Least Squares

Geometric Algorithms

Lecture 23

CAS CS 132

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Introduction

Recap Problem

$$\mathbf{u} = \begin{bmatrix} 1 \\ 3 \\ -2 \\ -1 \end{bmatrix} \qquad \mathbf{v} = \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix}$$

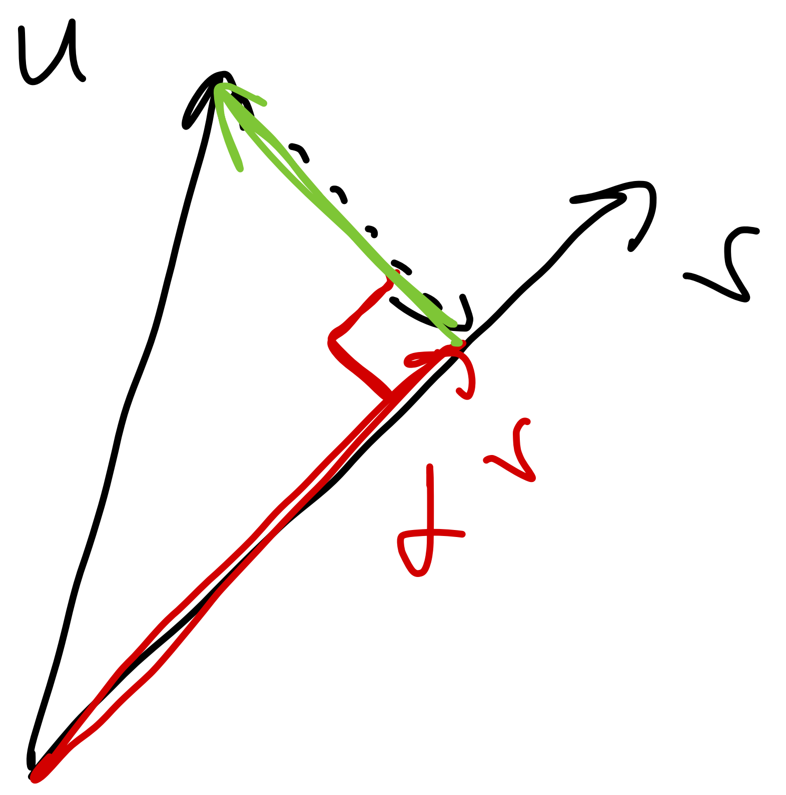
Find the orthogonal projection of $\mathbf{u}$ *onto the span of* $\mathbf{v}$*.*

Answer

$$\alpha \vec{r} = \frac{\langle u, r \rangle}{\langle r, r \rangle} \vec{r}$$

$$\begin{bmatrix} 0 \\ 5/2 \\ -5/2 \\ 0 \end{bmatrix}$$

$$\hat{\mathbf{u}} = \begin{bmatrix} 0 \\ 5/2 \\ -5/2 \\ 0 \end{bmatrix}$$



$$\alpha \vec{v} = \frac{5}{2} \begin{bmatrix} 0 \\ 1 \\ -1 \\ 1 \end{bmatrix}$$

$$u = \begin{bmatrix} 1 \\ 3 \\ -2 \\ -1 \end{bmatrix} \quad v = \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix}$$

$$\langle u - \alpha v, v \rangle = 0$$

$$\langle u, v \rangle - \langle \alpha v, v \rangle =$$

$$\langle u, v \rangle - \alpha \langle v, v \rangle = 0$$

$$\langle u, v \rangle = 0 + 3 + 2 + 0 = 5$$

$$\langle v, v \rangle = 0 + 1 + 1 + 0 = 2$$

$$\|v\|^2$$

Objectives

1. Introduce the least squares problem as a method of *approximating* solutions to matrix equations.

2. Learn how to solve the least squares problems.

3. Connect least squares solutions to projections.

Keywords

general least squares problem

sum of squares error (ℓ_2–error)

least squares solutions

orthogonal projections

normal equations

Orthogonal Matrices

Orthonormal Matrices

$m \times n$

Definition. A matrix is **orthonormal** if its columns form an orthonormal set.

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This is incredibly confusing, but we'll try to be consistent and clear.

Inverses of Orthogonal Matrices

Theorem. If an $n \times n$ matrix U is orthogonal (square orthonormal) then it is invertible and

$U = [\vec{u}_1 \ \ \vec{u}_2]$

$$U^{-1} = U^T$$

Verify: $\begin{bmatrix} \vec{u}_1 \\ \vec{u}_2 \end{bmatrix} [\vec{u}_1 \ \ \vec{u}_2] = \begin{bmatrix} \langle \vec{u}_1, \vec{u}_1 \rangle & \langle \vec{u}_1, \vec{u}_2 \rangle \\ \langle \vec{u}_2, \vec{u}_1 \rangle & \langle \vec{u}_2, \vec{u}_2 \rangle \end{bmatrix}$

$\langle \vec{u}_1, \vec{u}_1 \rangle = 1$, $\langle \vec{u}_1, \vec{u}_2 \rangle = 0$, $\langle \vec{u}_2, \vec{u}_1 \rangle = 0$, $\langle \vec{u}_2, \vec{u}_2 \rangle = 1$

$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Orthonormal Matrices and Inner Products

Theorem. For a $m \times n$ orthonormal matrix U, and any vectors x and y in R^n

$$\langle Ux, Uy \rangle = \langle x, y \rangle$$

Orthonormal matrices preserve inner products.

Verify: $\langle Ux, Uy \rangle = (Ux)^T(Uy) = x^T U^T U y$

$= x^T y = \langle x, y \rangle$

Length, Angle, Orthogonality Preservation

Since <u>lengths</u> and <u>angles</u> are defined in terms of inner products, they are also preserved by orthonormal matrices:

$$\|x\| = \sqrt{\langle x, x \rangle}$$

$$\cos\theta = \left\langle \frac{u}{\|u\|}, \frac{v}{\|v\|} \right\rangle$$

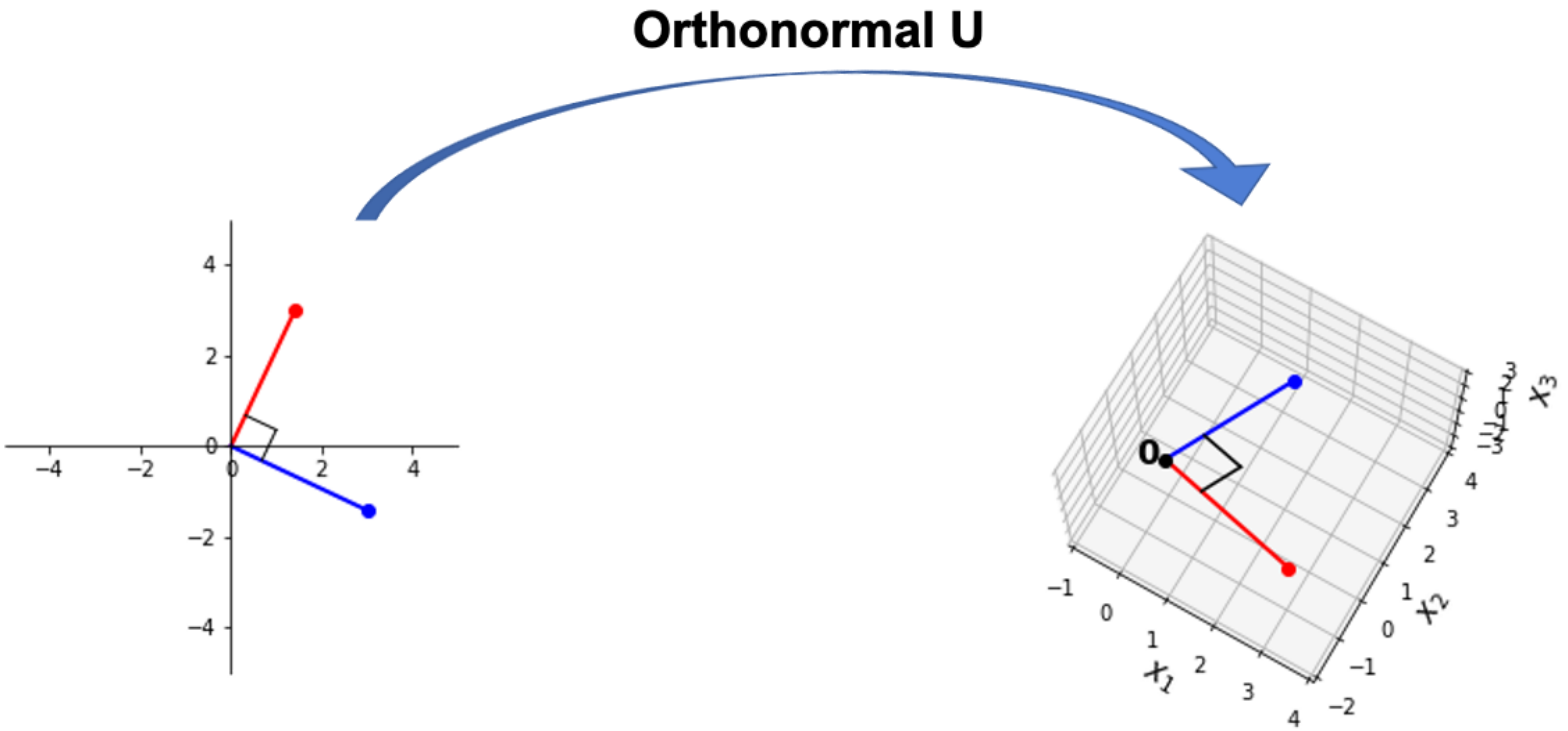
$$\|Ux\| = \sqrt{\langle Ux, Ux \rangle} = \sqrt{\langle x, x \rangle} = \|x\|$$

$$\left\langle \frac{Uu}{\|Uu\|}, \frac{Uv}{\|Uv\|} \right\rangle = \left\langle \frac{Uu}{\|u\|}, \frac{Uv}{\|v\|} \right\rangle$$

$$= \frac{1}{\|u\|\|v\|} \langle Uu, Uv \rangle = \frac{1}{\|u\|\|v\|} \langle u, v \rangle$$

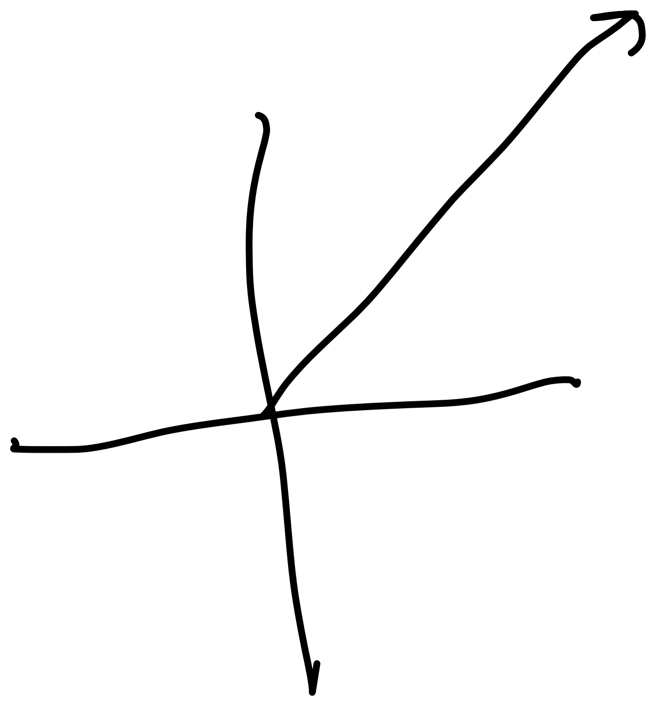
$$= \cos\theta$$

The Picture



Example

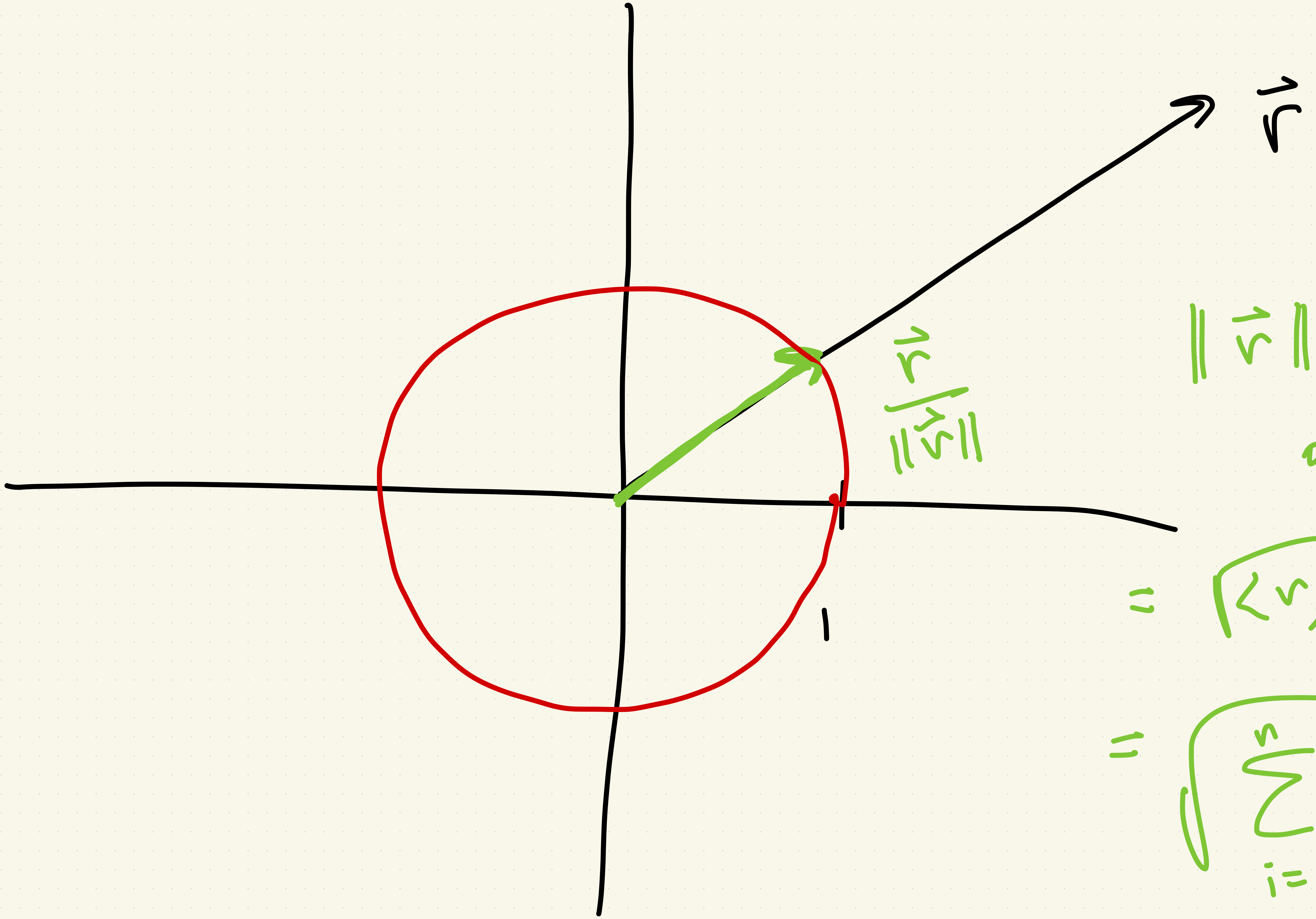
$$U = \begin{bmatrix} 1/\sqrt{2} & 2/3 \\ 1/\sqrt{2} & -2/3 \\ 0 & 1/3 \end{bmatrix} \qquad x = \begin{bmatrix} \sqrt{2} \\ 3 \end{bmatrix}$$



$$Ux = \begin{bmatrix} 1/\sqrt{2}\cdot\sqrt{2} + 2/3\cdot 3 \\ 1/\sqrt{2}\cdot\sqrt{2} - 2/3\cdot 3 \\ 0 + 1/3\cdot 3 \end{bmatrix} = \begin{bmatrix} 3 \\ -1 \\ 1 \end{bmatrix}$$

$$\|x\| = \sqrt{2+9} = \sqrt{11}$$

$$\|Ux\| = \sqrt{9+1+1} = \sqrt{11}$$



$\|\vec{r}\|$ = length of $\vec{r}$

$= \sqrt{\langle r, r \rangle}$

$= \sqrt{\sum_{i=1}^{n} r_i^2}$

Question (Conceptual)

Suppose A is an $m \times n$ matrix with orthogonal but ***not*** *orthonormal columns. What is $A^T A$?*

Remember: for orthonormal matrix

$$A^T A = I$$

Answer

If $A = [\mathbf{a}_1 \ \ \mathbf{a}_2 \ \ \ldots \ \ \mathbf{a}_n]$ then $A^T A$ is a diagonal matrix D where

$$D_{ii} = \|\mathbf{a}_i\|^2$$

$$\begin{bmatrix} \vec{u}_1 \\ \vec{u}_2 \end{bmatrix} \begin{bmatrix} \vec{u}_1 & \vec{u}_2 \end{bmatrix} = \begin{bmatrix} u_1 \cdot u_1 & u_1 \cdot u_2 \\ u_2 \cdot u_1 & u_2 \cdot u_2 \end{bmatrix}$$

$u_1 \cdot u_1 = \|u_1\|^2$, $u_1 \cdot u_2 = 0$, $u_2 \cdot u_1 = 0$, $u_2 \cdot u_2 = \|u_2\|^2$

Motivation

The story of an enterprising CS132 student

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Problem. Solve the equation $A\mathbf{x} = \mathbf{b}$.

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...     [0, 2, 2]])
>>> b = np.array([-1, 2, 3])
>>> np.linalg.solve(A, b)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
  File "/opt/homebrew/lib/python3.11/site-packages/numpy/linalg/linalg.py", line 409, in solve
    r = gufunc(a, b, signature=signature, extobj=extobj)
        ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^

  File "/opt/homebrew/lib/python3.11/site-packages/numpy/linalg/linalg.py", line 112, in _raise_linalgerror_singular
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This doesn't always work.

Reads the docs...

numpy.linalg.solve

`linalg.solve(a, b)` [source]

Solve a linear matrix equation, or system of linear scalar equations.

Computes the "exact" solution, *x*, of the well-determined, i.e., full rank, linear matrix equation *ax* = *b*.

Parameters: **a** : *(..., M, M) array_like*

Coefficient matrix.

b : *{(..., M,), (..., M, K)}, array_like*

Ordinate or "dependent variable" values.

Returns: **x** : *{(..., M,), (..., M, K)} ndarray*

Solution to the system a x = b. Returned shape is identical to *b*.

Raises: **LinAlgError**

If *a* is singular or not square.

See also

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Notes

> *New in version 1.8.0.*

Broadcasting rules apply, see the **`numpy.linalg`** documentation for details.

The solutions are computed using LAPACK routine `_gesv`.

a must be square and of full-rank, i.e., all rows (or, equivalently, columns) must be linearly independent; if either is not true, use **`lstsq`** for the least-squares best "solution" of the system/equation.

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where M and N are the input matrix dimensions.
To use the future default and silence this warning we advise to pass `rcond=None`, to keep using the old,
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(array([-0.11111111,  0.77777778,  0.22222222]), array([], dtype=float64), 2, array([6.84168488e+00,
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Answer: $\mathbf{x} = \begin{bmatrix} -1/9 \\ 7/9 \\ 2/9 \end{bmatrix}$

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Answer: $\mathbf{x} = \begin{bmatrix} -1/9 \\ 7/9 \\ 2/9 \end{bmatrix}$ **This is not correct**

This System is Inconsistent

$$\begin{bmatrix} 1 & 0 & 5 & -1 \\ 1 & -1 & 4 & 2 \\ 0 & 2 & 2 & 3 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 5 & -1 \\ 0 & -1 & -1 & 3 \\ 0 & 2 & 2 & 3 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 5 & -1 \\ 0 & -1 & -1 & 3 \\ 0 & 0 & 0 & 9 \end{bmatrix}$$

The "correct" answer: There is no solution.

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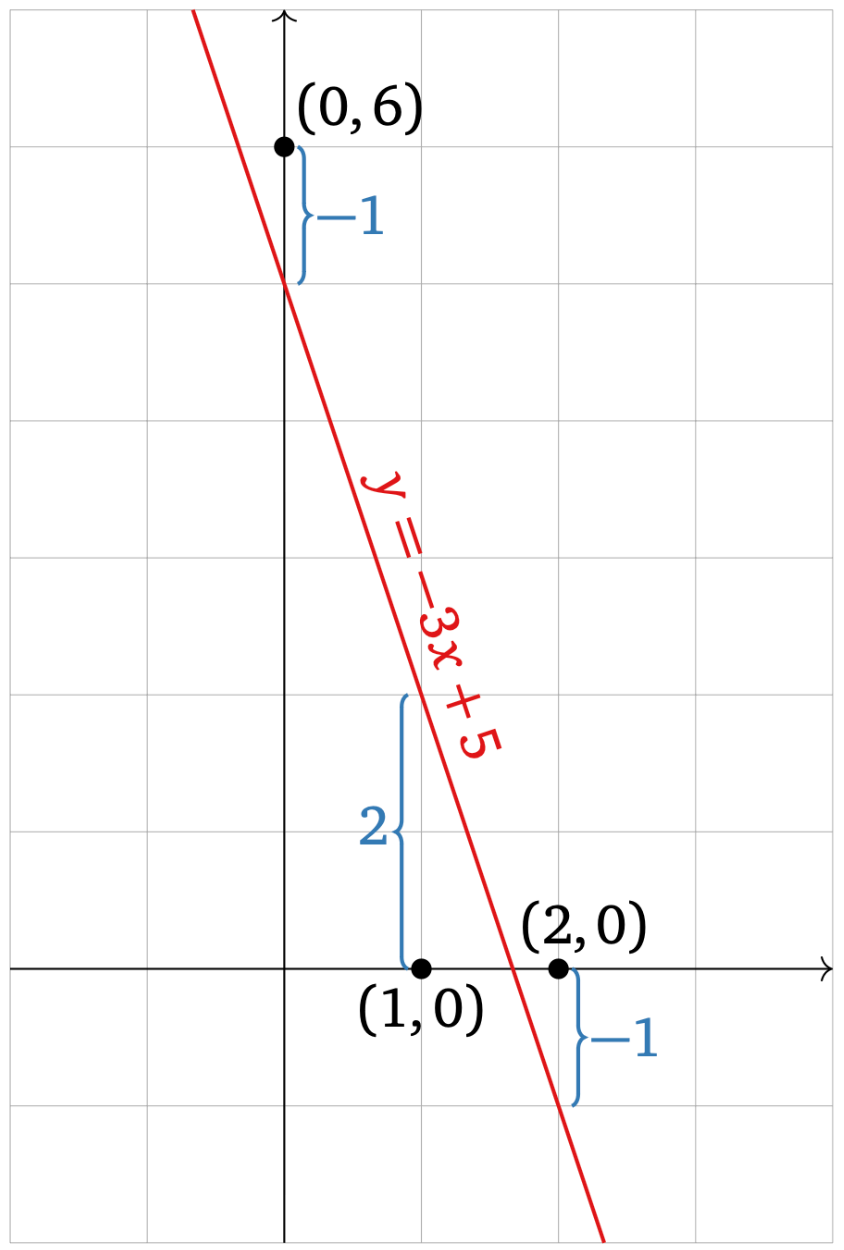
What's going on here?

