Least Squares

Geometric Algorithms
Lecture 23

CAS CS 132

Recap Problem

Project $\vec{y}$ onto span$\{\vec{u}\}$

$\hat{y} = \alpha \vec{u}$

$\alpha = \frac{\vec{y}^T \vec{u}}{\vec{u}^T \vec{u}}$

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

Find the orthogonal projection of **u** *onto the span of* **v**

$$\alpha = \frac{\vec{u}^T \vec{v}}{\vec{v}^T \vec{v}} = \frac{3+2}{1+1} = 5$$

$$\hat{u} = 5\vec{v} = \begin{bmatrix} 0 \\ 5 \\ -5 \\ 0 \end{bmatrix}$$

Answer

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

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

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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

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

Orthonormal Matrices and Inner Products

Theorem. For a $\underline{m \times n}$ 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

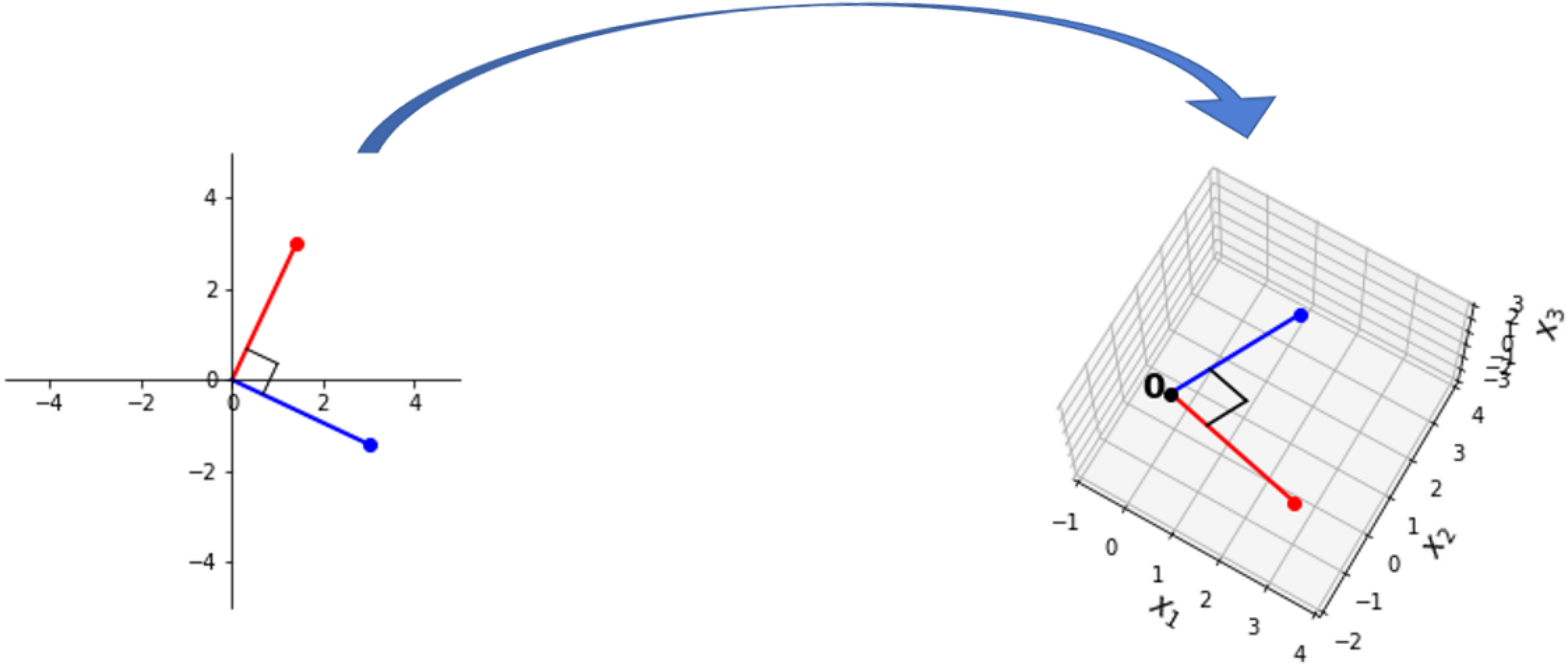
and thus lengths & angles

Verify:

Length, Angle, Orthogonality Preservation

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

The Picture



Orthonormal U

Example

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

moving on...

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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Answer. Use `np.linalg.solve(A, b)`

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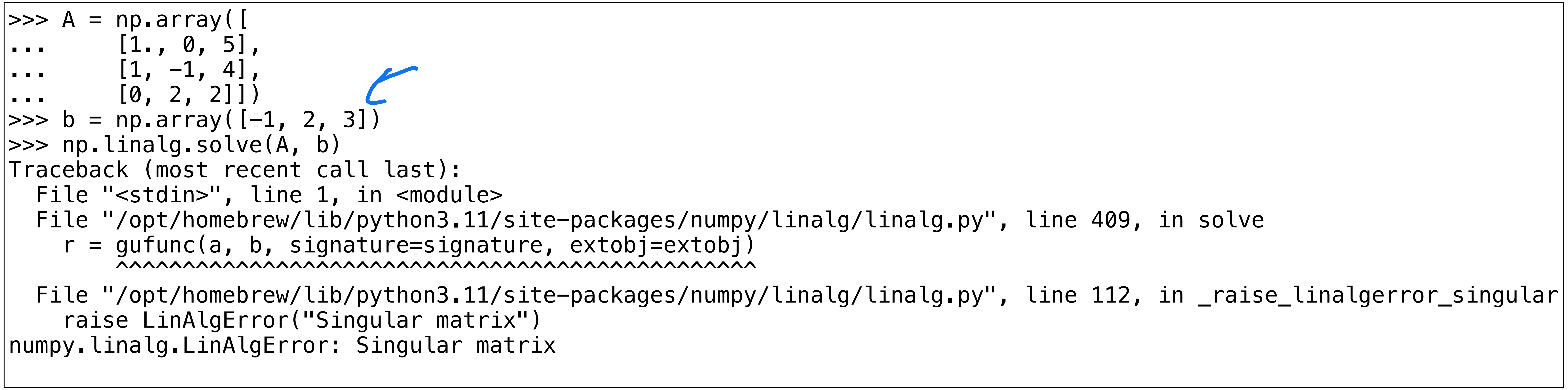

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        ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
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    raise LinAlgError("Singular matrix")
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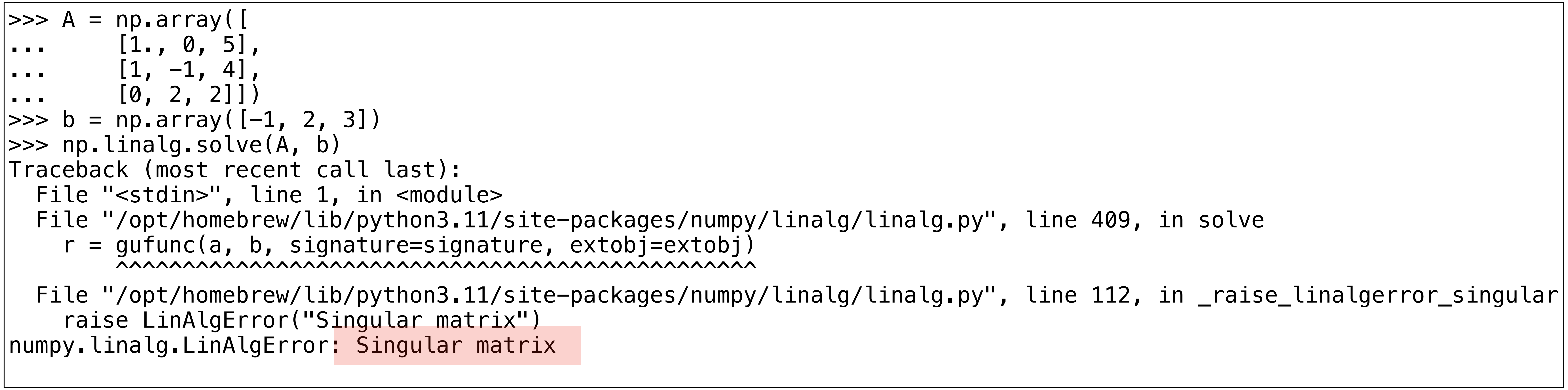

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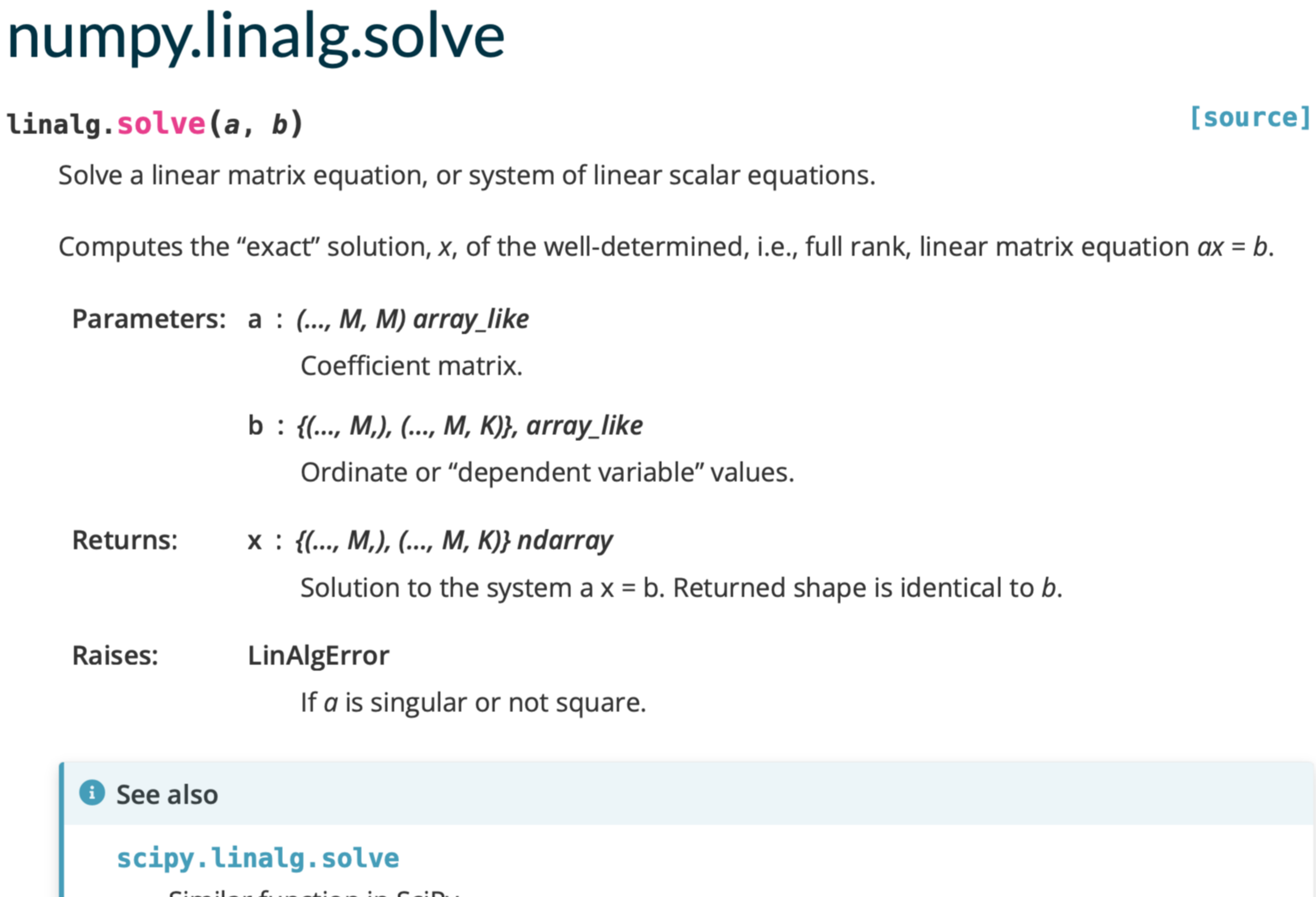
This doesn't always work

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

`scipy.linalg.solve`

Similar function in SciPy.

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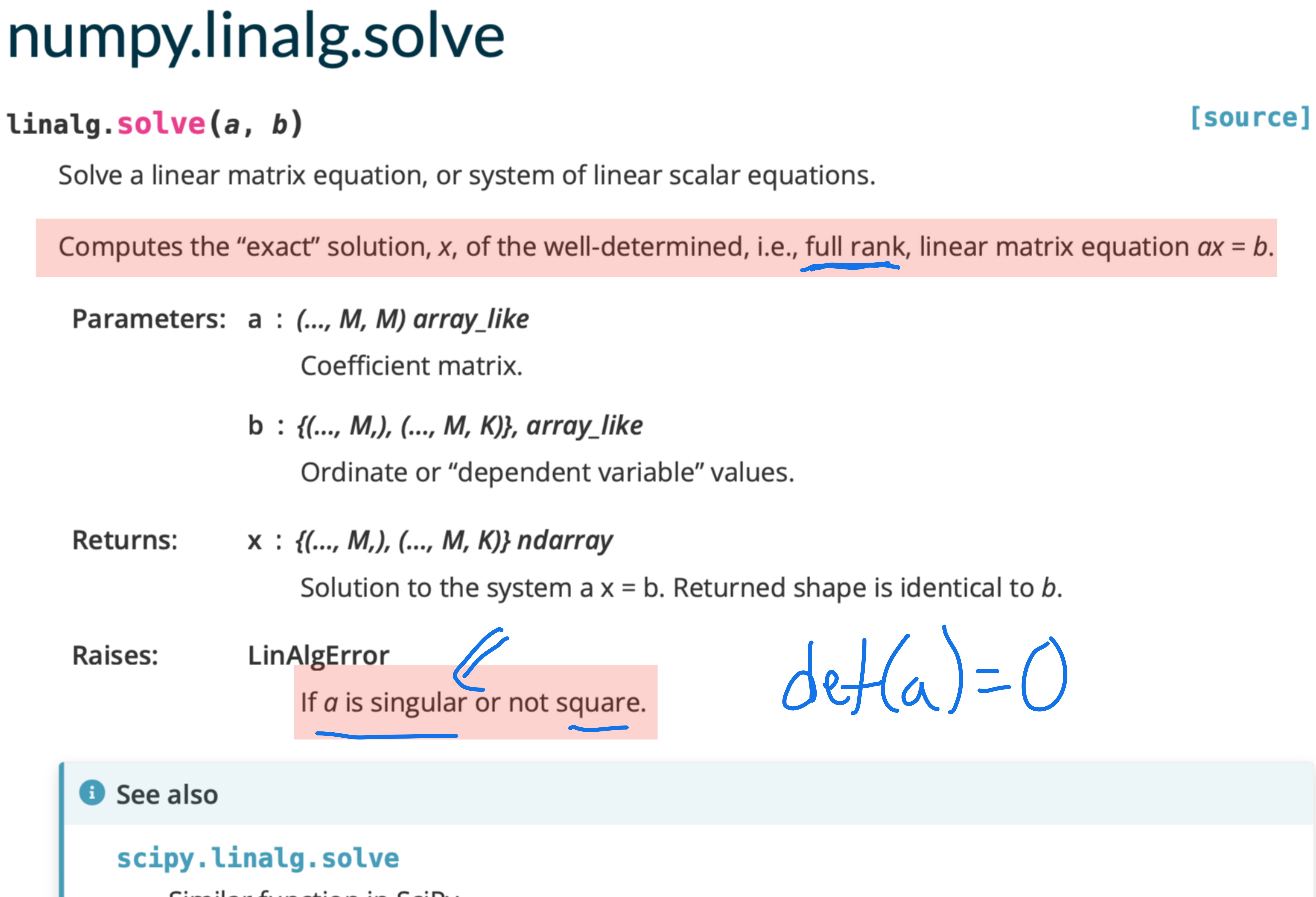

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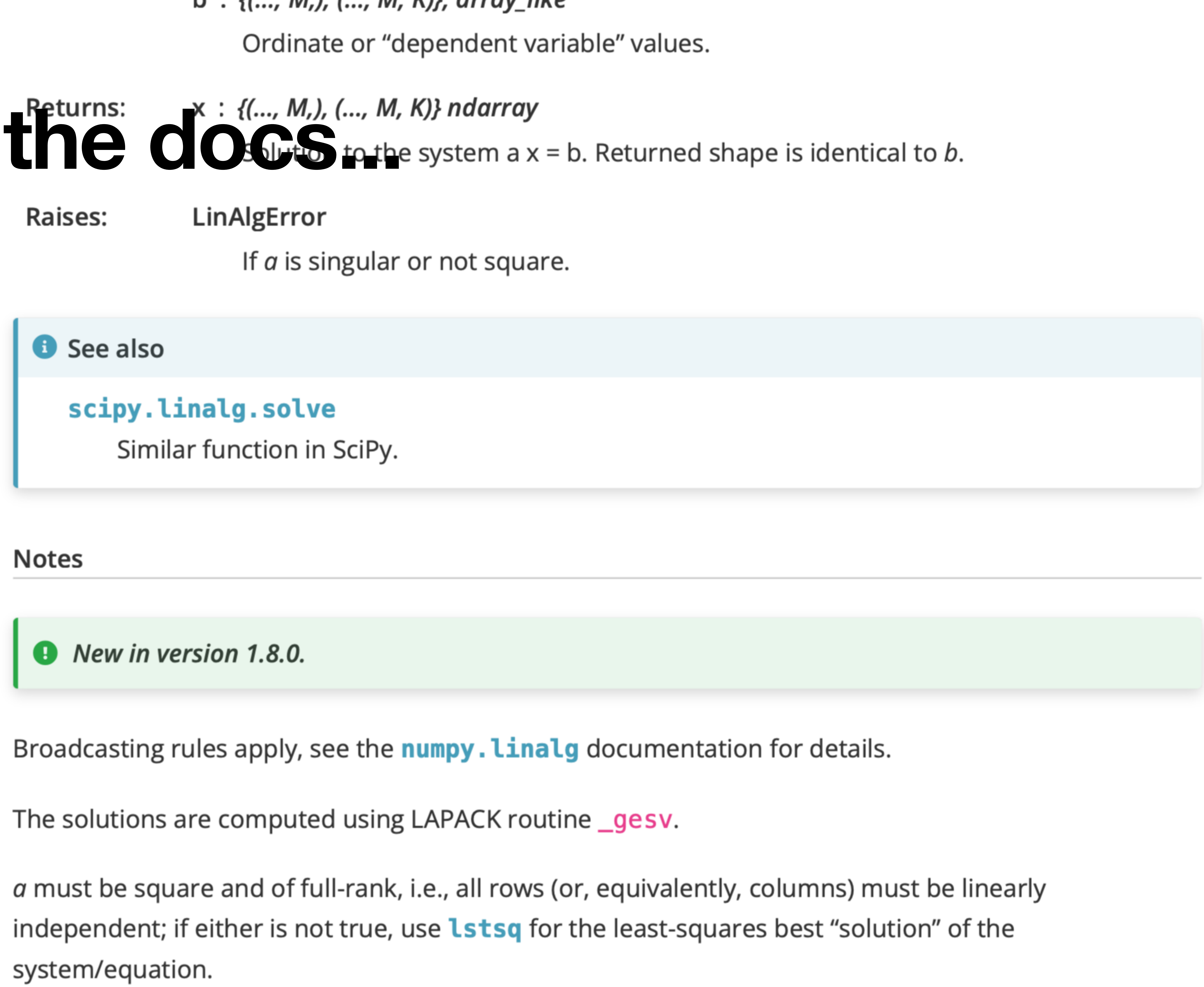

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Notes

❗ *New in version 1.8.0.*

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

The solutions are computed using LAPACK routine `_gesv`.

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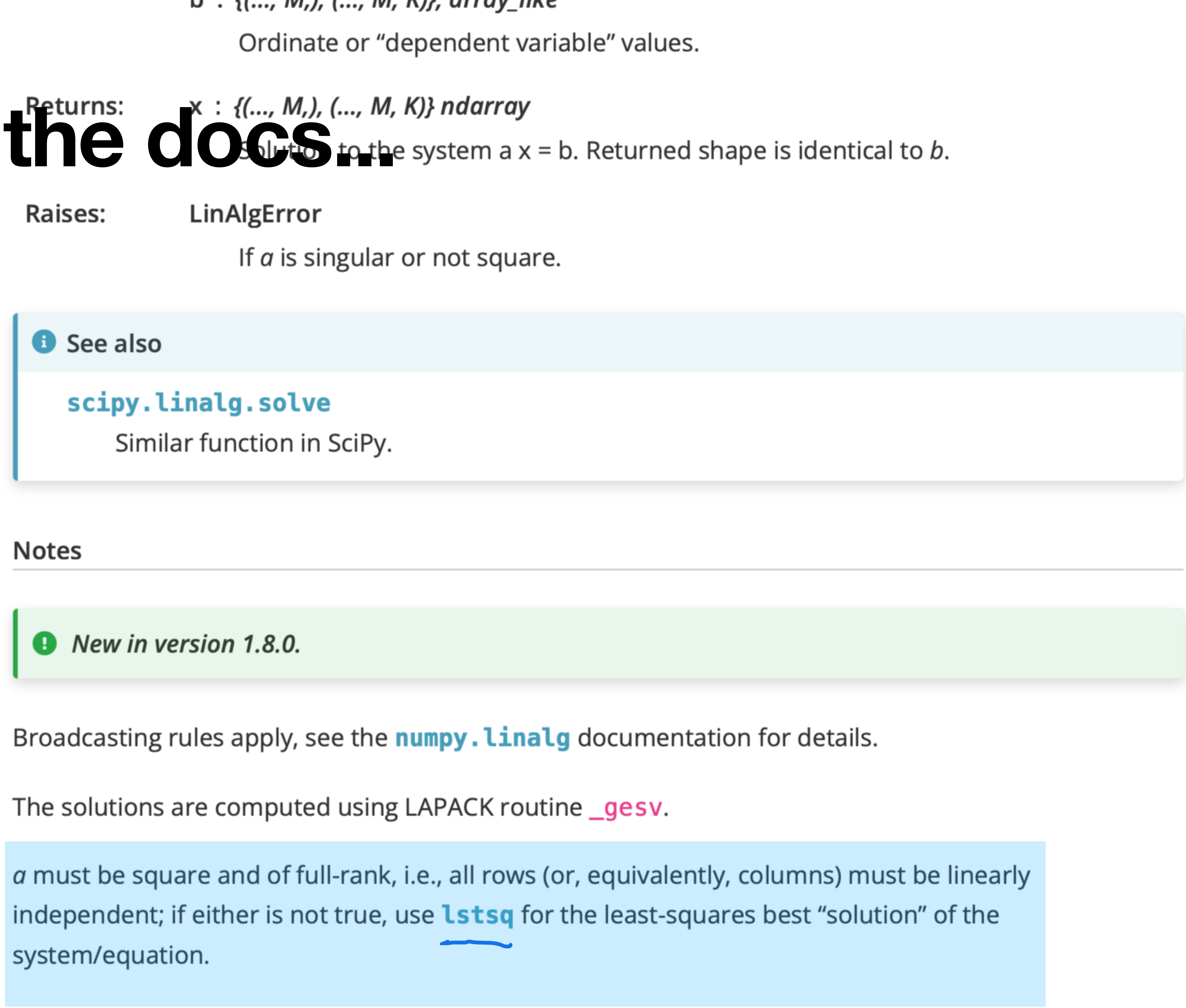

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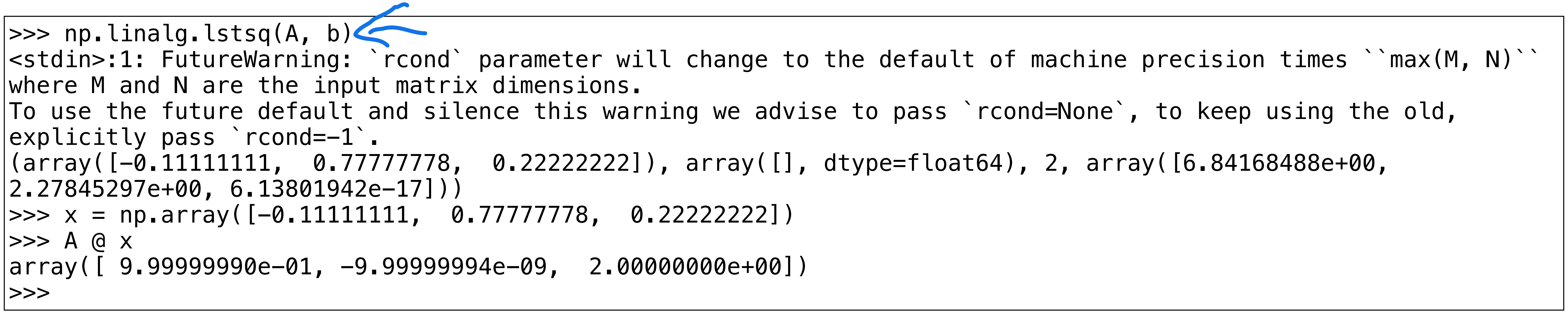

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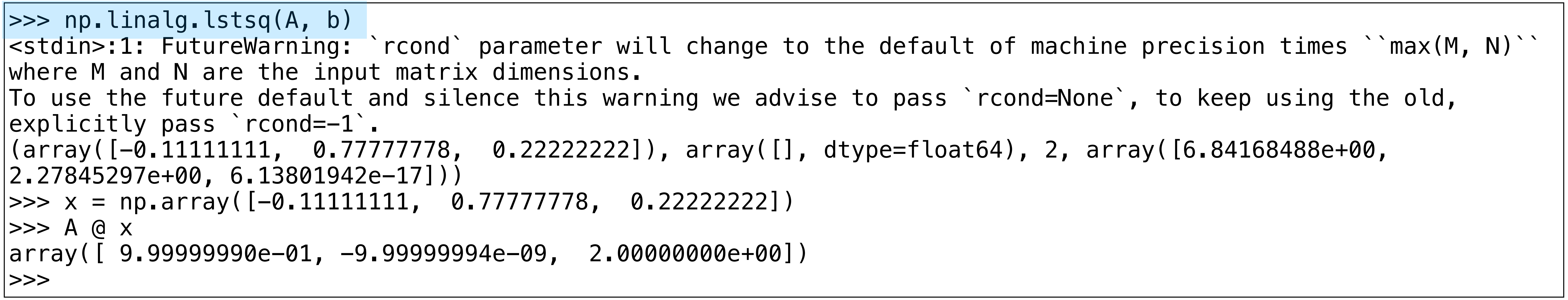

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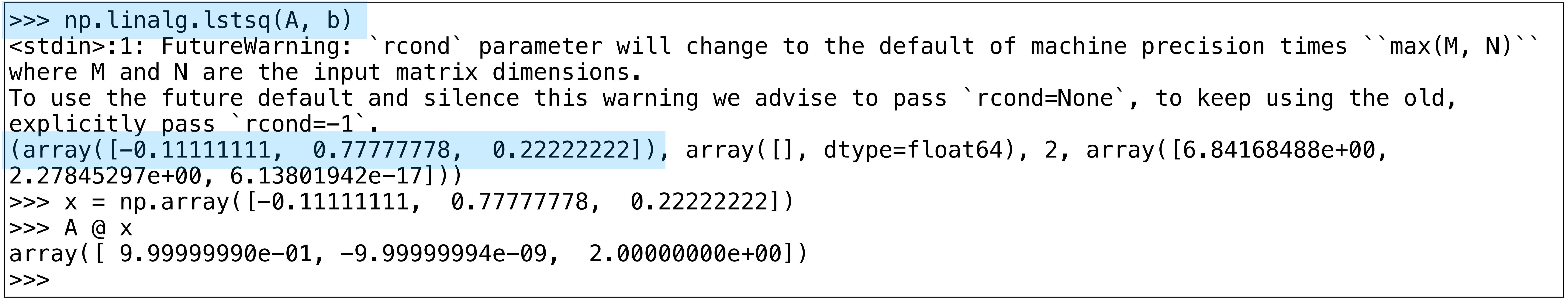

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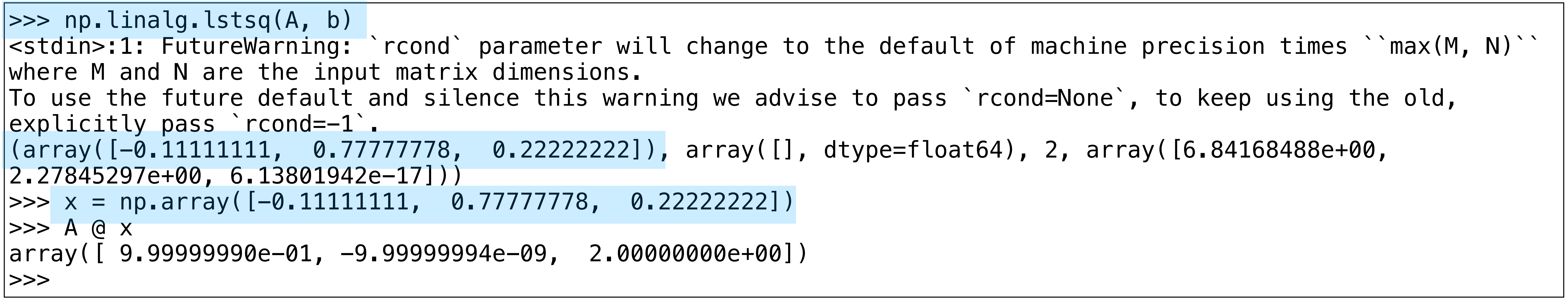

