San José State University
Math 250: Mathematical Data Visualization

## Generalized inverse and pseudoinverse

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## Outline

- Matrix generalized inverse
- Pseudoinverse
- Applications


## Generalized inverse and pseudoinverse

## 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

$$
\mathbf{A B}=\mathbf{B A}=\mathbf{I}
$$

In this case, $\mathbf{B}$ is called the matrix inverse of $\mathbf{A}$ and denoted as $\mathbf{B}=\mathbf{A}^{-1}$.
Remark. A square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is invertible if and only if

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


## Generalized inverse and pseudoinverse

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 $\mathbf{A x}=\mathbf{b}$ has a unique solution

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

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

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

## What about general matrices?

Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ be a square but singular matrix $(m=n, \operatorname{det}(\mathbf{A})=0)$, or a rectangular matrix $(m \neq n)$.

We would like to address the following questions:

- Is there some kind of inverse?
- Given a vector $\mathbf{b} \in \mathbb{R}^{m}$, does the linear system $\mathbf{A x}=\mathrm{b}$ have a solution?
- If yes, is the solution unique?
- Otherwise, is there some kind of approximate solution?


## More motivation: Least squares

In many practical tasks, the least squares problem arises naturally:

$$
\min _{\mathbf{x} \in \mathbb{R}^{n}}\|\mathbf{A x}-\mathbf{b}\|^{2} \quad\left(\text { where } \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{b} \in \mathbb{R}^{m}\right. \text { are fixed) }
$$

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

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

Proof. First, we rewrite the objective function as

$$
f(\mathbf{x})=\mathbf{x}^{T}\left(\mathbf{A}^{T} \mathbf{A}\right) \mathbf{x}-2 \mathbf{x}^{T}\left(\mathbf{A}^{T} \mathbf{b}\right)+\|\mathbf{b}\|^{2} \longleftarrow \text { Convex, differentiable }
$$

## Generalized inverse and pseudoinverse

Next, we find all critical points by setting the gradient to zero:

$$
\nabla f=2 \mathbf{A}^{T} \mathbf{A} \mathbf{x}-2 \mathbf{A}^{T} \mathbf{b}=0
$$

Since $\operatorname{rank}\left(\mathbf{A}^{T} \mathbf{A}\right)=\operatorname{rank}(\mathbf{A})=n$, the matrix $\mathbf{A}^{T} \mathbf{A} \in \mathbb{R}^{n \times n}$ is nonsingular, and consequently the above equation has one and only one solution

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

To show that it is a local minimizer (and thus also a global minimizer), we compute the Hessian of $f$ and obtain that

$$
\nabla^{2} f=2 \mathbf{A}^{T} \mathbf{A}
$$

which is a positive definite matrix (because $\mathbf{A}^{T} \mathbf{A}$ is nonsingular).

## Generalized inverse and pseudoinverse

We want to better understand the following two matrices:

- $\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T}$ (pseudoinverse): The least squares solution is

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

- $\mathbf{A}\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T}$ (projection matrix): Closest approximation of $\mathbf{b}$ is

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

## 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

$$
\mathbf{A G A}=\mathbf{A}
$$

Remark. If $\mathbf{A}$ is square and invertible, then (1) $\mathbf{A}^{-1}$ is a generalized inverse of $\mathbf{A}$ and (2) it is the only generalized inverse of $\mathbf{A}$ :

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

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 $\mathbf{G}=\left[\begin{array}{l}x \\ y\end{array}\right] \in \mathbb{R}^{2 \times 1}$ satisfying

$$
[1,2]=\mathbf{A}=\mathbf{A G A}=[1,2]\left[\begin{array}{l}
x \\
y
\end{array}\right][1,2]=(x+2 y) \cdot[1,2] .
$$

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

## Generalized inverse and pseudoinverse

The following theorem indicates a way to find the generalized inverse of any matrix.
Theorem 0.1. Let $\mathbf{A}=\left[\begin{array}{ll}A_{11} & A_{12} \\ A_{21} & A_{22}\end{array}\right] \in \mathbb{R}^{m \times n}$ be a matrix of rank $r$, and $A_{11} \in \mathbb{R}^{r \times r}$. If $A_{11}$ is invertible, then $\mathbf{G}=\left[\begin{array}{cc}A_{11}^{-1} & O \\ O & O\end{array}\right] \in \mathbb{R}^{n \times m}$ 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.

## Generalized inverse and pseudoinverse

Example 0.1. Consider the following matrix

$$
\mathbf{A}=\left[\begin{array}{lll}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{array}\right]
$$

Since $\operatorname{rank}(\mathbf{A})=2$ and the top-left $2 \times 2$ block happens to be invertible, we can easily find a generalized inverse

$$
\mathbf{G}=\left[\begin{array}{ccc}
-\frac{5}{3} & \frac{2}{3} & 0 \\
\frac{4}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0
\end{array}\right]
$$

You are asked to verify that $\mathbf{A G A}=\mathbf{A}$.