Non-Linearity



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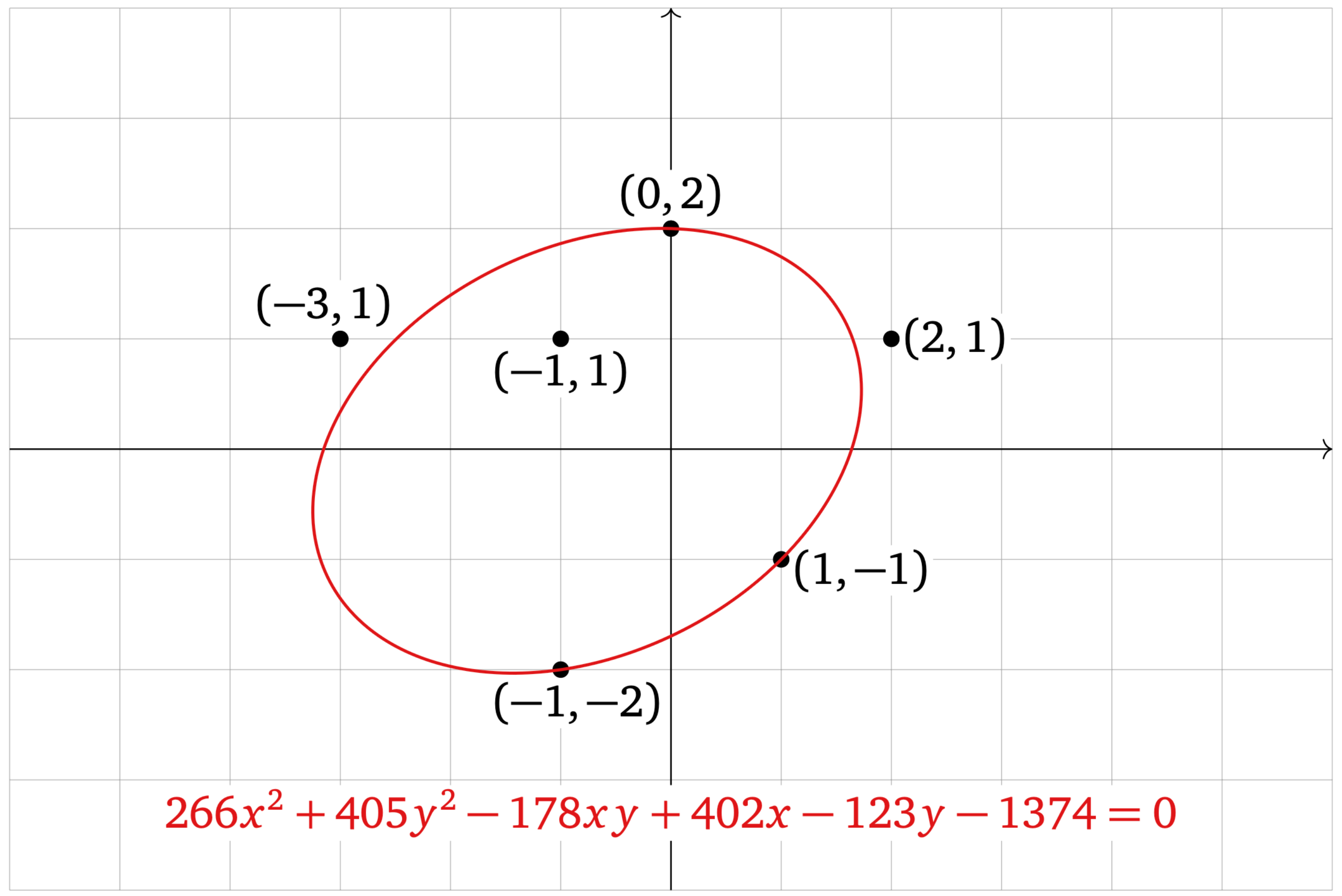
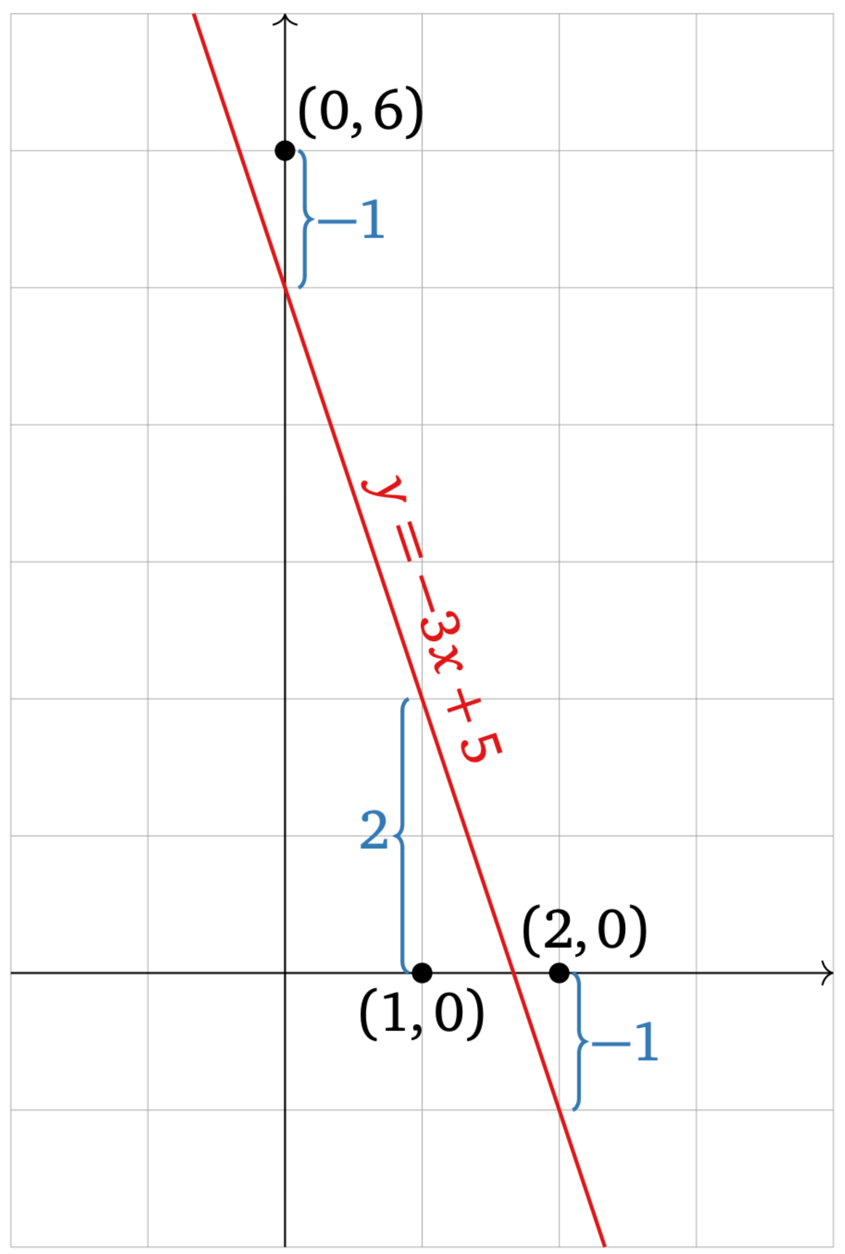


https://textbooks.math.gatech.edu/ila/least-squares.html

Non-Linearity

Linear algebra is very powerful and very clean, but **the world isn't linear**. There are non-linear relationships and sources of *noise*.



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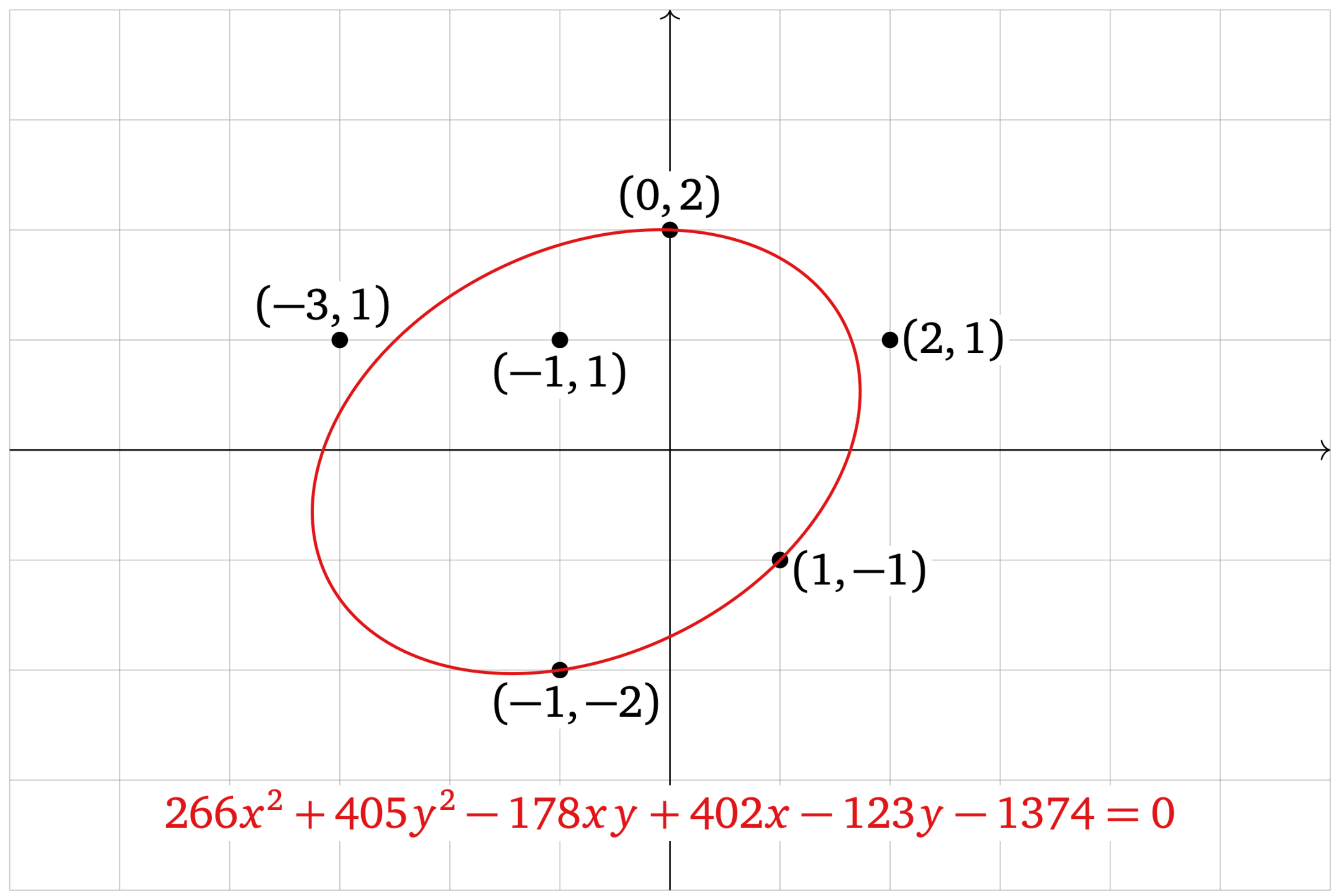

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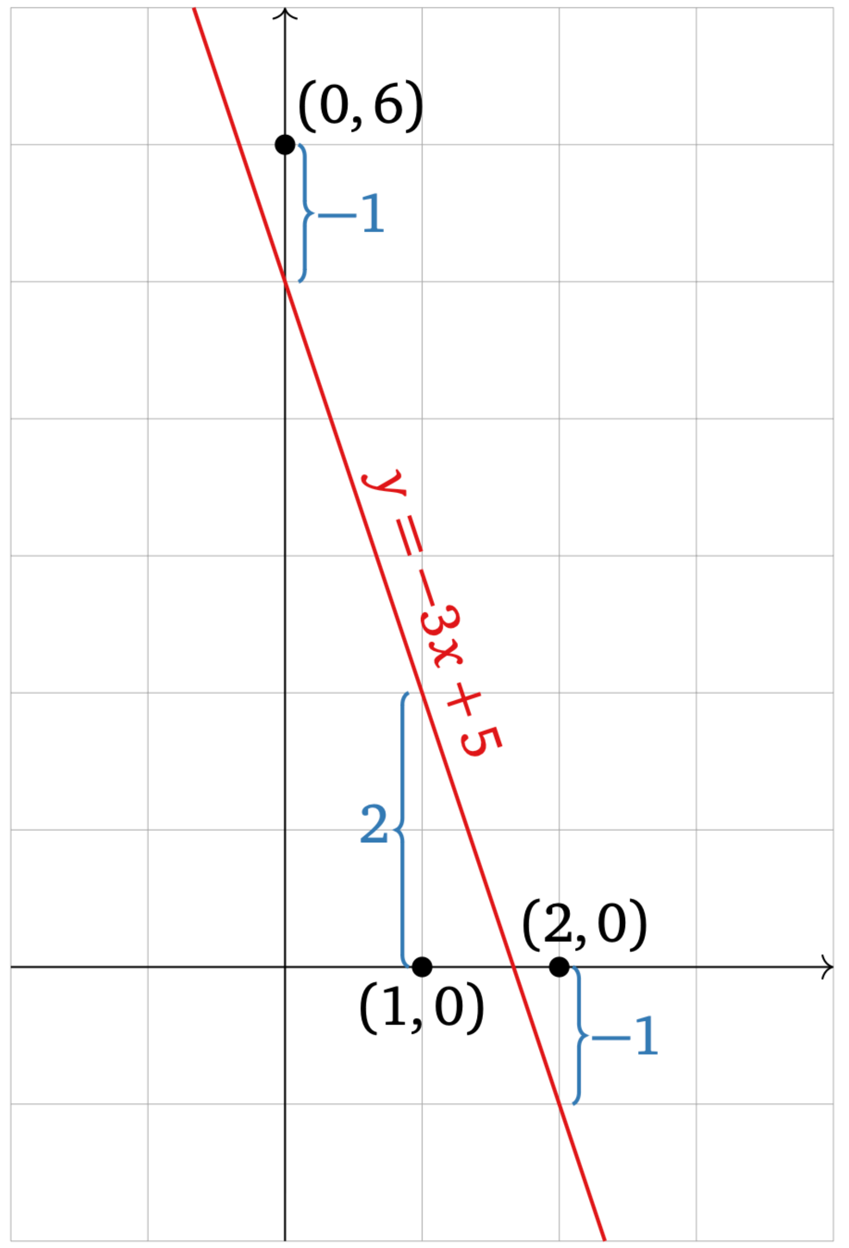

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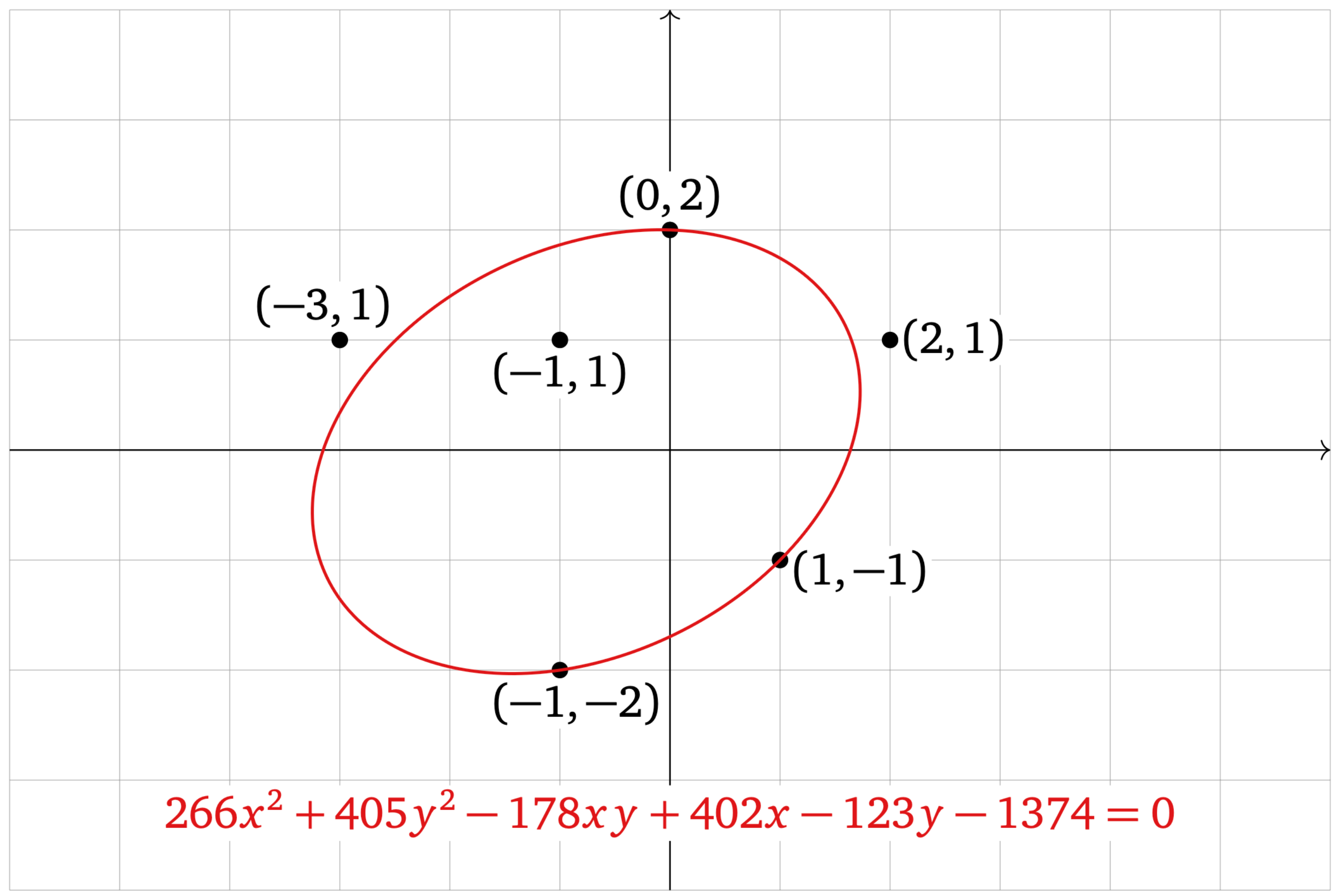

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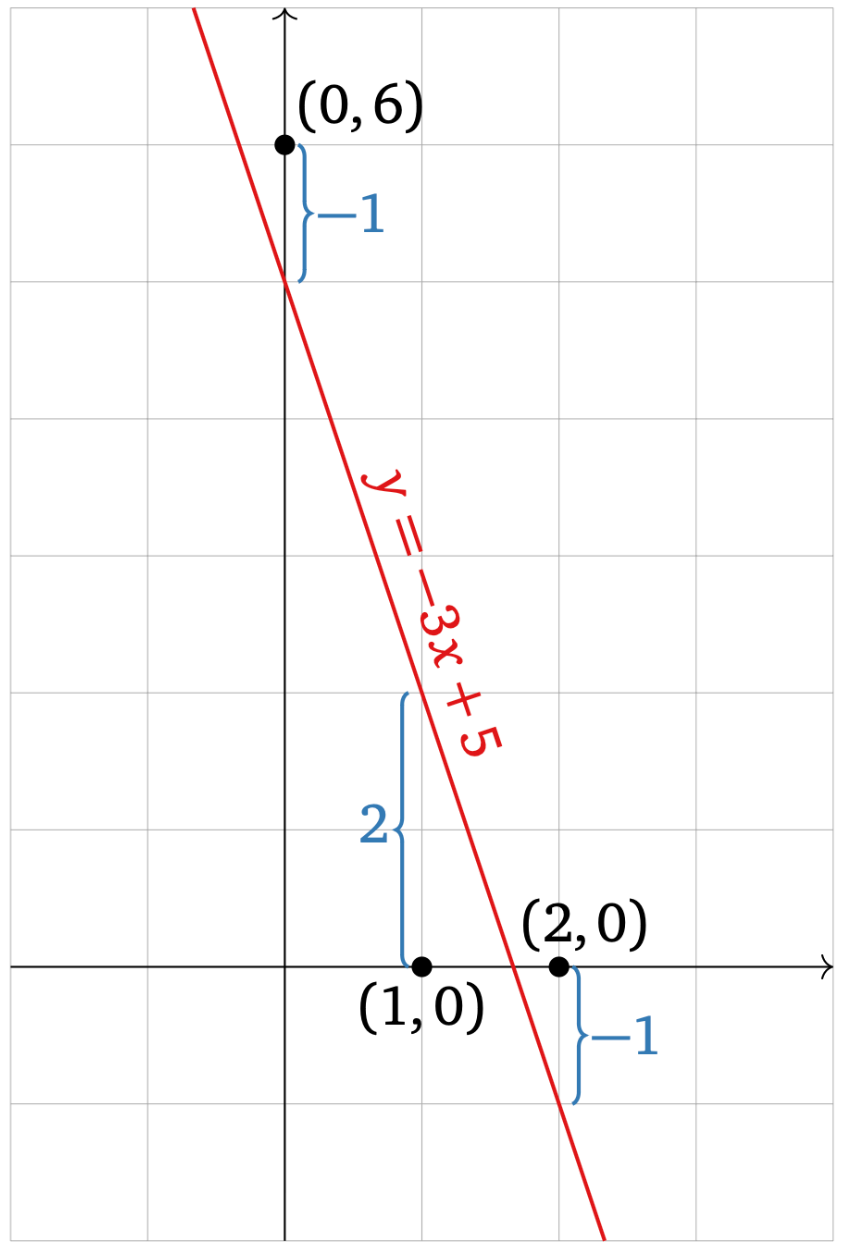
But we can try...



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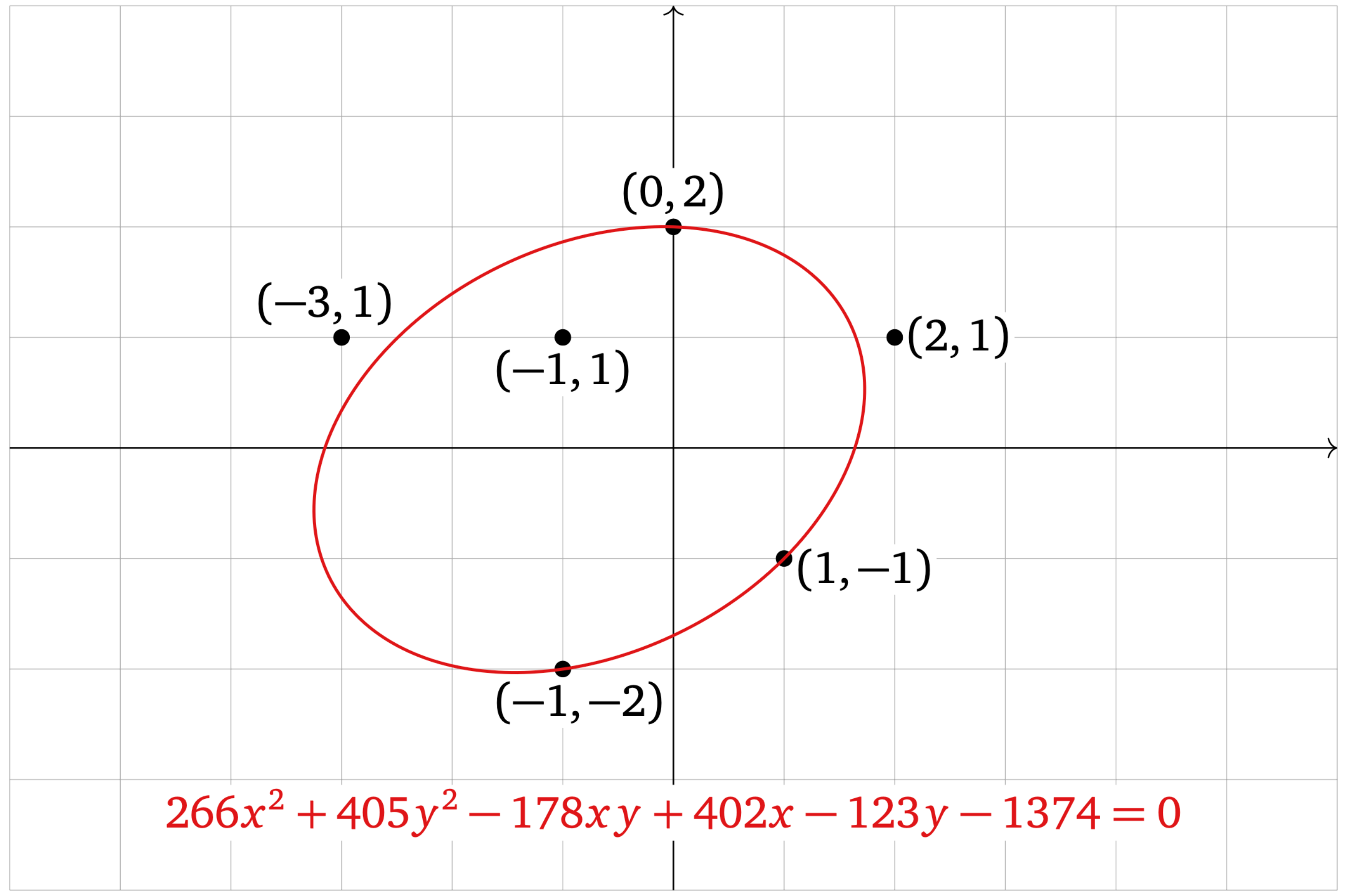

