Lecture 3

Linear Systems II

Conditioning & introduction to least squares problems

CS328 - Numerical Methods for Visual Computing and Machine Learning

Prof. Wenzel Jakob

Where are we now?

Veggies first, then the cake

MidJourney: *two plates next to each other. one contains heaps of carrots, cucumbers, and tomatoes. The other is full of sumptuous cake and candy. Hyper-realistic, f/1.4*

1. **Floating Point arithmetic & error**

2. **Linear systems, LU**

$$A = L\,U$$

3. **Conditioning & least squares basics**

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

4. **Least squares, QR**

$$A = Q\,R$$

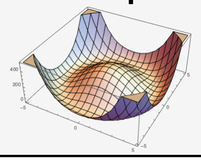
5. **Writing efficient numerical code**

```
vmovaps ymm5, cs:ymmword_100004840 ; Move aligned memory
vmovaps ymm3, cs:ymmword_100004860 ; Move aligned memory
vandnps ymm7, ymm5, ymm1 ; Bitwise logical AND NOT (256
vandnps ymm6, ymm5, ymm0 ; Bitwise logical AND NOT (256
vminps  ymm4, ymm7, ymm6 ; Packed FP minimum (8-wide)
vmaxps  ymm2, ymm6, ymm7 ; Packed FP maximum (8-wide)
vcmpgt_oqps ymm6, ymm6, ymm7 ; Packed FP comparison -- c
```

6. **Eigenanalysis, SVD**

$$A = U\,\Sigma\,V^T$$

7. **Nonlinear problems**

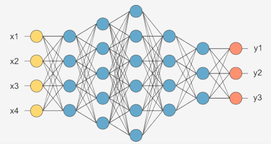


8. **Aut. differentiation**

PYTORCH

TensorFlow

9. **Neural networks**



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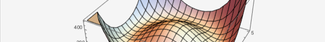

2. **Linear systems, LU**

$$A = LU$$

3. **Conditioning & least squares basics**

$$A^TA\,x = A^Tb$$

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$$A = QR$$

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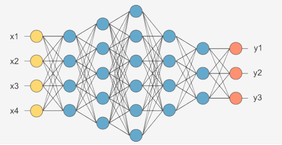

Solving a linear system using Gaussian Elimination

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{b} \end{array}\right] = \left[\begin{array}{cccc|c} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{array}\right]$$

Observation: None of the decisions taken by the algorithm depend on the right hand side.

Solving a linear system using Gaussian Elimination

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{b} \end{array}\right] = \left[\begin{array}{cccc|c} \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{array}\right]$$

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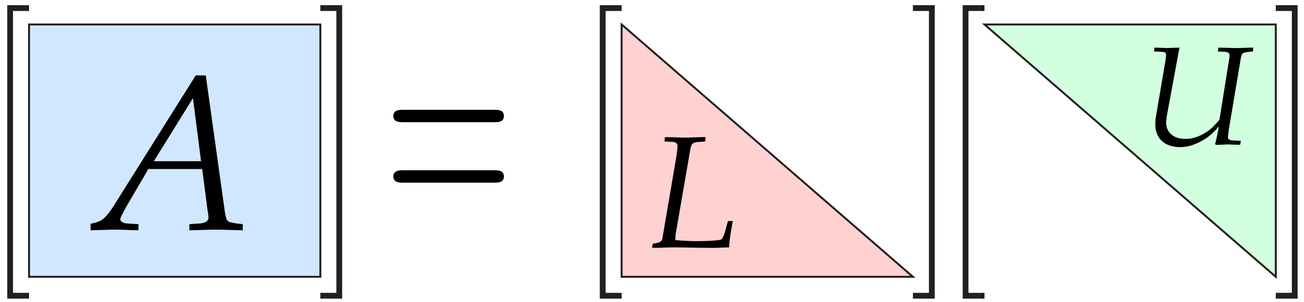
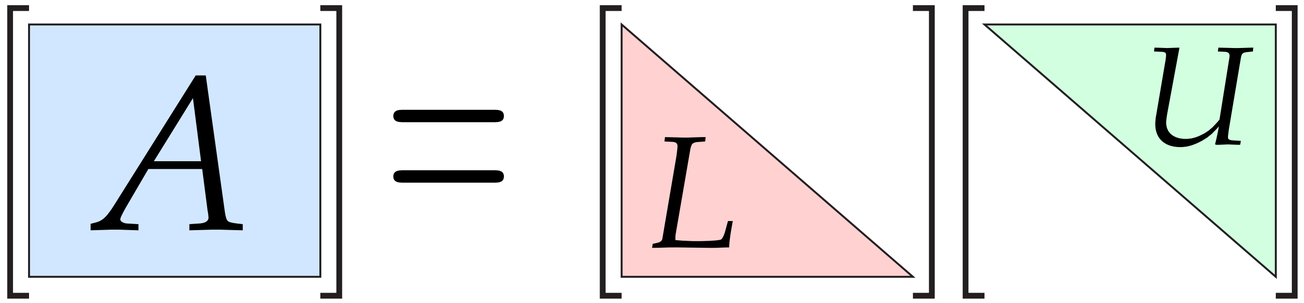
Recap: LU factorization



Recap: LU factorization



$$\mathbf{U} = \underbrace{\mathbf{E}_6\mathbf{E}_5\mathbf{E}_4\mathbf{E}_3\mathbf{E}_2\mathbf{E}_1\mathbf{A}}$$

$$\mathbf{A} = \mathbf{LU}$$

$$\underbrace{(\mathbf{E}_6\mathbf{E}_5\mathbf{E}_4\mathbf{E}_3\mathbf{E}_2\mathbf{E}_1)^{-1}}$$

$$= \mathbf{E}_1^{-1}\mathbf{E}_2^{-1}\mathbf{E}_3^{-1}\mathbf{E}_4^{-1}\mathbf{E}_5^{-1}\mathbf{E}_6^{-1}$$

Recap: don't invert (big) matrices

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

Usually this **does not mean** "compute an inverse of A". Read this as "call a linear system solver to solve $\mathbf{Ax} = \mathbf{b}$"

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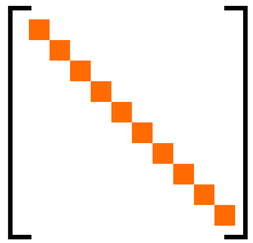

Diagonal

```
for i in range(n):
    x[i] = b[i] / A[i, i]
```

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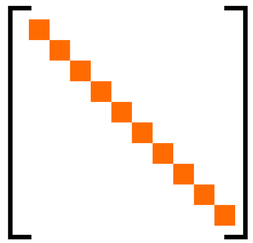

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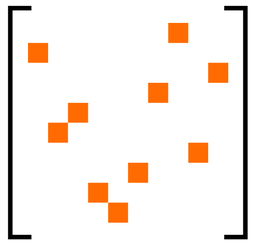

Permutation

```
for i in range(n):
    x[i] = b[i] / A[i, i]
```

```
for i in range(n):
    x[i] = b[perm[i]]
```

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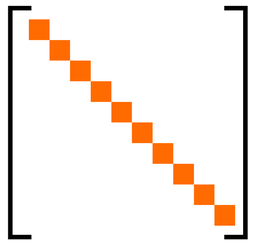

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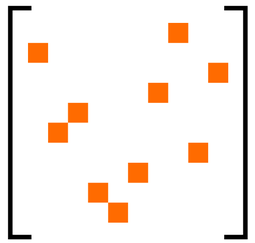

Permutation

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for i in range(n):
    x[i] = b[perm[i]]
```

Triangular

Forward/backward substitution

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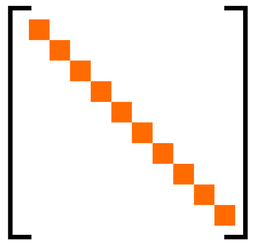

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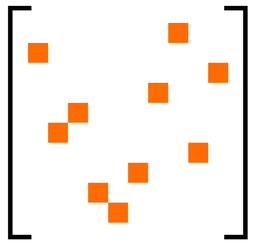

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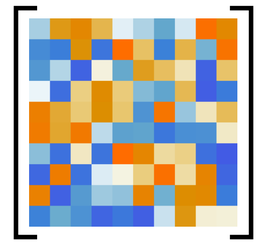

Dense

General solver, e.g. LU factorization

A worked out example

LU factorization of a 2x2 matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 2 & 4 \end{bmatrix}$$

A worked out example

LU factorization of a 2x2 matrix

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 2 & 4 \end{bmatrix} \begin{matrix} \\ *\,\text{-}2 \end{matrix}$$

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$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 2 & 4 \end{bmatrix} \begin{matrix} \\ *\,\text{-}2 \end{matrix}$$

(Elimination matrix that performs this operation)

$$\mathbf{E}_1 = \begin{bmatrix} 1 & 0 \\ -2 & 1 \end{bmatrix}$$

A worked out example

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A worked out example

LU factorization of a 2x2 matrix

(Elimination matrix that performs this operation)

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$$\mathbf{L} = \mathbf{E}_1^{-1} = \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix}$$

$$\longrightarrow \mathbf{A} = \mathbf{LU}$$ ✅

Cost of matrix operations

1. Matrix-vector multiplication

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b = A @ x
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$$\mathbf{b} \in \mathbb{R}^{10000}$$
$$\mathbf{A} \in \mathbb{R}^{10000 \times 10000}$$

100 million matrix entries!

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66 *ms* ~6x slower

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— 30'282 *ms* ~2'752x slower

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$$\mathcal{O}(n^2)$$

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```
C = A @ B
```

Cost of matrix operations

2. Matrix-matrix multiplication

```
C = A @ B
```

```
C = np.zeros((n, n))
for j in range(n):
    C[:, j] = A @ B[:, j]
```

Cost of matrix operations

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Cost of matrix operations

2. Matrix-matrix multiplication

$$\mathbf{A}, \mathbf{B} \in \mathbb{R}^{1000 \times 1000}$$

1 million matrix entries!

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341'495 *ms* ~17'973x slower

Cost of matrix operations

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$\mathcal{O}(n^3)$

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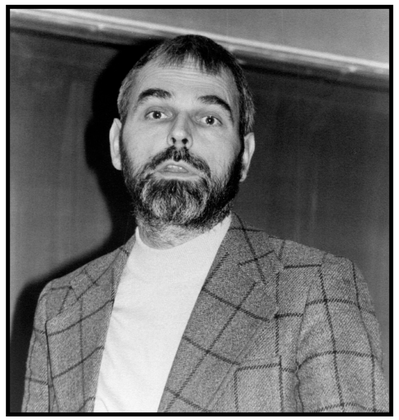
Cost of matrix operations

$O(n^3)$ time complexity.. is that really true?



Volker Strassen, *1969*
"Matrix multiplication has $O(n^{2.8074})$ time complexity."

MidJourney: *a galactic computer*

Cost of matrix operations

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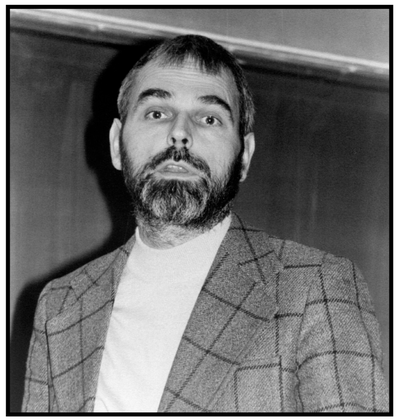

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"Matrix multiplication has $O(n^{2.8074})$ time complexity."

Still an active area of research

Virginia Williams et al., *2023*

"Matrix multiplication has $O(n^{2.371552})$ time complexity."

MidJourney: *a galactic computer*

Cost of matrix operations

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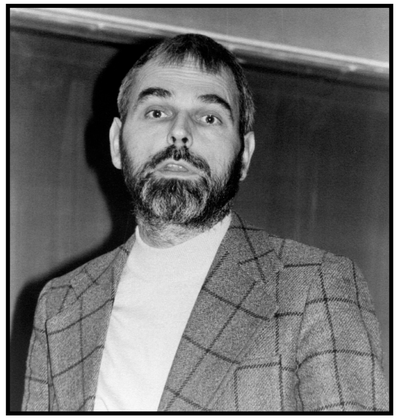

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"Matrix multiplication has $O(n^{2.8074})$ time complexity."

Still an active area of research

Virginia Williams et al., *2023*
"Matrix multiplication has $O(n^{2.371552})$ time complexity."

MidJourney: *a galactic computer*

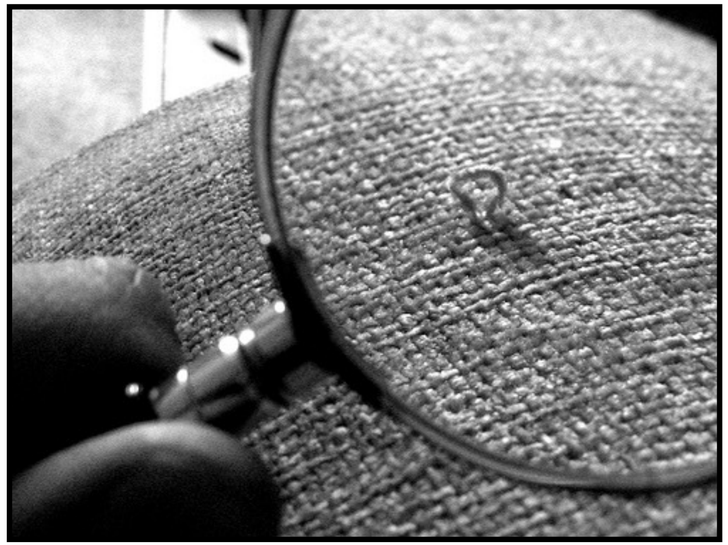
Quite possible that the true cost is $O(n^2)$. *Nobody knows!*

Many works are *galactic* algorithms. In practice, the naïve algorithm tends to be fastest.

Cost of matrix operations

Forward/backward substitution

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{b} \end{array}\right] = \left[\begin{array}{cccc|c} \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{array}\right]$$



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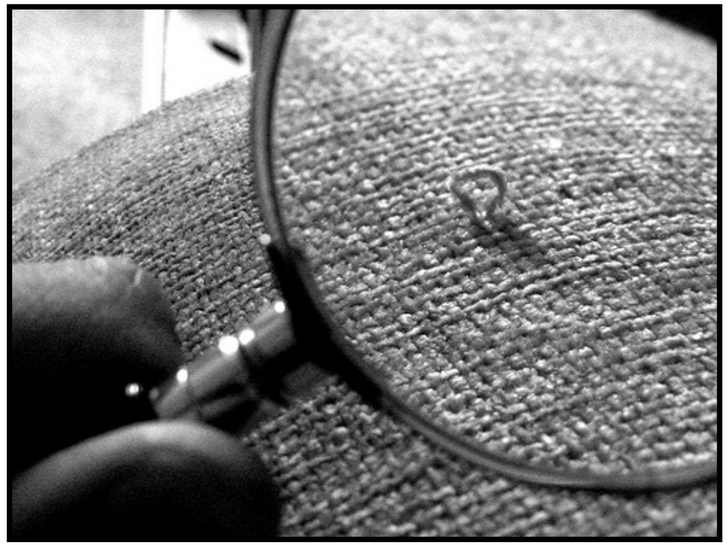

Cost of matrix operations

Triangular system solving *aka.* *"substitution"*.

LU permutation produces $\mathbf{PLU} = \mathbf{A}$

Usage: solve $\mathbf{P}\mathbf{x}_1 = \mathbf{b}$ (permute), solve $\mathbf{L}\mathbf{x}_2 = \mathbf{x}_1$ (forward subst.), solve $\mathbf{U}\mathbf{x}_3 = \mathbf{x}_2$ (backward subst.)

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```
lup = la.lu_factor(A)
x = la.lu_solve(lup, b)
```

Cost of matrix operations

$$\mathbf{b} \in \mathbb{R}^{10000}$$

$$\mathbf{A} \in \mathbb{R}^{10000 \times 10000}$$

100 million matrix entries!

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2'755 *ms* (measured on an M1 Mac)

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recommended

30 *ms*

```
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x1 = P.T @ b
x2 = la.solve_triangular(L, x1, lower=True)
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recommended: 2'755 *ms* (measured on an M1 Mac) + 30 *ms*

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manual: 102 *ms* ~3.4x slower

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# As above, but using the following function instead
def solve_triangular(M, y, lower):
    x = np.zeros(n)
    todo = range(n) if lower else reversed(range(n))
    for i in todo:
        x[i] = (y[i] - M[i, :] @ x) / M[i, i]
    return x
```

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not invented here syndrome! — 150 *ms* — 5x slower

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    return x
```

Factorization $\mathcal{O}(n^3)$

recommended	275 *ms*	(measured on an M1 Mac)
	30 *ms*	
manual	102 *ms*	3.4x slower
not invented here syndrome!	150 *ms*	5x slower

Substitution $\mathcal{O}(n^2)$

Examples of linear systems

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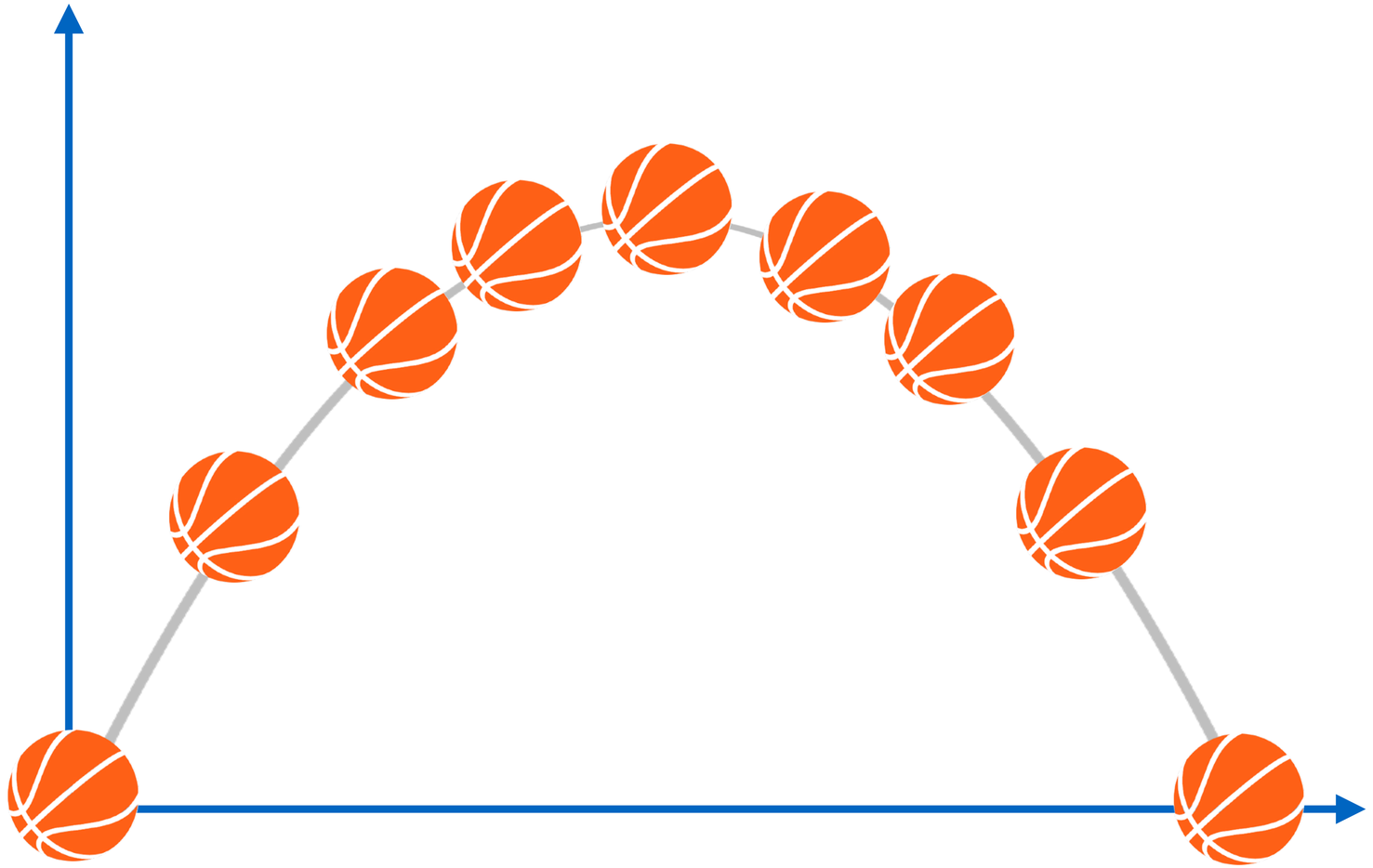
Examples of linear systems

How can we model this?

This kind of motion is well-understood! **(Ideal ballistic motion)**



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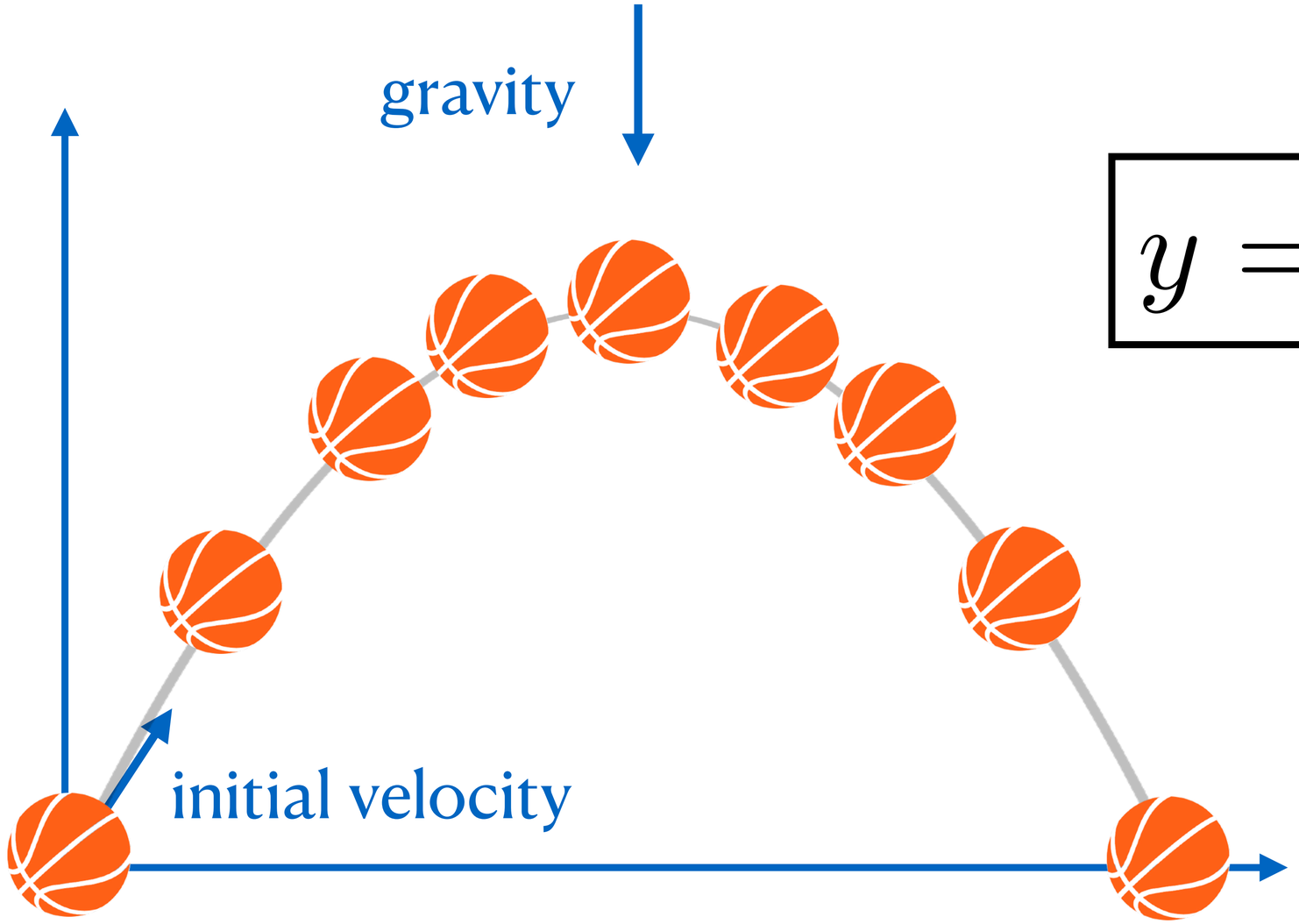
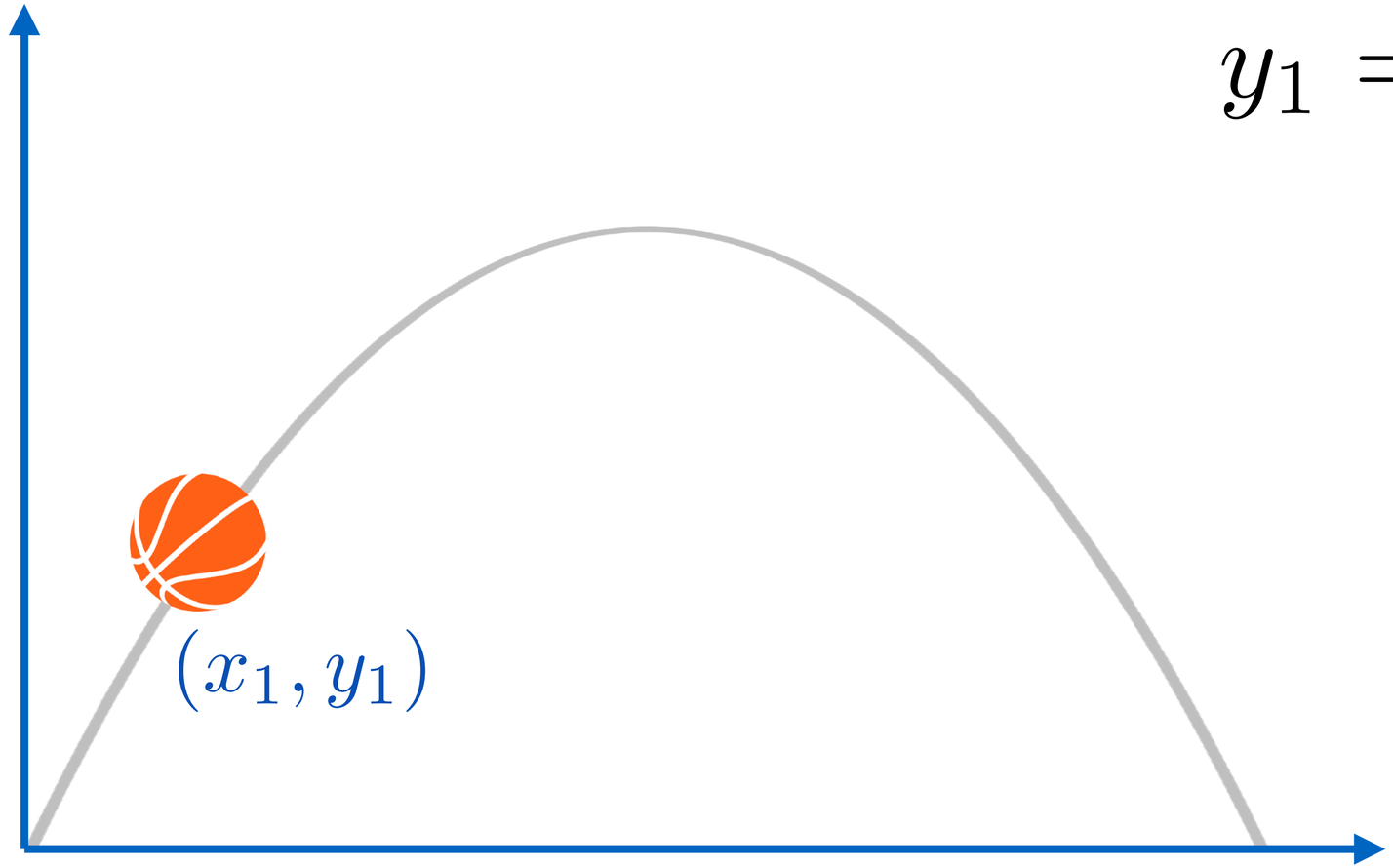


$$y = ax^2 + bx + c$$

Ideal Ballistic Motion

Step 1: Think about observables and unknowns



$$y_1 = ax_1^2 + bx_1 + c$$

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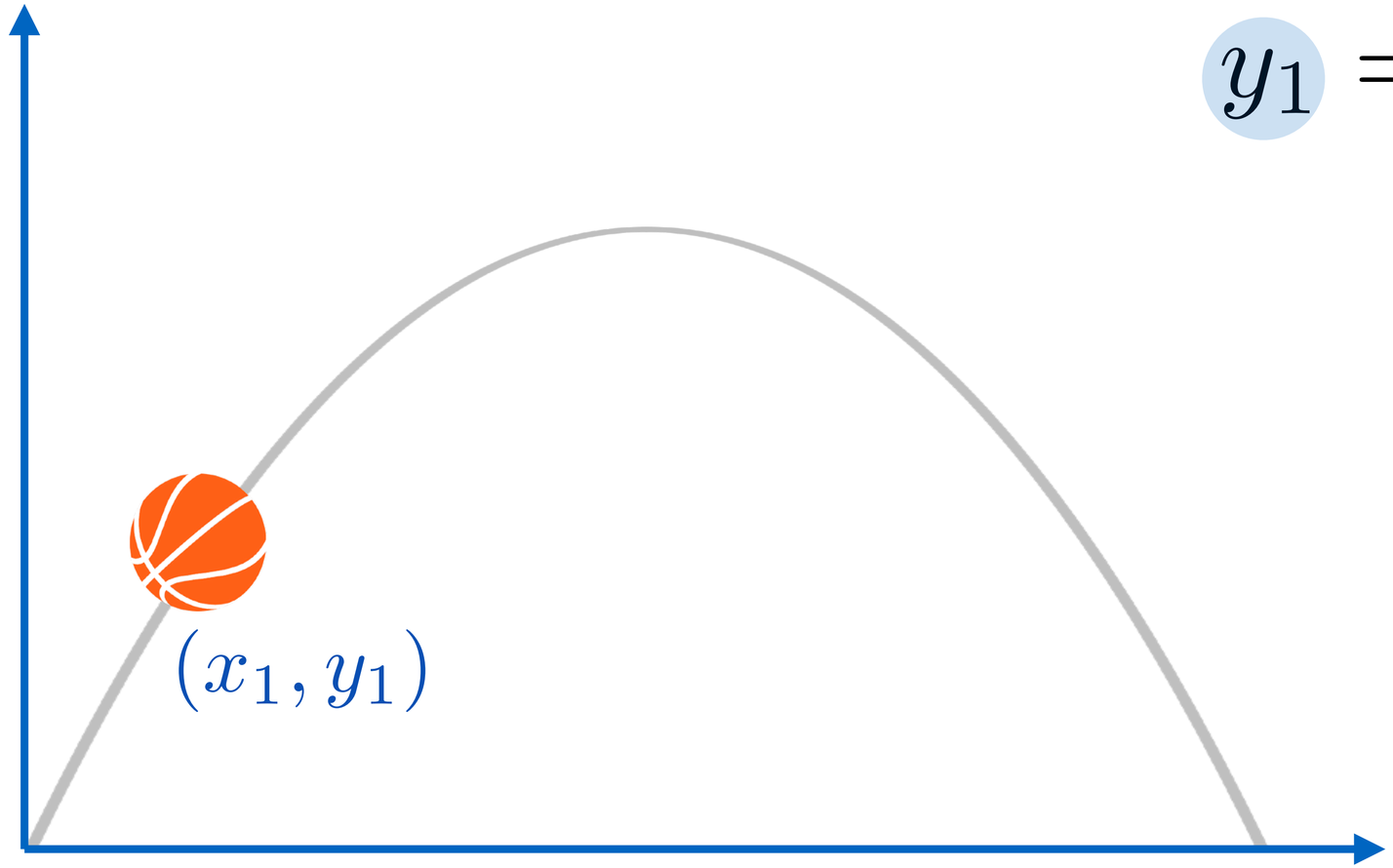

