Lecture 7

The Eigen- & Singular Value Decompositions

Nonlinear matrix algorithms

CS328 - Numerical Methods for Visual Computing and Machine Learning

Prof. Wenzel Jakob

EPFL RGL Realistic Graphics Lab

MATH-111 recap

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

MATH-111 recap

Eigenvalue Eigenvector

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Eigenvalue → λ

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where

$$\mathbf{A} \in \mathbb{R}^{n\times n}, \;\; \lambda \in \mathbb{R}$$
$$\mathbf{v} \in \mathbb{R}^{n}, \|\mathbf{v}\| = 1$$

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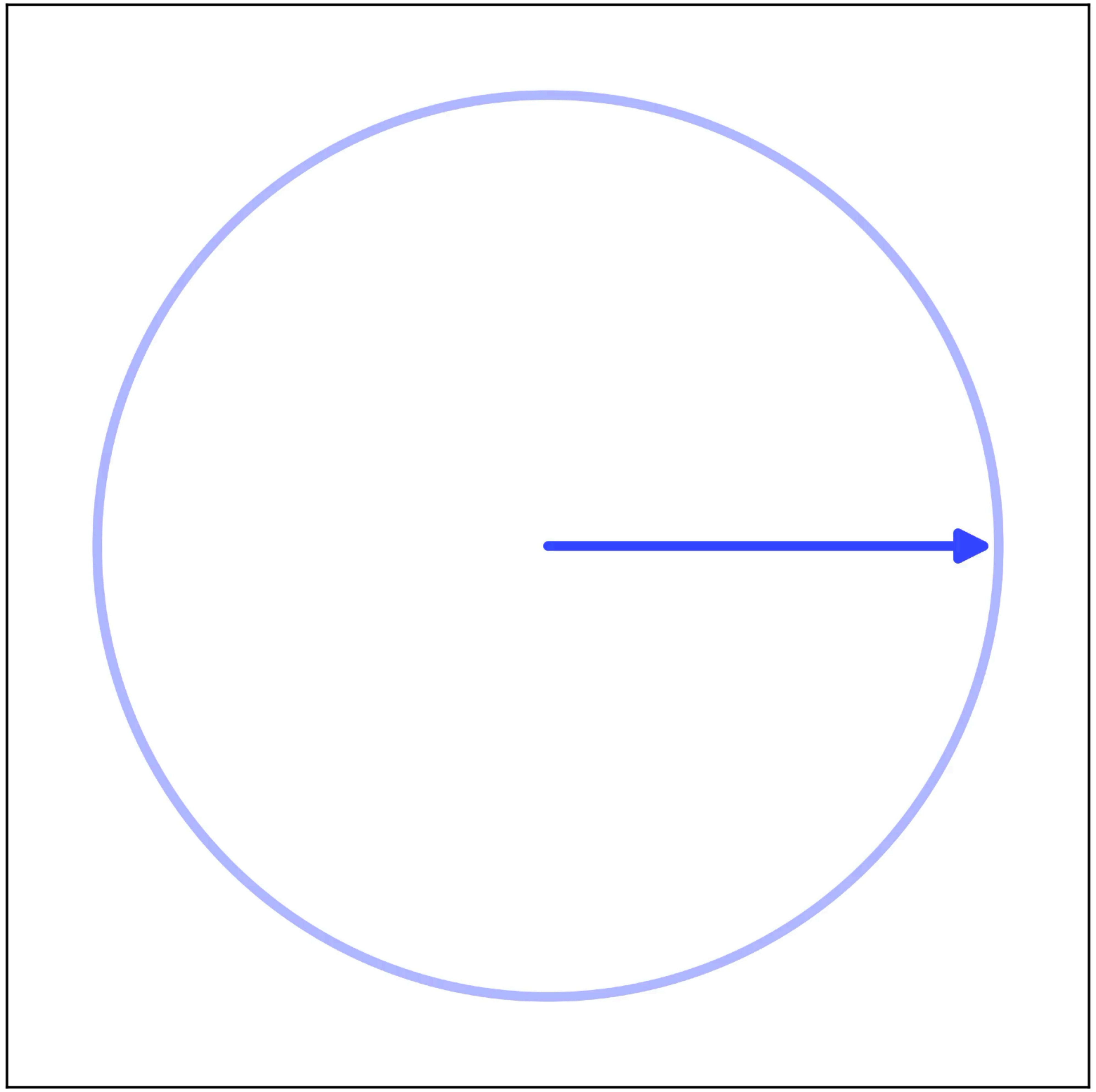
where

$$\mathbf{A} \in \mathbb{R}^{n\times n}, \ \ \lambda_i \in \mathbb{R}$$
$$\mathbf{v}_i \in \mathbb{R}^n, \|\mathbf{v}_i\| = 1$$

$$(i = 1, \ldots, n)$$

Eigendecomposition: the geometry



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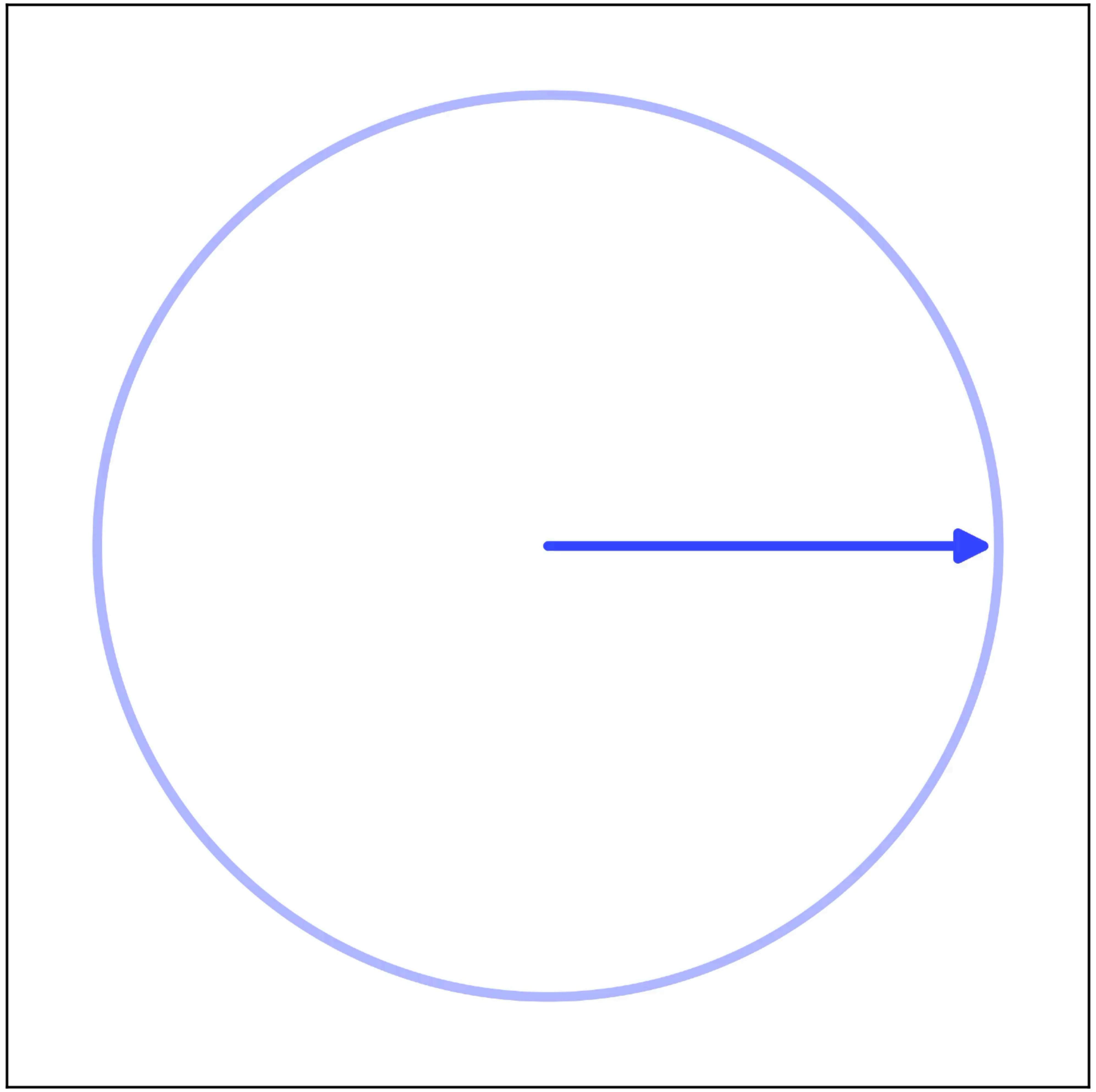

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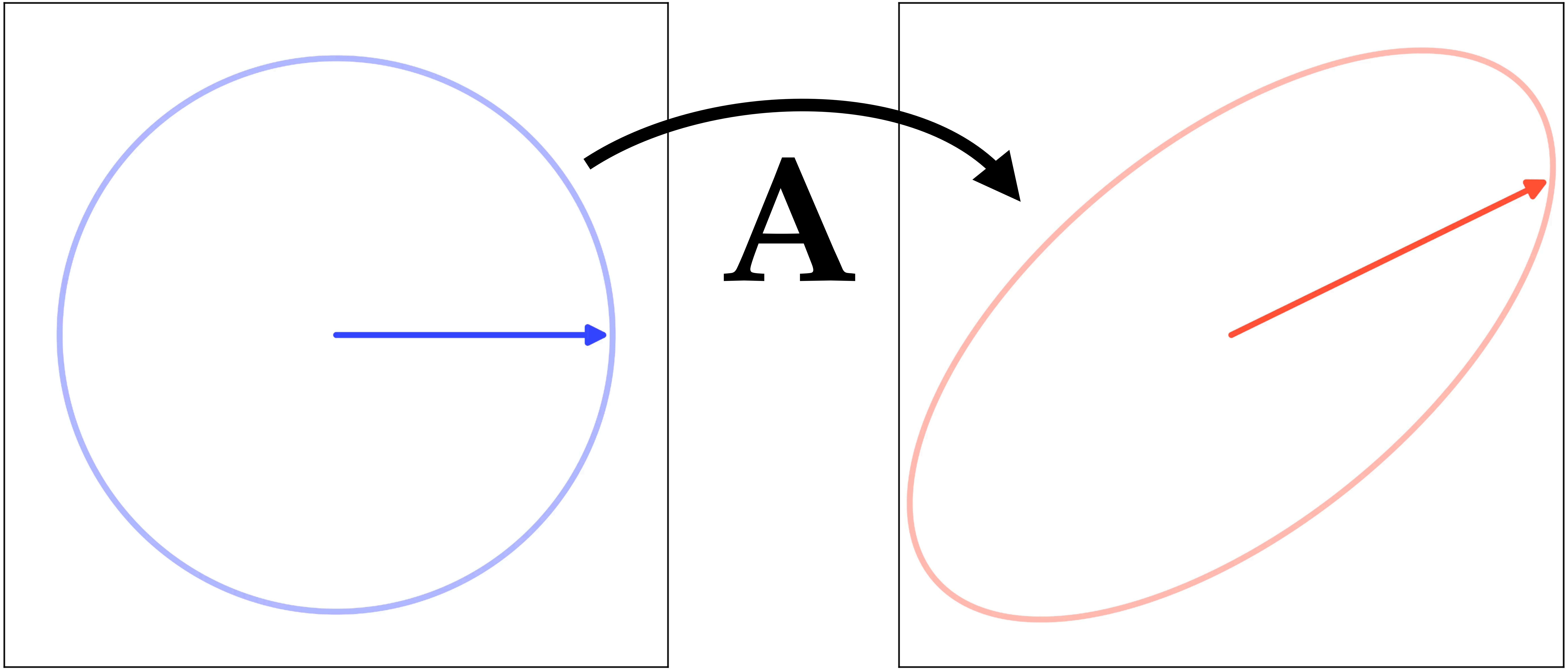

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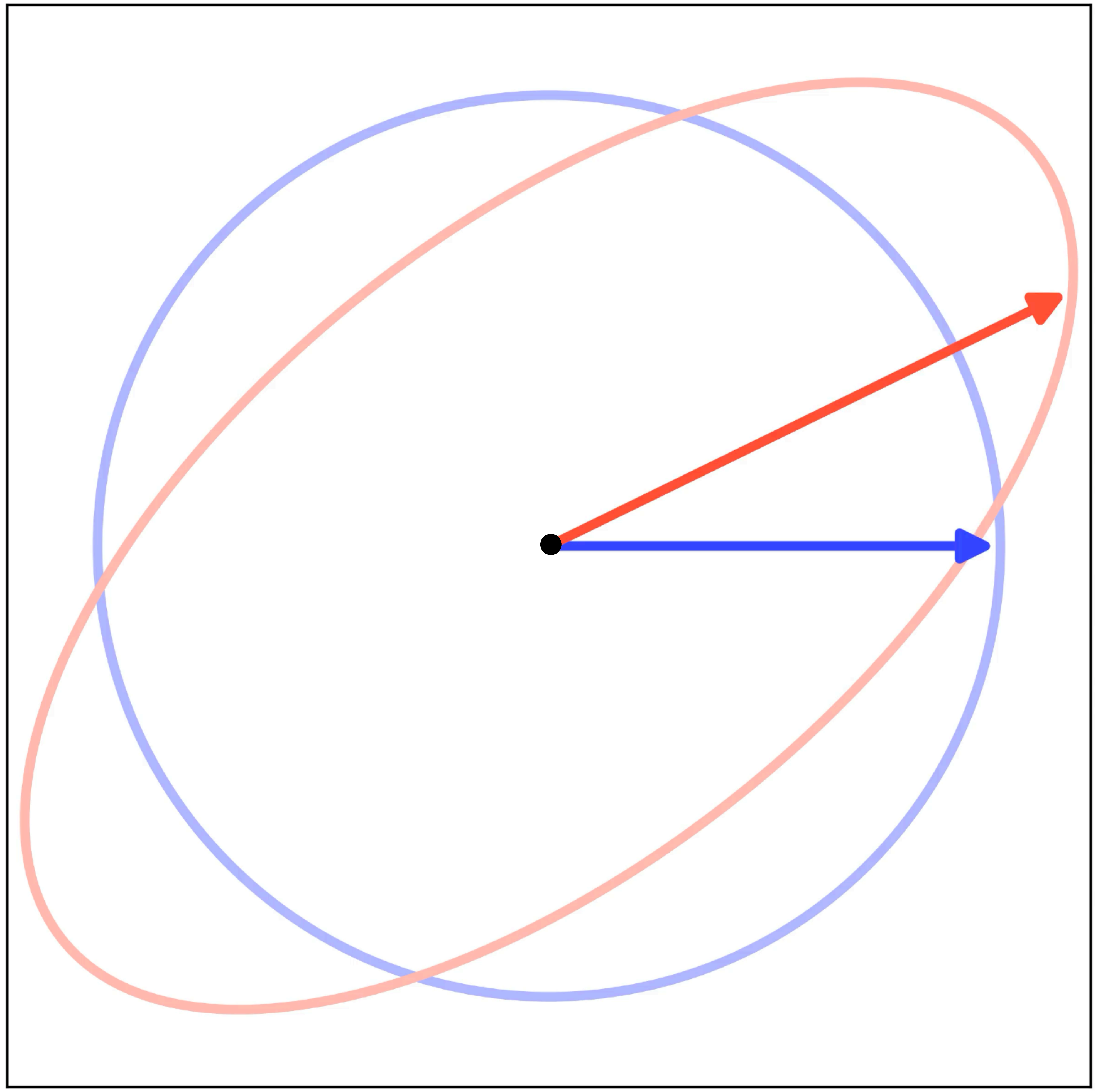