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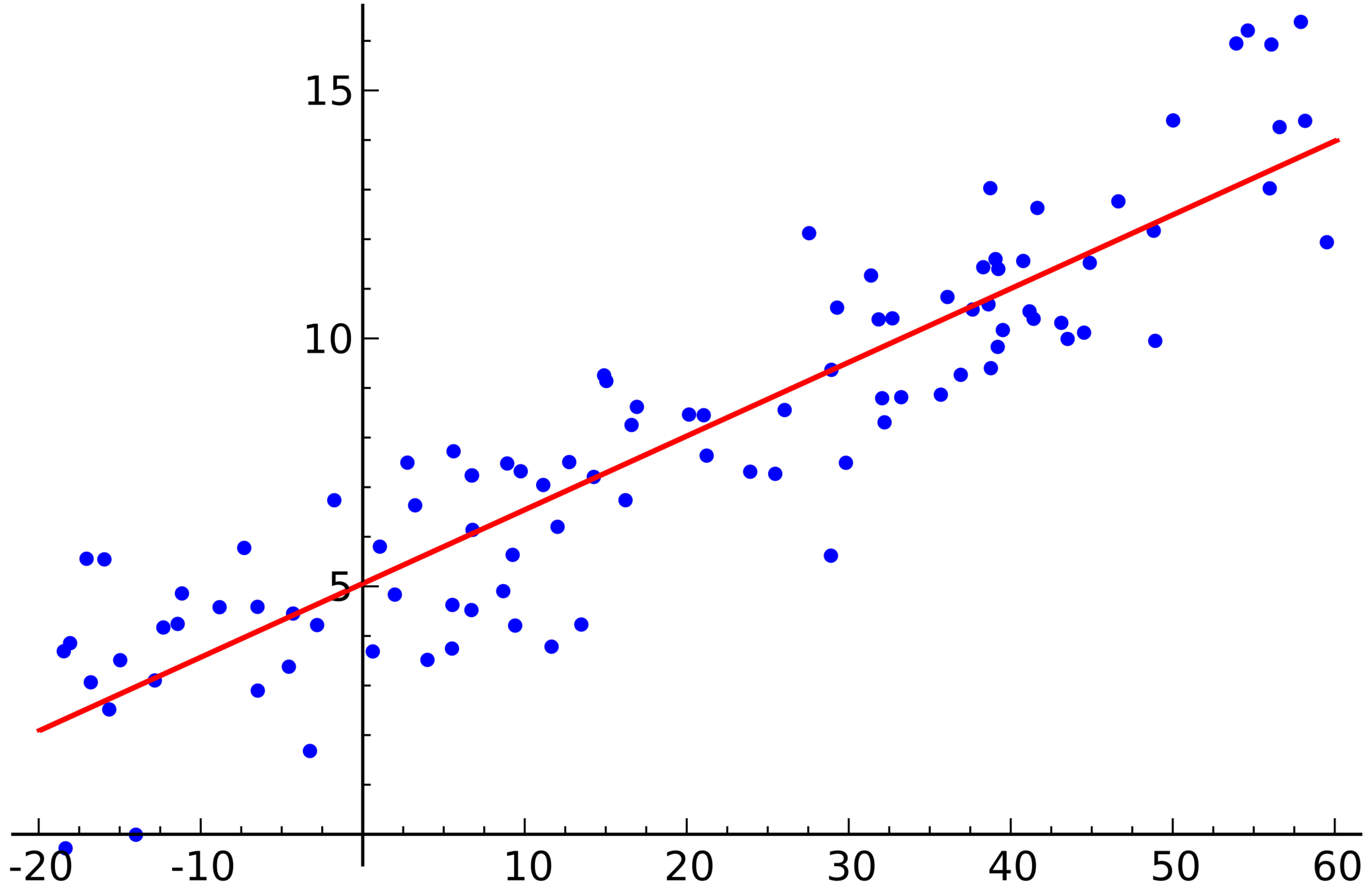
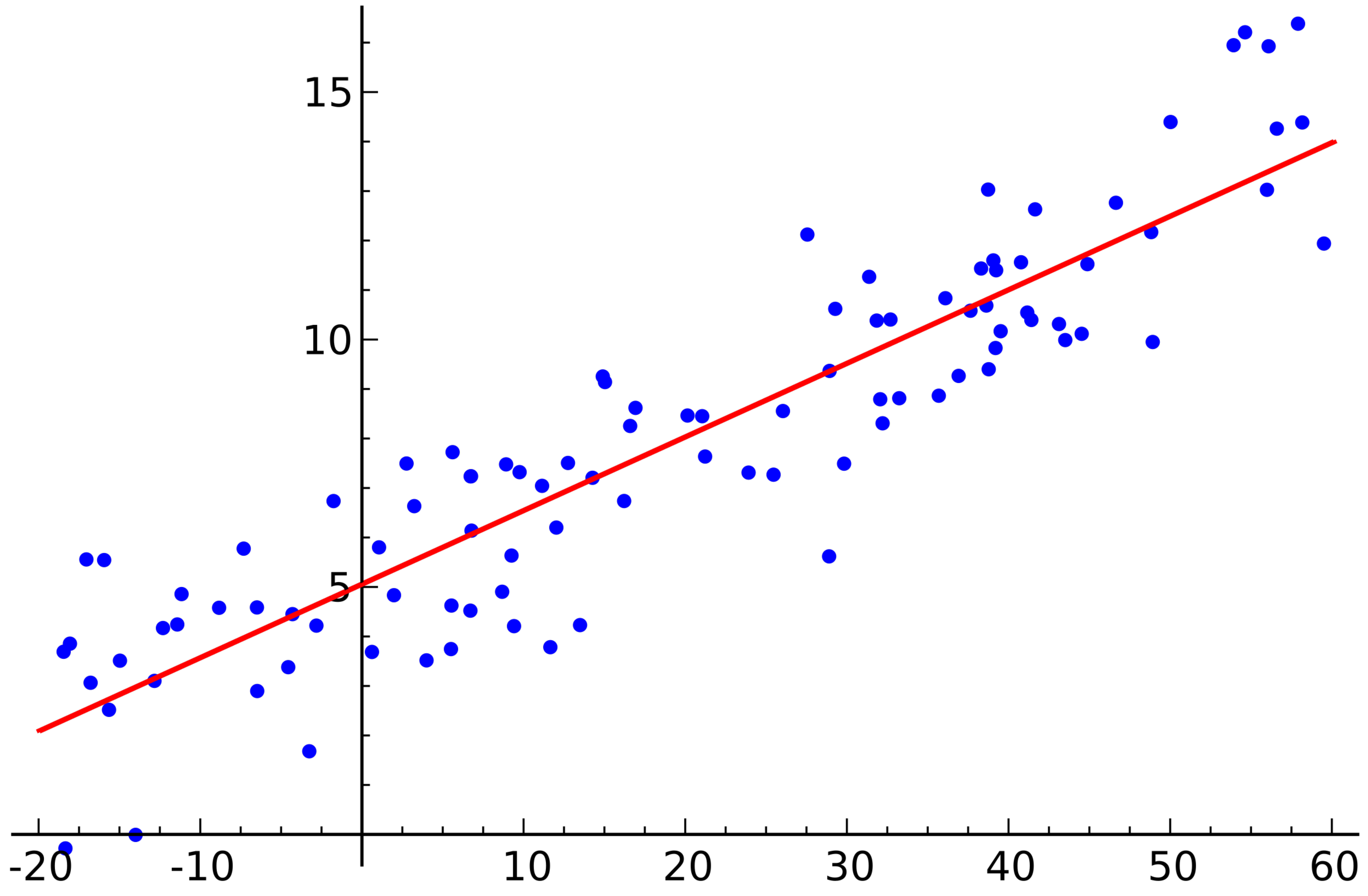
The Idea



https://commons.wikimedia.org/wiki/File:Linear_regression.svg

The Idea

Least Squares is a method for finding *approximate* solutions to systems of linear equations.



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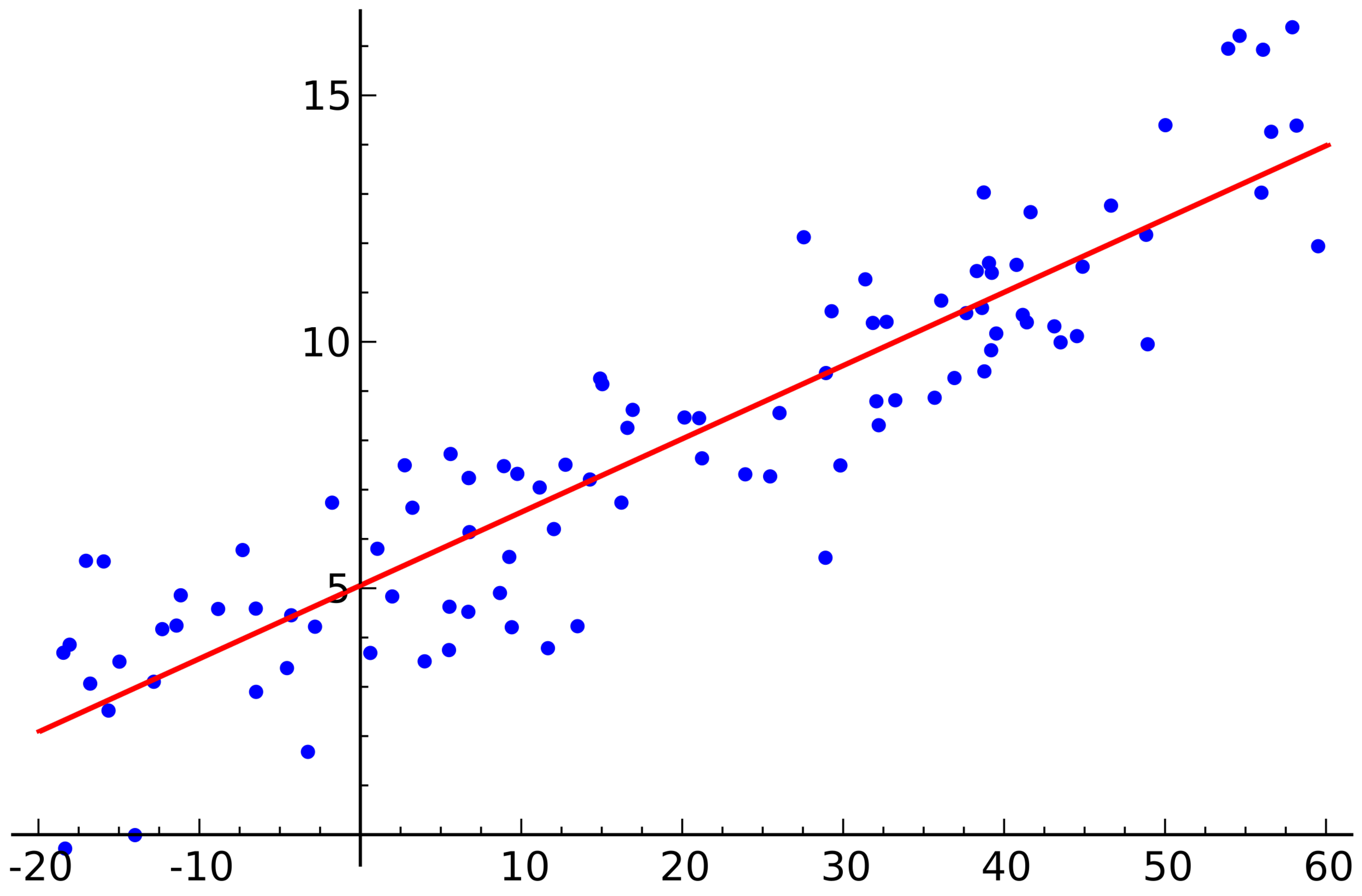
This is **a lot more useful in practice** than exact solutions.



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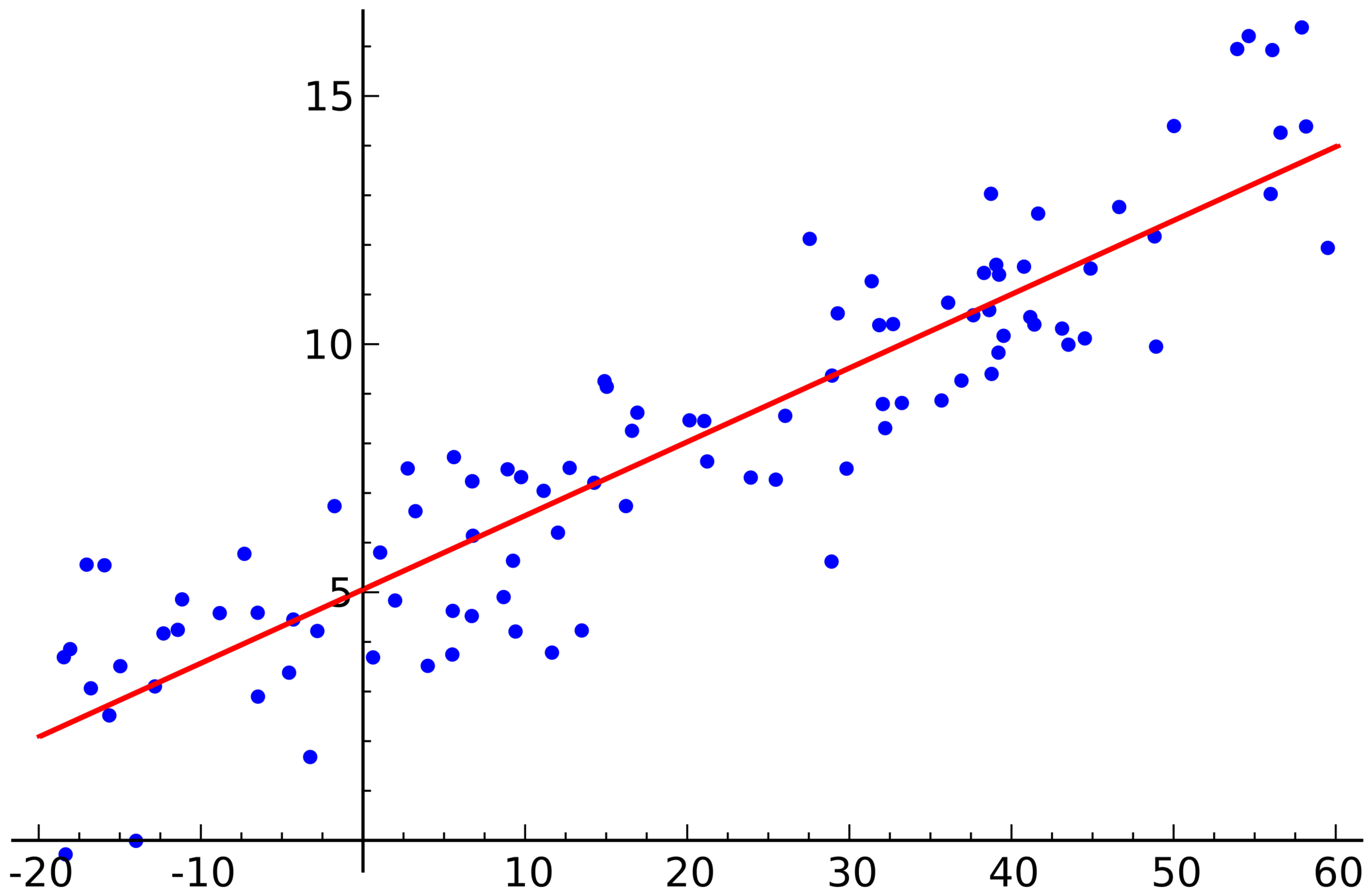
It can be used to do **linear regression** from stats class.



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General Least Squares Problem

The Picture

$A\vec{x} = \vec{b}$ has no solution

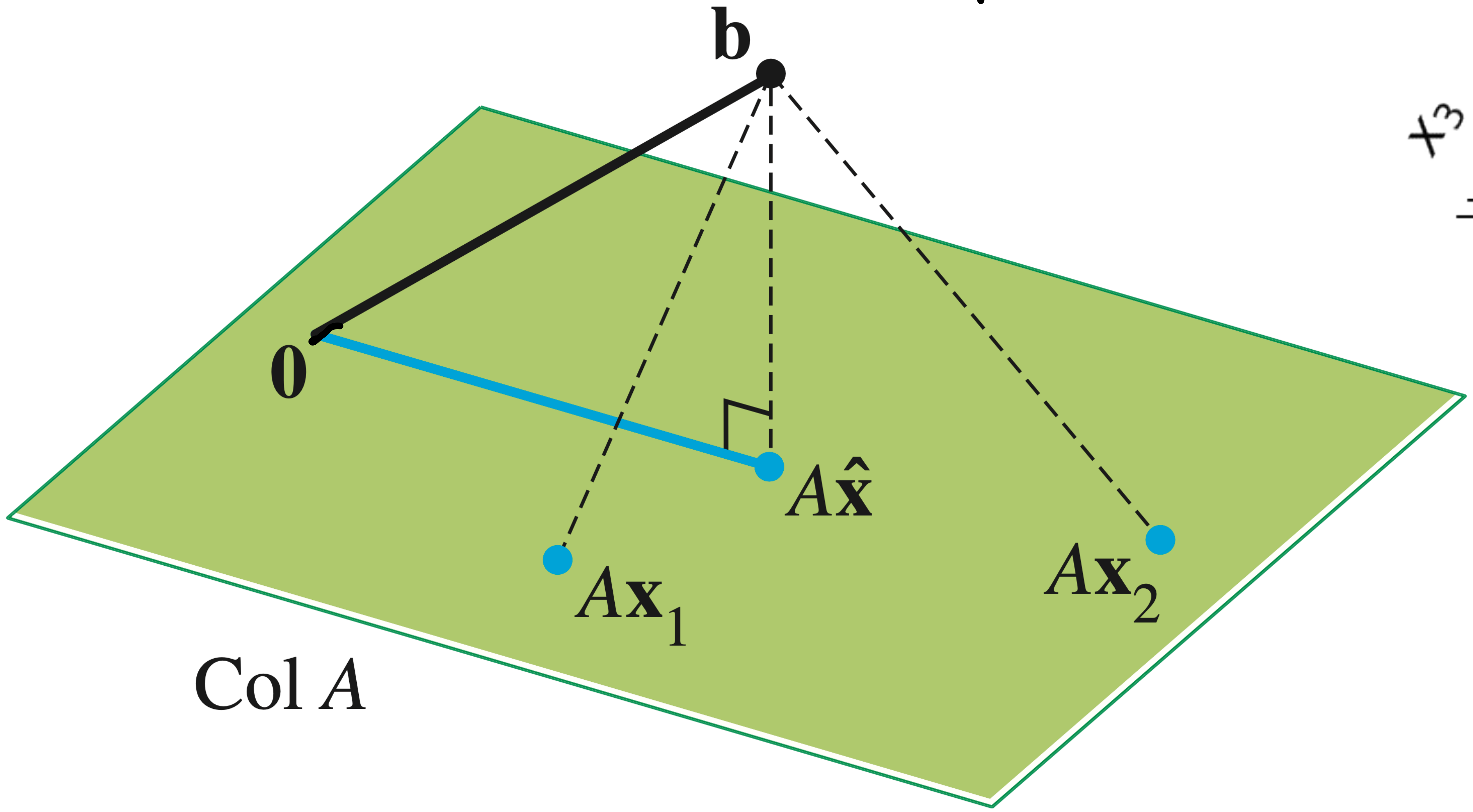
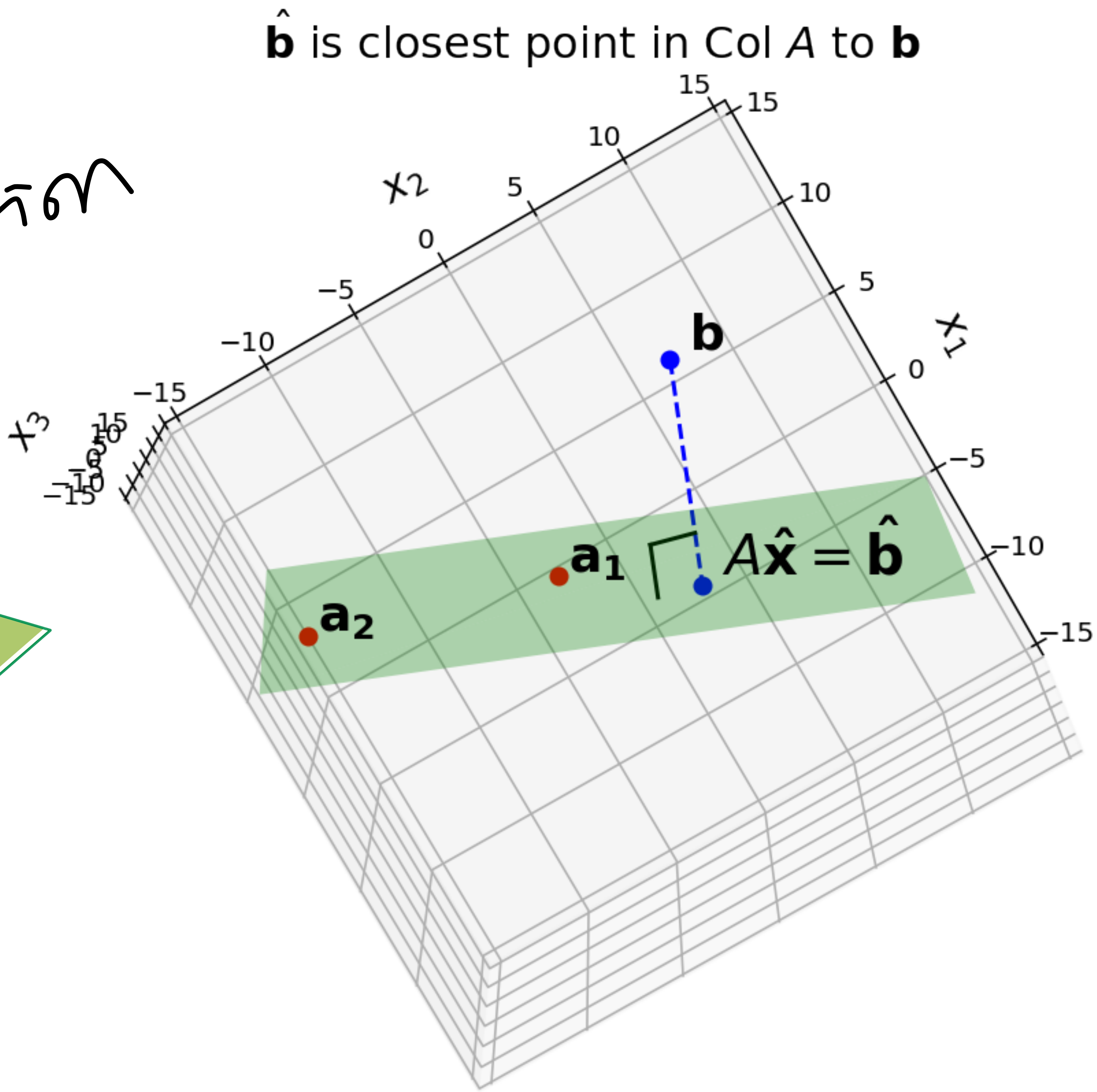
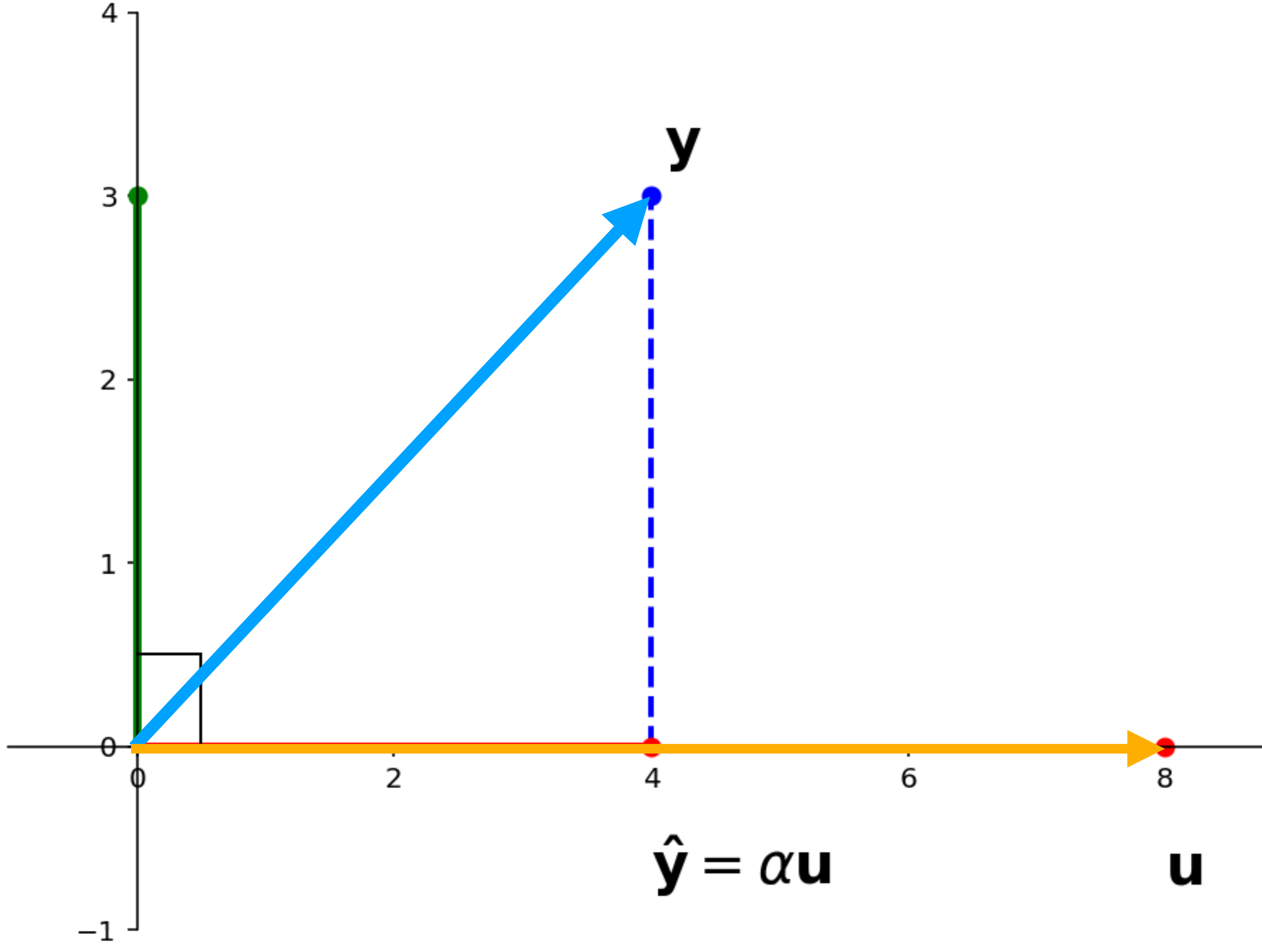


Figure 22.8

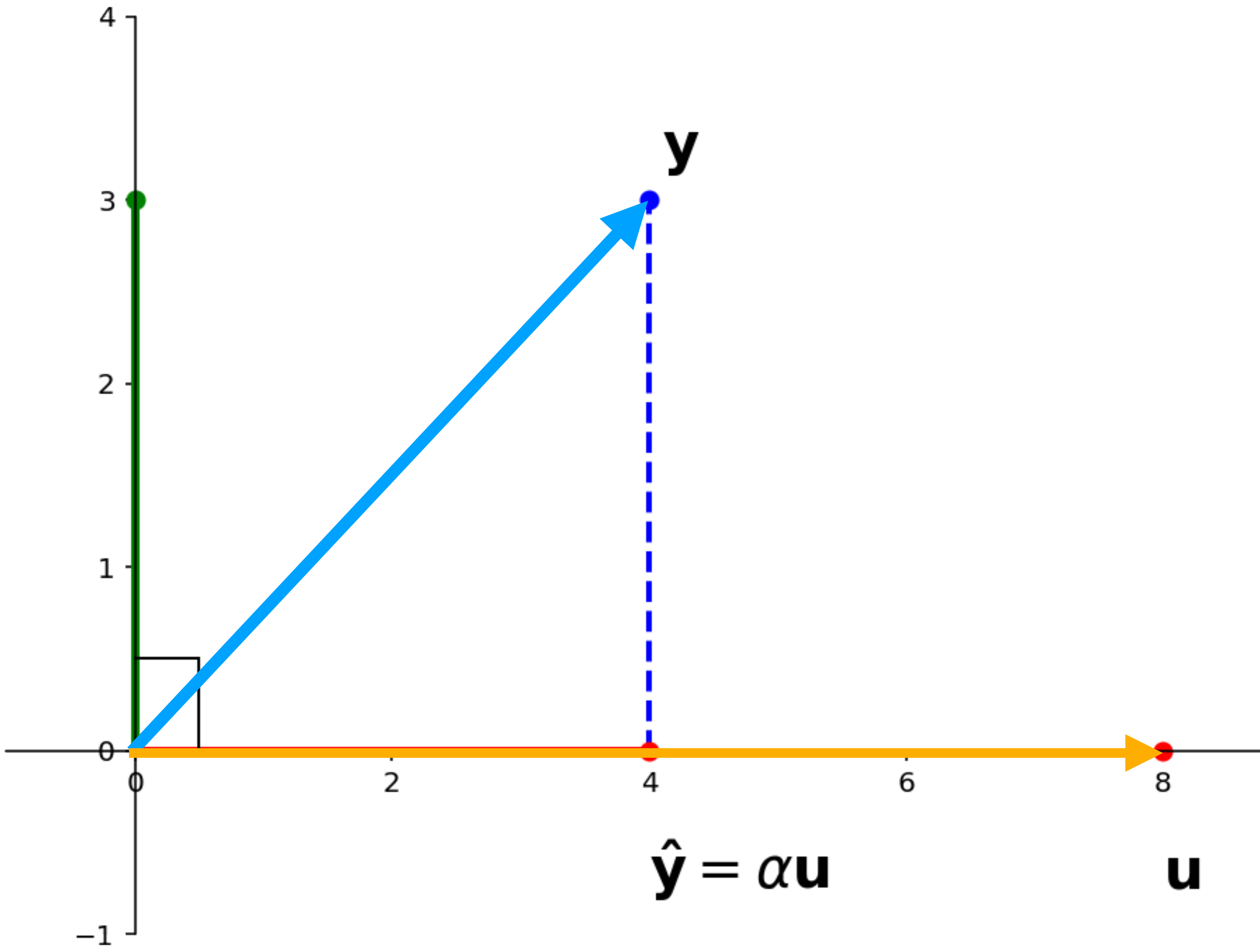


Recall: Orthogonal Projection



Recall: Orthogonal Projection

Question. Given vectors $\mathbf{y}$ and $\mathbf{u}$ in R^n, find vectors $\hat{\mathbf{y}}$ and $\mathbf{z}$ such that



