HW 5 due next Thurs Nov 5
before lecture.
Class on Tues Nov 3 (election day)
is optional. Please Vote!

Current Topic: "Least Squares"
e.g. fitting a line to data points.

General Theorem:
Consider a linear system $A\vec{x} = \vec{b}$.
If the system has no solution,
then will look for the "best" approximate
solution: $$A\hat{x} \approx \vec{b}.$$

"Best" in the sense that the length
$$\| A\hat{x} - \vec{b} \|$$
is MINIMIZED. This is called a
"least squares" approximation

because the (squared) length is the sum of the squares of the coordinates.

I claim that the solution $\hat{x}$ satisfies the "normal equation"

$$\boxed{A^T A \hat{x} = A^T \vec{b}}$$

Today I will explain how this works.

Jargon: Let A be $m \times n$ matrix.

We define the <u>column space</u> of A:

$$C(A) = \{ \text{set of vectors } A\vec{x} \}$$

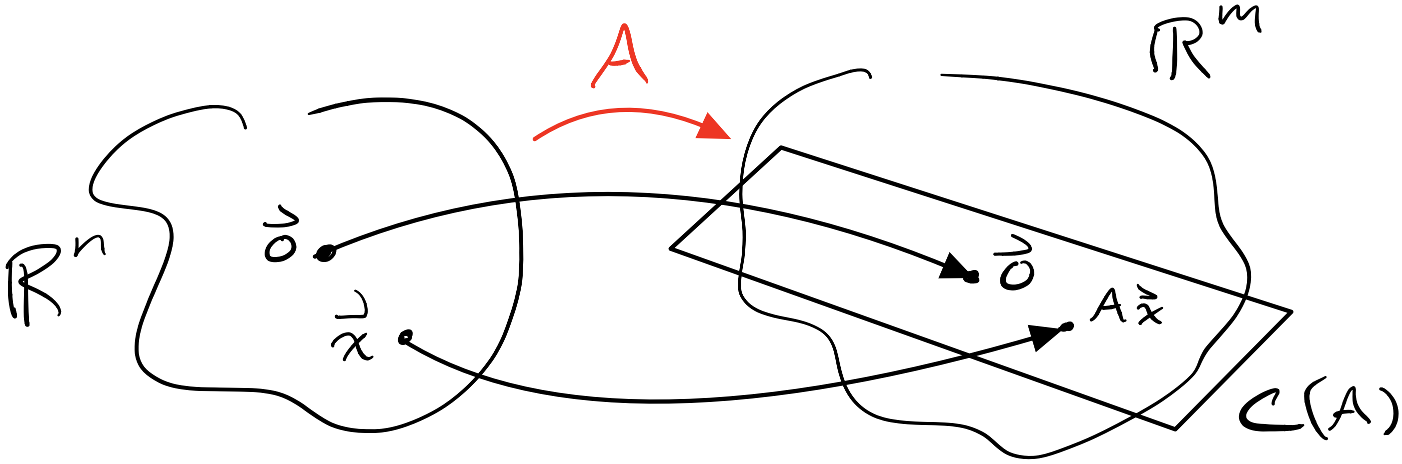
If $A = \begin{pmatrix} | & | & & | \\ \vec{a}_1 & \vec{a}_2 & \cdots & \vec{a}_n \\ | & | & & | \end{pmatrix}$ then

this becomes

$$C(A) = \{ x_1 \vec{a}_1 + x_2 \vec{a}_2 + \cdots + x_n \vec{a}_n \}$$

= the set of all linear combinations of the columns of A.