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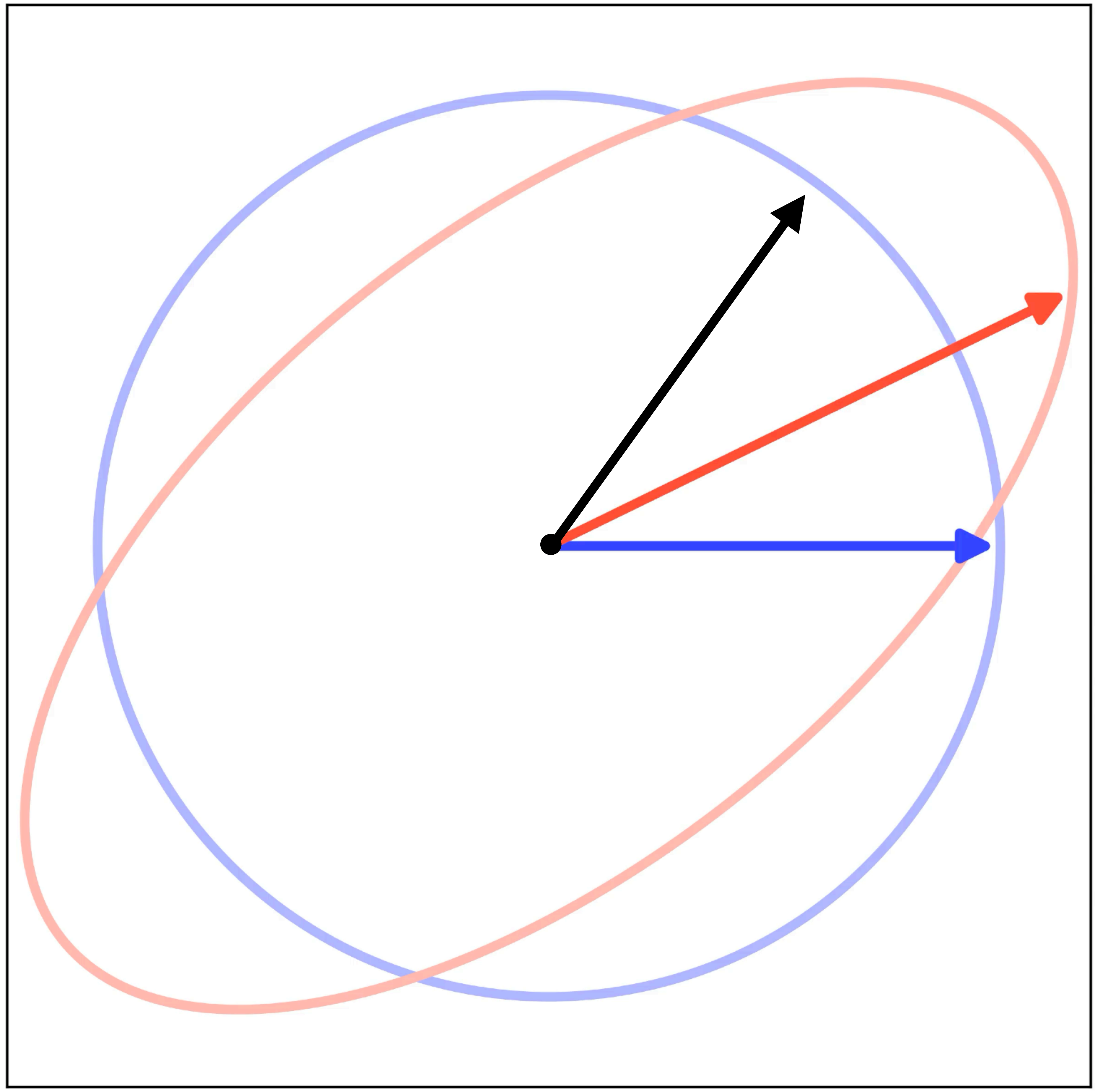

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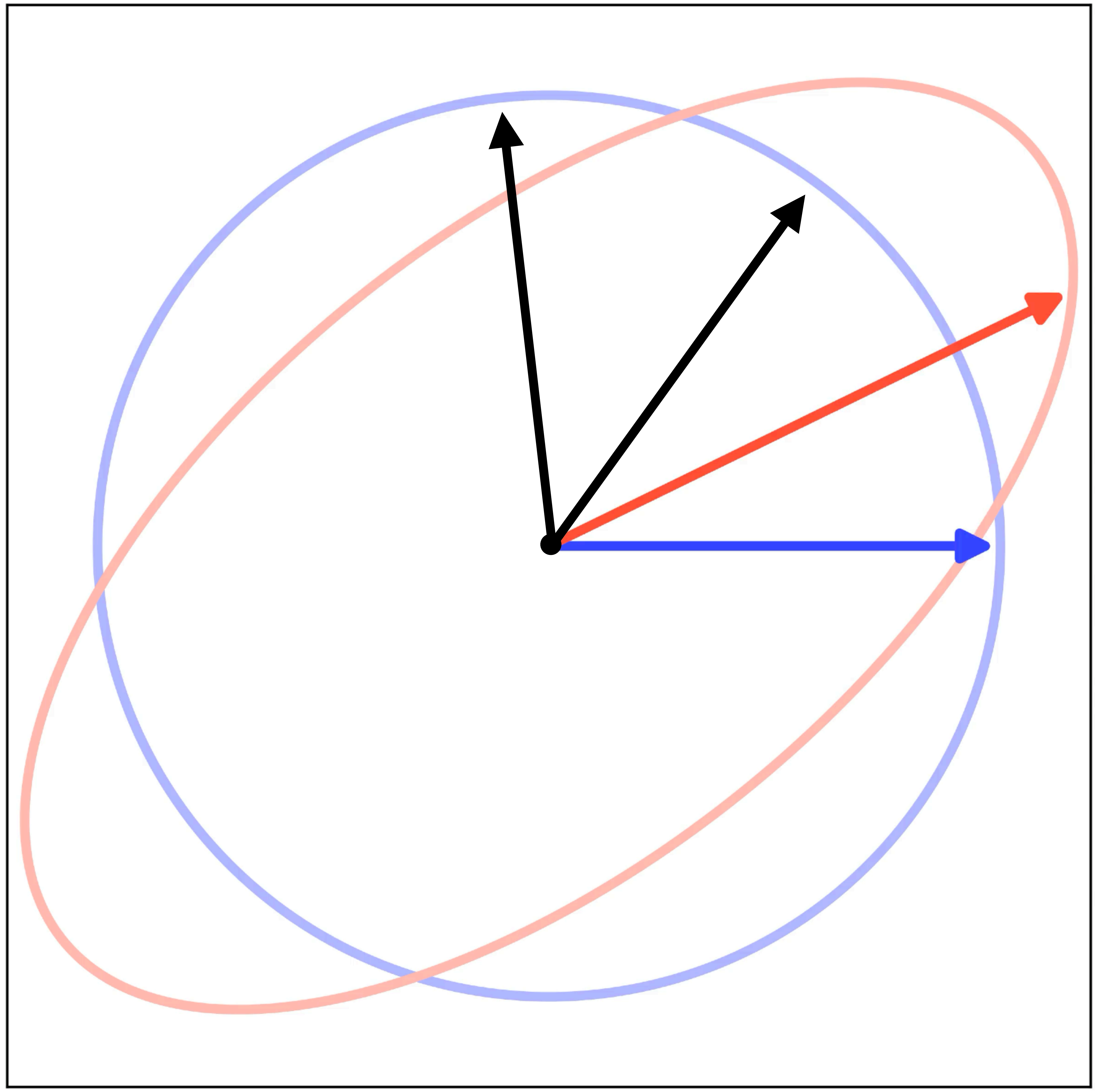

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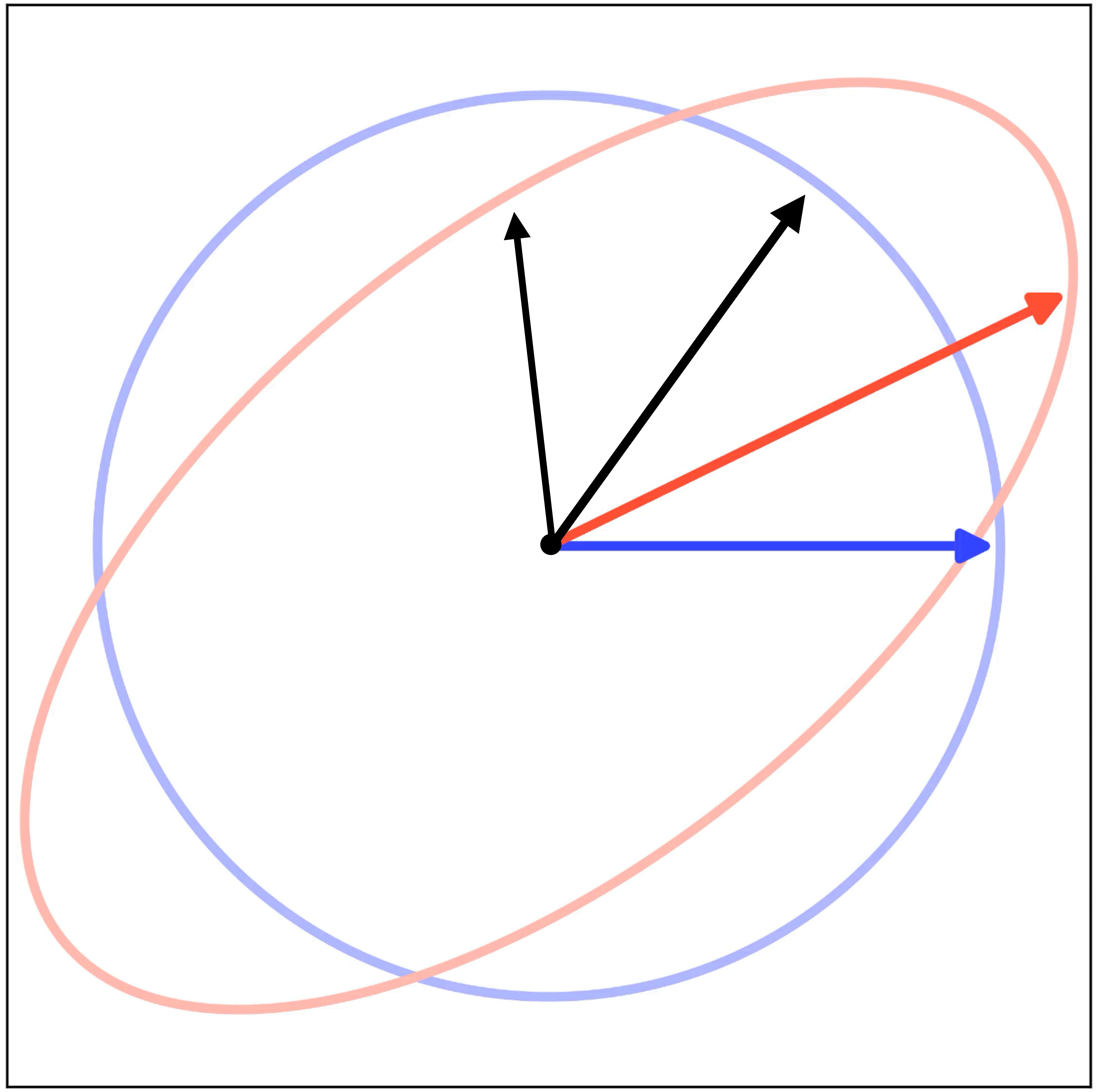

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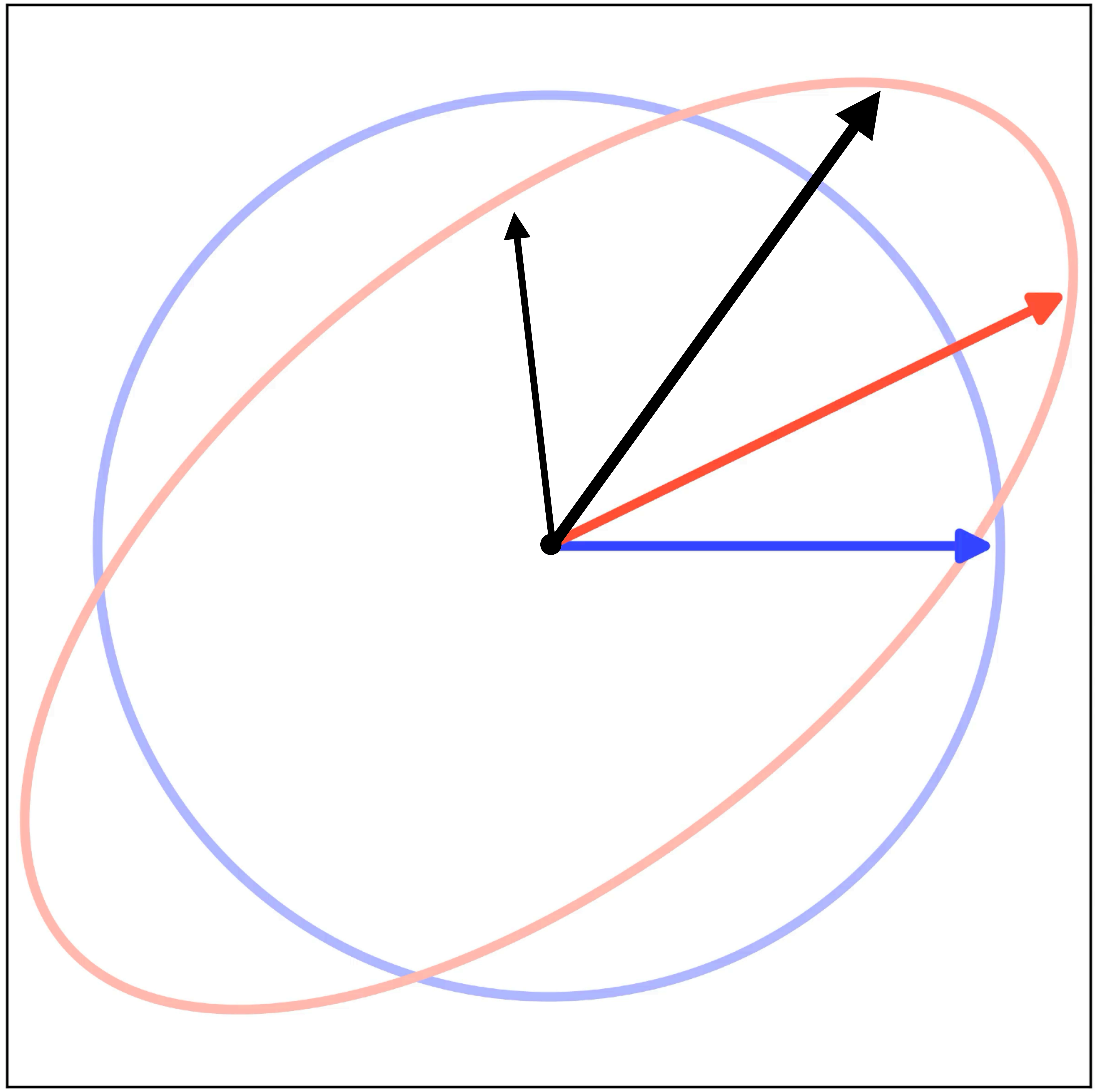

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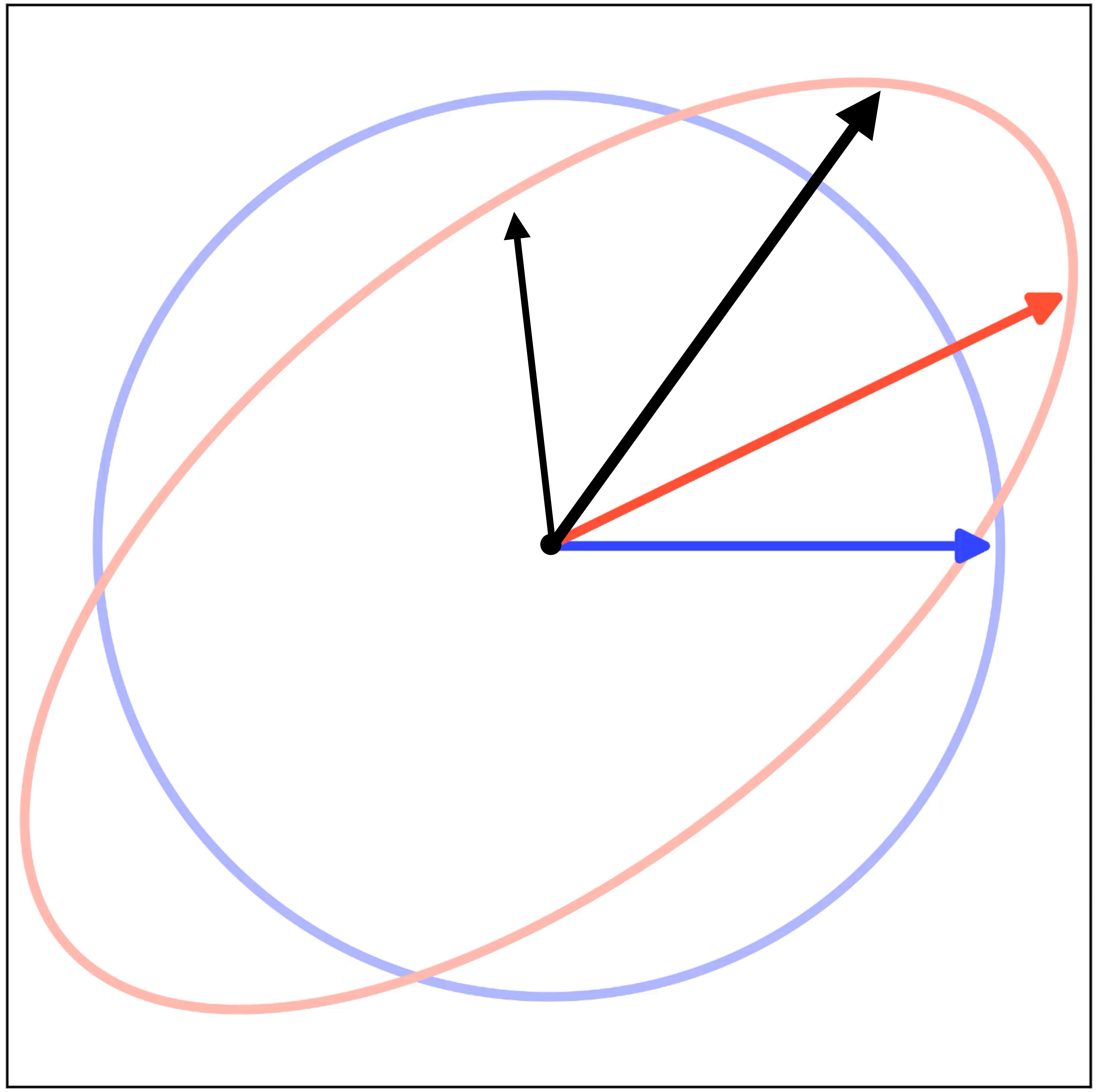