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known

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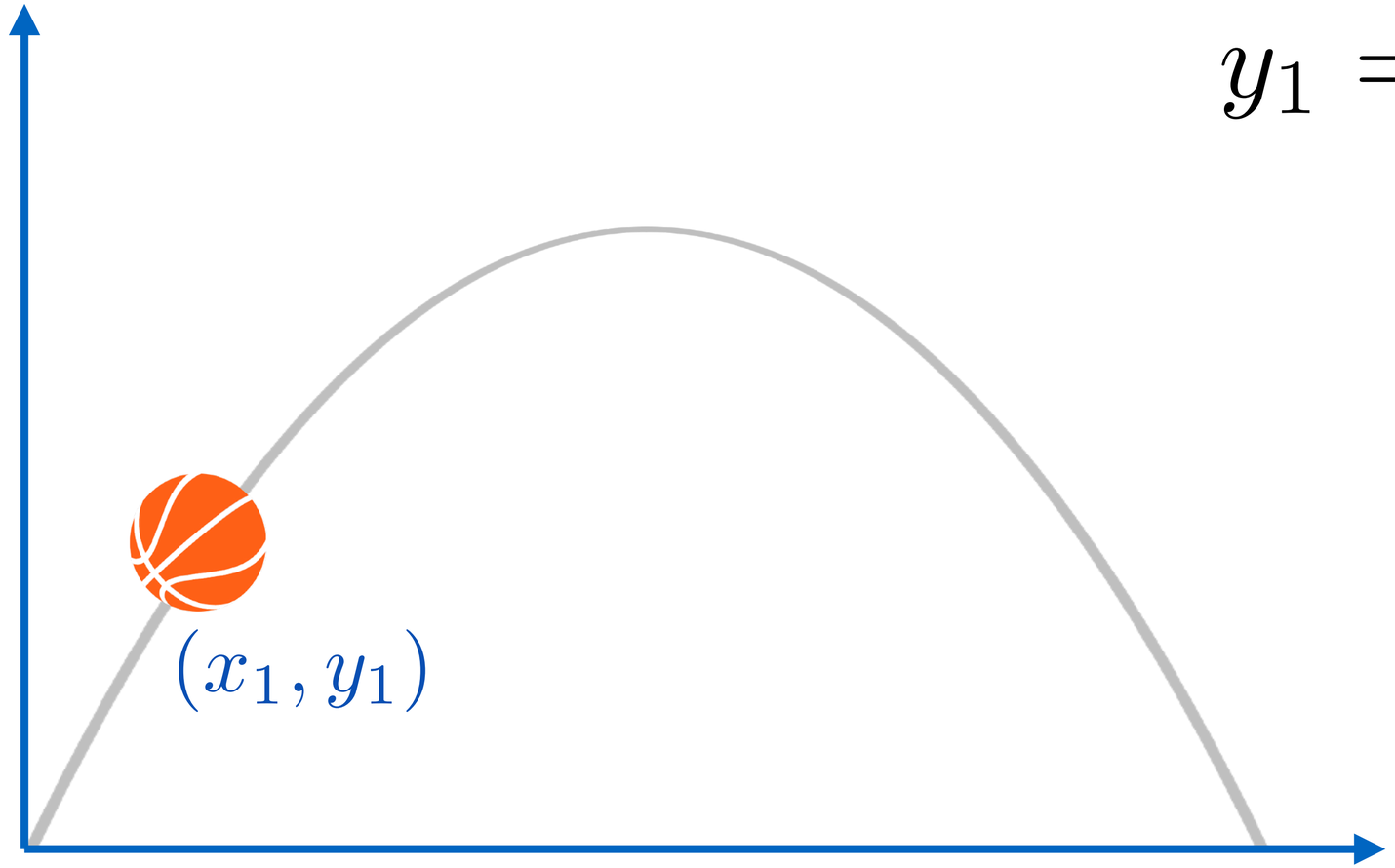

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unknown

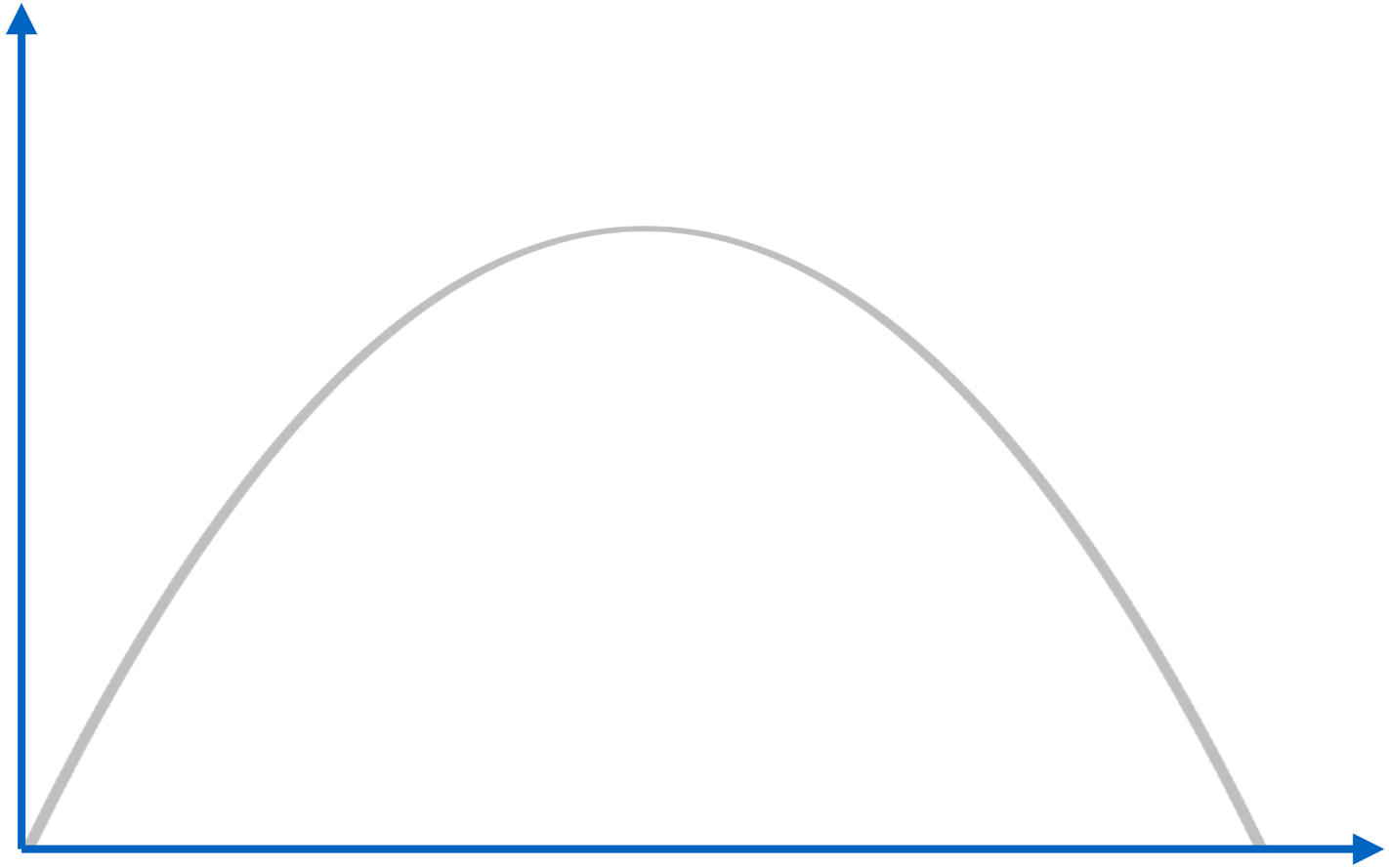
Regression

- We have a model of the **expected behaviour**.
- The model contains unknown parameter values.
- We have data / measurements that *may* be supported by the model.
- **Goal**: find parameters that best support the data.

- Can we express this as a solution to a linear system?
  - In that case, this is called **linear regression**.

Ideal Ballistic Motion

How many data points (i.e., *measurements*) do we need to solve this system?



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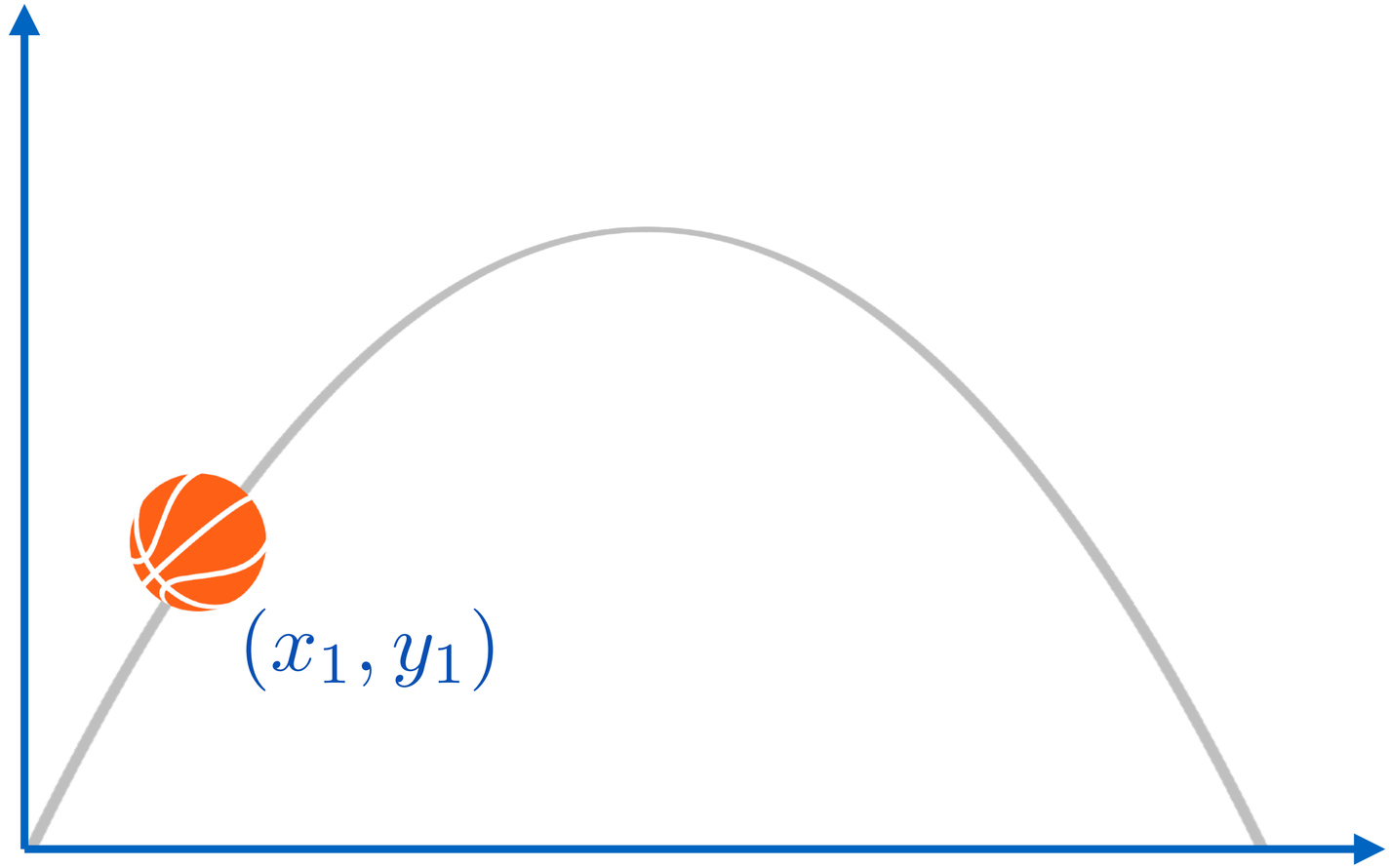

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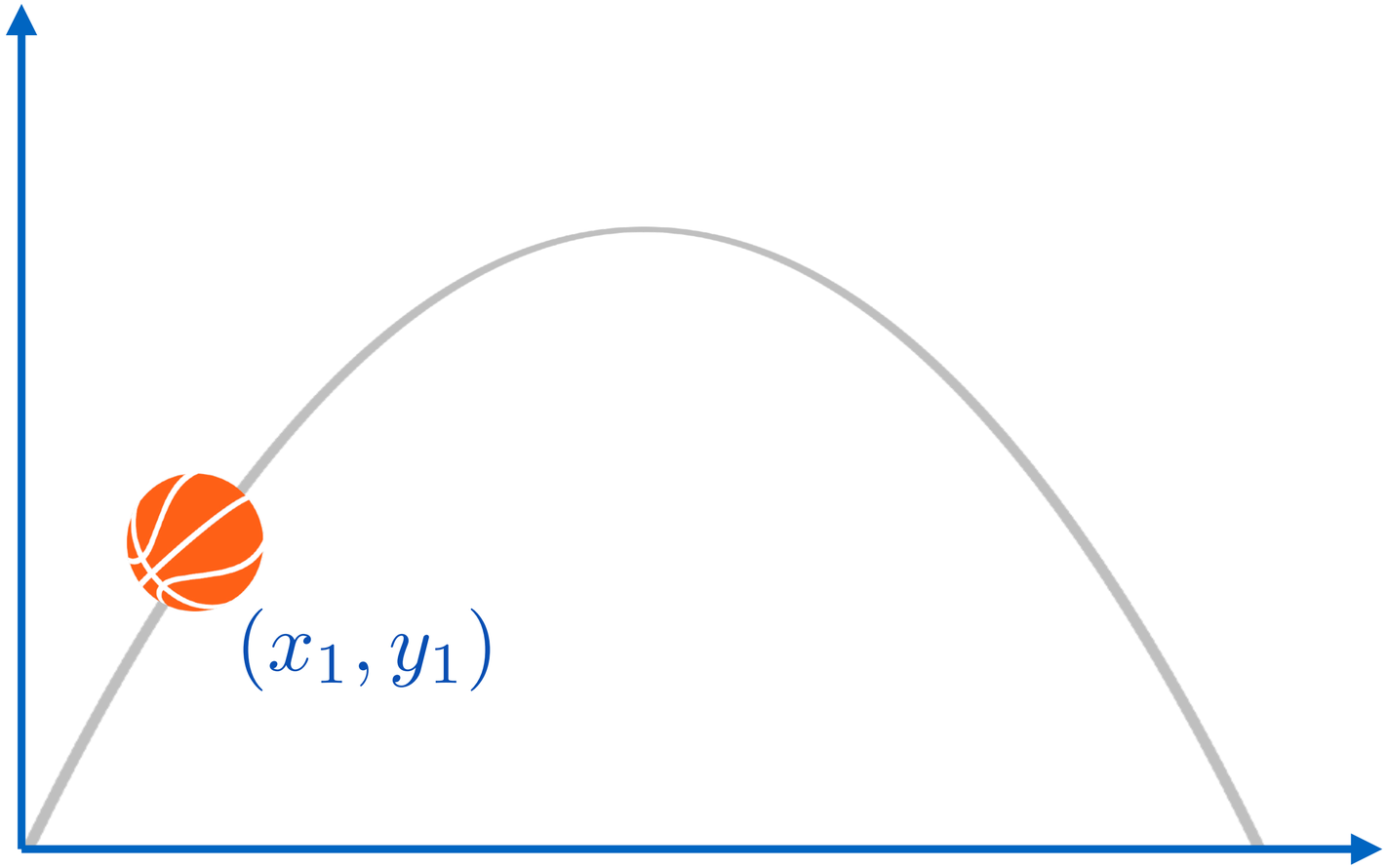

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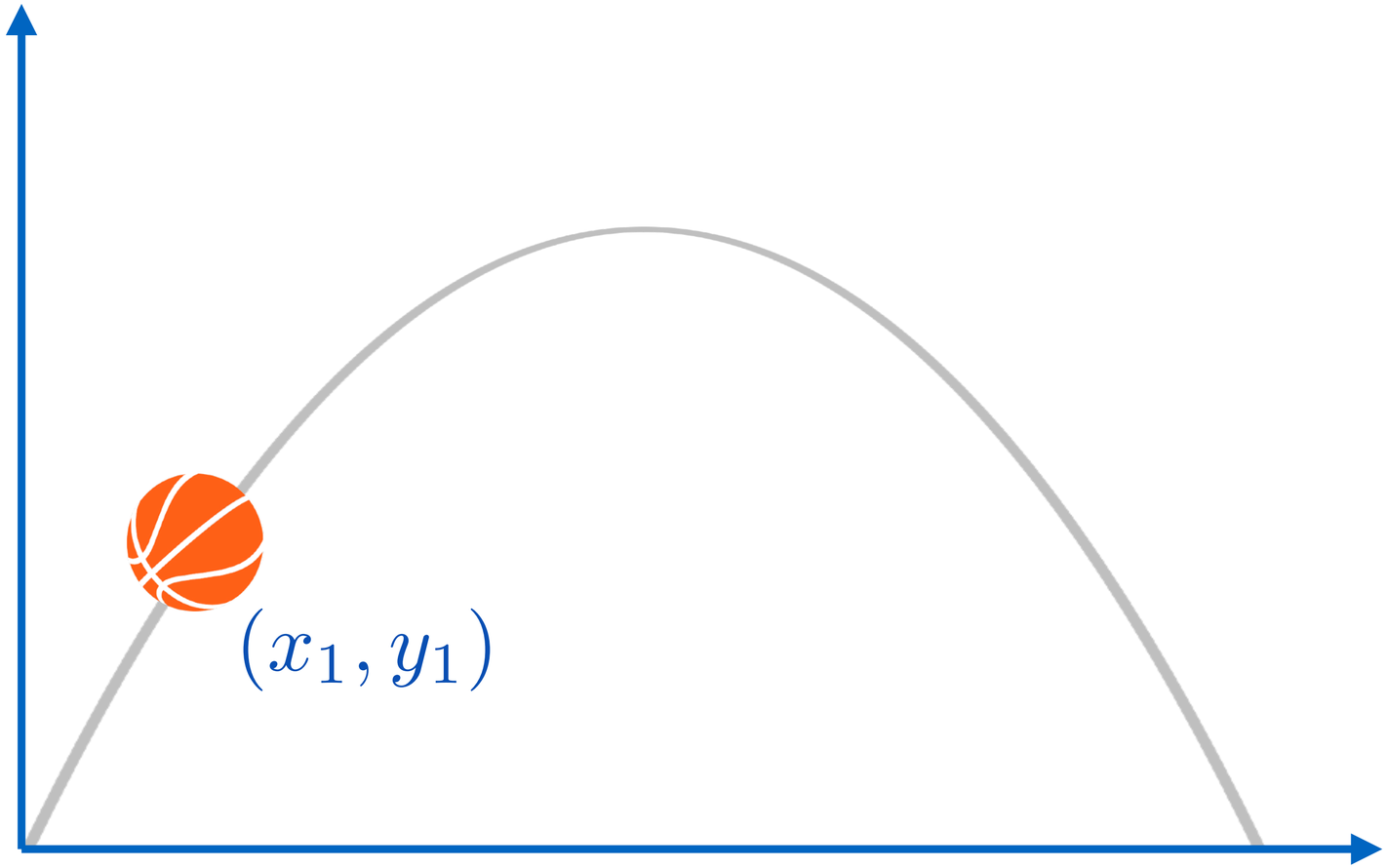

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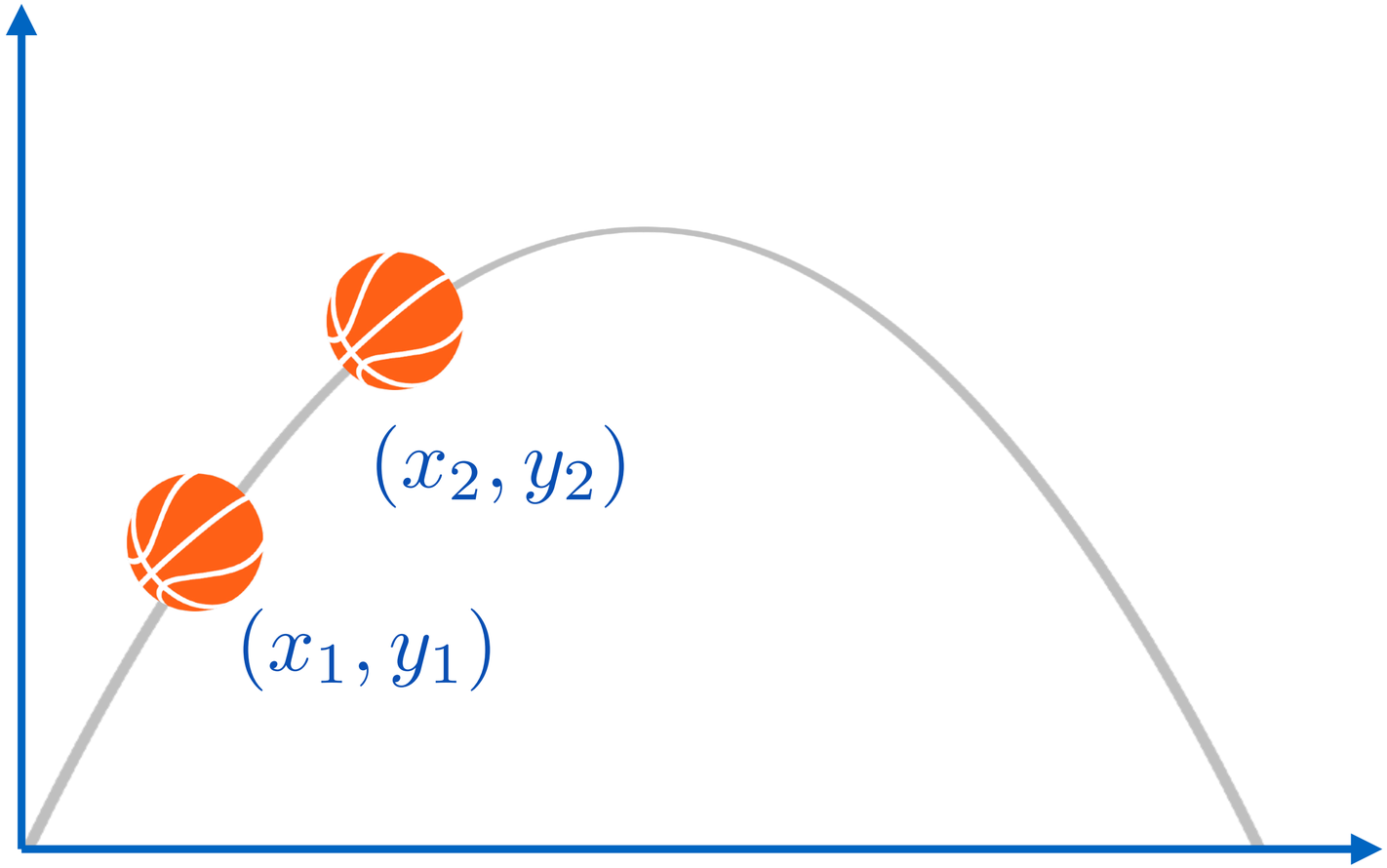

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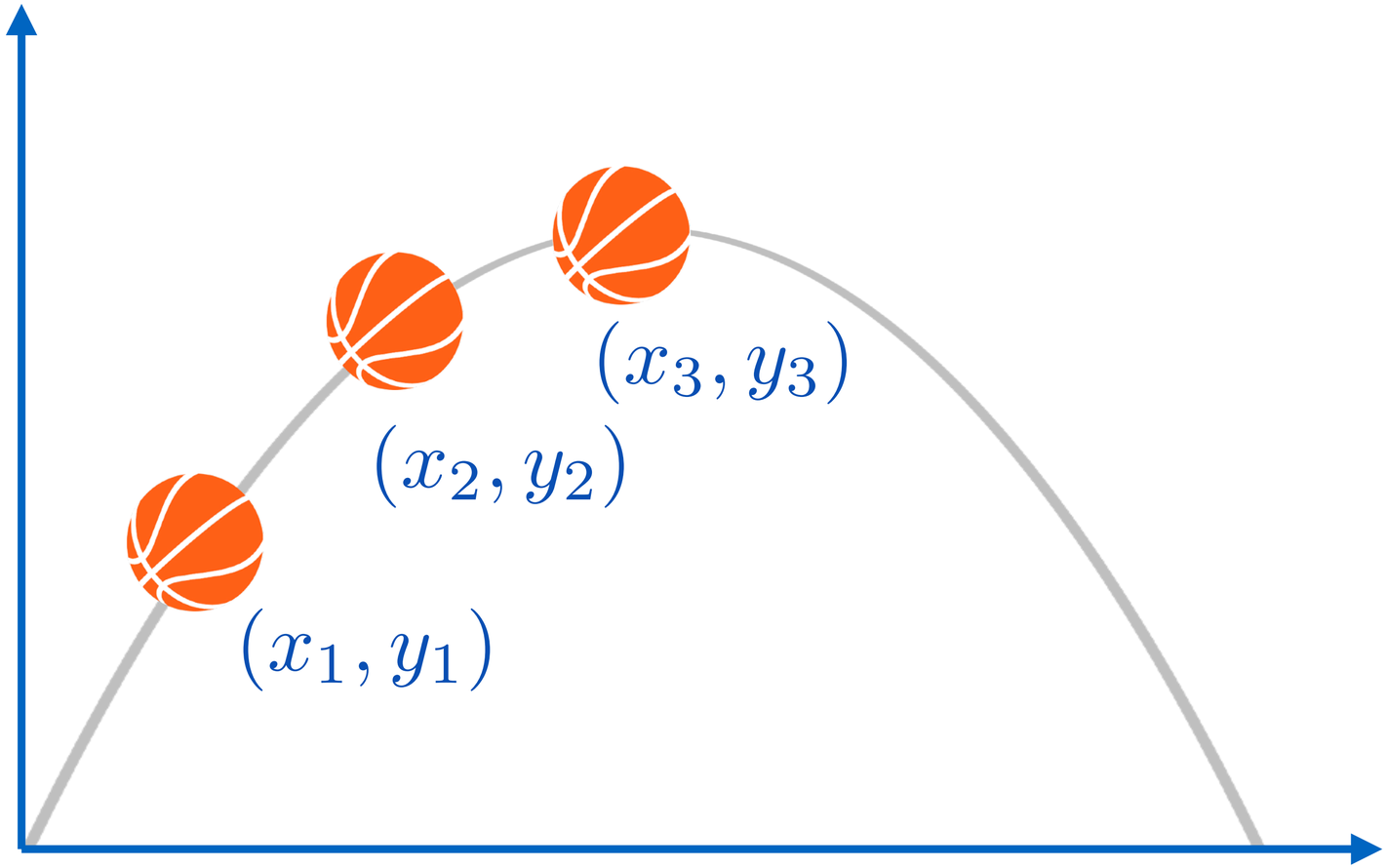