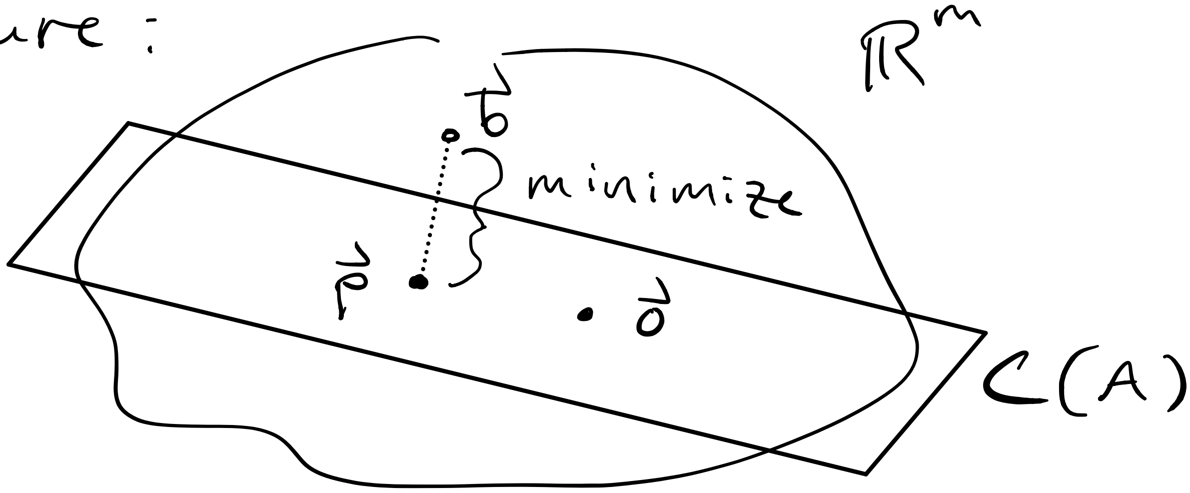
Picture:



Maybe the column space does not fill up all of $\mathbb{R}^m$.

If system $A\vec{x} = \vec{b}$ has no solution $\vec{x}$, then this just means that point $\vec{b}$ <u>is not in column space</u> $C(A)$.

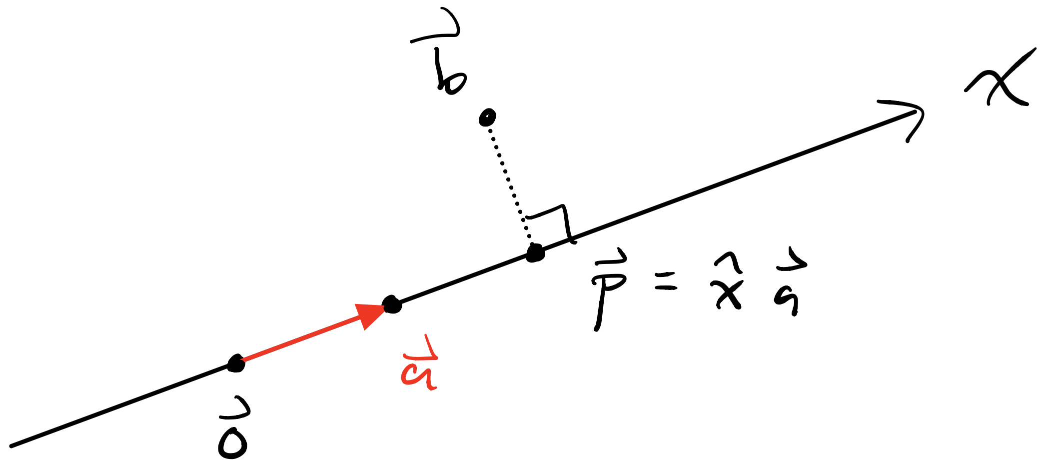
Picture:



In this case we want to find the point $\vec{p}$ in the column space that is closest to $\vec{b}$.

Example when $C(A)$ is a line.

Let $A = \vec{a} \in \mathbb{R}^m$, $C(A) = x\vec{a}$.



Distance $\|\vec{p} - \vec{b}\|$ is minimized when $\vec{p} - \vec{b}$ is $\perp$ to the line, i.e., $\perp$ to vector $\vec{a}$. Furthermore, since $\vec{p}$ is on the line we must have $\vec{p} = \hat{x}\vec{a}$ for some $\hat{x} \in \mathbb{R}$.

Solve for $\hat{x}$. Two key facts:

- $\vec{p} = \hat{x}\,\vec{a}$,
- $\vec{a}^T(\vec{p} - \vec{b}) = 0$.

Combine:

$$\vec{a}^T(\hat{x}\,\vec{a} - \vec{b}) = 0$$

$$\hat{x}\,\vec{a}^T\vec{a} - \vec{a}^T\vec{b} = 0$$

$$\hat{x}\,\vec{a}^T\vec{a} = \vec{a}^T\vec{b}$$

$$\hat{x} = \frac{\vec{a}^T\vec{b}}{\vec{a}^T\vec{a}} \left(= \frac{\vec{a}\cdot\vec{b}}{\vec{a}\cdot\vec{a}} \right)$$

Conclusion: The <u>projection</u> $\vec{p}$ of the <u>point</u> $\vec{b}$ onto the <u>line</u> $t\vec{a}$ is

$$\vec{p} = \hat{x}\,\vec{a} = \underbrace{\left(\frac{\vec{a}\cdot\vec{b}}{\vec{a}\cdot\vec{a}}\right)}_{\text{scalar}} \underset{\uparrow \atop \text{vector.}}{\vec{a}}$$