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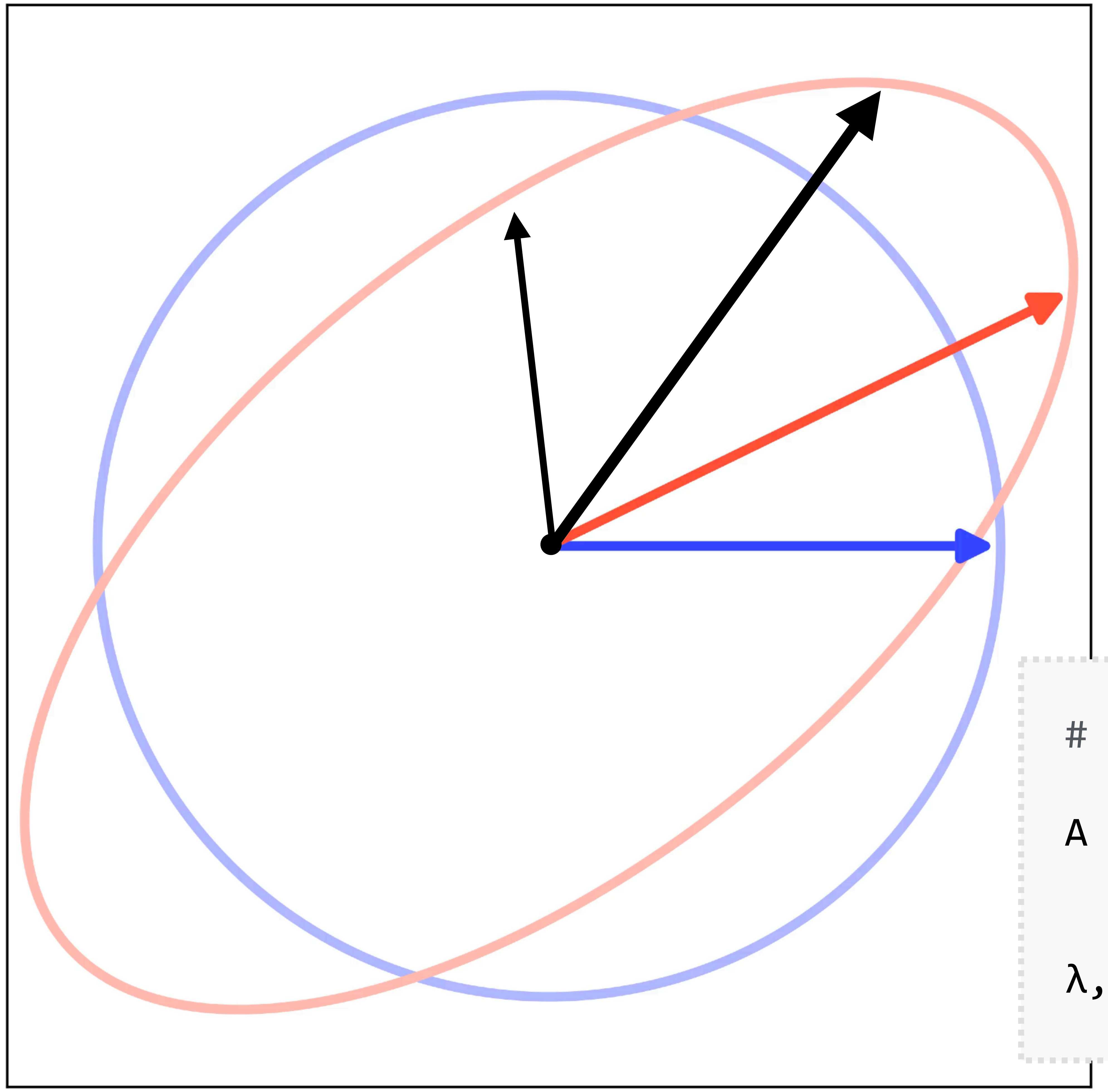

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```
# Randomly generated matrix

A = array([[ 1.16043581,  0.0566787 ],
           [ 0.56722123,  0.85777919]])