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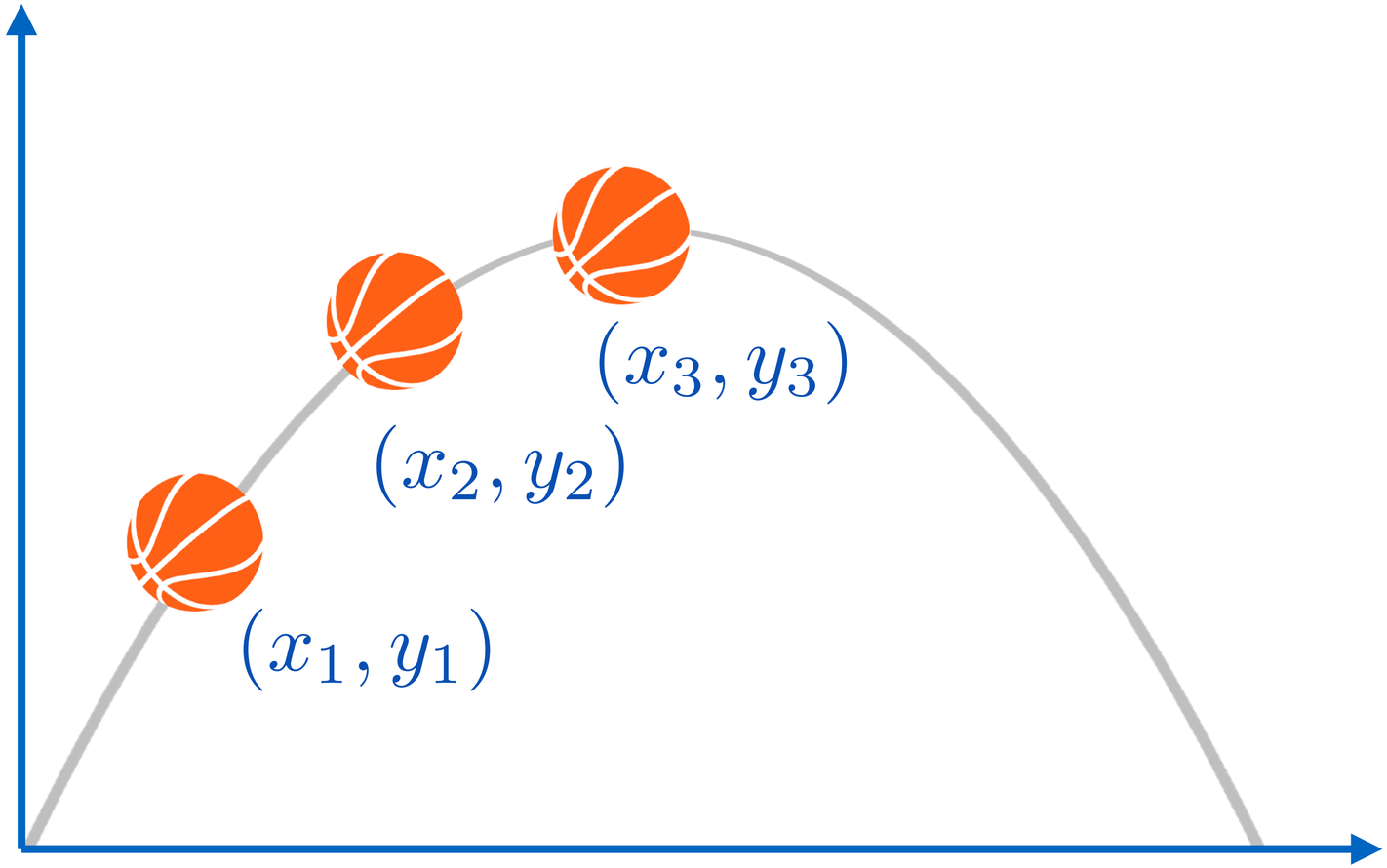

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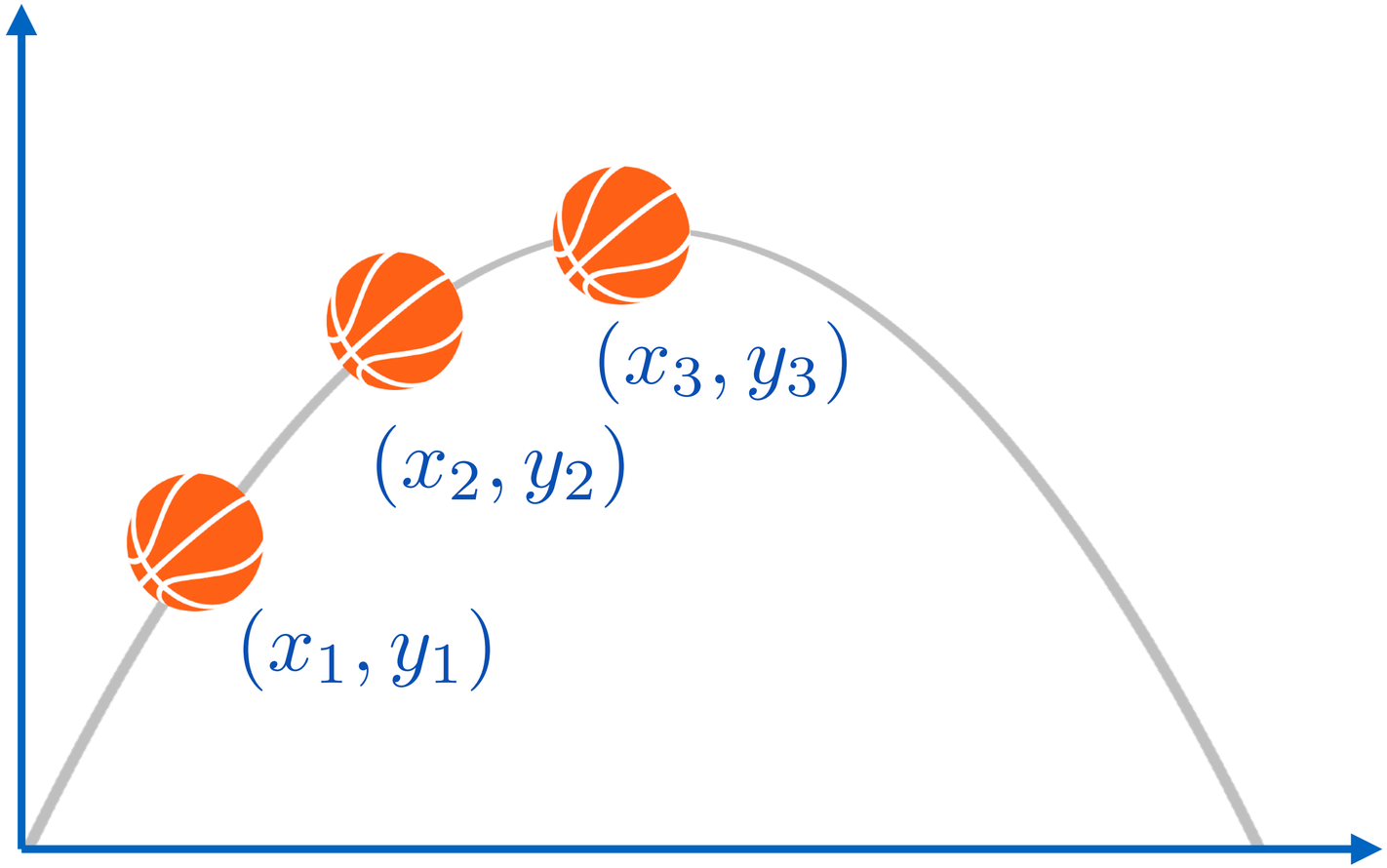

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$$\begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

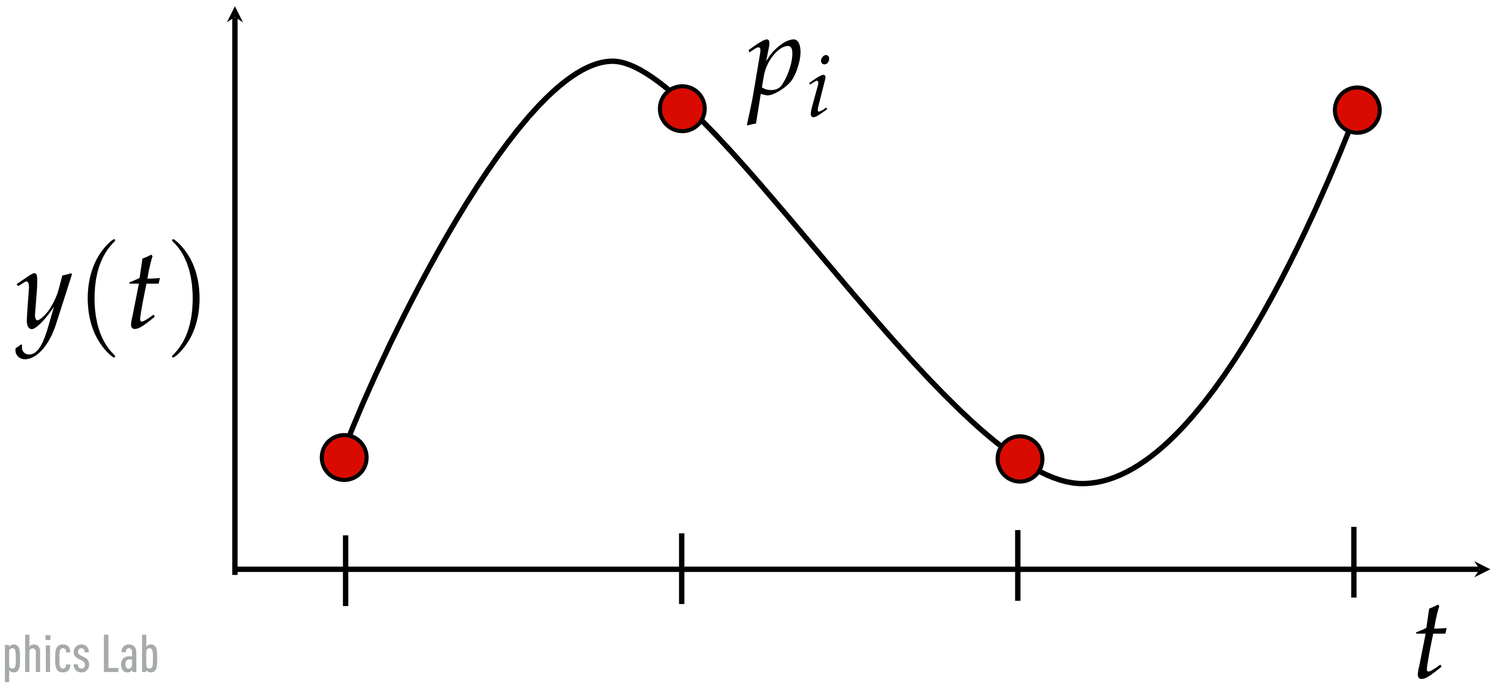
(identical, but using matrix-vector notation)

Polynomial regression

The basketball example is a representative of this larger class

Find a polynomial that *perfectly interpolates* a given set of points so that

$$y(t_i) = p_i$$



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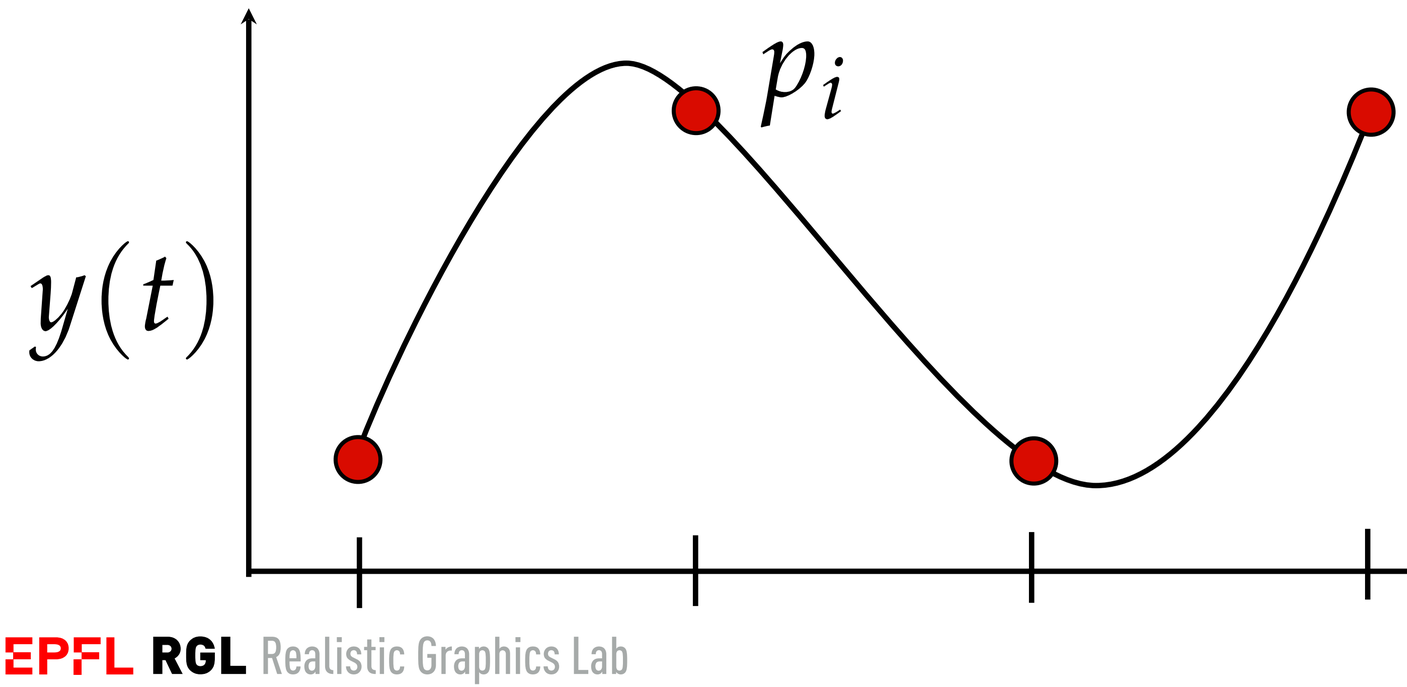
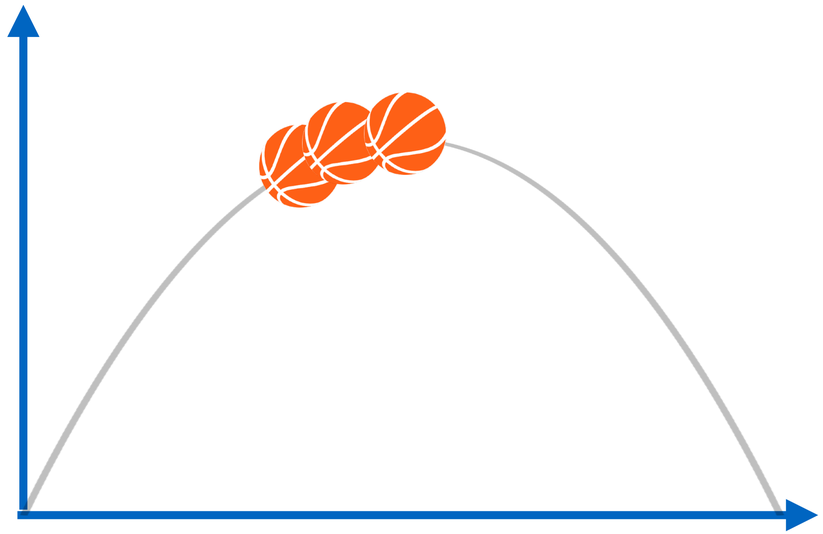


$$\begin{bmatrix} t_0^3 & t_0^2 & t_0 & 1 \\ t_1^3 & t_1^2 & t_1 & 1 \\ t_2^3 & t_2^2 & t_2 & 1 \\ t_3^3 & t_3^2 & t_3 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix}$$

"Vandermonde matrix"

Food for thought

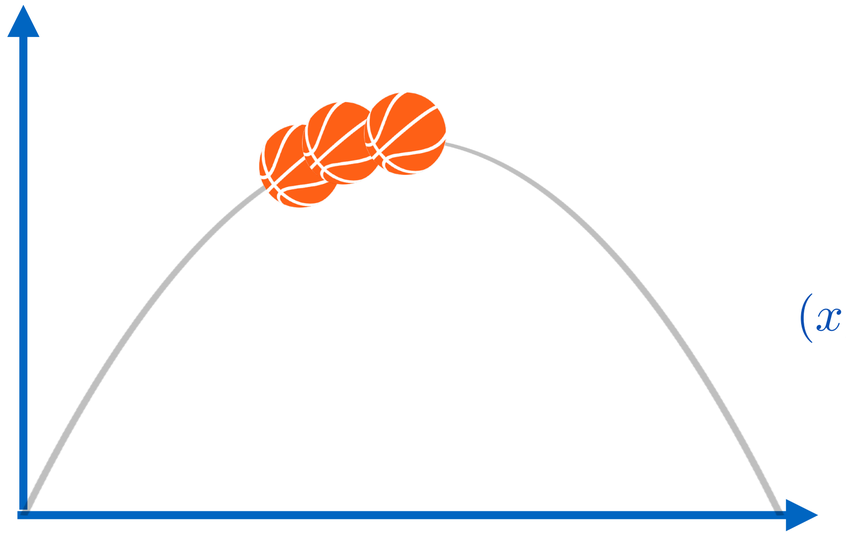
What could possibly go wrong?



What if the observations are *weak*?

Food for thought

What could possibly go wrong?



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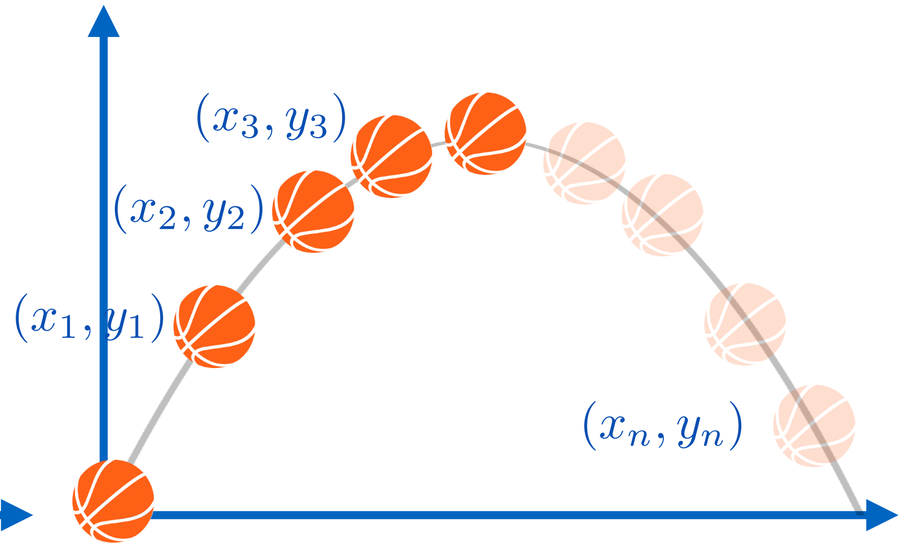

What if there are > 3 observations?

Use subset? Which ones? Use all somehow?

Food for thought

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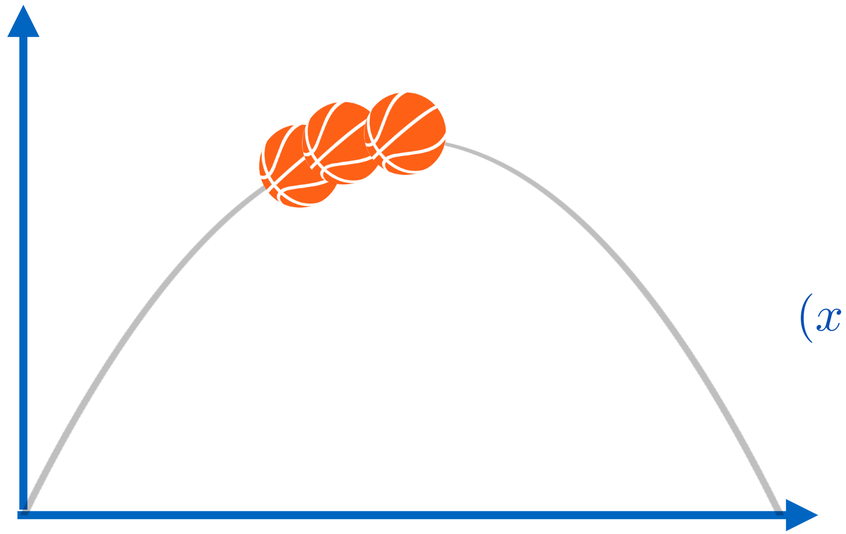

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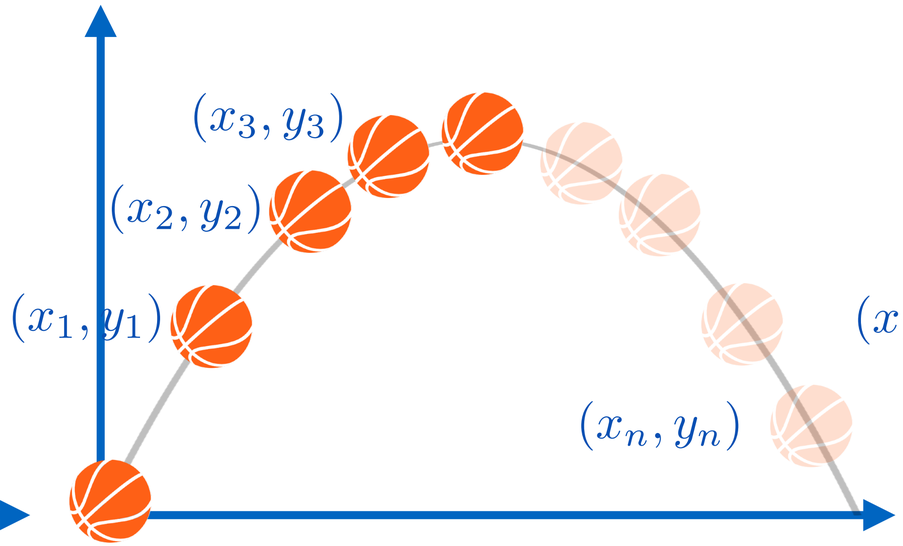

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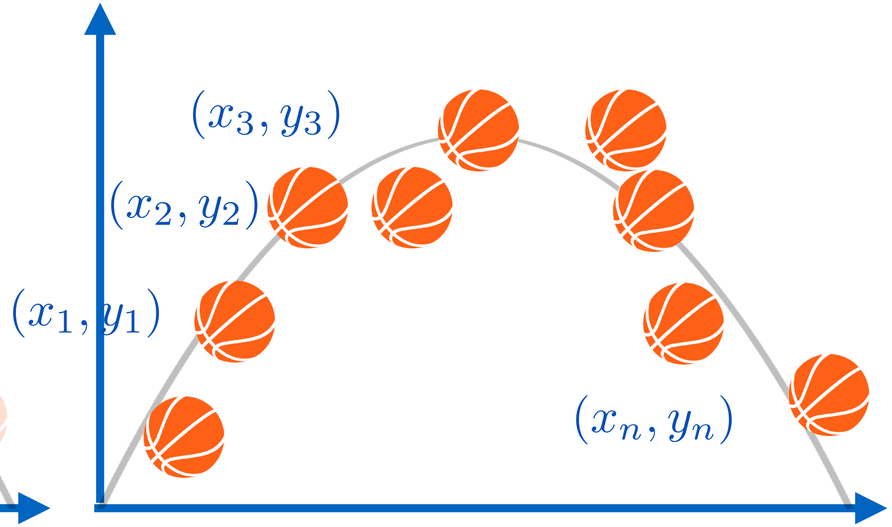


What if there is noise?

What if the model violates the assumptions?

Demo time

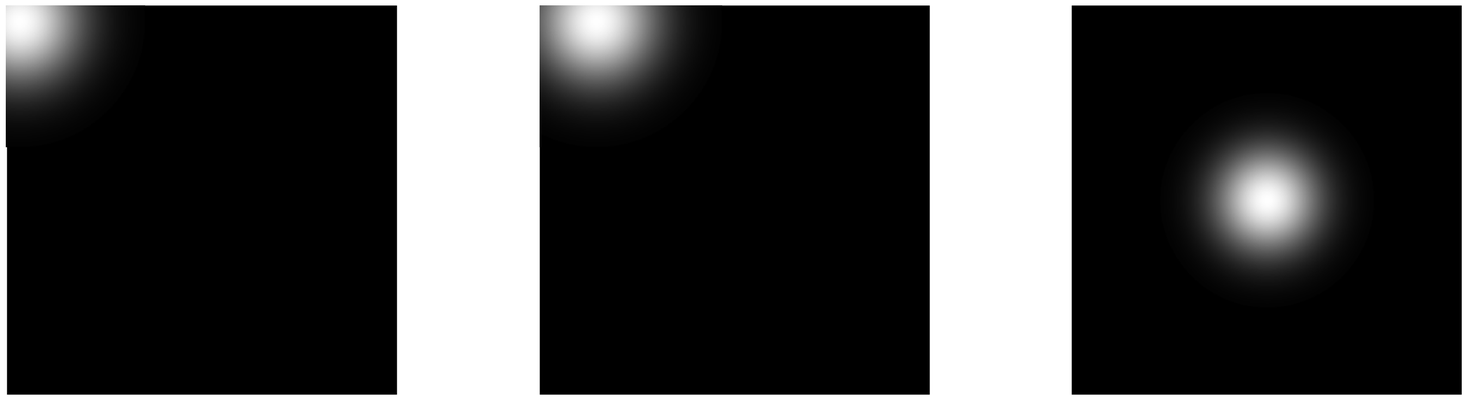

KABOOM!