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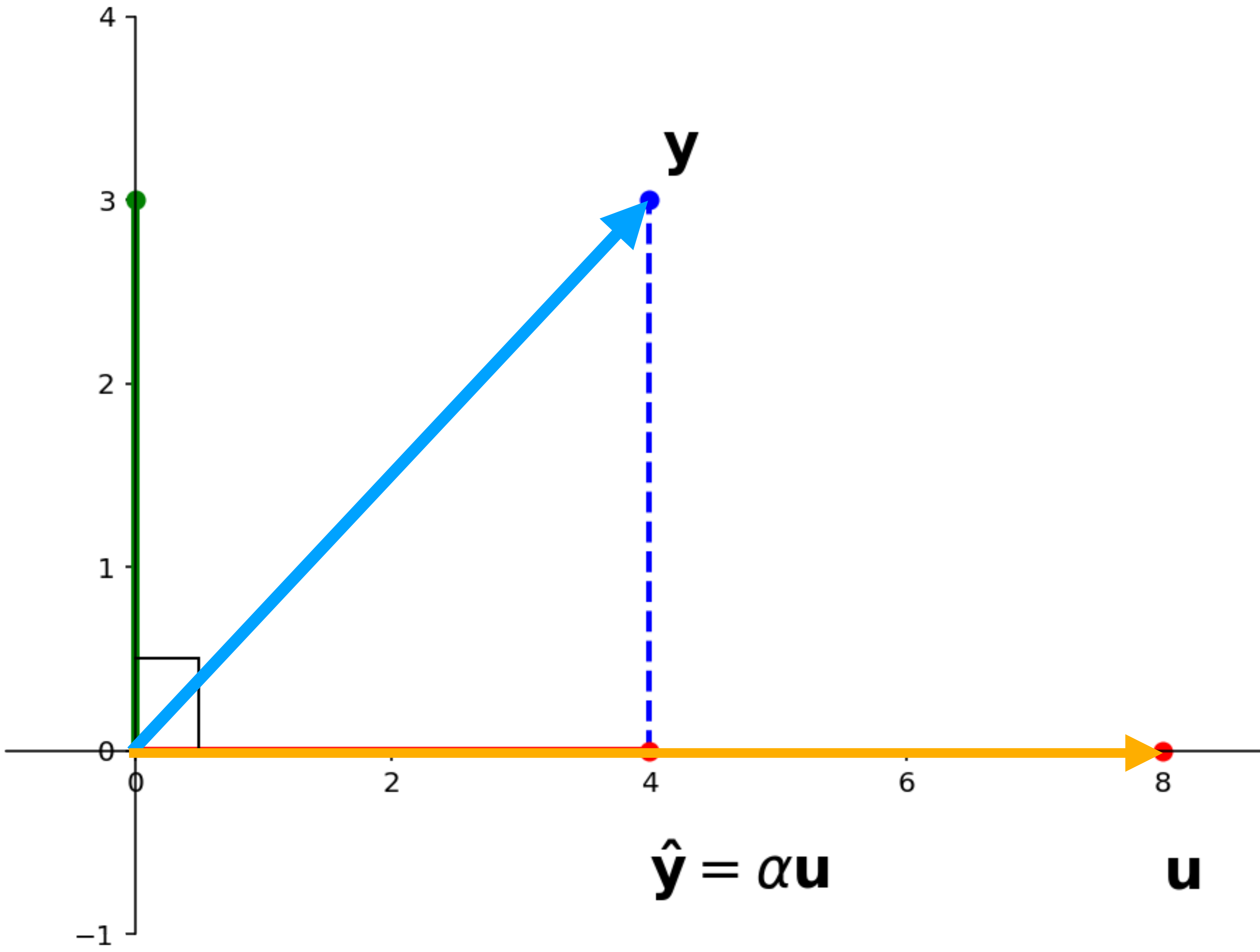

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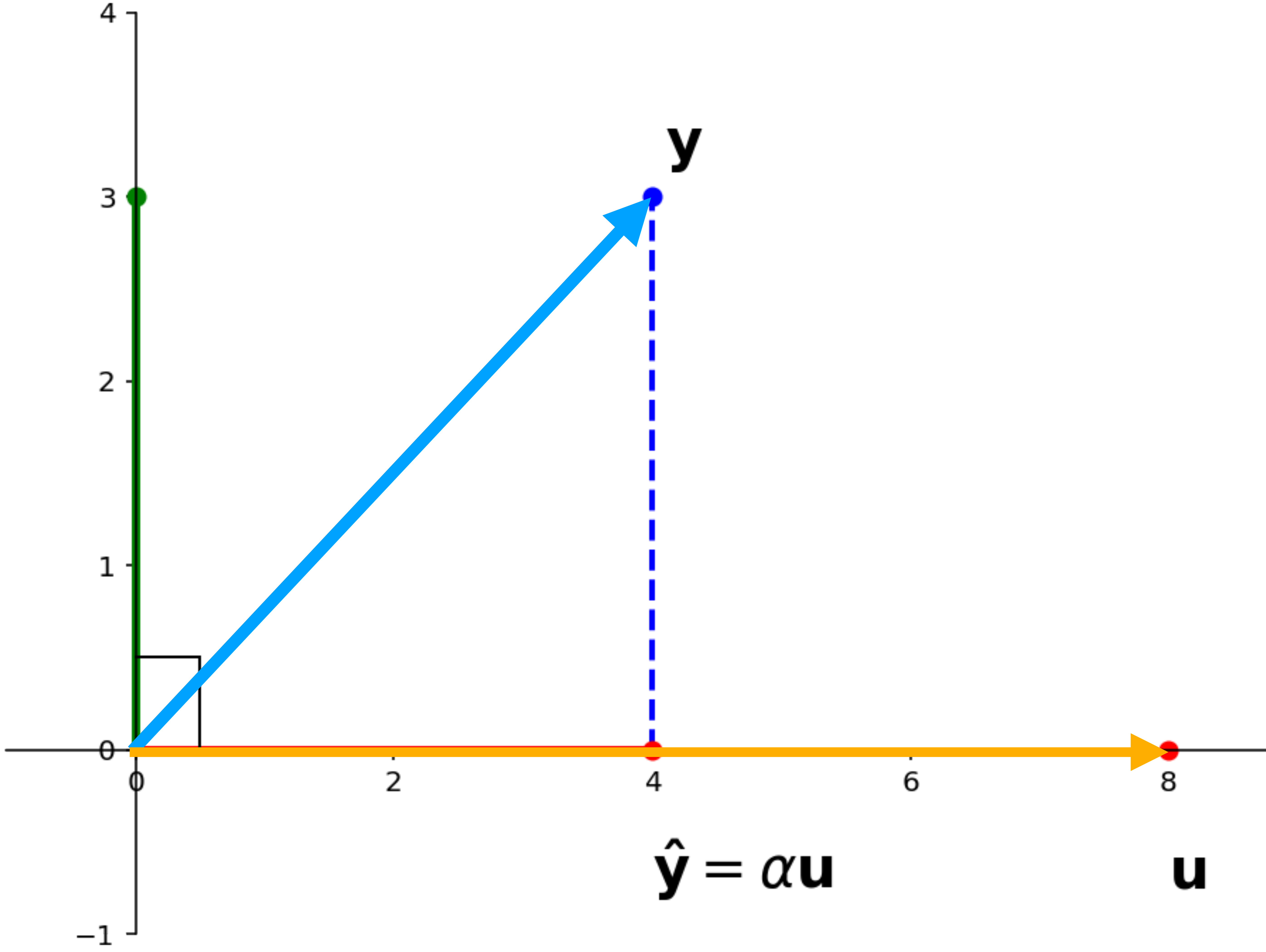
» $\hat{\mathbf{y}} \in span\{\mathbf{u}\}$



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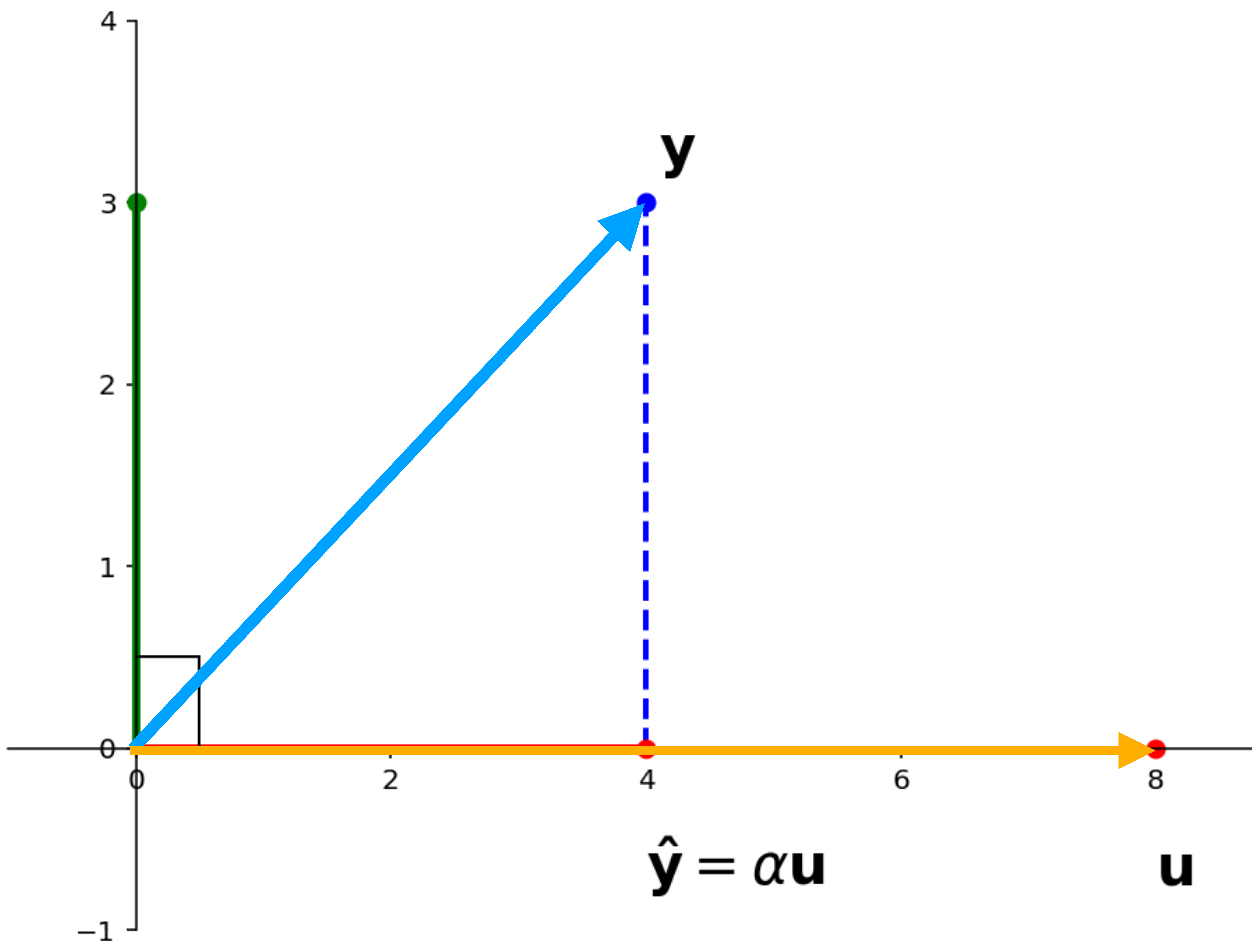
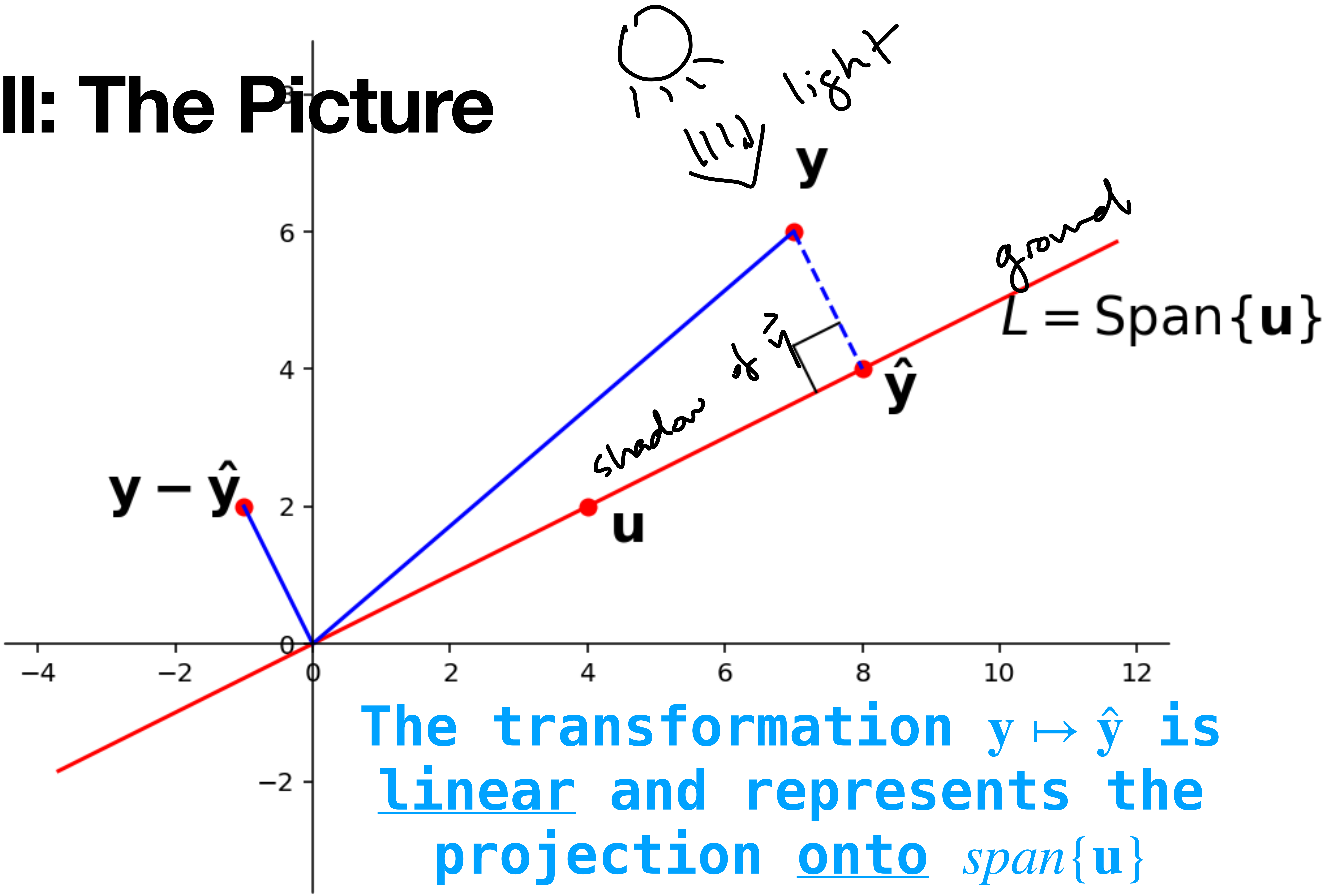
- $\hat{\mathbf{y}} \in span\{\mathbf{u}\}$
- $\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}$



Recall: The Picture



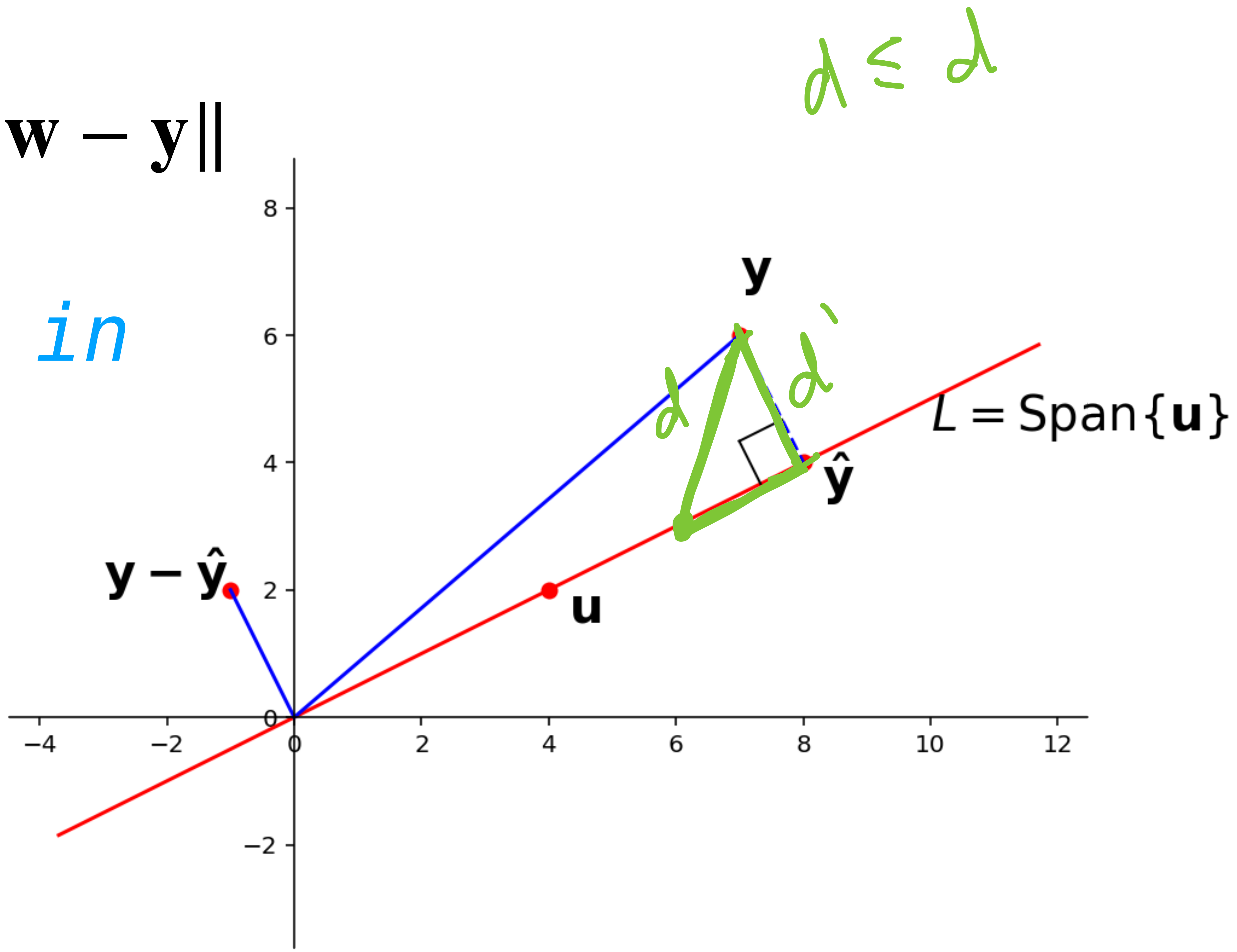
The transformation $\mathbf{y} \mapsto \hat{\mathbf{y}}$ is linear and represents the projection onto $span\{\mathbf{u}\}$

Recall: $\hat{\mathbf{y}}$ and Distance

Theorem. $\|\hat{\mathbf{y}} - \mathbf{y}\| = \min_{\mathbf{w} \in span\{\mathbf{u}\}} \|\mathbf{w} - \mathbf{y}\|$

$\hat{\mathbf{y}}$ is the closest vector in $span\{\mathbf{u}\}$ to $\mathbf{y}$.

"Proof" by inspection:



The Equational Perspective

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We know the equation $x\mathbf{u} = \mathbf{y}$ may have no solution.

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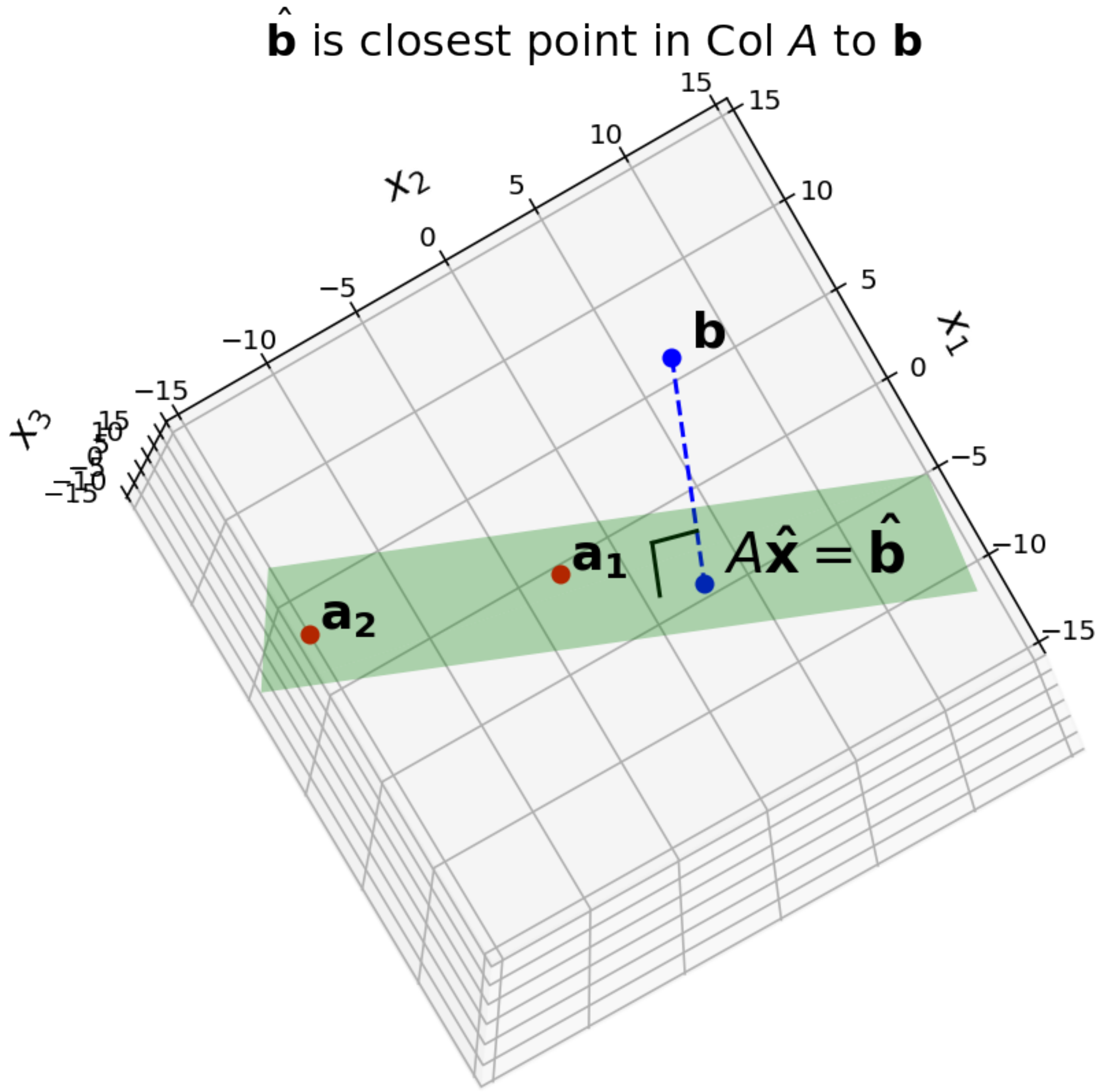
We need to generalize this to arbitrary matrix equations.