λ, V  = scipy.linalg.eig(A)
```

Eigenvectors (.. of non-singular matrices)

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- Therefore, a matrix with those $\mathbf{v}_i$ as its columns

$$\mathbf{V} = \begin{pmatrix} | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_n \\ | & & | \end{pmatrix}$$

has rank n (i.e., *full rank*) and so is non-singular

What happens when we multiply A and V?

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In other words:

$$\mathbf{AV} = \mathbf{V\Lambda}$$

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The Eigendecomposition

$$\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$$

Geometric summary

The eigendecomp. expresses a linear transformation $\mathbf{A}$ as product of 3 transforms

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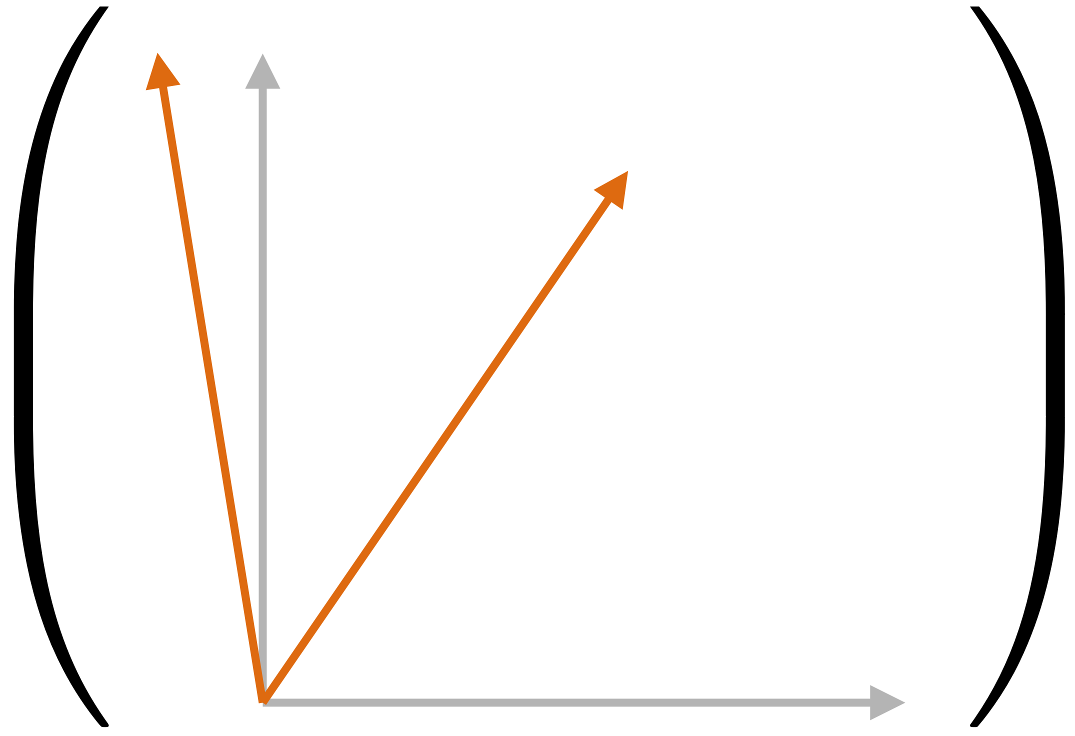

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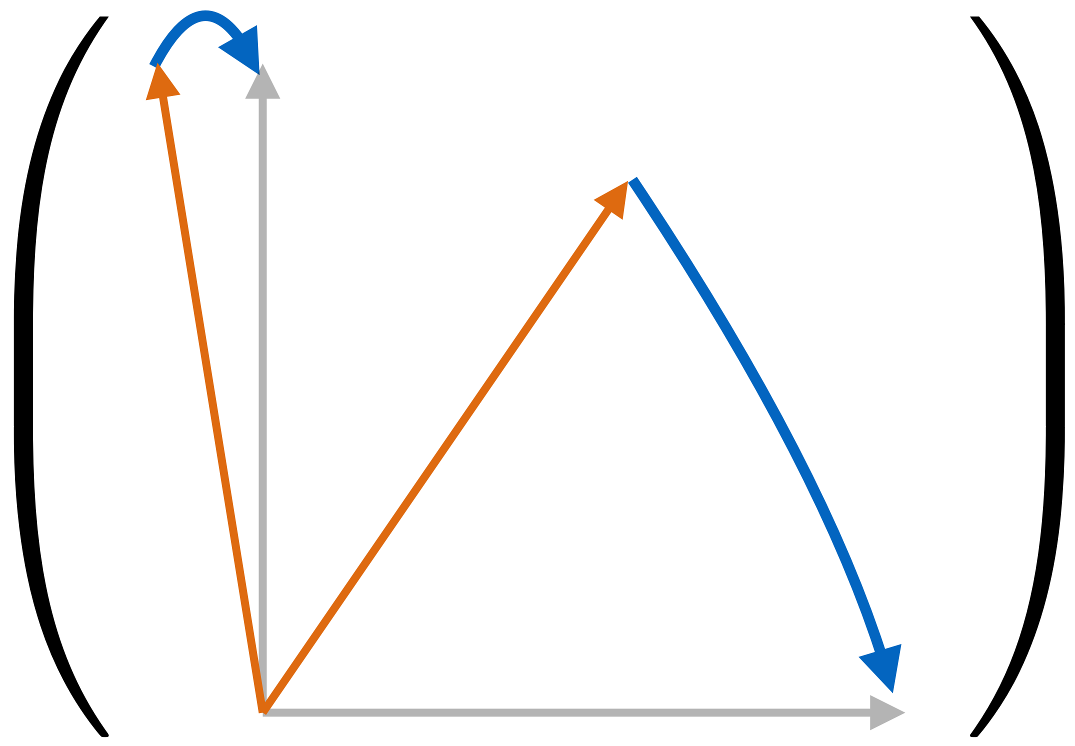

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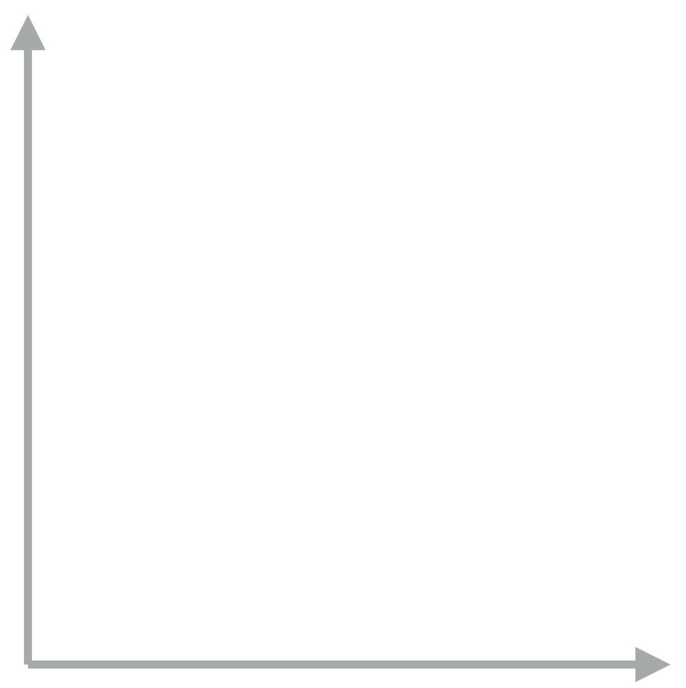
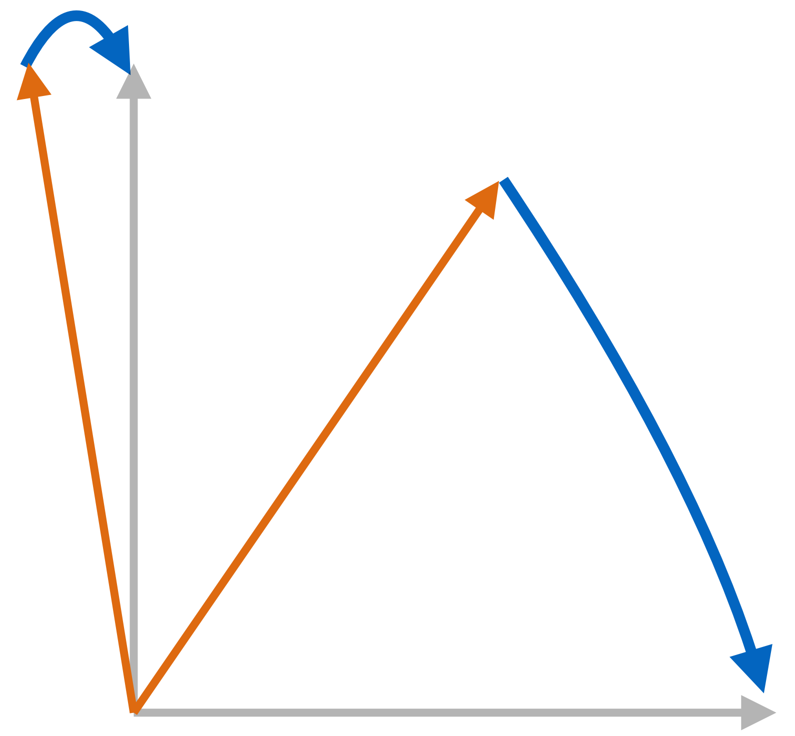


non-uniform scale



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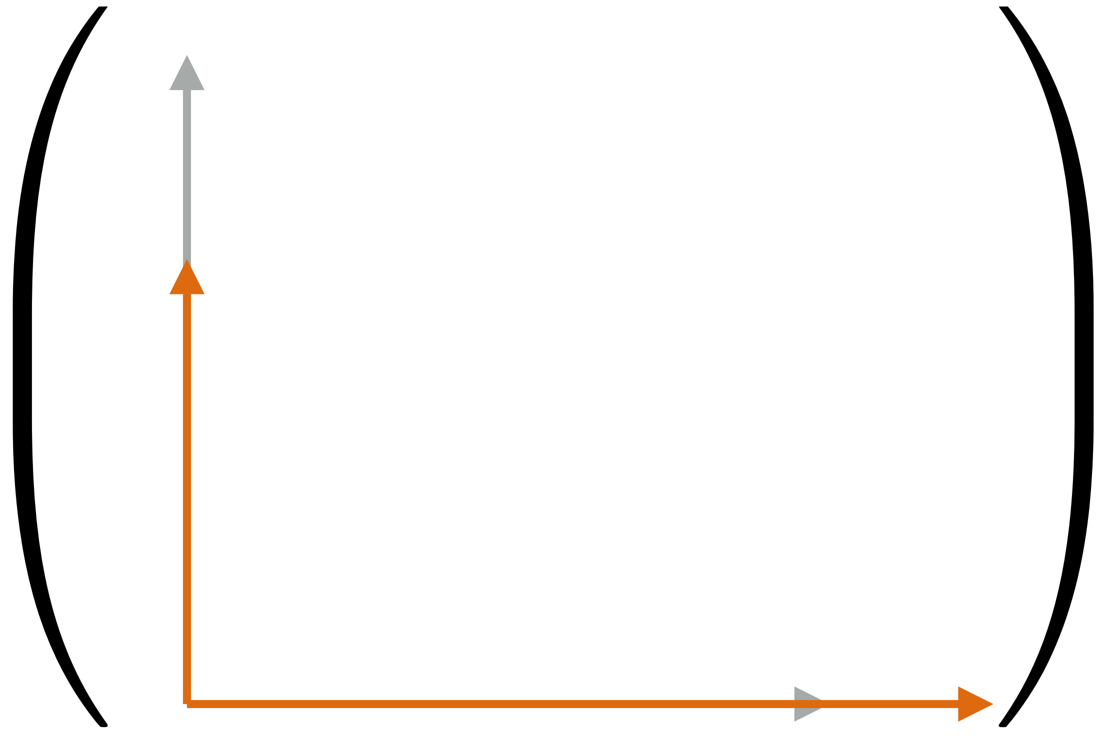

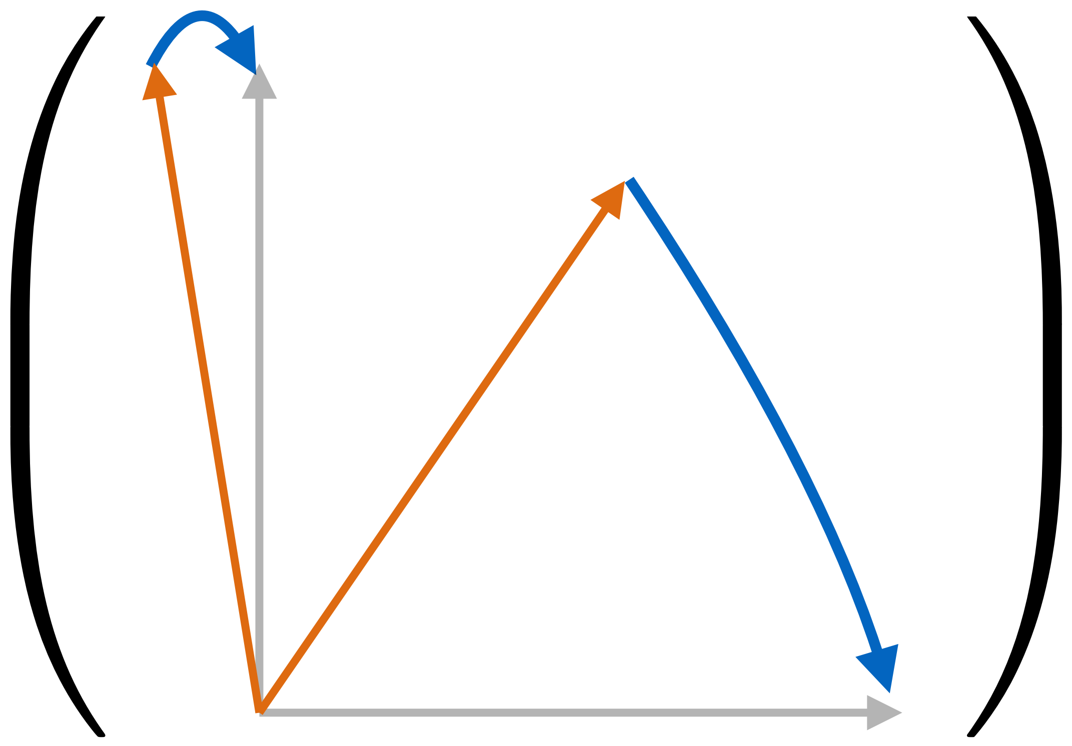

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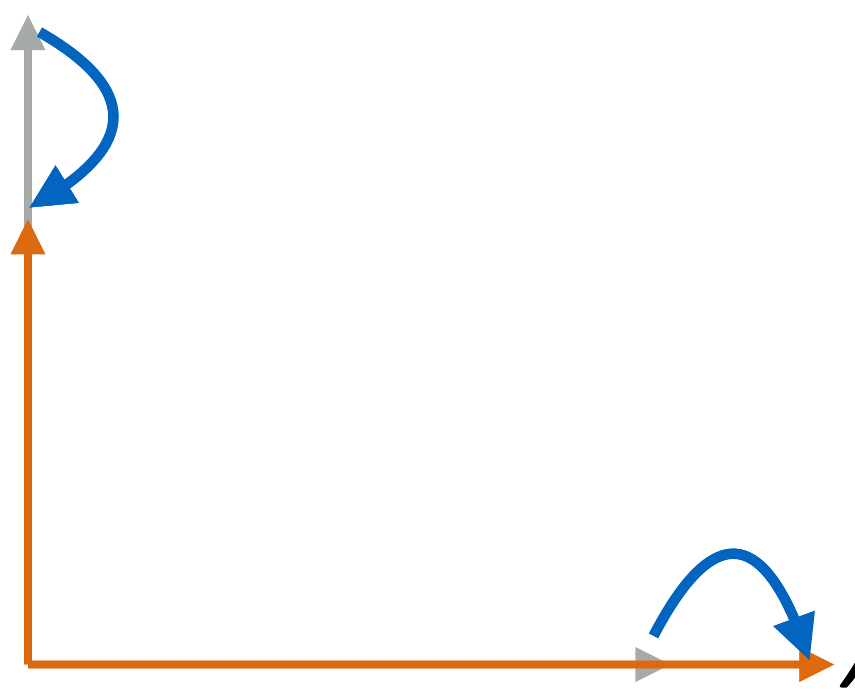

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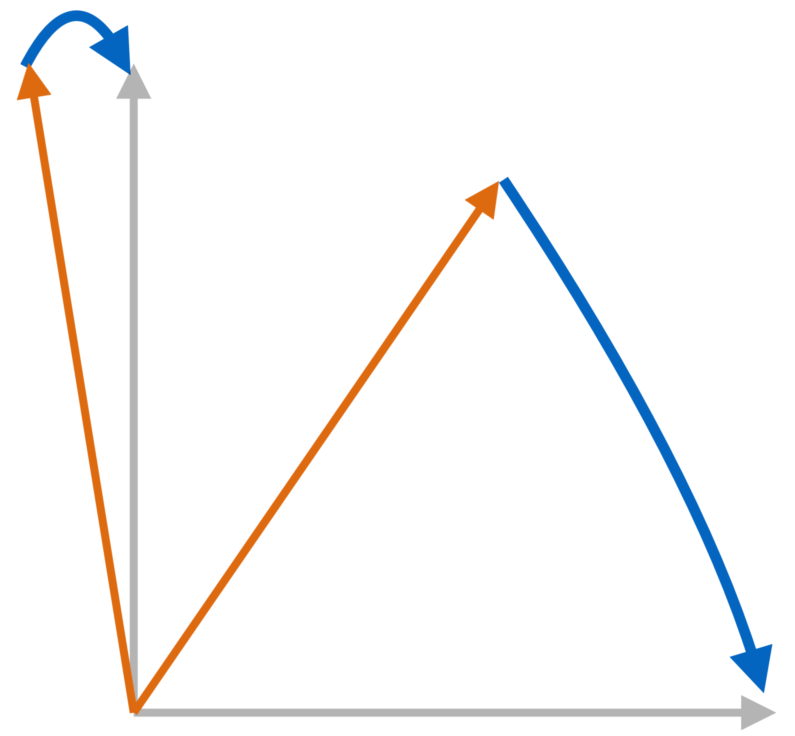

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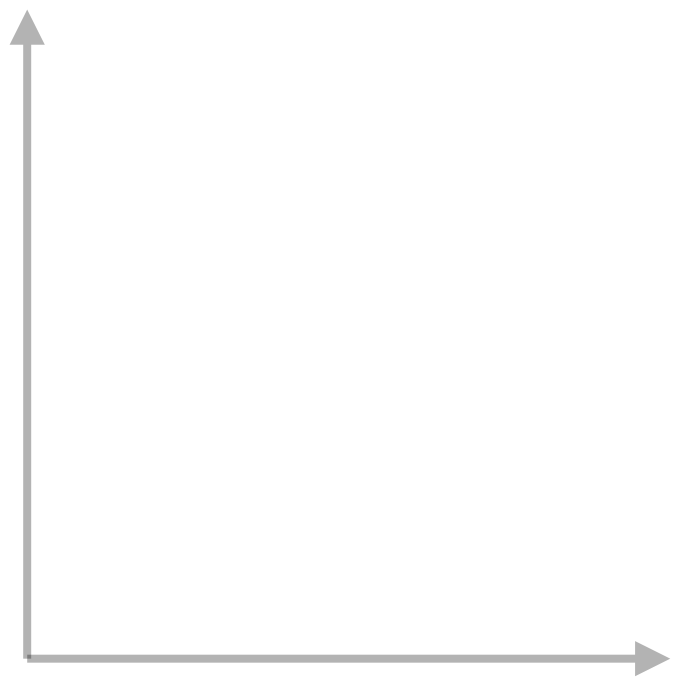

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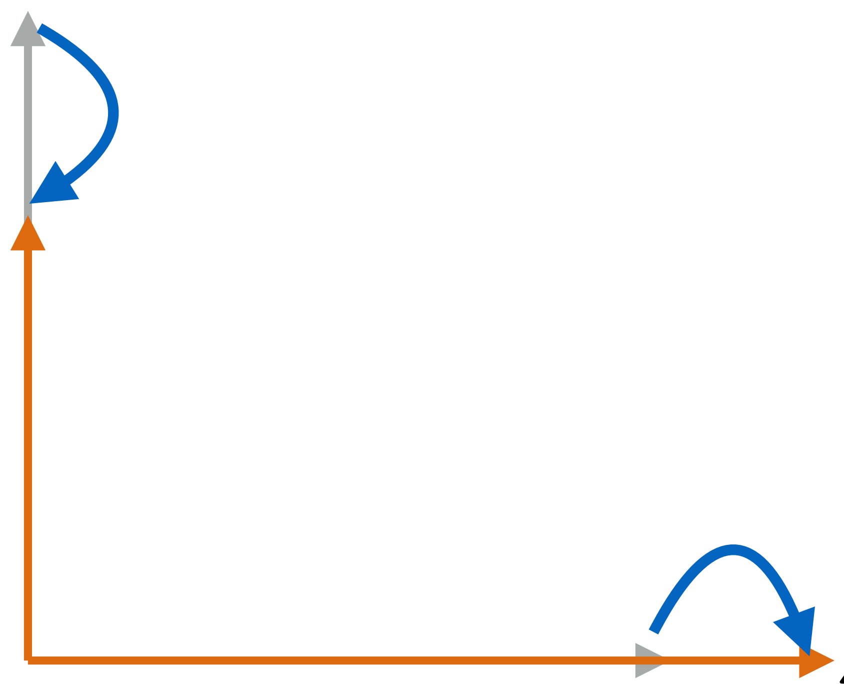

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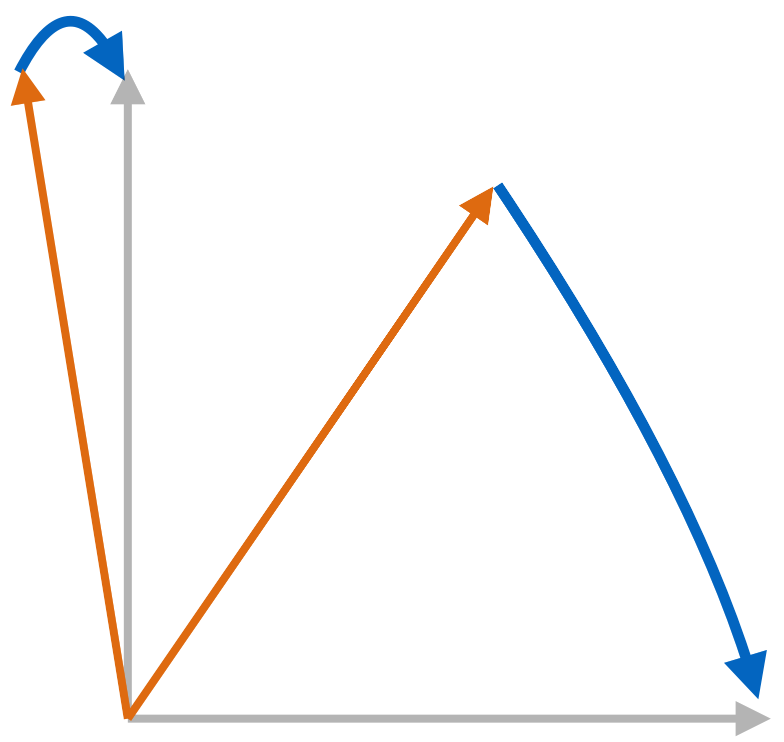

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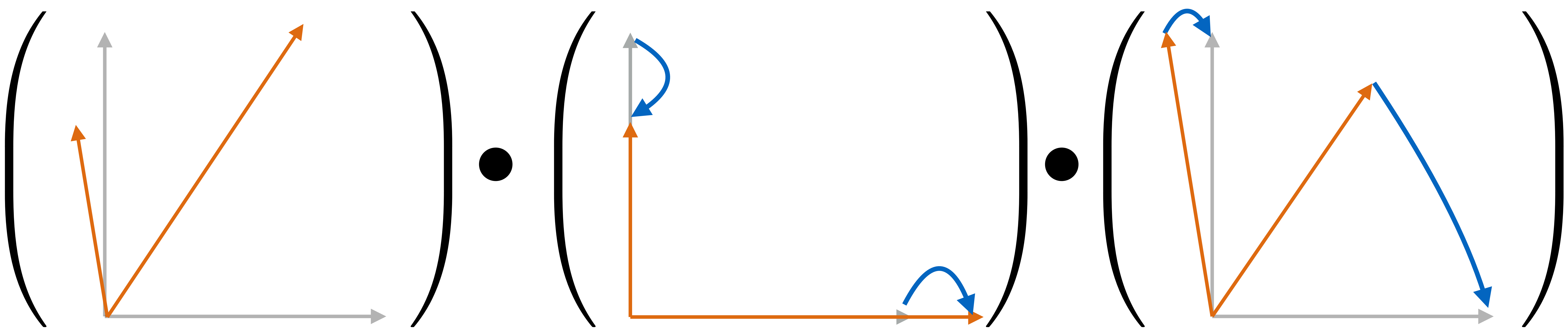

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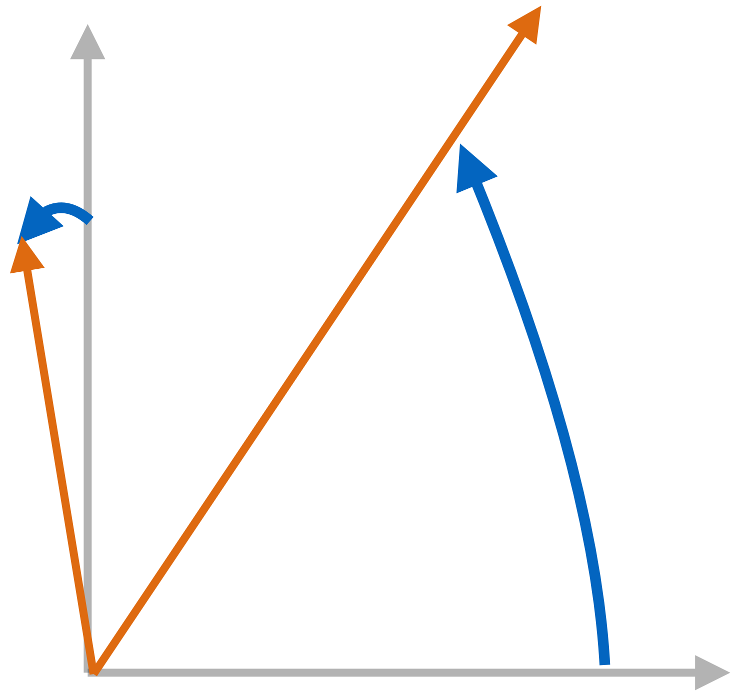

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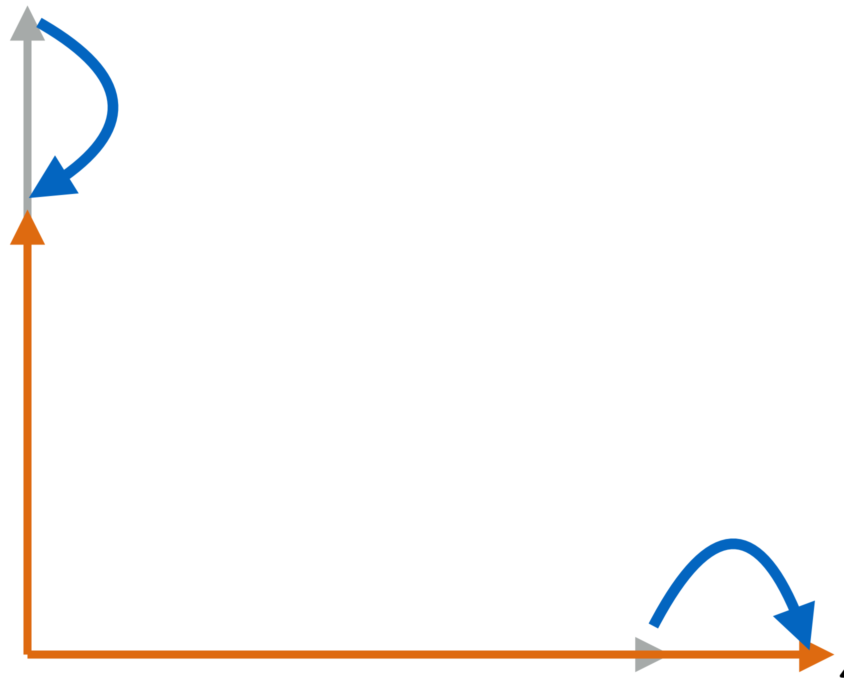

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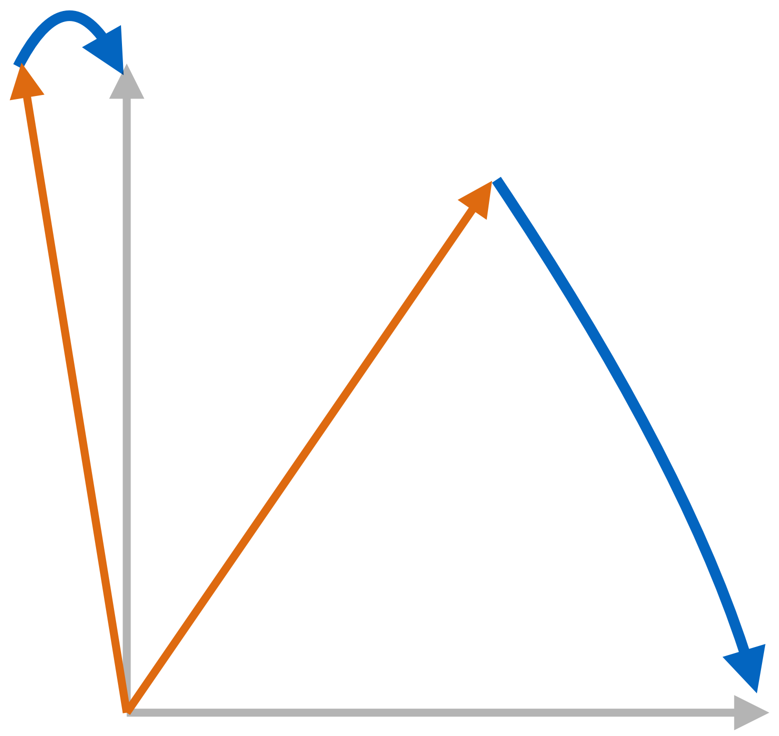

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Will see examples of all of these.
(Some in the context of SVD)

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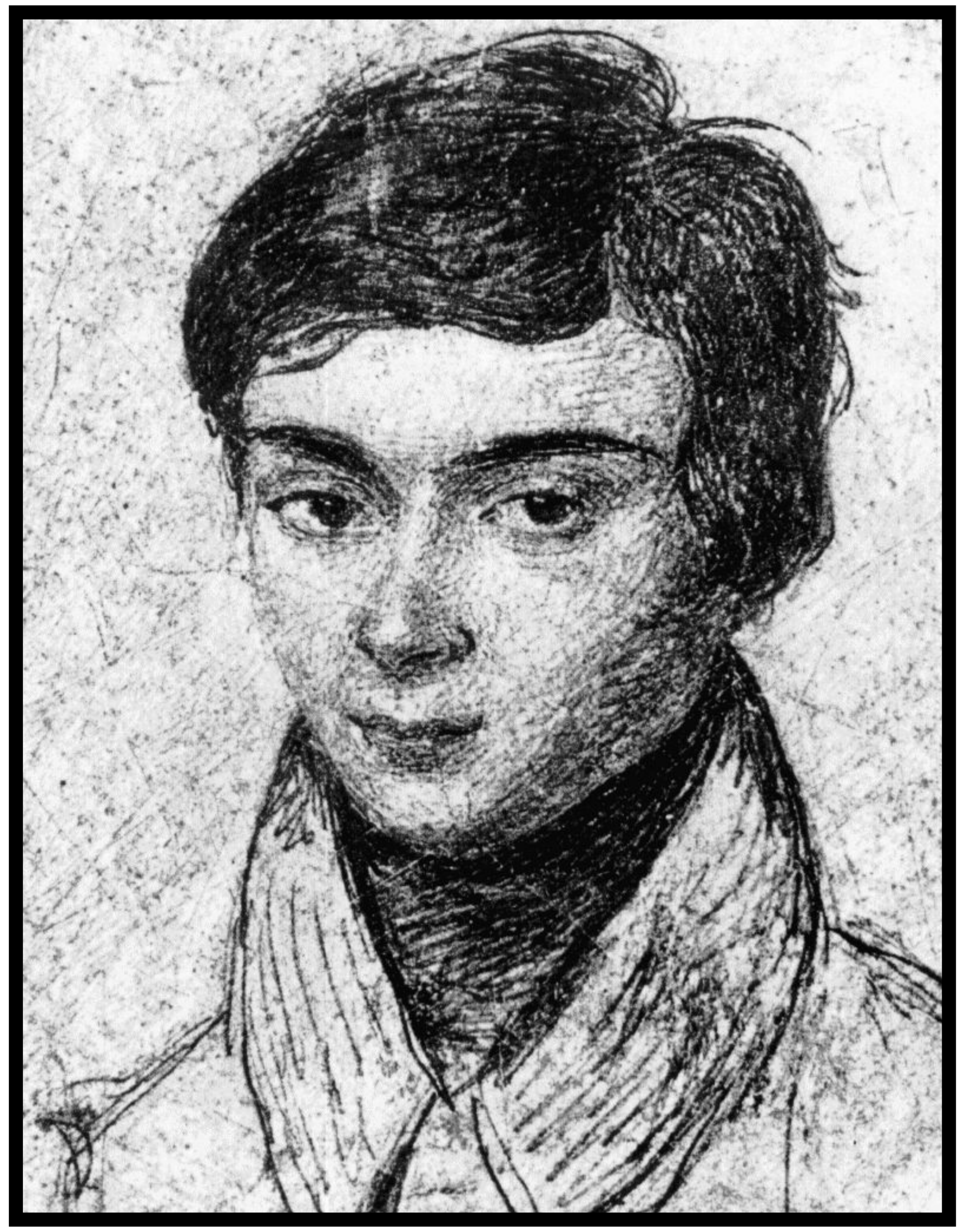

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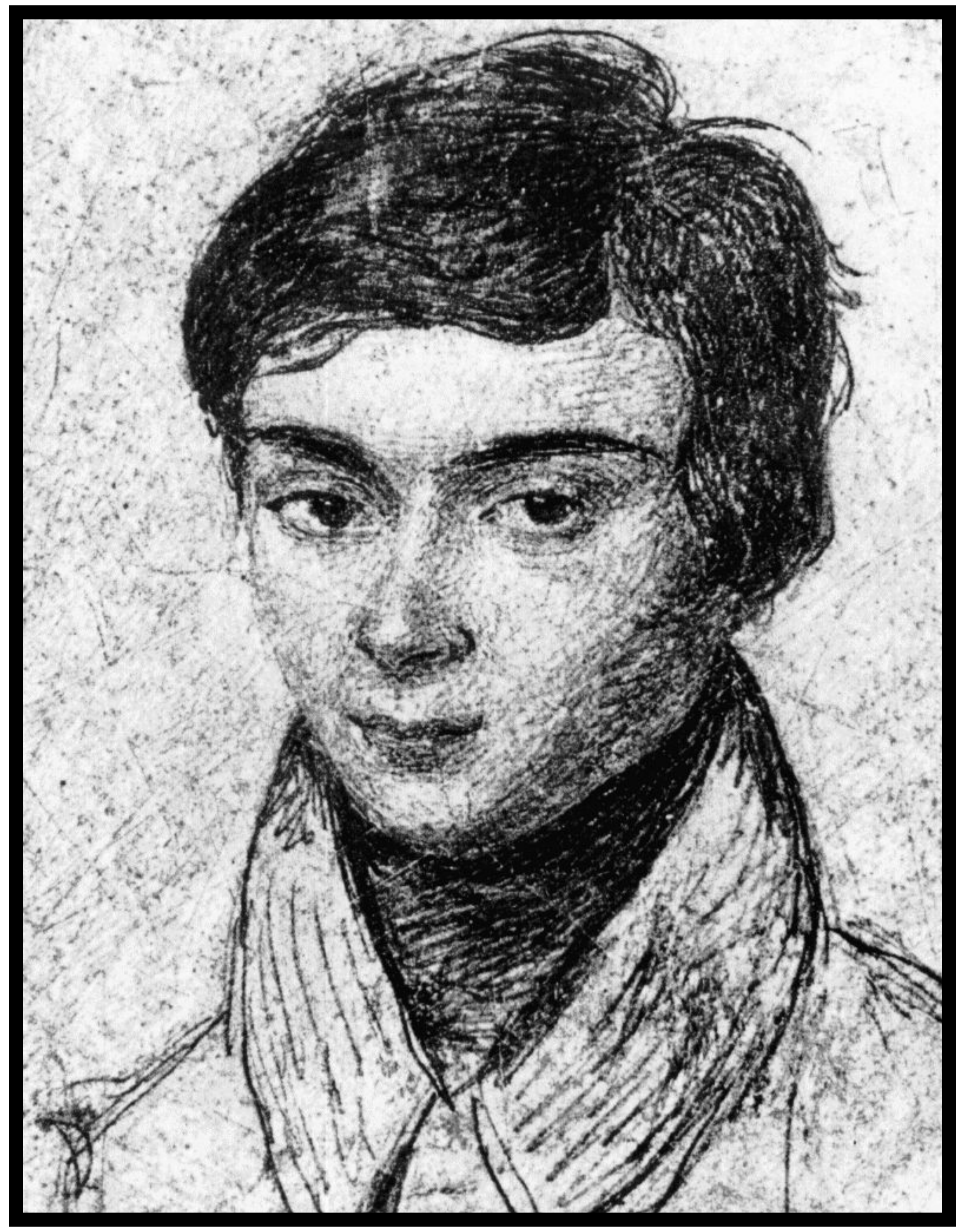

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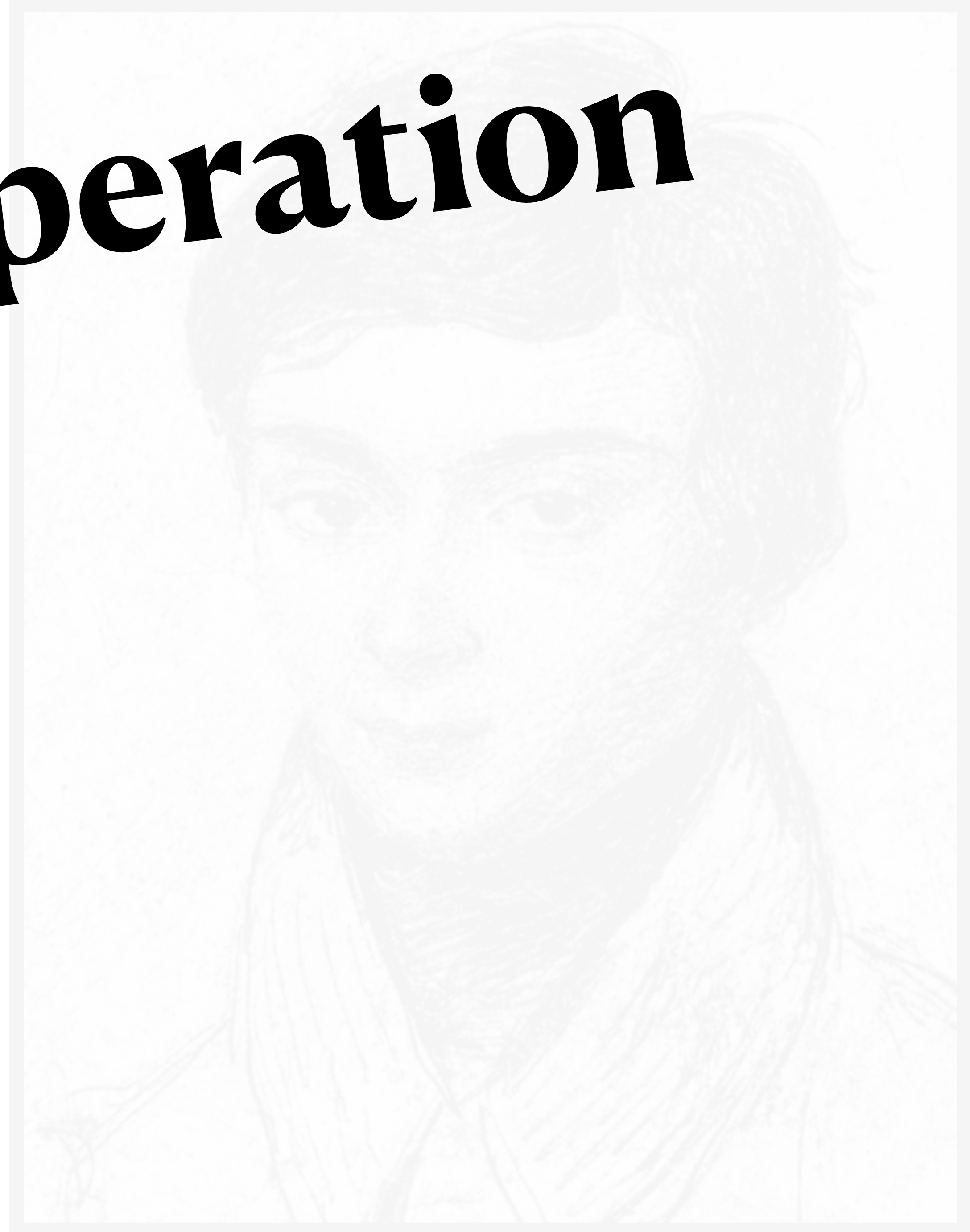

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Eigendecomposition is a **nonlinear operation** (our very first one!)

- Approximate result
- No guarantees on computation time

Matrix powers

The following works for both integer and fractional powers

- Let's compute

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$$\mathbf{A}^2 =$$

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- That includes the inverse as well:

$$\mathbf{A}^{-1} = \mathbf{V}\boldsymbol{\Lambda}^{-1}\mathbf{V}^{-1}$$

Observation when taking high powers of a matrix

(Building on the power identity from the previous slide)

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$$\mathbf{\Lambda}^k = \begin{pmatrix} \lambda_1^k & & \\ & \ddots & \\ & & \lambda_n^k \end{pmatrix}$$

As $k \to \infty$, first entry becomes **huge** compared to others.

Observation when taking high powers of a matrix

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$$\mathbf{\Lambda}^k \approx \begin{pmatrix} \lambda_1^k & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix}$$

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Power iteration

A simple method to compute the dominant eigenvector

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for i in range(num_iterations):
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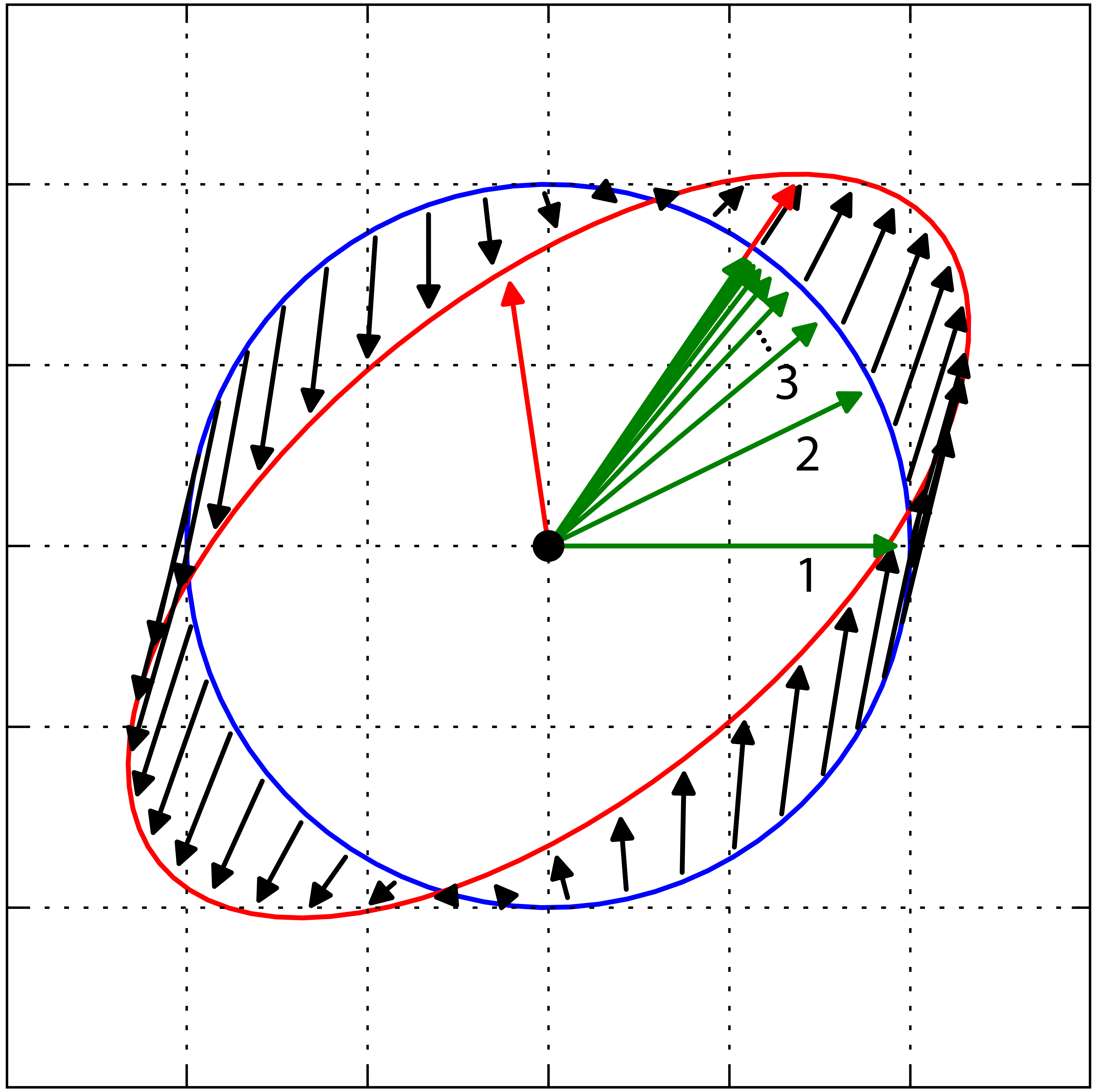

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Inverse iteration:

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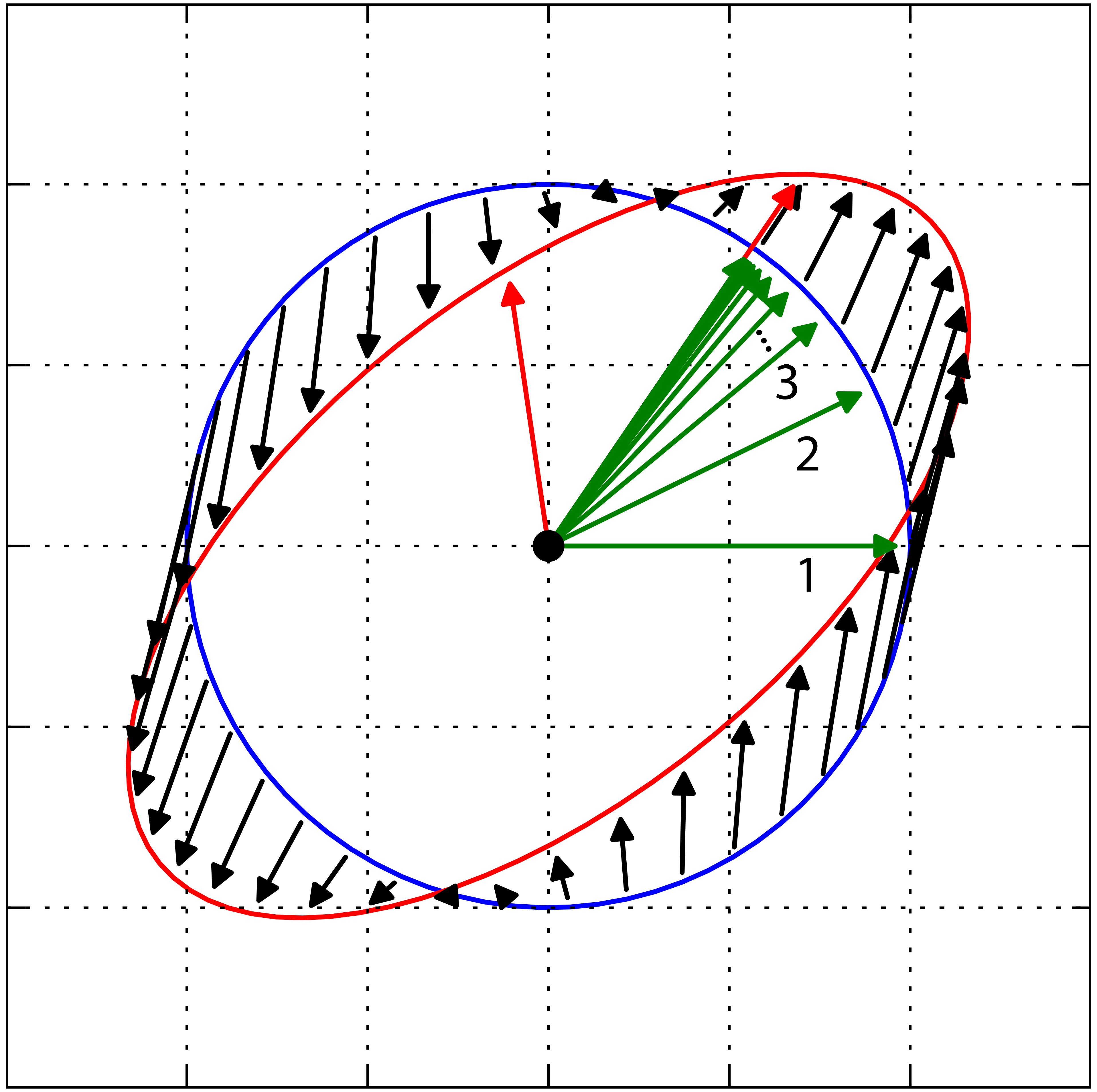
x = np.random.random(size)
A_lup = la.lu_factor(A)

for i in range(num_iterations):
    x = la.lu_solve(A_lup, x)
    x /= np.linalg.norm(x)
```