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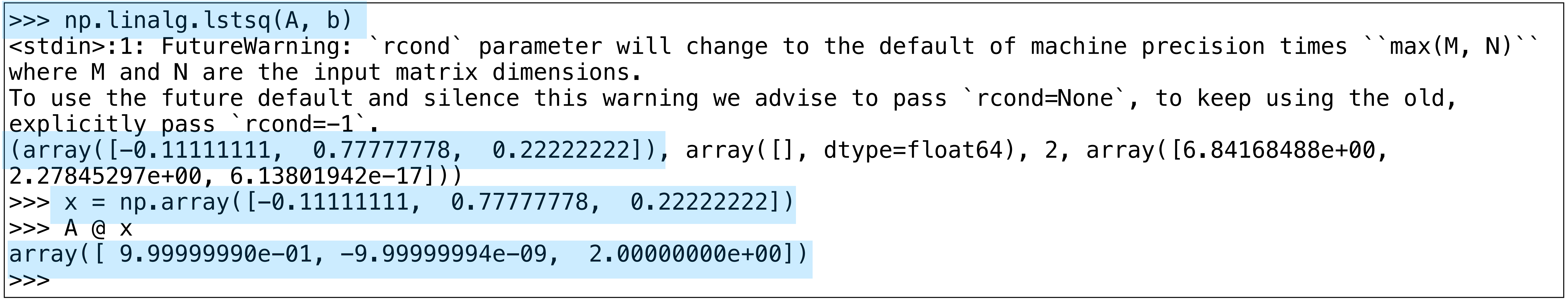

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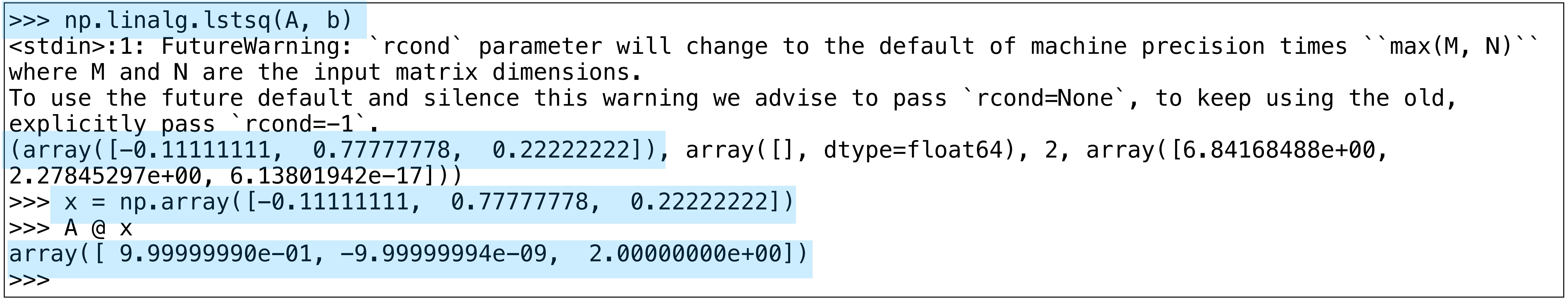
0.1 , -0.0000... , 2

↑

$[0.1, 0, 2]^T$

np.linalg.lstsq



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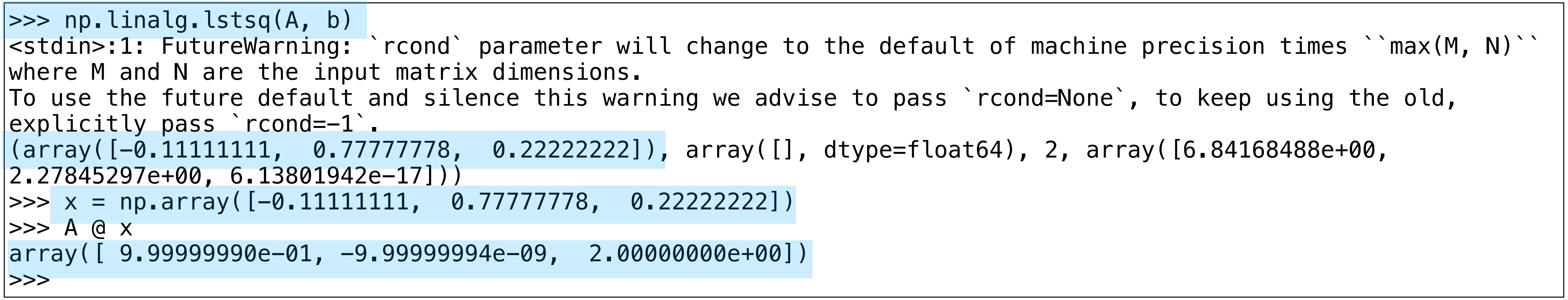
uh...probably numerical errors...

Answer: $\mathbf{x} = \begin{bmatrix} -1/9 \\ 7/9 \\ 2/9 \end{bmatrix}$

np.linalg.lstsq



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This is not correct

This System is Inconsistent

$$\begin{bmatrix} 1 & 0 & 5 & -1 \\ 1 & -1 & 4 & 2 \\ 0 & 2 & 2 & 3 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 5 & -1 \\ 0 & -1 & -1 & 3 \\ 0 & 2 & 2 & 3 \end{bmatrix} \sim \left[\begin{array}{ccc:c} 1 & 0 & 5 & -1 \\ 0 & -1 & -1 & 3 \\ 0 & 0 & 0 & 9 \end{array}\right]$$

The "correct" answer: There is no solution

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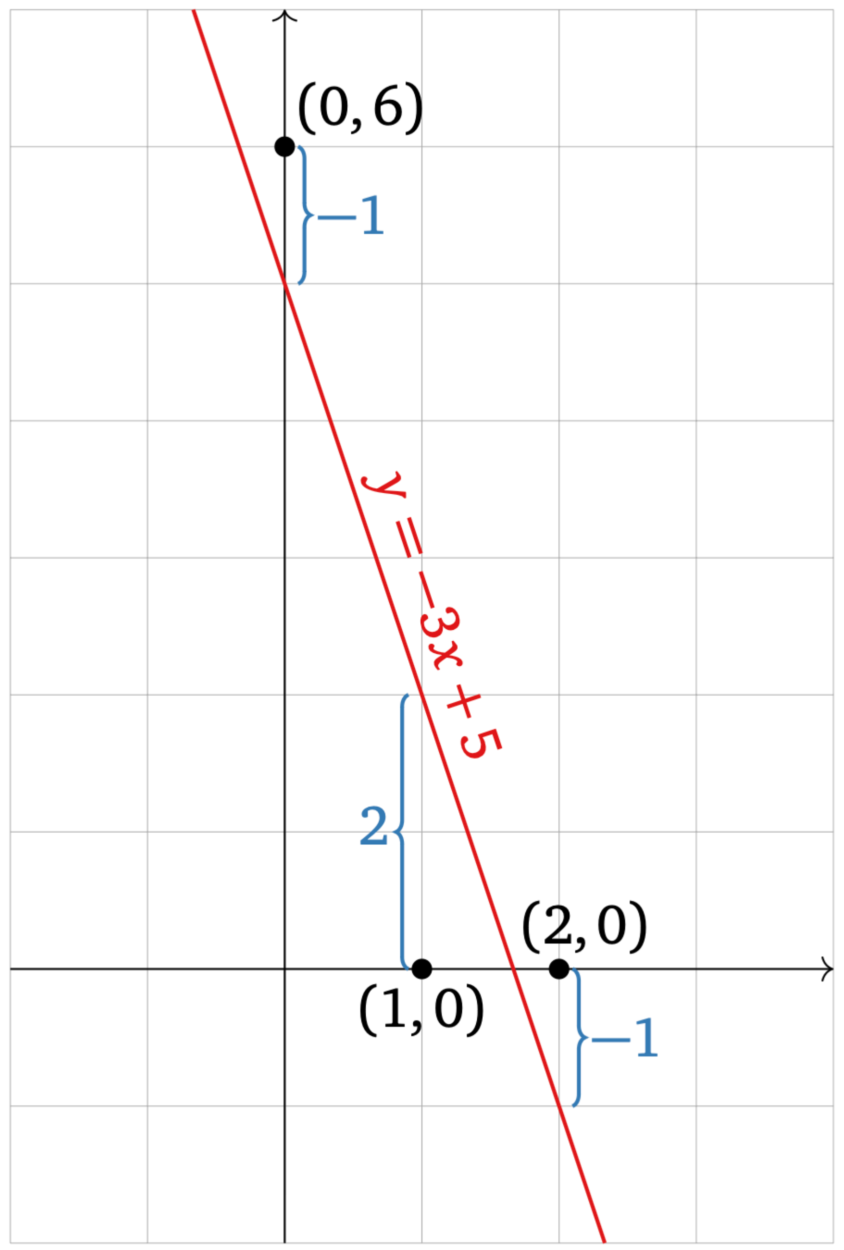
What's going on here?

Non-Linearity



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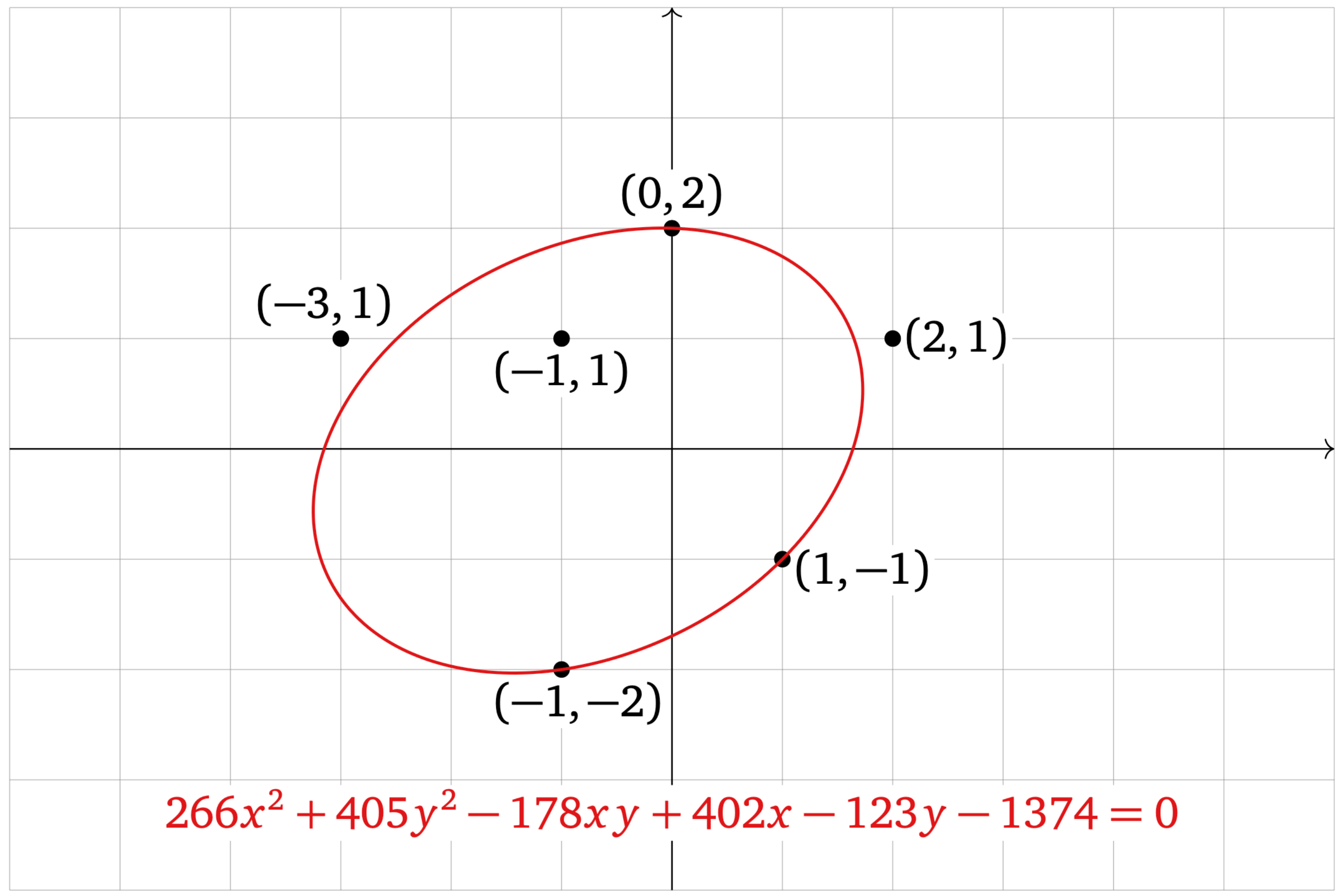
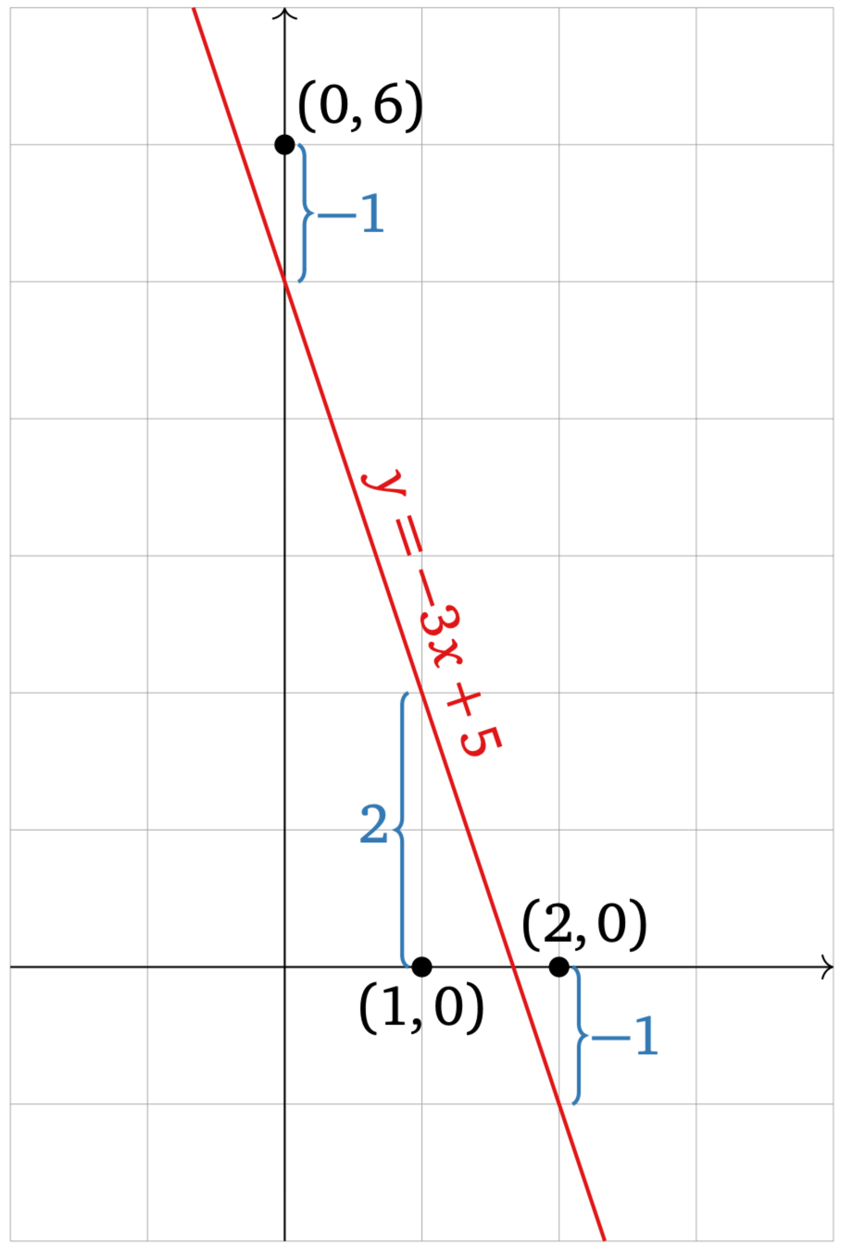


https://textbooks.math.gatech.edu/ila/least-squares.html

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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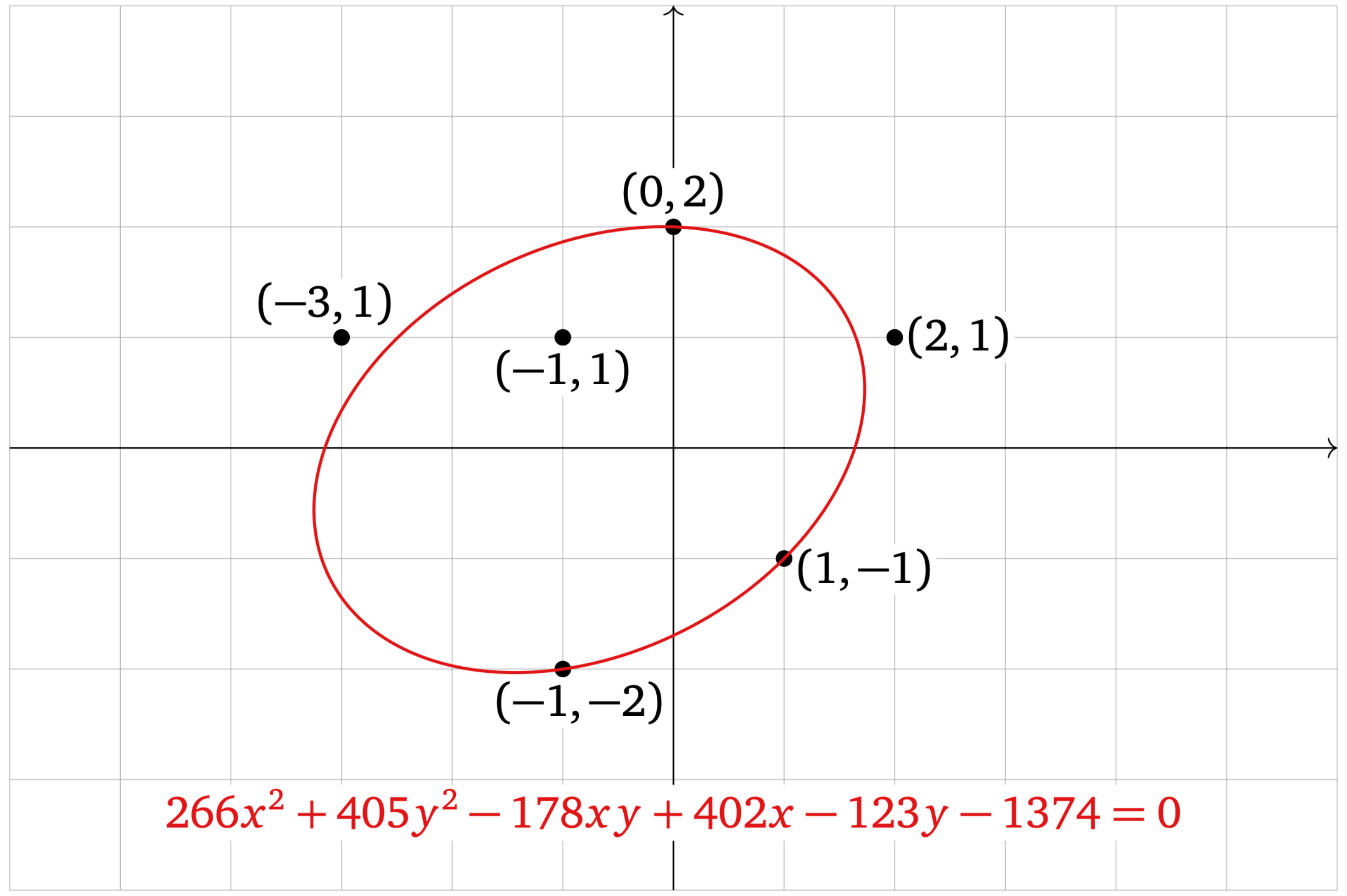

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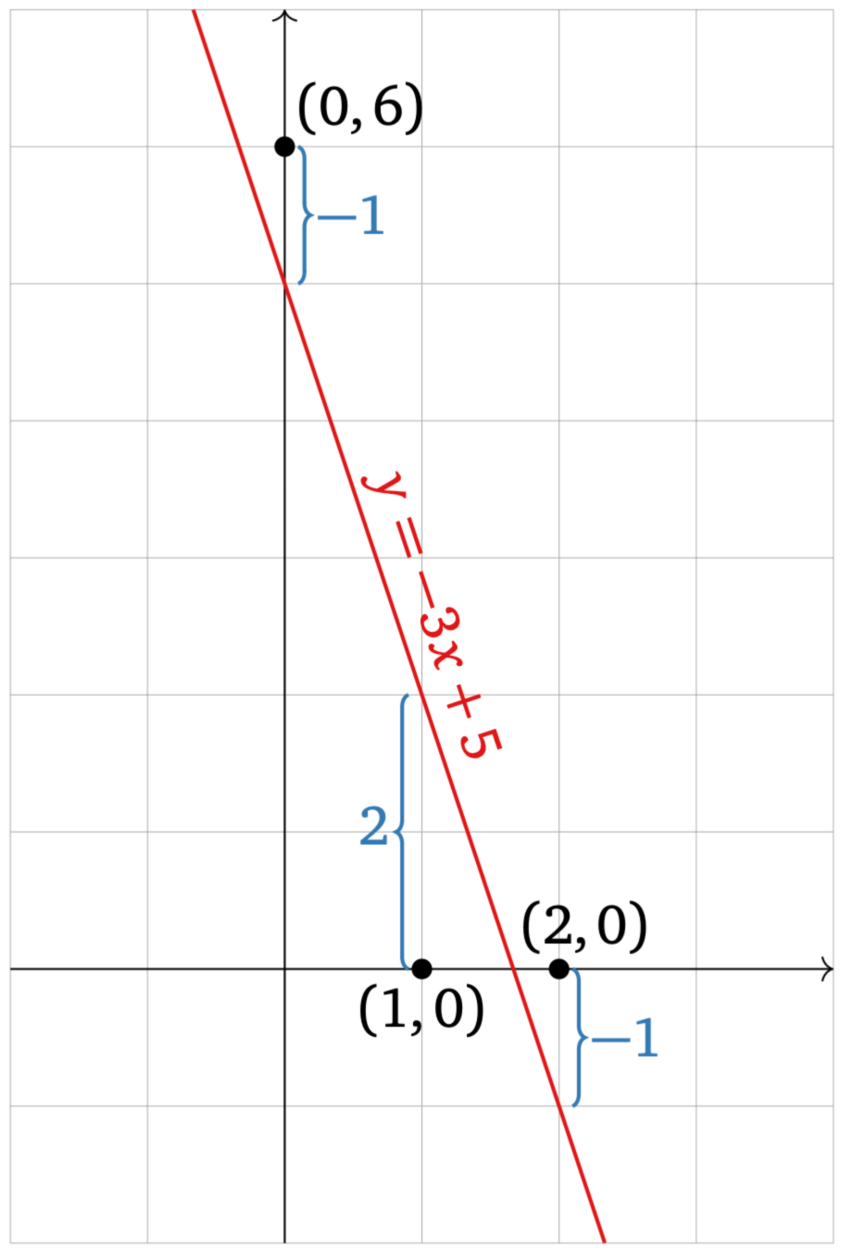

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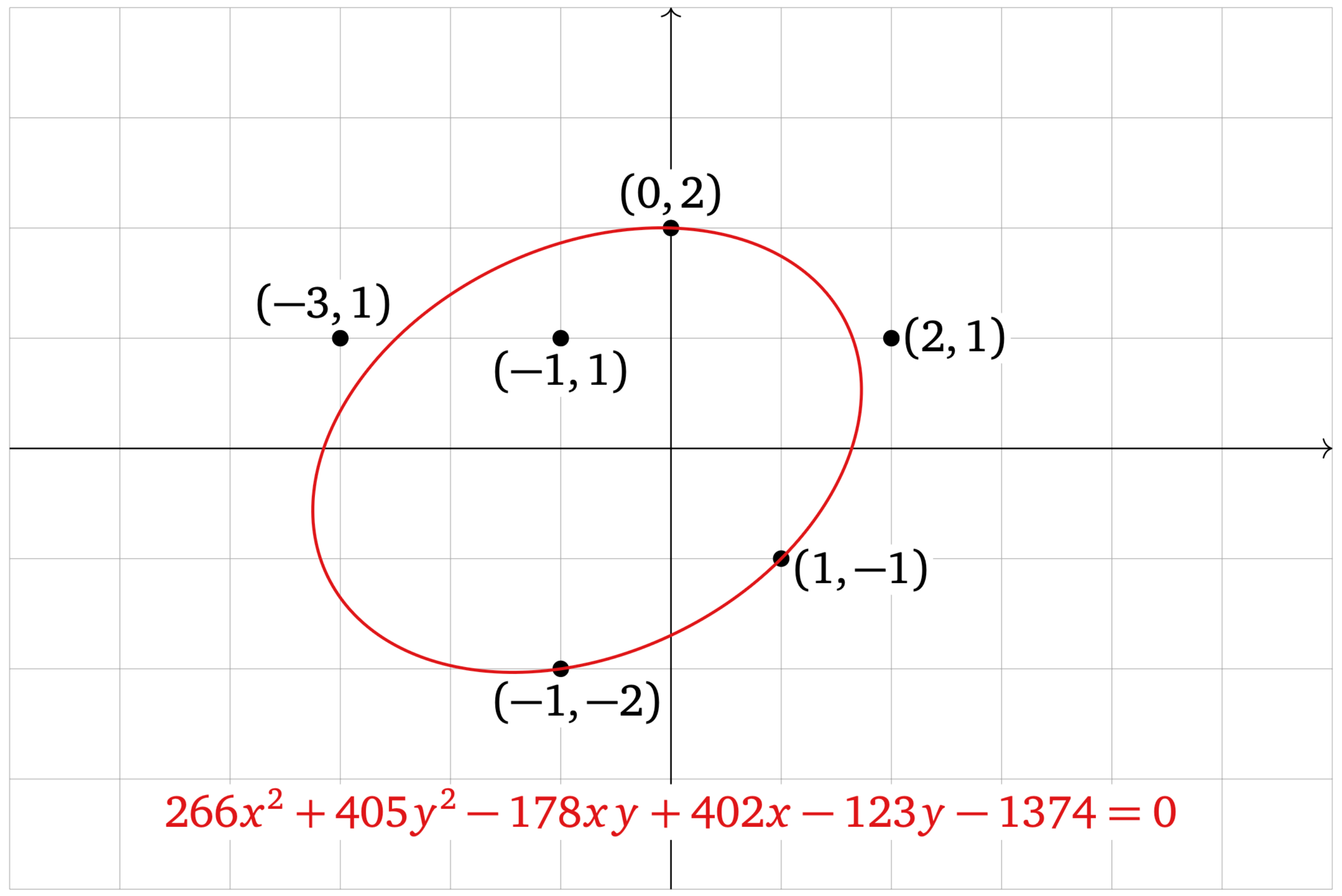

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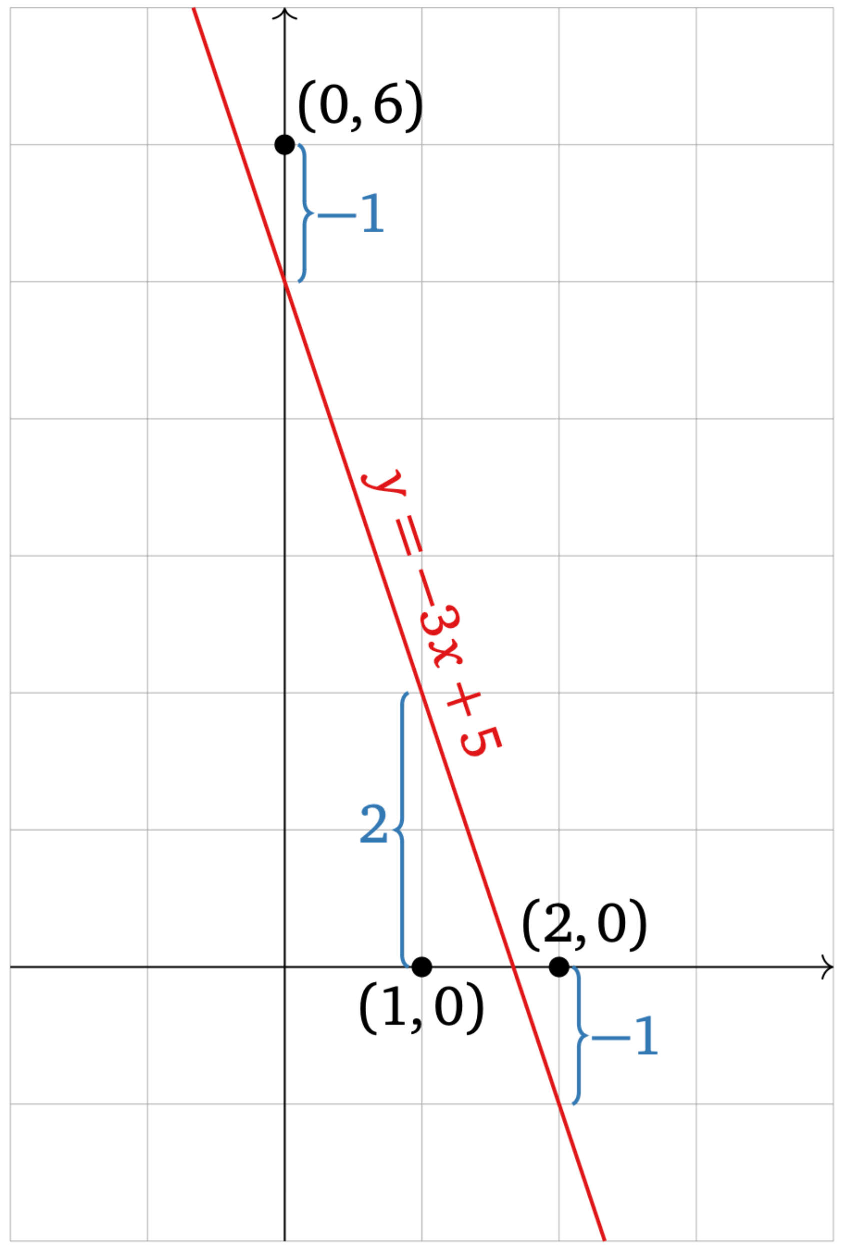
But we can try...