The General Least Squares Problem

Figure 22.8



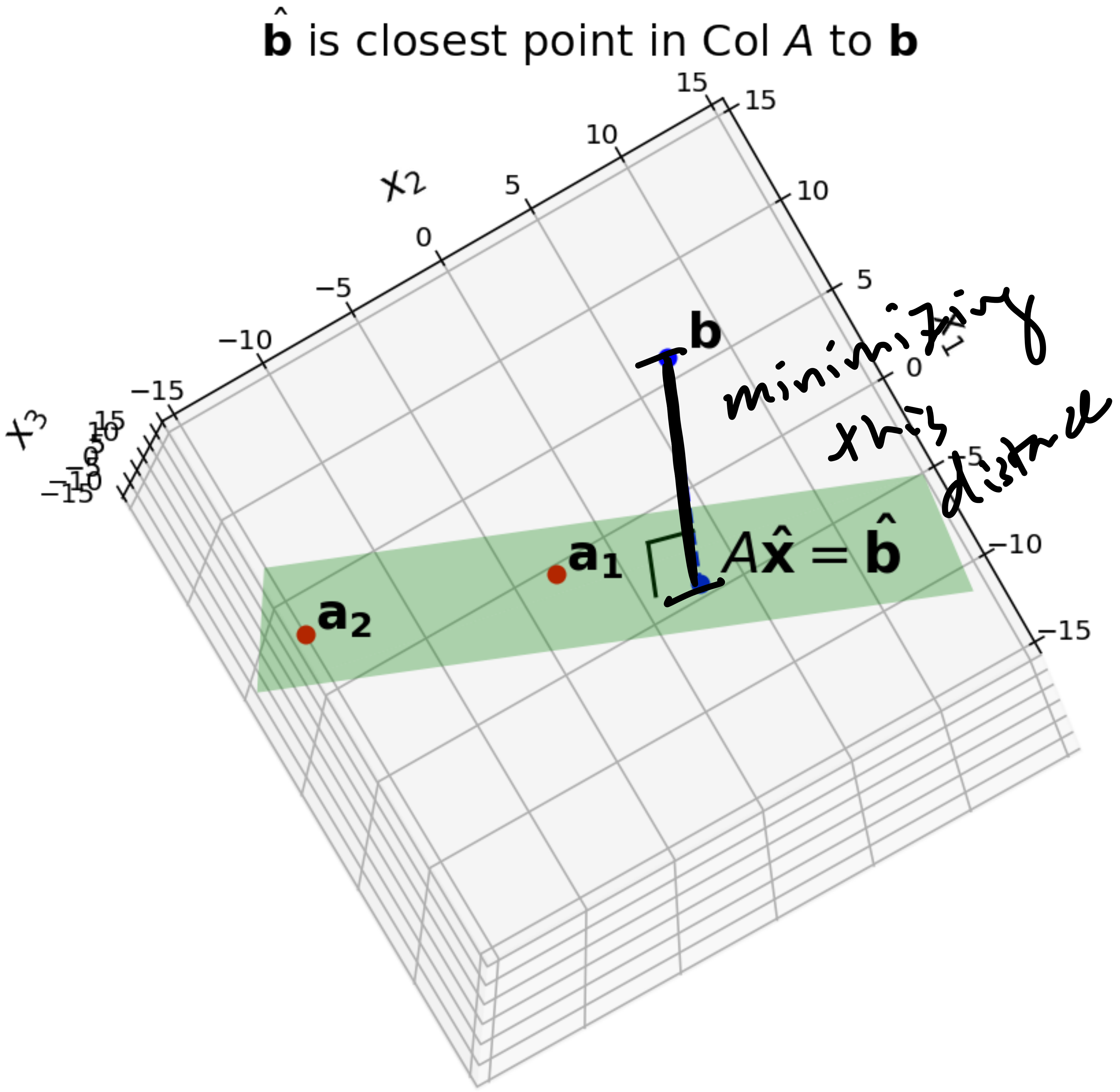
The General Least Squares Problem

$A\vec{x} = \vec{b}$

Problem. Given a $m \times n$ matrix A and a vector $\mathbf{b}$ from $\mathbb{R}^m$, find a vector $\mathbf{x}$ in $\mathbb{R}^n$ which minimizes

$$dist(A\mathbf{x}, \mathbf{b}) = \|A\mathbf{x} - \mathbf{b}\|$$

Figure 22.8



The General Least Squares Problem

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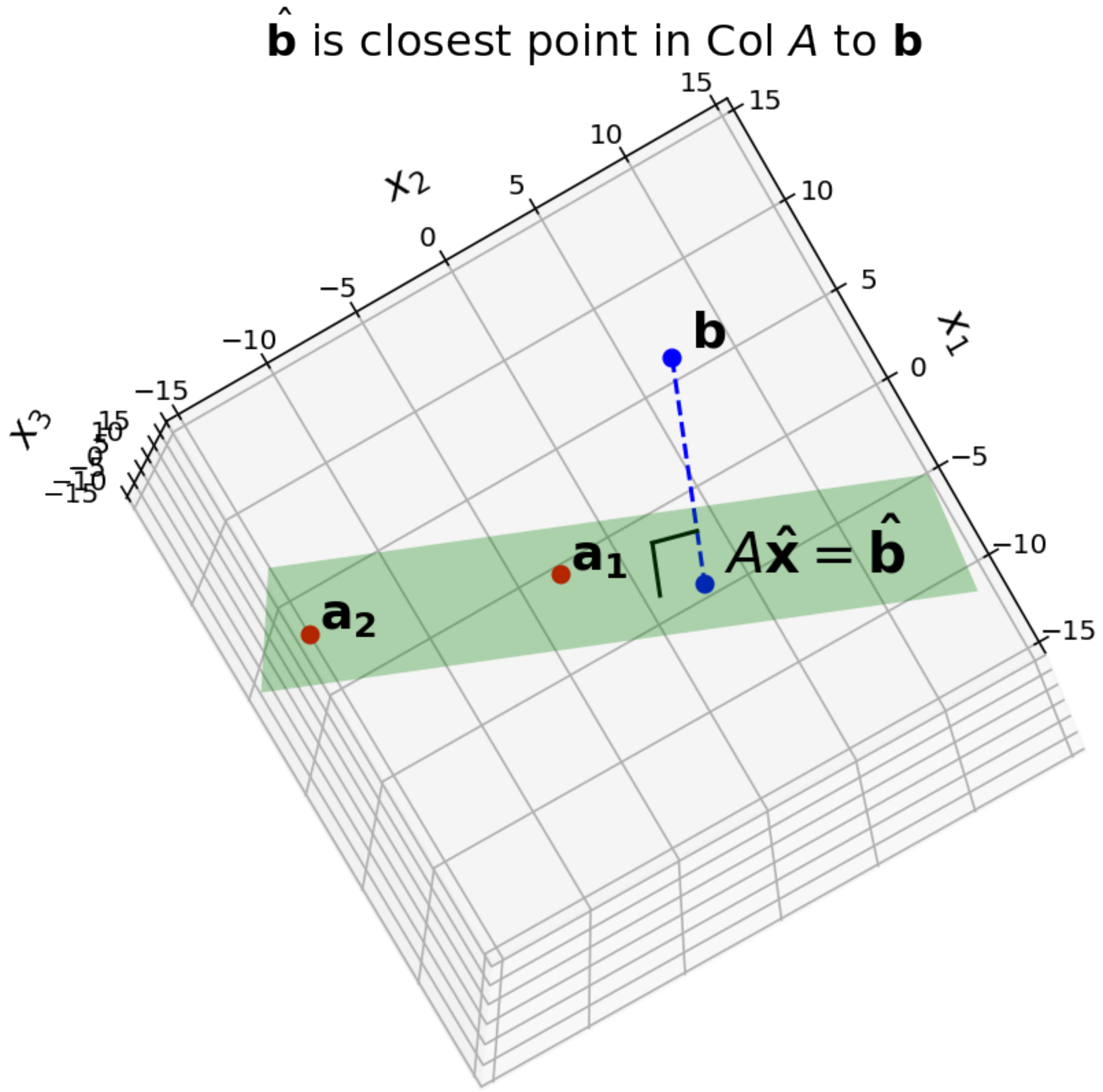
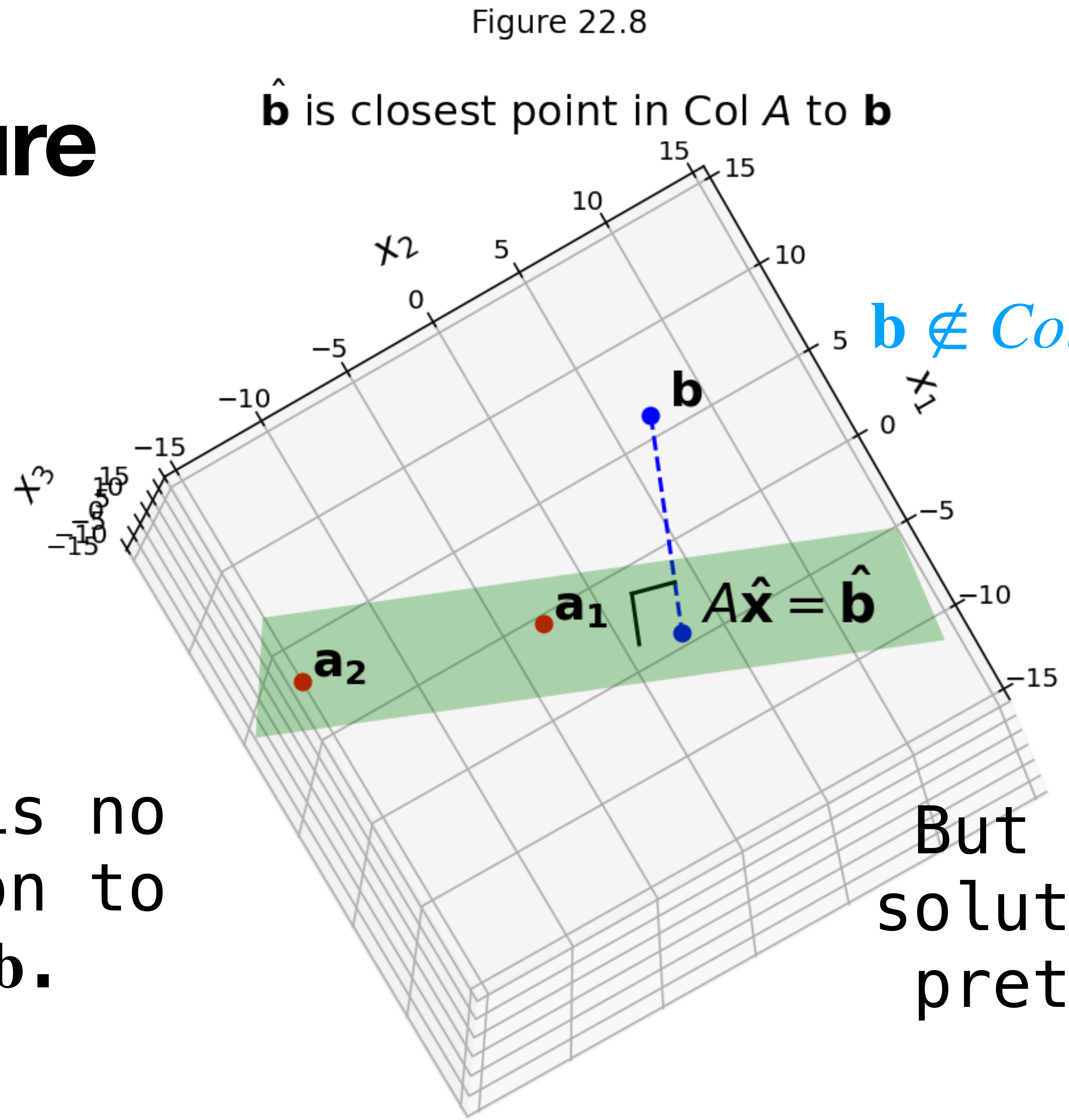
Find a vector $\mathbf{x}$ *which makes* $\|A\mathbf{x} - \mathbf{b}\|$ *as small as possible.*

Figure 22.8



The Picture



There is no solution to $A\mathbf{x} = \mathbf{b}$.

But there's a solution that's pretty close.

Sum of Squares

$$\|A\mathbf{x} - \mathbf{b}\|^2 = \sum_{i=1}^{n} ((A\mathbf{x})_i - \mathbf{b}_i)^2$$

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It is equivalent to minimize $\|A\mathbf{x} - \mathbf{b}\|^2$, which can be viewed as a **sum of squares.**

These things come up everywhere.

(Advanced.) This error is everywhere differentiable, whereas $\sum_{i=1}^{n} |(A\mathbf{x})_i - b_i|$ *is not.*

Least Squares Solution

Definition. Given a $m \times n$ matrix A and a vector $\mathbf{b}$ in $\mathbb{R}^m$, a **least squares solution** of $A\mathbf{x} = \mathbf{b}$ is a vector $\hat{\mathbf{x}}$ from $\mathbb{R}^n$ such that

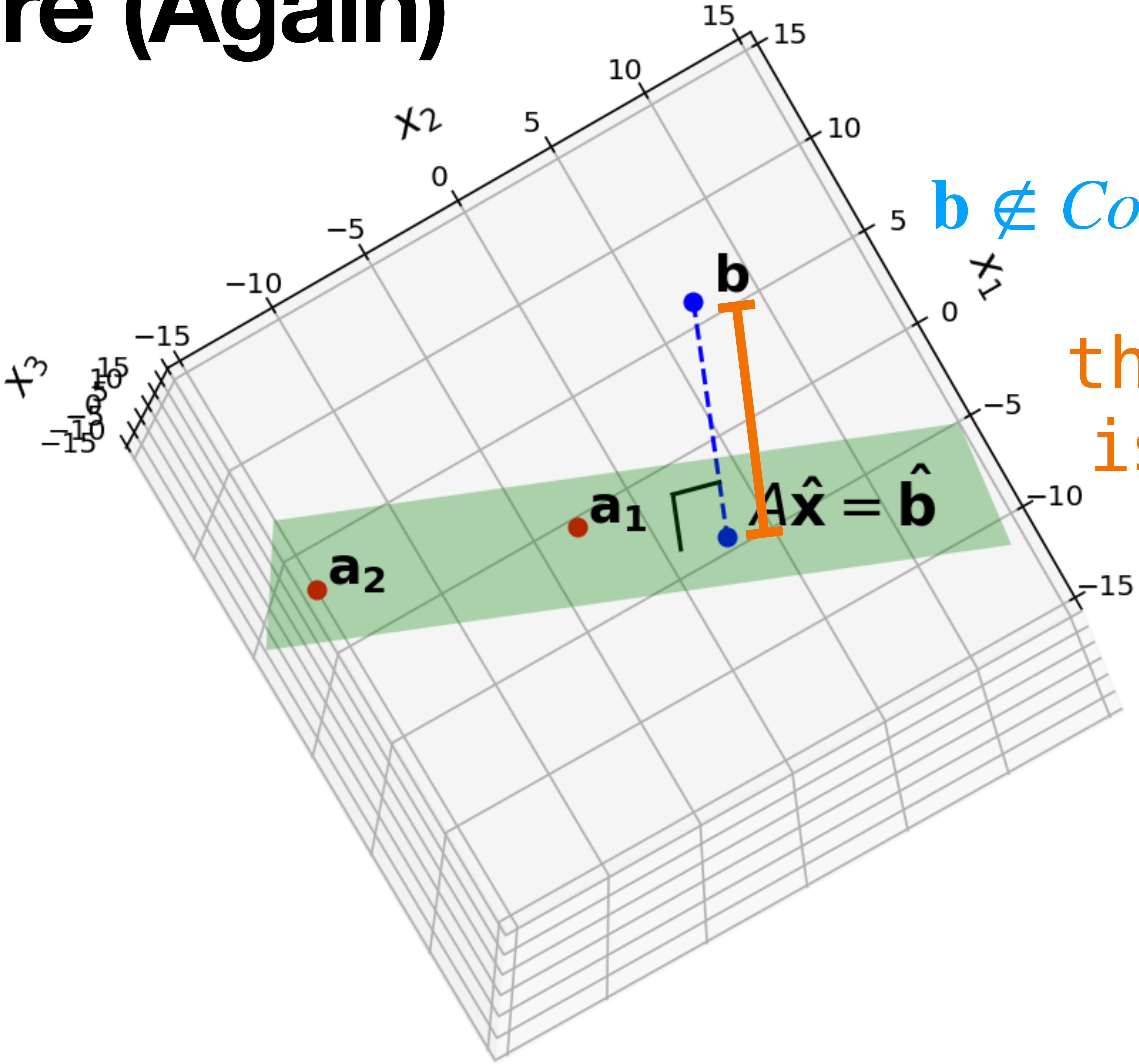
$$\|A\hat{\mathbf{x}} - \mathbf{b}\| \leq \|A\mathbf{x} - \mathbf{b}\|$$

for any $\mathbf{x}$ in $\mathbb{R}^n$.

Again, $\|A\hat{\mathbf{x}} - \mathbf{b}\|$ is as small as possible.

Figure 22.8

The Picture (Again)



$\mathbf{b} \notin Col(A)$

this distance is minimized

Argmin

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

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Another way of framing this is via $\arg\min$.

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Defintion. $\arg\min_{x \in X} f(x) = \hat{x}$ where $f(\hat{x}) = \min_{x \in X} f(x)$

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$\hat{x}$ is the ***arg****ument* that ***min****imizes* f.

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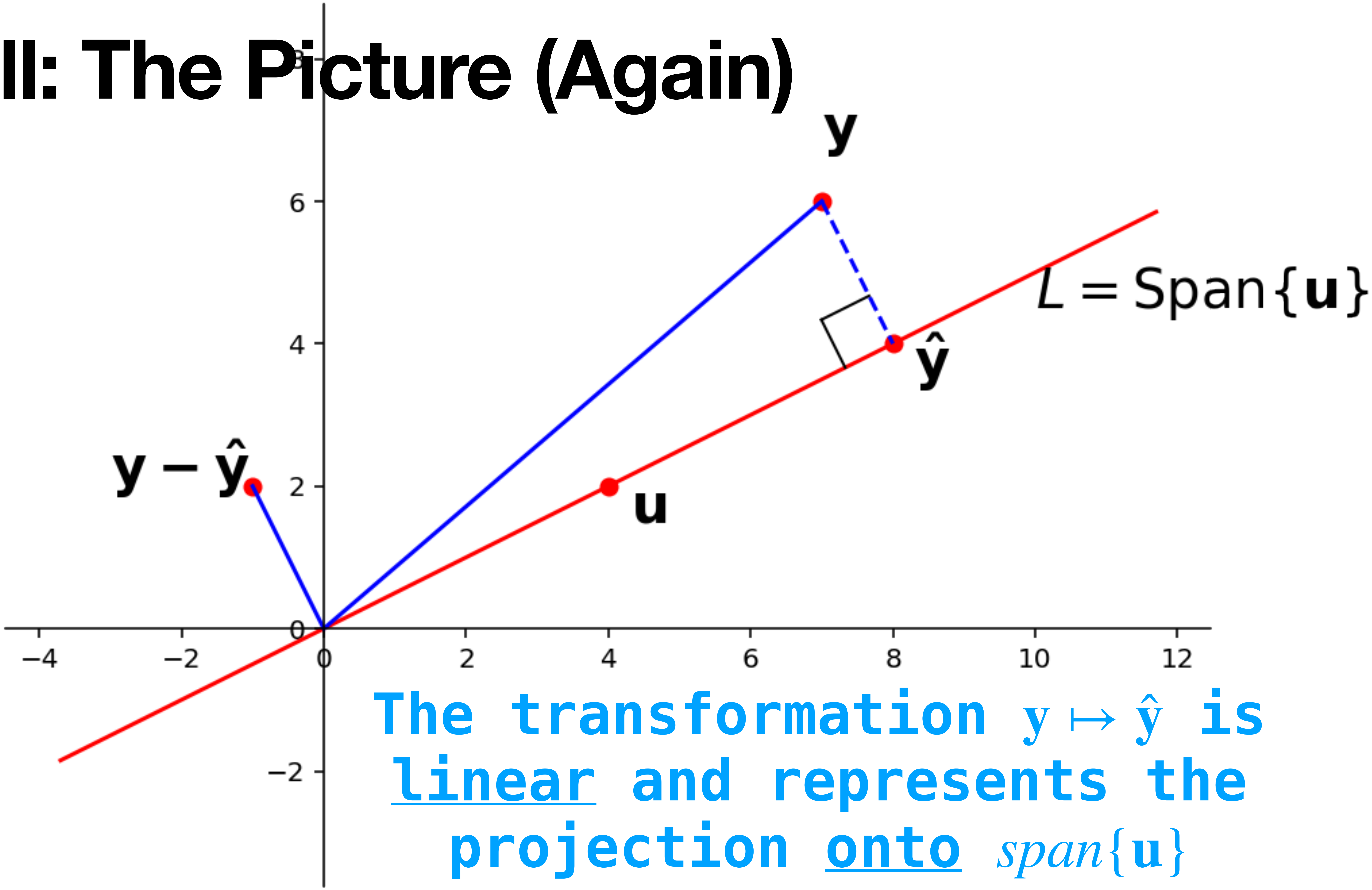
This is now an <u>optimization problem</u>.

Solving the General Least Squares Problems

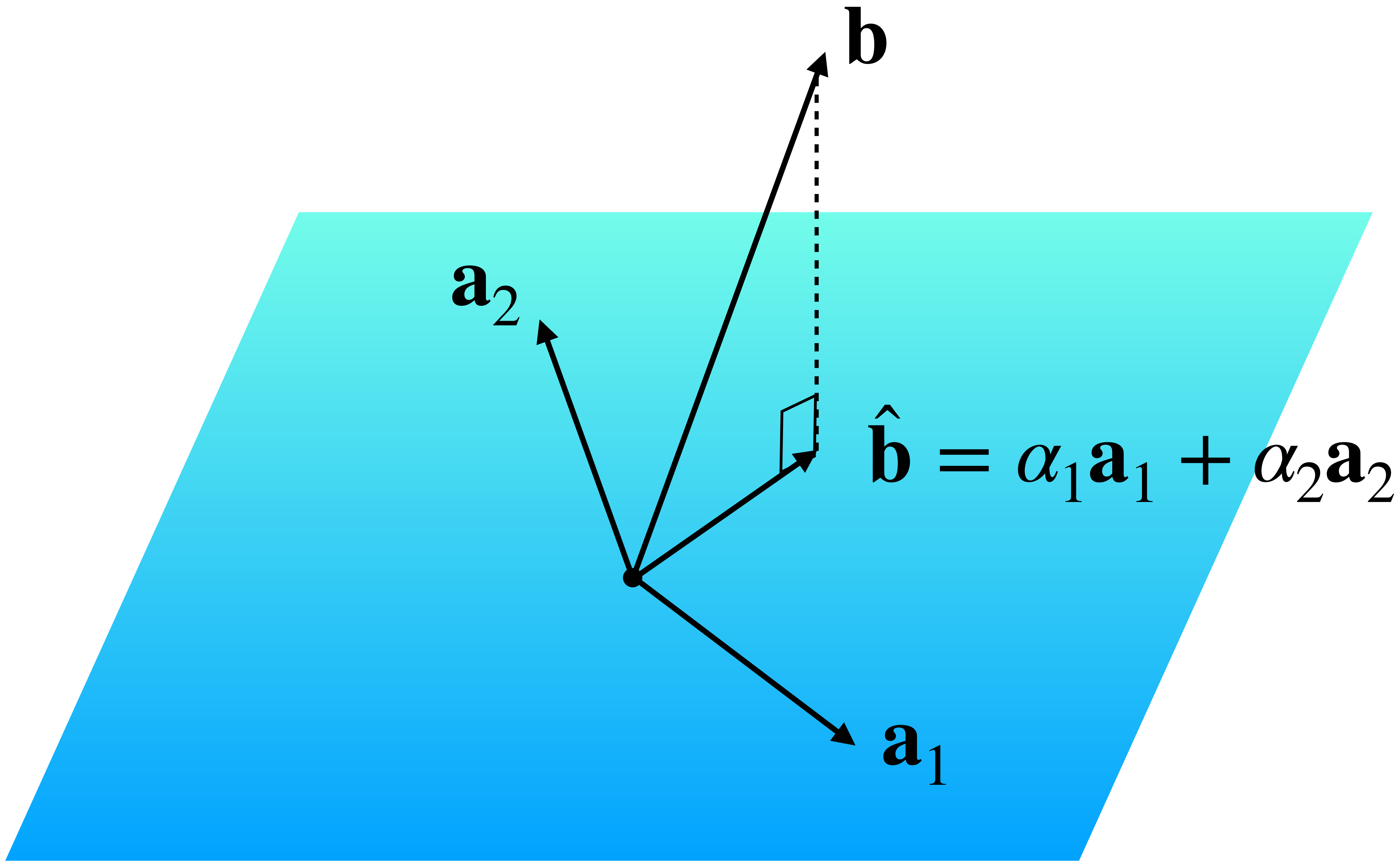
Recall: The Picture (Again)



The transformation $\mathbf{y} \mapsto \hat{\mathbf{y}}$ is linear and represents the projection onto $span\{\mathbf{u}\}$

Projects onto other Spans

The transformation $\mathbf{b} \mapsto \hat{\mathbf{b}}$ is the projection of $\mathbf{b}$ onto $\mathrm{span}\{\mathbf{a}_1, \mathbf{a}_2\}$



The High Level Approach.

Question. Find a least squares solutions to $A\mathbf{x} = \mathbf{b}$

Solution.