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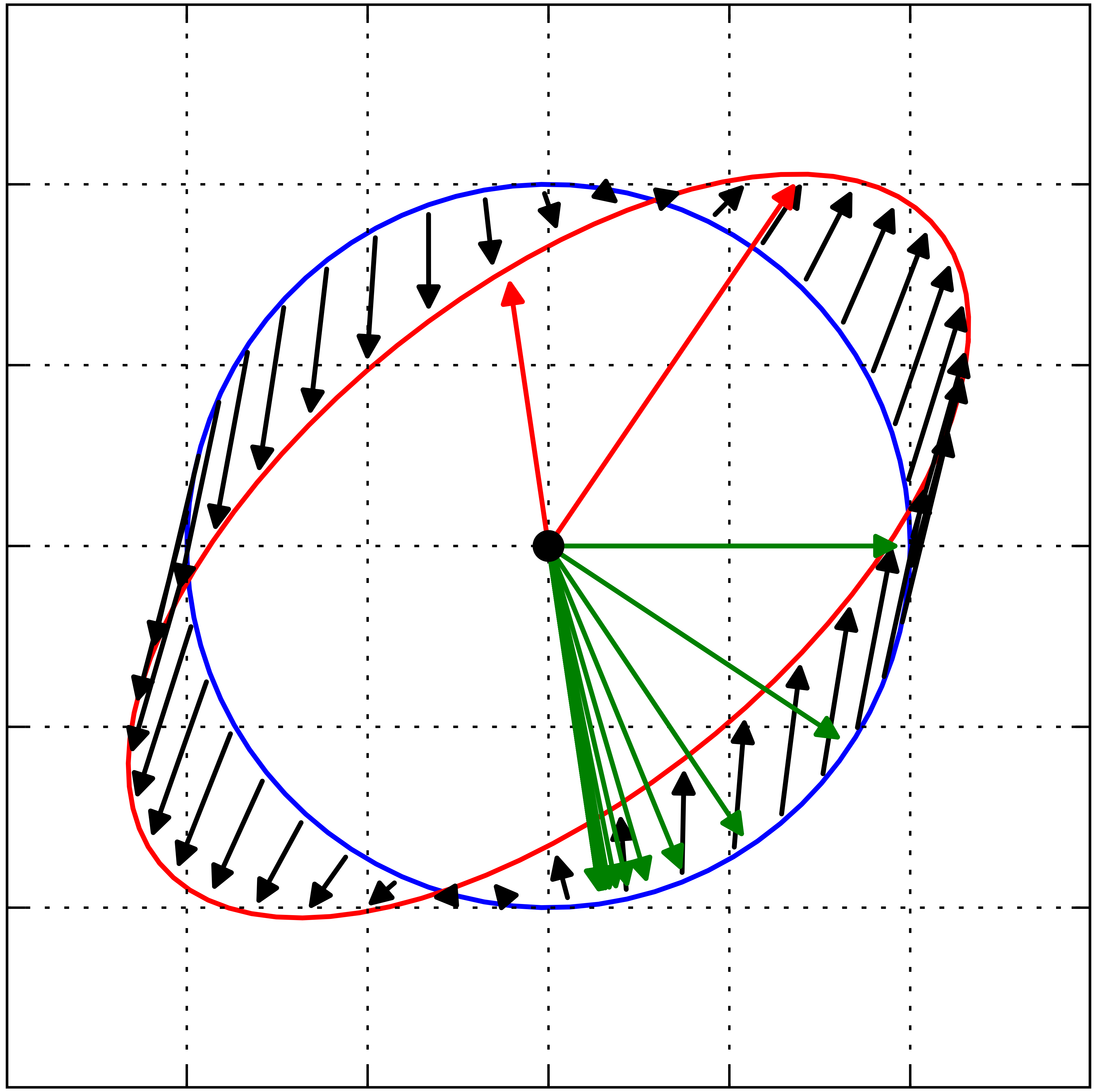