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

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

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

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

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

Example 0.2. Consider the linear system $\mathbf{A x}=\mathbf{b}$, where

$$
\mathbf{A}=\left[\begin{array}{lll}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{array}\right], \quad \mathbf{b}=\left[\begin{array}{c}
6 \\
15 \\
24
\end{array}\right]
$$

It is consistent because $\mathbf{x}=\mathbf{1}$ is a solution.
According to the theorem, a particular solution to the system is

$$
\mathbf{x}^{*}=\mathbf{G} \mathbf{b}=\left[\begin{array}{ccc}
-\frac{5}{3} & \frac{2}{3} & 0 \\
\frac{4}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0
\end{array}\right]\left[\begin{array}{c}
6 \\
15 \\
24
\end{array}\right]=\left[\begin{array}{l}
0 \\
3 \\
0
\end{array}\right]
$$

## Generalized inverse and pseudoinverse

## Projection matrices

Def 0.2. A square matrix $\mathbf{P}$ is called a projection matrix if it is idempotent, i.e., $\mathbf{P}=\mathbf{P}^{2}$.

Remark. Let $\mathbf{P}$ be a projection matrix. Then

- $\mathbf{P}$ must be digonalizable;
- $\mathbf{P}$ have eigenvalues of 0 and/or 1 . Moreover, the algebraic multiplicity of 1 is equal to the rank and trace of $\mathbf{P}$.


## Generalized inverse and pseudoinverse

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 column space. To see this, let $\mathbf{x} \in \mathbb{R}^{n}$. Then

$$
\mathbf{P} \mathbf{x}=\left[\mathbf{p}_{1} \ldots \mathbf{p}_{n}\right]\left[\begin{array}{c}
x_{1} \\
\vdots \\
x_{n}
\end{array}\right]=\sum x_{i} \mathbf{p}_{i} \in \operatorname{Col}(\mathbf{P})
$$



## Generalized inverse and pseudoinverse

- A projection matrix projects every vector already in its column space onto itself.

To see this, let $\mathbf{v} \in \operatorname{Col}(\mathbf{P})$. Then there exists some $\mathbf{x} \in \mathbb{R}^{n}$ such that $\mathbf{v}=\mathbf{P x}$.

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


## Generalized inverse and pseudoinverse

Example 0.3. Below are two projection matrices:

$$
\mathbf{P}_{1}=\left(\begin{array}{cc}
1 & 0 \\
1 & 0
\end{array}\right), \quad \mathbf{P}_{2}=\left(\begin{array}{cc}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{array}\right)
$$

They have the same column space, which is the 45 degree line through the origin in $\mathbb{R}^{2}$, and thus both project points in $\mathbb{R}^{2}$ onto the same line. However, the ways they project points are different: For any $\mathbf{x} \in \mathbb{R}^{2}$,

$$
\begin{aligned}
& \mathbf{P}_{1} \mathbf{x}=\left(\begin{array}{ll}
1 & 0 \\
1 & 0
\end{array}\right)\binom{x_{1}}{x_{2}}=\binom{x_{1}}{x_{1}} \\
& \mathbf{P}_{2} \mathbf{x}=\left(\begin{array}{ll}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{array}\right)\binom{x_{1}}{x_{2}}=\binom{\frac{x_{1}+x_{2}}{2}}{\frac{x_{1}+x_{2}}{2}}
\end{aligned}
$$

## Generalized inverse and pseudoinverse



## Generalized inverse and pseudoinverse

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 $\mathbf{P}=\mathbf{A G} \in \mathbb{R}^{m \times m}$ is a projection matrix.

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

$$
(\mathbf{A G})(\mathbf{A G})=(\mathbf{A G A}) \mathbf{G}=\mathbf{A G}
$$

This shows that AG is a projection matrix.

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

$$
(\mathbf{G A})(\mathbf{G A})=\mathbf{G}(\mathbf{A G A})=\mathbf{G A}
$$

## Generalized inverse and pseudoinverse

Remark. AG and A must have the same column space. To see this,
(1) For any $\mathbf{y} \in \operatorname{Col}(\mathbf{A G})$, there exists some $\mathbf{x} \in \mathbb{R}^{m}$ such that $\mathbf{y}=$ $(\mathbf{A G}) \mathbf{x}$. It follows that $\mathbf{y}=\mathbf{A}(\mathbf{G x}) \in \operatorname{Col}(\mathbf{A})$. This shows that $\operatorname{Col}(\mathbf{A G}) \subseteq \operatorname{Col}(\mathbf{A})$.
(2) For any $\mathbf{y} \in \operatorname{Col}(\mathbf{A})$, there exists some $\mathbf{x} \in \mathbb{R}^{n}$ such that $\mathbf{y}=\mathbf{A x}$. Write $\mathbf{y}=(\mathbf{A G A}) \mathbf{x}=(\mathbf{A G})(\mathbf{A x})$. This shows that $\mathbf{y} \in \operatorname{Col}(\mathbf{A G})$. Thus, $\operatorname{Col}(\mathbf{A}) \subseteq \operatorname{Col}(\mathbf{A G})$.