Example: $\vec{a} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

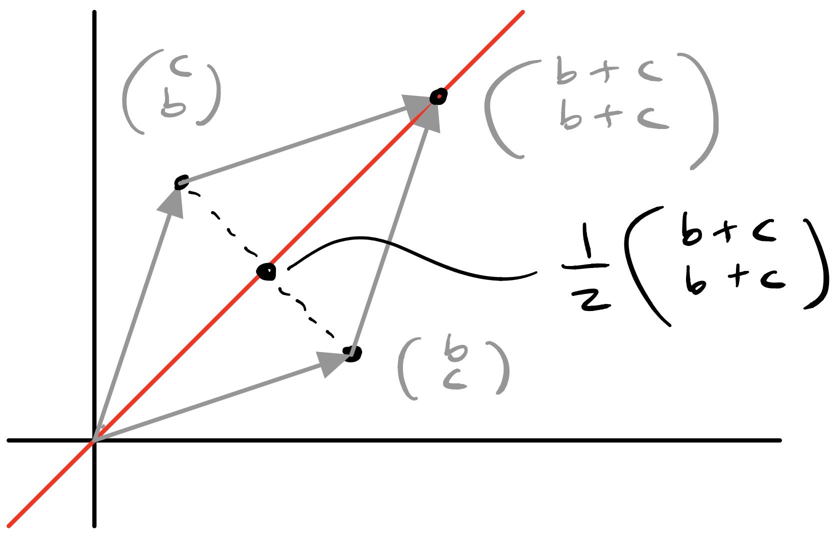
Project a general point $\vec{b} = \begin{pmatrix} b \\ c \end{pmatrix}$ onto the line $t\begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

From above formula:

$$\vec{p} = \left(\frac{\vec{a} \circ \vec{b}}{\vec{a} \circ \vec{a}} \right) \vec{a}$$

$$= \frac{b+c}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} (b+c)/2 \\ (b+c)/2 \end{pmatrix}.$$

Picture: Makes sense ✓



Furthermore, let P be the 2×2 matrix that projects onto this line:

$$P\begin{pmatrix} b \\ c \end{pmatrix} = \begin{pmatrix} (b+c)/2 \\ (b+c)/2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}b + \frac{1}{2}c \\ \frac{1}{2}b + \frac{1}{2}c \end{pmatrix}$$

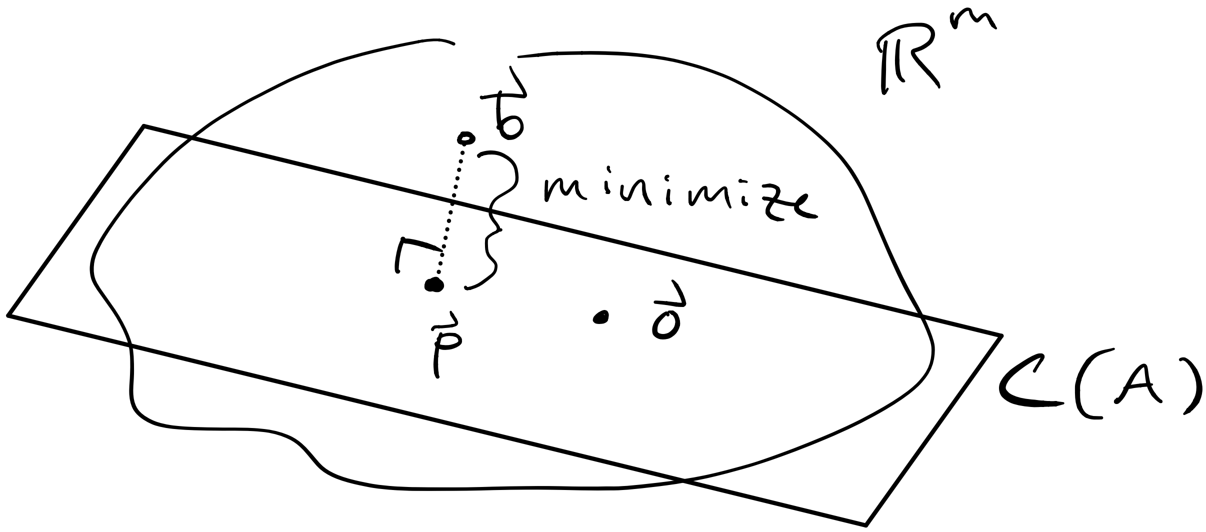
What is P?