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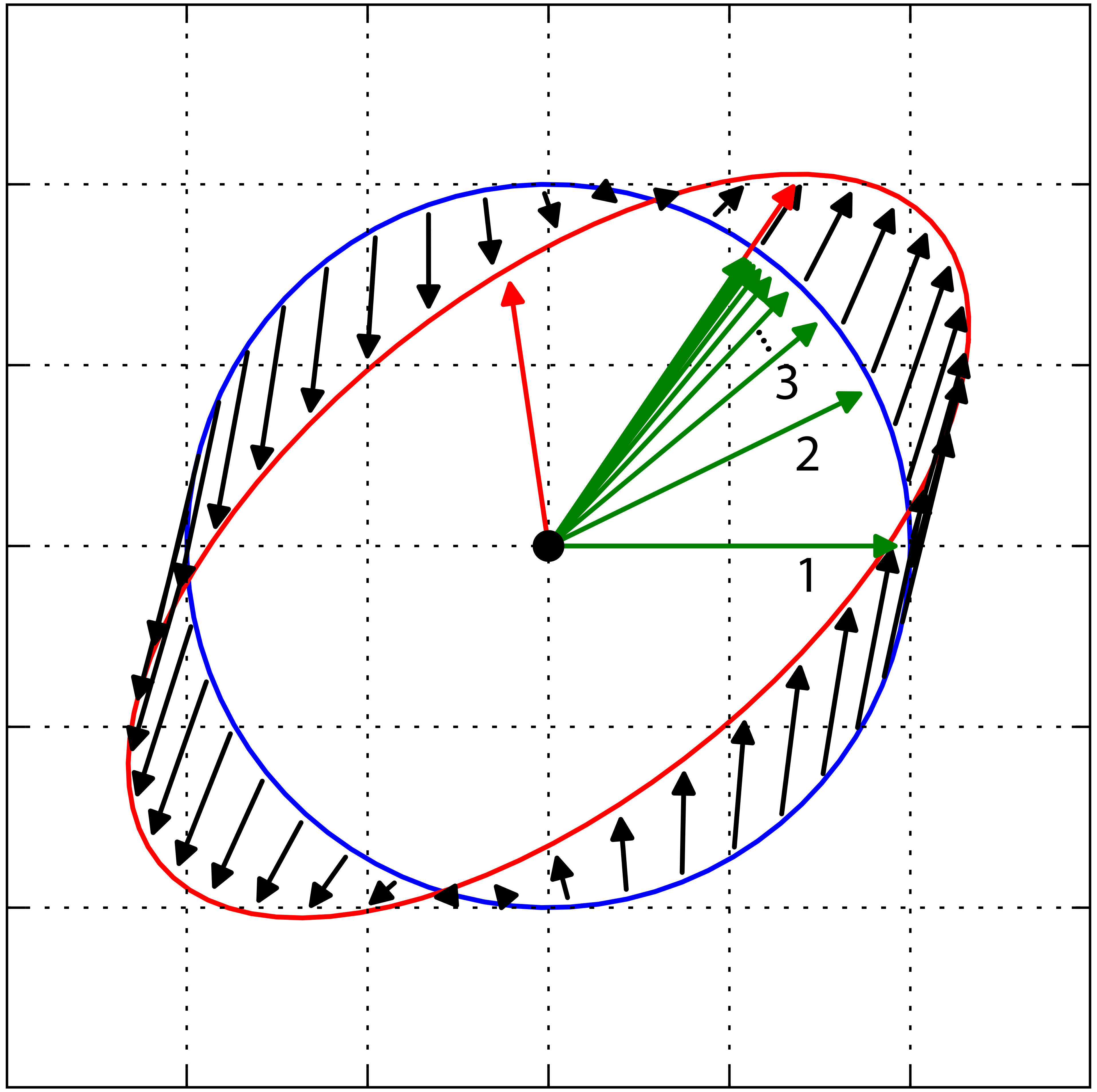

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QR algorithm

[Link: Detailed explanation]

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$$\mathbf{A}_{k+1} = \mathbf{R}_k \mathbf{Q}_k$$

[Link: Detailed explanation]

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Demo time

QR algorithm

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- Intuition: Run n instances of the power iteration at the same time.
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- **In practice**: many subtleties, use libraries and don't build your own version.

Application: Solving linear ODEs

Simple homogeneous ODE: $x'(t) = ax(t)$

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A way to evaluate $\exp(\mathrm{A})$ when A is a matrix.

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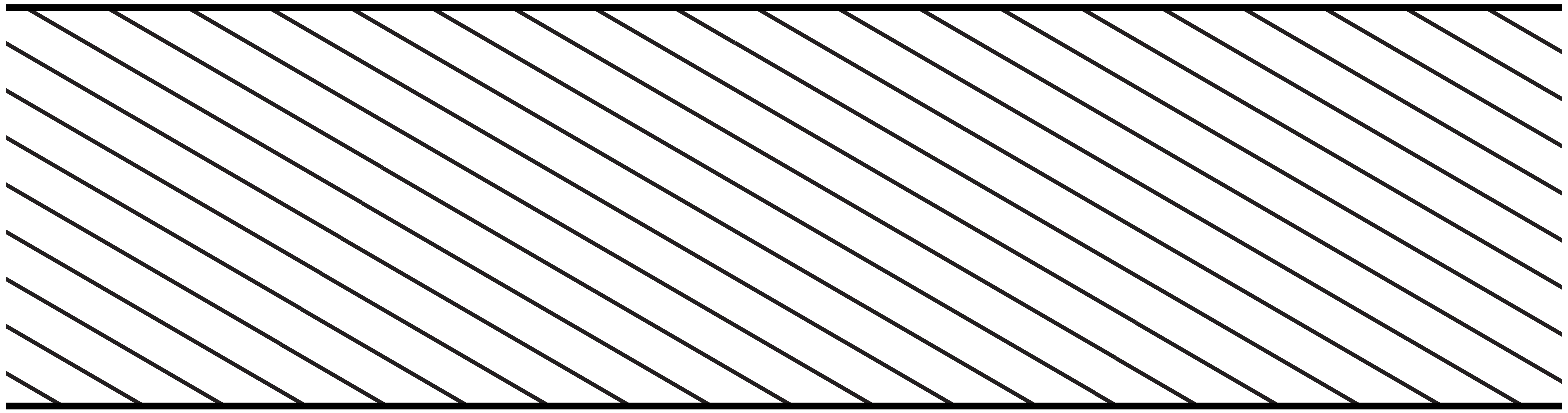
$$e^{\mathbf{\Lambda}} = \begin{pmatrix} e^{\lambda_1} & & \\ & \ddots & \\ & & e^{\lambda_n} \end{pmatrix}$$

A random example from my own research

Scattering in dusty layers



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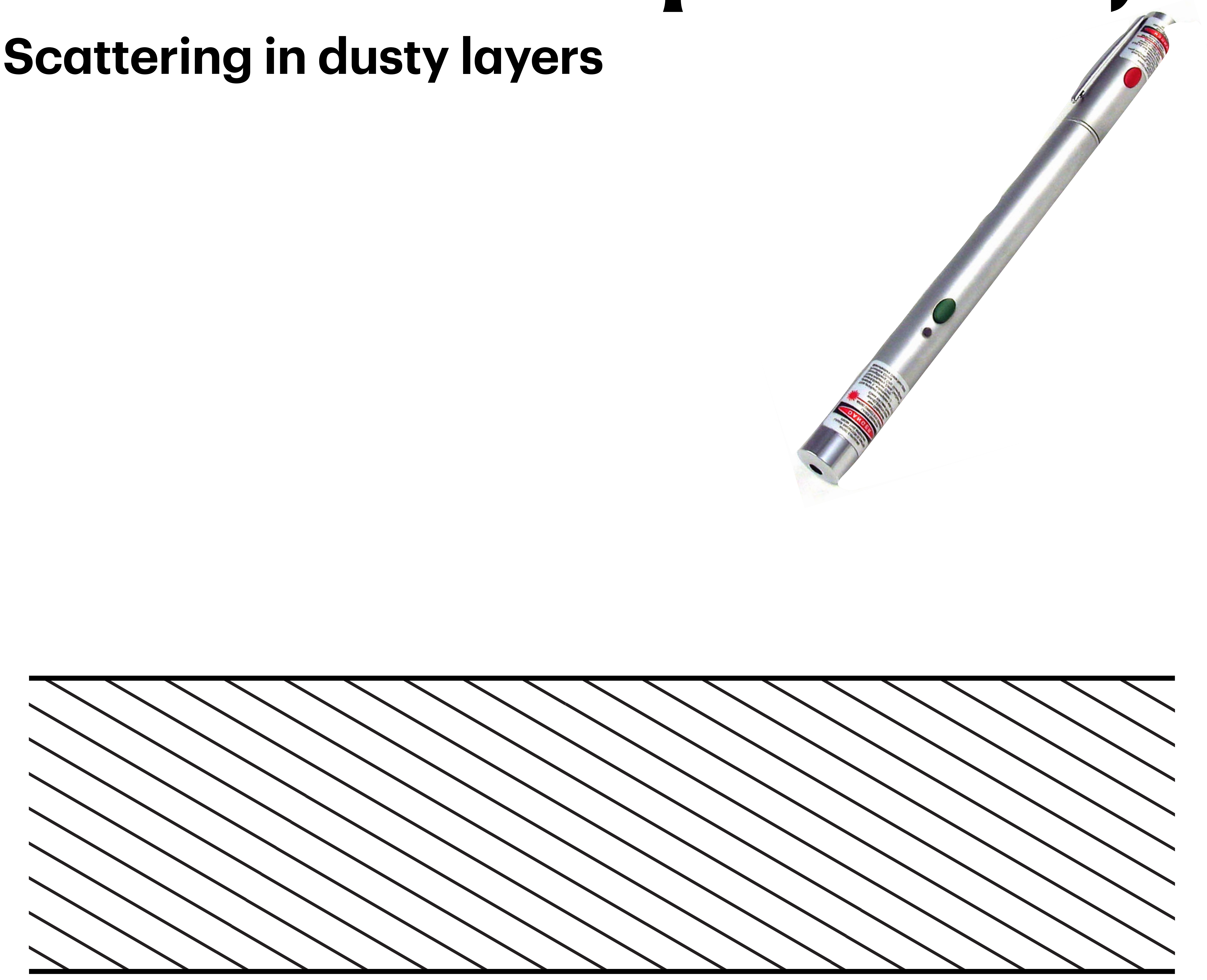