## Generalized inverse and pseudoinverse

Therefore, AG is a projection matrix onto the column space of $\mathbf{A}$.
$\mathbf{A} \in \mathrm{R}^{m \times n}$


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

Example 0.4. Consider the matrix $\mathbf{A}$ and its generalized inverse $\mathbf{G}$ :

$$
\mathbf{A}=\left[\begin{array}{lll}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{array}\right], \quad \mathbf{G}=\left[\begin{array}{ccc}
-\frac{5}{3} & \frac{2}{3} & 0 \\
\frac{4}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0
\end{array}\right]
$$

We have

$$
\mathbf{A G}=\left[\begin{array}{lll}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{array}\right]\left[\begin{array}{ccc}
-\frac{5}{3} & \frac{2}{3} & 0 \\
\frac{4}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0
\end{array}\right]=\left[\begin{array}{ccc}
1 & 0 & 0 \\
0 & 1 & 0 \\
-1 & 2 & 0
\end{array}\right]
$$

which represents 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) $\mathbf{A B A}=\mathbf{A} \longleftarrow \mathbf{B}$ is a generalized inverse of $\mathbf{A}$
(2) $\mathbf{B A B}=\mathbf{B} \quad \longleftarrow \mathbf{A}$ is a generalized inverse of $\mathbf{B}$
(3) $(\mathbf{A B})^{T}=\mathbf{A B} \longleftarrow \mathbf{A B}$ is symmetric
(4) $(\mathbf{B A})^{T}=\mathbf{B A} \longleftarrow \mathbf{B A}$ is symmetric

## Remark.

- If $\mathbf{B}$ only satisfies (1), it is known as a generalized inverse of $\mathbf{A}$; if $\mathbf{B}$ only satisfies (1) and (2), it is called a reflexive generalized inverse.
- 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, $\mathbf{A}=\left(\mathbf{A}^{\dagger}\right)^{\dagger}$.


## Generalized inverse and pseudoinverse

Example 0.5. 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 $x+2 y=1$ is a generalized inverse of $\mathbf{A}$ :

$$
[1,2]=\mathbf{A}=\mathbf{A G A}=[1,2]\left[\begin{array}{l}
x \\
y
\end{array}\right][1,2]=(x+2 y) \cdot[1,2] .
$$

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

$$
\begin{gathered}
{\left[\begin{array}{l}
x \\
y
\end{array}\right]=\mathbf{G}=\mathbf{G A G}=\left[\begin{array}{l}
x \\
y
\end{array}\right][1,2]\left[\begin{array}{l}
x \\
y
\end{array}\right]=(x+2 y) \cdot\left[\begin{array}{l}
x \\
y
\end{array}\right]} \\
x+2 y=(\mathbf{A G})^{T}=\mathbf{A G}=[1,2]\left[\begin{array}{l}
x \\
y
\end{array}\right]=x+2 y \\
{\left[\begin{array}{cc}
x & y \\
2 x & 2 y
\end{array}\right]=(\mathbf{G A})^{T}=\mathbf{G A}=\left[\begin{array}{l}
x \\
y
\end{array}\right][1,2]=\left[\begin{array}{ll}
x & 2 x \\
y & 2 y
\end{array}\right] \longrightarrow 2 x=y}
\end{gathered}
$$

## Generalized inverse and pseudoinverse

Solving the two equations together gives that

$$
x=\frac{1}{5}, y=\frac{2}{5} .
$$

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

$$
\mathbf{A}^{\dagger}=\left[\begin{array}{c}
\frac{1}{5} \\
\frac{2}{5}
\end{array}\right] .
$$