Another classical example of a "bad" linear system

***Deconvolution*:** removing blur from a signal (e.g., an image)

Blurry

$$\mathbf{b} = \begin{pmatrix} | & | & \cdots & | \\ \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_n \\ | & | & \cdots & | \end{pmatrix} \mathbf{x}$$



Original

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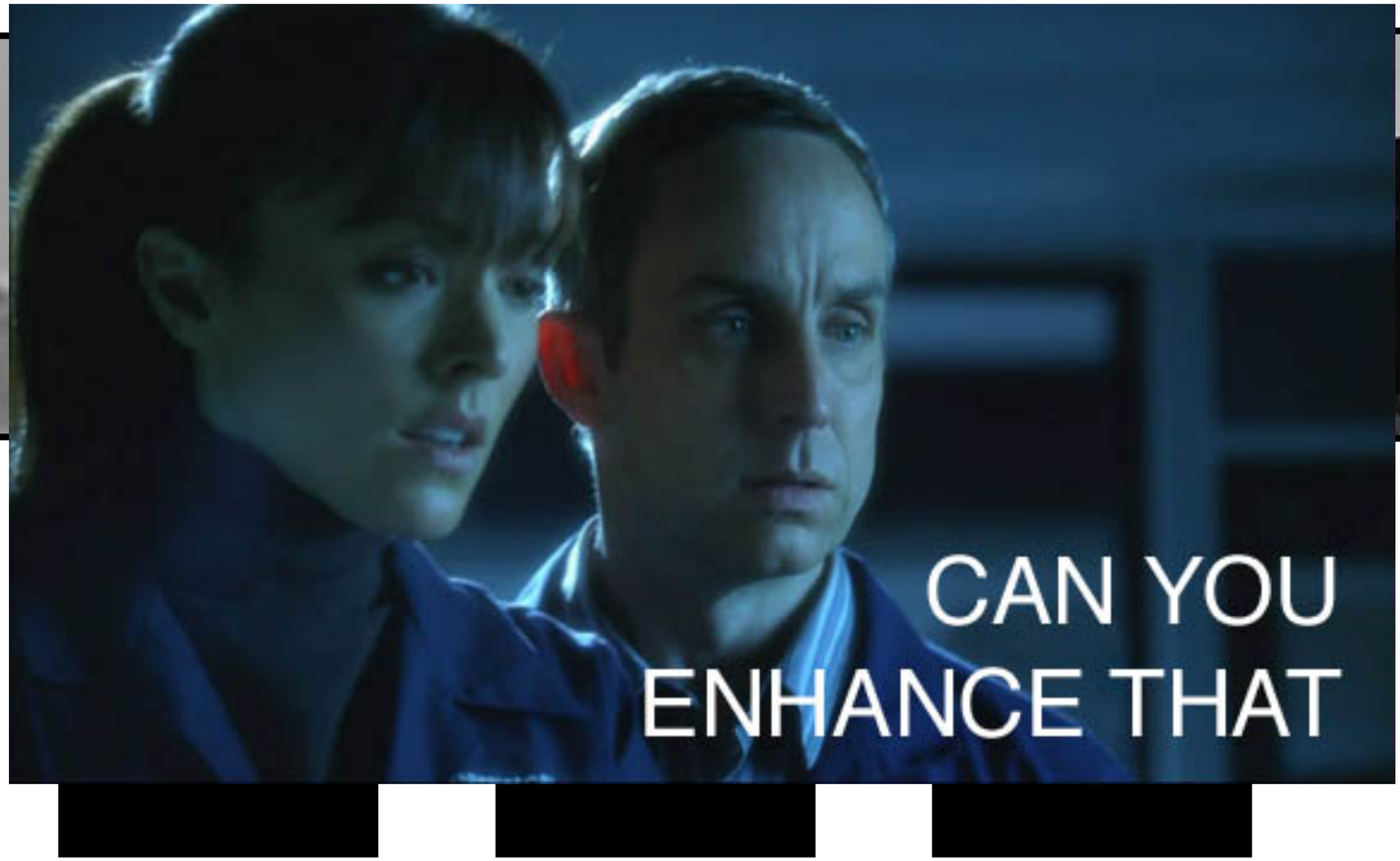

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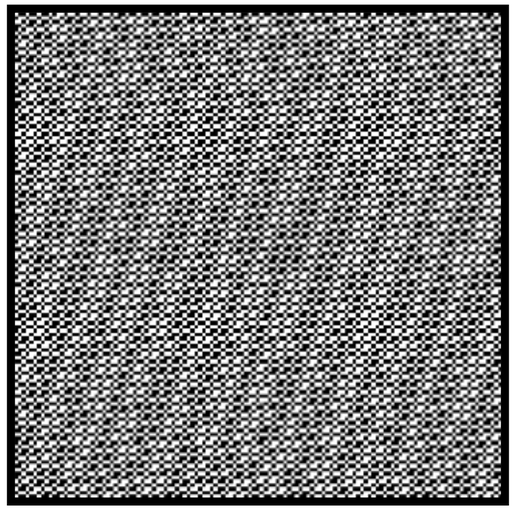
Recovered



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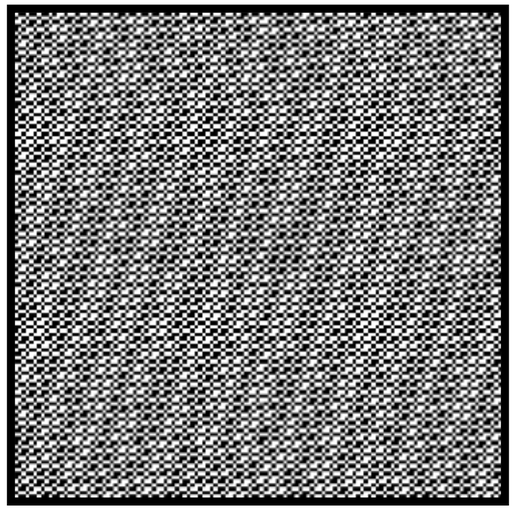


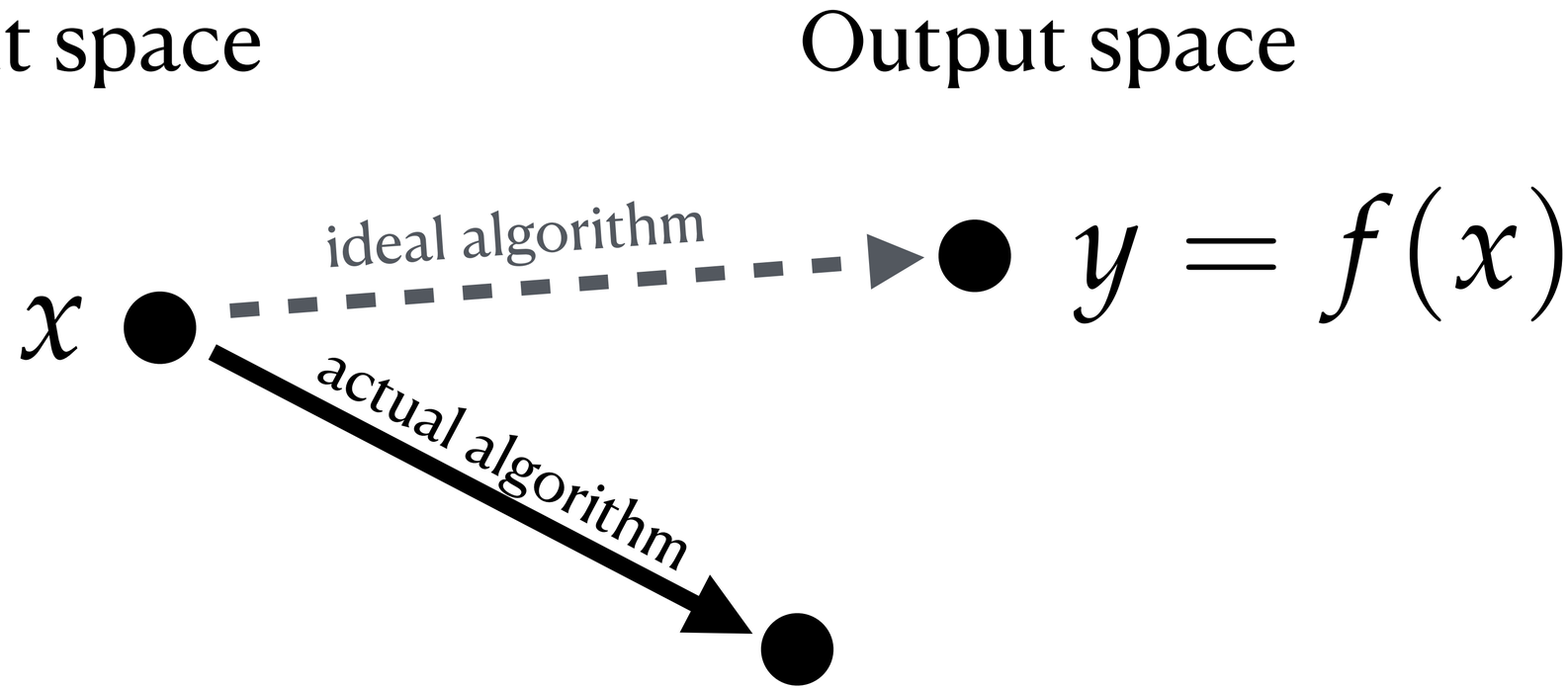
Regularized

Forward and Backward Error

Recap

Forward and Backward Error

Recap



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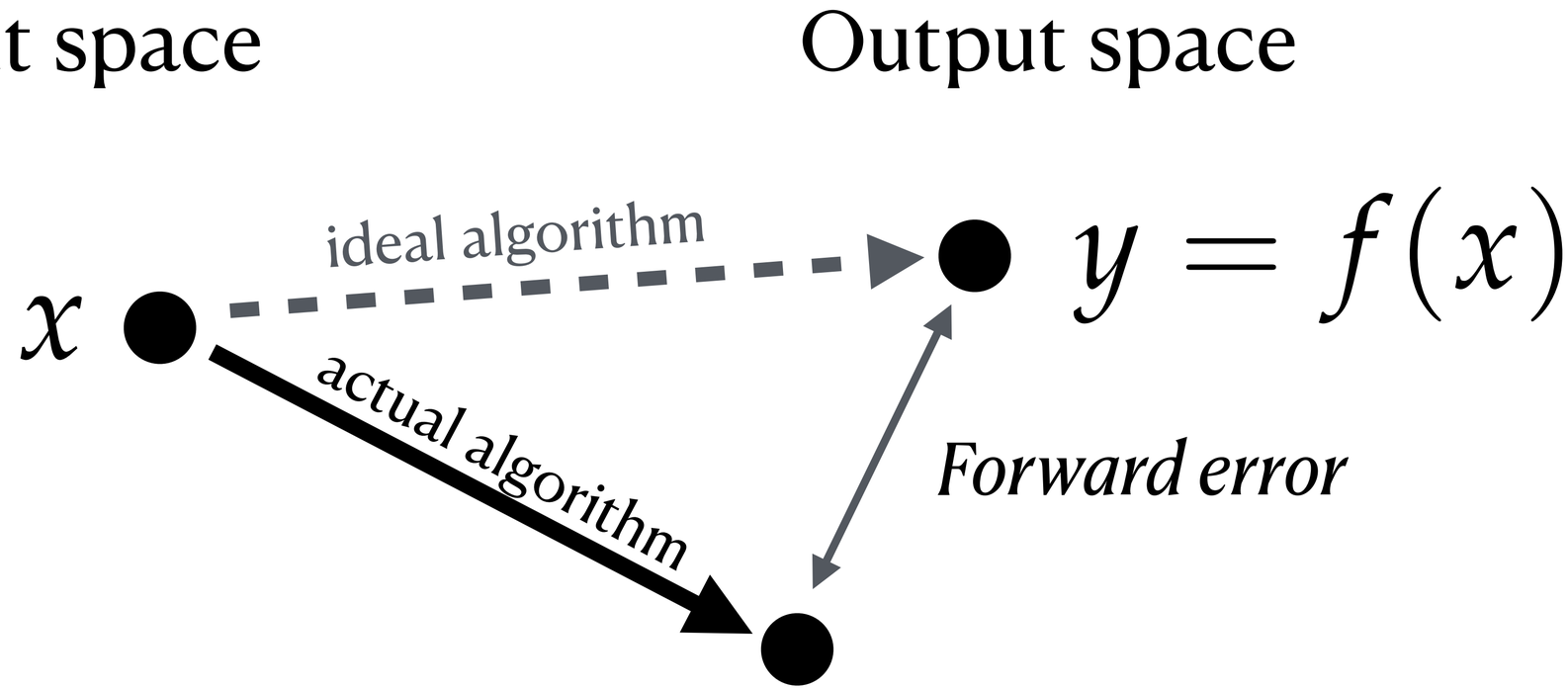

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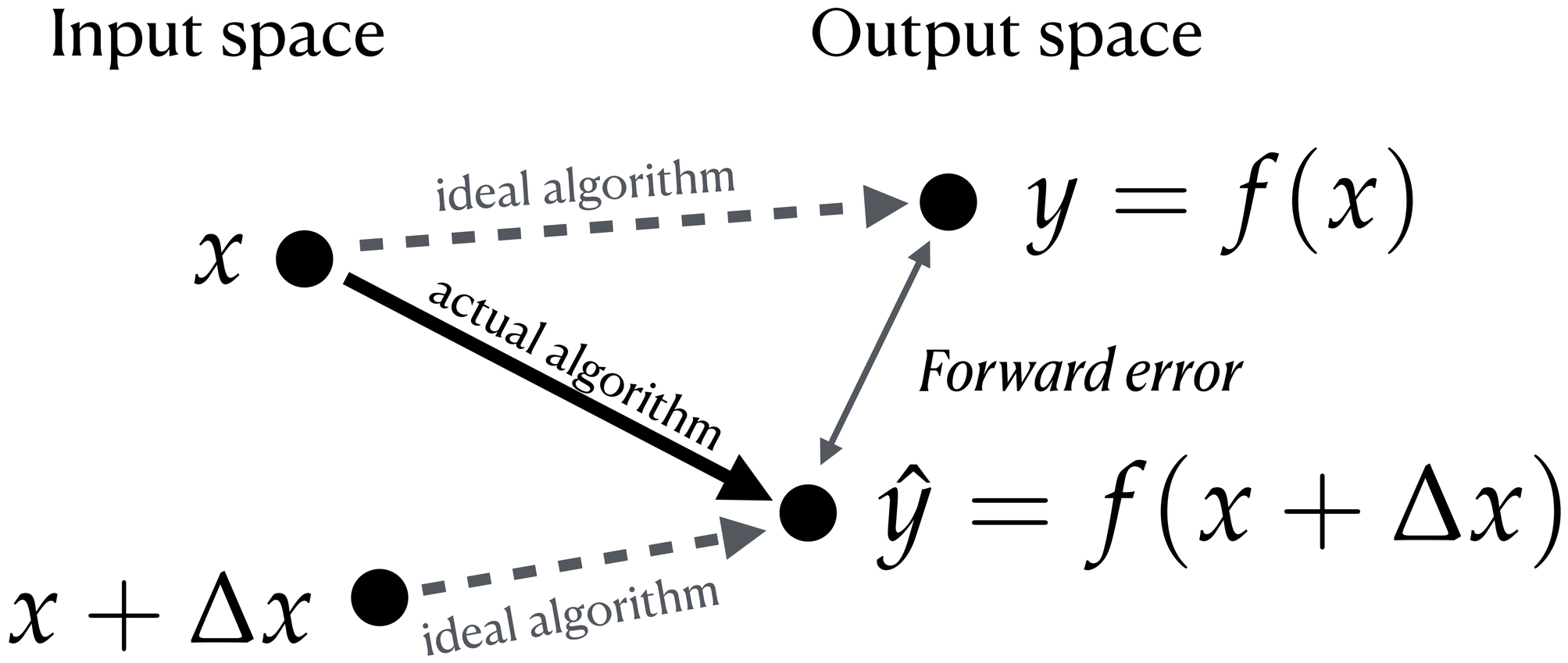

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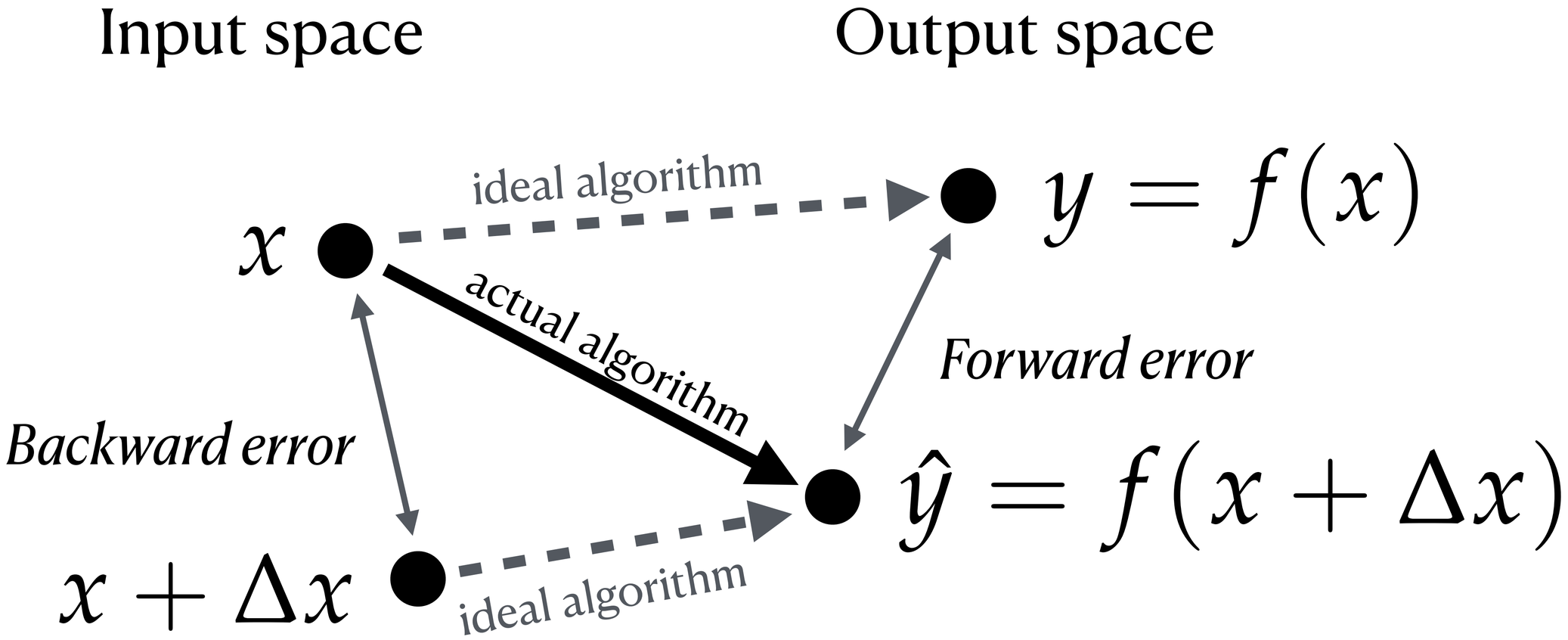
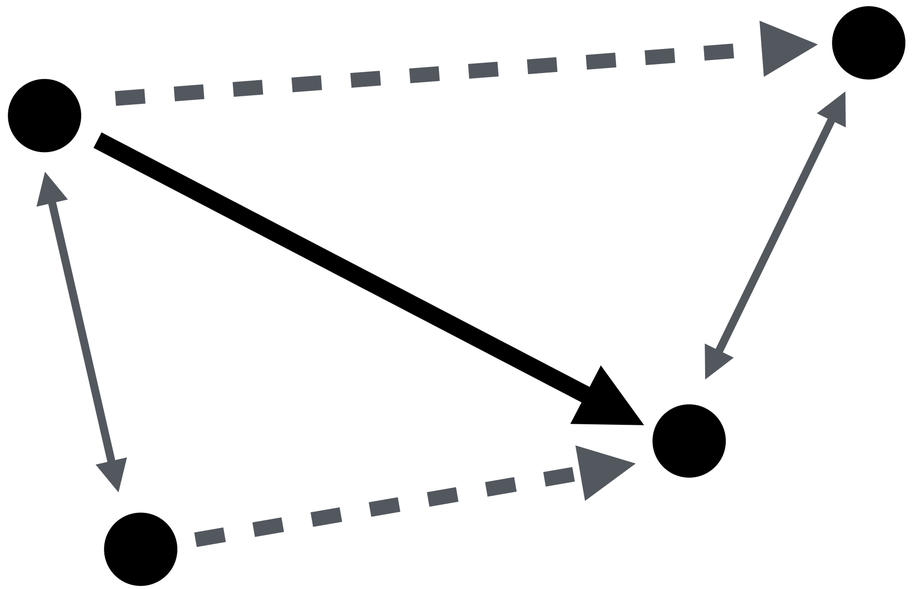


Conditioning of linear systems



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Condition number: ratio $\dfrac{\text{forward error}}{\text{backward error}}$

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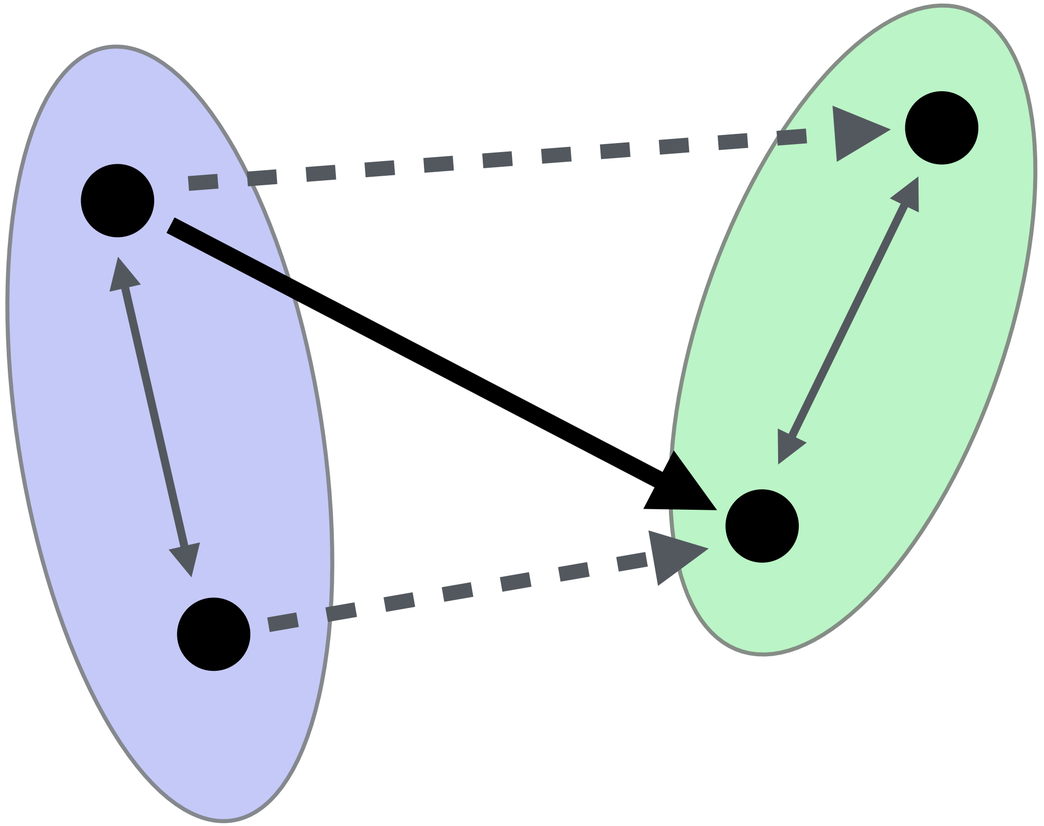

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.. applied to linear system solving

Theoretical infinite precision solver

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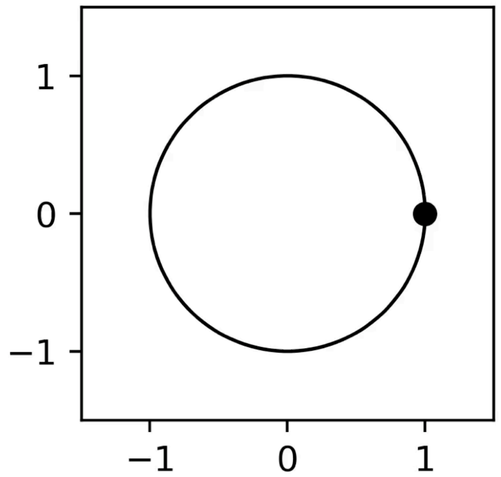
$$r(\hat{\mathbf{x}}) = \mathbf{A}\hat{\mathbf{x}} - \mathbf{b}$$

The *residual* gives an approximation of the backward error of a linear system solver.

Interlude: Matrix-vector multiplication, ellipses, and ellipsoids

Four randomly generated matrices — how do they transform points on a circle?



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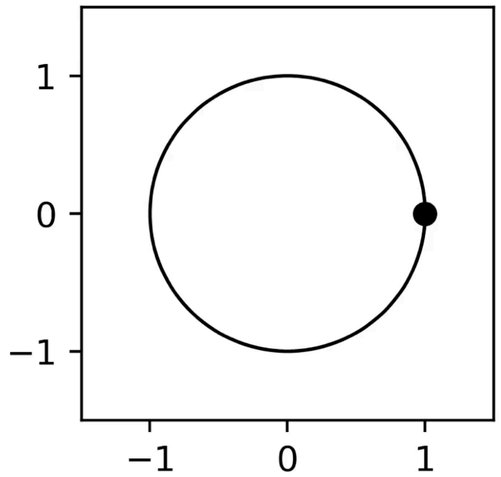

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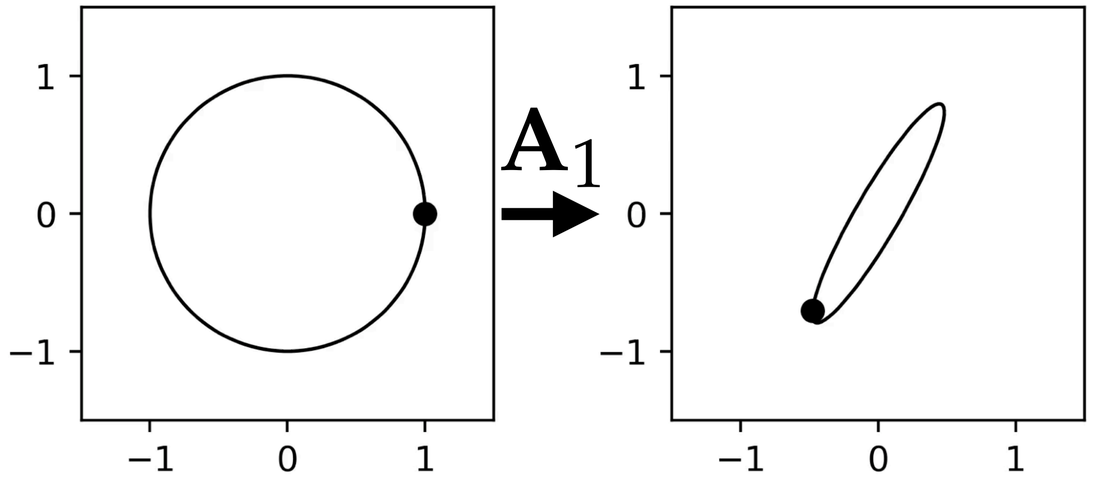

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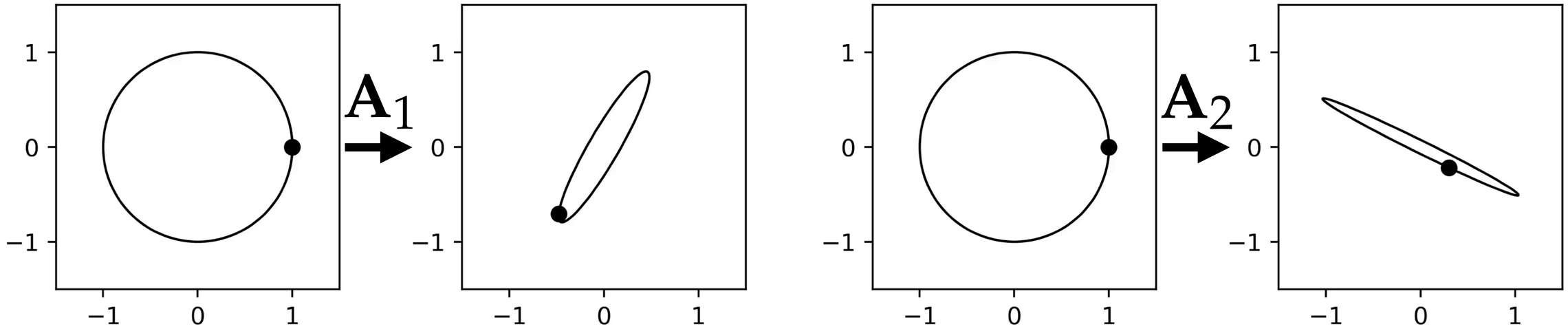