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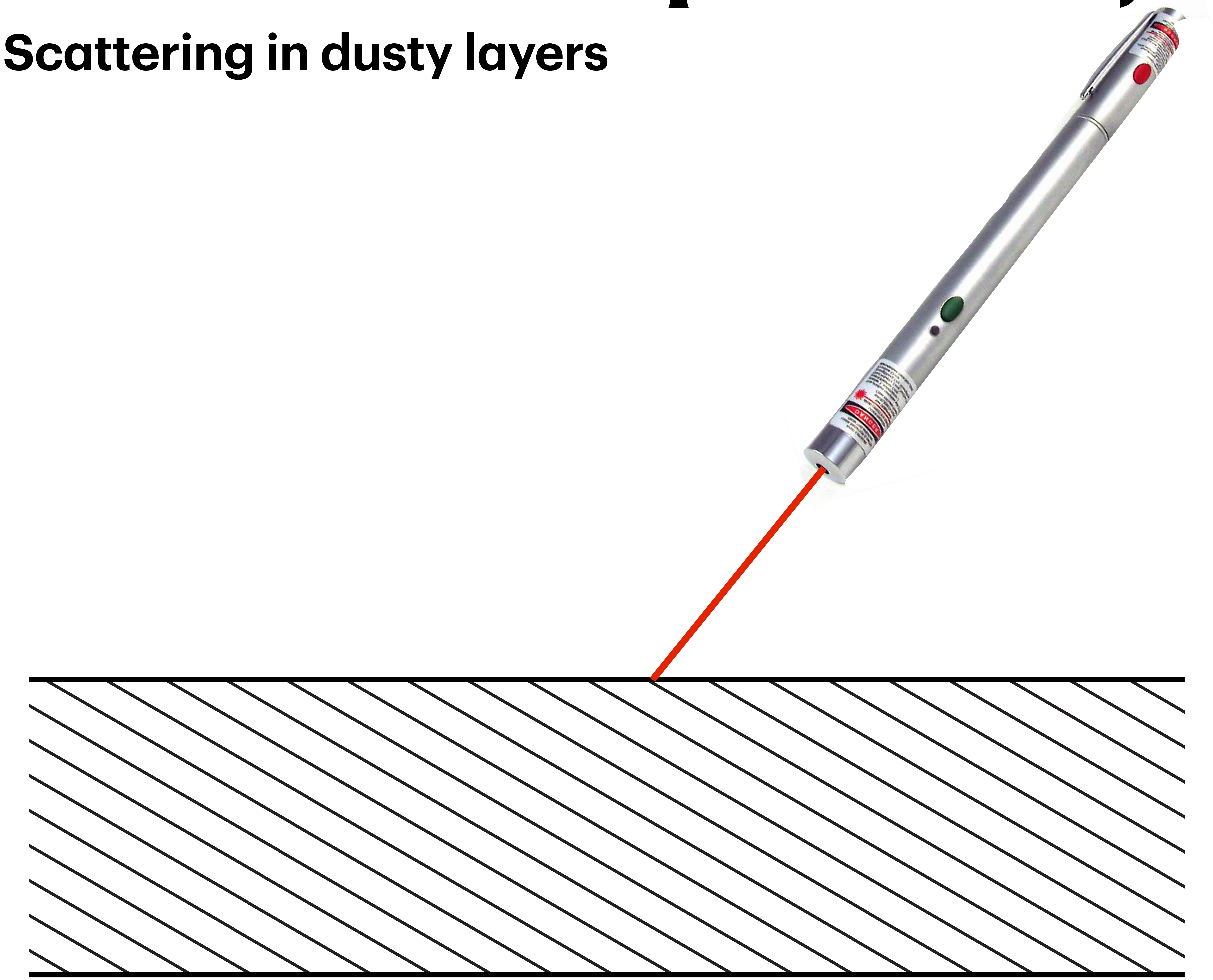

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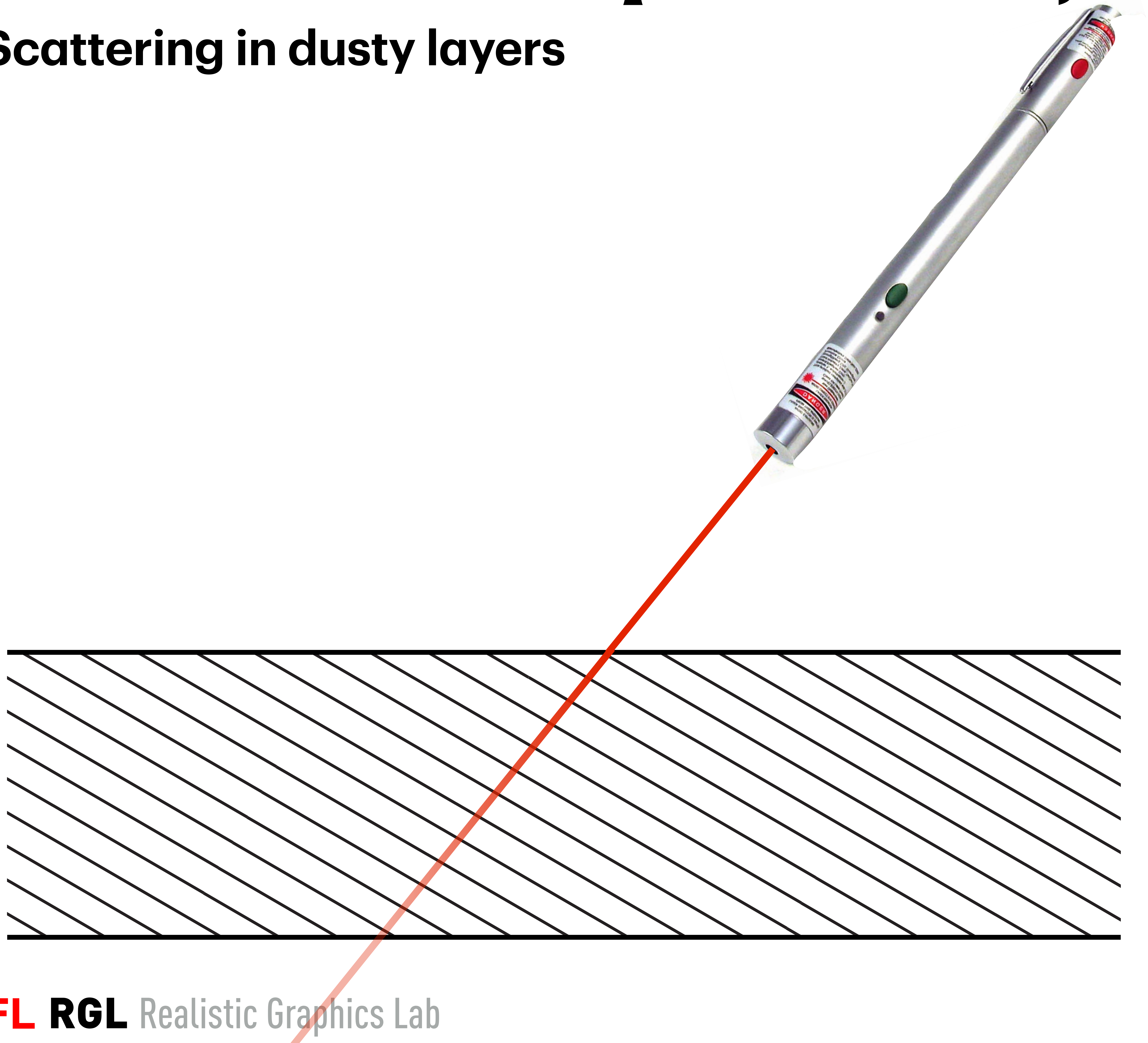

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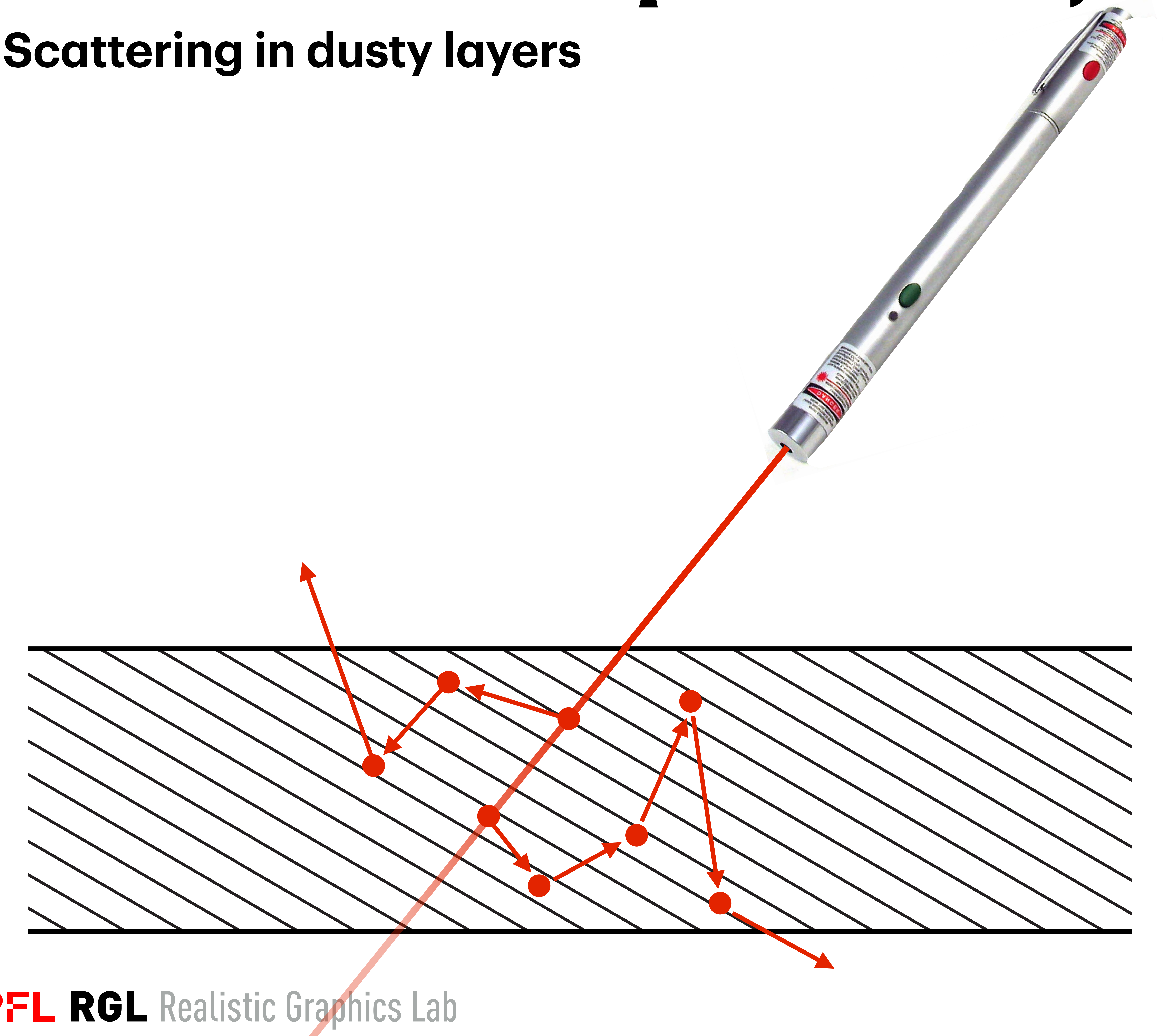

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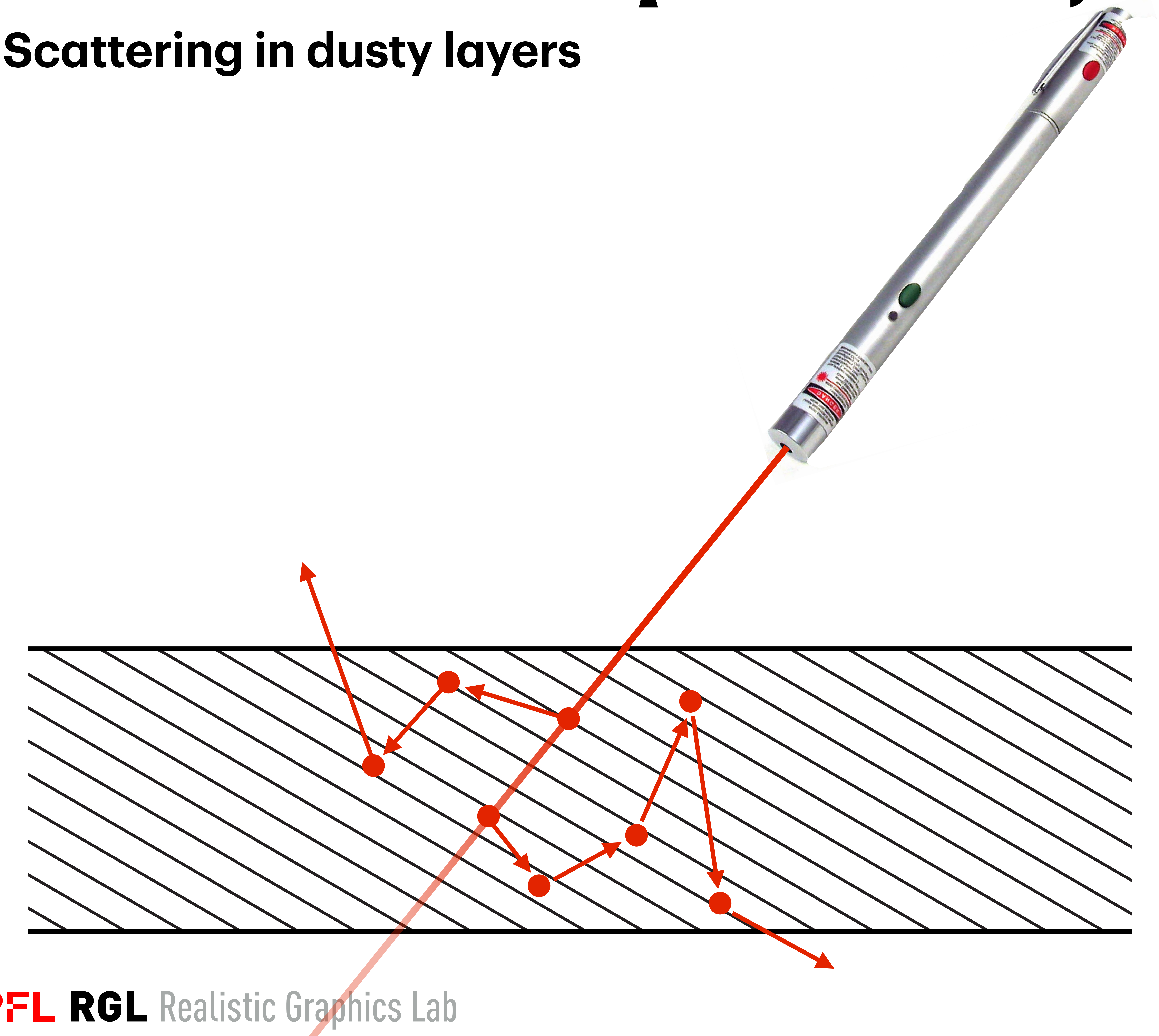

Problem has the form

$$\mathbf{x}'(t) = \mathbf{A}\mathbf{x}(t)$$

$\mathbf{x}(t)$ is the light traveling in different directions.

t is the depth within the layer.


α=0.02
τ=0.000, g=0.900

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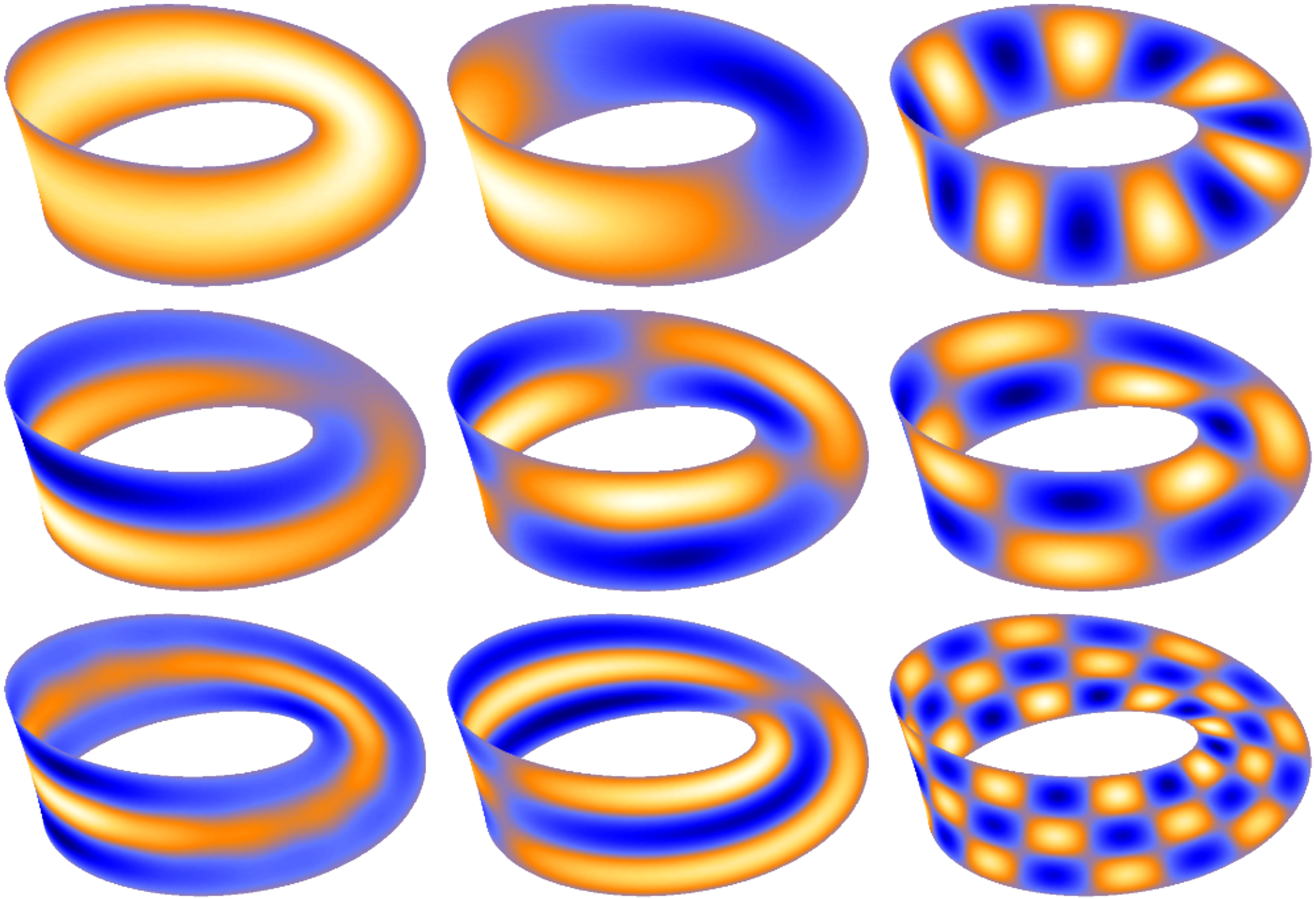
Oscillations on surfaces