Example 0.6. Let $\mathbf{A}=\left[\begin{array}{ll}1 & 0 \\ 1 & 0\end{array}\right]$. Verify that $\mathbf{A}^{\dagger}=\left[\begin{array}{cc}\frac{1}{2} & \frac{1}{2} \\ 0 & 0\end{array}\right]$. By direct calculation,

$$
\begin{array}{rlr}
\mathbf{A A}^{\dagger} & =\left[\begin{array}{ll}
1 & 0 \\
1 & 0
\end{array}\right]\left[\begin{array}{ll}
\frac{1}{2} & \frac{1}{2} \\
0 & 0
\end{array}\right]=\left[\begin{array}{ll}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{array}\right] & \text { (symmetric) } \\
\mathbf{A}^{\dagger} \mathbf{A} & =\left[\begin{array}{ll}
\frac{1}{2} & \frac{1}{2} \\
0 & 0
\end{array}\right]\left[\begin{array}{ll}
1 & 0 \\
1 & 0
\end{array}\right]=\left[\begin{array}{cc}
1 & 0 \\
0 & 0
\end{array}\right] & \\
\mathbf{A A}^{\dagger} \mathbf{A} & =\left[\begin{array}{ll}
1 & 0 \\
1 & 0
\end{array}\right]\left[\begin{array}{ll}
\frac{1}{2} & \frac{1}{2} \\
0 & 0
\end{array}\right]\left[\begin{array}{ll}
1 & 0 \\
1 & 0
\end{array}\right]=\left[\begin{array}{cc}
1 & 0 \\
1 & 0
\end{array}\right] & =\mathbf{A} \\
\mathbf{A}^{\dagger} \mathbf{A} \mathbf{A}^{\dagger} & =\left[\begin{array}{ll}
\frac{1}{2} & \frac{1}{2} \\
0 & 0
\end{array}\right]\left[\begin{array}{ll}
1 & 0 \\
1 & 0
\end{array}\right]\left[\begin{array}{cc}
\frac{1}{2} & \frac{1}{2} \\
0 & 0
\end{array}\right]=\left[\begin{array}{cc}
\frac{1}{2} & \frac{1}{2} \\
0 & 0
\end{array}\right] & =\mathbf{A}^{\dagger}
\end{array}
$$

## Generalized inverse and pseudoinverse

Example 0.7 (Cont'd). Consider the matrix again

$$
\mathbf{A}=\left[\begin{array}{lll}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{array}\right]
$$

which has the following generalized inverse (i.e., $\mathbf{A G A}=\mathbf{A}$ ):

$$
\mathbf{G}=\left[\begin{array}{ccc}
-\frac{5}{3} & \frac{2}{3} & 0 \\
\frac{4}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0
\end{array}\right]
$$

It can be verified that $\mathbf{A}$ is also a generalized inverse of $\mathbf{G}$ :

$$
\mathbf{G A G}=\mathbf{G}
$$

Thus, $\mathbf{G}$ is (at least) a reflexive generalized inverse of $\mathbf{A}$.

## Generalized inverse and pseudoinverse

However, neither AG nor GA is symmetric:

$$
\begin{aligned}
\mathbf{A G} & =\left[\begin{array}{lll}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{array}\right]\left[\begin{array}{ccc}
-\frac{5}{3} & \frac{2}{3} & 0 \\
\frac{4}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0
\end{array}\right]=\left[\begin{array}{ccc}
1 & 0 & 0 \\
0 & 1 & 0 \\
-1 & 2 & 0
\end{array}\right] \\
\mathbf{G A} & =\left[\begin{array}{ccc}
-\frac{5}{3} & \frac{2}{3} & 0 \\
\frac{4}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0
\end{array}\right]\left[\begin{array}{lll}
1 & 2 & 3 \\
4 & 5 & 6 \\
7 & 8 & 9
\end{array}\right]=\left[\begin{array}{ccc}
1 & 0 & -1 \\
0 & 1 & 2 \\
0 & 0 & 0
\end{array}\right]
\end{aligned}
$$

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

## Orthogonal projection matrices

Def 0.4. A square matrix $\mathbf{P}$ is called a orthogonal projection matrix if it is both symmetric and idempotent, i.e., $\mathbf{P}=\mathbf{P}^{T}$ and $\mathbf{P}=\mathbf{P}^{2}$.


## Generalized inverse and pseudoinverse

Let $\mathbf{P} \in \mathbb{R}^{n \times n}$ be any orthogonal projection matrix. Because it is still a projection matrix, it must project any vector $\mathbf{b} \in \mathbb{R}^{n}$ onto its column space, i.e., $\mathbf{P b} \in \operatorname{Col}(\mathbf{P})$.

This leads to the following decomposition of $\mathbf{b}$ :

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

Since $\mathbf{P}=\mathbf{P}^{T}$ by definition, we have

$$
(\mathbf{P b})^{T}(\mathbf{I}-\mathbf{P}) \mathbf{b}=\mathbf{b}^{T} \mathbf{P}(\mathbf{I}-\mathbf{P}) \mathbf{b}=\mathbf{b}^{T}\left(\mathbf{P}-\mathbf{P}^{2}\right) \mathbf{b}=0 .
$$

This shows that the two components, $\mathbf{P b}$ and $(\mathbf{I}-\mathbf{P}) \mathbf{b}$, are orthogonal to each other.