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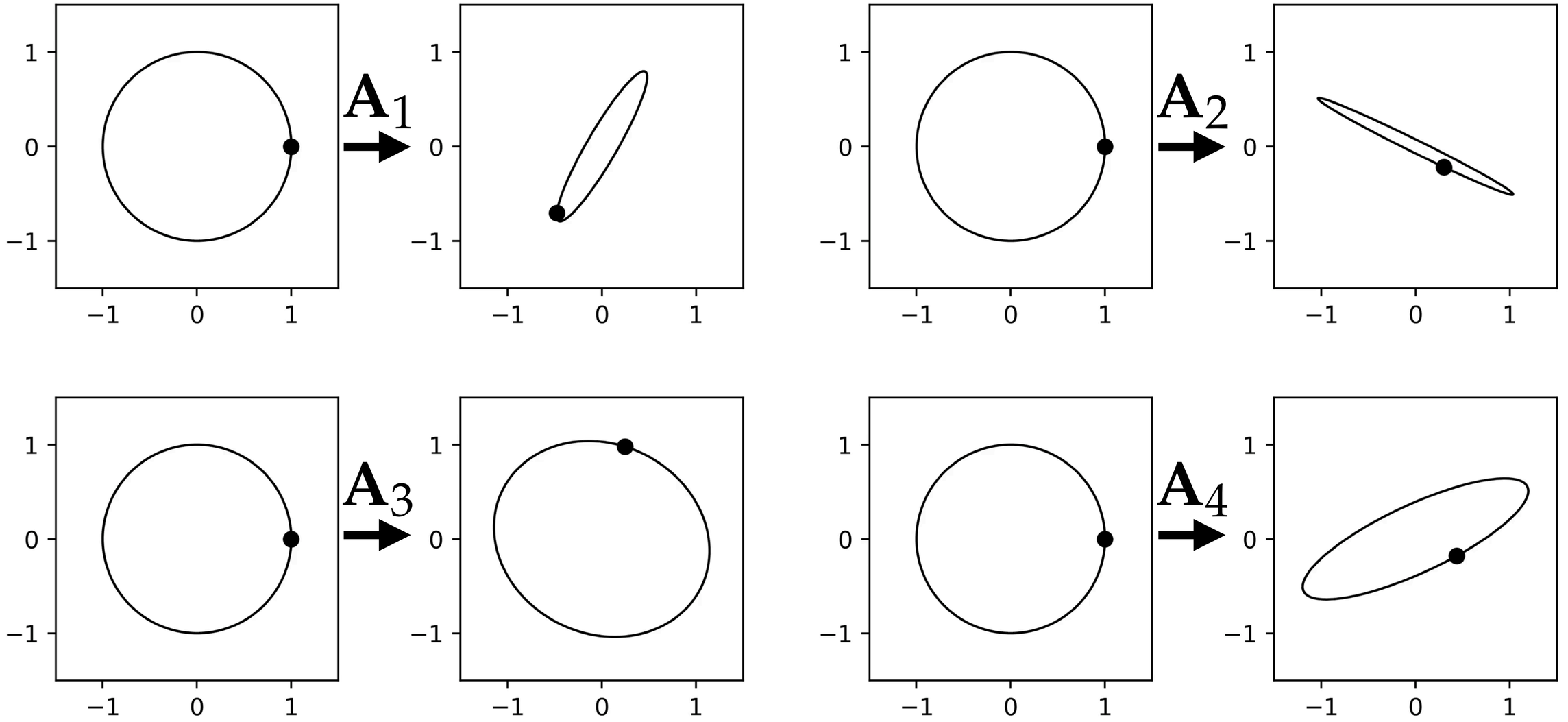
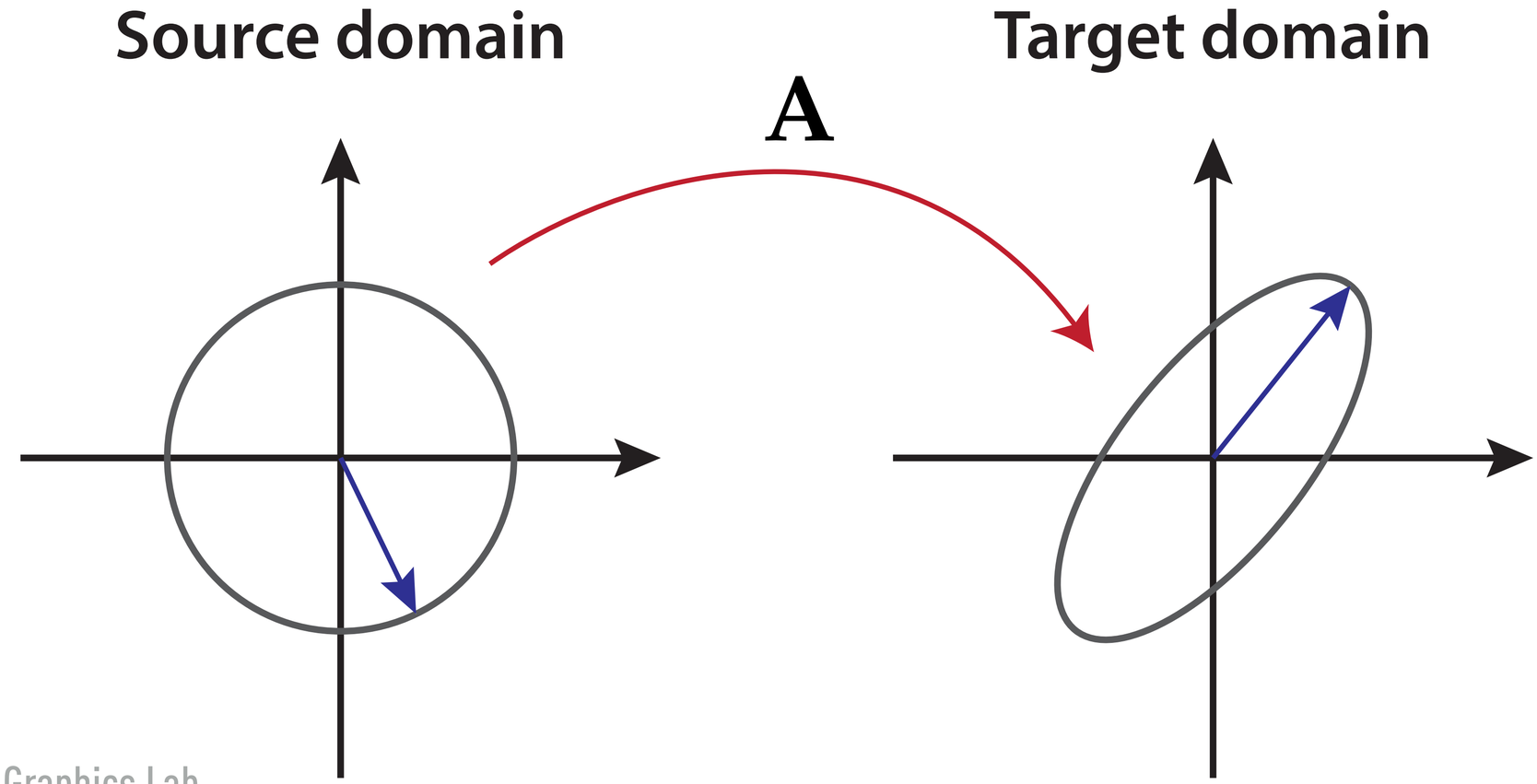


The matrix norm (aka. operator norm)

Determines the maximum radius of this ellipse

$$\|\mathbf{A}\| = \max\{\|\mathbf{Ax}\|, \text{where } \|\mathbf{x}\| = 1\}$$



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Putting it together: $$\frac{\|\Delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \|\mathbf{A}^{-1}\| \cdot \|\Delta\mathbf{b}\| \cdot \frac{\|\mathbf{A}\|}{\|\mathbf{b}\|}$$

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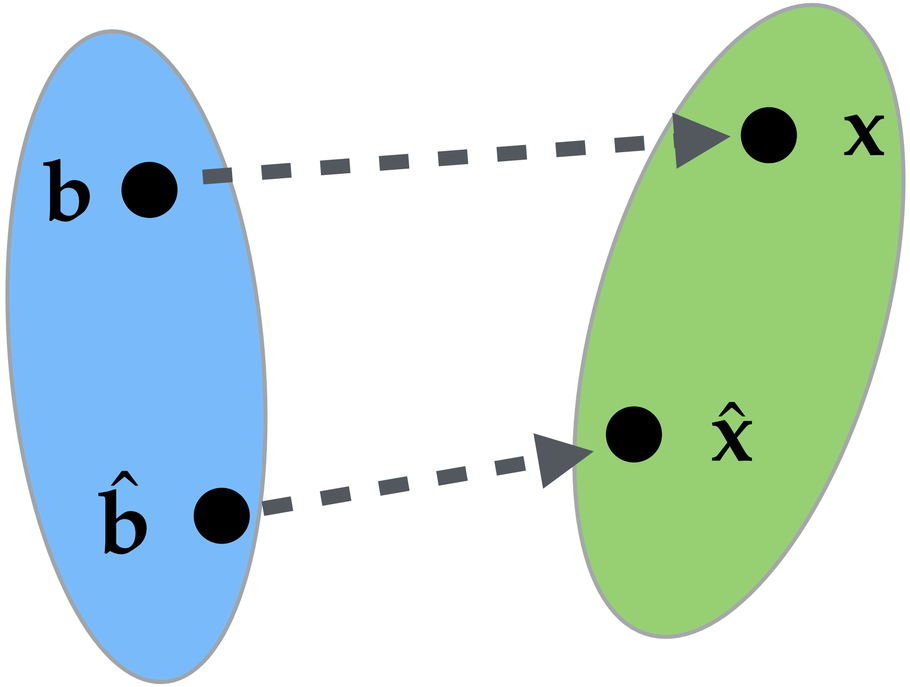

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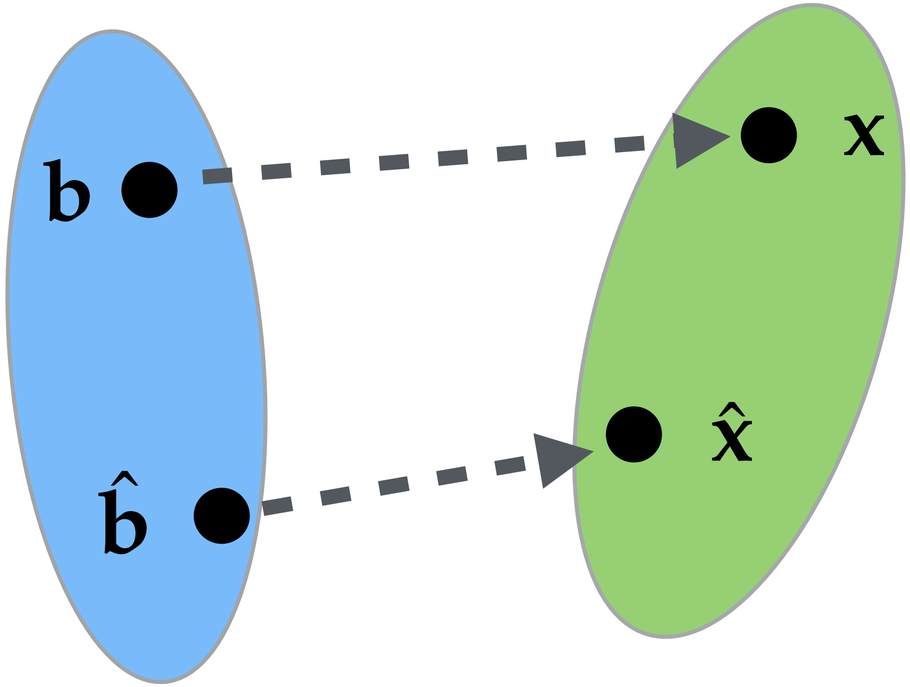

$$\frac{\|\Delta \mathbf{x}\|}{\|\mathbf{x}\|} \leq \underbrace{\|\mathbf{A}^{-1}\| \cdot \|\mathbf{A}\|}_{= \operatorname{cond}(A) = \kappa(A)} \cdot \frac{\|\Delta \mathbf{b}\|}{\|\mathbf{b}\|}$$

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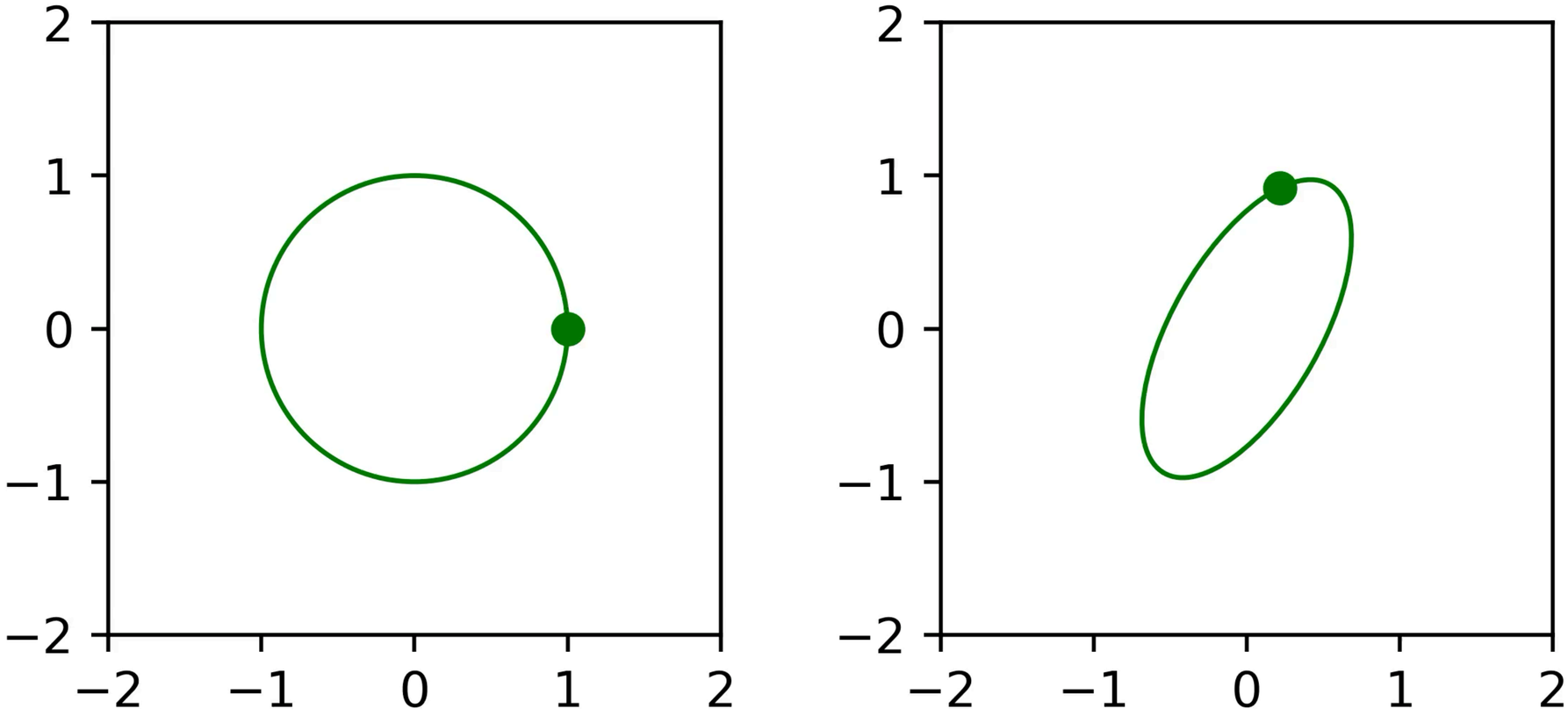

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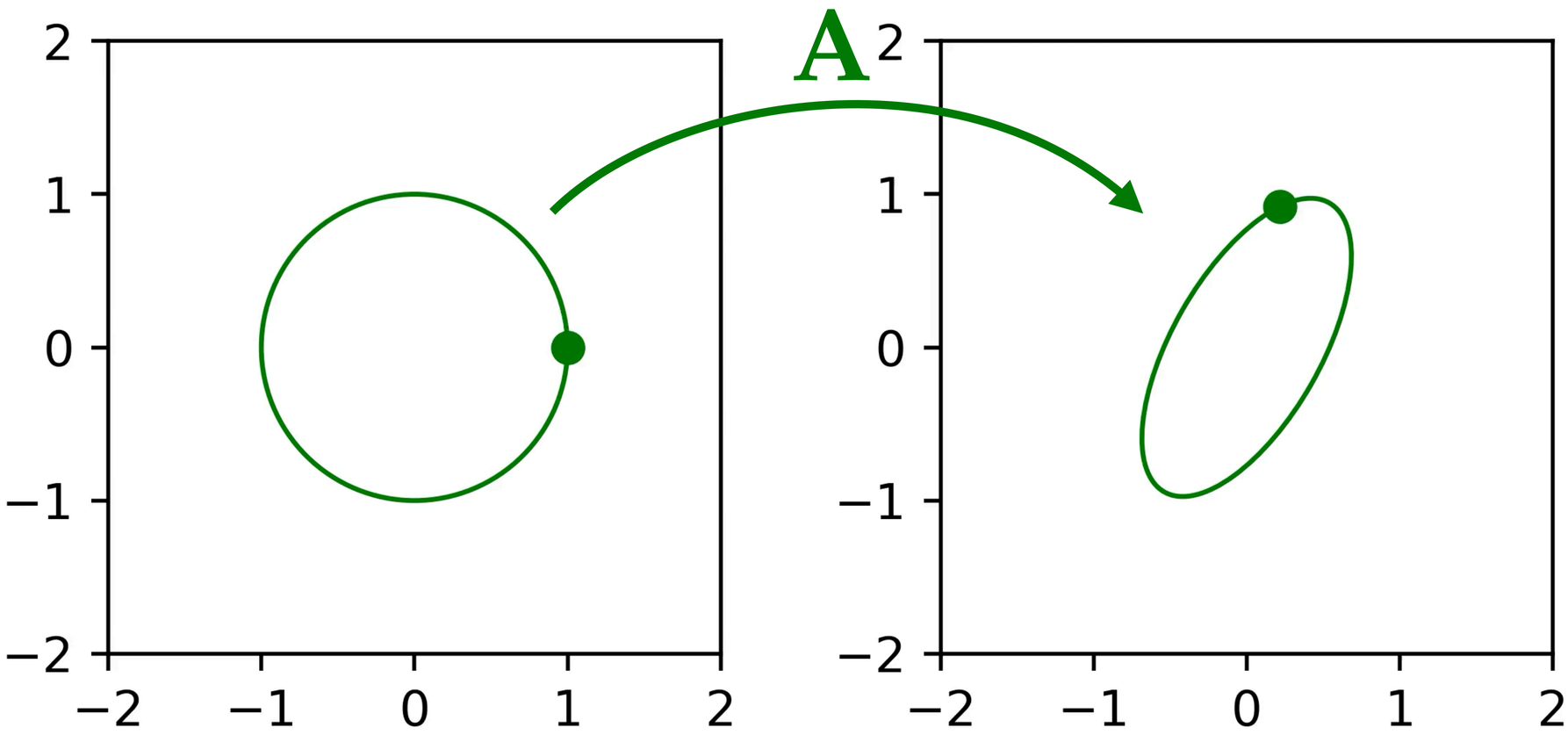

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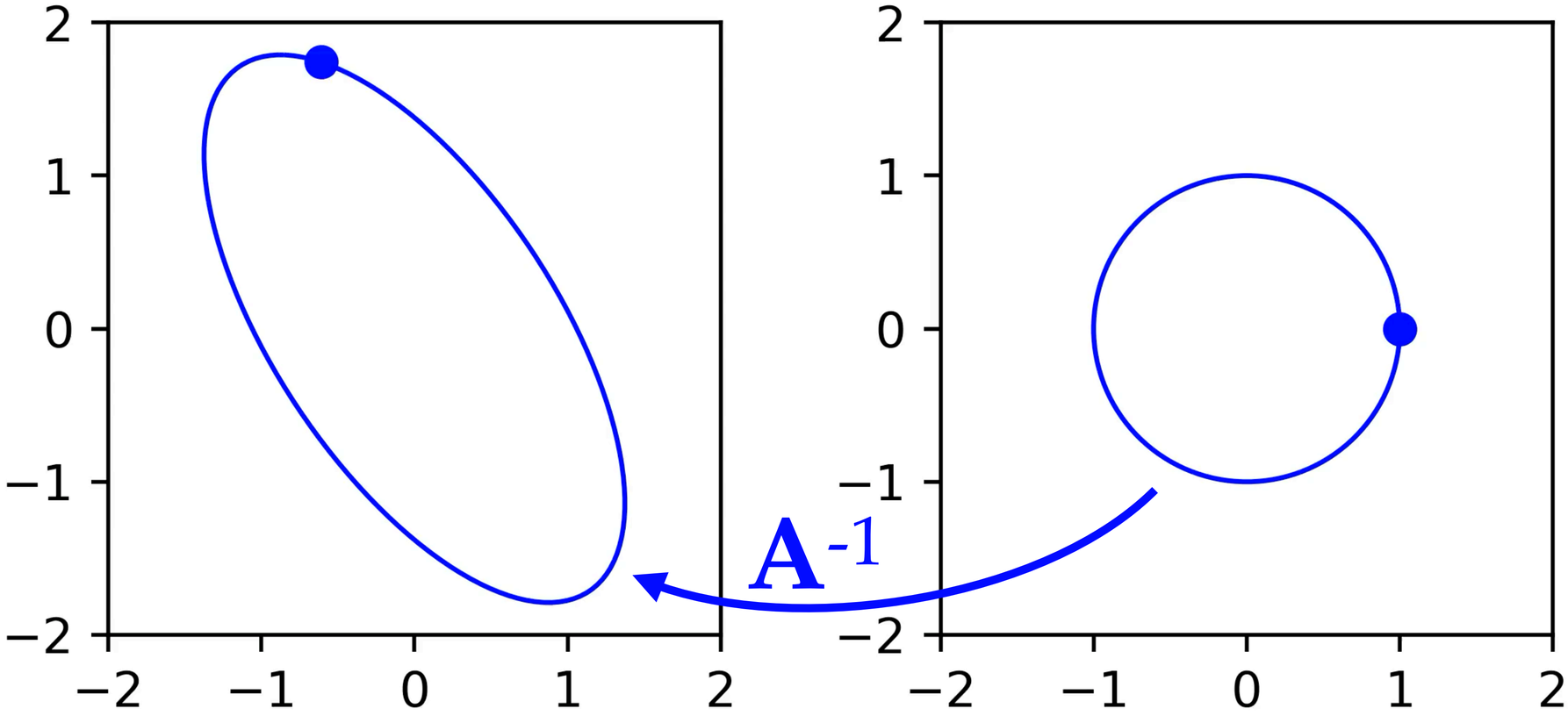

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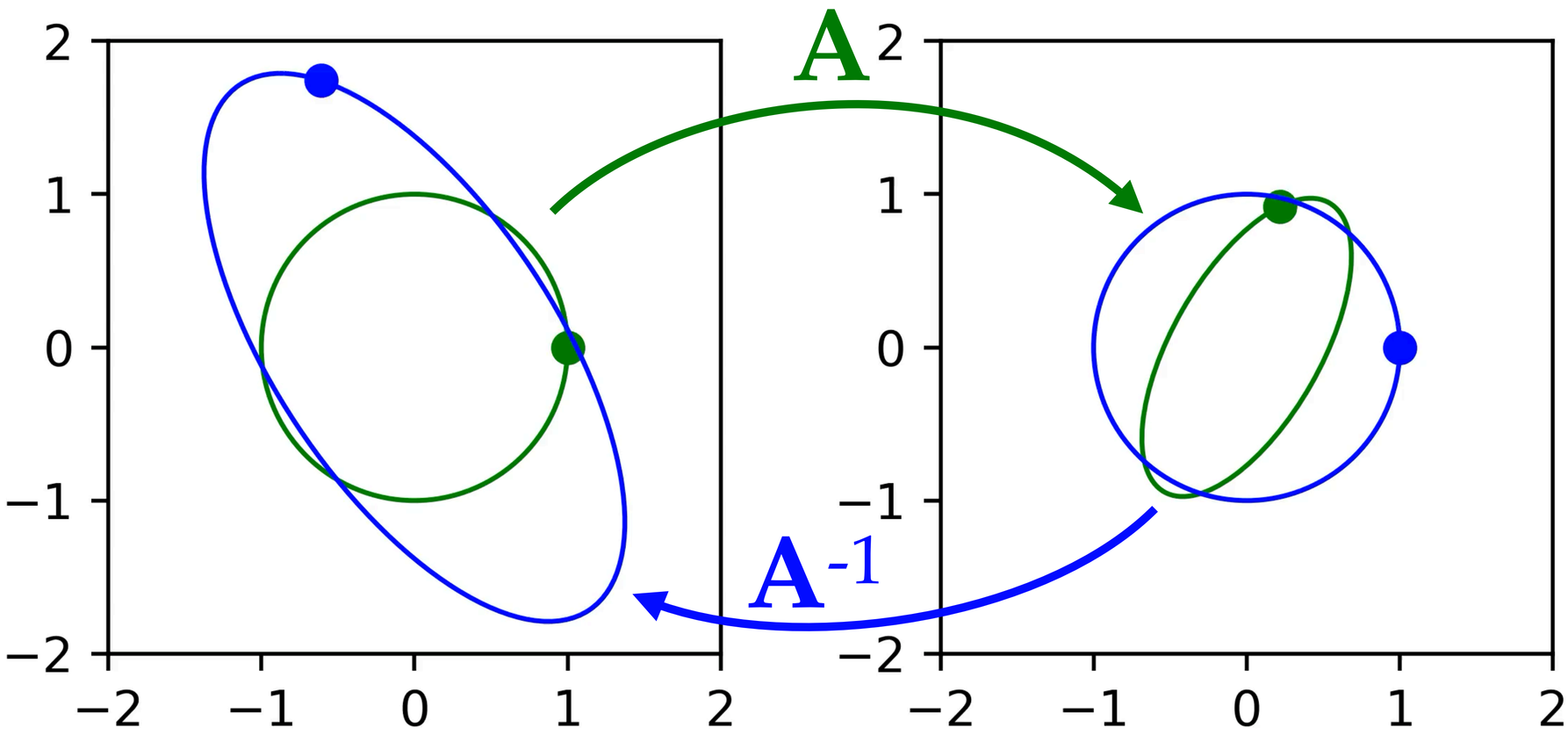

The condition number

Some useful properties

$$\mathrm{cond}(\mathbf{A}) = \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\|$$

- $\mathrm{cond}(\mathbf{A}) = \infty$ iff $\mathbf{A}$ is singular
- $\mathrm{cond}(\mathbf{A}) = 1$ if $\mathbf{A}$ is the identity matrix
- $\mathrm{cond}(\gamma\mathbf{A}) = \mathrm{cond}(\mathbf{A}) \quad \gamma \in \mathbb{R}$
- $\mathrm{cond}(\mathbf{QA}) = \mathrm{cond}(\mathbf{A})$ where $\mathbf{Q}$ is a rotation matrix

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- On the other hand, $\text{cond}(\mathbf{A}) = 1$ (!)

Implications

Stated without proof.

If you are using a good linear system solver, and if $\mathbf{b}$ can be assumed to be accurate, then

$$\frac{\|\Delta \mathbf{x}\|}{\|\mathbf{x}\|} \lesssim \operatorname{cond}(\mathbf{A})\,\operatorname{ulp}(1)$$

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Where ulp(1)

$\approx 2^{-23}$ (*single precision*)

$\approx 2^{-52}$ (*double precision*)

A Chicken-and-Egg problem

- Inverting matrices is expensive.
- We want to know the condition number to find out if this is *even possible?*

Midjourney: *chicken and egg problem*

- Our definition of $\mathrm{cond}(\mathbf{A})$ requires inverting a matrix and computing a matrix norm (*how*?!)

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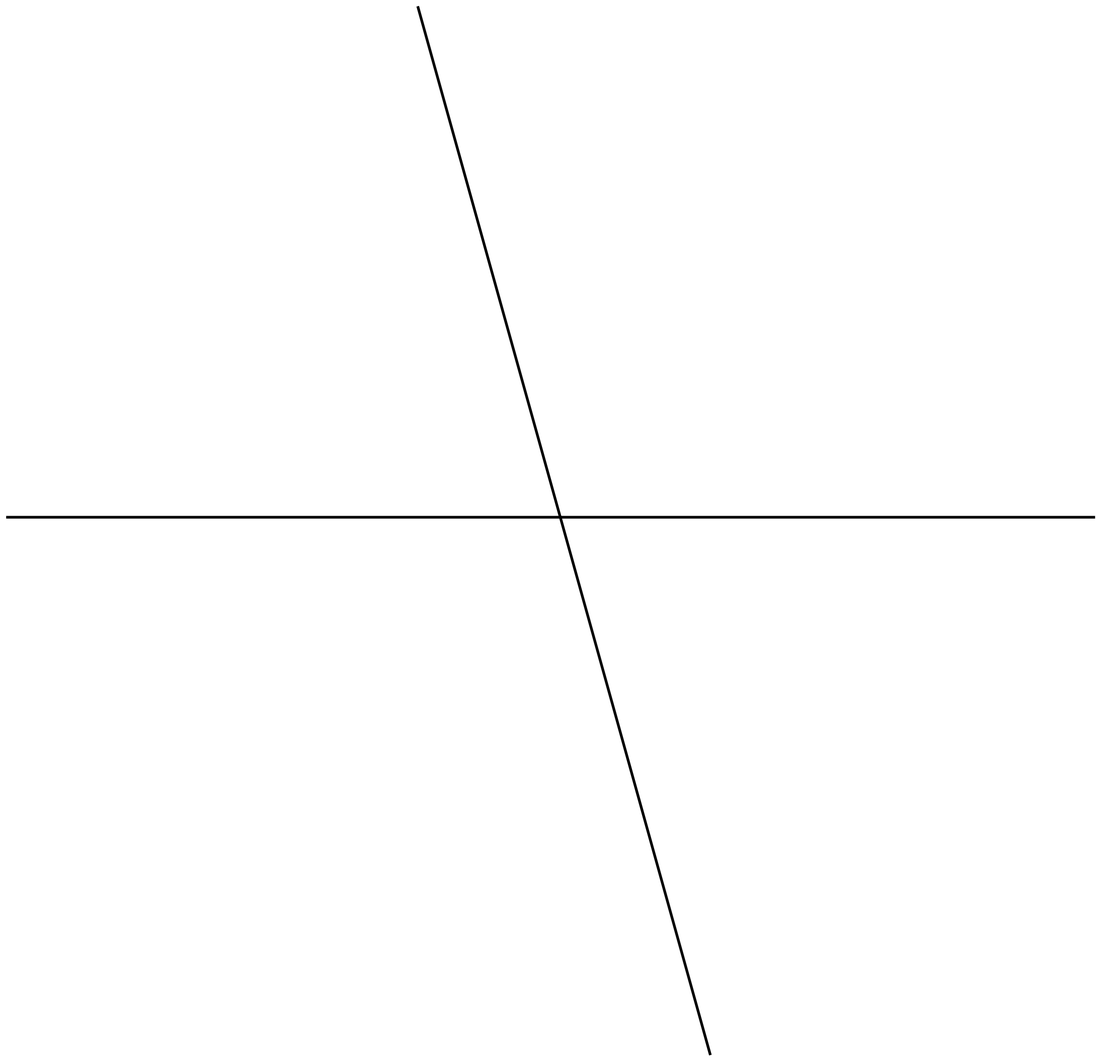
Stay tuned!