$$P = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}.$$

Check:

$$\begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \begin{pmatrix} b \\ c \end{pmatrix} = \begin{pmatrix} \frac{1}{2}b + \frac{1}{2}c \\ \frac{1}{2}b + \frac{1}{2}c \end{pmatrix} \checkmark$$

General Case:



In this case, every point of

the column space looks like $A\hat{x}$ for some vector $\hat{x} \in \mathbb{R}^n$, so

$$\vec{p} = A\hat{x} \text{ for some } \hat{x}.$$

To minimize the length $\|\vec{p}-\vec{b}\|$, want vector $\vec{p}-\vec{b}$ to be perpendicular to the column space.

How can we say that $\vec{p}-\vec{b}$ is $\perp$ to a whole space?

Let $A = \begin{pmatrix} \vec{a}_1 & \vec{a}_2 & \cdots & \vec{a}_n \end{pmatrix}$. Then

$\vec{v}$ is $\perp$ to $C(A)$

$\iff$ $\vec{v}$ $\perp$ to every column of A.

$\iff$ $\vec{a}_i^T \vec{v} = 0$ for all i.

Note: This is the same as saying that $A^T \vec{v} = \vec{0}$!

$$A^T\vec{v} = \begin{pmatrix} \text{---}\ \vec{a}_1^T\ \text{---} \\ \vdots \\ \text{---}\ \vec{a}_n^T\ \text{---} \end{pmatrix}\vec{v}$$

$$= \begin{pmatrix} \vec{a}_1^T\vec{v} \\ \vdots \\ \vec{a}_n^T\vec{v} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix} = \vec{0}.$$

Repeat:

$$\boxed{\vec{v} \perp C(A) \iff A^T\vec{v} = \vec{0}}$$

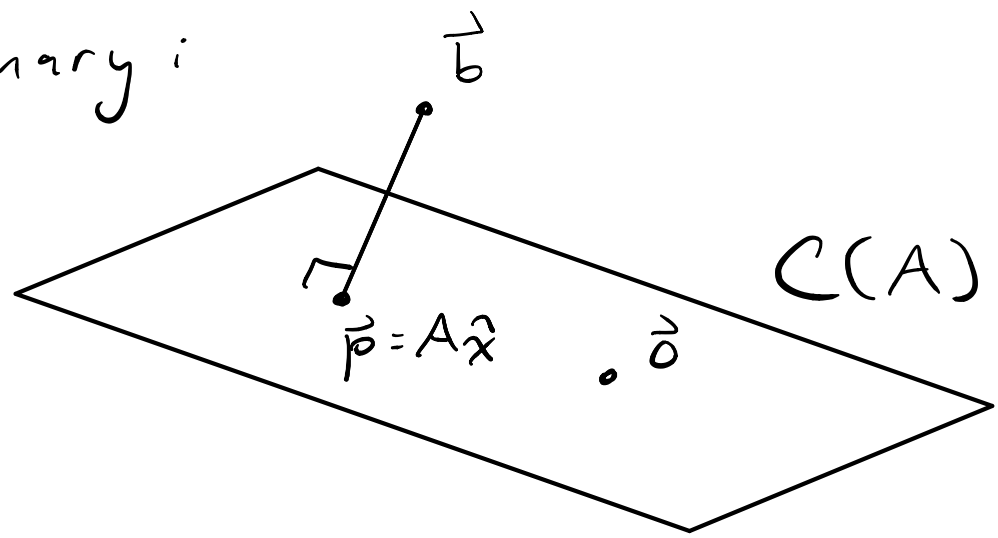
Let's use this. We have

- $\vec{p} = A\hat{x}$
- $A^T(\vec{p} - \vec{b}) = \vec{0}$.

Combine:
$$A^T(A\hat{x} - \vec{b}) = \vec{0}$$
$$A^TA\hat{x} - A^T\vec{b} = \vec{0}$$
$$A^TA\hat{x} = A^T\vec{b}$$

Just as I claimed. ✓

Summary:



Distance $\| A\hat{x} - \vec{b} \|$ minimized

when $A^T A \hat{x} = A^T \vec{b}$.

This is called the "normal equation"

(because of all the right angles).

Example: Project onto the

plane $s(1,1,1) + t(1,2,3)$.

Express the plane as the column

space of $A = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}$.