1. Find the closest point $\hat{\mathbf{b}}$ in $Col(A)$ to $\mathbf{b}$.

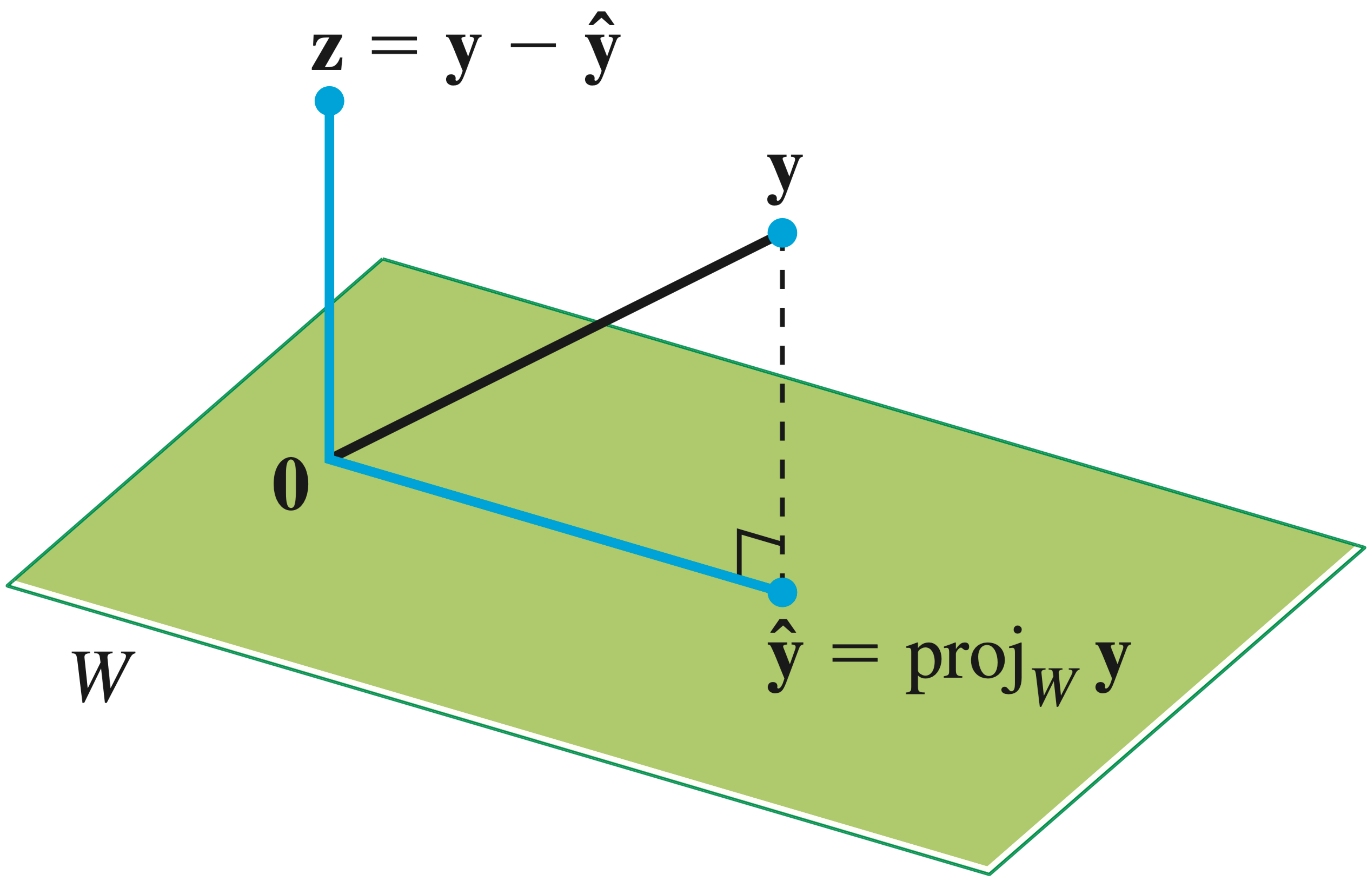
2. Solve the equation $A\mathbf{x} = \hat{\mathbf{b}}$ instead.

Orthogonal Decomposition Theorem

Theorem. Let W be a subspace of $\mathbb{R}^n$. Every vector $\mathbf{y}$ in $\mathbb{R}^n$ can be written uniquely as

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{z}$$

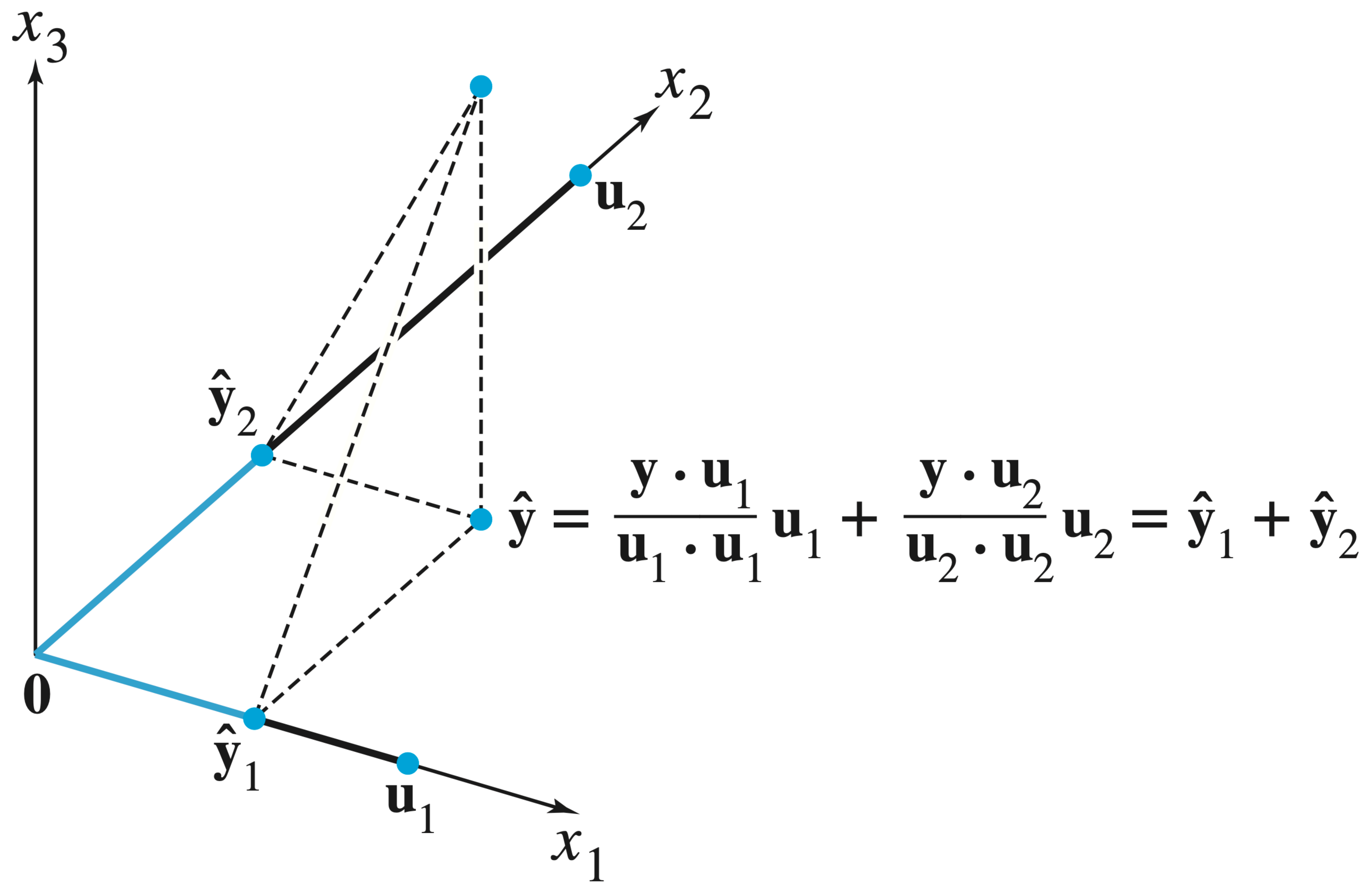
where $\hat{\mathbf{y}} \in W$ and $\mathbf{z}$ is orthogonal to every vector in W.



Projection via Orthogonal Bases

We can determine $\hat{\mathbf{y}}$ by projecting onto an orthogonal basis.

Every subspace has an orthogonal basis (we won't prove this)



Linear Algebra and its Applications, Lay, Lay, McDonald

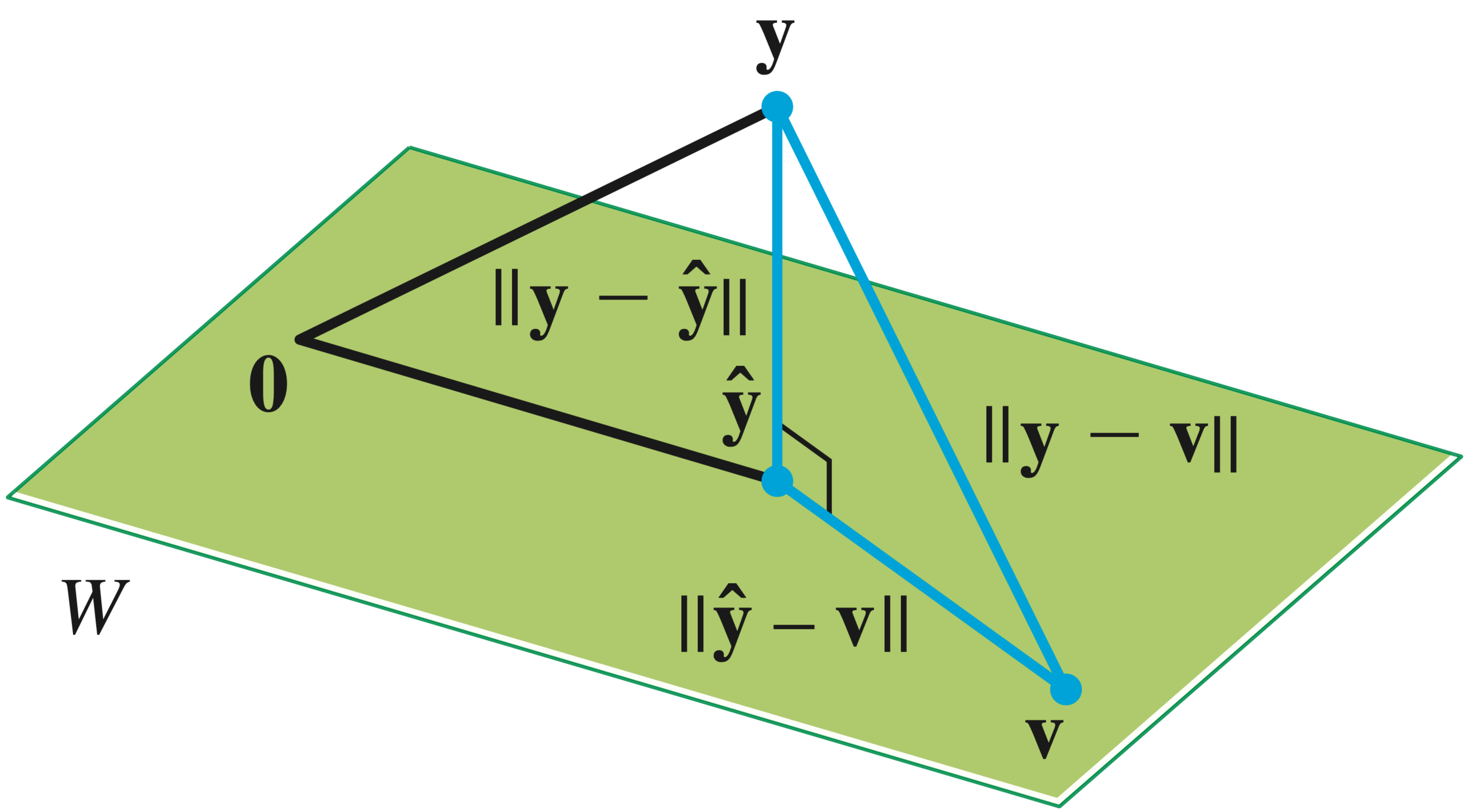
The Best-Approximation Theorem

Theorem. Let W be a subspace of $\mathbb{R}^n$, and let $\hat{\mathbf{y}}$ be the orthogonal projection of $\mathbf{y}$ onto W. Then

$$\|\mathbf{y} - \hat{\mathbf{y}}\| \leq \|\mathbf{y} - \mathbf{w}\|$$

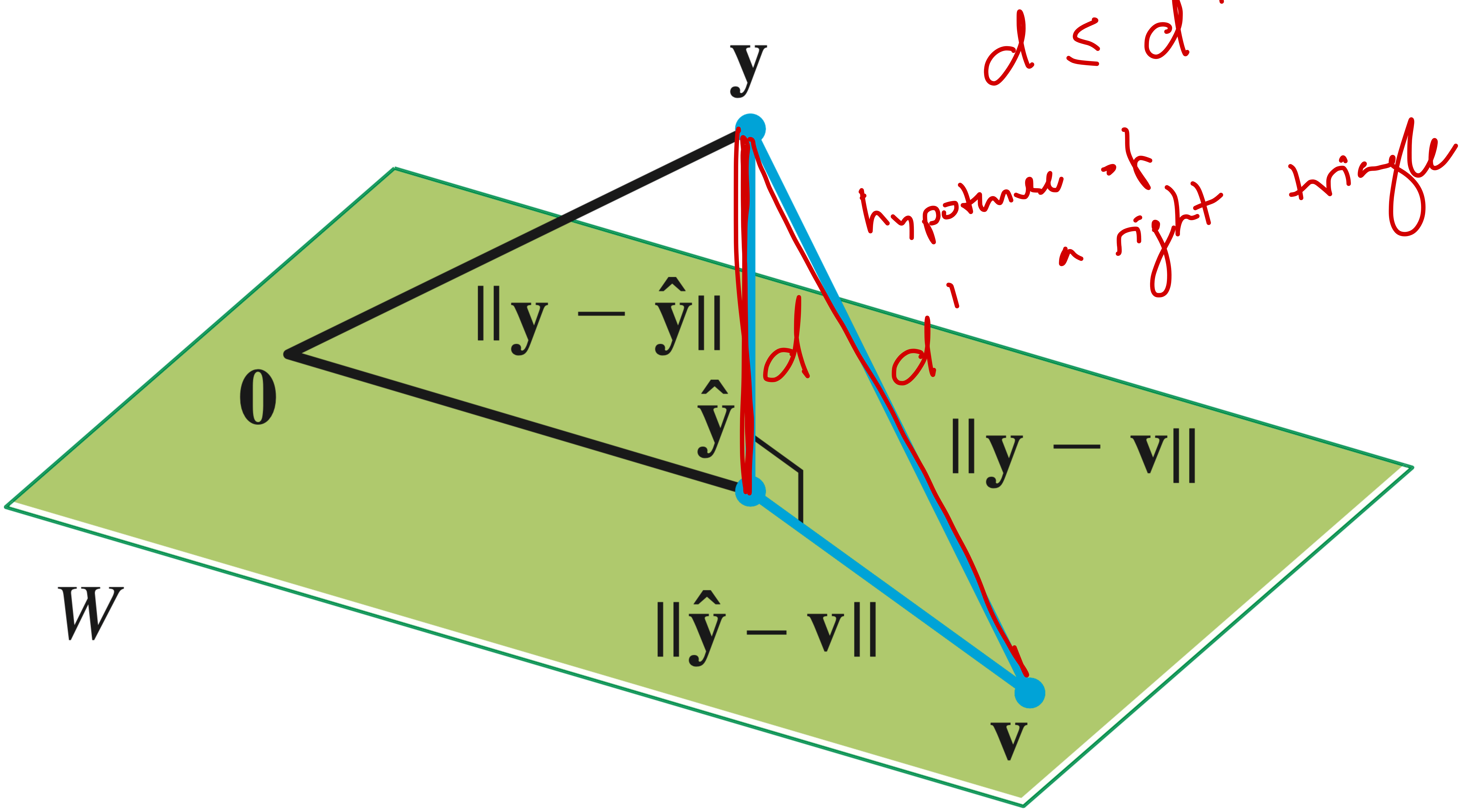
for <u>any</u> vector $\mathbf{w}$ in W.

$\hat{\mathbf{y}}$ is the closest point in W to $\mathbf{y}$



Linear Algebra and its Applications, Lay, Lay, McDonald

Proof by Inspection



Proof by Algebra

Verify:

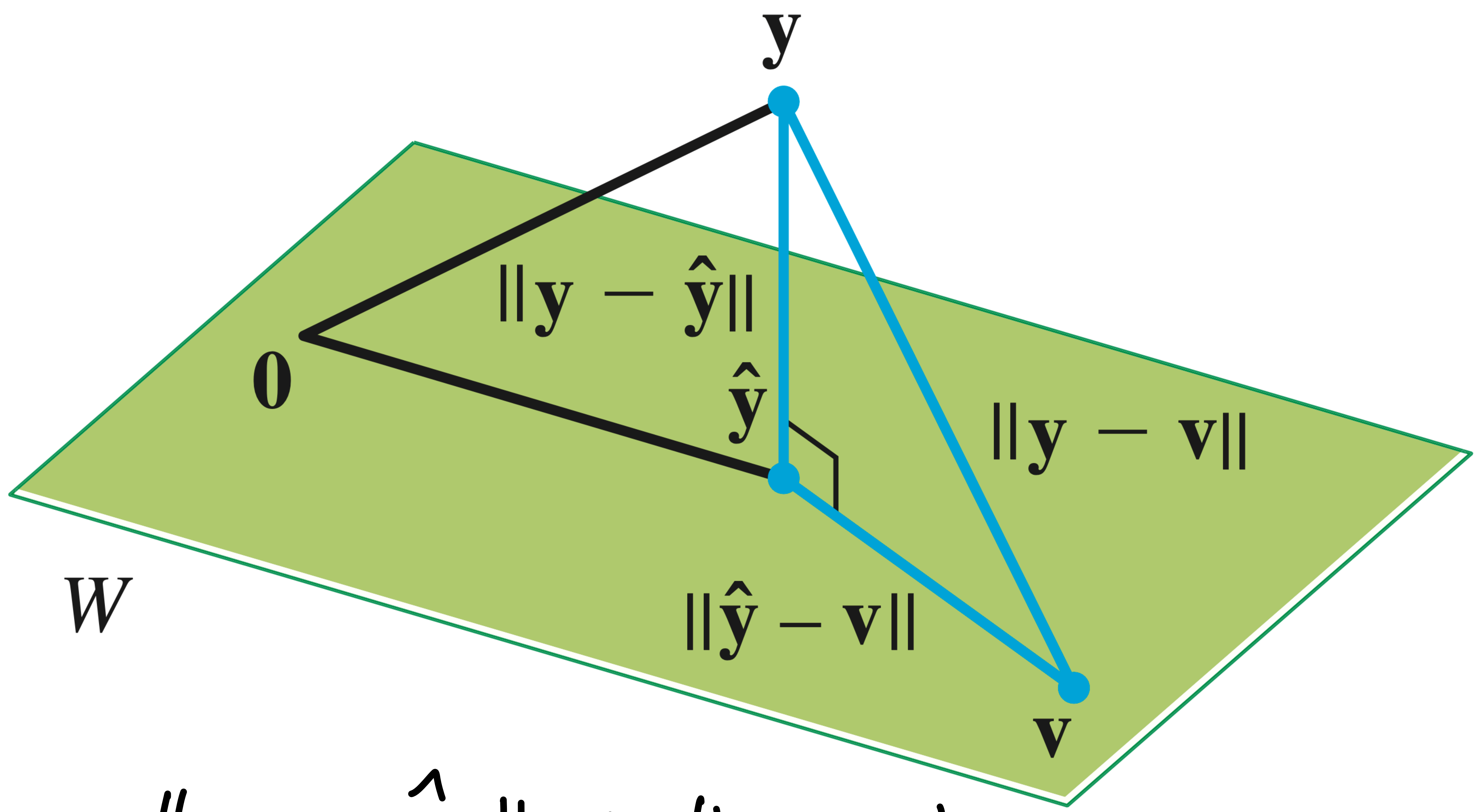
$$\|\hat{y}-v\|^2 + \|y-\hat{y}\|^2 = \|y-v\|^2$$

by Pythagorean theorem,

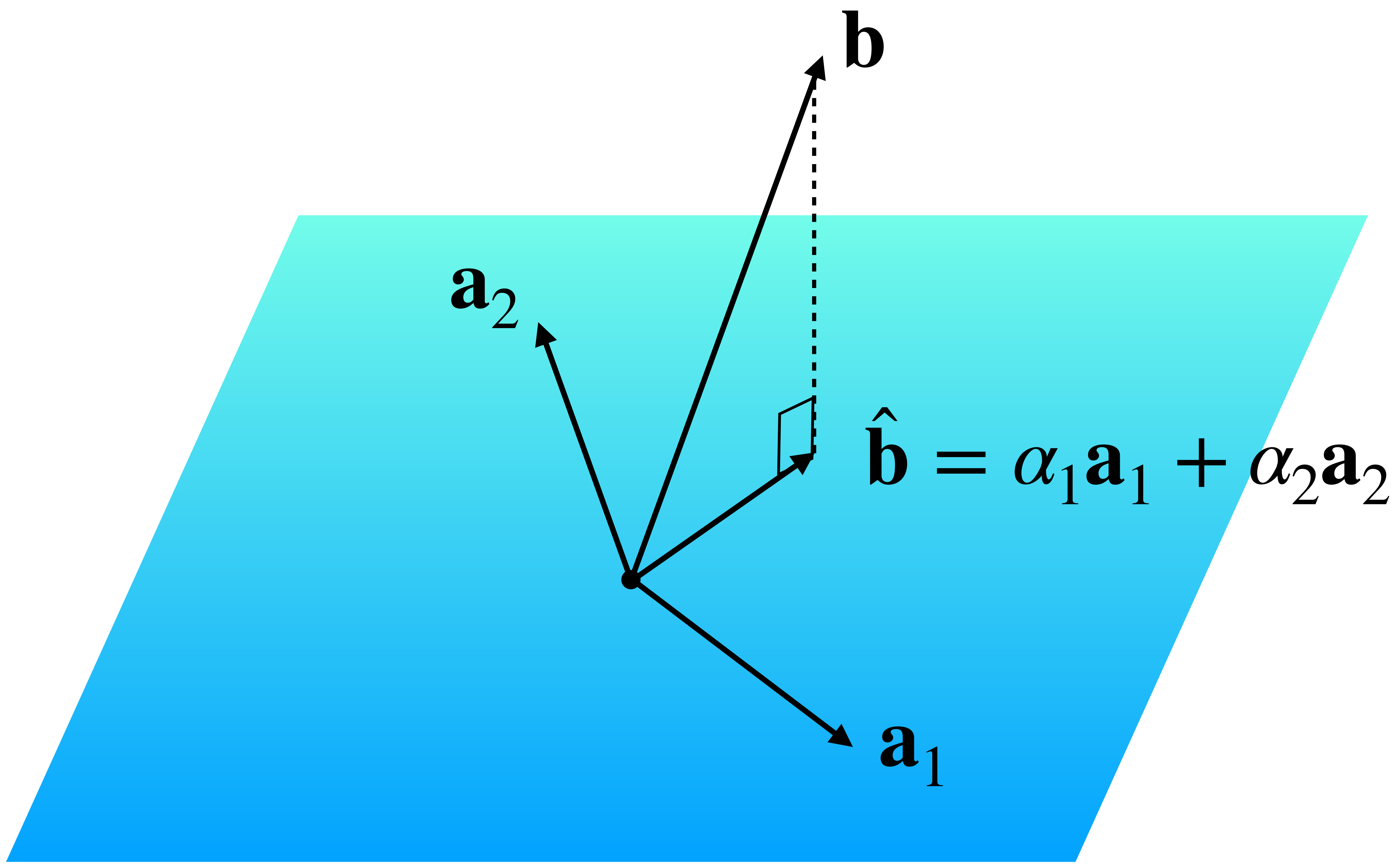
$$\|\hat{y}-\vec{v}\|^2 > 0$$

(no negative distances)

$$\|y-\hat{y}\|^2 \le \|y-v\|^2 \Rightarrow \|y-\hat{y}\| \le \|y-v\|$$



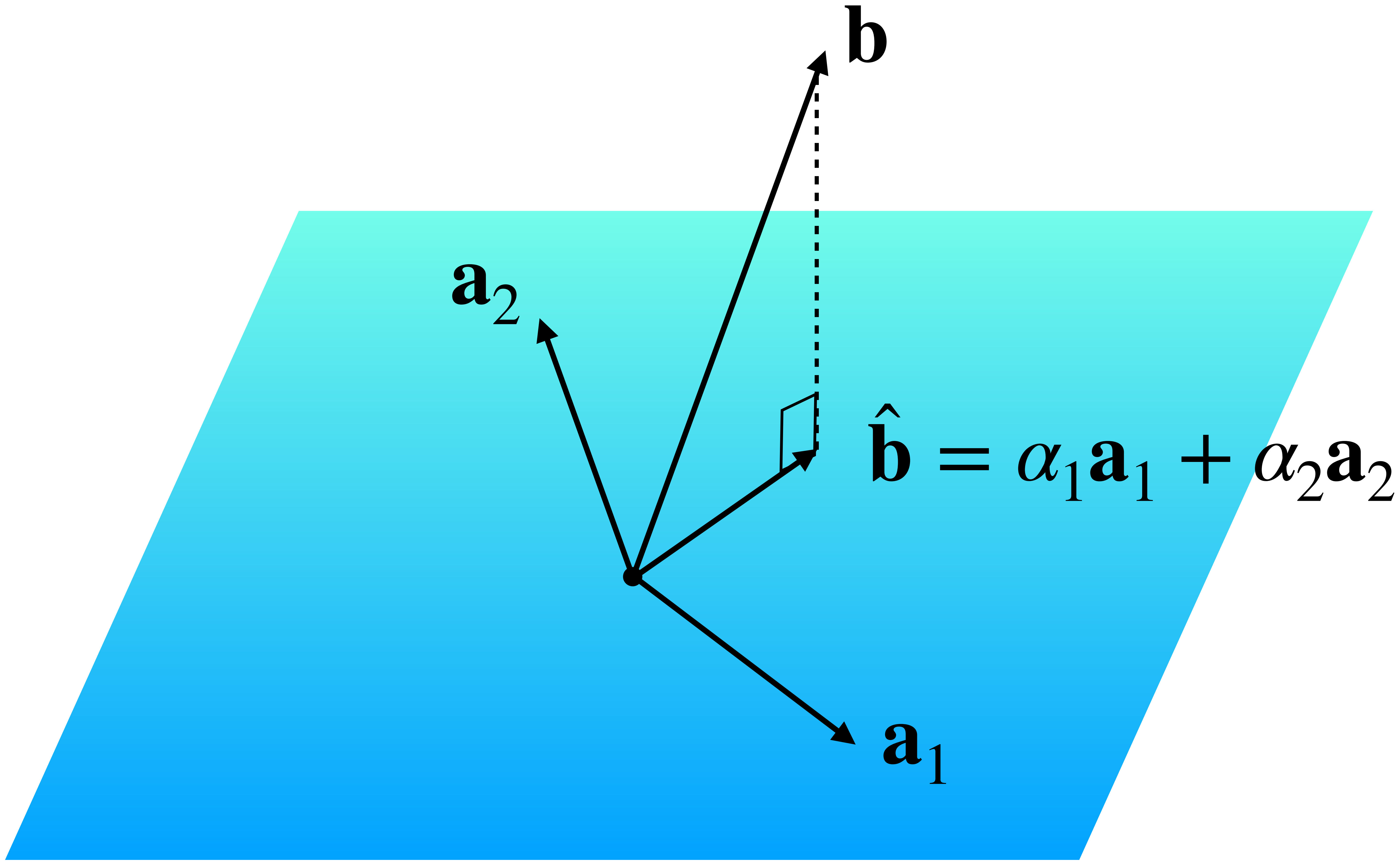
The Point



$\mathbf{b}$
$\mathbf{a}_2$
$\hat{\mathbf{b}} = \alpha_1\mathbf{a}_1 + \alpha_2\mathbf{a}_2$
$\mathbf{a}_1$