Geometry of badly conditioned systems

Noise & errors may be greatly magnified. Row-based interpretation.



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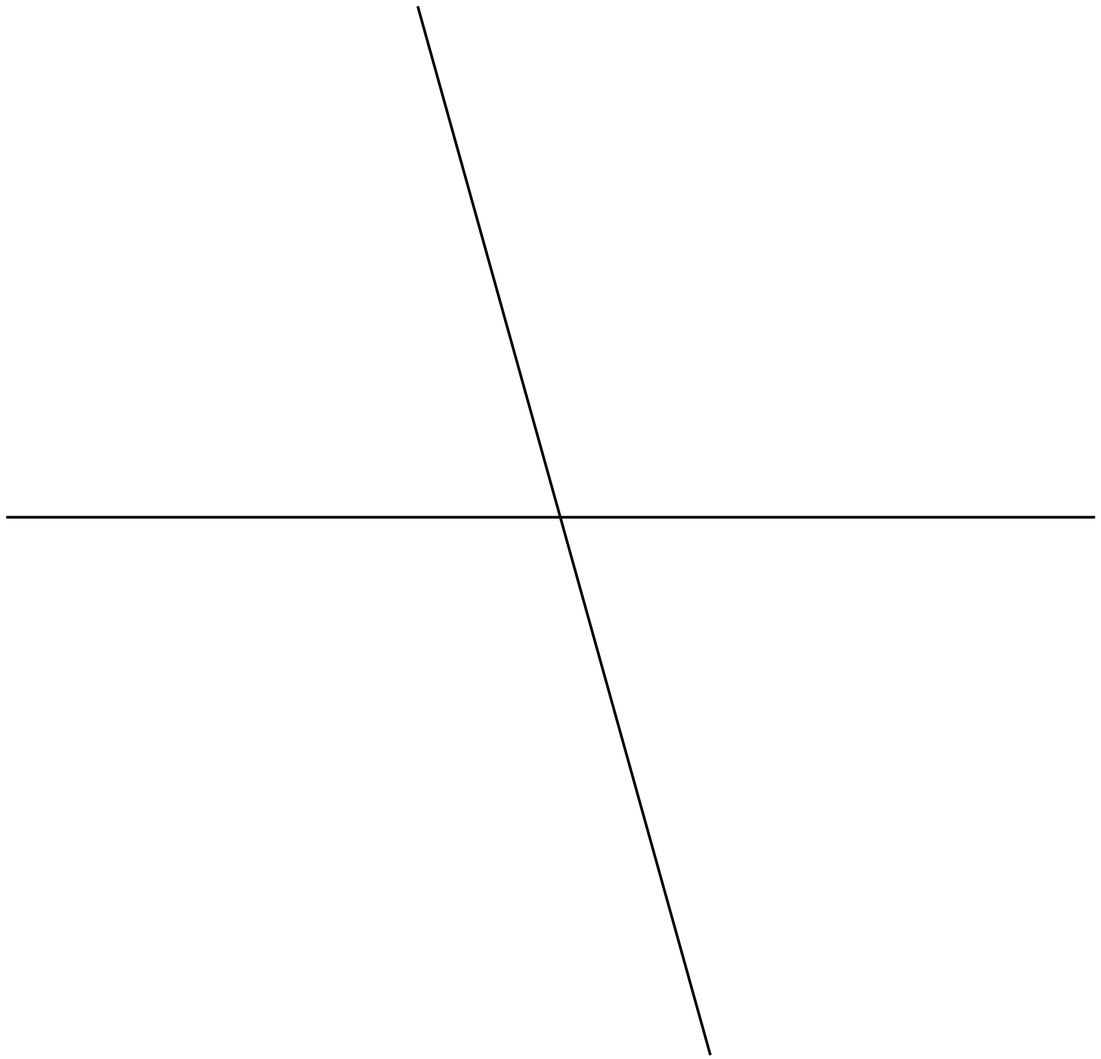

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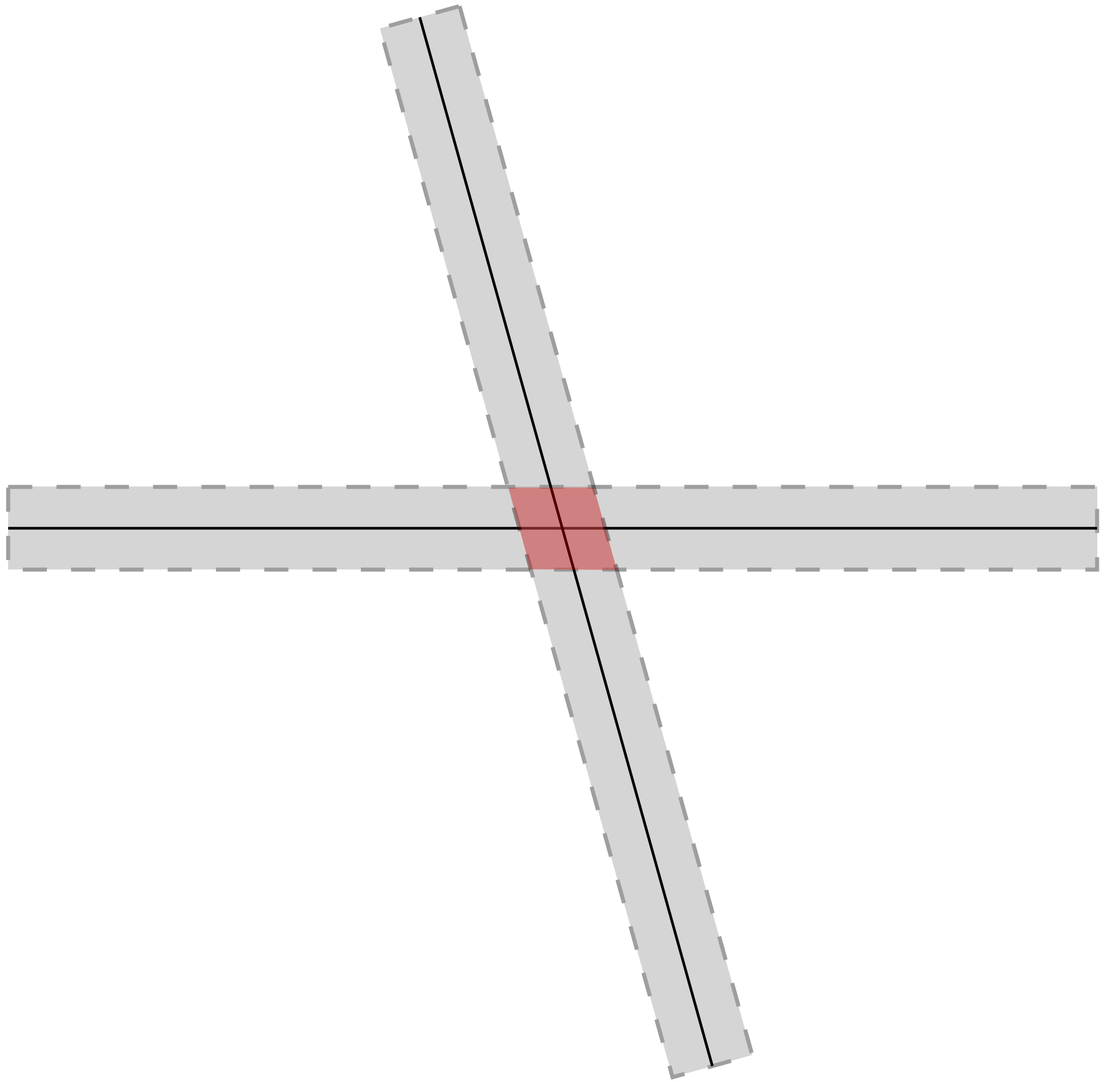

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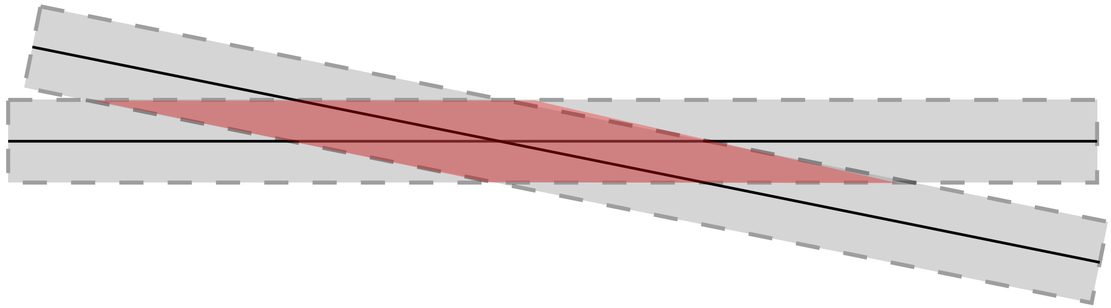
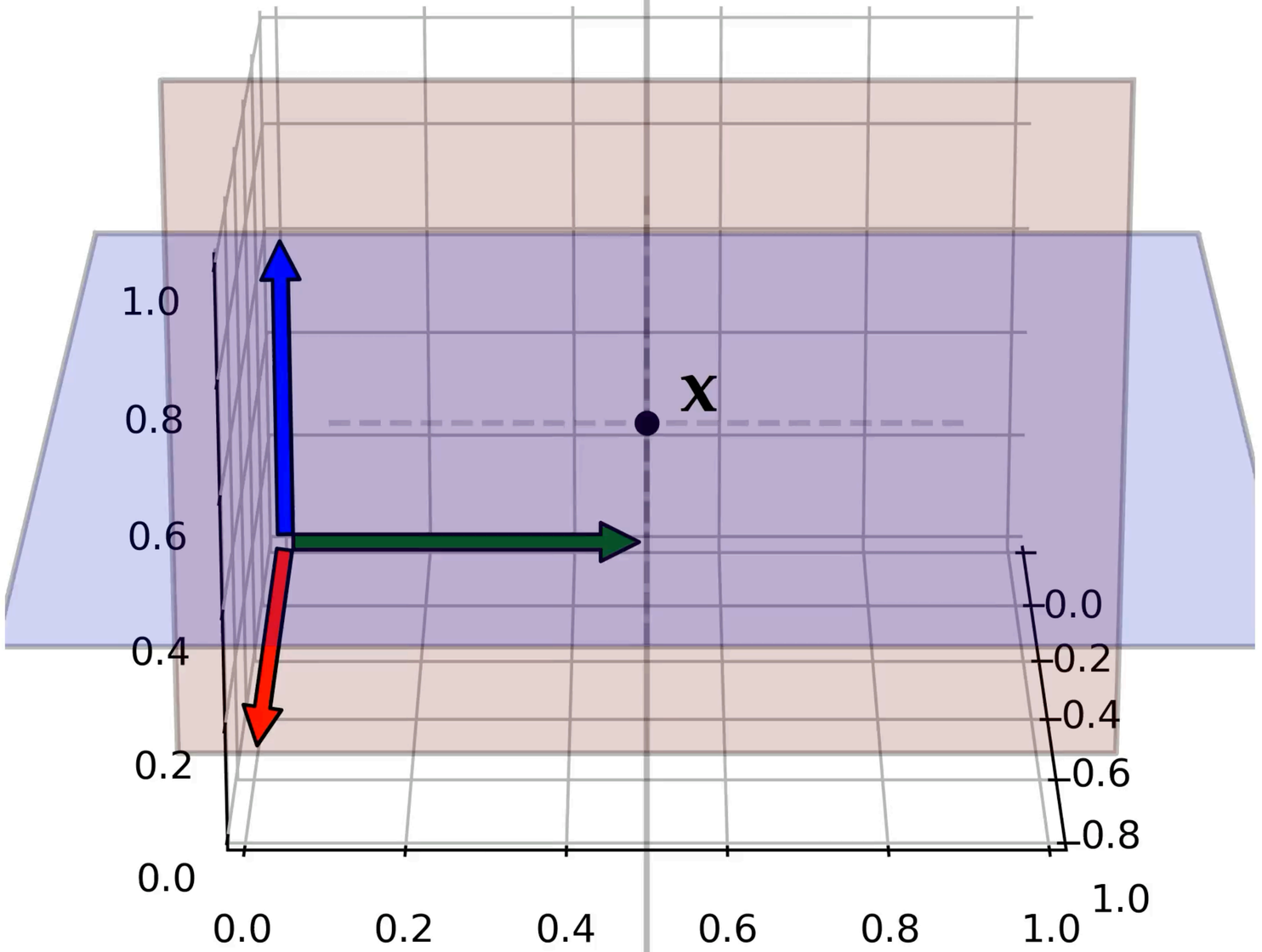


Geometric interpretation of linear systems

Row-based view



$$\mathbf{A} = \begin{pmatrix} — & \mathbf{a}^{(1)} & — \\ — & \mathbf{a}^{(2)} & — \\ — & \mathbf{a}^{(3)} & — \end{pmatrix}$$

Interpretation: Compute the intersection of planes with normals $\mathbf{a}^{(i)}$ and offset b_i

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

$$\Leftrightarrow \quad \begin{aligned} \mathbf{a}^{(1)} \cdot \mathbf{x} &= b_1 \\ \mathbf{a}^{(2)} \cdot \mathbf{x} &= b_2 \\ \mathbf{a}^{(3)} \cdot \mathbf{x} &= b_3 \end{aligned}$$

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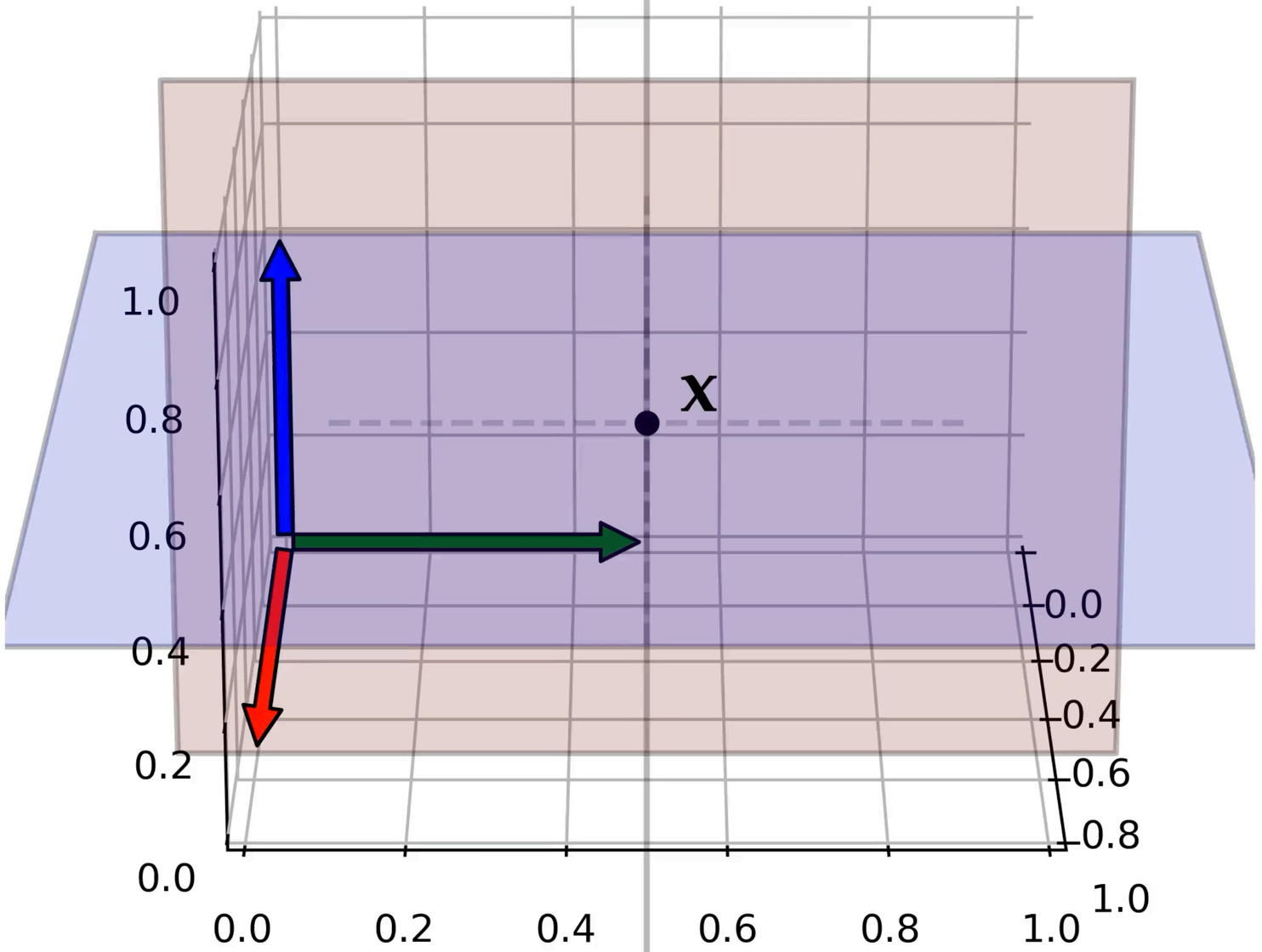

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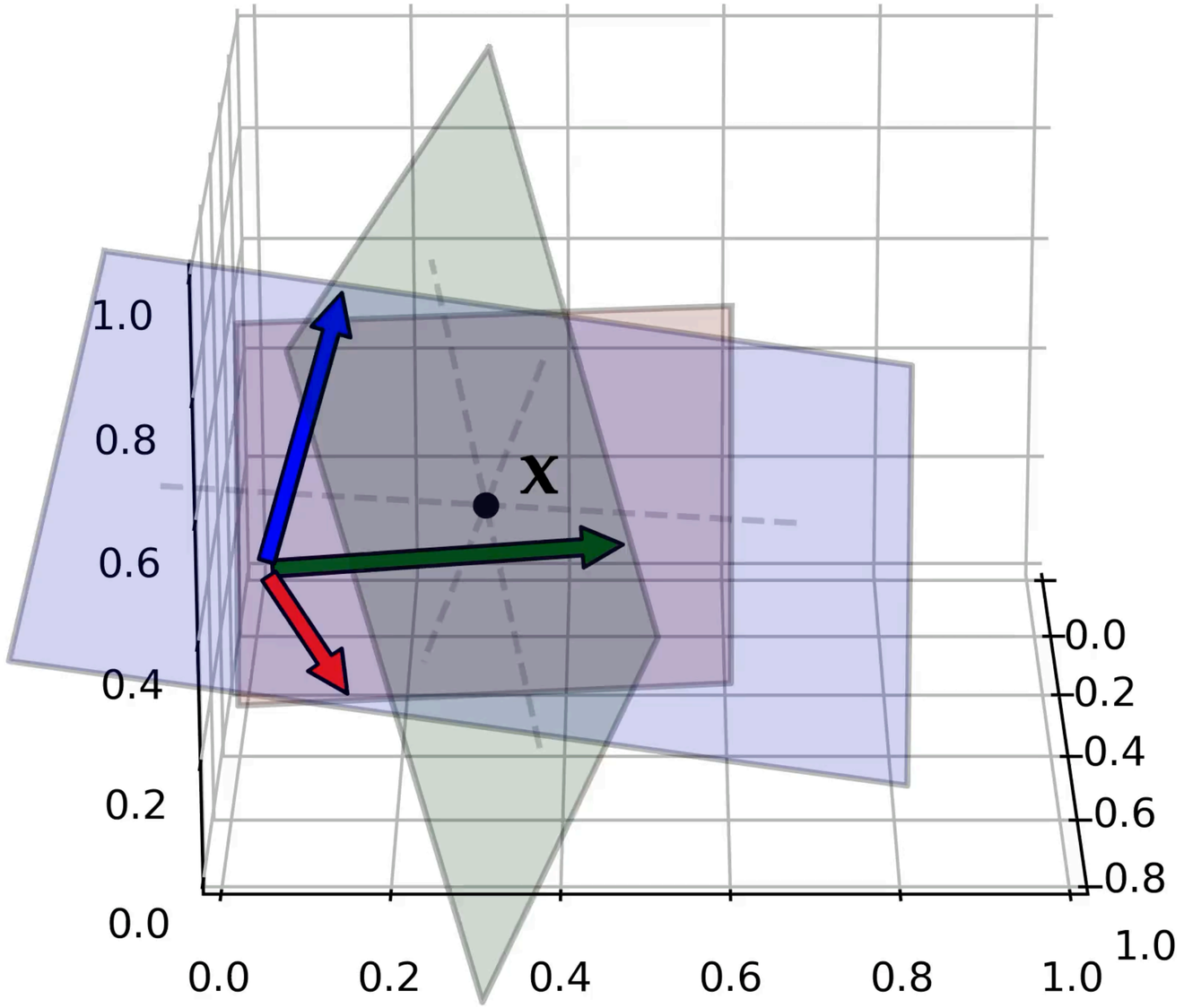

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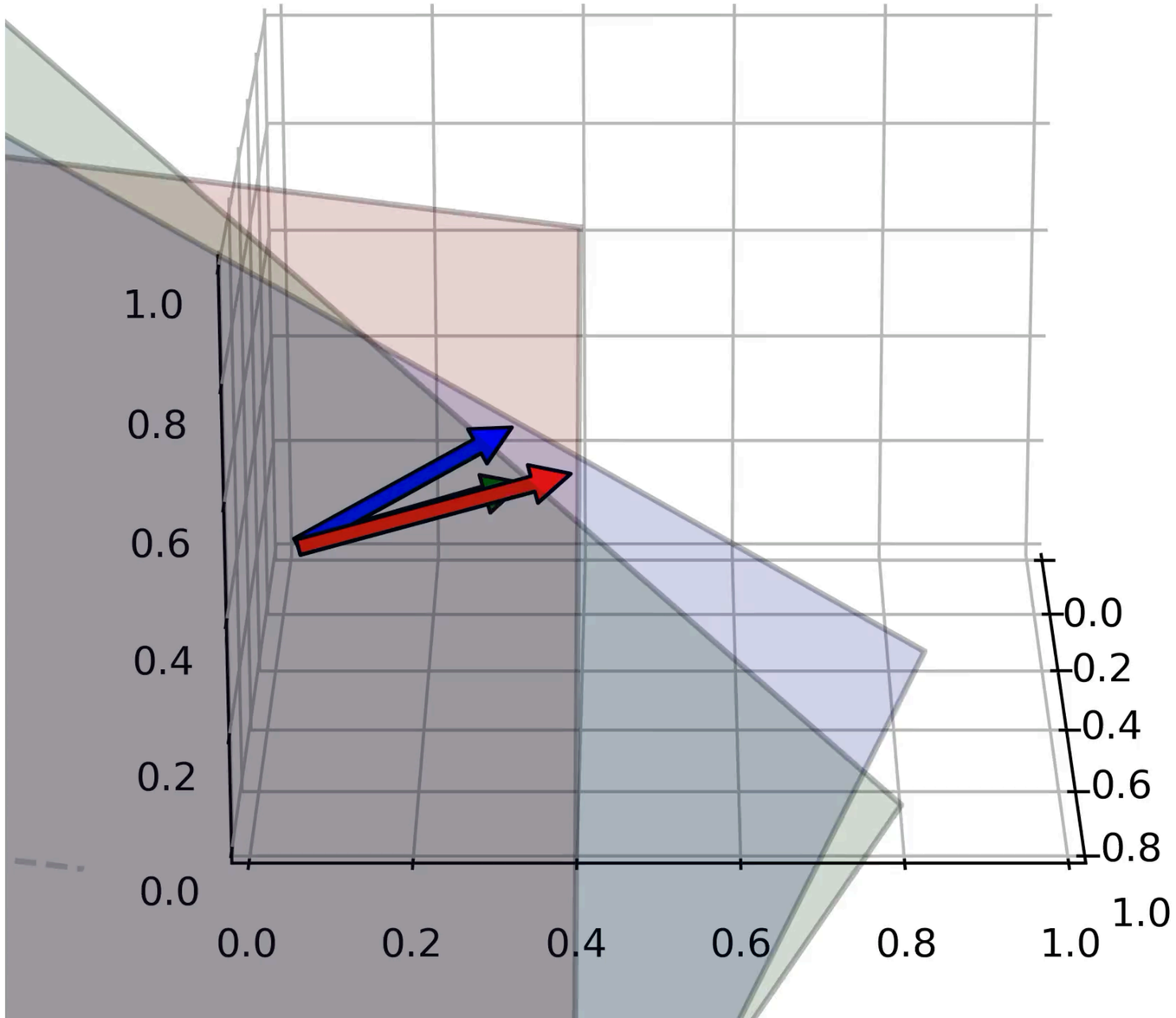
Geometric interpretation of linear systems

Row-based view



$$\mathbf{A} = \begin{pmatrix} — & \mathbf{a}^{(1)} & — \\ — & \mathbf{a}^{(2)} & — \\ — & \mathbf{a}^{(3)} & — \end{pmatrix}$$

Interpretation: Compute the intersection of planes with normals $\mathbf{a}^{(i)}$ and offset b_i

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

$$\Leftrightarrow \quad \begin{aligned} \mathbf{a}^{(1)} \cdot \mathbf{x} &= b_1 \\ \mathbf{a}^{(2)} \cdot \mathbf{x} &= b_2 \\ \mathbf{a}^{(3)} \cdot \mathbf{x} &= b_3 \end{aligned}$$

Conditioning of the Vandermonde Matrix

Maps from polynomial coefficients to polynomial evaluations.

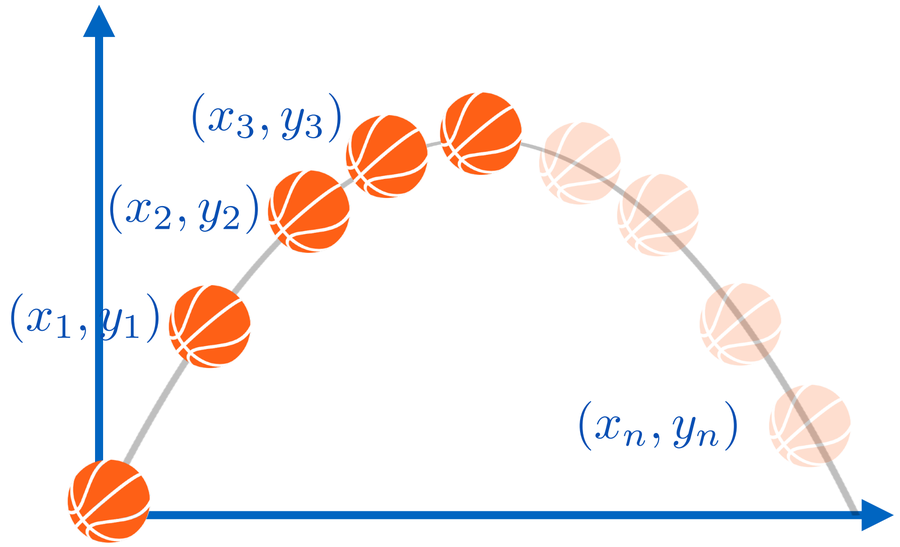
$$\mathbf{A} = \begin{pmatrix} \alpha_1^n & \dots & \alpha_1^2 & \alpha_1 & 1 \\ \alpha_2^n & \dots & \alpha_2^2 & \alpha_2 & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \alpha_3^n & \dots & \alpha_3^2 & \alpha_3 & 1 \\ \alpha_m^n & \dots & \alpha_m^2 & \alpha_m & 1 \end{pmatrix}$$

Condition number for n = 100 (for uniformly spaced positions on [0, 1]):

$$\mathrm{cond}(\mathbf{A}) = 7.31 \cdot 10^{19} \text{ (!!!!!!)}$$

Linear Least Squares

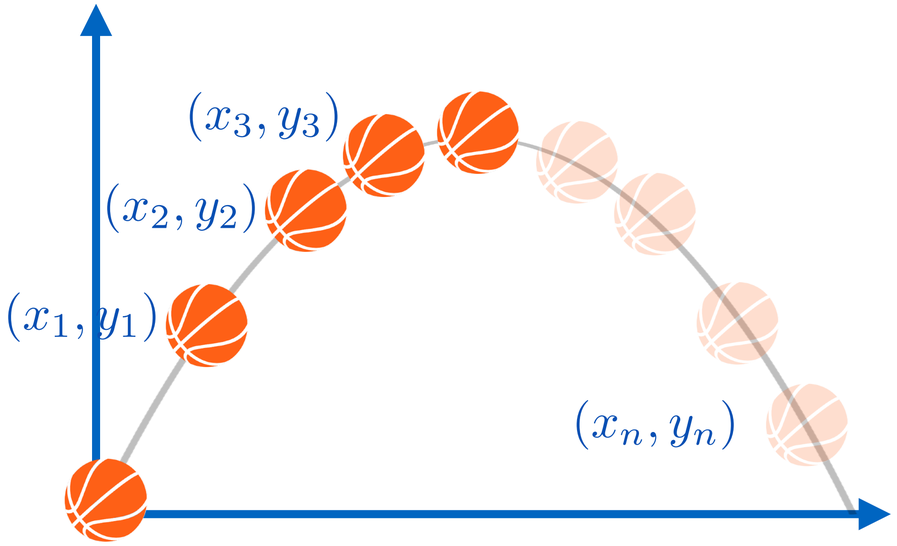
Linear Least Squares



What if there are > 3 observations?