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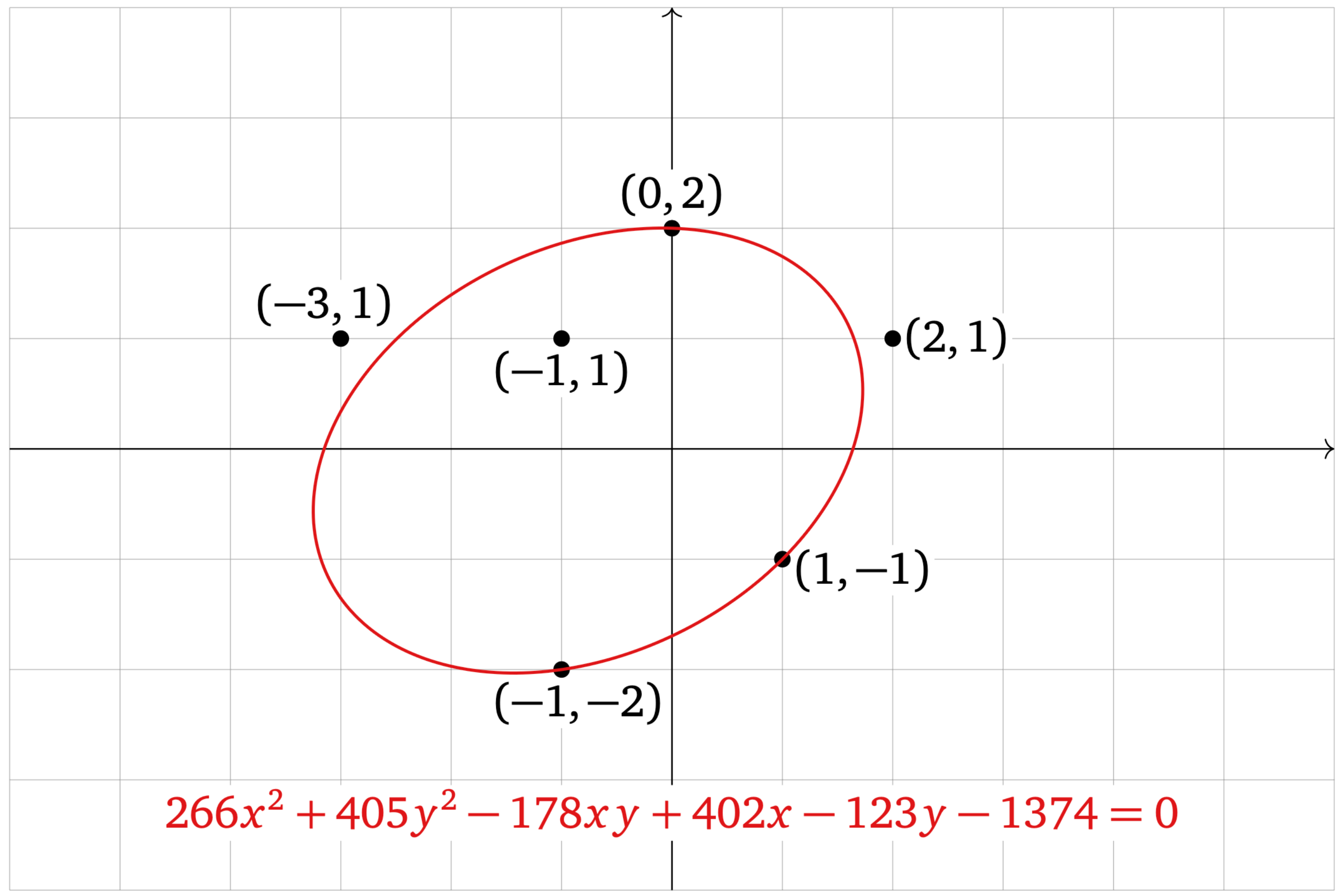

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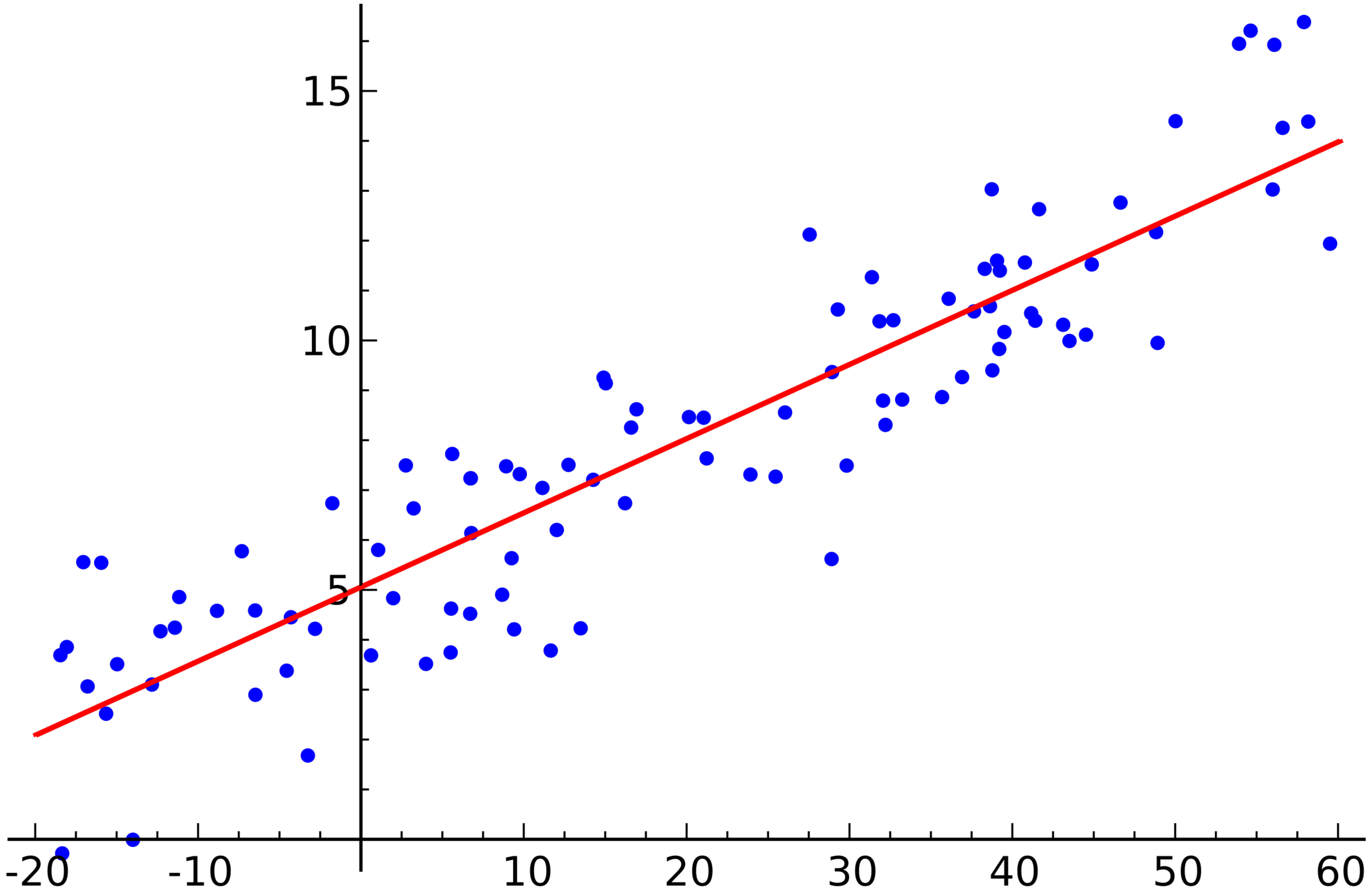
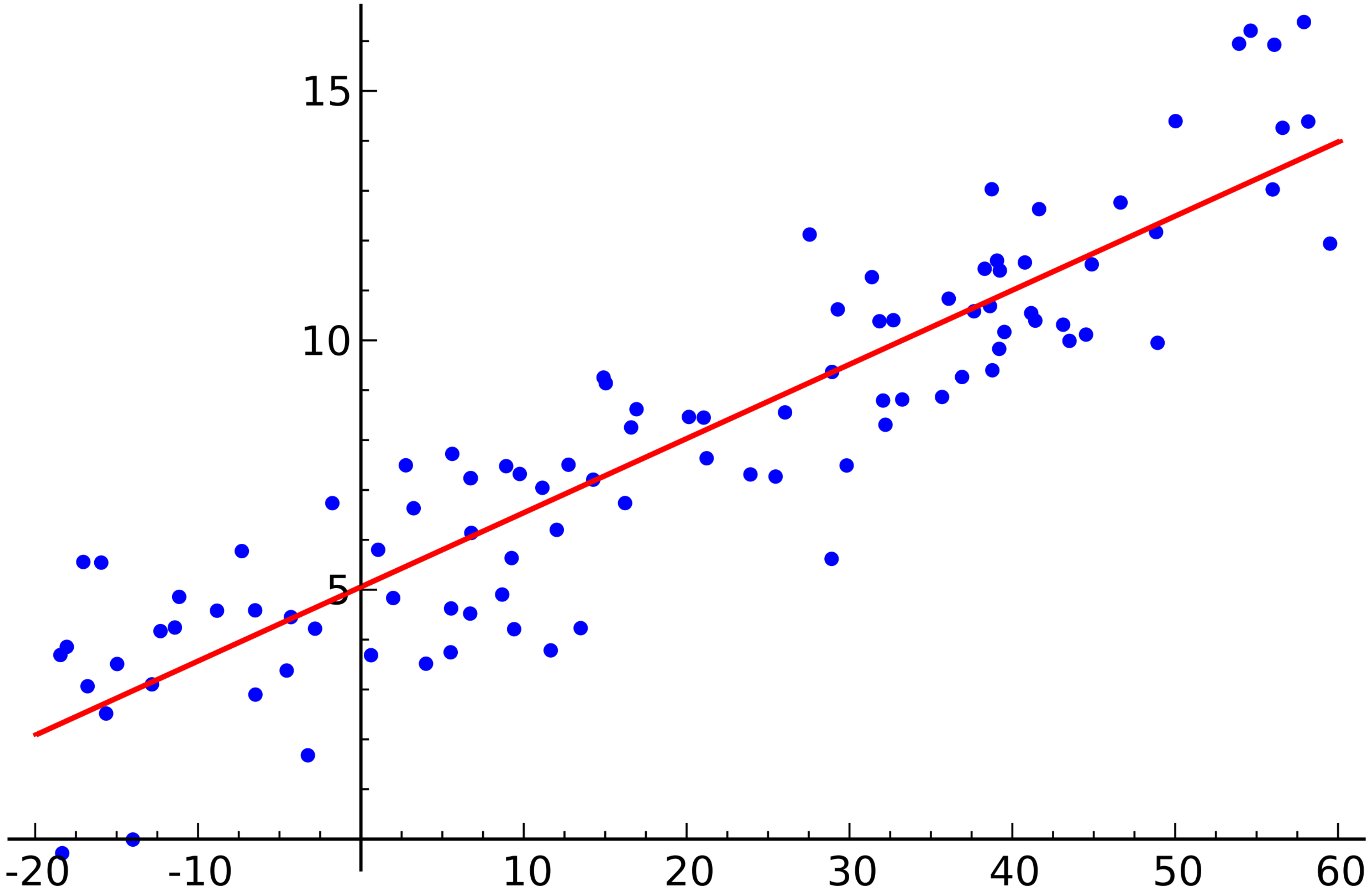
The Idea



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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The Idea

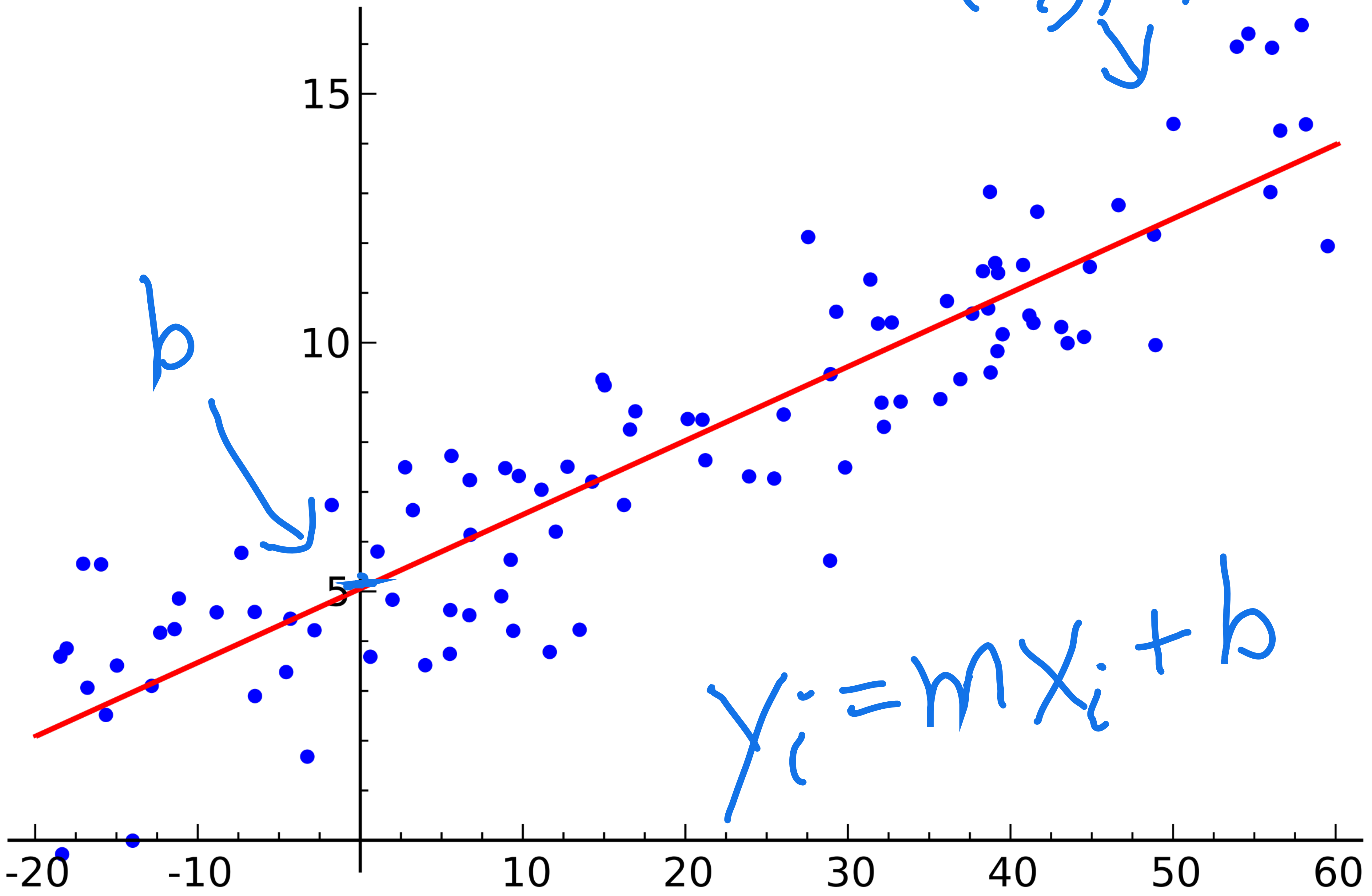
Least Squares is a method for finding *approximate* solutions to systems of linear equations

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

slope y-intercept

$$y = mx + b$$

(x_i, y_i)



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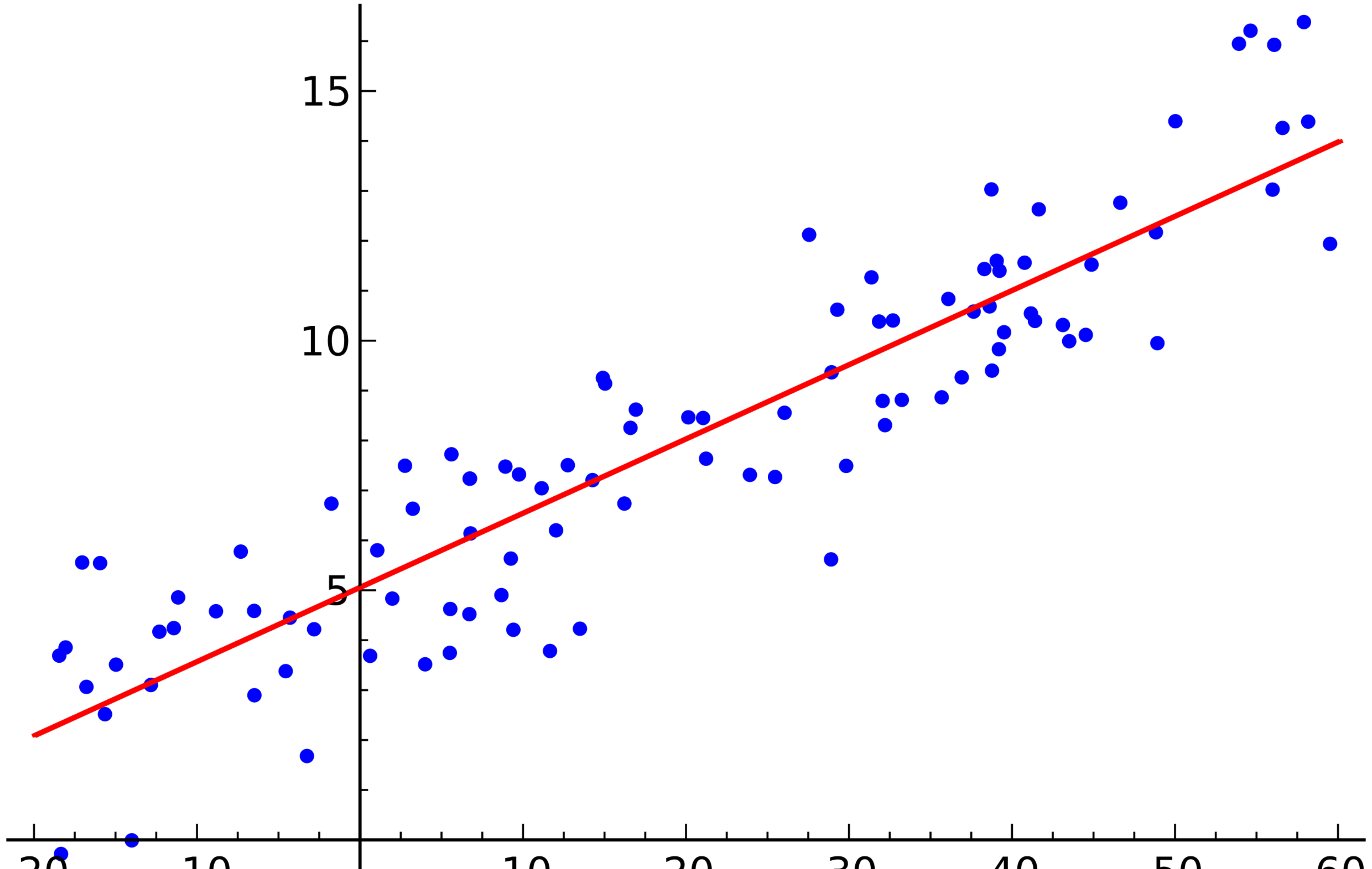
It can be used to do **linear regression** from stats class



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General Least Squares Problem

The Picture

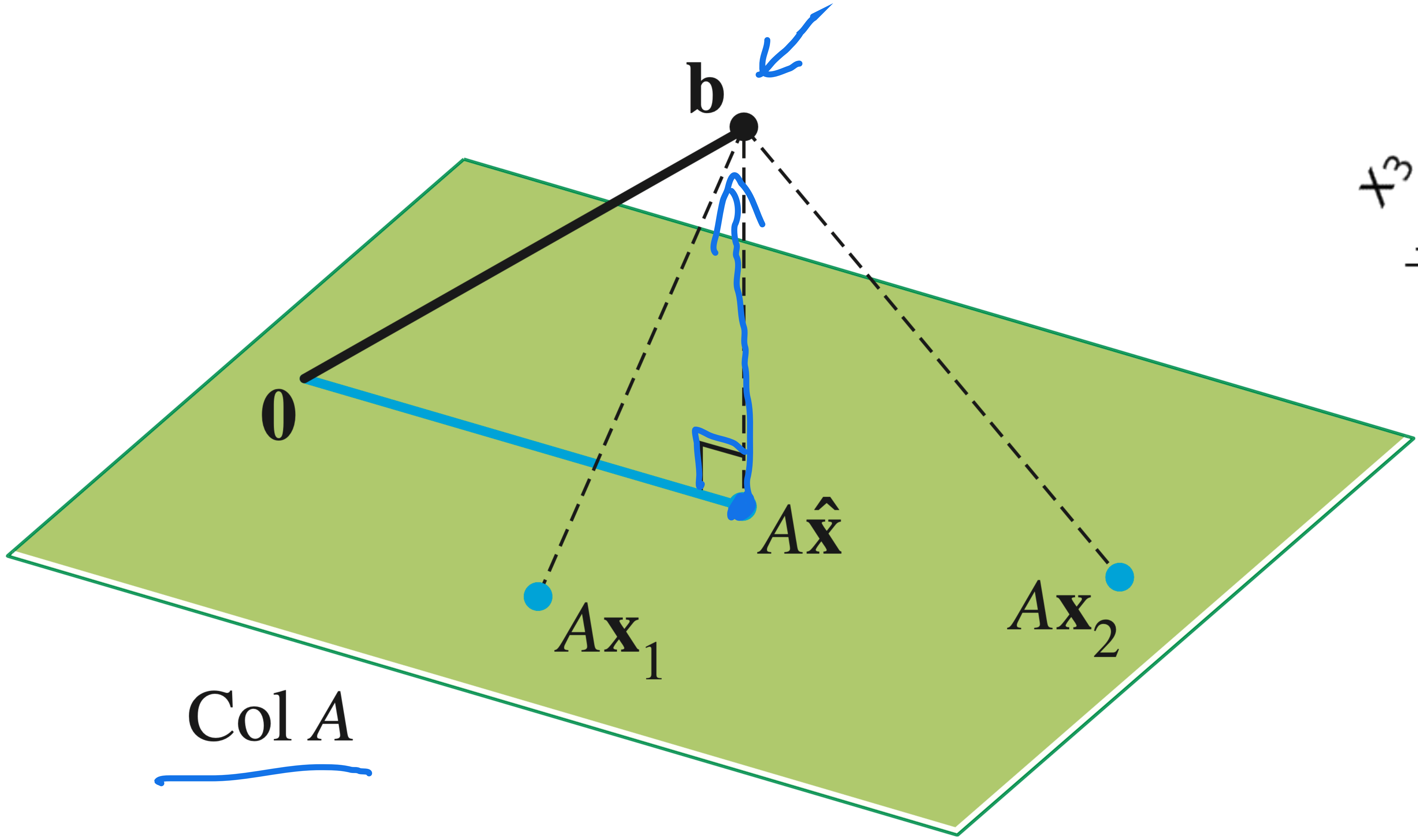
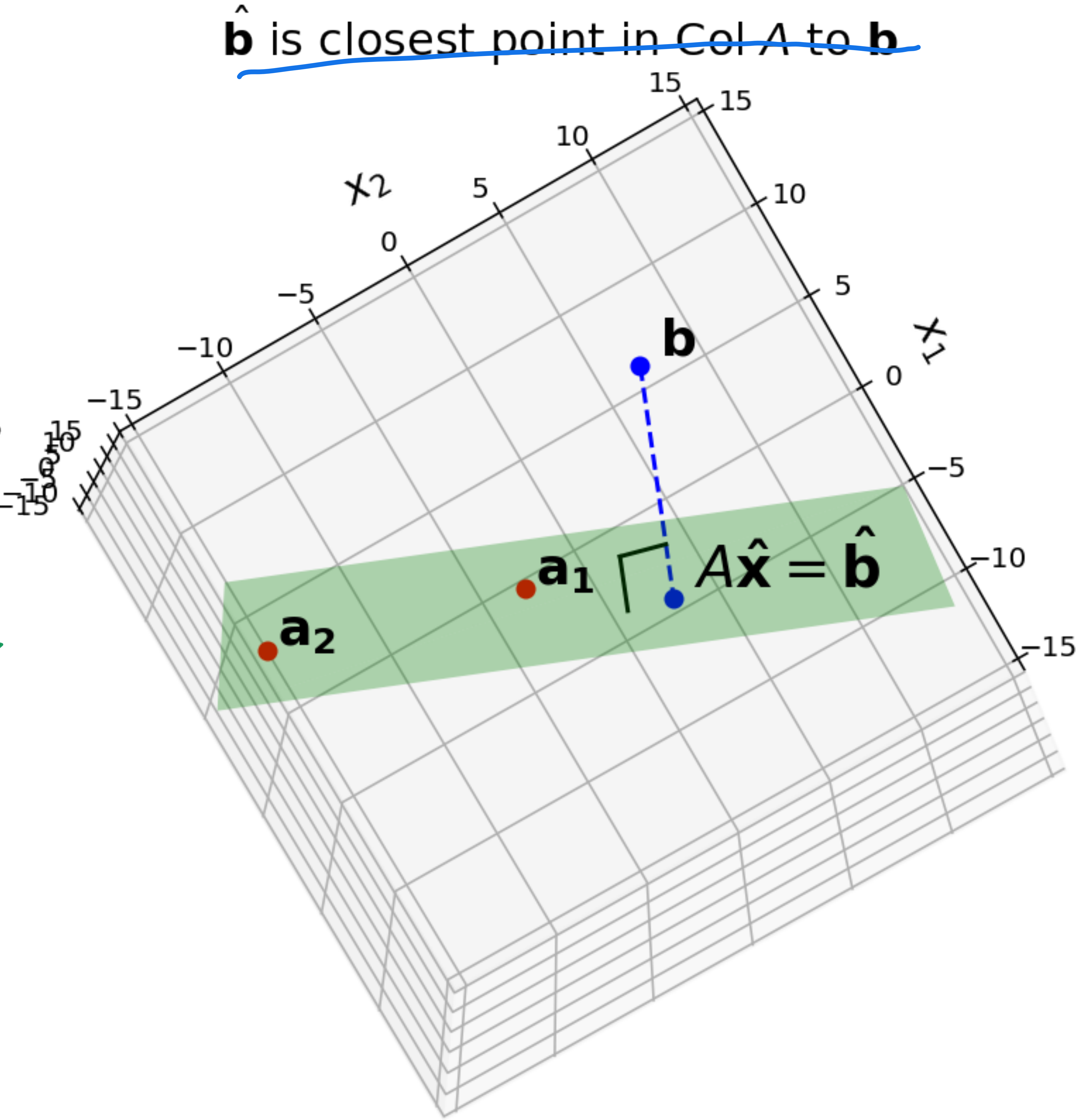
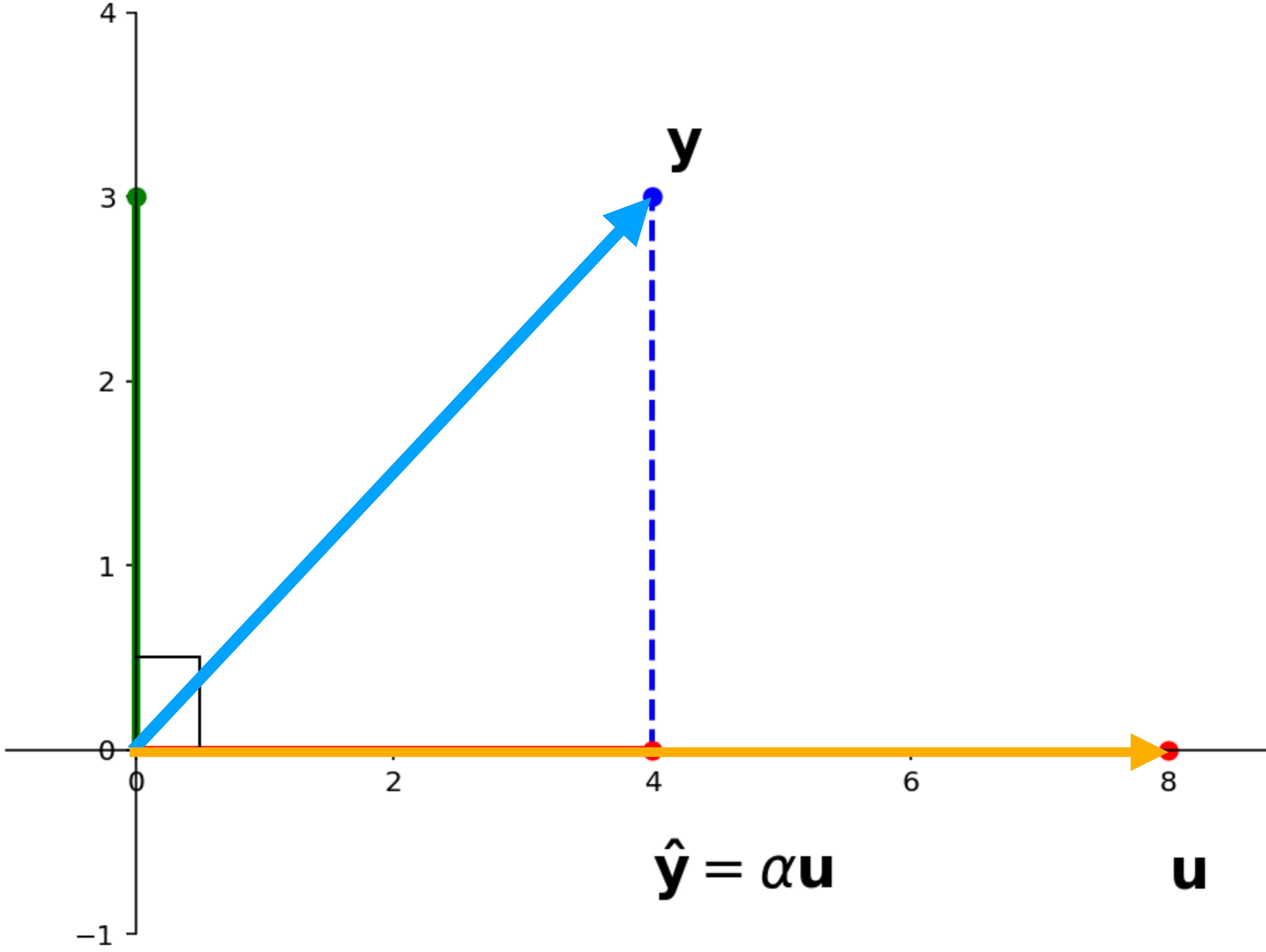