To project $\vec{b} = (b, c, d)$ onto the plane, let $\vec{p} = A\hat{x}$, so

$$A^T A \hat{x} = A^T \vec{b}$$

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \hat{x} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} b \\ c \\ d \end{pmatrix}$$

$$\begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix} \hat{x} = \begin{pmatrix} b+c+d \\ b+2c+3d \end{pmatrix}$$

$$\hat{x} = \frac{1}{6} \begin{pmatrix} 14 & -6 \\ -6 & 3 \end{pmatrix} \begin{pmatrix} b+c+d \\ b+2c+d \end{pmatrix}.$$

Conclusion: The projection of $\vec{b} = (b, c, d)$ onto the plane is

$$\vec{p} = A\hat{x} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \frac{1}{6} \begin{pmatrix} 14 & -6 \\ -6 & 3 \end{pmatrix} \begin{pmatrix} b+c+d \\ b+2c+3d \end{pmatrix}$$

That's a mess! ☹

Let's try to simplify. We have

- $\vec{p} = A\hat{x}$
- $A^T A \hat{x} = A^T \vec{b}$.

Assuming that $A^T A$ is invertible then we have

$$A^T A \hat{x} = A^T \vec{b}$$

$$\cancel{(A^T A)^{-1} A^T A} \hat{x} = (A^T A)^{-1} A^T \vec{b}$$

$$\hat{x} = (A^T A)^{-1} A^T \vec{b}$$

$$A\hat{x} = A(A^T A)^{-1} A^T \vec{b}$$

$$\vec{p} = \underbrace{A(A^T A)^{-1} A^T}_{\text{this is the matrix that does the projection.}} \vec{b}.$$

Summary: The matrix that projects any point onto column space of A is

$$\boxed{P = A(A^T A)^{-1} A^T}$$

Check our first Example:

- $A = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$P = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \left[\begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right]^{-1} \begin{pmatrix} 1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 1 \end{pmatrix} [2]^{-1} \begin{pmatrix} 1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & 1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \checkmark$$

More generally, for any column vector $\vec{a}$, the matrix that projects onto the <u>Line</u> $t\vec{a}$ is

$$P = \vec{a}\left(\vec{a}^T\vec{a}\right)^{-1}\vec{a}^T$$

$$= \vec{a}\,\underbrace{\left(\vec{a}\cdot\vec{a}\right)}_{\text{scalar}}^{-1}\vec{a}^T$$

$$= \frac{1}{\underbrace{\vec{a}\cdot\vec{a}}_{\text{scalar}}}\,\underbrace{\vec{a}\,\vec{a}^T}_{\text{matrix}} = \frac{1}{\|\vec{a}\|^2}\,\vec{a}\,\vec{a}^T.$$

Example: To project onto the line $t(1,-2,1)$ in $\mathbb{R}^3$:

$$P = \frac{1}{\left\|\begin{pmatrix}1\\-2\\1\end{pmatrix}\right\|^2}\begin{pmatrix}1\\-2\\1\end{pmatrix}\begin{pmatrix}1 & -2 & 1\end{pmatrix}$$

$$= \frac{1}{6}\begin{pmatrix}1 & -2 & 1\\-2 & 4 & -2\\1 & -2 & 1\end{pmatrix}.$$

Return to previous example:

- To project onto the plane

$$C(A) = C\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} = s\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + t\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix},$$

the matrix is:

$$Q = A(A^T A)^{-1} A^T$$

$$= \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix}^{-1} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \frac{1}{6} \begin{pmatrix} 14 & -6 \\ -6 & 3 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}$$

$\vdots$ compute

$$= \frac{1}{6}\begin{pmatrix} 5 & 2 & -1 \\ 2 & 2 & 2 \\ -1 & 2 & 5 \end{pmatrix}.$$

That was a bit of work, but I claim there is a shortcut!

Let P = project onto <u>line</u> $t(1,-2,1)$

Q = proj. onto <u>plane</u> $s(1,1,1) + t(1,2,3)$.

Since this line and plane are "orthogonal complements" of each other, I claim that we must have

$$P + Q = I$$

Check: $P + Q$

$$= \frac{1}{6}\begin{pmatrix} 1 & -2 & 1 \\ -2 & 4 & -2 \\ 1 & -2 & 1 \end{pmatrix} + \frac{1}{6}\begin{pmatrix} 5 & 2 & -1 \\ 2 & 2 & 2 \\ -1 & 2 & 5 \end{pmatrix}$$

$$= \frac{1}{6}\begin{pmatrix} 6 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 6 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \checkmark$$

I'll explain later why this works.