## Generalized inverse and pseudoinverse

Example 0.8. $\left[\begin{array}{lll}1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0\end{array}\right],\left[\begin{array}{cc}\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2}\end{array}\right]$ are orthogonal projection matrices,
but $\left[\begin{array}{ccc}1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 2 & 0\end{array}\right]$ is not (it is just a projection matrix).

Example 0.9. The centering matrix $\mathbf{C}_{n}=\mathbf{I}_{n}-\frac{1}{n} \mathbf{J}_{n}$ is also an orthogonal projection matrix (see notes for details).

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

Proof. First, $\mathbf{A}^{\dagger}$ is still a generalized inverse. Thus, $\mathbf{A A}^{\dagger}$ 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 $\mathbf{A}$ ).

## Generalized inverse and pseudoinverse




## 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:

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

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

## Generalized inverse and pseudoinverse

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

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

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

$$
\begin{array}{rlr}
\mathbf{A} \mathbf{A}^{\dagger} \mathbf{A} & =\mathbf{A} \cdot\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T} \cdot \mathbf{A}=\mathbf{A} \\
\mathbf{A}^{\dagger} \mathbf{A} \mathbf{A}^{\dagger} & =\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T} \cdot \mathbf{A} \cdot\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T}=\mathbf{A}^{\dagger} \\
\mathbf{A}^{\dagger} & =\mathbf{A}\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T} & (\text { symmetric) } \\
\mathbf{A}^{\dagger} \mathbf{A} & =\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T} \cdot \mathbf{A}=\mathbf{I}_{n} & \text { (symmetric) }
\end{array}
$$

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

## Generalized inverse and pseudoinverse

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

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

## Generalized inverse and pseudoinverse

Example 0.10. Find the pseudoinverse of $\mathbf{A}=\left(\begin{array}{cc}1 & -1 \\ 0 & 1 \\ 1 & 0\end{array}\right)$.
Solution: Observe that this matrix has full column rank (i.e., 2).
Since

$$
\mathbf{A}^{T} \mathbf{A}=\left(\begin{array}{ccc}
1 & 0 & 1 \\
-1 & 1 & 0
\end{array}\right)\left(\begin{array}{cc}
1 & -1 \\
0 & 1 \\
1 & 0
\end{array}\right)=\left(\begin{array}{cc}
2 & -1 \\
-1 & 2
\end{array}\right)
$$

we have

$$
\mathbf{A}^{\dagger}=\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T}=\frac{1}{3}\left(\begin{array}{ll}
2 & 1 \\
1 & 2
\end{array}\right)\left(\begin{array}{ccc}
1 & 0 & 1 \\
-1 & 1 & 0
\end{array}\right)=\frac{1}{3}\left(\begin{array}{ccc}
1 & 1 & 2 \\
-1 & 2 & 1
\end{array}\right)
$$

## Generalized inverse and pseudoinverse

It follows that the orthogonal projection matrix onto $\operatorname{Col}(\mathbf{A})$ is

$$
\mathbf{A A}^{\dagger}=\left(\begin{array}{cc}
1 & -1 \\
0 & 1 \\
1 & 0
\end{array}\right) \cdot \frac{1}{3}\left(\begin{array}{ccc}
1 & 1 & 2 \\
-1 & 2 & 1
\end{array}\right)=\frac{1}{3}\left(\begin{array}{ccc}
2 & -1 & 1 \\
-1 & 2 & 1 \\
1 & 1 & 2
\end{array}\right)
$$

For instance, the orthogonal projection of 1 onto $\operatorname{Col}(\mathbf{A})$ is

$$
\mathbf{A} \mathbf{A}^{\dagger} \mathbf{1}=\frac{1}{3}\left(\begin{array}{l}
2 \\
2 \\
4
\end{array}\right)=\mathbf{A} \cdot \underbrace{\frac{1}{3}\binom{4}{2}}_{\mathbf{A}^{\dagger} \mathbf{1}}
$$

## Generalized inverse and pseudoinverse

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

$$
\mathbf{U}^{T} \mathbf{U}=\left[\begin{array}{c}
\mathbf{u}_{1}^{T} \\
\vdots \\
\mathbf{u}_{n}^{T}
\end{array}\right]\left[\mathbf{u}_{1} \ldots \mathbf{u}_{n}\right]=\left[\begin{array}{ccc}
1 & & \\
& \ddots & \\
& & 1
\end{array}\right]=\mathbf{I}_{n}
$$

It follows that

- $\mathbf{U}^{\dagger}=\left(\mathbf{U}^{T} \mathbf{U}\right)^{-1} \mathbf{U}^{T}=\mathbf{U}^{T}$ (pseudoinverse), and
- $\mathbf{U U}^{\dagger}=\mathbf{U U}^{T}$ (orthogonal projection matrix).