Figure 22.8

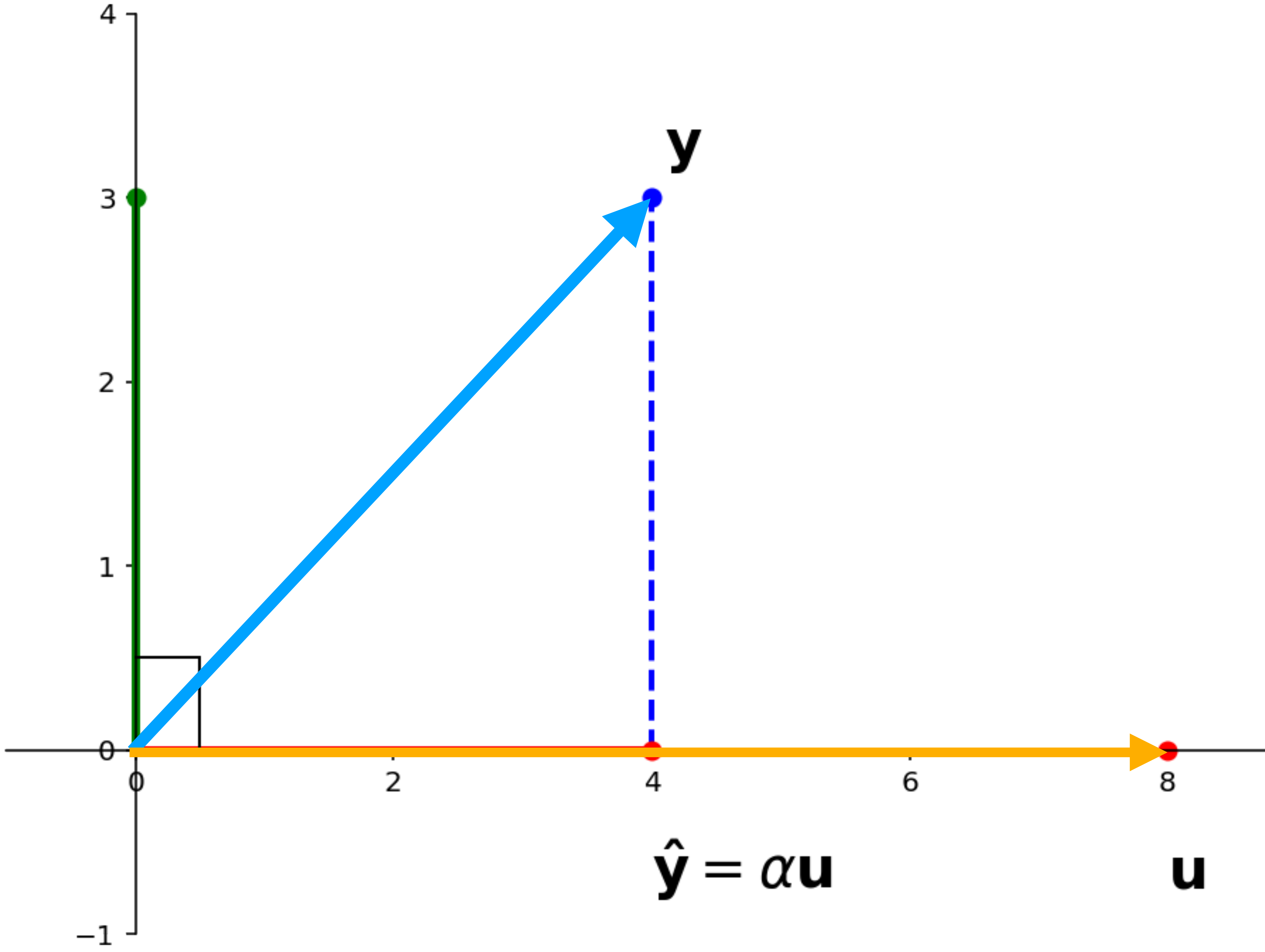


Recall: Orthogonal Projection



Recall: Orthogonal Projection

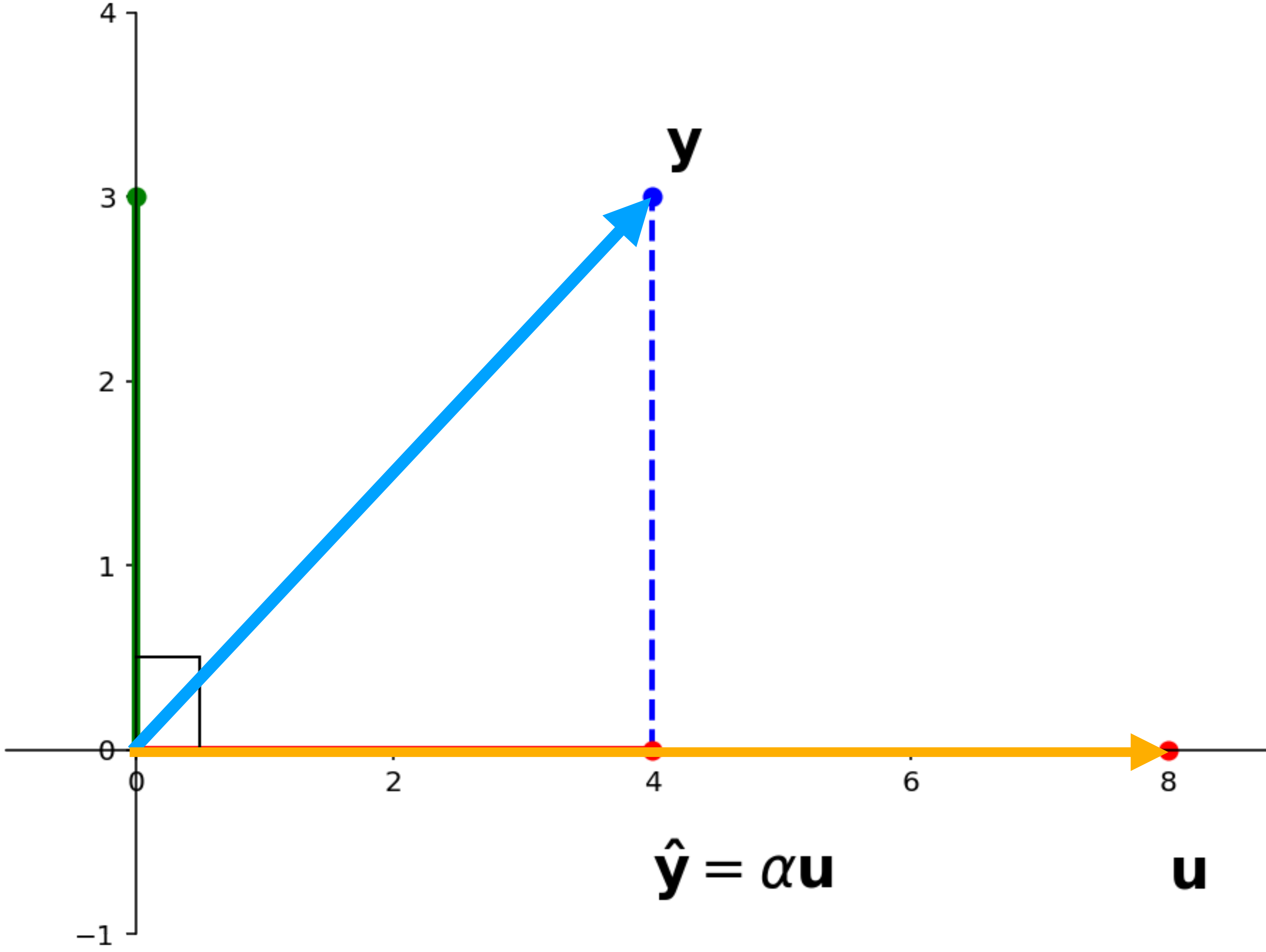
Question. Given vectors $\mathbf{y}$ and $\mathbf{u}$ in R^n, find vectors $\hat{\mathbf{y}}$ and $\mathbf{z}$ such that



Recall: Orthogonal Projection

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

- $\mathbf{z}$ is orthogonal to $\mathbf{u}$ (i.e., $\mathbf{z} \cdot \mathbf{u} = 0$)



Recall: Orthogonal Projection

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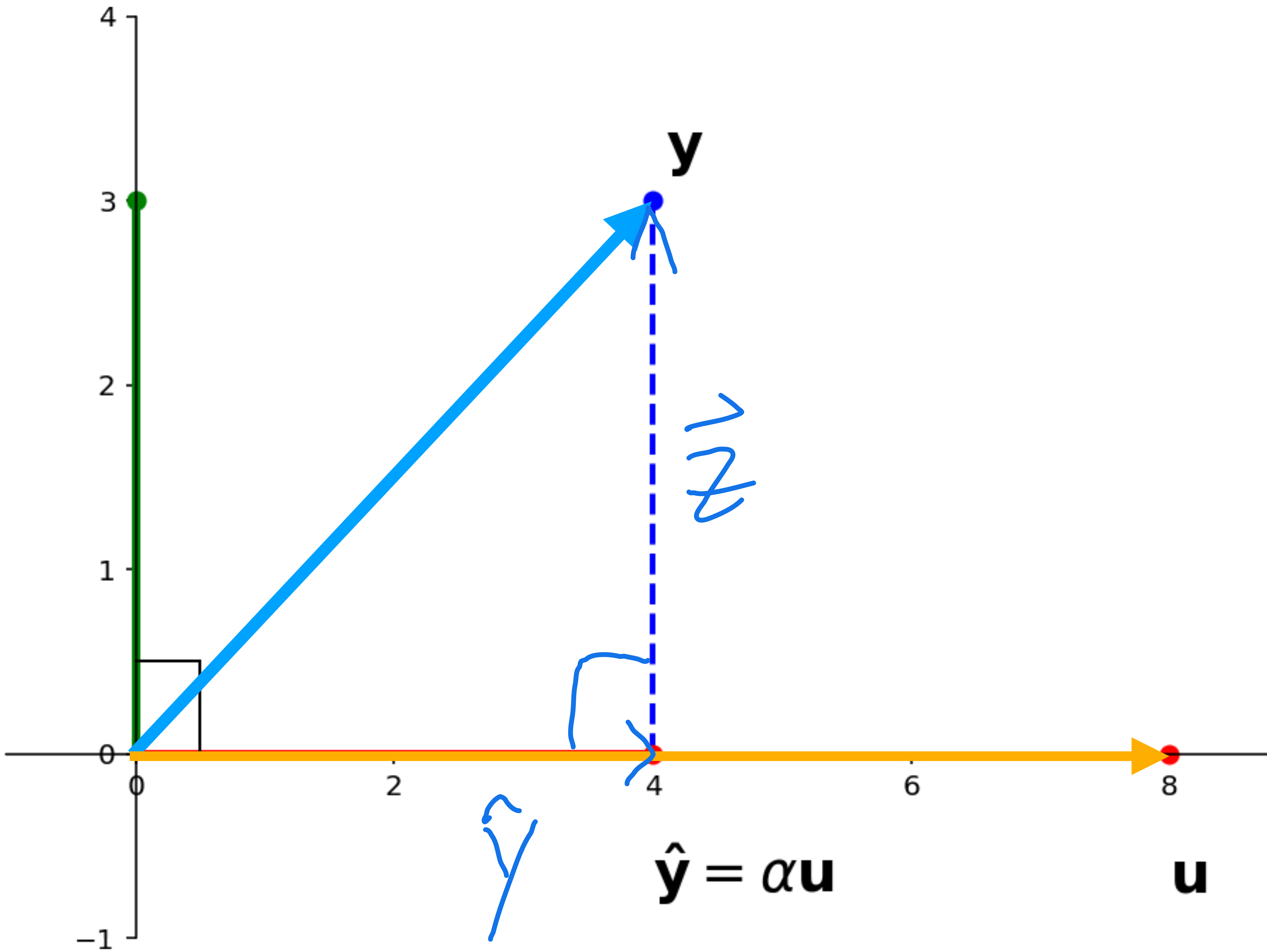
» $\mathbf{z}$ is orthogonal to $\mathbf{u}$ (i.e., $\mathbf{z} \cdot \mathbf{u} = 0$)

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



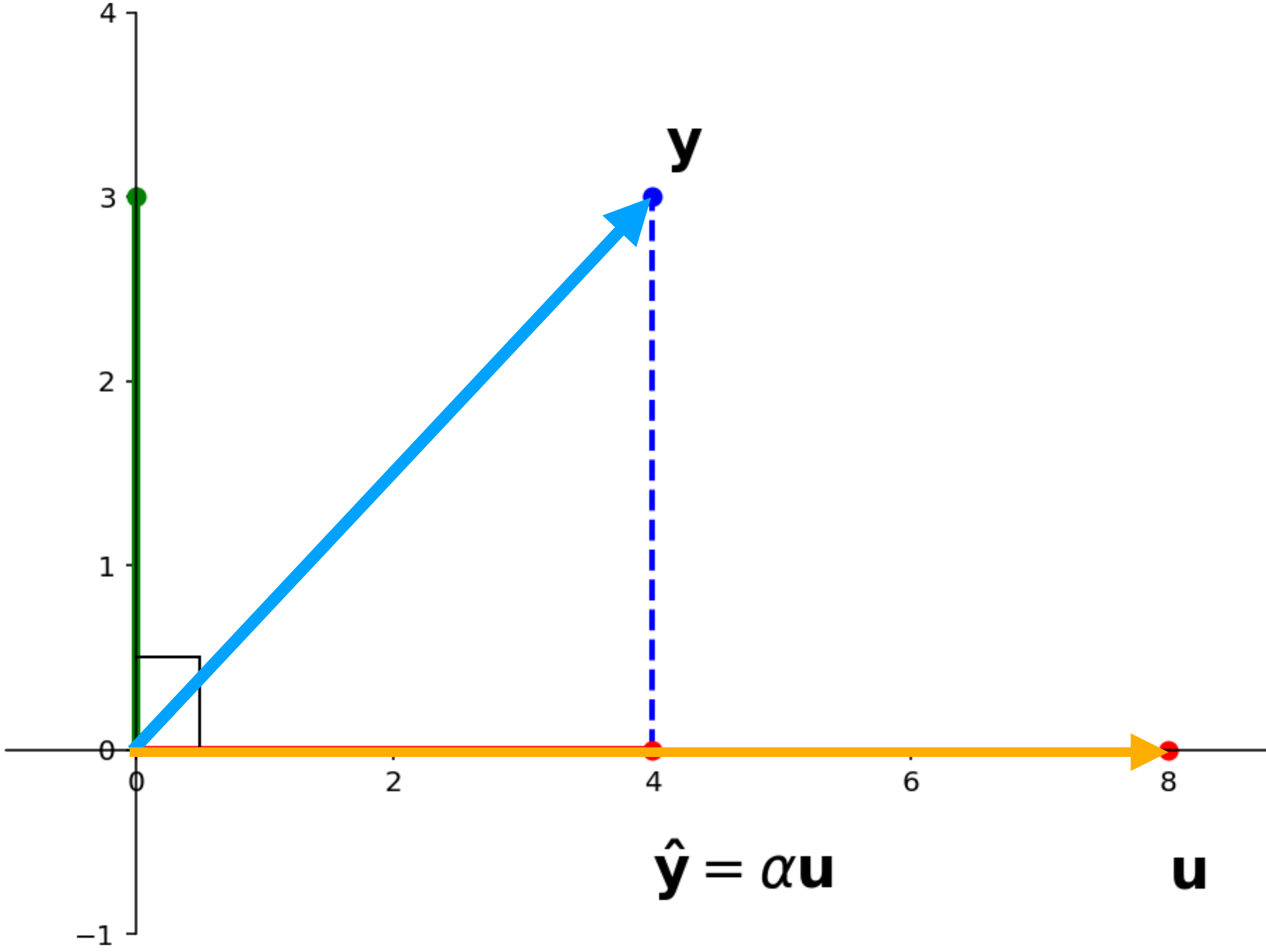
Recall: Orthogonal Projection

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

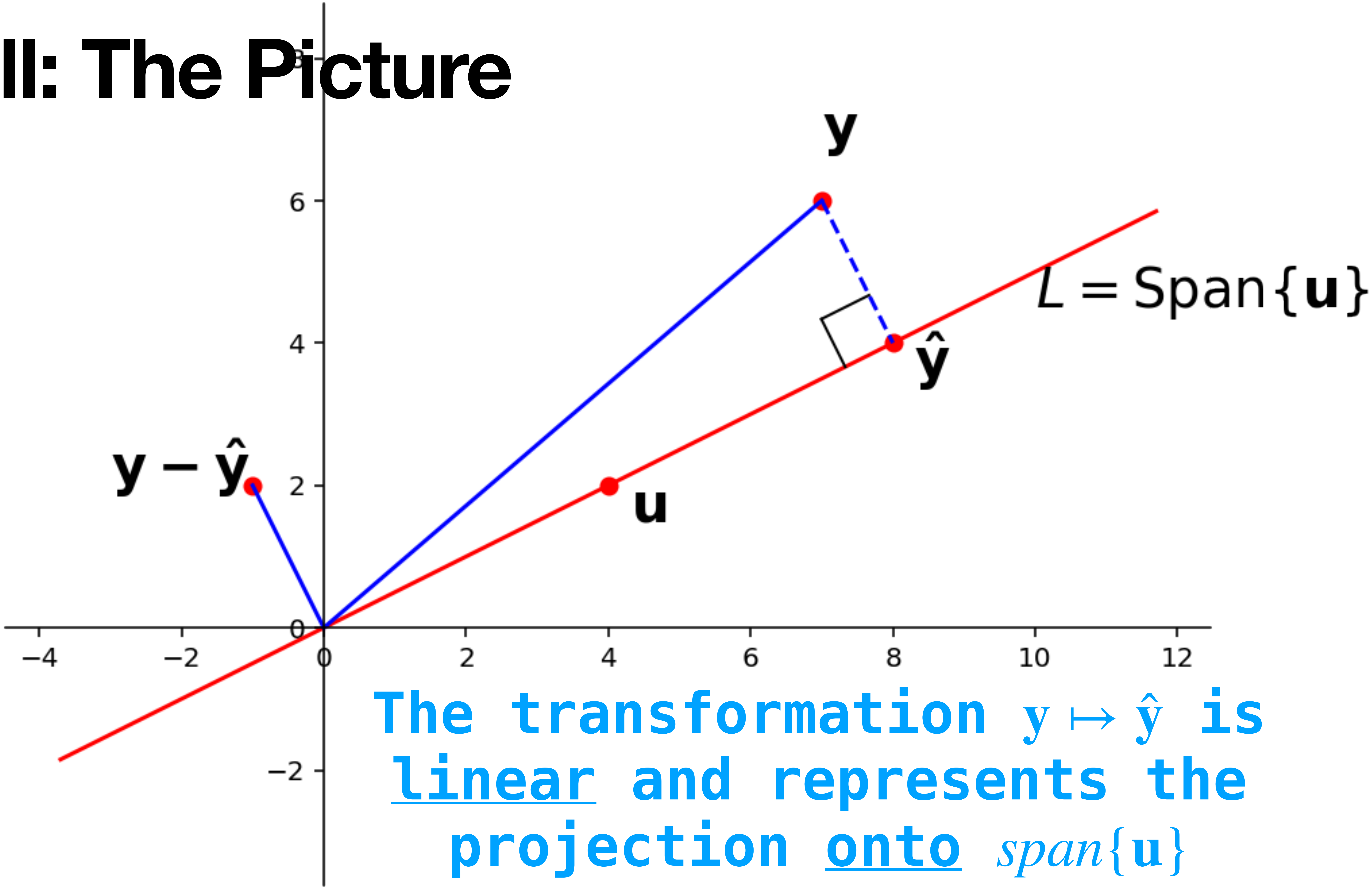
» $\mathbf{z}$ is orthogonal to $\mathbf{u}$ (i.e., $\mathbf{z} \cdot \mathbf{u} = 0$)

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

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



Recall: The Picture



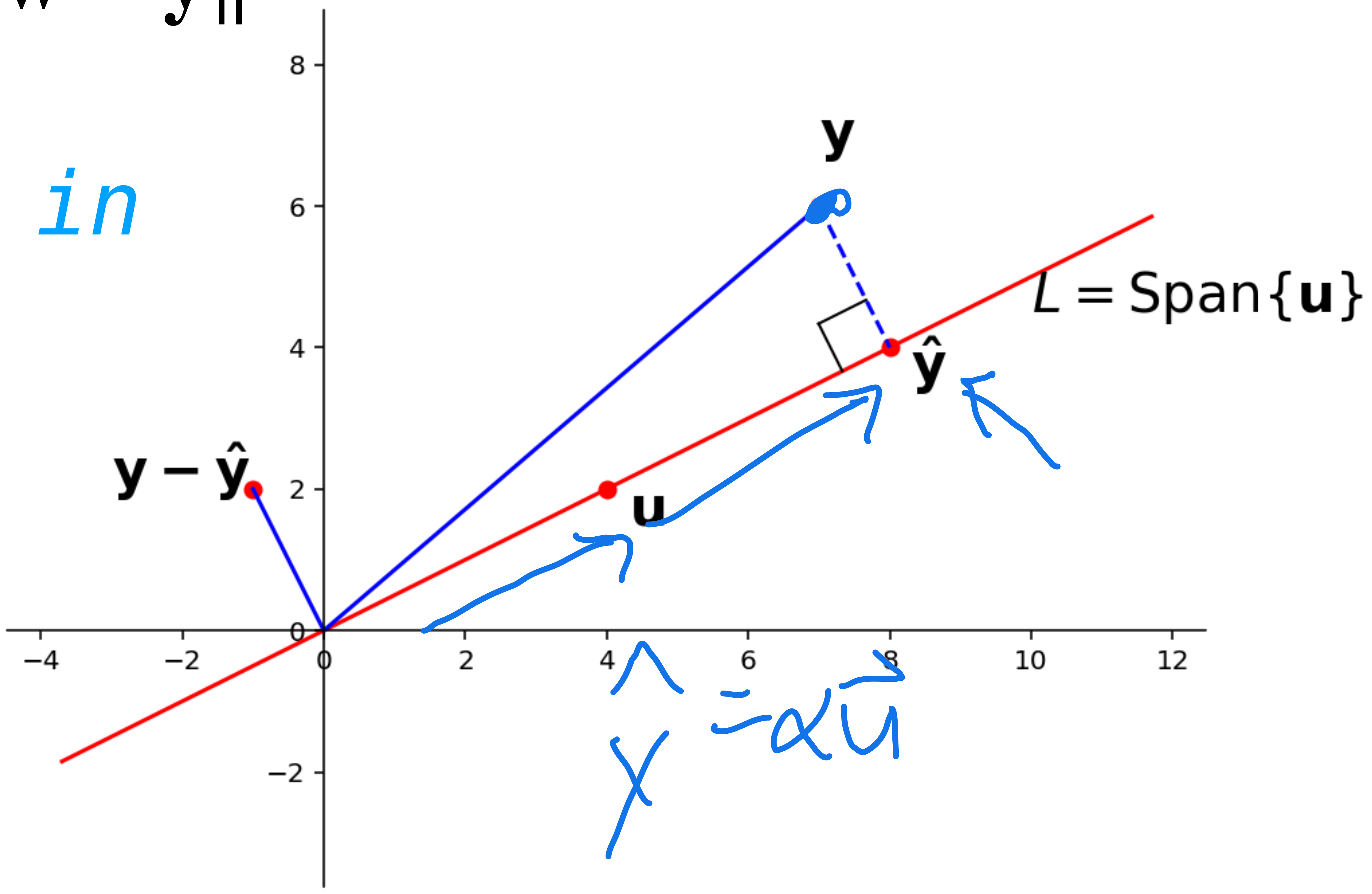
The transformation $\mathbf{y} \mapsto \hat{\mathbf{y}}$ is linear and represents the projection onto $span\{\mathbf{u}\}$

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

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

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

"Proof" by inspection:



$\hat{y} = \alpha\vec{u}$

The Equational Perspective

The Equational Perspective

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

The Equational Perspective

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

Question. Find a value α such that $\alpha\mathbf{u}$ is as close as possible to $\mathbf{y}$

The Equational Perspective

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

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That is, the distance $dist(\mathbf{y}, \alpha\mathbf{u}) = \underline{\|\mathbf{y} - \alpha\mathbf{u}\|}$ is as small as possible

The Equational Perspective

We know the equation $\overset{A}{\cancel{\alpha}}\mathbf{u} = \mathbf{y}$ may have no solution

