dagger\boldsymbol{\Sigma}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T = \mathbf{V}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T = \mathbf{A}^\dagger\\
\mathbf{A}\mathbf{A}^\dagger &= \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T \cdot \mathbf{V}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T = \mathbf{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T \qquad \text{(symmetric)}\\
\mathbf{A}^\dagger\mathbf{A} &= \mathbf{V}\boldsymbol{\Sigma}^\dagger\mathbf{U}^T \cdot \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{V}\boldsymbol{\Sigma}^\dagger\boldsymbol{\Sigma}\mathbf{V}^T \qquad \text{(symmetric)}
\end{aligned}$$

This completes the proof. □

Example 0.9. Consider again the matrix

$$\mathbf{X} = \begin{pmatrix} 1 & -1 \\ 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

We have previously found its SVD:

$$\mathbf{X} = \begin{pmatrix} \frac{2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} \end{pmatrix} \cdot \begin{pmatrix} \sqrt{3} & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}^T$$

By the last theorem,

$$\mathbf{X}^\dagger = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} \end{pmatrix}^T = \frac{1}{3} \begin{pmatrix} 1 & 1 & 2 \\ -1 & 2 & 1 \end{pmatrix}$$

MATLAB function for computing pseudoinverse

pinv Pseudoinverse.

$X = pinv(A)$ produces a matrix X of the same dimensions as A' so that $A * X * A = A, X * A * X = X$ and $A * X$ and $X * A$ are Hermitian. The computation is based on $SVD(A)$ and any singular values less than a tolerance are treated as zero.

$pinv(A, TOL)$ treats all singular values of A that are less than TOL as zero. By default, $TOL = max(size(A)) * eps(norm(A))$.

Applications of matrix pseudoinverse

- Linear least squares

- Minimum norm solution to a consistent linear system

Linear least squares

Consider a system of linear equations $\mathbf{A}\mathbf{x} = \mathbf{b}$ where $\mathbf{A} \in \mathbb{R}^{m\times n}$ and $\mathbf{b} \in \mathbb{R}^m$.

In general, a vector $\mathbf{x}$ that solves the system may not exist, or if one does exist, it may not be unique.

In either case, we seek a least squares solution instead by solving the following least squares problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|$$

This problem always has a solution, as the next slide shows.

Theorem 0.8. A minimizer of the above least squares problem is

$$\mathbf{x}^* = \mathbf{A}^\dagger \mathbf{b}.$$

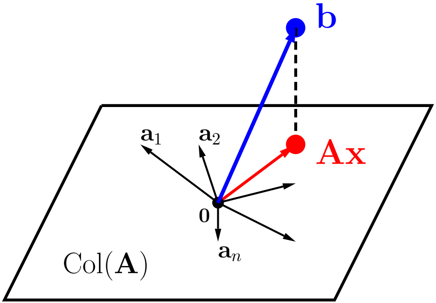
Proof. Since

$$\mathbf{A}\mathbf{x} \in \mathrm{Col}(\mathbf{A}),$$

the optimal $\mathbf{x}$ should be such that

$$\mathbf{A}\mathbf{x} = (\mathbf{A}\mathbf{A}^\dagger)\mathbf{b}$$

Obviously, $\mathbf{x}^* = \mathbf{A}^\dagger \mathbf{b}$ solves this equation and thus is a solution of the least squares problem (but it might not be the only solution). □



Remark. If $\mathbf{A}$ has full column rank (i.e., $\mathrm{rank}(\mathbf{A}) = n \le m$), then the least squares solution exits and is unique: $\mathbf{x}^* = \mathbf{A}^\dagger \mathbf{b} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{b}$.

Minimum-norm solution to a consistent linear system

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

Theorem 0.9. Let $\mathbf{A} \in \mathbb{R}^{m\times n}$ and $\mathbf{b} \in \mathbb{R}^m$. If the linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ has solutions, then $\mathbf{x}^* = \mathbf{A}^\dagger\mathbf{b}$ is an exact solution and has the smallest possible norm, i.e., $\|\mathbf{x}^*\| \le \|\mathbf{x}\|$ for all solutions $\mathbf{x}$.

Proof. First, since $\mathbf{A}^\dagger$ is a generalized inverse, it must be a solution to $\mathbf{Ax} = \mathbf{b}$. To show that it has the smallest possible norm, for any solution $\mathbf{x} \in \mathbb{R}^n$, consider its orthogonal decomposition via $\mathbf{A}^\dagger\mathbf{A} \in \mathbb{R}^{n\times n}$:

$$\mathbf{x} = (\mathbf{A}^\dagger\mathbf{A})\mathbf{x} + (\mathbf{I} - \mathbf{A}^\dagger\mathbf{A})\mathbf{x} = \mathbf{A}^\dagger\mathbf{b} + (\mathbf{I} - \mathbf{A}^\dagger\mathbf{A})\mathbf{x}$$

It follows that

$$\|\mathbf{x}\|^2 = \|\mathbf{A}^\dagger\mathbf{b}\|^2 + \|(\mathbf{I} - \mathbf{A}^\dagger\mathbf{A})\mathbf{x}\|^2 \geq \|\mathbf{A}^\dagger\mathbf{b}\|^2$$

This shows that $\|\mathbf{x}\| \geq \|\mathbf{A}^\dagger\mathbf{b}\|$. $\square$

Summary

- **Generalized inverse** $\mathbf{G} \in \mathbb{R}^{n\times m}$ for a matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$:
  - *Definition*: $\mathbf{AGA} = \mathbf{A}$
  - *Existence*: $\mathbf{G}$ always exists but might not be unique
  - *Computing*: How to find a generalized inverse (see slide 9 for formula)
  - *Property*: $\mathbf{AG}$ is a projection matrix onto $\mathrm{Col}(\mathbf{A})$
  - *Application*: $\mathbf{x} = \mathbf{Gb}$ is a solution to $\mathbf{Ax} = \mathbf{b}$ (if consistent)

- **Pseudoinverse** $\mathbf{A}^\dagger \in \mathbb{R}^{n\times m}$ for a matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$:
  - *Definition*: $\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}^\dagger$, and $\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}$, and both $\mathbf{A}\mathbf{A}^\dagger, \mathbf{A}^\dagger\mathbf{A}$ are symmetric
  - *Existence*: $\mathbf{A}^\dagger$ always exists and is unique
  - *Computing*: How to find the pseudoinverse:
    * If $\mathbf{A}$ has full column rank: $\mathbf{A}^\dagger = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$
    * If $\mathbf{A}$ is "diagonal": $\mathbf{A}^\dagger \in \mathbb{R}^{n\times m}$ is also "diagonal" with reciprocals of nonzero diagonals of $\mathbf{A}$
    * In general: $\mathbf{A}^\dagger = \mathbf{V}\mathbf{\Sigma}^\dagger\mathbf{U}^T$ (if $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$)
  - *Property*: $\mathbf{A}\mathbf{A}^\dagger$ is an orthogonal projection matrix onto $\mathrm{Col}(\mathbf{A})$

- *Application*: For any $\mathbf{A} \in \mathbb{R}^{m\times n}, \mathbf{b} \in \mathbb{R}^m$, $\mathbf{A}^\dagger \mathbf{b}$ solves the least squares problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|$$

  If $\mathbf{A}\mathbf{x} = \mathbf{b}$ has exact solutions, then $\mathbf{A}^\dagger \mathbf{b}$ is the minimum-norm solution.