Use subset? Which ones? Use all somehow?

Linear Least Squares



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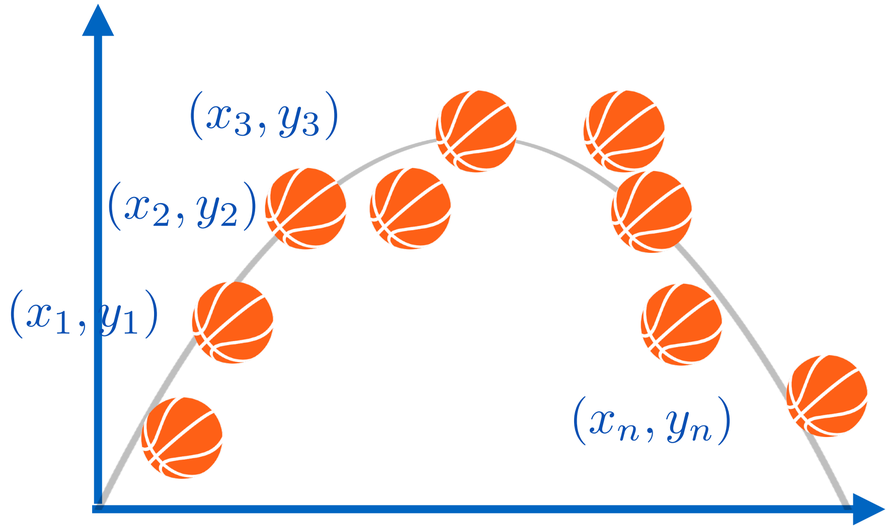


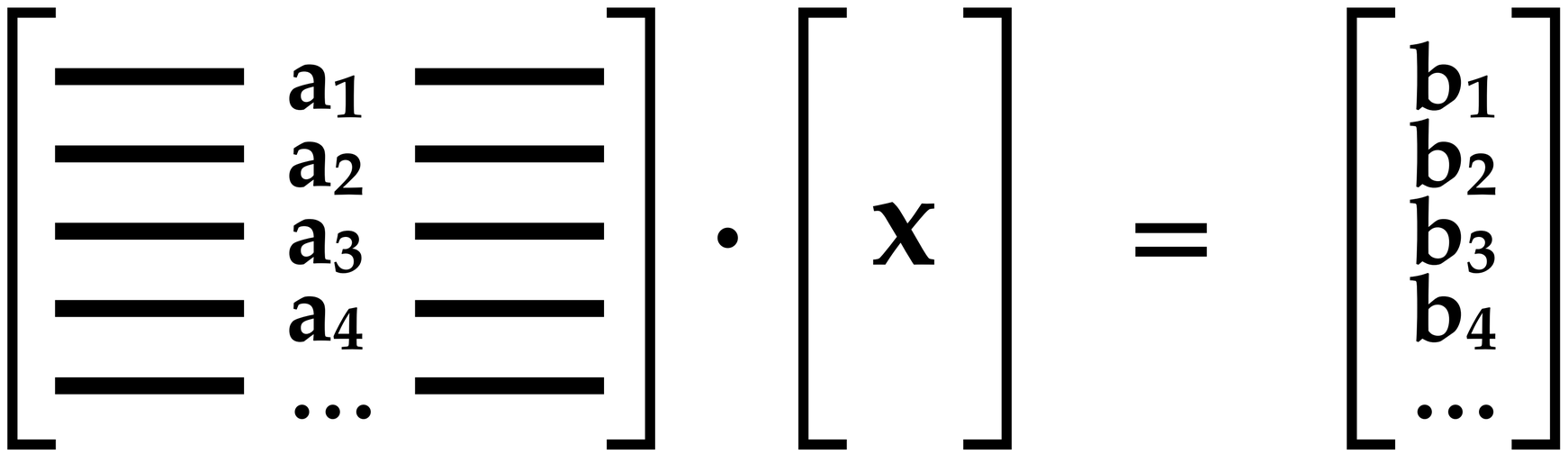
What if there is noise?

What if the model violates the assumptions?

From linear systems to least squares

$$\begin{bmatrix} & \mathbf{A} & \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \end{bmatrix}$$

From linear systems to least squares



n constraint equations (many)

m parameters (few)

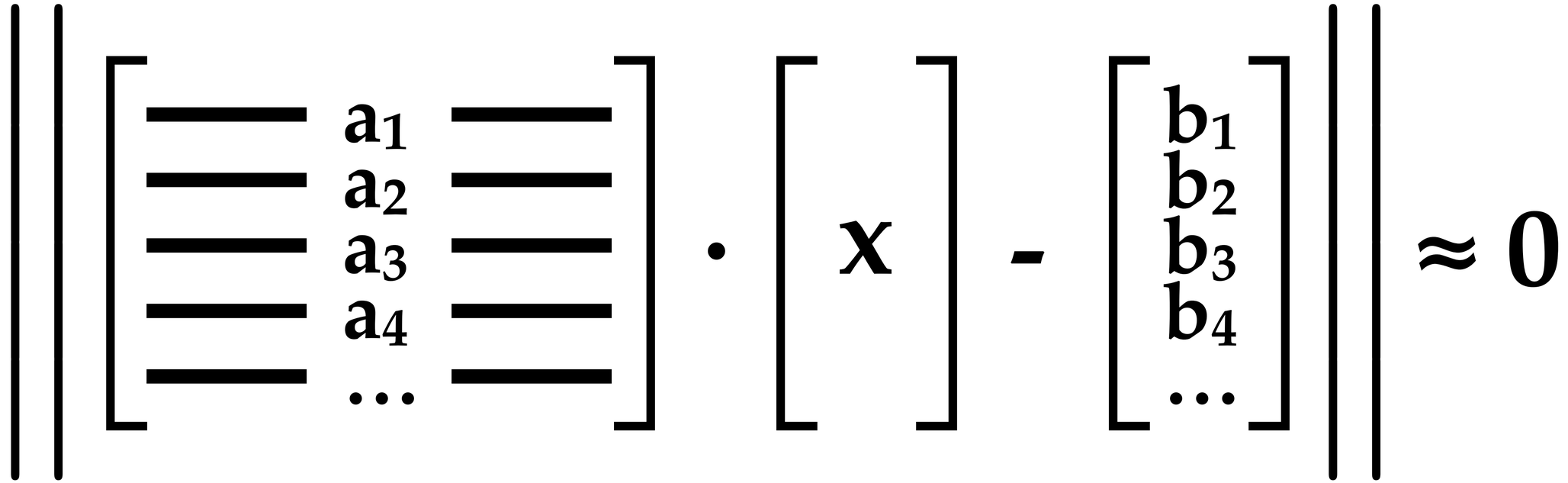
From linear systems to least squares

$$\begin{bmatrix} \text{—} & \mathbf{a}_1 & \text{—} \\ \text{—} & \mathbf{a}_2 & \text{—} \\ \text{—} & \mathbf{a}_3 & \text{—} \\ \text{—} & \mathbf{a}_4 & \text{—} \\ \text{—} & \dots & \text{—} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x} \end{bmatrix} - \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \\ \mathbf{b}_4 \\ \dots \end{bmatrix} \approx \mathbf{0}$$

n constraint equations (many)

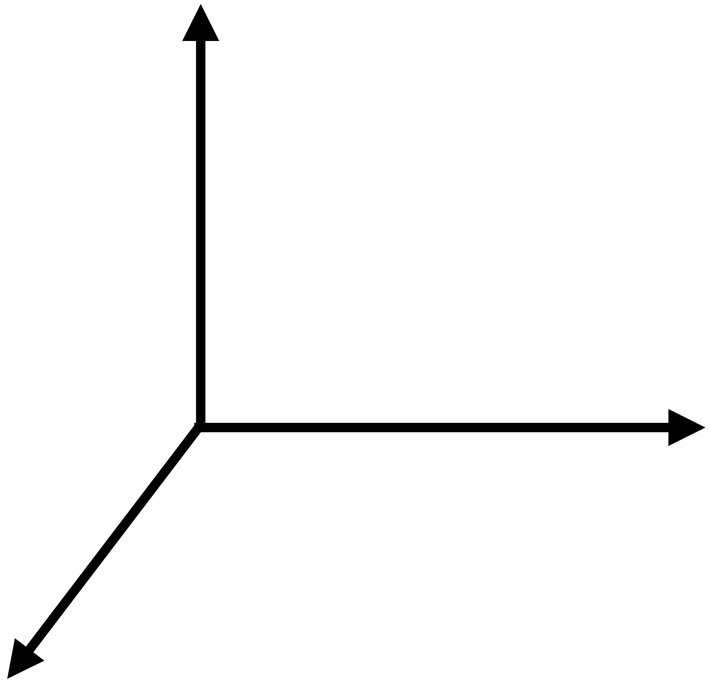
m parameters (few)

From linear systems to least squares



Geometric intuition

For almost all values of $\mathbf{b}$, $\mathbf{A}\mathbf{x} = \mathbf{b}$ is not solvable. Try to get as close as possible.



$$\mathbf{A} = \left(\begin{array}{cc} | & | \\ \mathbf{a}_1 & \mathbf{a}_2 \\ | & | \end{array} \right) \Bigg\} \text{ 3 rows}$$

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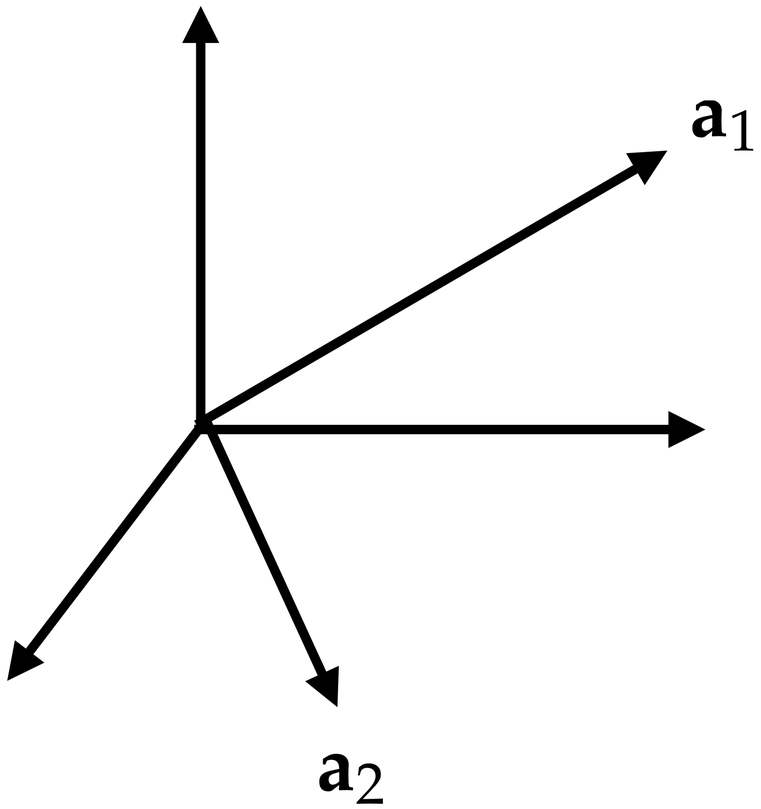

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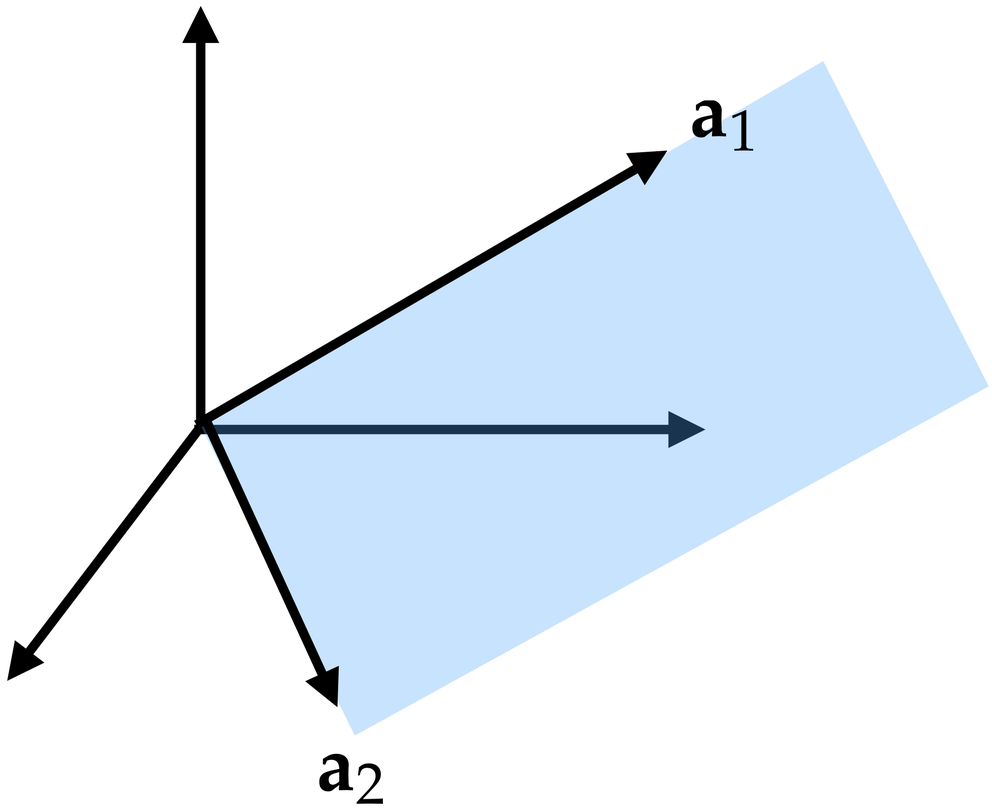

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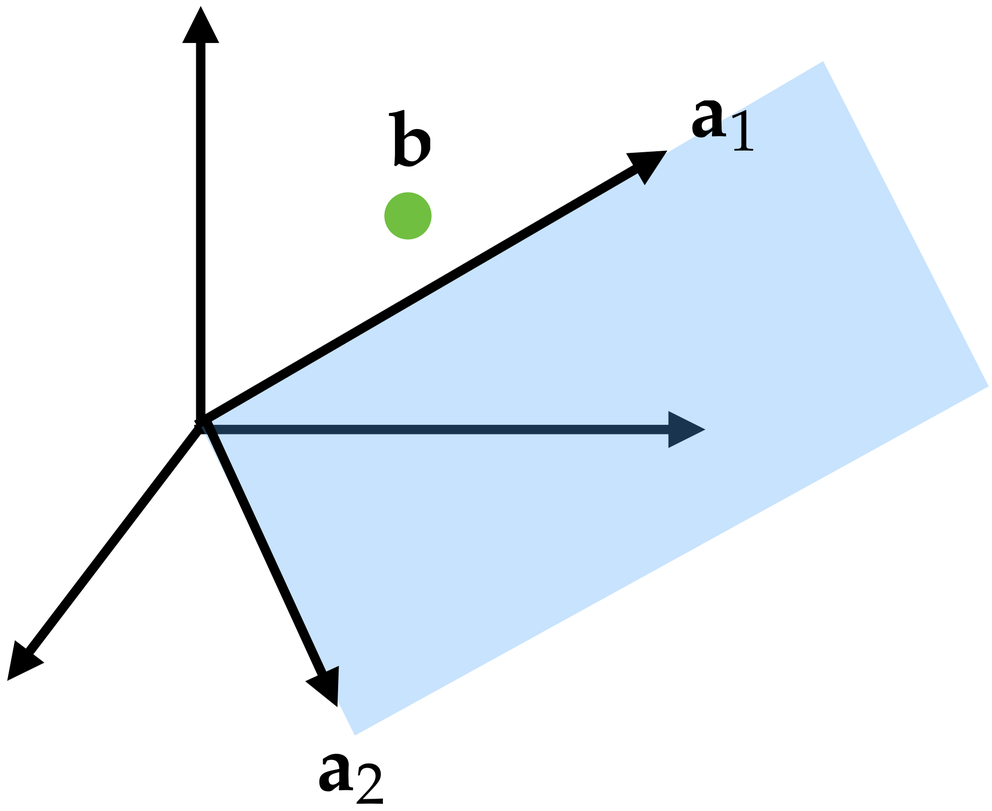

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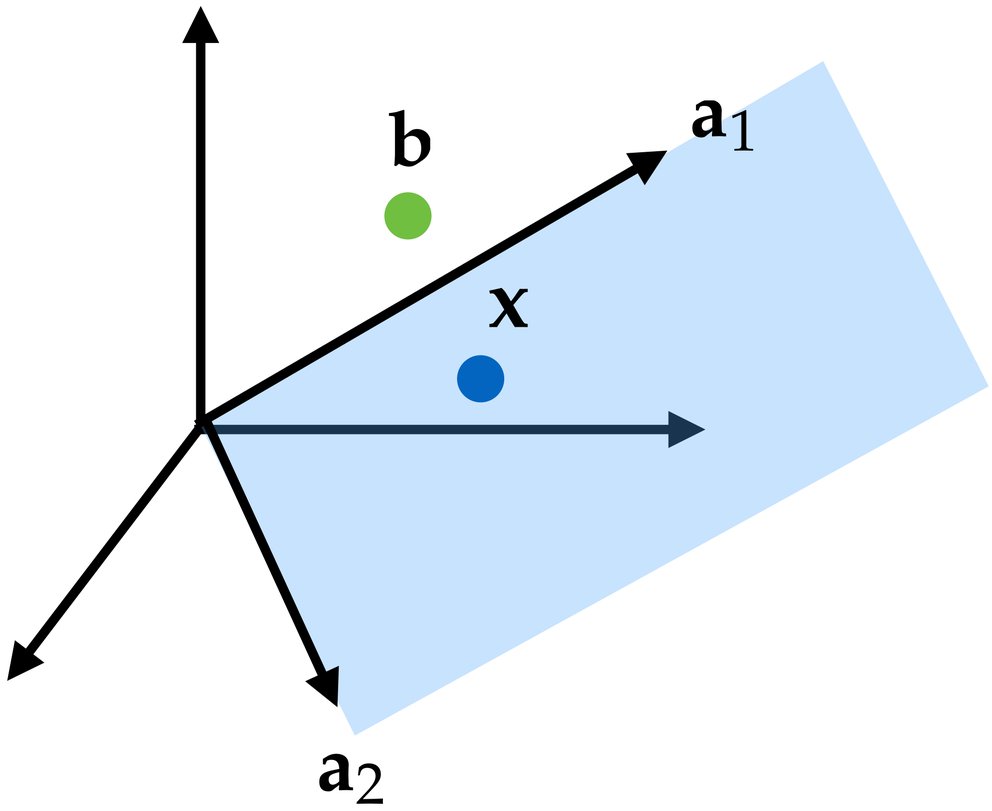

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Compromise: minimize the residual

Want: $\|\mathbf{r}(\mathbf{x})\| = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|$ to be as *small as possible*

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Ingredient: the ***squared*** length of a vector is just the inner product with itself:

$$\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 = \langle \mathbf{A}\mathbf{x} - \mathbf{b}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle$$

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&= \mathbf{x}^T \mathbf{A}^T \mathbf{A}\mathbf{x} - 2\mathbf{b}^T \mathbf{A}\mathbf{x} + \|\mathbf{b}\|^2
\end{aligned}
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$$= 2\mathbf{A}^T \mathbf{A}\mathbf{x} - 2\mathbf{A}^T \mathbf{b}$$

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

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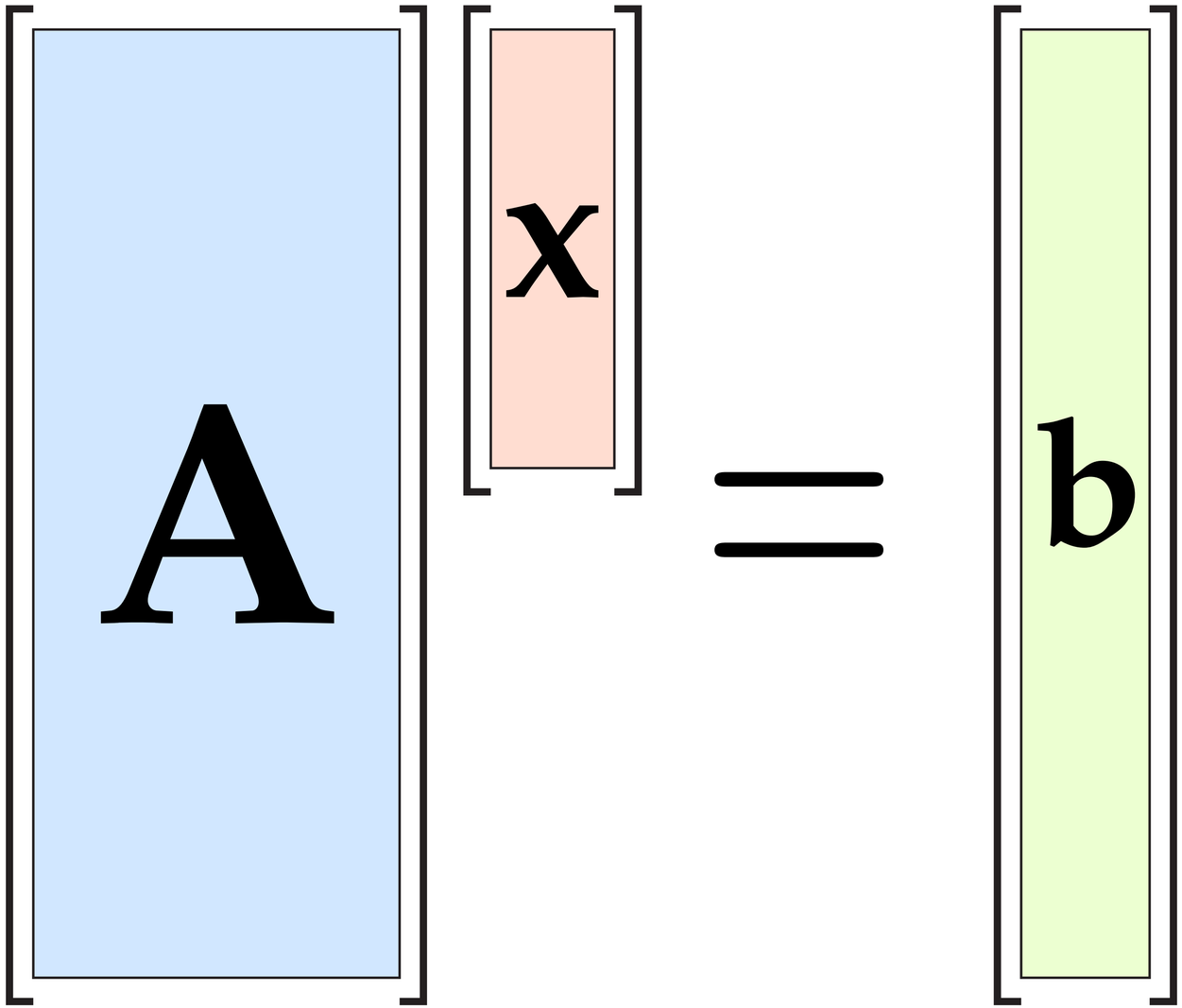
Carl Friedrich Gauss

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

Normal equations

Tall linear system

Generally ill-defined



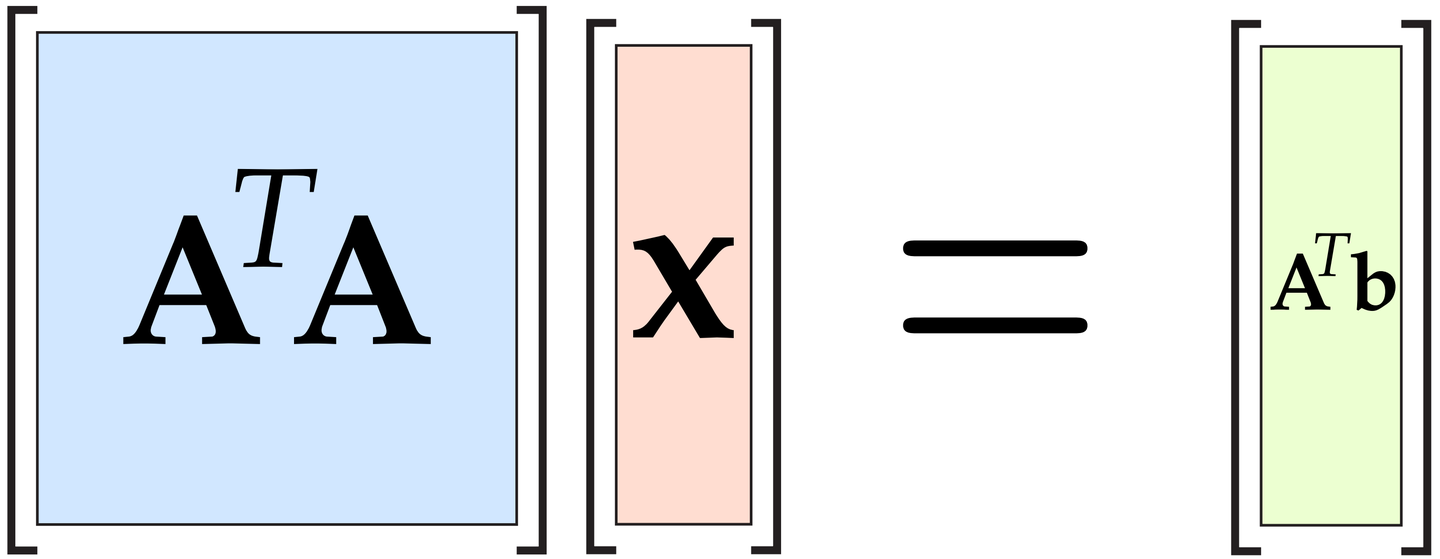
Linear least squares via the normal equations

The "best" solution (in the L_2 sense) is given by:

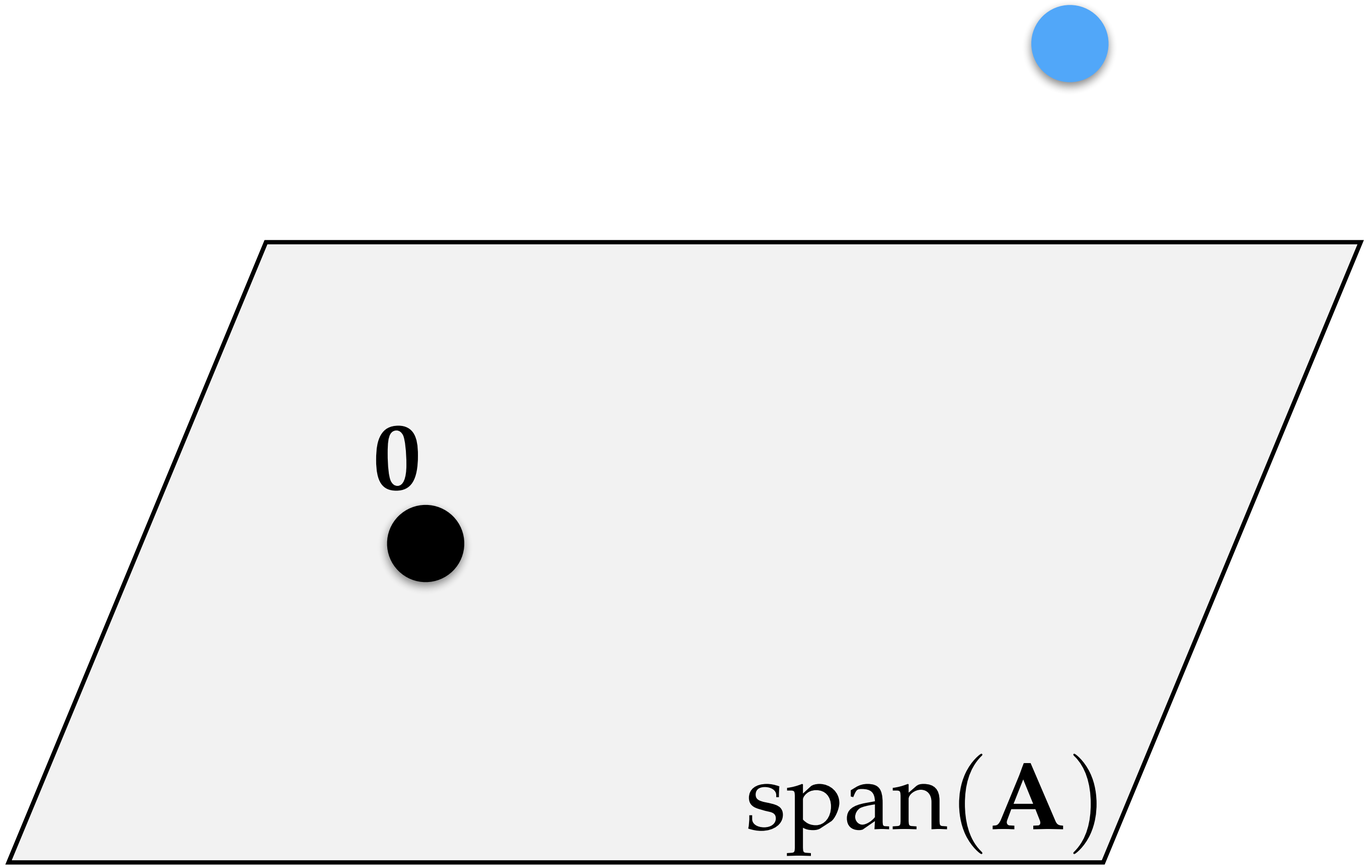
$$\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$$

Linear least squares via the normal equations

.. which is equivalent to a smaller square linear system



Why are they called normal equations?