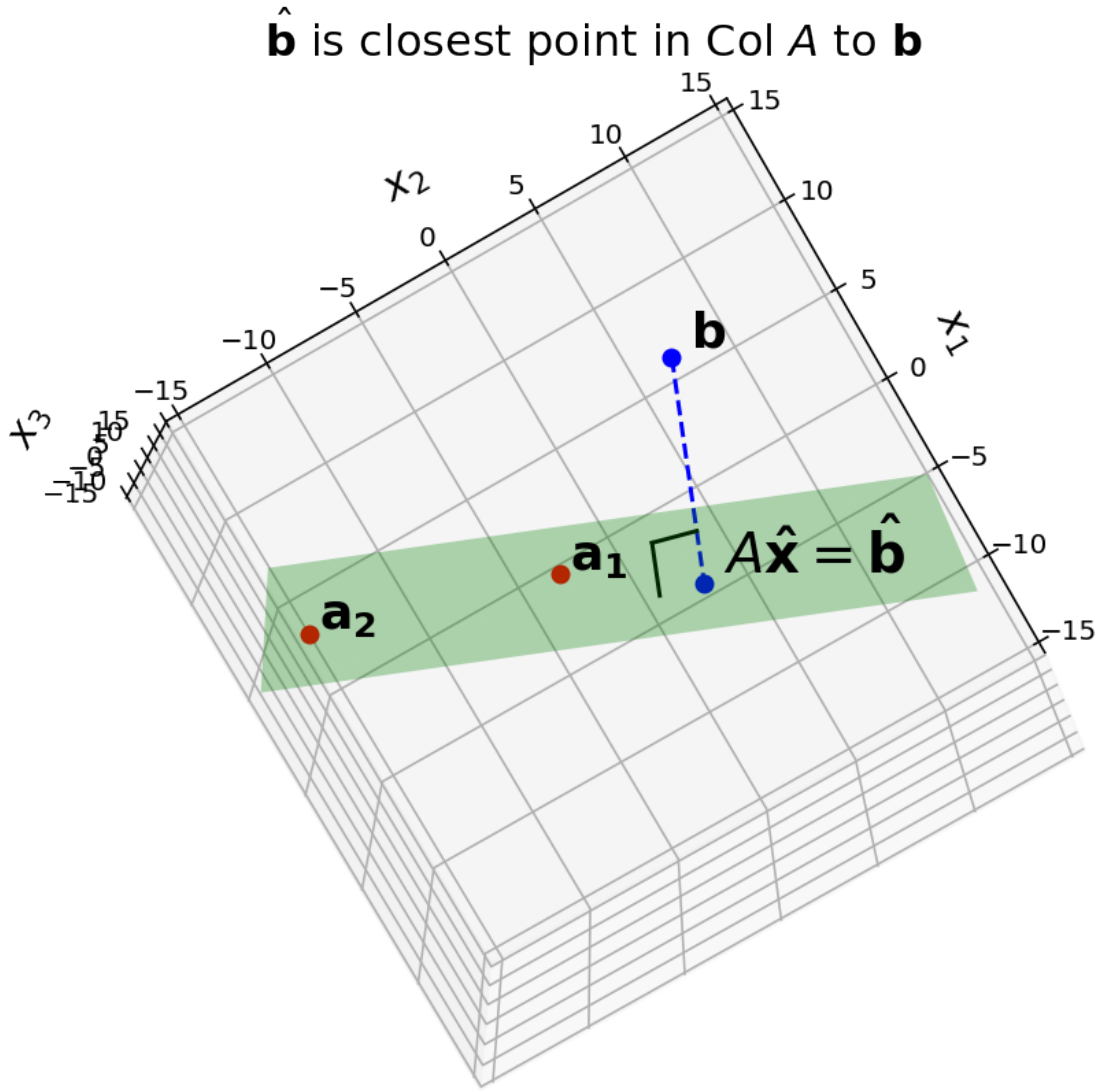
Question. Find a value α such that $\alpha\mathbf{u}$ is as close as possible to $\mathbf{y}$

That is, the distance $dist(\mathbf{y}, \alpha\mathbf{u}) = \|\mathbf{y} - \alpha\mathbf{u}\|$ is as small as possible

We need to generalize this to arbitrary matrix equations

The General Least Squares Problem

Figure 22.8



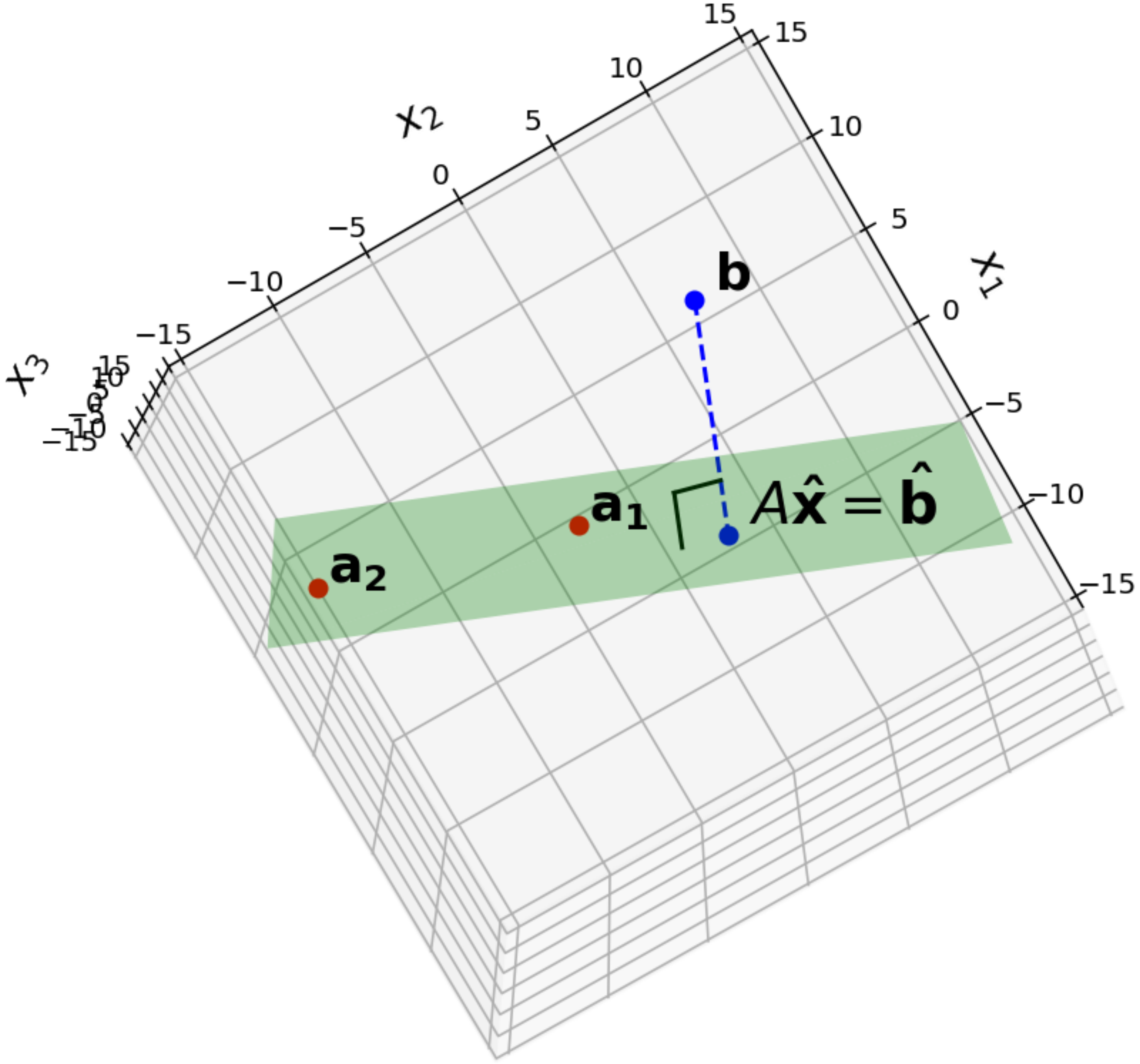
The General Least Squares Problem

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 <u>minimizes</u>

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

Figure 22.8

$\hat{\mathbf{b}}$ is closest point in Col A to $\mathbf{b}$



The General Least Squares Problem

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

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

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

Figure 22.8

$\hat{\mathbf{b}}$ is closest point in Col A to $\mathbf{b}$

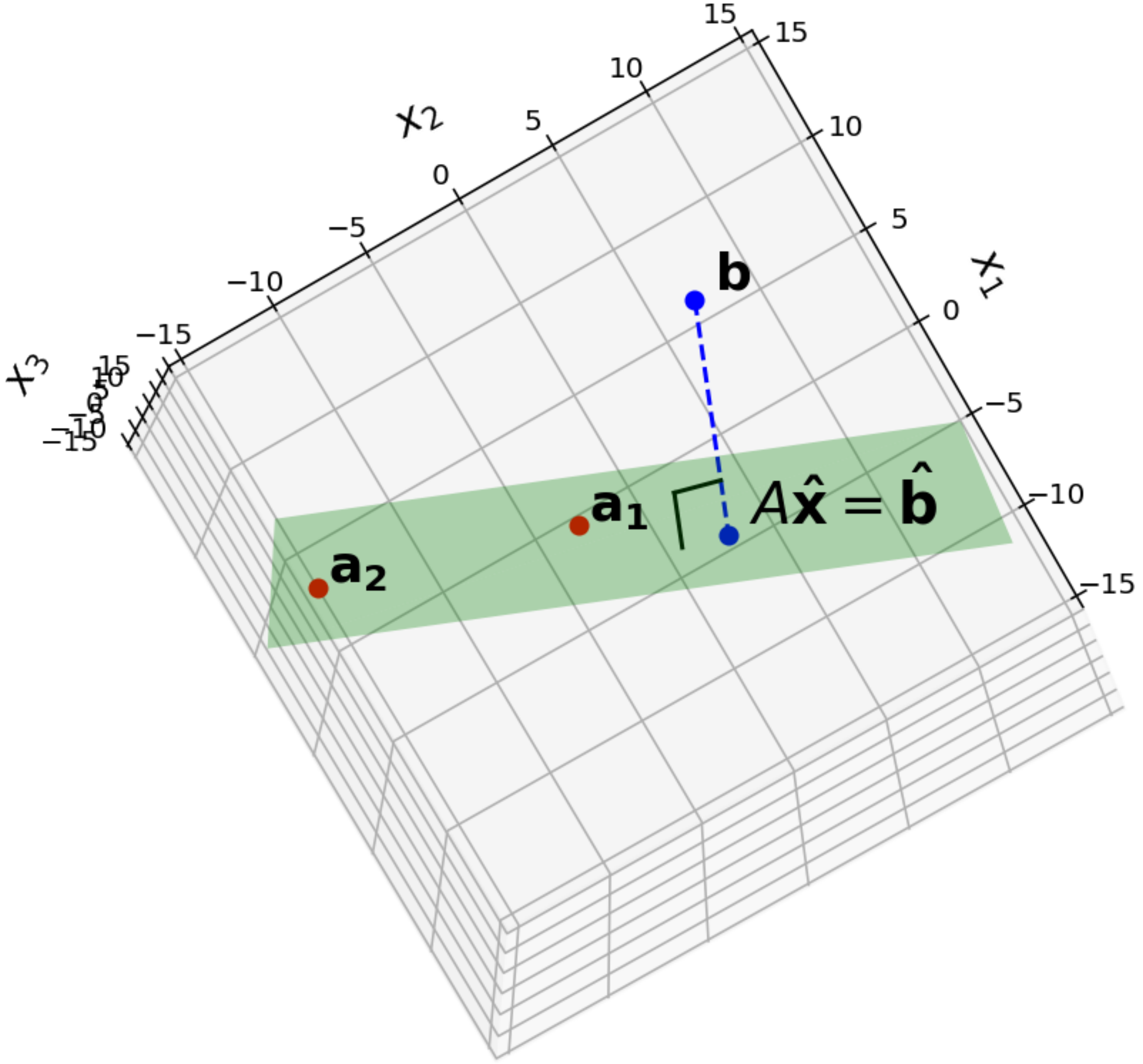
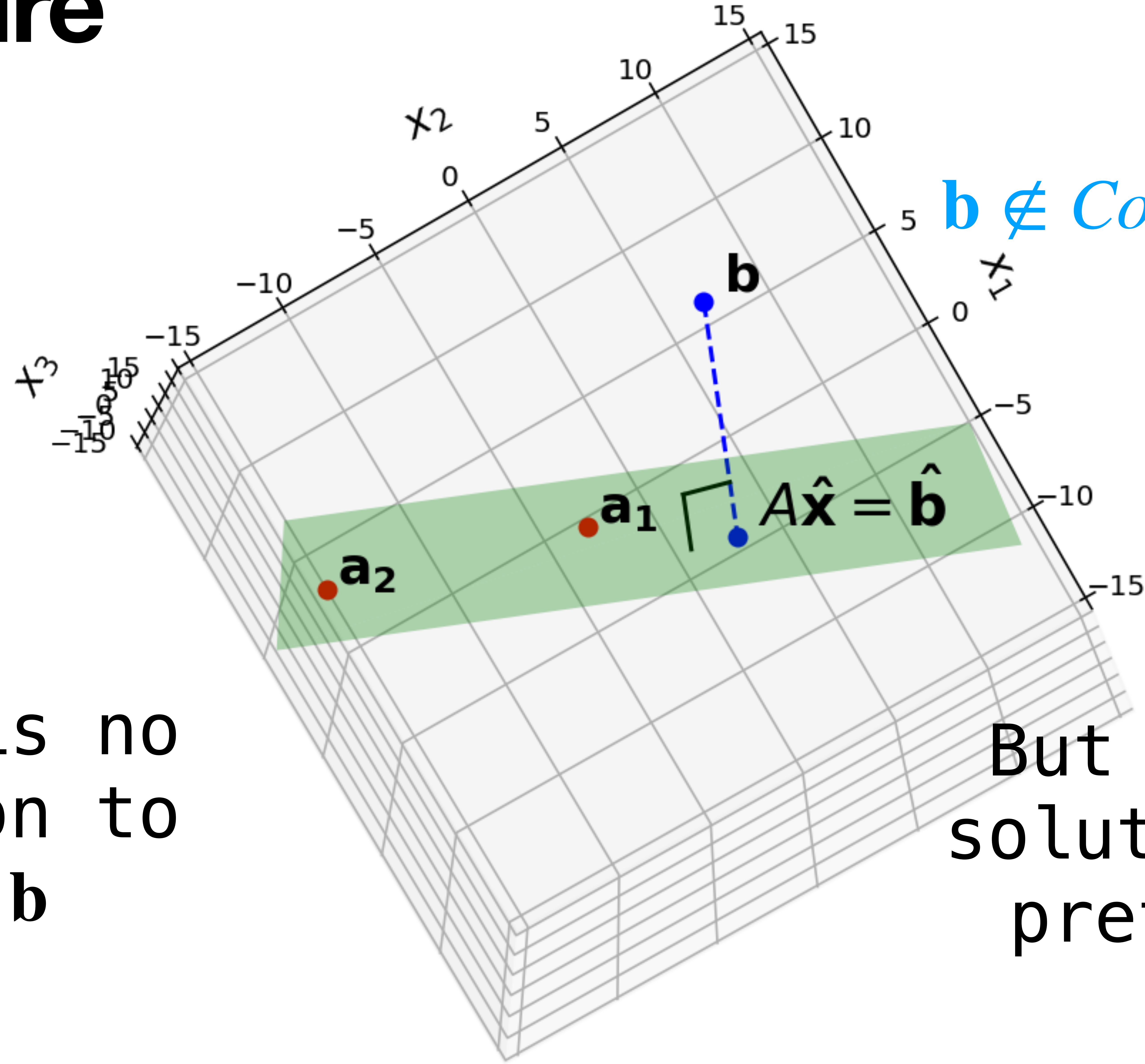


Figure 22.8

The Picture



$\hat{\mathbf{b}}$ is closest point in Col A to $\mathbf{b}$

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

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

But there's a solution that's pretty close

Sum of Squares

$$\|Ax - b\|$$

$$\downarrow$$

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

Sum of Squares

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

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

Sum of Squares

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

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

Sum of Squares

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

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

These things come up everywhere

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

L^1 error

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 $\underline{\hat{\mathbf{x}}}$ from $\mathbb{R}^n$ such that

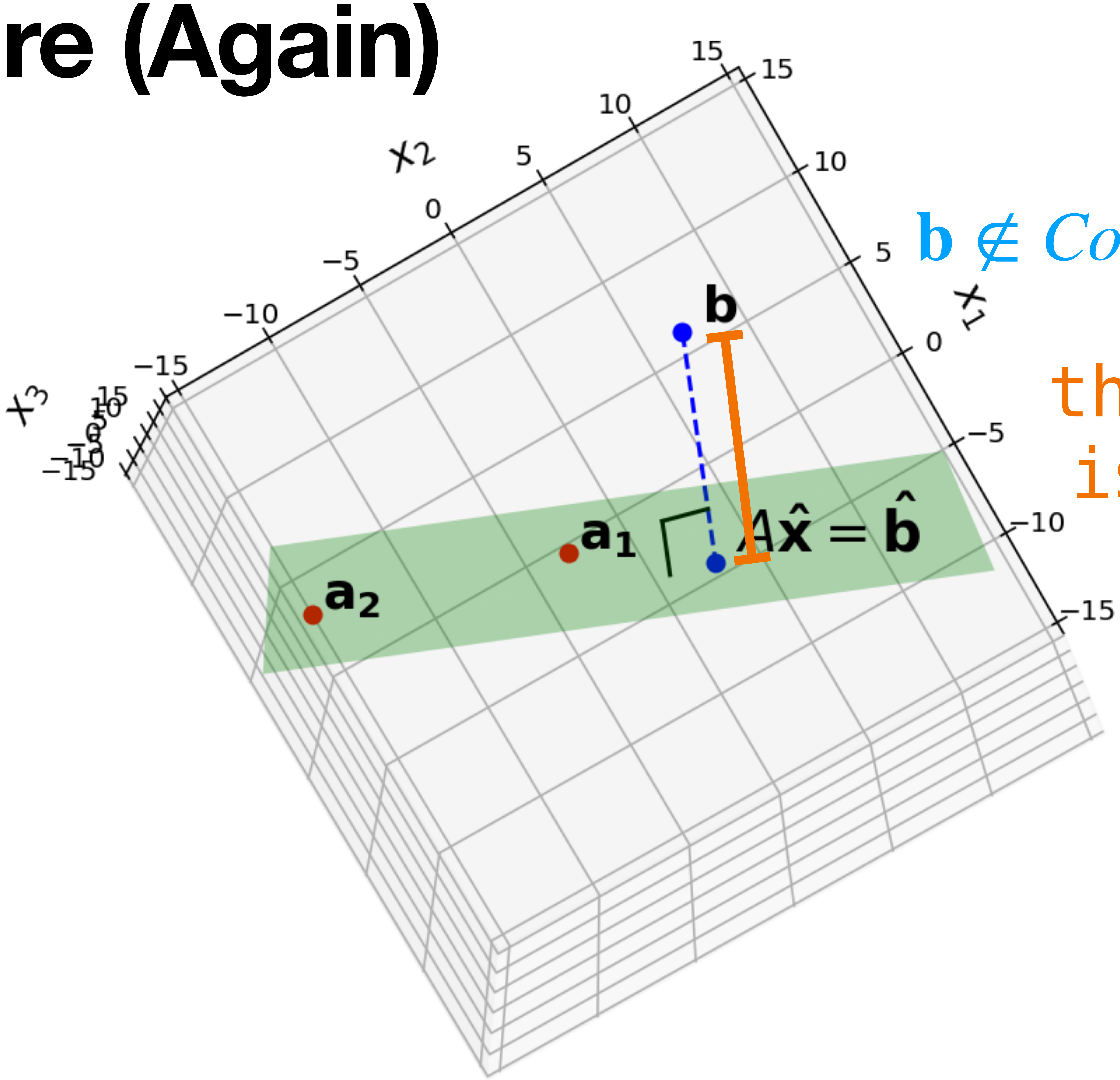
$$\underline{\|A\hat{\mathbf{x}} - \mathbf{b}\|} \leq \underline{\|A\mathbf{x} - \mathbf{b}\|}$$

for $\underline{\text{any}}$ $\mathbf{x}$ 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

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

Argmin

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

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

Argmin

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

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

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

Argmin

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

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

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

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

Argmin

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

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

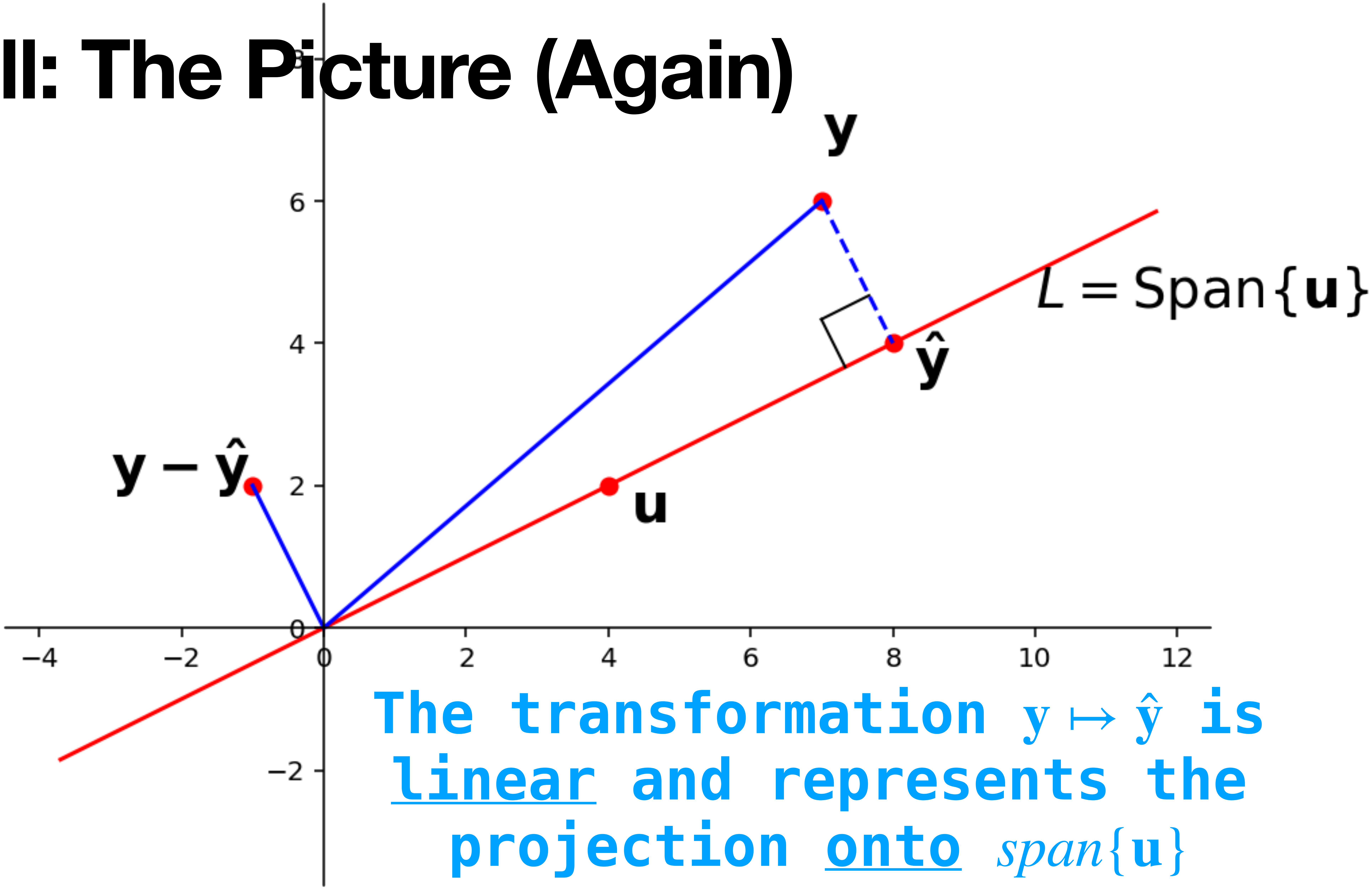
Defintion. $\arg\min_{x\in X} f(x) = \hat{x}$ where $f(\hat{x}) = \min_{x\in X} f(x)$

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

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

Solving the General Least Squares Problems

Recall: The Picture (Again)

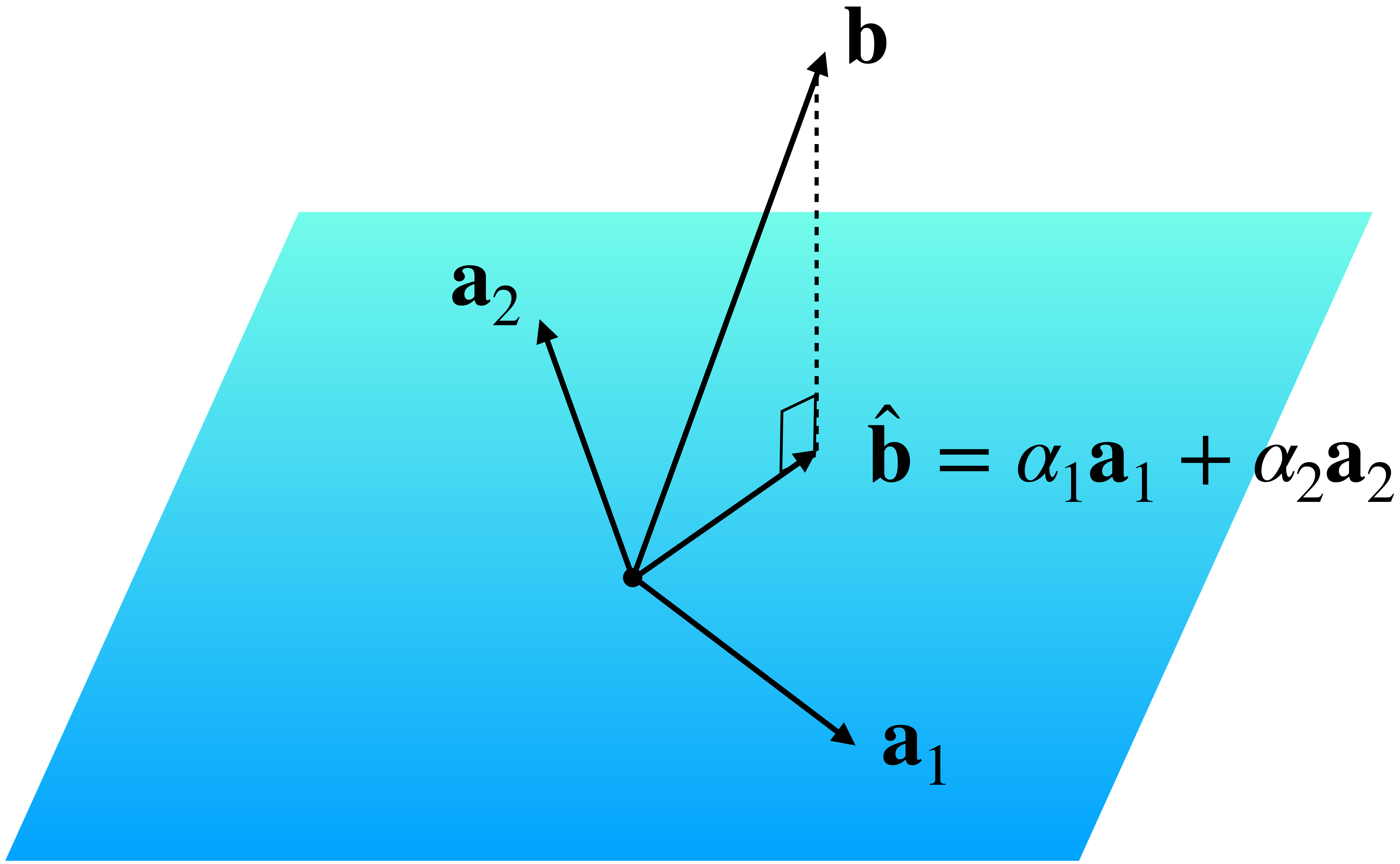


$\mathbf{y}$
$L = \mathrm{Span}\{\mathbf{u}\}$
$\hat{\mathbf{y}}$
$\mathbf{y} - \hat{\mathbf{y}}$
$\mathbf{u}$
8
6
4
2
0
−2
−4
−2
0
2
4
6
8
10
12

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 $\text{span}\{\mathbf{a}_1, \mathbf{a}_2\}$


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

The High Level Approach.

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

Solution.