## Generalized inverse and pseudoinverse

## Example 0.11. Let

$$
\mathbf{A}=\left(\begin{array}{cc}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & -\frac{1}{2} \\
\frac{1}{2} & -\frac{1}{2}
\end{array}\right)
$$

which has orthonormal columns. Therefore, the pseudoinverse of $\mathbf{A}$ is $\mathbf{A}^{\dagger}=\mathbf{A}^{T}$ and the orthogonal projection matrix is

$$
\mathbf{A} \mathbf{A}^{\dagger}=\mathbf{A} \mathbf{A}^{T}=\left(\begin{array}{cc}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & -\frac{1}{2} \\
\frac{1}{2} & -\frac{1}{2}
\end{array}\right)\left(\begin{array}{cccc}
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2}
\end{array}\right)=\left(\begin{array}{cccc}
\frac{1}{2} & \frac{1}{2} & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 \\
0 & 0 & \frac{1}{2} & \frac{1}{2} \\
0 & 0 & \frac{1}{2} & \frac{1}{2}
\end{array}\right)
$$

## Generalized inverse and pseudoinverse

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

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

Proof. We verify this result using an example. Let

$$
\mathbf{A}=\left[\begin{array}{lll}
0 & 0 & 0 \\
0 & 3 & 0
\end{array}\right] \quad \text { and } \quad \mathbf{B}=\left[\begin{array}{cc}
0 & 0 \\
0 & \frac{1}{3} \\
0 & 0
\end{array}\right]
$$

Then

$$
\mathbf{A B}=\left[\begin{array}{ll}
0 & 0 \\
0 & 1
\end{array}\right] \quad \text { and } \quad \mathbf{B A}=\left[\begin{array}{lll}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0
\end{array}\right]
$$

both of which are symmetric. Furthermore,

$$
\begin{aligned}
& \mathbf{A B A}=\left[\begin{array}{ll}
0 & 0 \\
0 & 1
\end{array}\right]\left[\begin{array}{lll}
0 & 0 & 0 \\
0 & 3 & 0
\end{array}\right]=\left[\begin{array}{lll}
0 & 0 & 0 \\
0 & 3 & 0
\end{array}\right]=\mathbf{A} \\
& \mathbf{B A B}=\left[\begin{array}{lll}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0
\end{array}\right]\left[\begin{array}{ll}
0 & 0 \\
0 & \frac{1}{3} \\
0 & 0
\end{array}\right]=\left[\begin{array}{ll}
0 & 0 \\
0 & \frac{1}{3} \\
0 & 0
\end{array}\right]=\mathbf{B} .
\end{aligned}
$$

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

## Generalized inverse and pseudoinverse

Theorem 0.7. Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ be an arbitrary 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:

$$
\left.\begin{array}{rl}
\mathbf{A} \mathbf{A}^{\dagger} \mathbf{A} & =\mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T} \cdot \mathbf{V} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T} \cdot \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T}=\mathbf{U} \boldsymbol{\Sigma} \boldsymbol{\Sigma}^{\dagger} \boldsymbol{\Sigma} \mathbf{V}^{T}=\mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T}=\mathbf{A} \\
\mathbf{A}^{\dagger} \mathbf{A} \mathbf{A}^{\dagger} & =\mathbf{V} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T} \cdot \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T} \cdot \mathbf{V} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T}=\mathbf{V} \boldsymbol{\Sigma}^{\dagger} \boldsymbol{\Sigma} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T}=\mathbf{V} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T}=\mathbf{A}^{\dagger} \\
\mathbf{A A}^{\dagger} & =\mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T} \cdot \mathbf{V} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T}=\mathbf{U} \boldsymbol{\Sigma} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T} \\
\mathbf{A}^{\dagger} \mathbf{A} & =\mathbf{V} \boldsymbol{\Sigma}^{\dagger} \mathbf{U}^{T} \cdot \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{T}=\mathbf{V} \boldsymbol{\Sigma}^{\dagger} \boldsymbol{\Sigma} \mathbf{V}^{T}
\end{array} \quad \text { (symmetric) }\right) \text { (symmetric) }
$$

## Generalized inverse and pseudoinverse

Remark. The formula for $\mathbf{A}^{\dagger}$ is also in (full) SVD form:

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

It can be simplified to the compact SVD form

$$
\mathbf{A}^{\dagger}=\mathbf{V}_{r} \boldsymbol{\Sigma}_{r}^{-1} \mathbf{U}_{r}^{T}
$$

Thus, it suffices to find the compact SVD of $\mathbf{A}$ and use it to find $\mathbf{A}^{\dagger}$.
This simplified formula is computationally more efficient, as it avoids computing the redundant left/right singular vectors.