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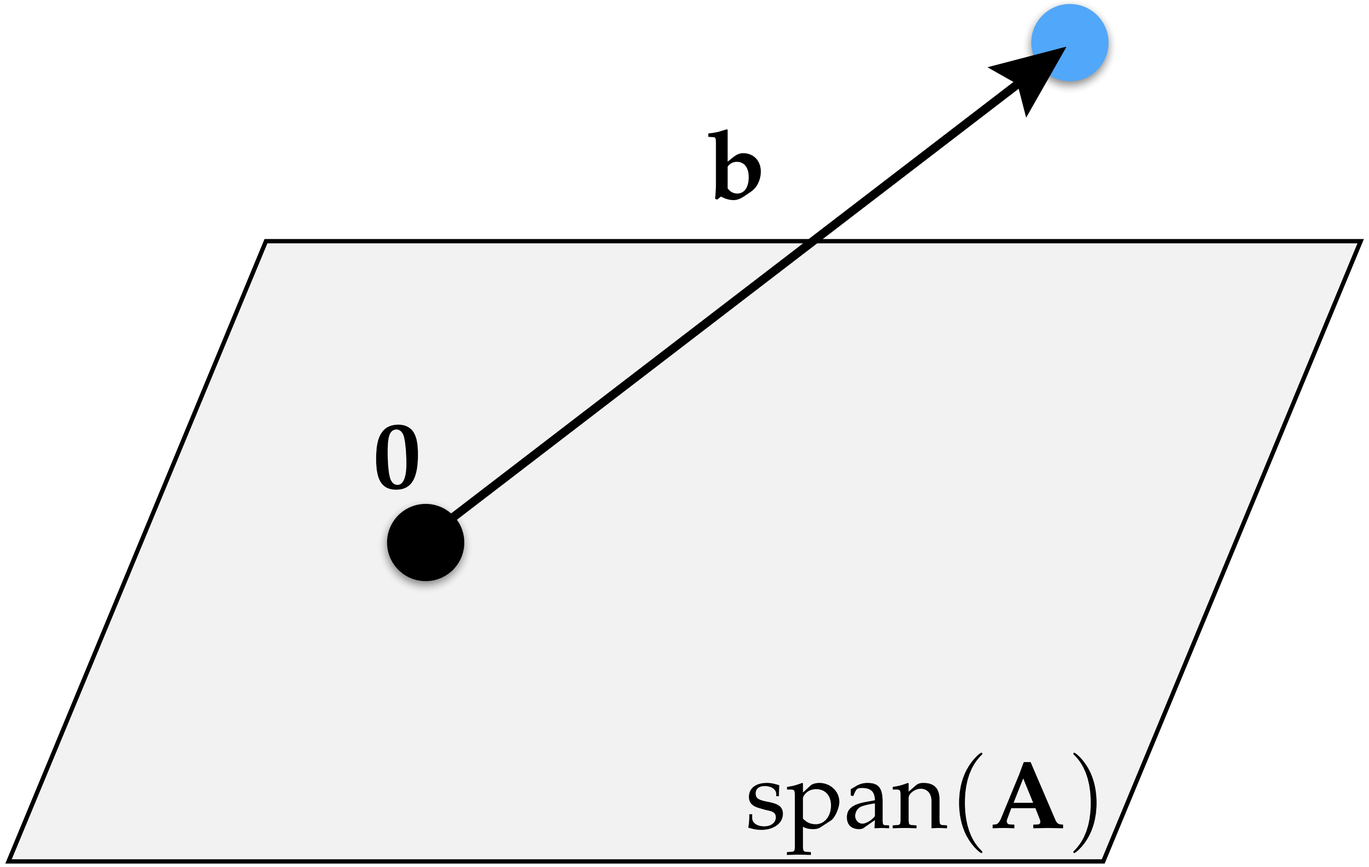

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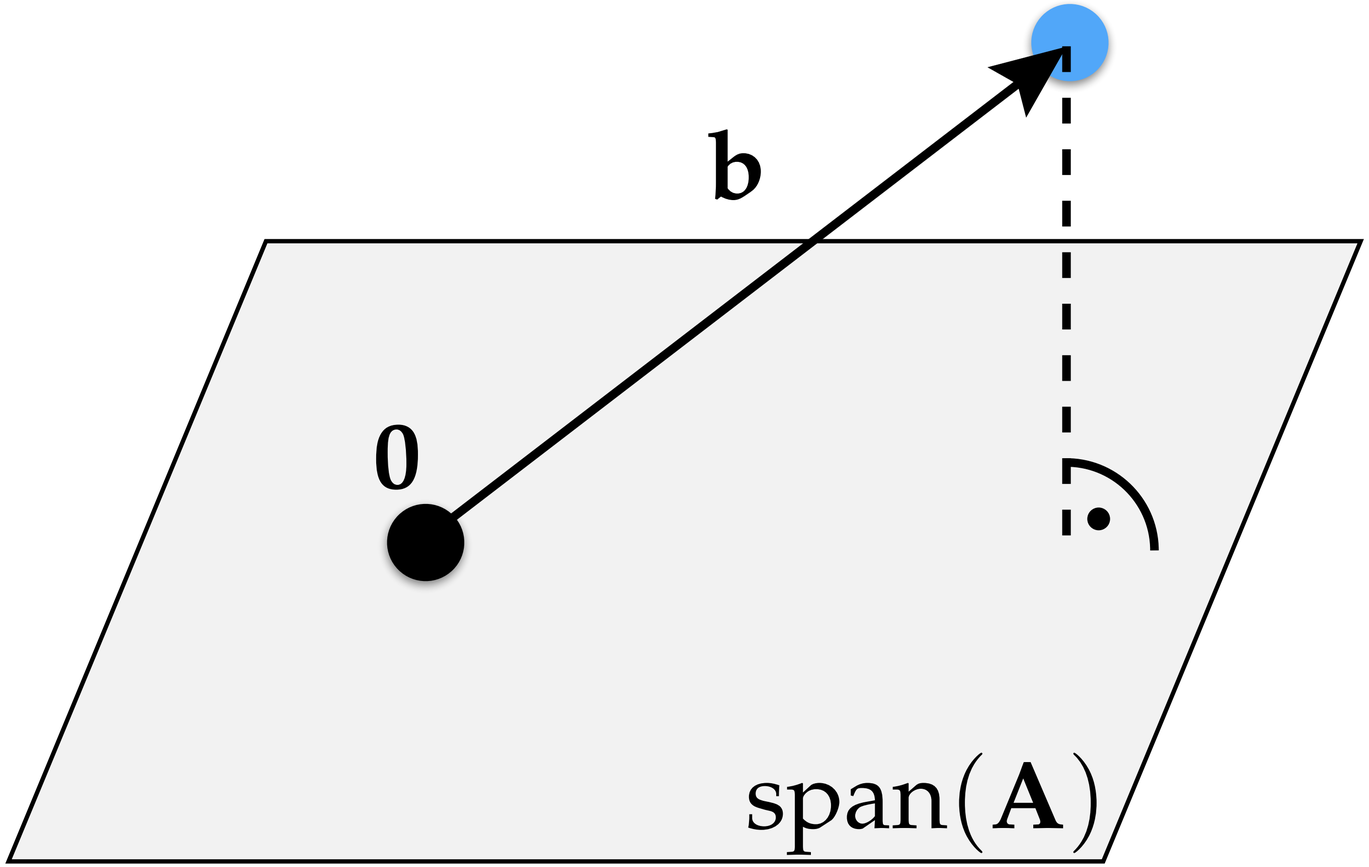

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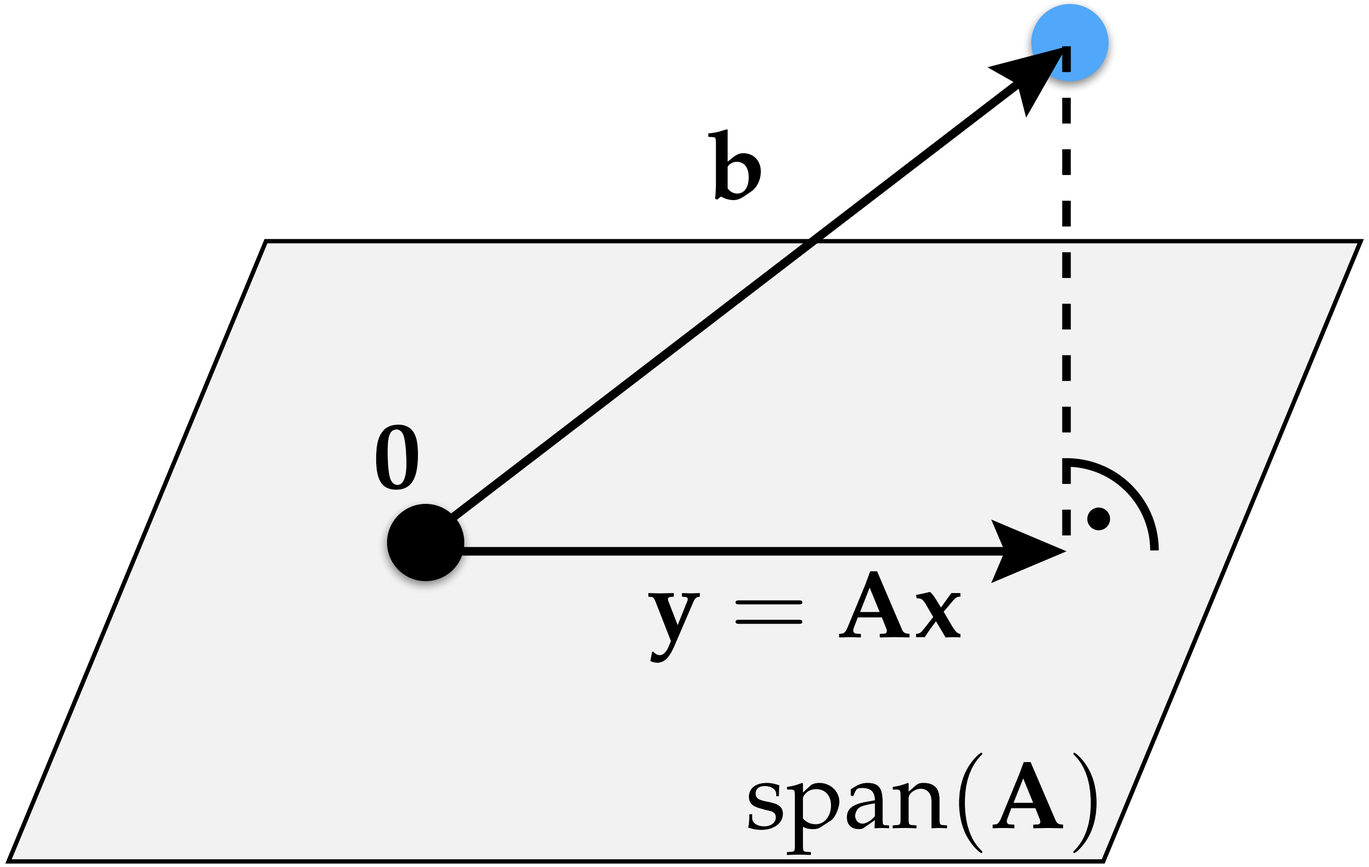

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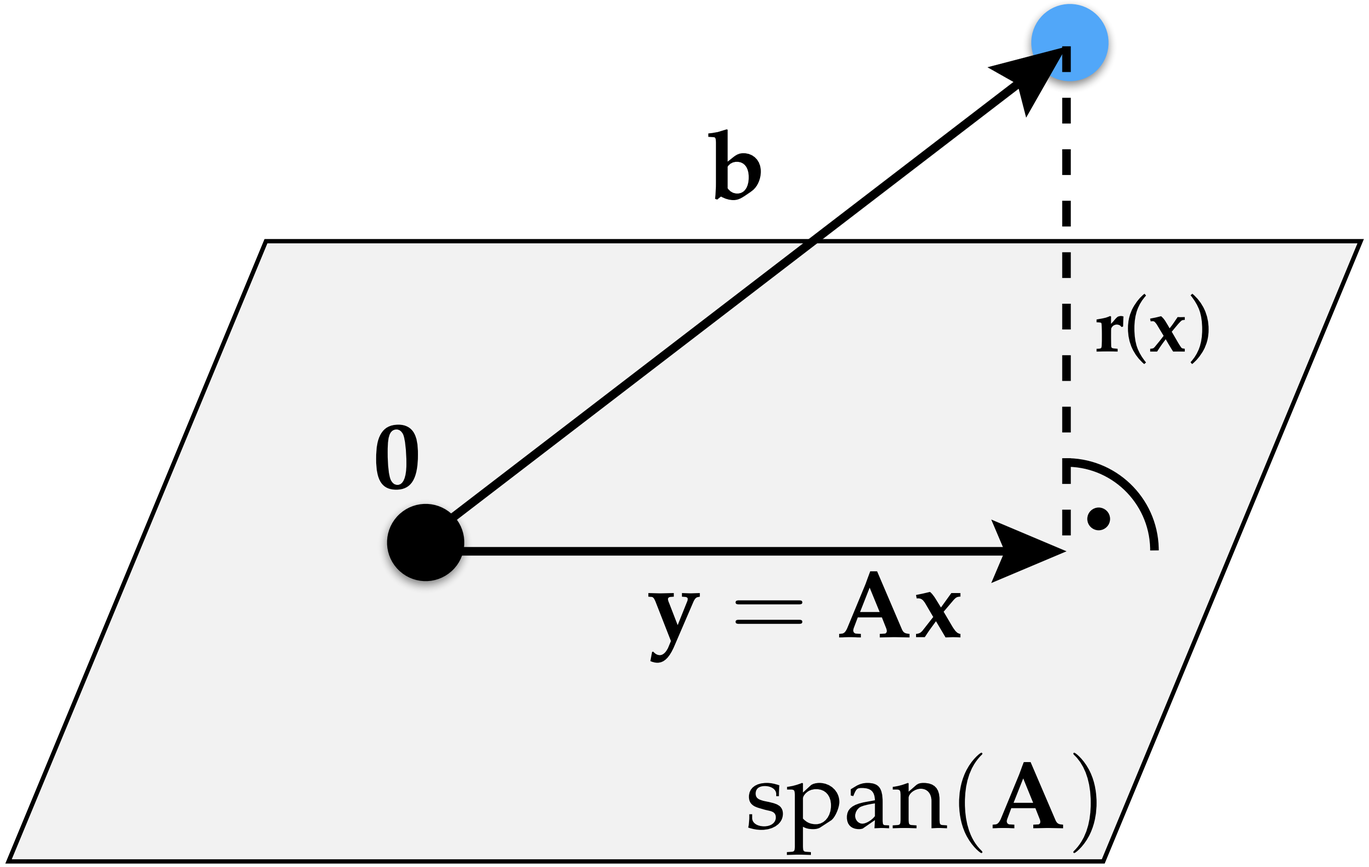

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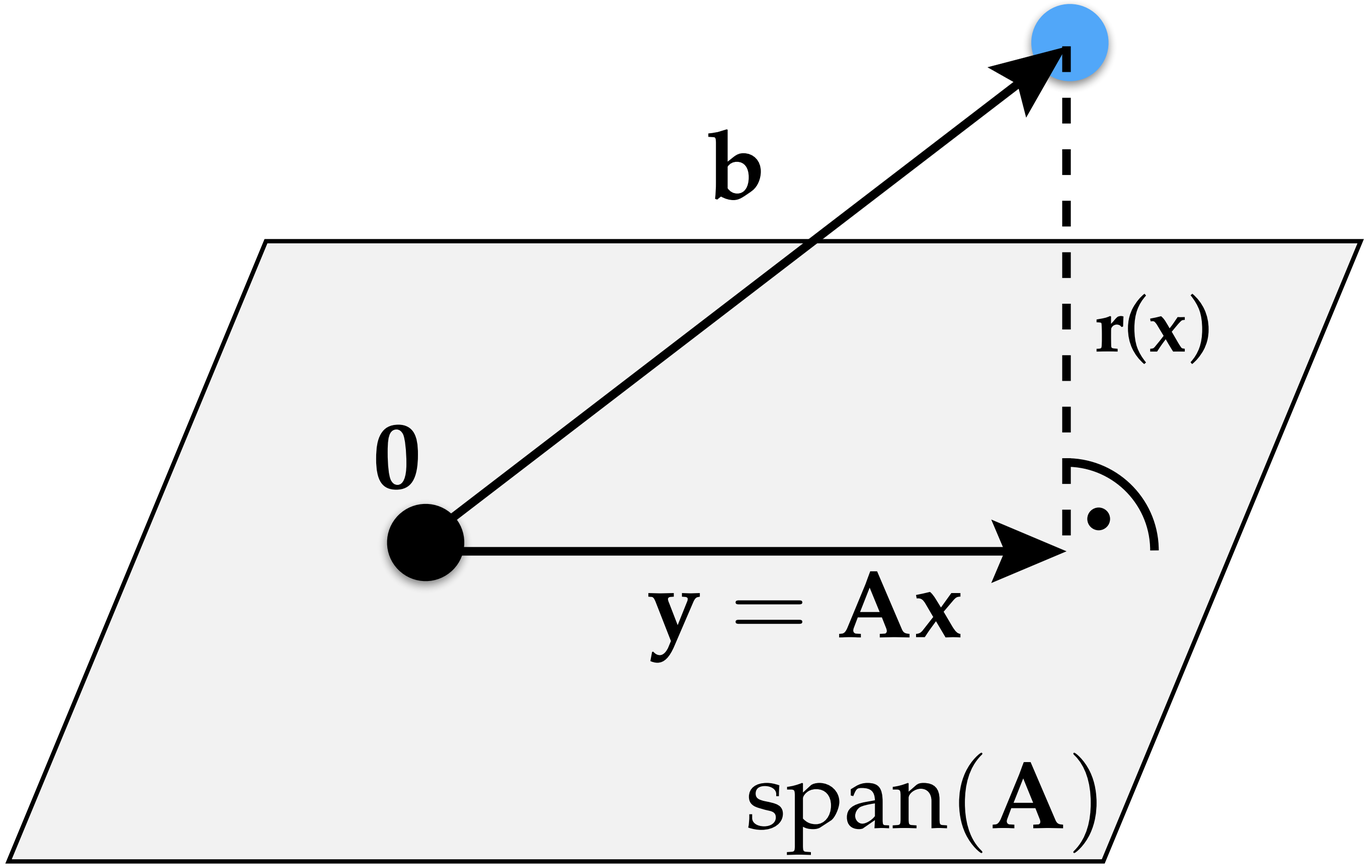

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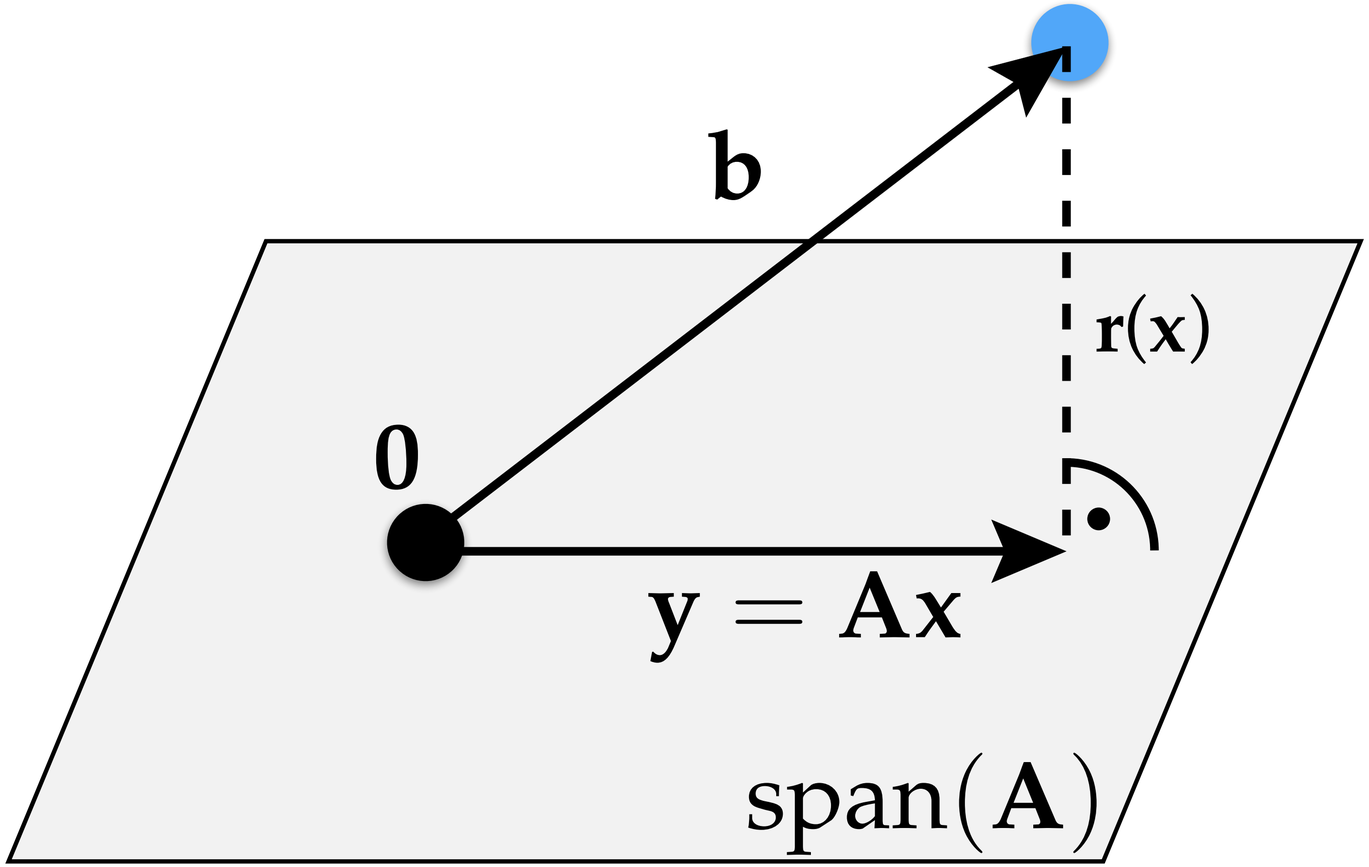

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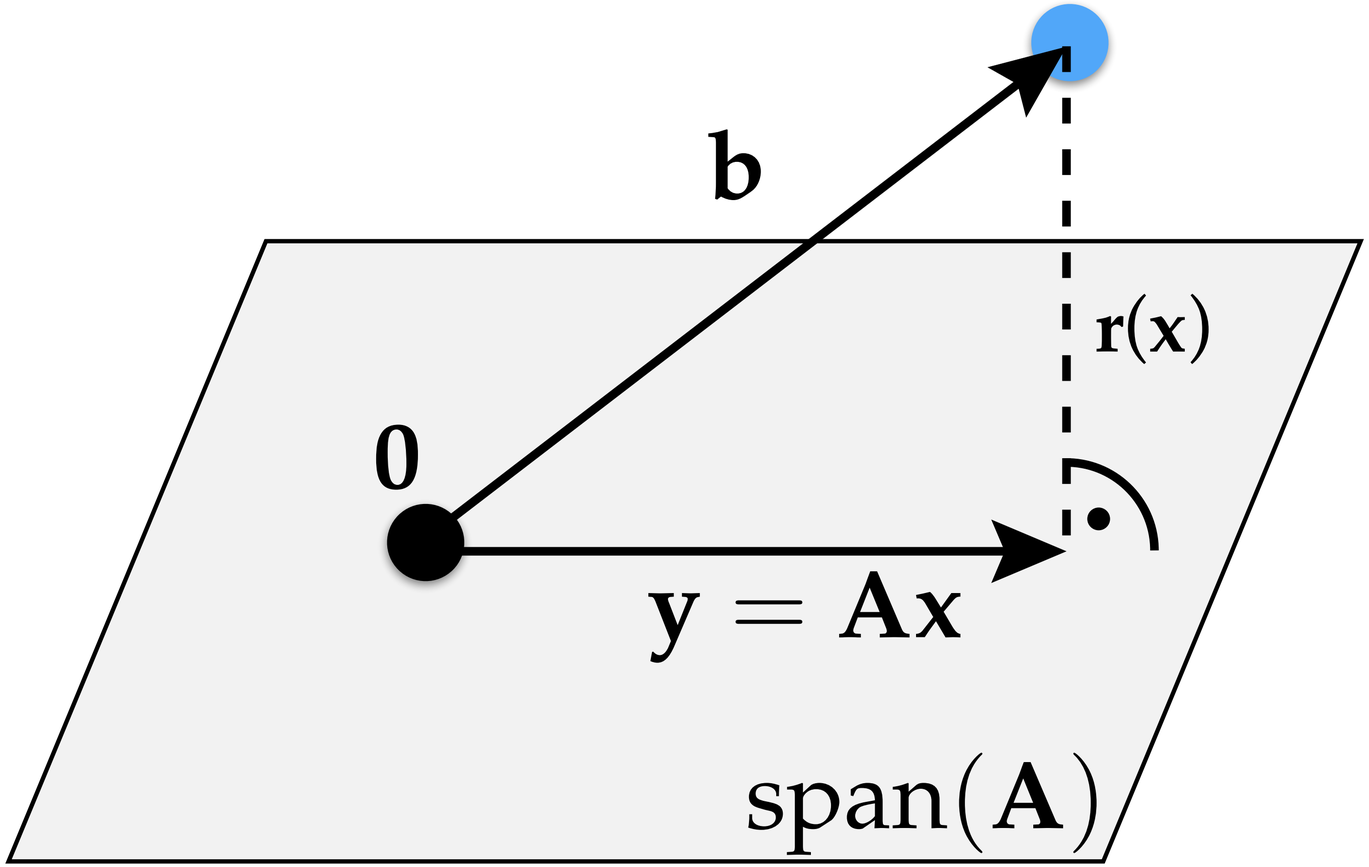

$$\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b} \;\Leftrightarrow\; \mathbf{A}^T(\mathbf{A}\mathbf{x} - \mathbf{b}) = \mathbf{0} \;\Leftrightarrow\; \mathbf{A}^T\mathbf{r}(\mathbf{x}) = \mathbf{0}.$$