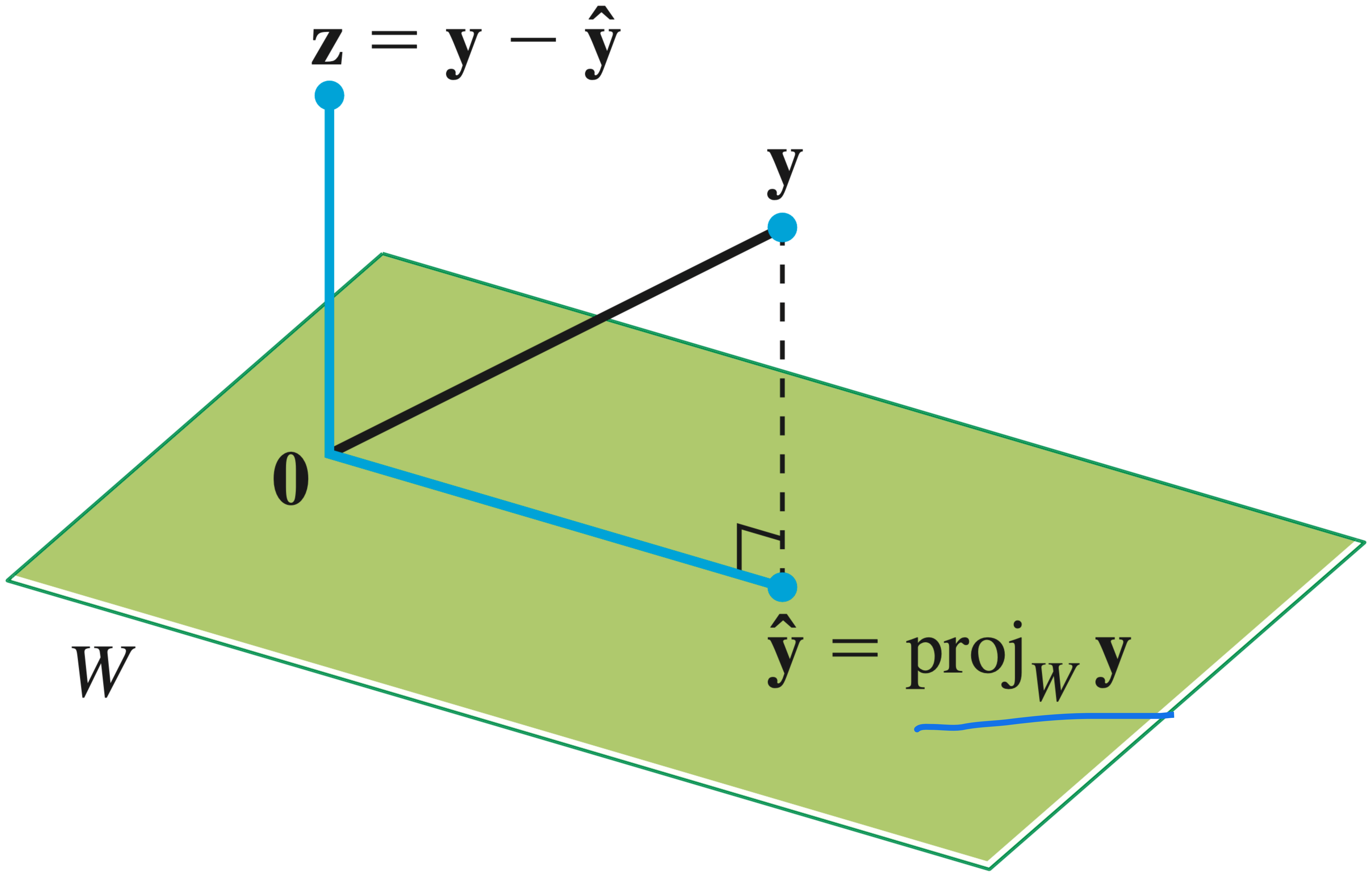
1. Find the closest point $\underline{\hat{\mathbf{b}} \text{ in } Col(A) \text{ to } \mathbf{b}}$
2. Solve the equation $\underline{A\mathbf{x} = \hat{\mathbf{b}}}$ instead

Orthogonal Decomposition Theorem

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

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

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


$\mathbf{z} = \mathbf{y} - \hat{\mathbf{y}}$
$\mathbf{y}$
$\mathbf{0}$
$\hat{\mathbf{y}} = \operatorname{proj}_W \mathbf{y}$
W

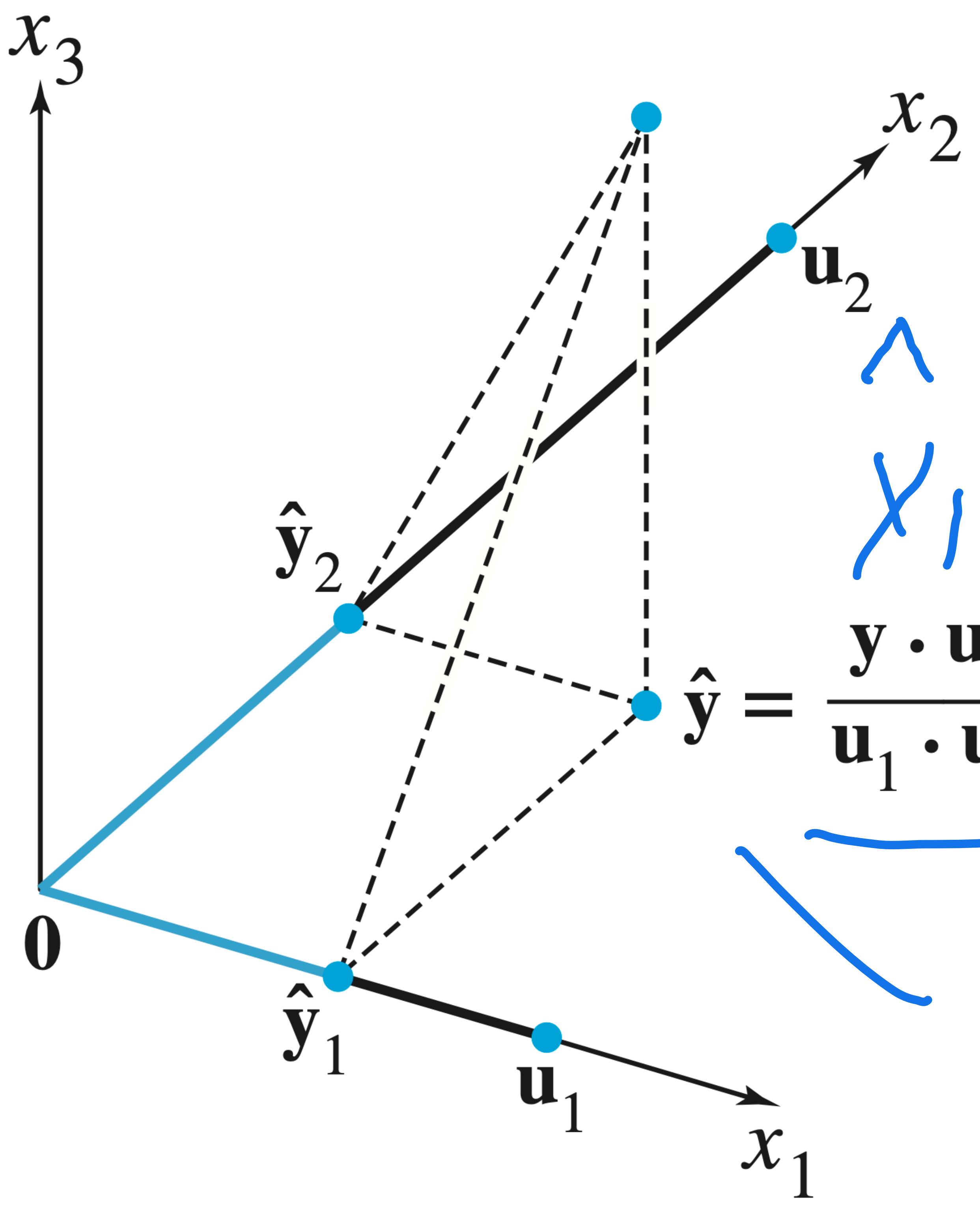
Linear Algebra and its Applications, Lay, Lay, McDonald

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)

Gram-Schmidt



$$\hat{\mathbf{y}} = \underbrace{\overset{\hat{y}_1}{\frac{\mathbf{y}\cdot\mathbf{u}_1}{\mathbf{u}_1\cdot\mathbf{u}_1}}\mathbf{u}_1 + \overset{\hat{y}_2}{\frac{\mathbf{y}\cdot\mathbf{u}_2}{\mathbf{u}_2\cdot\mathbf{u}_2}}\mathbf{u}_2}_{\text{projection onto span}\{\vec{u}_1,\vec{u}_2\}} = \hat{\mathbf{y}}_1 + \hat{\mathbf{y}}_2$$

Linear Algebra and its Applications, Lay, Lay, McDonald

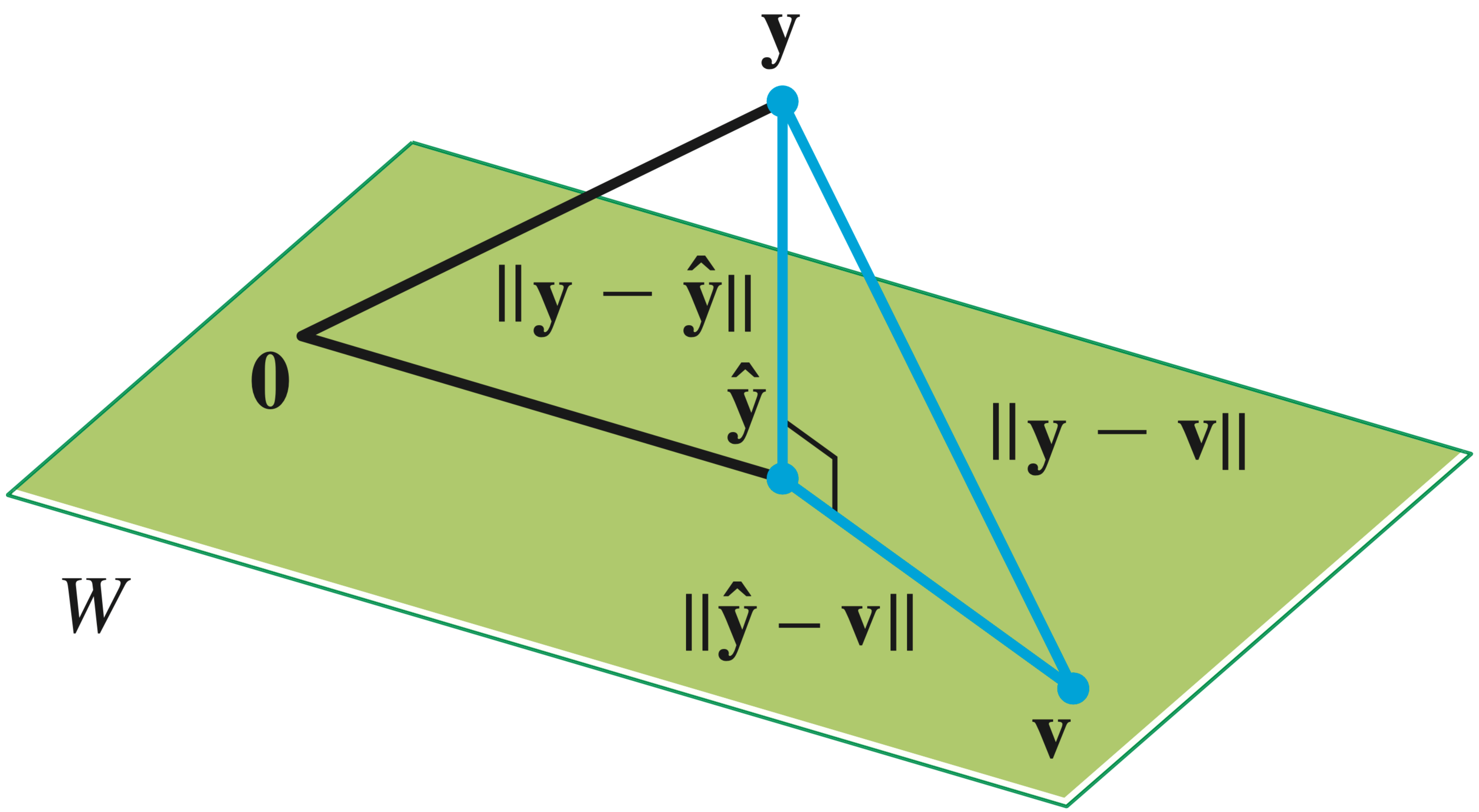
The Best-Approximation Theorem

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

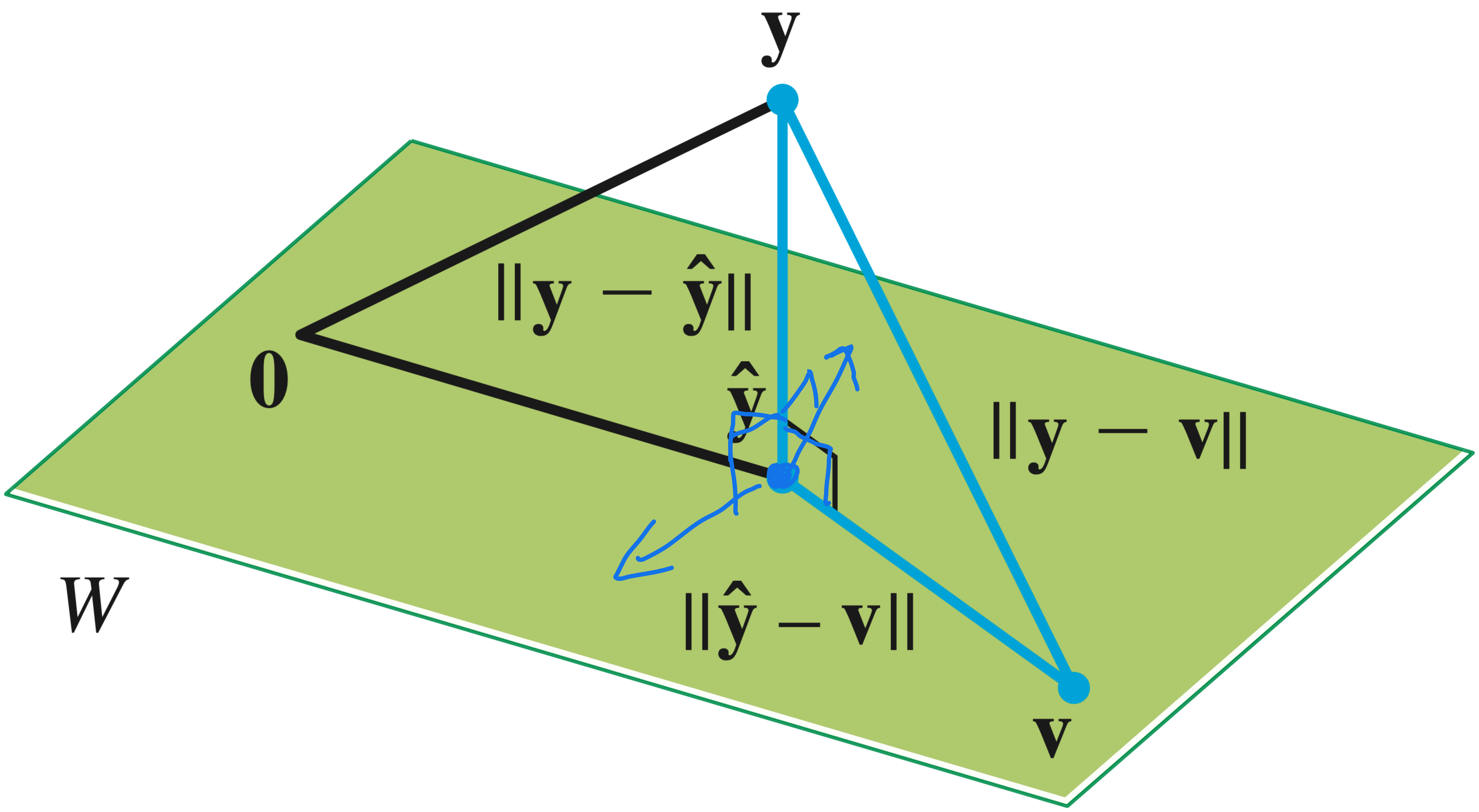
$\hat{\mathbf{y}}$ is the closest point in W to $\mathbf{y}$



$\mathbf{y}$
$\|\mathbf{y}-\hat{\mathbf{y}}\|$
$\mathbf{0}$
$\hat{\mathbf{y}}$
$\|\mathbf{y}-\mathbf{v}\|$
W
$\|\hat{\mathbf{y}}-\mathbf{v}\|$
$\mathbf{v}$

Linear Algebra and its Applications, Lay, Lay, McDonald

Proof by Inspection


$\mathbf{y}$
$\|\mathbf{y} - \hat{\mathbf{y}}\|$
$\mathbf{0}$
$\hat{\mathbf{y}}$
$\|\mathbf{y} - \mathbf{v}\|$
W
$\|\hat{\mathbf{y}} - \mathbf{v}\|$
$\mathbf{v}$

Proof by Algebra

Verify: For any $\vec{v}$ in W

goal: $\|\vec{y}-\vec{v}\| \geq \|\vec{y}-\hat{y}\|$

$$\Updownarrow$$

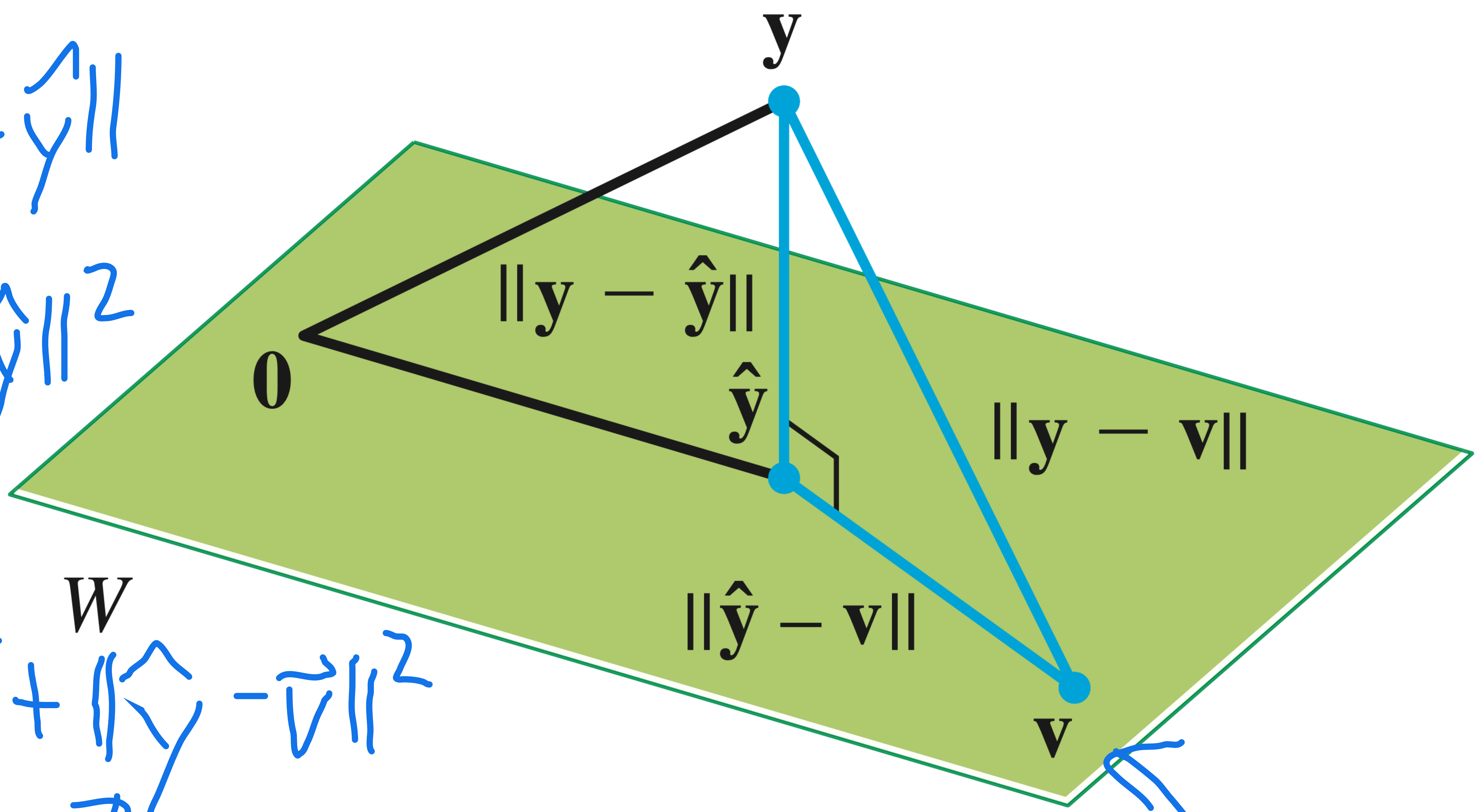
$$\|\vec{y}-\vec{v}\|^2 \geq \|\vec{y}-\hat{y}\|^2$$

$$\Uparrow$$

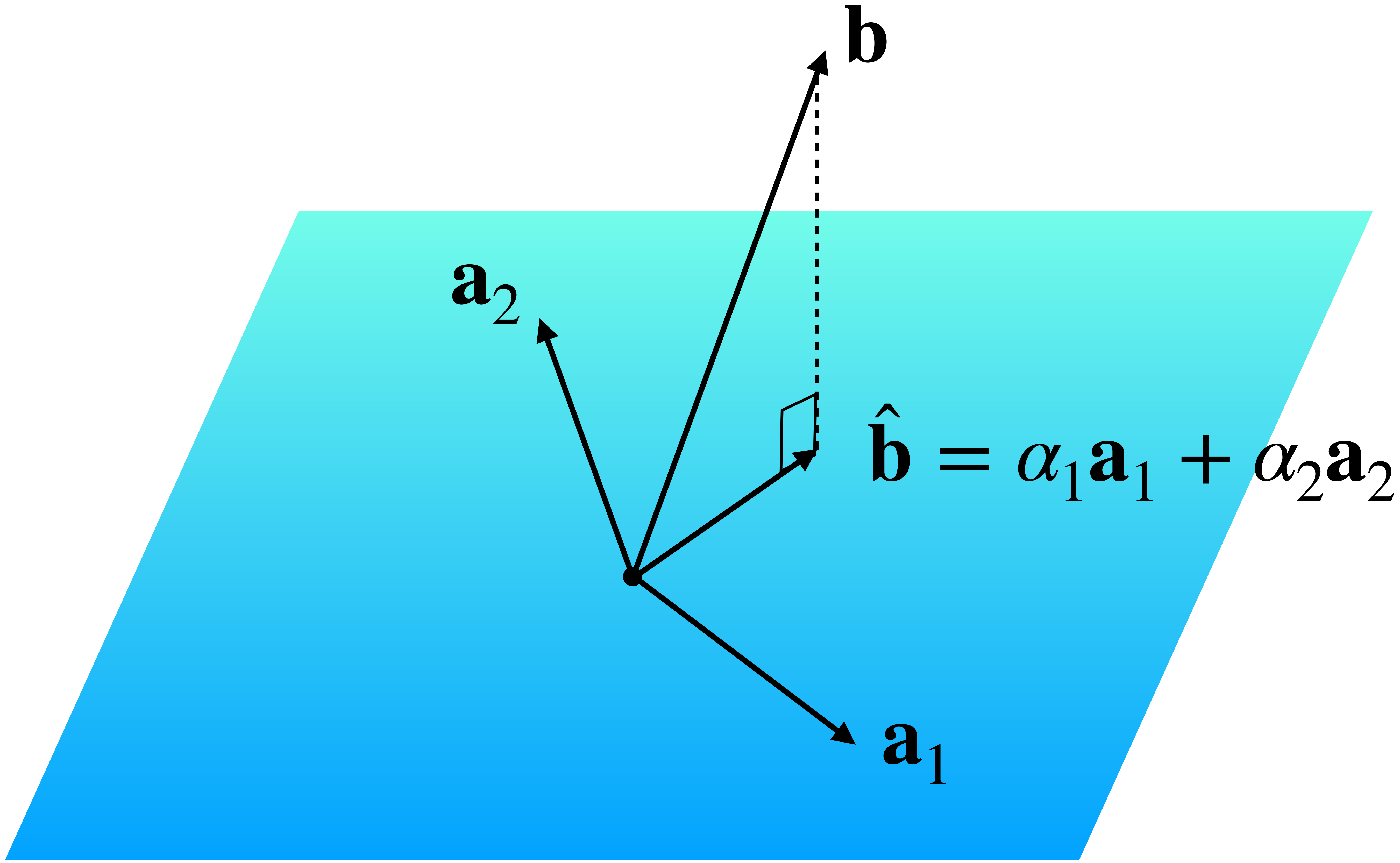
$$\|\vec{y}-\vec{v}\|^2 = \|\vec{y}-\hat{y}\|^2 + \|\hat{y}-\vec{v}\|^2$$

≥ 0

equality when $\vec{v} = \hat{y}$

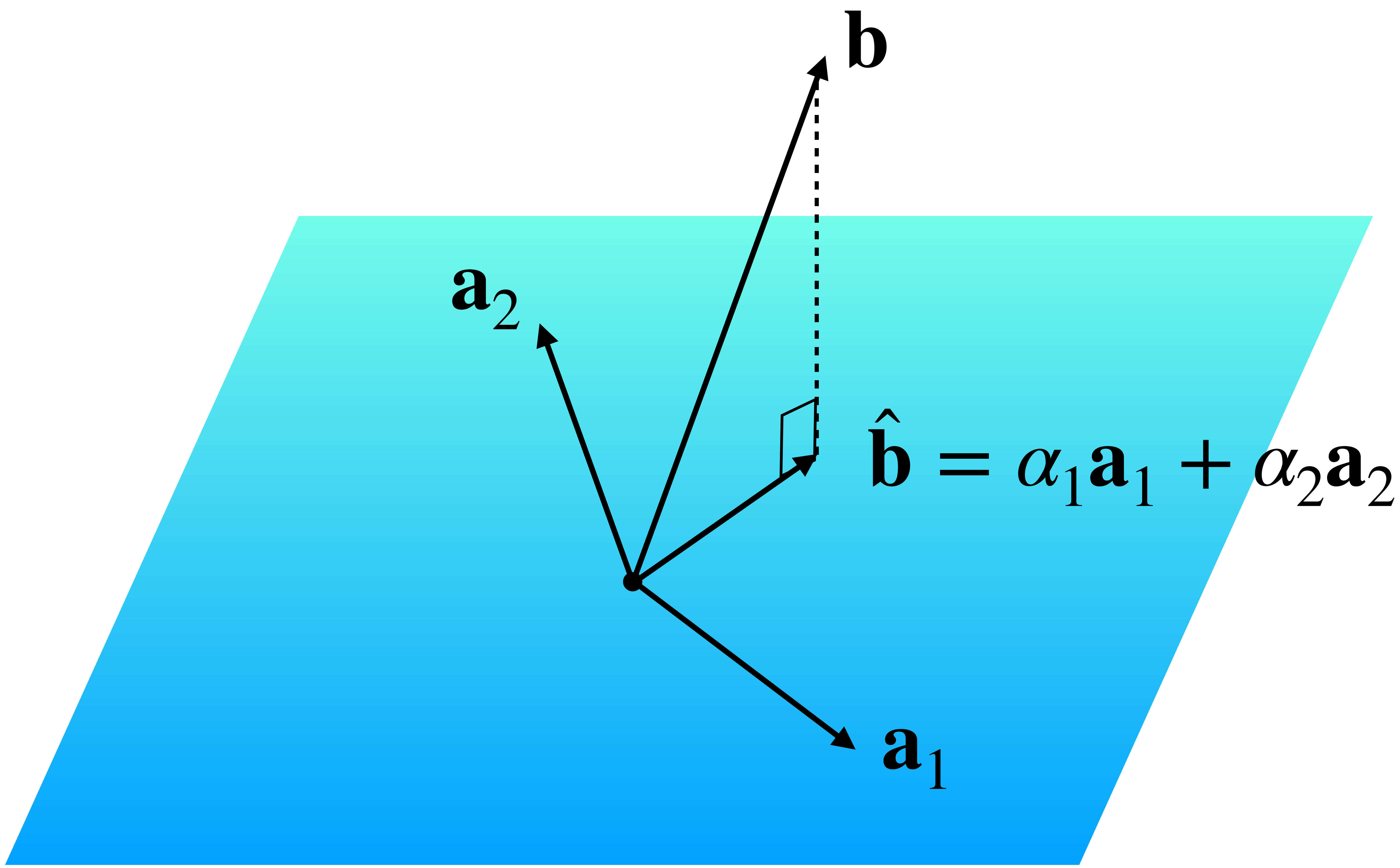


The Point


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

The Point

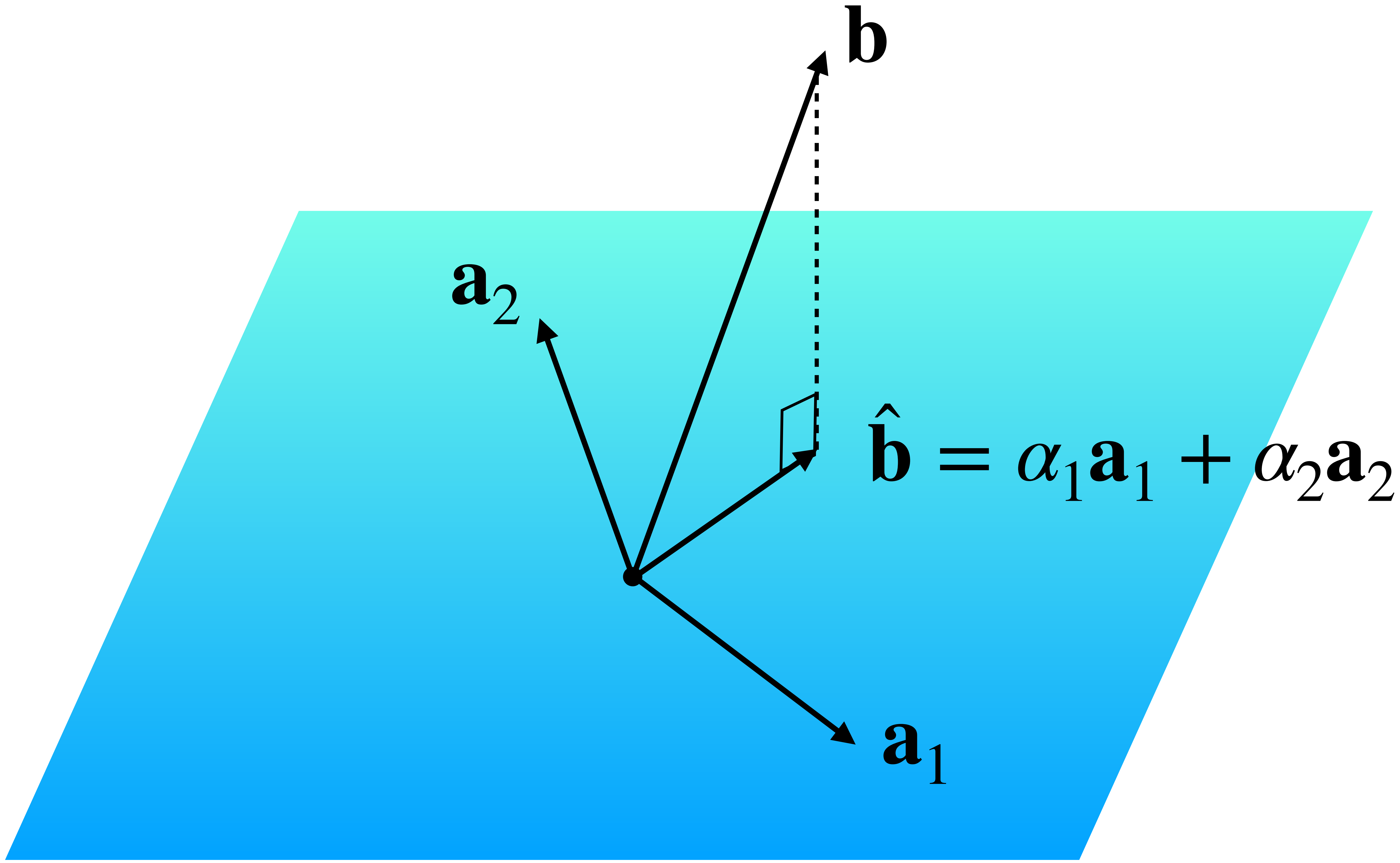
$\hat{\mathbf{b}}$ is in $Col(A)$ so $A\mathbf{x} = \hat{\mathbf{b}}$ has a solution