## Generalized inverse and pseudoinverse

Example 0.12. Consider again the matrix (with compact SVD)

$$
\underbrace{\left(\begin{array}{cc}
1 & -1 \\
0 & 1 \\
1 & 0
\end{array}\right)}_{\mathbf{A}}=\underbrace{\left(\begin{array}{cc}
\frac{2}{\sqrt{6}} & 0 \\
-\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}}
\end{array}\right)}_{\mathbf{U}_{2}} \cdot \underbrace{\left(\begin{array}{cc}
\sqrt{3} & 0 \\
0 & 1
\end{array}\right)}_{\boldsymbol{\Sigma}_{2}} \cdot \underbrace{\left(\begin{array}{cc}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{array}\right)^{T}}_{\mathbf{V}_{2}^{T}}
$$

By the last theorem,

$$
\mathbf{A}^{\dagger}=\underbrace{\left(\begin{array}{cc}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{array}\right)}_{\mathbf{V}_{2}} \cdot \underbrace{\left(\begin{array}{cc}
\frac{1}{\sqrt{3}} & 0 \\
0 & 1
\end{array}\right)}_{\boldsymbol{\Sigma}_{2}^{-1}} \cdot \underbrace{\left(\begin{array}{cc}
\frac{2}{\sqrt{6}} & 0 \\
-\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}}
\end{array}\right)^{T}}_{\mathbf{U}_{2}^{T}}=\frac{1}{3}\left(\begin{array}{ccc}
1 & 1 & 2 \\
-1 & 2 & 1
\end{array}\right)
$$

## Generalized inverse and pseudoinverse

Let $\mathbf{A}=\mathbf{U}_{r} \boldsymbol{\Sigma}_{r} \mathbf{V}_{r}^{T}$ be the compact SVD of a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$. We already know that the columns of $\mathbf{U}_{r}$ form an orthonormal basis for $\operatorname{Col}(\mathbf{A})$, and thus $\operatorname{Col}\left(\mathbf{U}_{r}\right)=\operatorname{Col}(\mathbf{A})$. Intuitively, the orthogonal projection matrices onto them must be the same, i.e.,

$$
\mathbf{A} \mathbf{A}^{\dagger}=\mathbf{U}_{r} \mathbf{U}_{r}^{T}
$$

Consequently, we could just use the matrix $\mathbf{U}_{r}$ (which has orthonormal columns) to compute the orthogonal projection matrix.

This idea can be verified as follows:

$$
\mathbf{A} \mathbf{A}^{\dagger}=\mathbf{U}_{r} \boldsymbol{\Sigma}_{r} \underbrace{\mathbf{V}_{r}^{T} \cdot \mathbf{V}_{r}}_{\mathbf{I}_{r}} \boldsymbol{\Sigma}_{r}^{-1} \mathbf{U}_{r}^{T}=\mathbf{U}_{r} \boldsymbol{\Sigma}_{r} \boldsymbol{\Sigma}_{r}^{-1} \mathbf{U}_{r}^{T}=\mathbf{U}_{r} \mathbf{U}_{r}^{T} .
$$

## Generalized inverse and pseudoinverse

Example 0.13. In the preceding example, we have already obtained the compact SVD of the matrix $\mathbf{A}=\left(\begin{array}{cc}1 & -1 \\ 0 & 1 \\ 1 & 0\end{array}\right)$.

Thus, we could compute the orthogonal projection matrix onto the column space of A as follows:

$$
\mathbf{U}_{2} \mathbf{U}_{2}^{T}=\left(\begin{array}{cc}
\frac{2}{\sqrt{6}} & 0 \\
-\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\
\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{2}}
\end{array}\right)\left(\begin{array}{ccc}
\frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{array}\right)=\frac{1}{3}\left(\begin{array}{ccc}
2 & -1 & 1 \\
-1 & 2 & 1 \\
1 & 1 & 2
\end{array}\right)
$$

It is the same with that obtained in Example 0.10.

## Generalized inverse and pseudoinverse

Example 0.14. Find the pseudoinverse of $\mathbf{A}=\left[\begin{array}{ll}1 & 0 \\ 1 & 0\end{array}\right]$.
Observe that $\operatorname{rank}(\mathbf{A})=1$. Thus, we can obtain its compact SVD easily:

$$
\mathbf{A}=\binom{1}{1}\left(\begin{array}{ll}
1 & 0
\end{array}\right)=\binom{\frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{2}}} \cdot \sqrt{2} \cdot\left(\begin{array}{ll}
1 & 0
\end{array}\right)
$$

It follows that the orthogonal projection matrix is

$$
\mathbf{A A}^{\dagger}=\binom{\frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{2}}}\left(\begin{array}{ll}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{array}\right)=\left(\begin{array}{cc}
\frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2}
\end{array}\right)
$$

How to find $\mathbf{A}^{\dagger}$ by using the compact SVD?