The Point

$\hat{\mathbf{b}}$ is in $Col(A)$ so $A\mathbf{x} = \hat{\mathbf{b}}$ **has a solution.**



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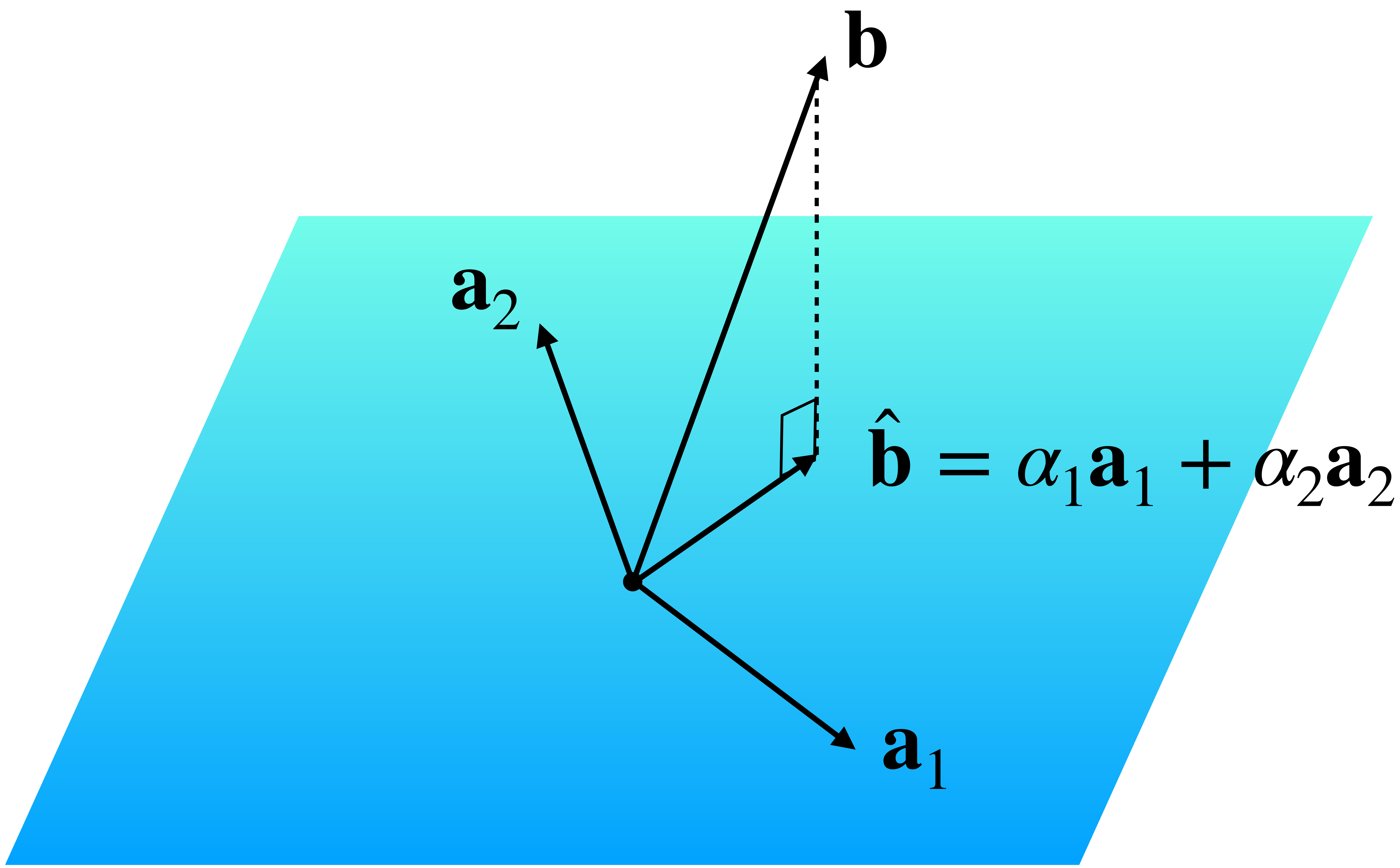
At this point, we could call it a day:



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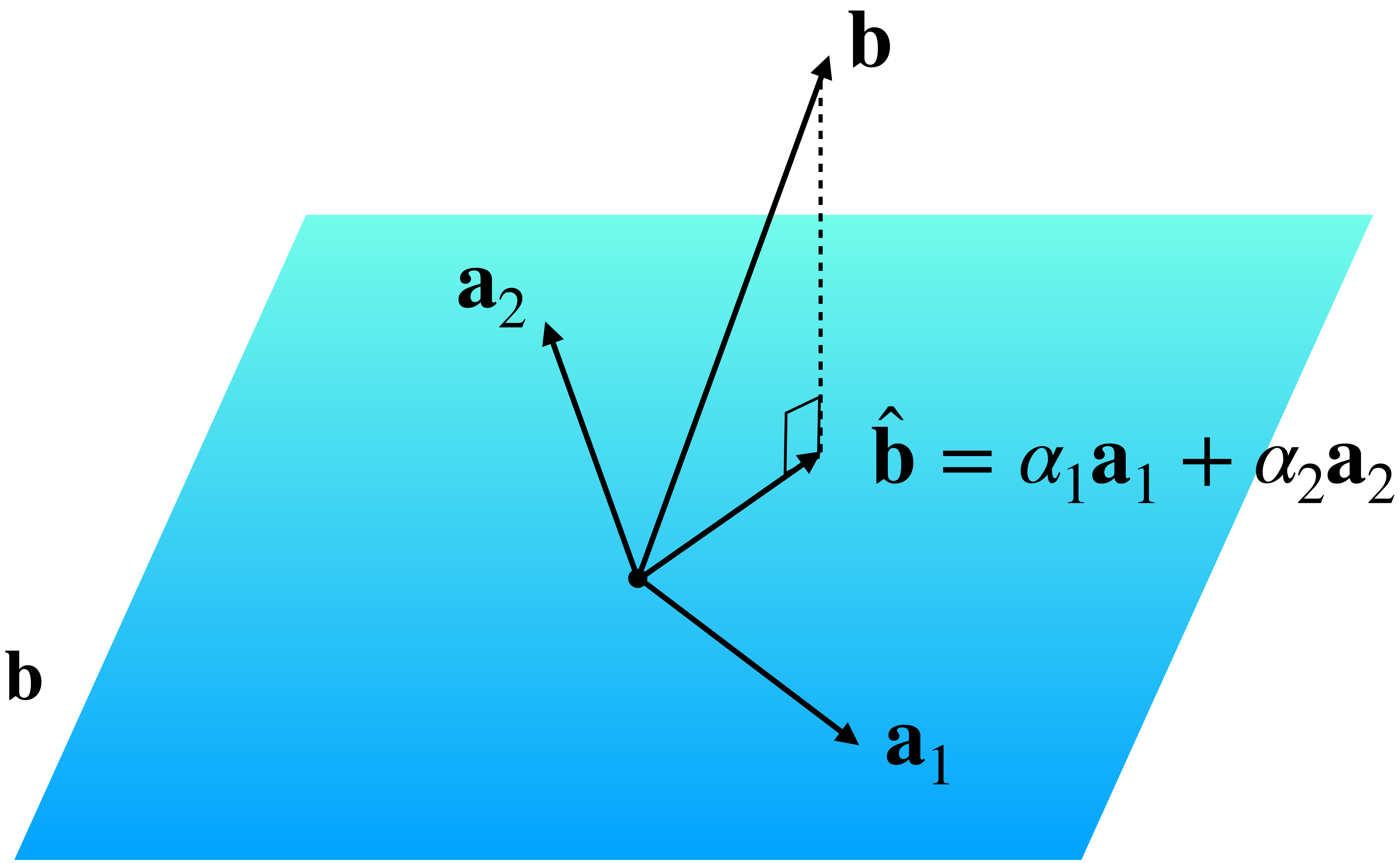
Question. Find a least squares solution to $A\mathbf{x} = \mathbf{b}$



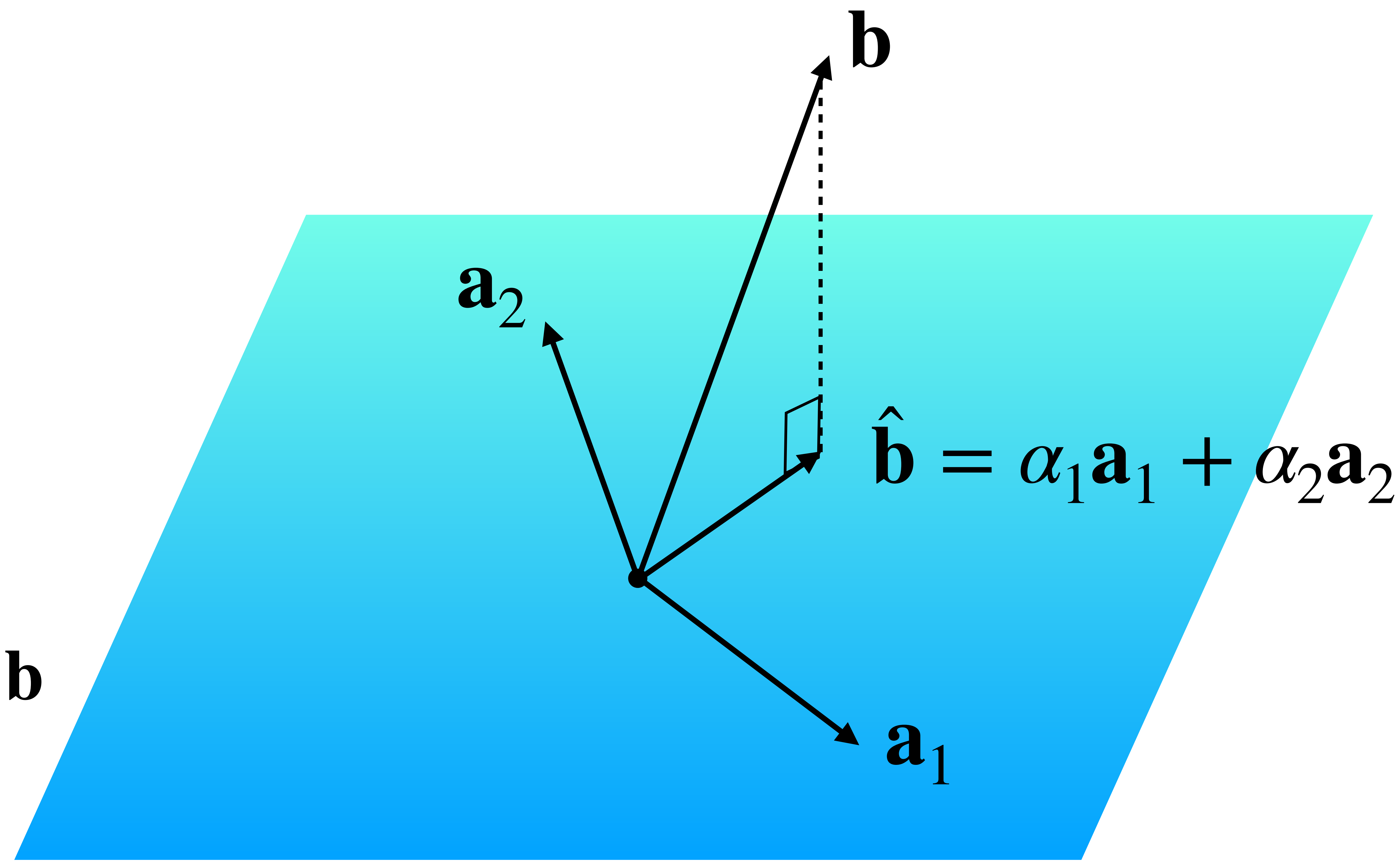
The Point

$\hat{\mathbf{b}}$ is in $Col(A)$ so $A\mathbf{x} = \hat{\mathbf{b}}$ **has a solution.**

At this point, we could call it a day:

Question. Find a least squares solution to $A\mathbf{x} = \mathbf{b}$

Solution. Find $\hat{\mathbf{b}}$, then solve $A\mathbf{x} = \hat{\mathbf{b}}$



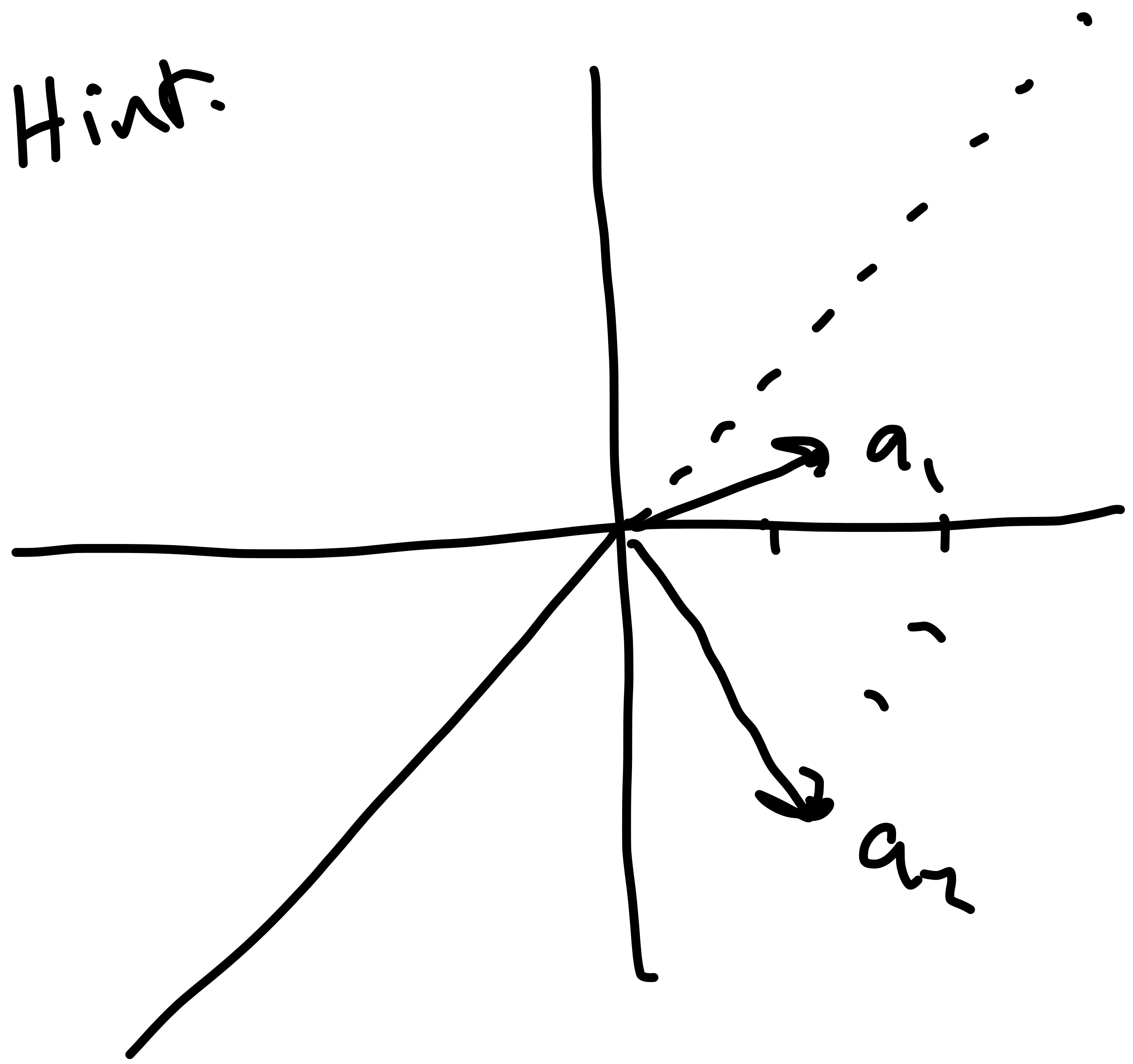
Question

Find the least square solution for the equation

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

a_1 a_2

Hint:



Col(A) = ? xy-plane

projection of $\begin{bmatrix} 4 \\ 1 \\ 4 \end{bmatrix}$ onto xy-plane = ? $\begin{bmatrix} 4 \\ 1 \\ 0 \end{bmatrix}$

Answer

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

$$\begin{bmatrix} 1 & 2 \\ -1 & 3 \\ 0 & 0 \end{bmatrix} x = \begin{pmatrix} 4 \\ 1 \\ 0 \end{pmatrix}$$

$$\begin{matrix} 2 & 1 & \\ \end{matrix}$$

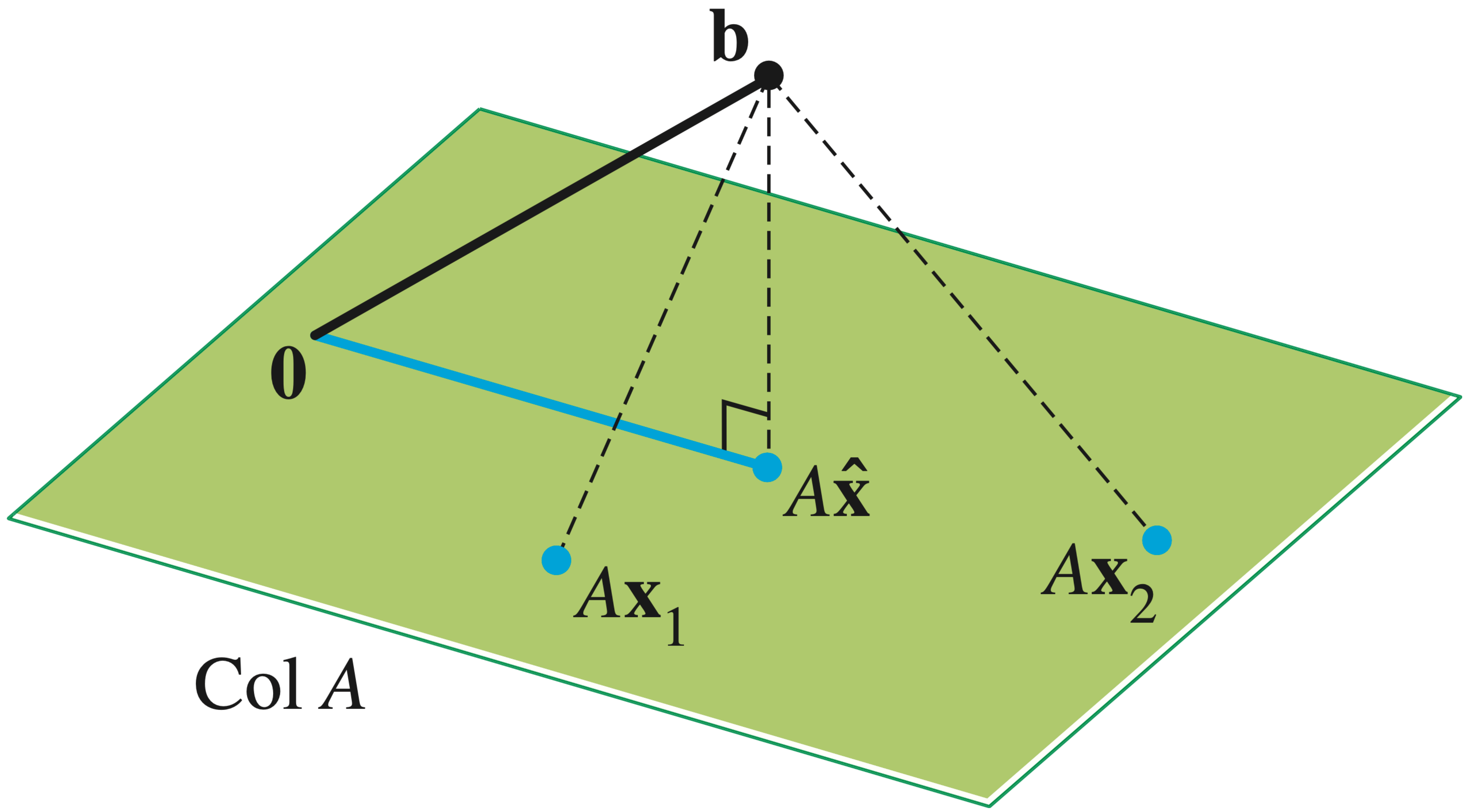
$$\begin{bmatrix} 1 & 2 & 4 \\ -1 & 3 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

$$2\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} + \begin{bmatrix} 2 \\ 3 \\ 0 \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \\ 0 \end{bmatrix}$$

$$\hat{x} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

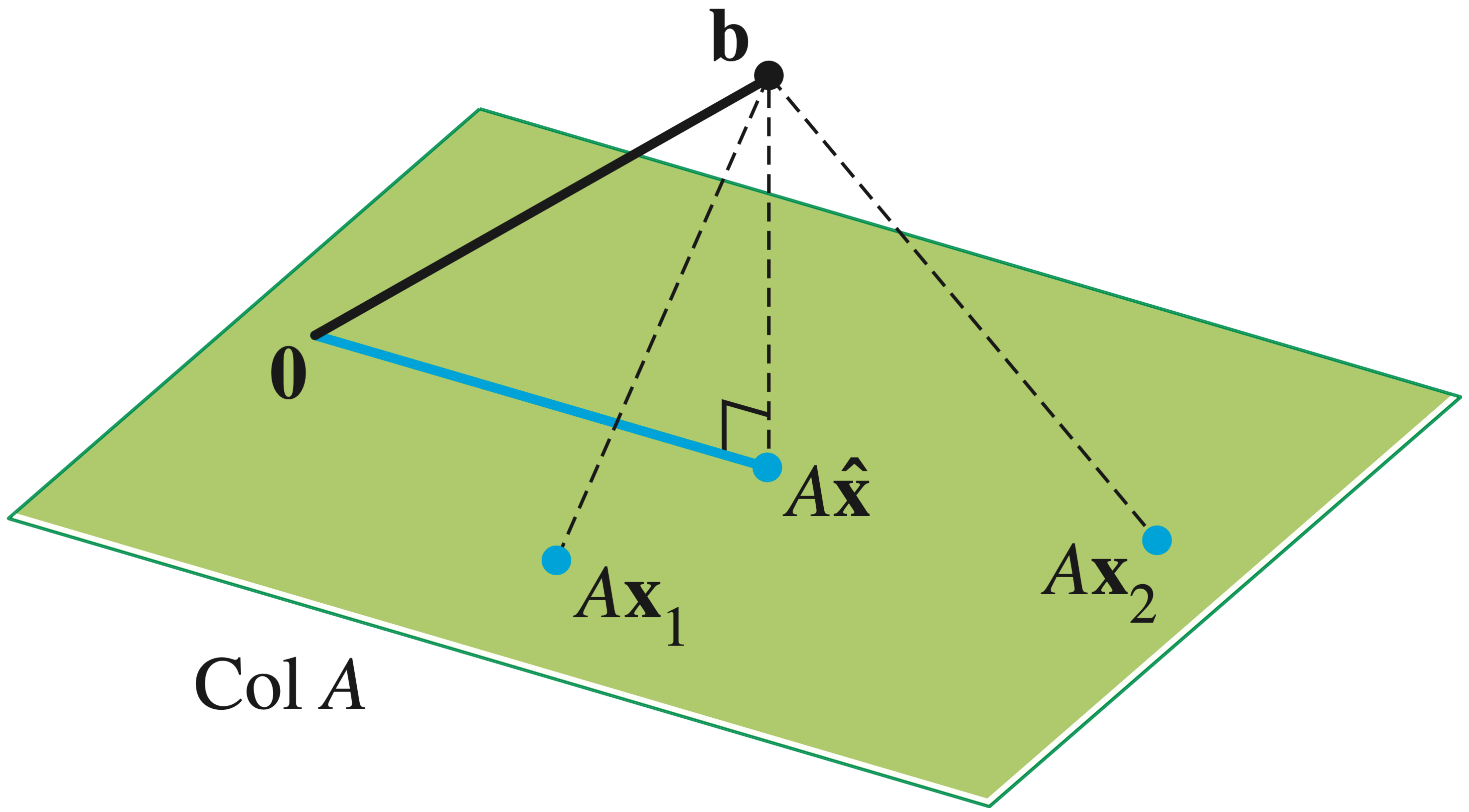
The Normal Equations

A Couple Observations



A Couple Observations

Suppose that $\hat{\mathbf{x}}$ is a least squares solution to A, so $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$