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

The Point

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

At this point, we could call it a day:


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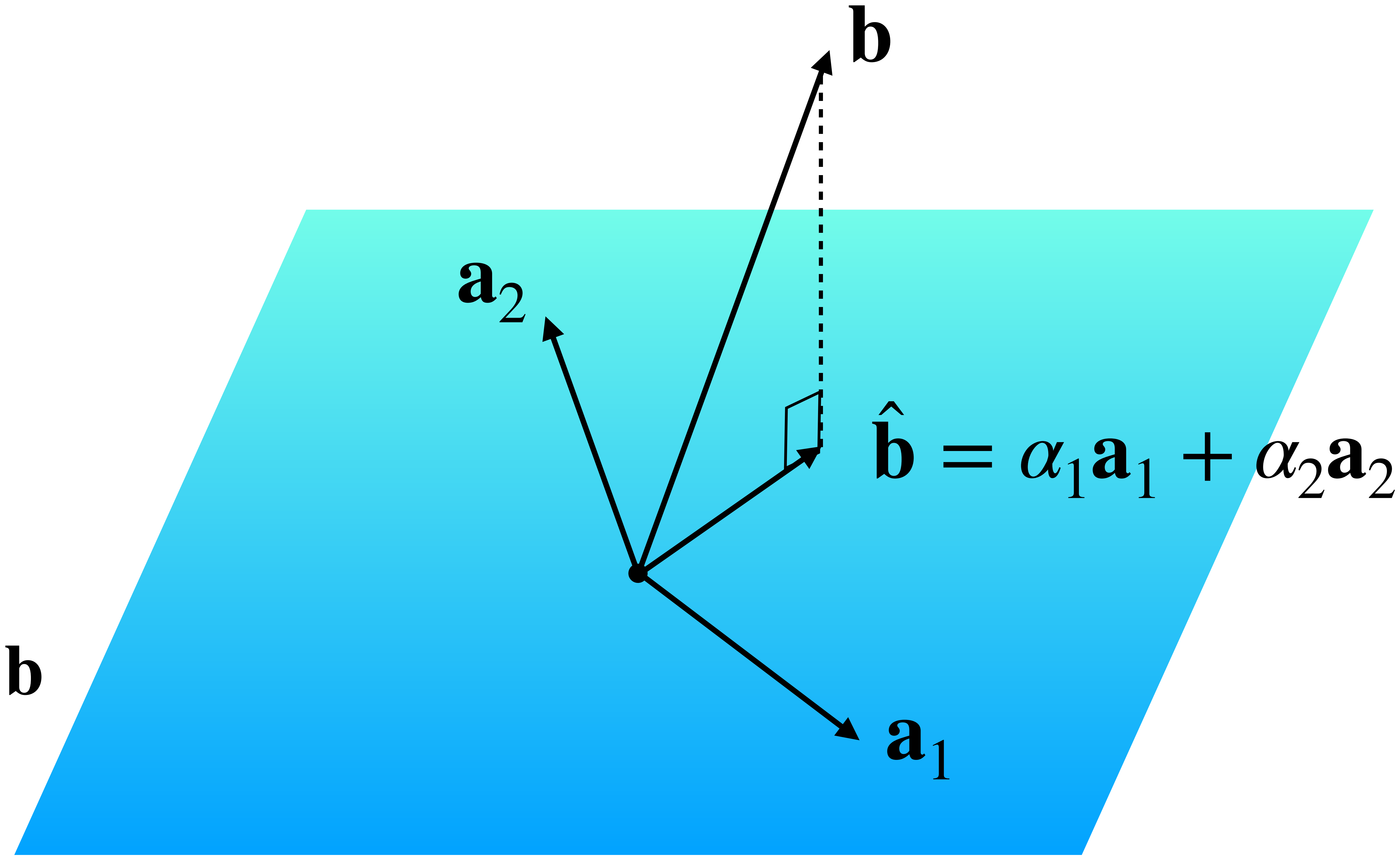
The Point

$\hat{\mathbf{b}}$ 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 $A\mathbf{x} = \mathbf{b}$


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

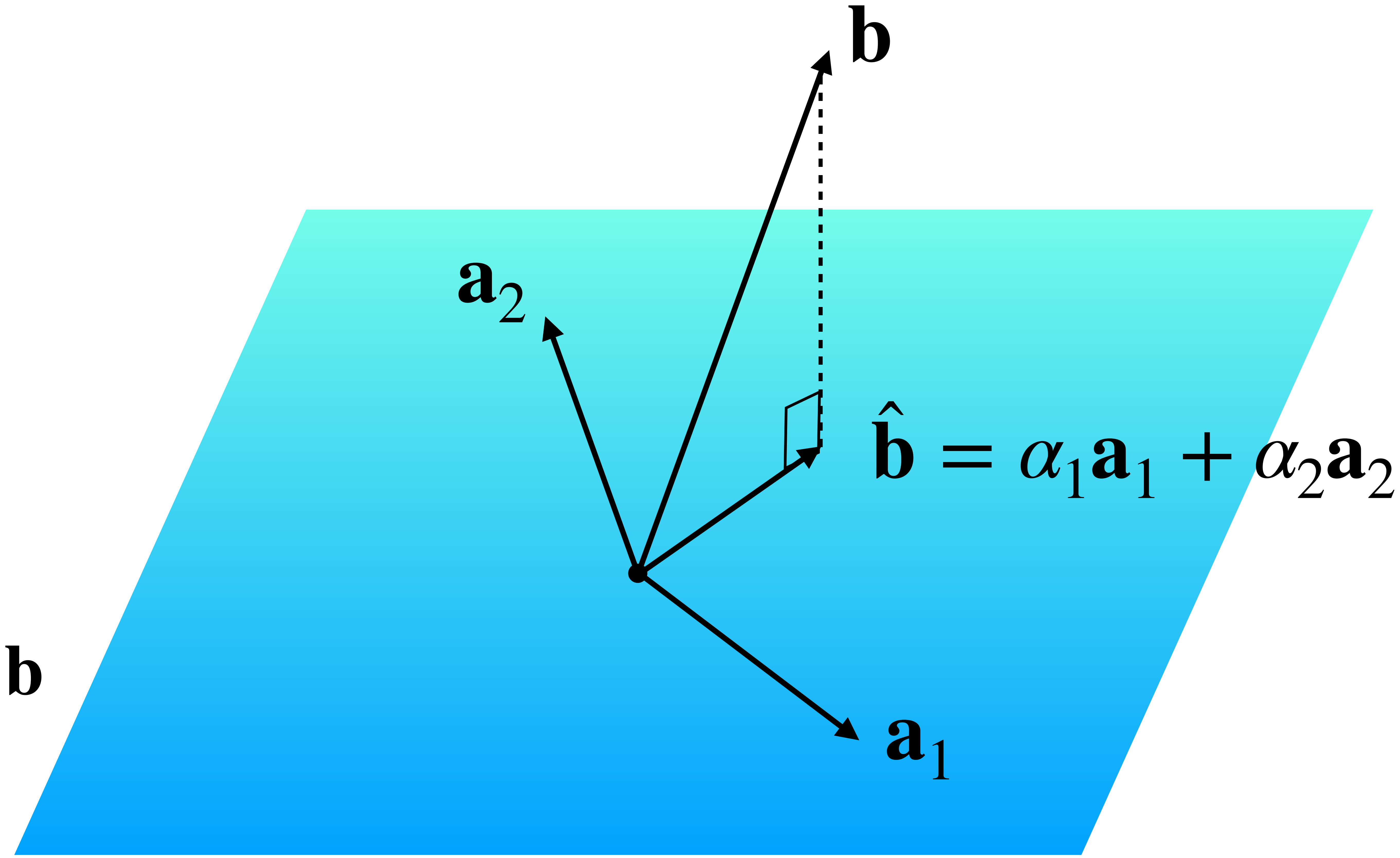
The Point

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

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 $\underline{A\mathbf{x} = \hat{\mathbf{b}}}$


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

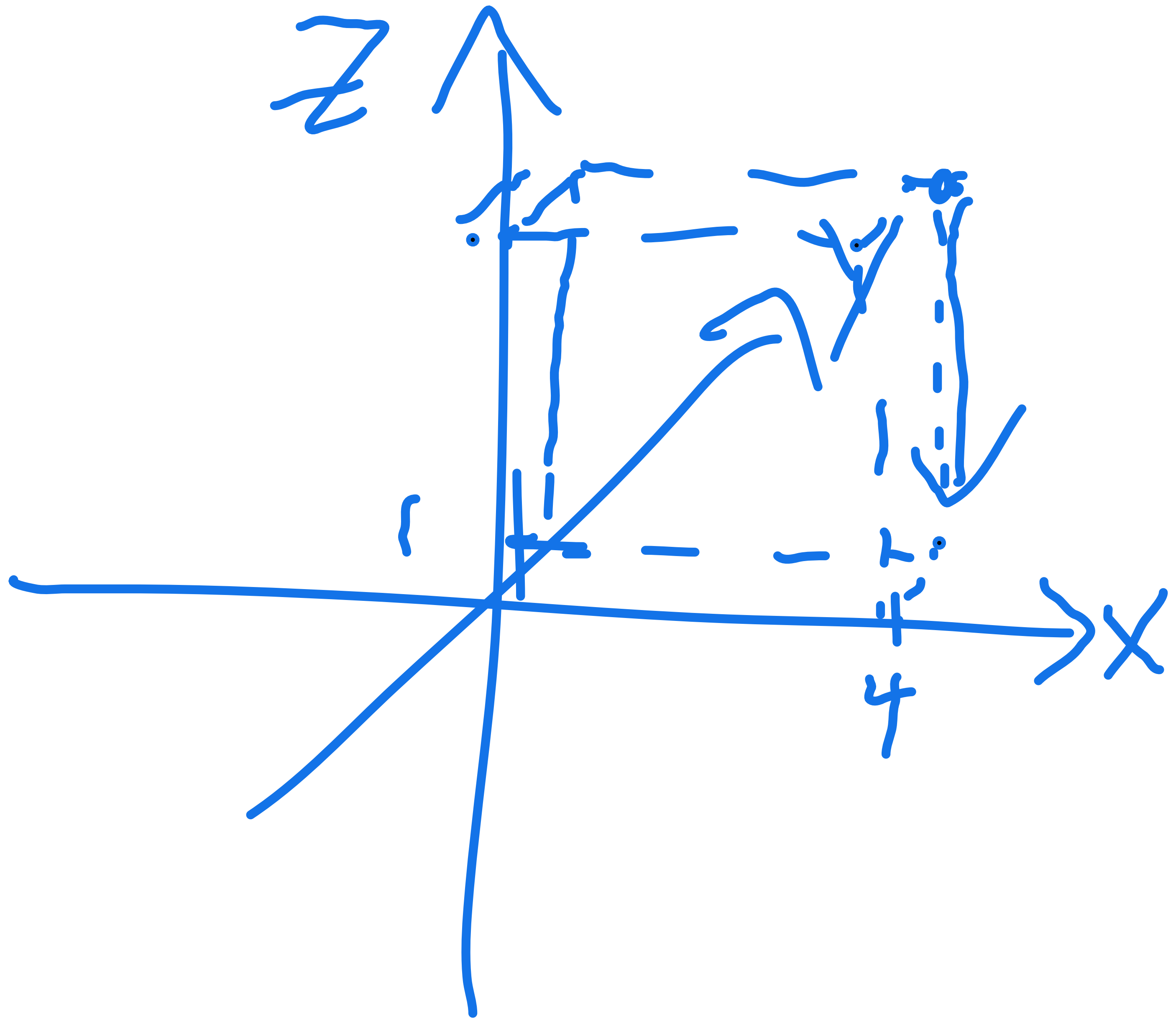
Example

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

$$\text{Col}A = \left\{ \begin{bmatrix} x \\ x \\ 0 \end{bmatrix} \middle| \, x,y \in \mathbb{R} \right\}$$

z entries are all 0

Let's determine the least squares solution for the above system:



$$\underline{\hat{b}} = \begin{bmatrix} 4 \\ 1 \\ 0 \end{bmatrix}$$

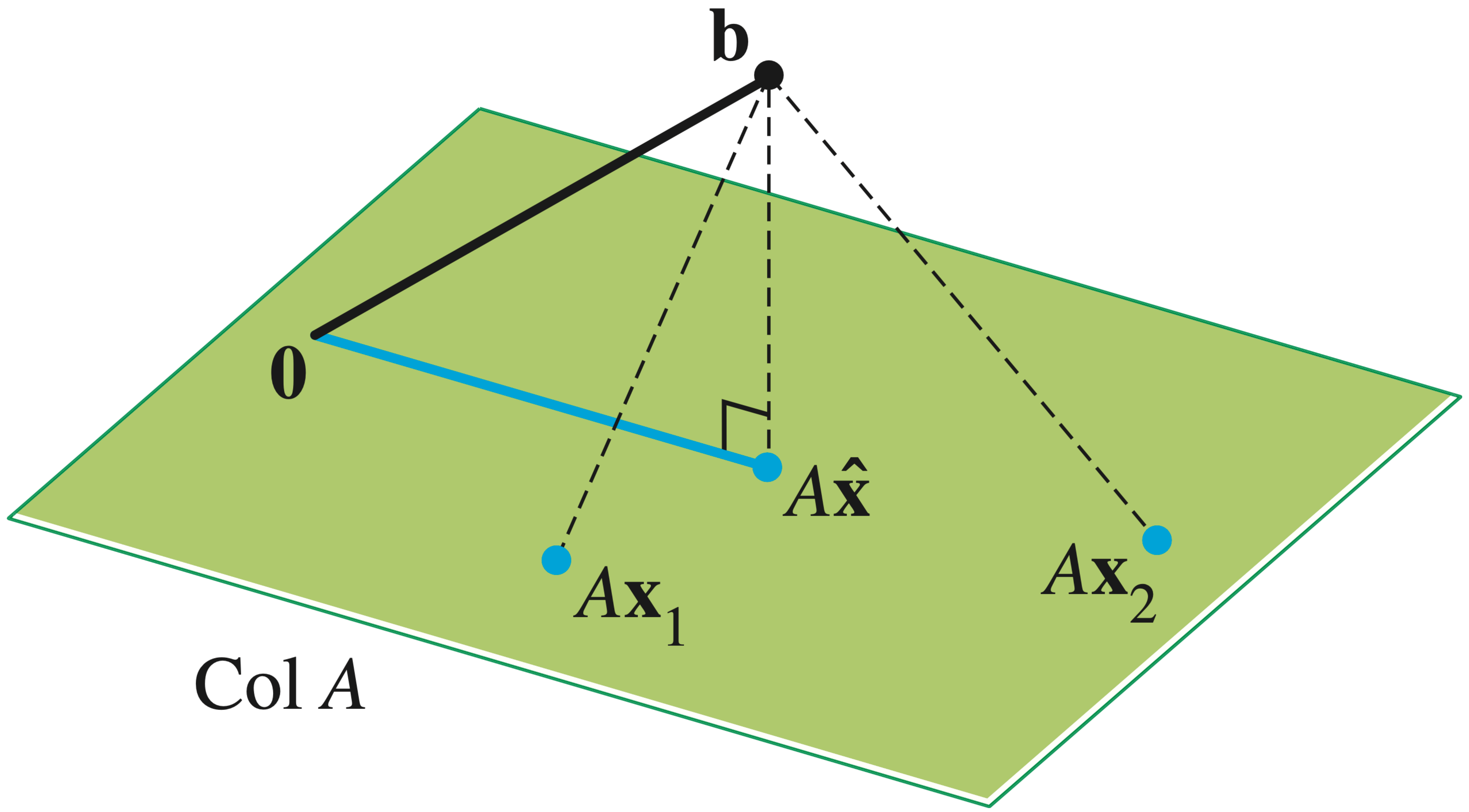
$$\left[\begin{array}{cc|c} 1 & 2 & 4 \\ -1 & 3 & 1 \end{array}\right] \sim \begin{bmatrix} 1 & 2 & 4 \\ 0 & 5 & 5 \end{bmatrix} \sim \begin{bmatrix} 1 & 2 & 4 \\ 0 & 1 & 1 \end{bmatrix}$$

$$\left[\begin{array}{cc|c} 1 & 0 & 2 \\ 0 & 1 & 1 \end{array}\right]$$

$$x = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \leftarrow \text{least-squares sol'n}$$

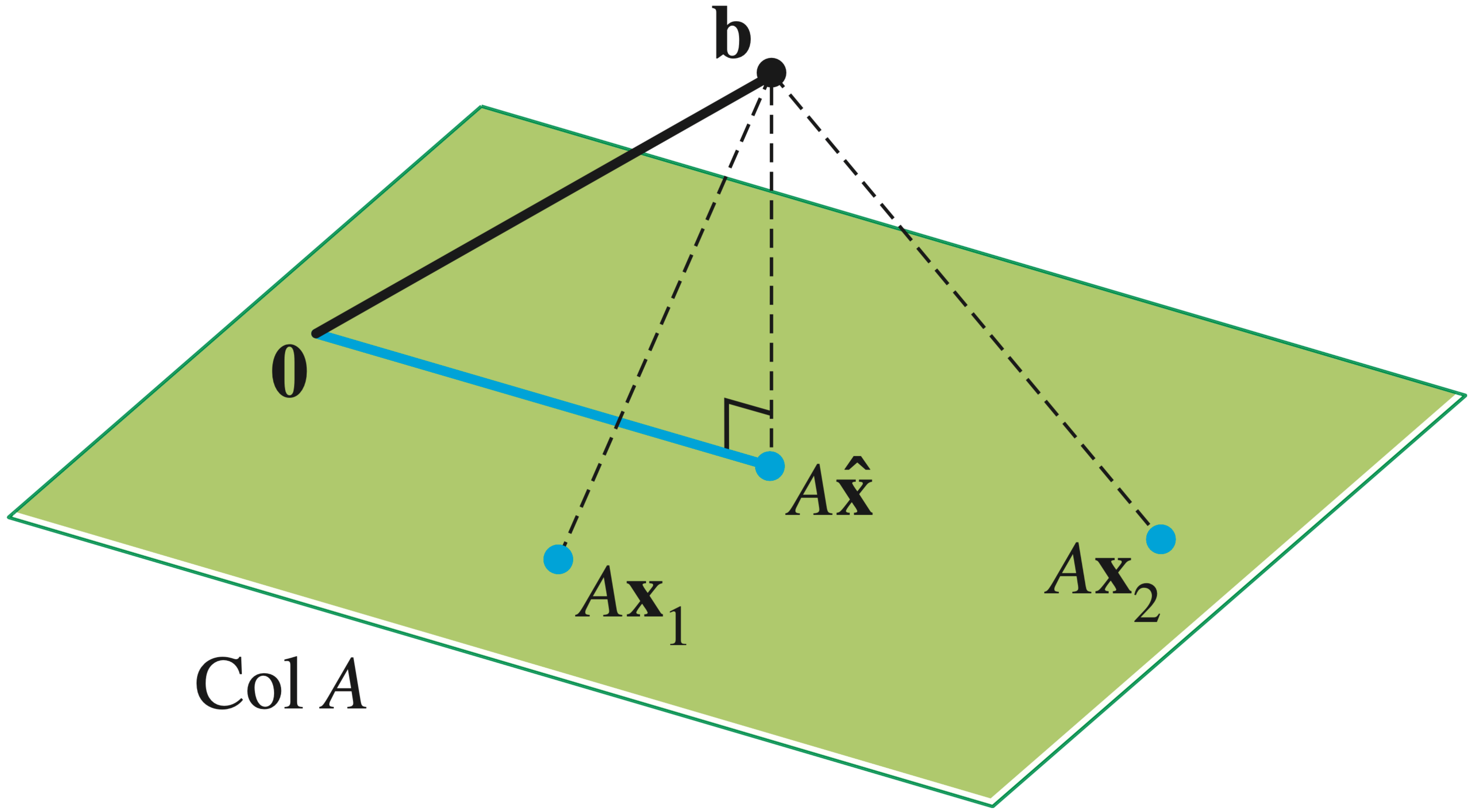
The Normal Equations

A Couple Observations



A Couple Observations

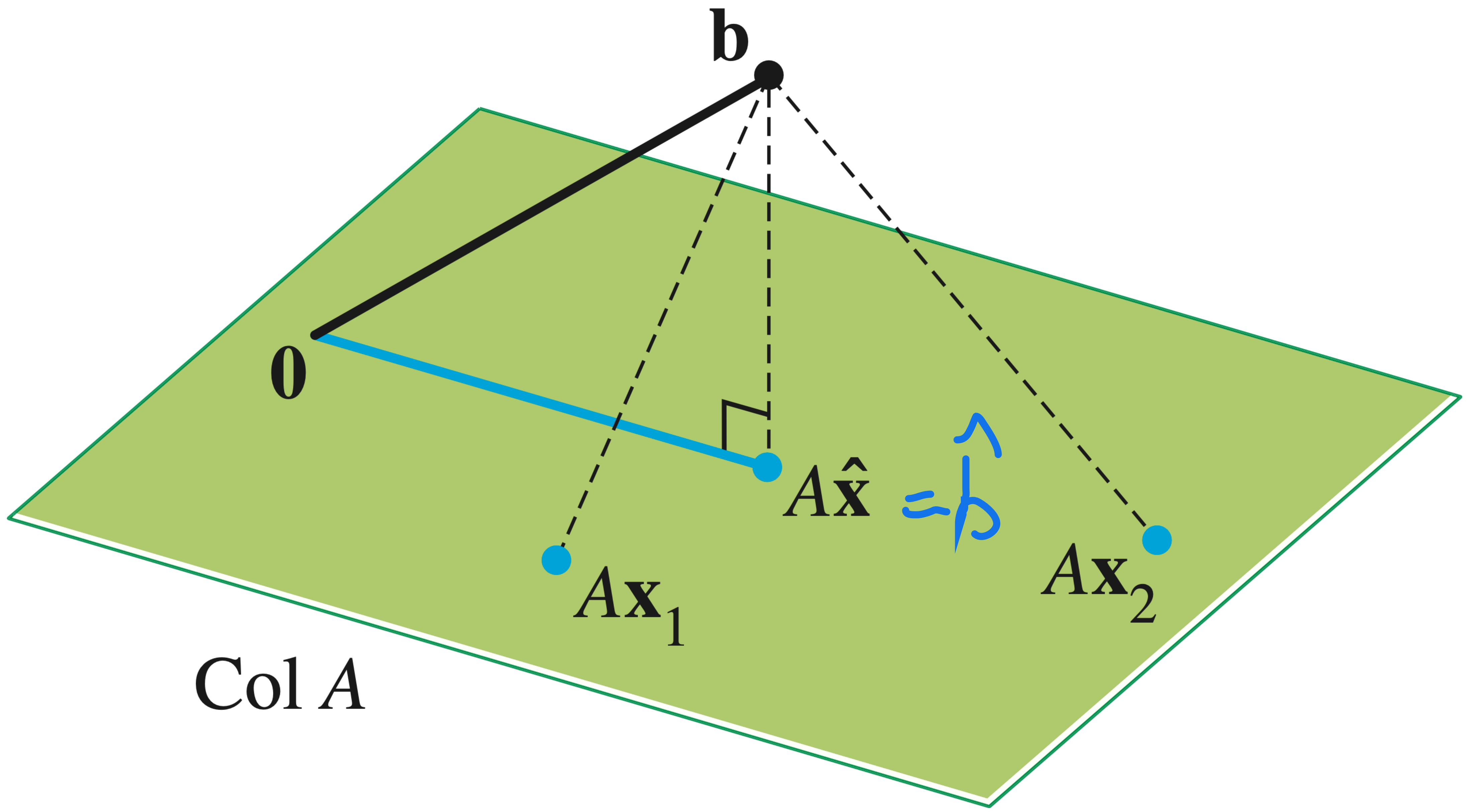
Suppose that $\hat{\mathbf{x}}$ is a least squares solution to A, so $A\hat{\mathbf{x}} = \hat{\mathbf{b}}$



A Couple Observations

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

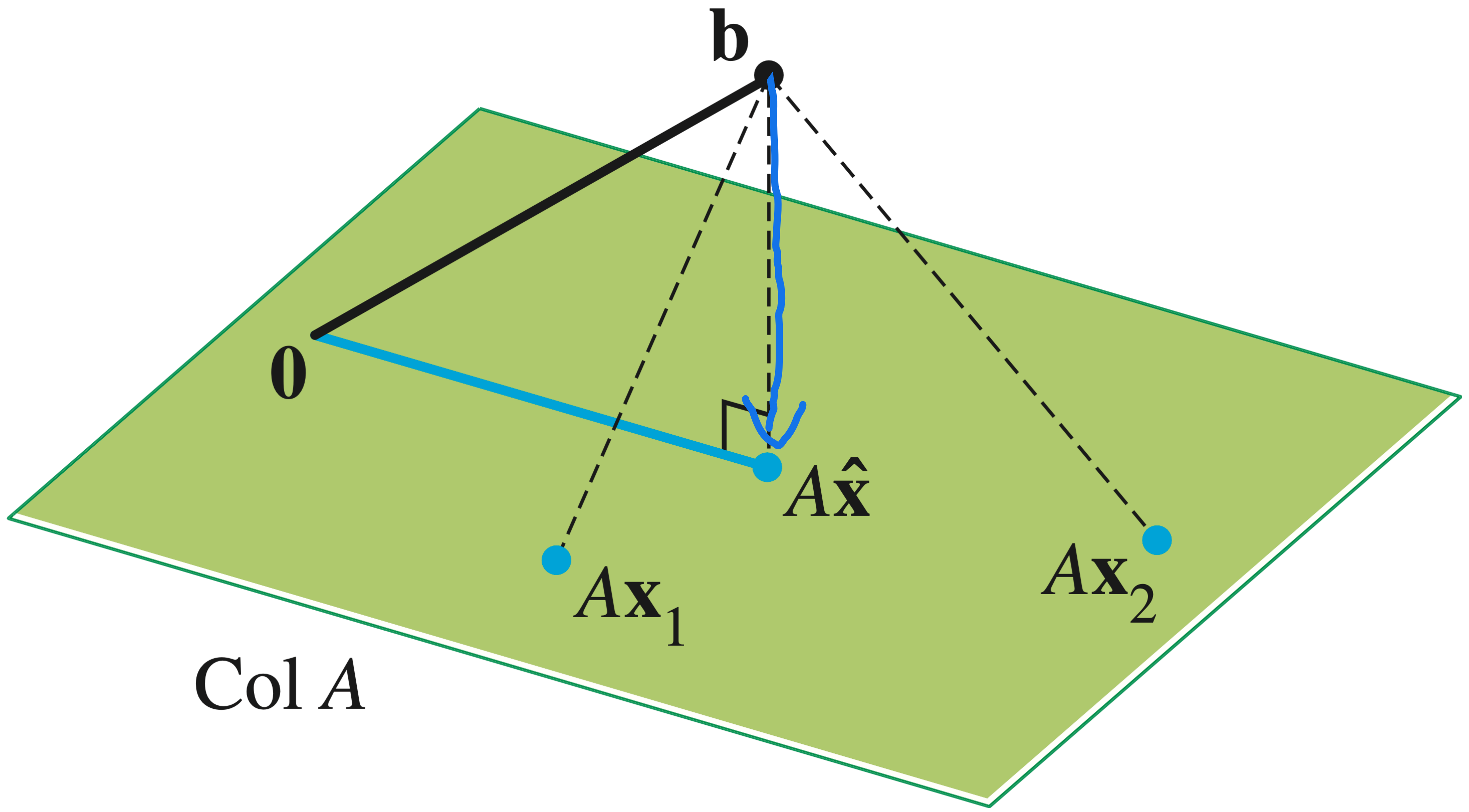
- $\hat{\mathbf{b}} - \mathbf{b}$ is orthogonal to $Col(A)$