## MATLAB function for computing pseudoinverse

pinv Pseudoinverse.
$X=\operatorname{pinv}(A)$ produces a matrix $X$ of the same dimensions as $A^{\prime}$ so that $A * X * A=A, X * A * X=X$ and $A * X$ and $X * A$ are Hermitian. The computation is based on $\operatorname{SVD}(A)$ and any singular values less than a tolerance are treated as zero.
$\operatorname{pinv}(A, T O L)$ treats all singular values of $A$ that are less than $T O L$ as zero. By default, $T O L=\max (\operatorname{size}(A)) * \operatorname{eps}(\operatorname{norm}(A))$.

## Applications of matrix pseudoinverse

- Linear least squares
- Minimum-norm solution to a consistent linear system


## Linear least squares

Consider a system of linear equations $\mathbf{A x}=\mathbf{b}$ where $\mathbf{A} \in \mathbb{R}^{m \times n}$ (not necessarily of full column rank) 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 general 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.

## Generalized inverse and pseudoinverse

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

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

Proof. Since $\mathbf{A x} \in \operatorname{Col}(\mathbf{A})$, the optimal x should be such that

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

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

## Generalized inverse and pseudoinverse

## Minimum-norm solution to a consistent linear system

For under-determined systems $\mathbf{A x}=\mathbf{b}$, 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 $\mathbf{A x}=\mathbf{b}$ has solutions, then $\mathbf{x}^{*}=\mathbf{A}^{\dagger} \mathbf{b}$ is an exact solution and has the smallest possible norm, i.e., $\left\|\mathrm{x}^{*}\right\| \leq\|\mathrm{x}\|$ for all solutions x .


## Generalized inverse and pseudoinverse

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

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

It follows that

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

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

## Summary

- Generalized inverse $\mathbf{G} \in \mathbb{R}^{n \times m}$ for a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$.
- Definition: AGA = A
- Existence: G always exists but might not be unique
- Computing: $\mathbf{A}=\left[\begin{array}{ll}A_{11} & A_{12} \\ A_{21} & A_{22}\end{array}\right] \rightarrow \mathbf{G}=\left[\begin{array}{cc}A_{11}^{-1} & O \\ O & O\end{array}\right]$, if $A_{11} \in \mathbb{R}^{r \times r}, r=\operatorname{rank}(\mathbf{A})$ is invertible.
- Property: AG is a projection matrix onto $\operatorname{Col}(\mathbf{A})$
- Application: $\mathbf{x}=\mathbf{G b}$ is a solution to $\mathbf{A x}=\mathbf{b}$ (if consistent)


## Generalized inverse and pseudoinverse

- Pseudoinverse $\mathbf{A}^{\dagger} \in \mathbb{R}^{n \times m}$ for a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$.
- Definition: $\mathbf{A A}^{\dagger} \mathbf{A}=\mathbf{A}^{\dagger}$, and $\mathbf{A}^{\dagger} \mathbf{A} \mathbf{A}^{\dagger}=\mathbf{A}$, and both $\mathbf{A A}^{\dagger}, \mathbf{A}^{\dagger} \mathbf{A}$ are symmetric
- Existence: $\mathbf{A}^{\dagger}$ always exists and is unique
- Computing:
* If $\mathbf{A}$ has full column rank: $\mathbf{A}^{\dagger}=\left(\mathbf{A}^{T} \mathbf{A}\right)^{-1} \mathbf{A}^{T}$
* If $\mathbf{A}$ is "diagonal": $\mathbf{A}^{\dagger} \in \mathbb{R}^{n \times m}$ is also "diagonal" with reciprocals of nonzero diagonals of $\mathbf{A}$


## Generalized inverse and pseudoinverse

* In general: $\mathbf{A}^{\dagger}=\mathbf{V}_{r} \boldsymbol{\Sigma}_{r}^{-1} \mathbf{U}_{r}^{T}$ (using compact SVD $\mathbf{A}=$ $\left.\mathbf{U}_{r} \boldsymbol{\Sigma}_{r} \mathbf{V}_{r}^{T}\right)$
- Property: $\mathbf{A A}^{\dagger}$ is an orthogonal projection matrix onto $\operatorname{Col}(\mathbf{A})$, and $\mathbf{A} \mathbf{A}^{\dagger}=\mathbf{U}_{r} \mathbf{U}_{r}^{T}$
- Application: For any $\mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{b} \in \mathbb{R}^{m}$, the vector $\mathbf{A}^{\dagger} \mathbf{b}$ solves the least squares problem

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

* If $\mathbf{A}$ has full column rank, then the solution is unique.
* If $\mathbf{A x}=\mathbf{b}$ has exact solutions, then $\mathbf{A}^{\dagger} \mathbf{b}$ is the minimumnorm solution.


# Next time: Matrix norm and low-rank approximation 

Read the book chapter on the topic.