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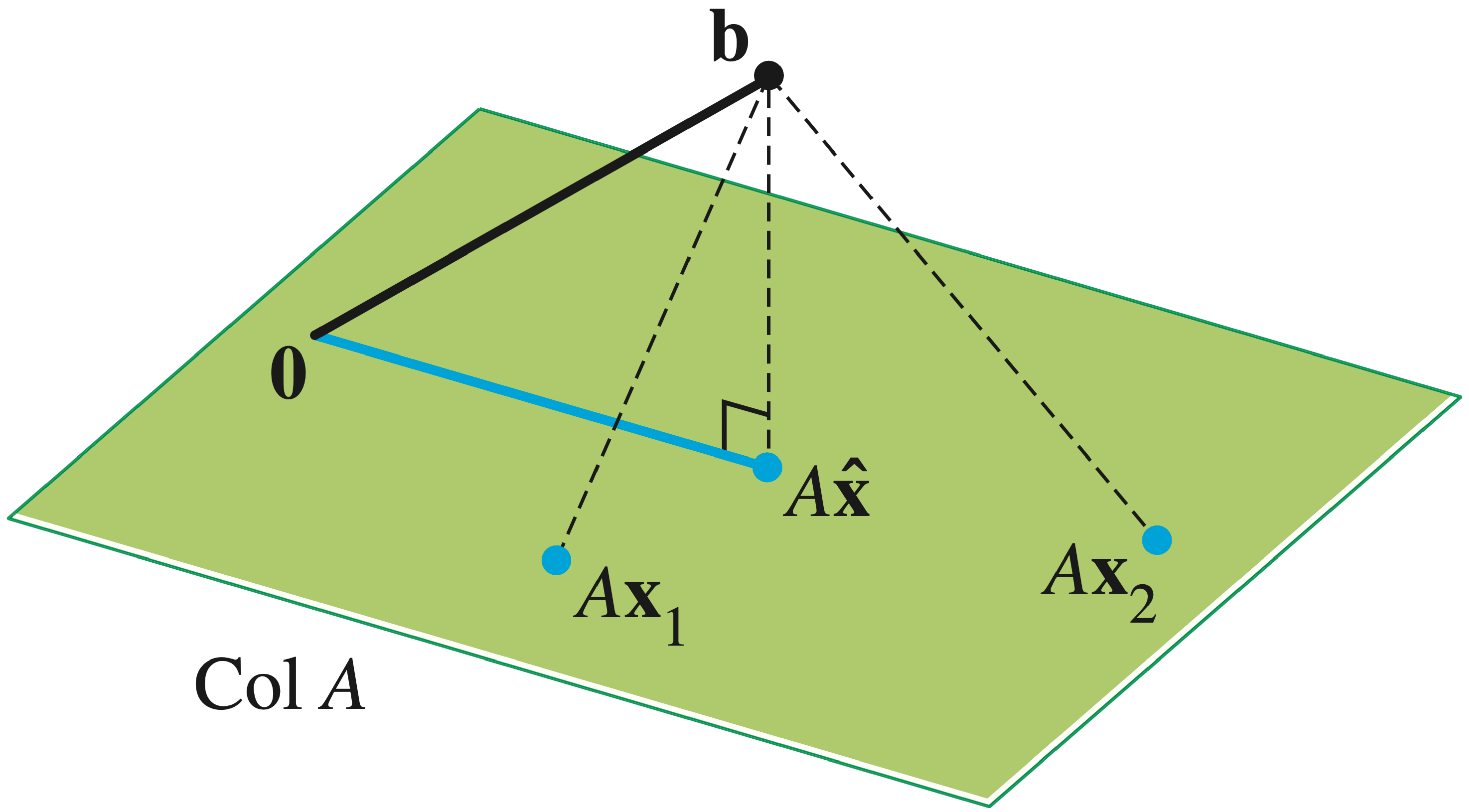
Suppose that $\hat{\mathbf{x}}$ is a least squares solution to A, so $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$

- $\hat{\mathbf{b}} - \mathbf{b}$ is orthogonal to $Col(A)$



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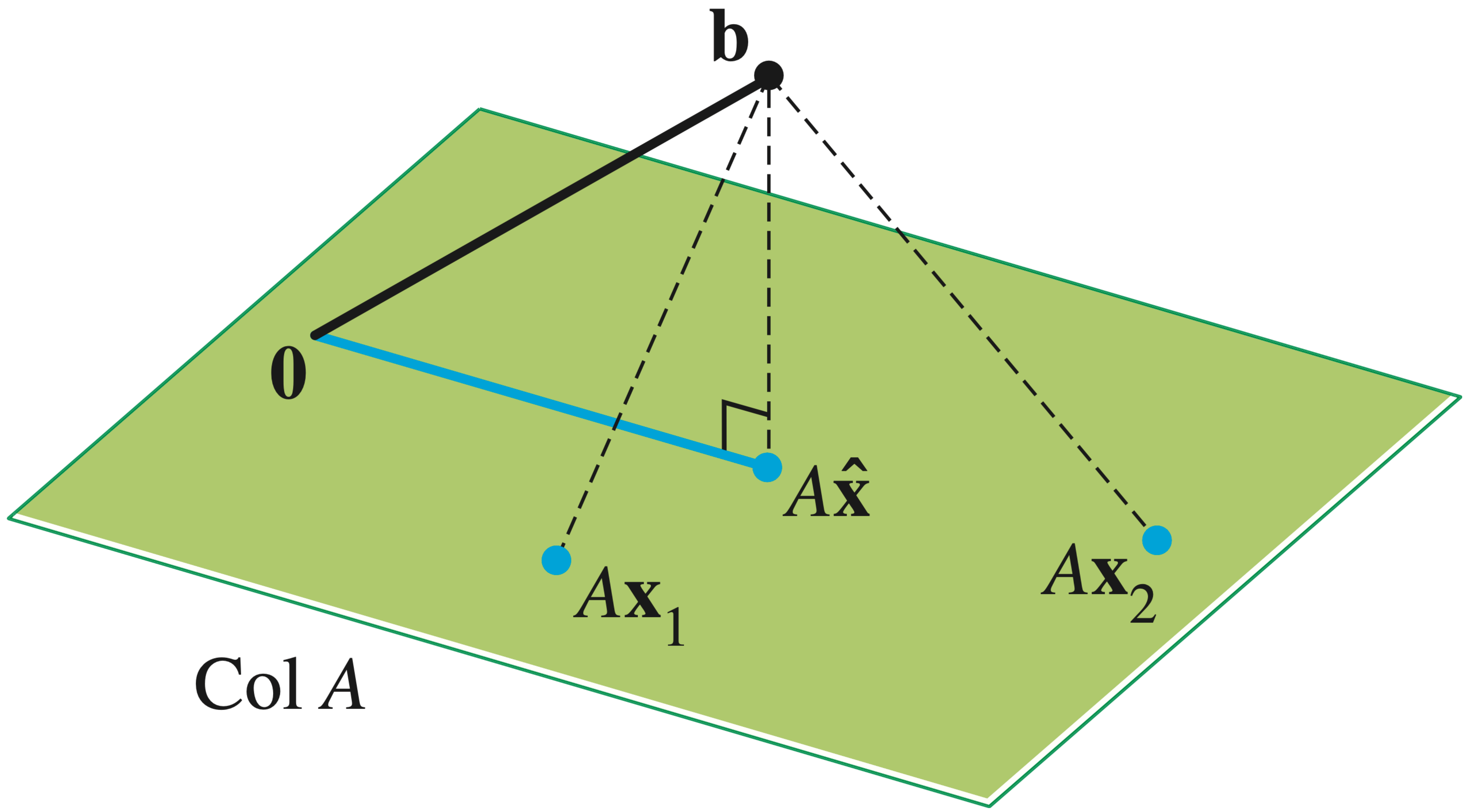

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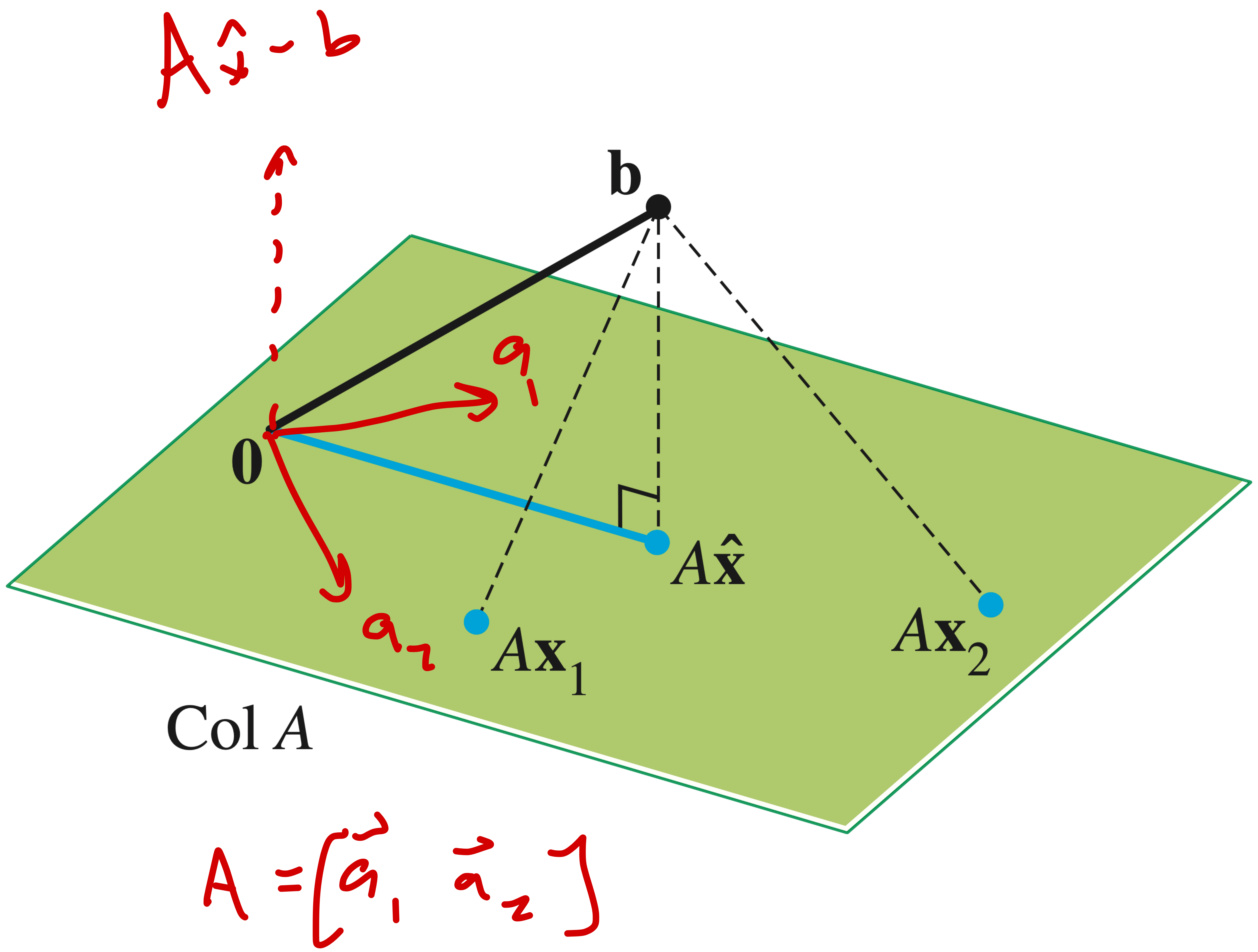
Suppose that $\hat{\mathbf{x}}$ is a least squares solution to A, so $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$

- $\hat{\mathbf{b}} - \mathbf{b}$ is orthogonal to $Col(A)$
- $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to $Col(A)$
- If $A = [\mathbf{a}_1 \ \ \mathbf{a}_2 \ \ \dots \ \ \mathbf{a}_n]$ then $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to each $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$



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Suppose that $\hat{\mathbf{x}}$ is a least squares solution to A, so $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$

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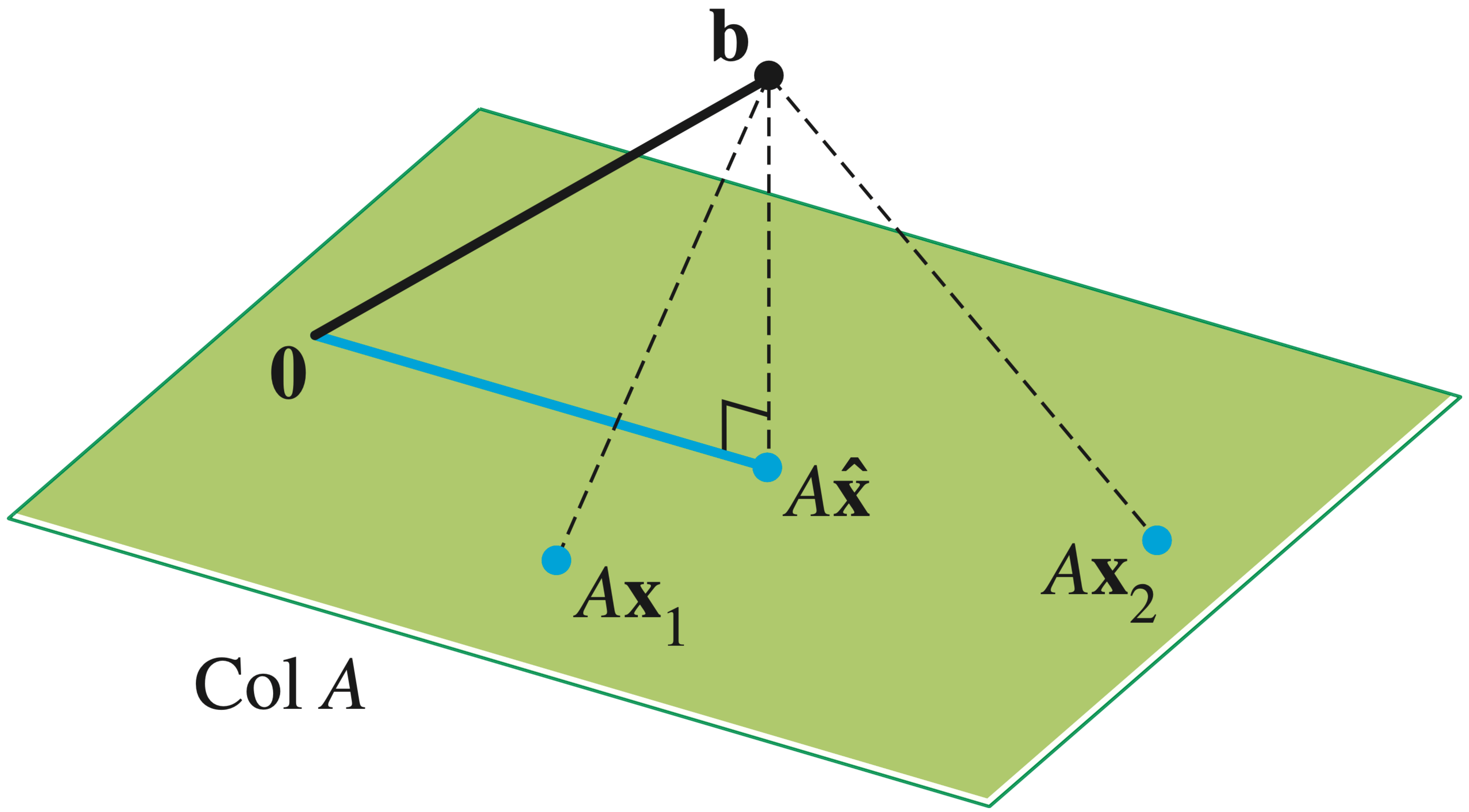
- $\mathbf{a}_i^T(A\hat{\mathbf{x}} - \mathbf{b}) = 0$



A Couple Observations

Suppose that $\hat{\mathbf{x}}$ is a least squares solution to A, so $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$

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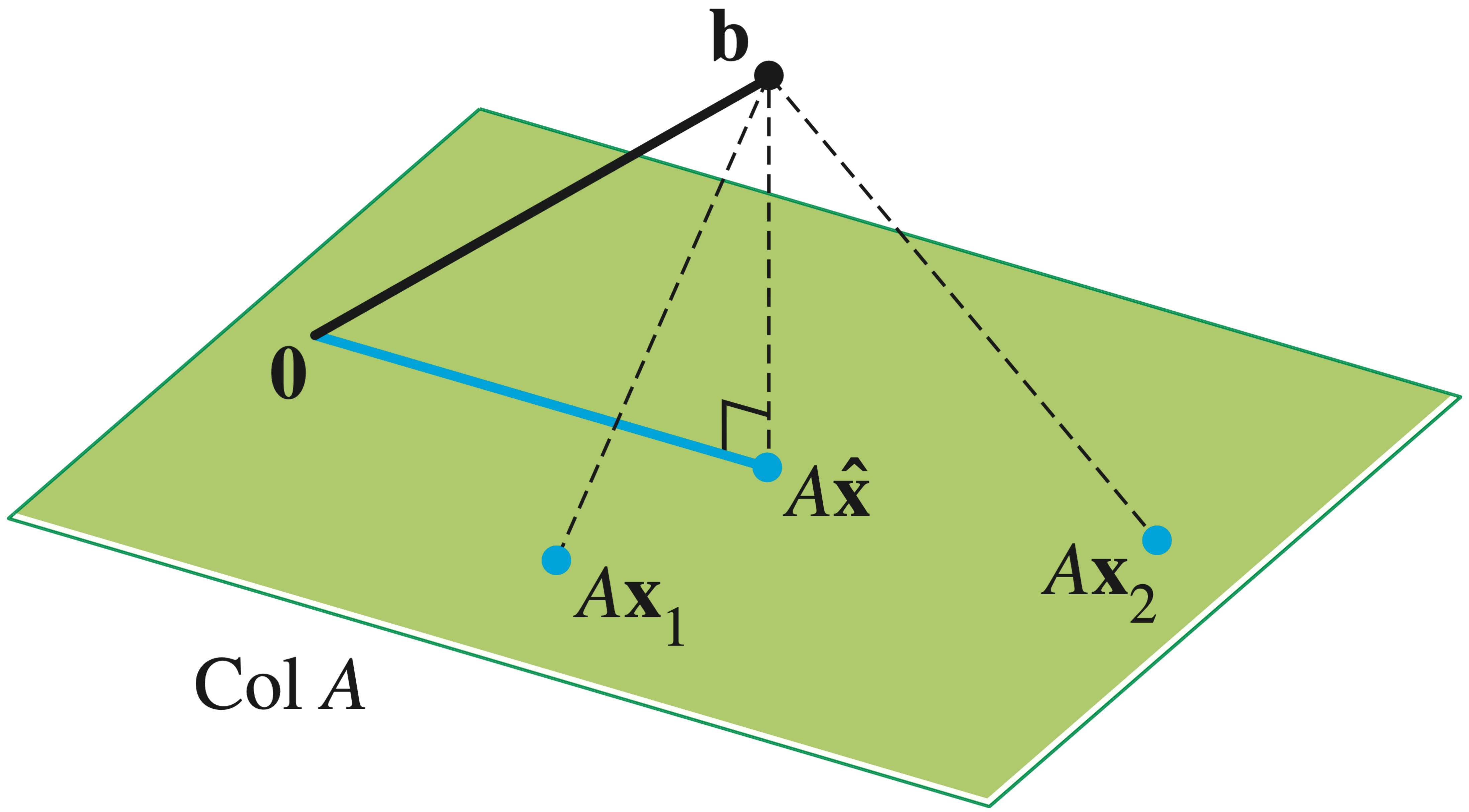
- $\mathbf{a}_i^T(A\hat{\mathbf{x}} - \mathbf{b}) = 0$
- $A^T(A\hat{\mathbf{x}} - \mathbf{b}) = \mathbf{0}$



A bit more magic

Let's simplify $A^T(A\hat{\mathbf{x}} - \mathbf{b})$:

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

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

The Normal Equations

The Normal Equations

Theorem. The set of least-squares solutions of $A\mathbf{x} = \mathbf{b}$ is the same as the set of solutions to

$$A^T A\mathbf{x} = A^T\mathbf{b}$$

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In particular, this set of solutions is nonempty.

We just showed that if $\hat{\mathbf{x}}$ is a least squares solution then $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$.

The Normal Equations

In the other direction, suppose $A^TA\mathbf{x} = A^T\mathbf{b}$:

$$A^T(Ax - b) = \vec{0}$$

$A\vec{x} - \vec{b}$ is perpendicular to Col(A)

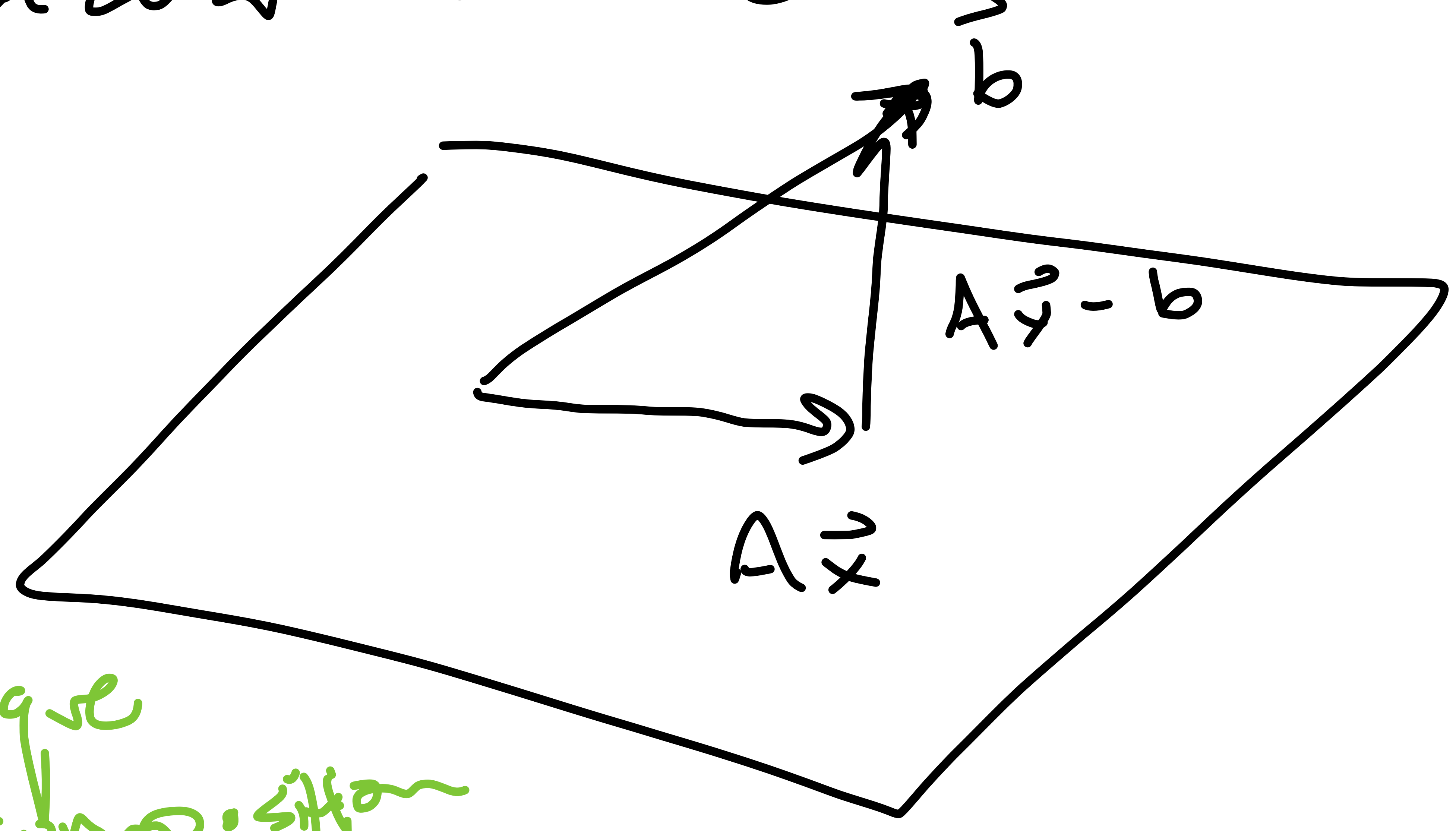
$$A\vec{x} = \vec{b} + (A\vec{x} - \vec{b})$$

$$\vec{b} = A\vec{x} - (A\vec{x} - \vec{b})$$

unique decomposition

$\therefore A\vec{x} = \hat{b}$

$\vec{x}$ is a LS-solution



Example

$$A = \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix}$$

Let's find the normal equations for $A\mathbf{x} = \mathbf{b}$:

Example

$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

Let's solve the normal equations for $A\mathbf{x} = \mathbf{b}$:

Question

Find the normal equations for the equation

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

Answer

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

Unique Least Squares Solutions

Question (Conceptual)

Is a least squares solution unique?

Answer: No

Remember that if $\mathbf{b} \in Col(A)$ then $\hat{\mathbf{b}} = \mathbf{b}$ and then we're asking if $A\mathbf{x} = \mathbf{b}$ has a unique solution for any choice of A.

When is there a unique solution?

The least squares method gives us to find an approximate solution when there is no exact solution.

But it doesn't help us choose a solution in the case that there are many.

Practically Speaking

numpy.linalg.lstsq

`linalg.lstsq(a, b, rcond='warn')` [source]

Return the least-squares solution to a linear matrix equation.

Computes the vector *x* that approximately solves the equation `a @ x = b`. The equation may be under-, well-, or over-determined (i.e., the number of linearly independent rows of *a* can be less than, equal to, or greater than its number of linearly independent columns). If *a* is square and of full rank, then *x* (but for round-off error) is the "exact" solution of the equation. Else, *x* minimizes the Euclidean 2-norm $||b - ax||$. If there are multiple minimizing solutions, the one with the smallest 2-norm $||x||$ is returned.

Parameters: **a** : *(M, N) array_like*

"Coefficient" matrix.

b : *{(M,), (M, K)} array_like*

Ordinate or "dependent variable" values. If *b* is two-dimensional, the least-squares solution is calculated for each of the *K* columns of *b*.

rcond : *float, optional*

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NumPy chooses the shortest vector

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(why?...)

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Unique Least Squares Solutions

Theorem. For a $m \times n$ matrix A the following are equivalent:

» $A\mathbf{x} = \mathbf{b}$ has a unique least squares solution for any choice of $\mathbf{b}$

» The columns of A are linearly independent.

» $A^T A$ is invertible.

Unique Least Squares Solutions

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

If A has linearly independent columns, then its unique least squares solution is defined as above:

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

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

Projecting onto a subspace

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

If the columns of A are linearly independent, then **they form a basis**.

Said another way: if $\mathscr{B}$ is a basis, then we can construct a matrix A whose columns are the vectors in $\mathscr{B}$.

This means we can find arbitrary projections.

Summary

Not all matrix equations have solutions, but every equation has a least squares solution

The least squares solution is an approximate solution, so it is close to an "actual" solution.

The normal equations give us a convenient way to compute least squares solutions.