A Couple Observations

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

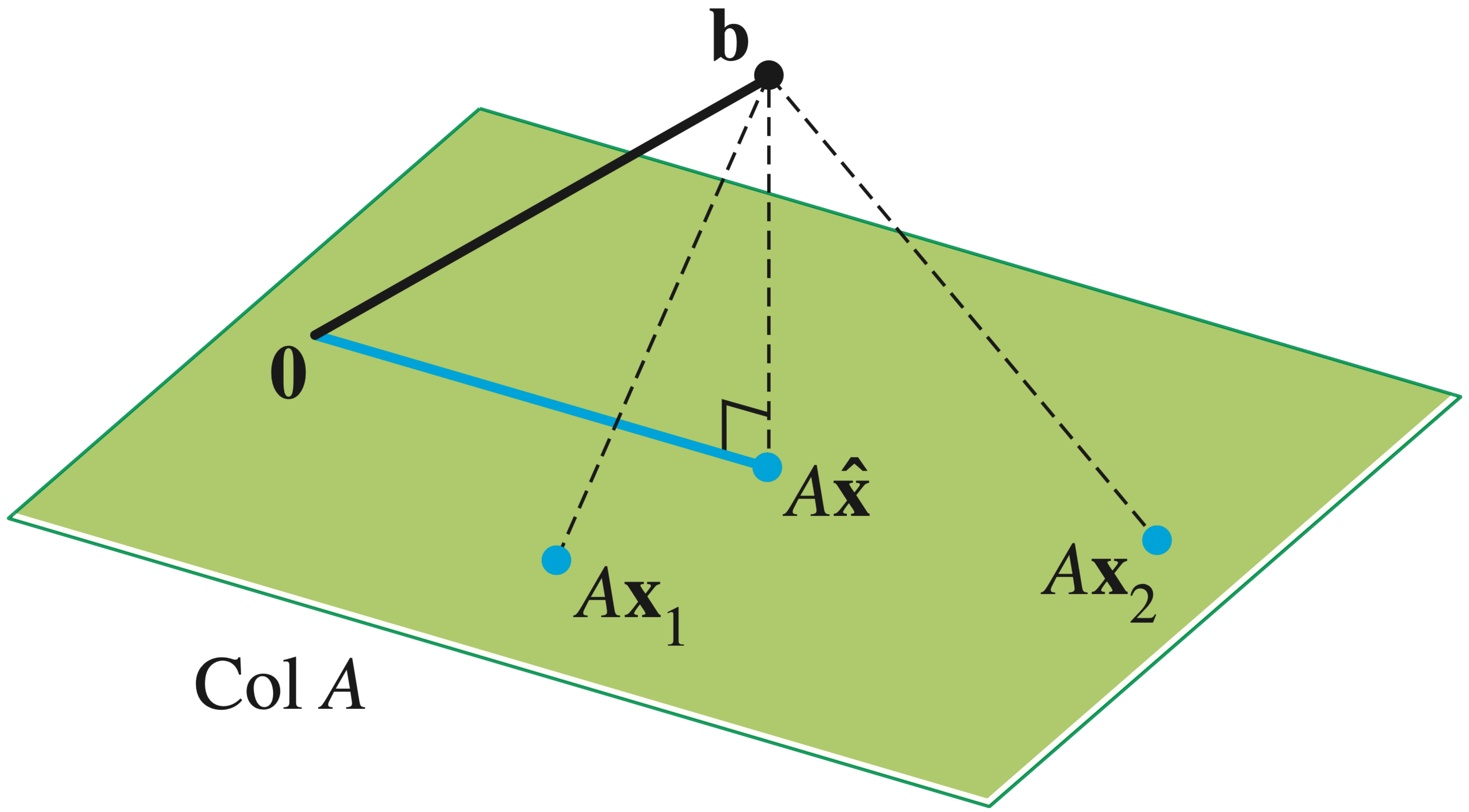
- $\hat{\mathbf{b}} - \mathbf{b}$ is orthogonal to $Col(A)$
- $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to $Col(A)$



A Couple Observations

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

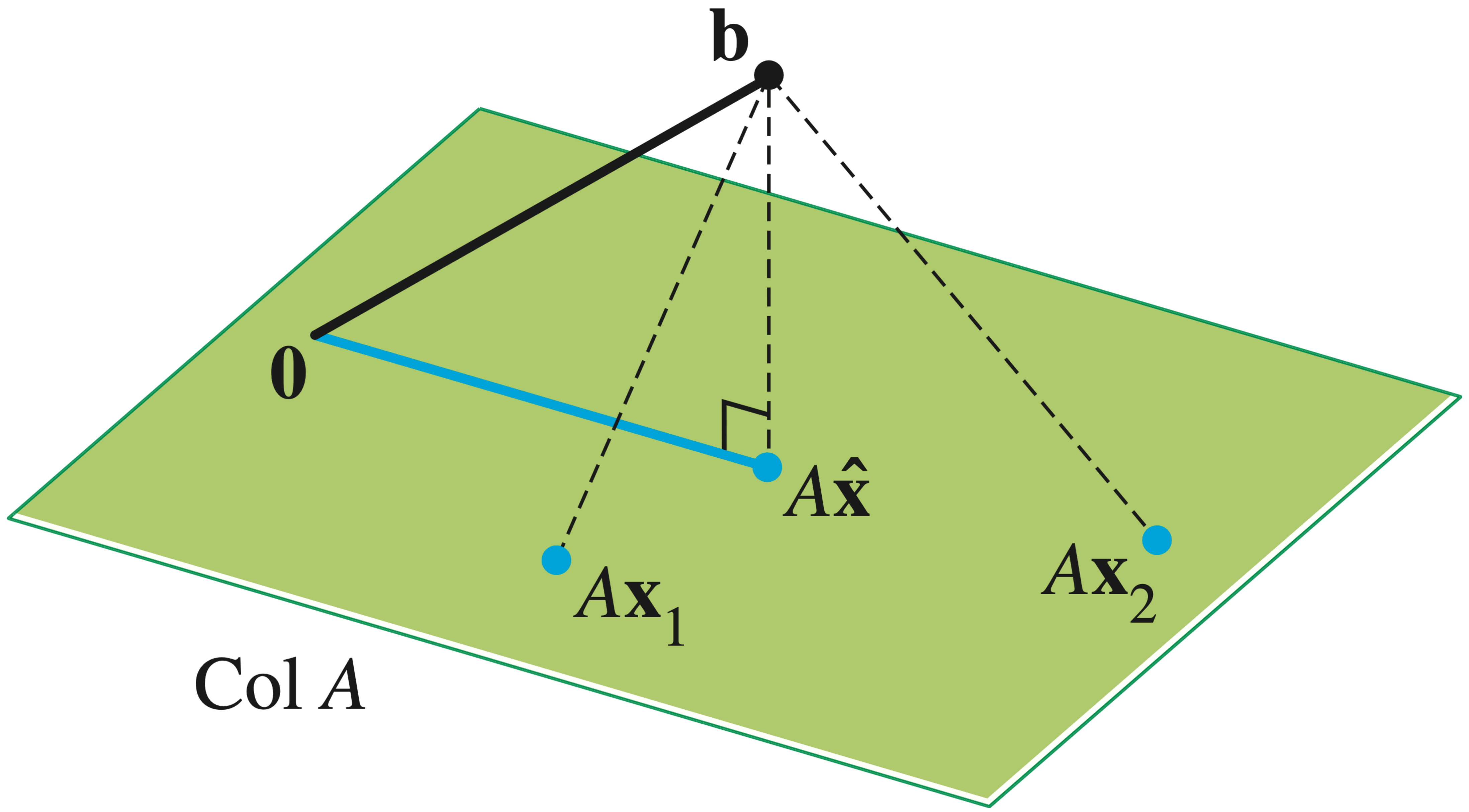
- $\hat{\mathbf{b}} - \mathbf{b}$ is orthogonal to $Col(A)$
- $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to $Col(A)$
- If $A = [\mathbf{a}_1 \;\; \mathbf{a}_2 \;\; \dots \;\; \mathbf{a}_n]$ then $A\hat{\mathbf{x}} - \mathbf{b}$ is orthogonal to each $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$



A Couple Observations

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 $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$
- $\mathbf{a}_i^T(A\hat{\mathbf{x}} - \mathbf{b}) = 0$



A Couple Observations

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

- $\hat{\mathbf{b}} - \mathbf{b}$ is orthogonal to $Col(A)$
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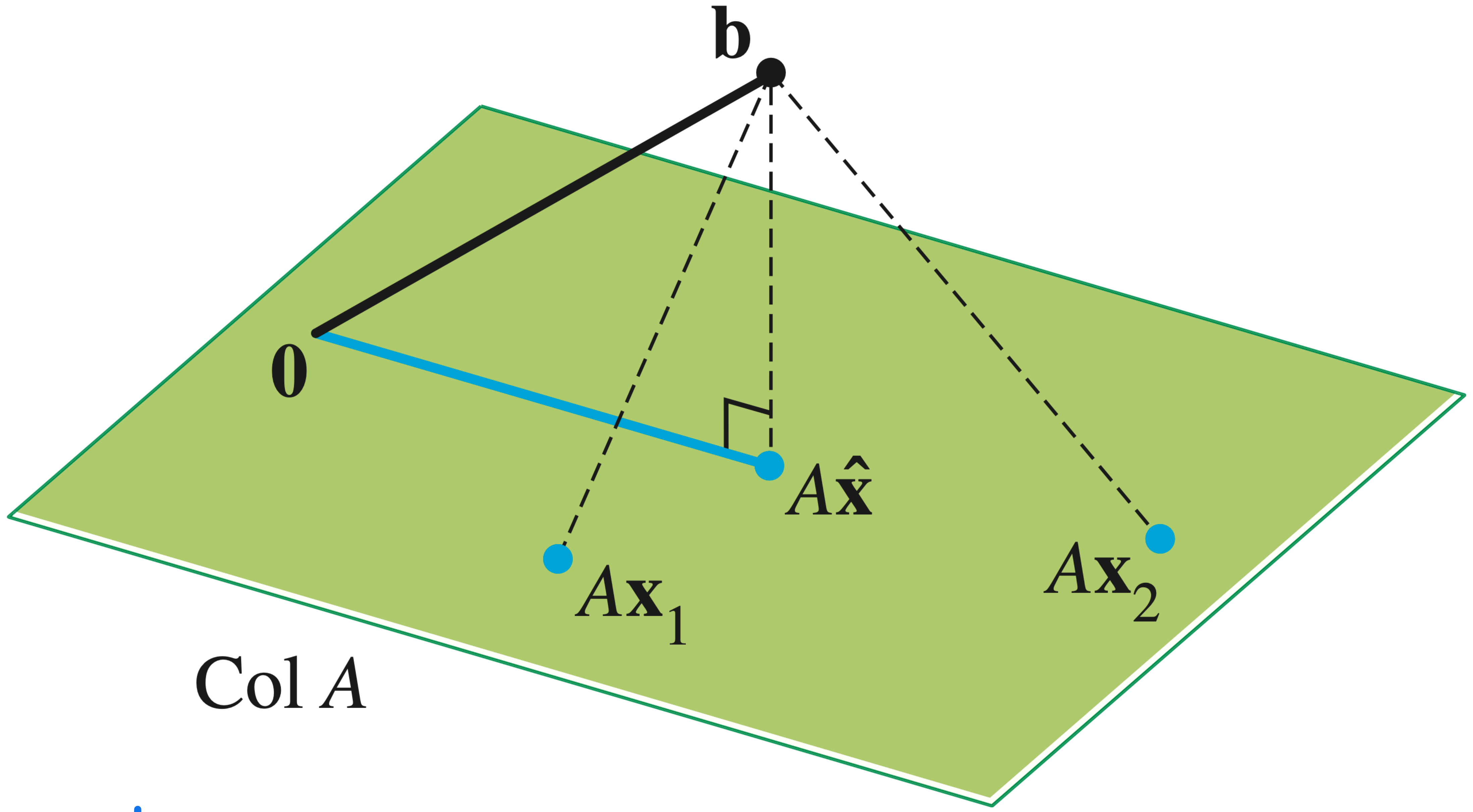
- $\mathbf{a}_i^T(A\hat{\mathbf{x}} - \mathbf{b}) = 0$
- $A^T(A\hat{\mathbf{x}} - \mathbf{b}) = \mathbf{0}$ ← matrix-vector equation



A bit more magic

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

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

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

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

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

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

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 $A\mathbf{x} = \mathbf{b}$:

$$A^T A = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 2 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix}$$

$$A^T \vec{b} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 0 \\ 11 \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

$$\begin{bmatrix} 17 & 1 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} \vec{x} \end{bmatrix} = \begin{bmatrix} 19 \\ 11 \end{bmatrix}$$

Example

$$\underbrace{\begin{bmatrix}17 & 1\\ 1 & 5\end{bmatrix}}_{A^TA}\begin{bmatrix}x_1\\ x_2\end{bmatrix} = \begin{bmatrix}19\\ 11\end{bmatrix}$$

$$\det(A^TA) = (17)(5) - 1$$
$$= 84$$

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

$$\begin{bmatrix}x_1\\ x_2\end{bmatrix} = \begin{bmatrix}17 & 1\\ 1 & 5\end{bmatrix}^{-1}\begin{bmatrix}19\\ 11\end{bmatrix} = \frac{1}{\det(A^TA)}\begin{bmatrix}5 & -1\\ -1 & 17\end{bmatrix}\begin{bmatrix}19\\ 11\end{bmatrix}$$

$$= \frac{1}{84}\begin{bmatrix}95-11\\ -19+187\end{bmatrix} = \frac{1}{84}\begin{bmatrix}84\\ 168\end{bmatrix}$$

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

$$\underline{A^TA\vec{x}}$$

$$\hat{b} = A\vec{x} = \begin{bmatrix}4 & 0\\ 0 & 2\\ 1 & 1\end{bmatrix}\begin{bmatrix}1\\ 2\end{bmatrix} = \begin{bmatrix}4\\ 4\\ 3\end{bmatrix} \leftarrow \text{orthogonal proj. onto Col } A$$

Example

$$\underset{\overset{\shortparallel}{A}}{\begin{bmatrix} 1 & 2 \\ -1 & 3 \\ 0 & 0 \end{bmatrix}} \mathbf{x} = \underset{\overset{\shortparallel}{b}}{\begin{bmatrix} 4 \\ 1 \\ 4 \end{bmatrix}}$$

$$\hat{b} = \begin{bmatrix} 4 \\ 1 \\ 0 \end{bmatrix} \overset{\checkmark}{\overset{?}{=}} A\vec{x} = \begin{bmatrix} 2+2 \\ -2+3 \\ 0 \end{bmatrix}$$

Let's do it again...

$$A^TA = \begin{bmatrix} 2 & -1 \\ -1 & 13 \end{bmatrix}$$

$$A^T\vec{b} = \begin{bmatrix} 1 & -1 & 0 \\ 2 & 3 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ 1 \\ 4 \end{bmatrix} = \begin{bmatrix} 3 \\ 11 \end{bmatrix}$$

$$\hat{b} \overset{?}{=} \vec{b} \quad \boxed{\text{NO}}$$

$$\left[\begin{array}{cc|c} 2 & -1 & 3 \\ -1 & 13 & 11 \end{array}\right] \sim \left[\begin{array}{cc|c} 0 & 25 & 25 \\ -1 & 13 & 11 \end{array}\right] \sim \left[\begin{array}{cc|c} 1 & -13 & -11 \\ 0 & 1 & 1 \end{array}\right] \sim \left[\begin{array}{cc|c} 1 & 0 & 2 \\ 0 & 1 & 1 \end{array}\right]$$

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

least-squares sol'n

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

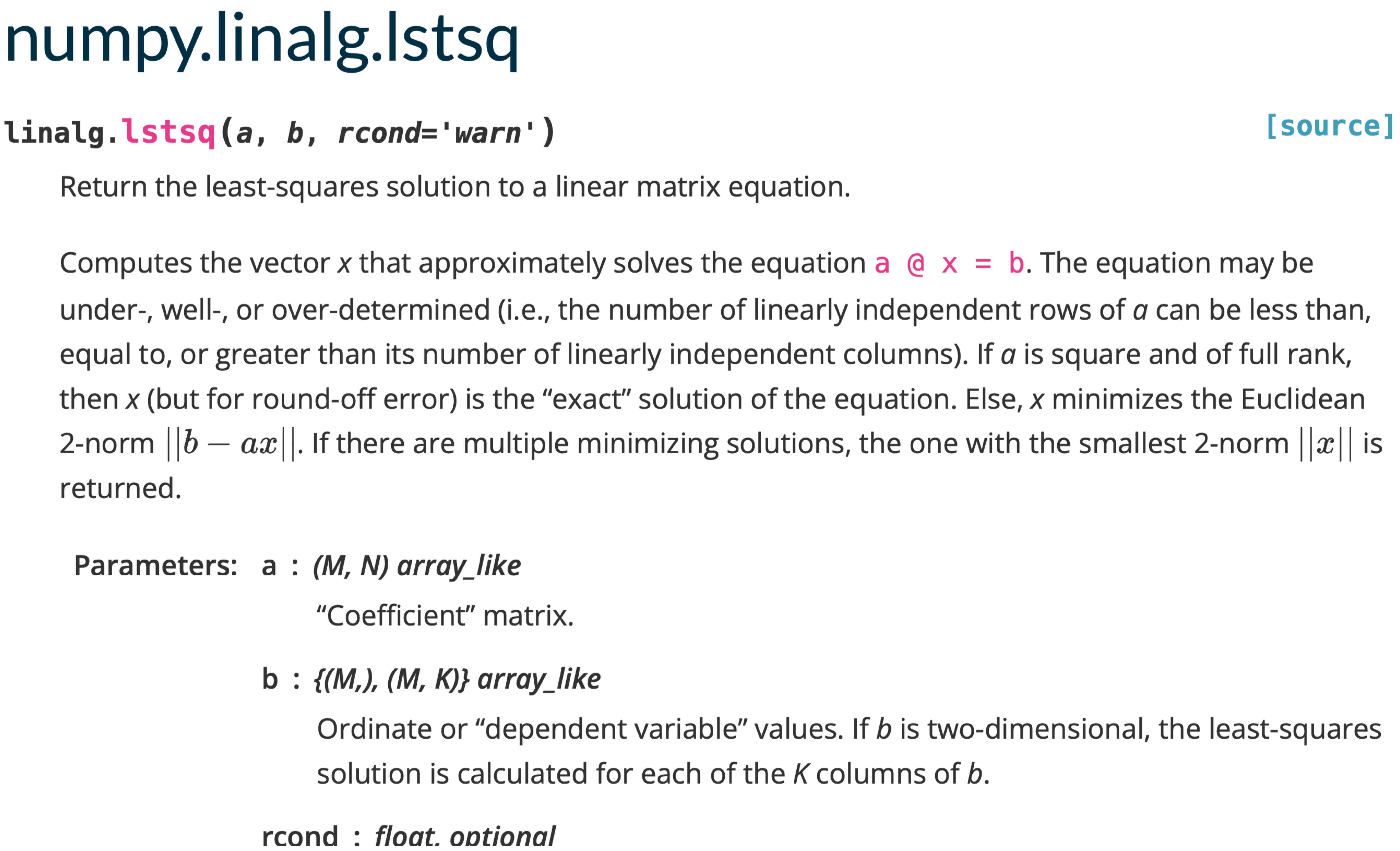
↑ may have many solutions

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***

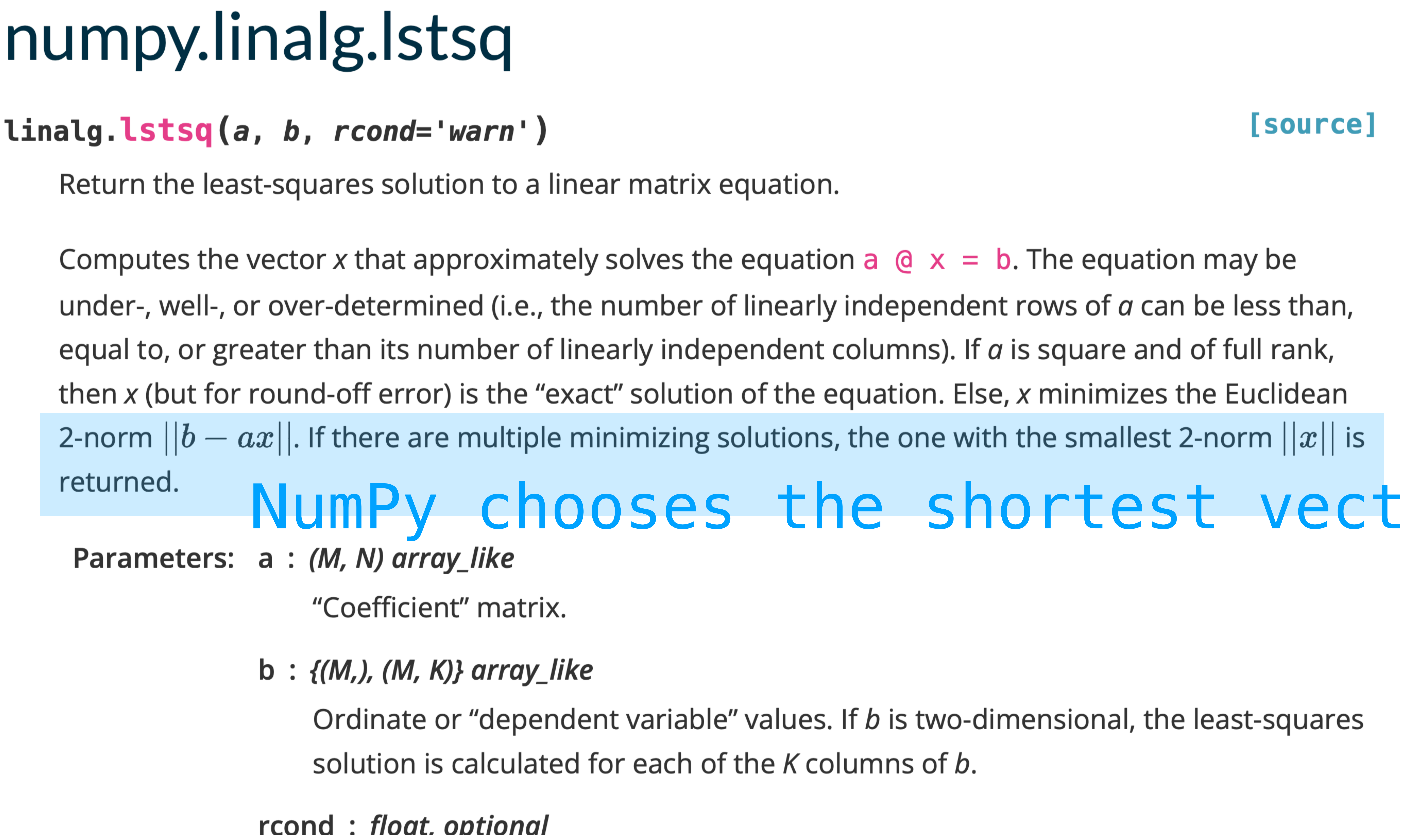
“Coefficient” matrix.

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*

Practically Speaking



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NumPy chooses the shortest vector

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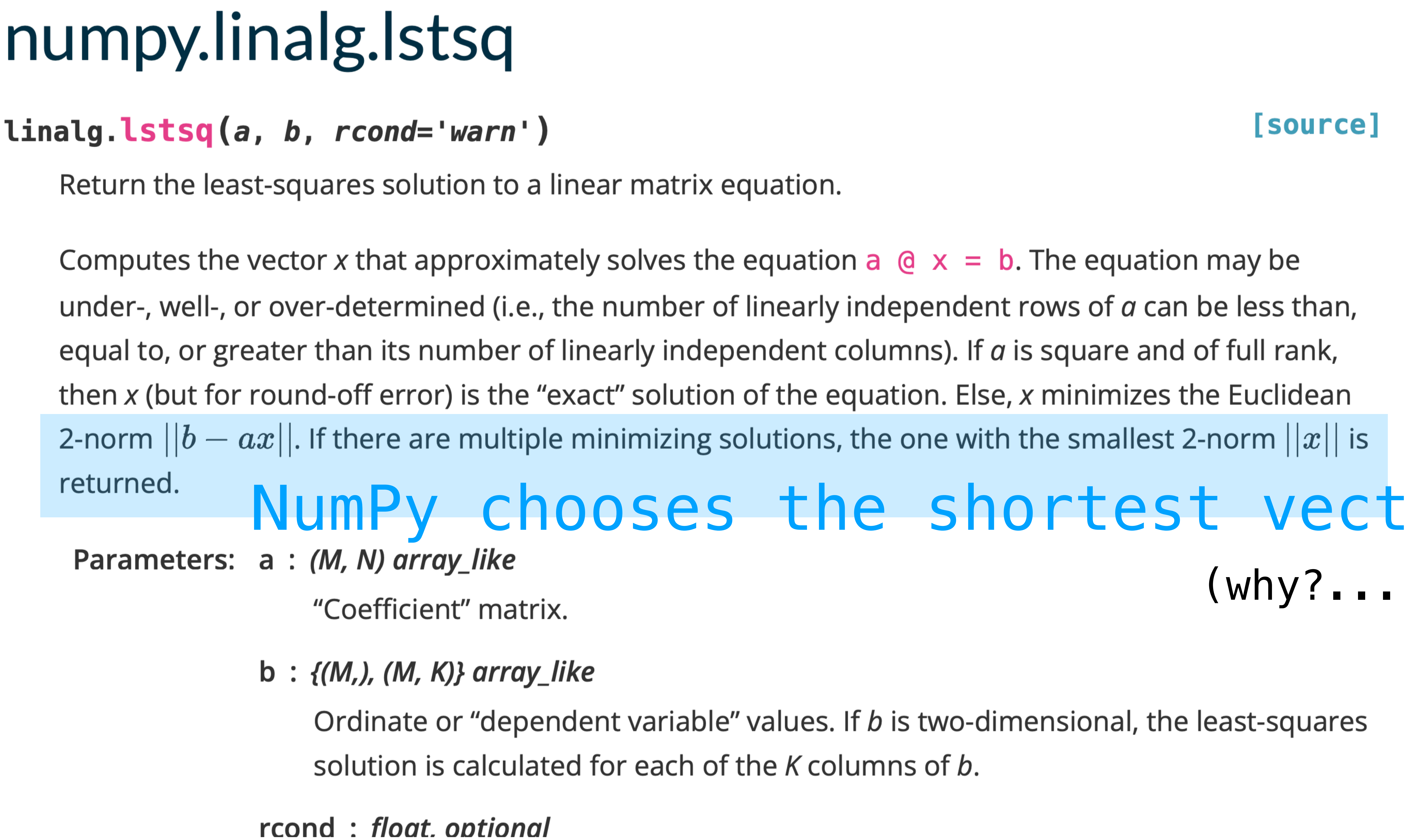
Practically Speaking



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NumPy chooses the shortest vector

(why?...)

Unique Least Squares Solutions

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

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

» The columns of A are <u>linearly independent</u>

» $A^T A$ is <u>invertible</u>

Unique Least Squares Solutions

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

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

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

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

Projecting onto a subspace

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

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