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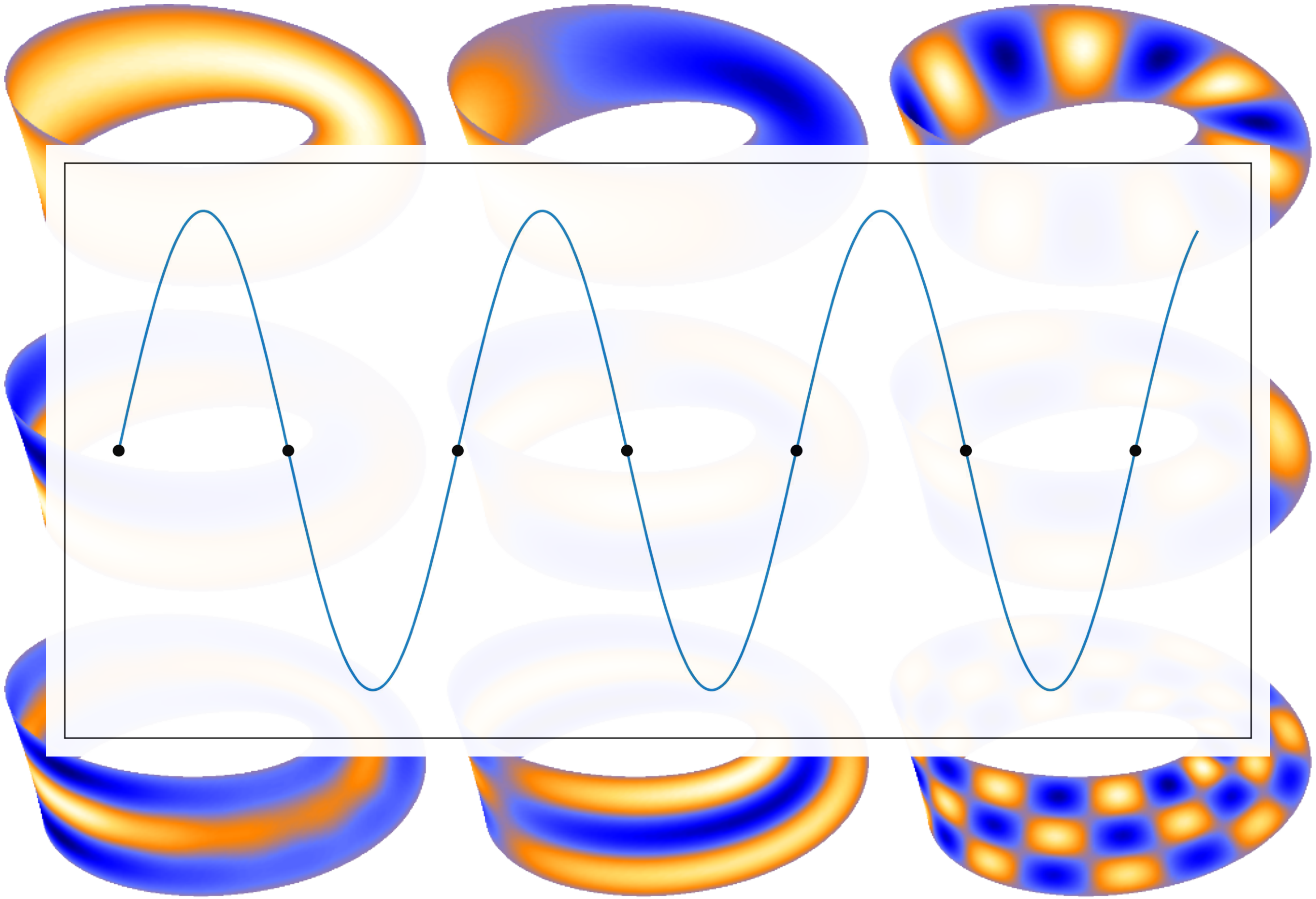

[Langlois, An, Jin, and James, SIGGRAPH 2014]

Diameter: 19 cm
Vertices: 51434
Compressed: 26 kB
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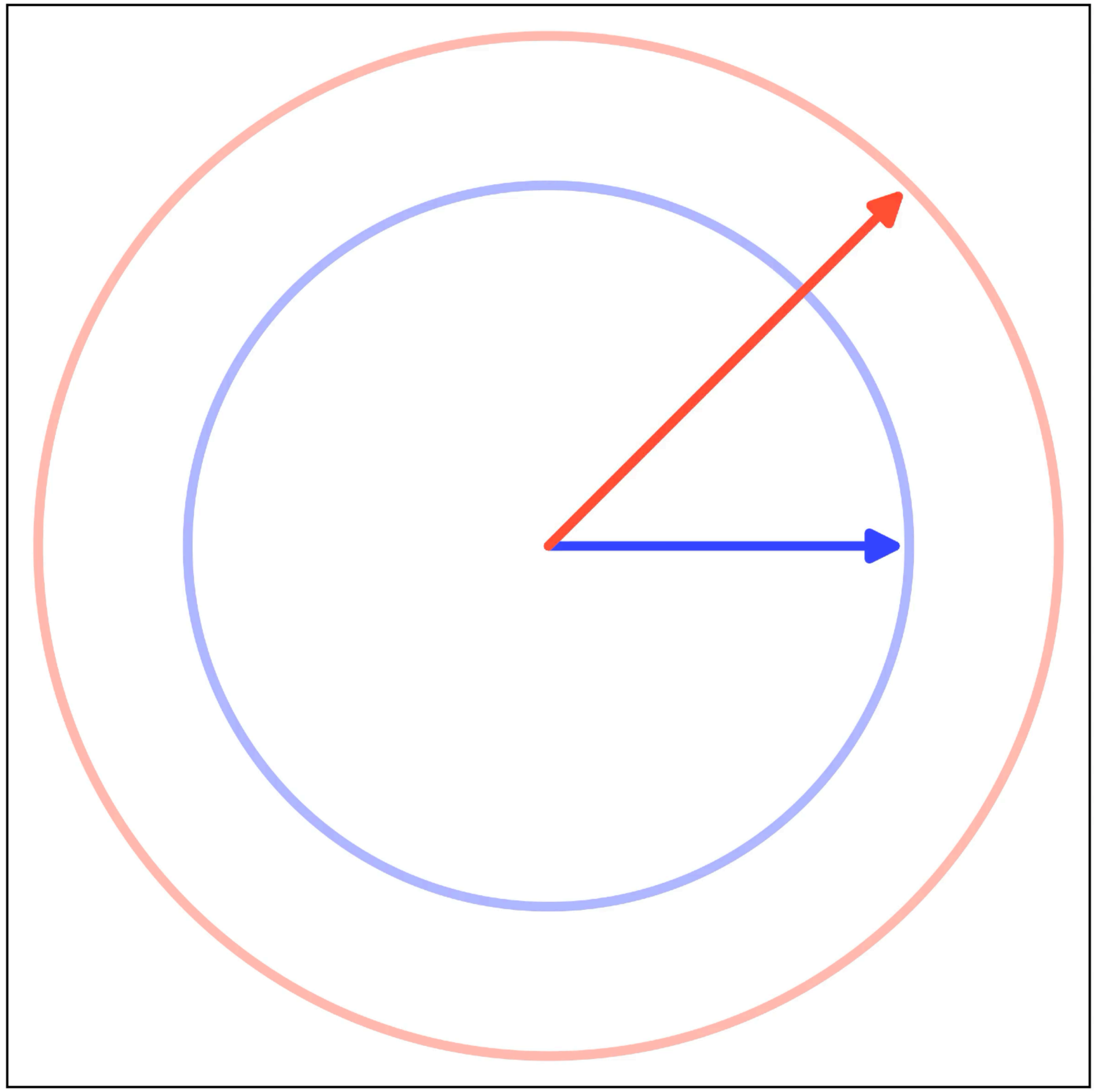

Eigenanalysis in practice: it's complicated..

1. an eigenvalue/eigenvector "pair" is actually a *triple* $(\mathbf{x}, \mathbf{y}, \lambda)$

where $\mathbf{y}^T\mathbf{A} = \lambda\mathbf{y}^T$ $\qquad$ $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$

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4. Doesn't make sense for non-square **A**!

The Singular Value Decomposition

LU $$A = LU$$

QR $$A = QR$$

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

The Singular Value Decomposition

The Singular Value Decomposition

- Can be computed for **any** matrix (non-square, non-symmetric, singular, ..)
- Involves only orthogonal and diagonal matrices.
- **Impeccable** numerical properties.
- No complex arithmetic necessary.
- Expensive to compute (~5-10 times the cost of LU)
- SVD and Eigendecomposition are *identical** when **A** is symmetric.

* Except for tiny differences: ordering of entries, etc.

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

Terminology

Let's look at the m=n case first.

$$\mathbf{V} = \begin{pmatrix} | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_n \\ | & & | \end{pmatrix}$$

"*Right singular vectors*"
Orthogonal.

$$\mathbf{U} = \begin{pmatrix} | & & | \\ \mathbf{u}_1 & \cdots & \mathbf{u}_n \\ | & & | \end{pmatrix}$$

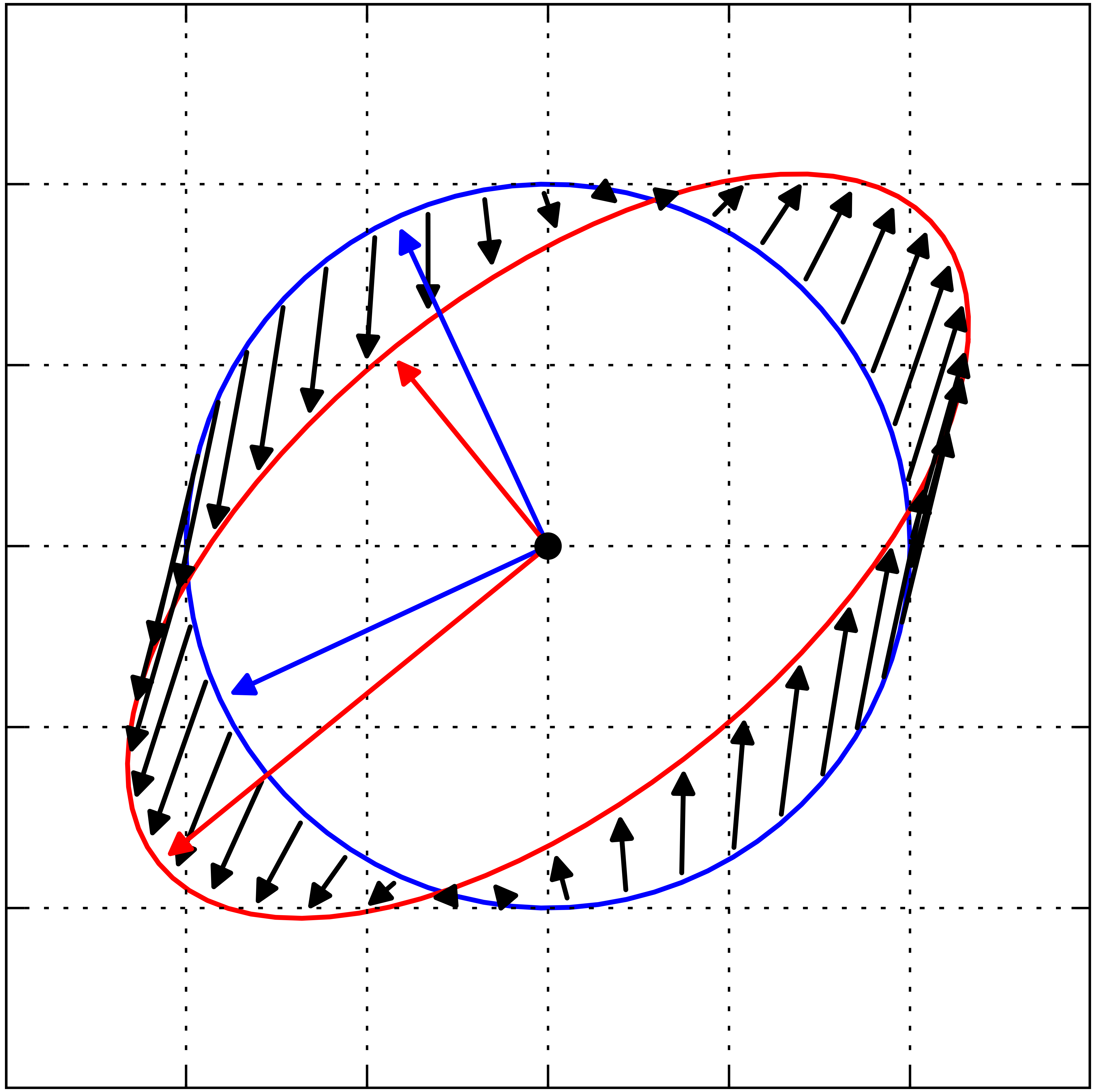
"*Left singular vectors*"
Orthogonal.

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix}$$

"*Singular values*"
Positive, sorted in decreasing order

SVD

```
U, Σ, V = scipy.linalg.svd(A)
```



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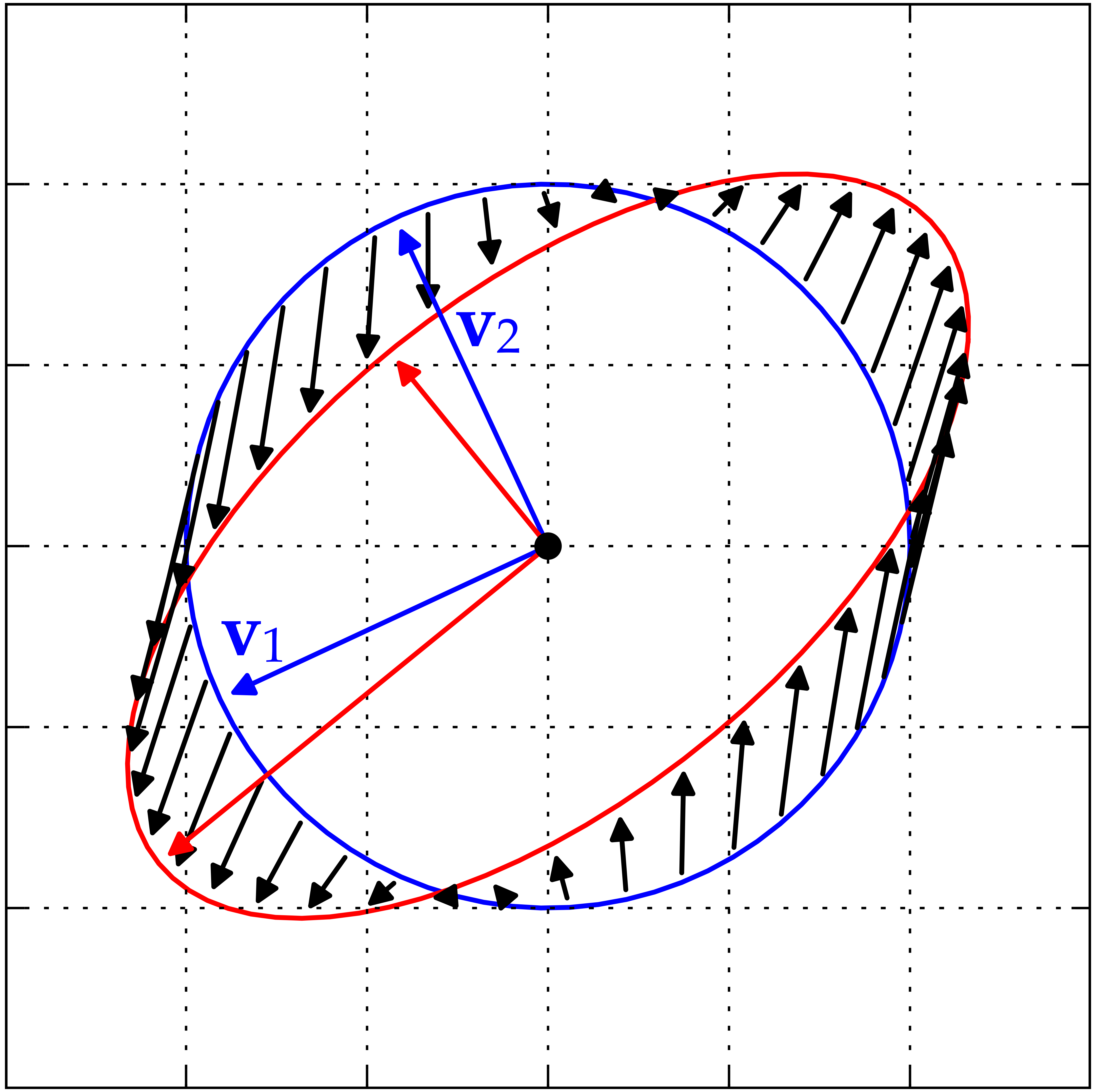

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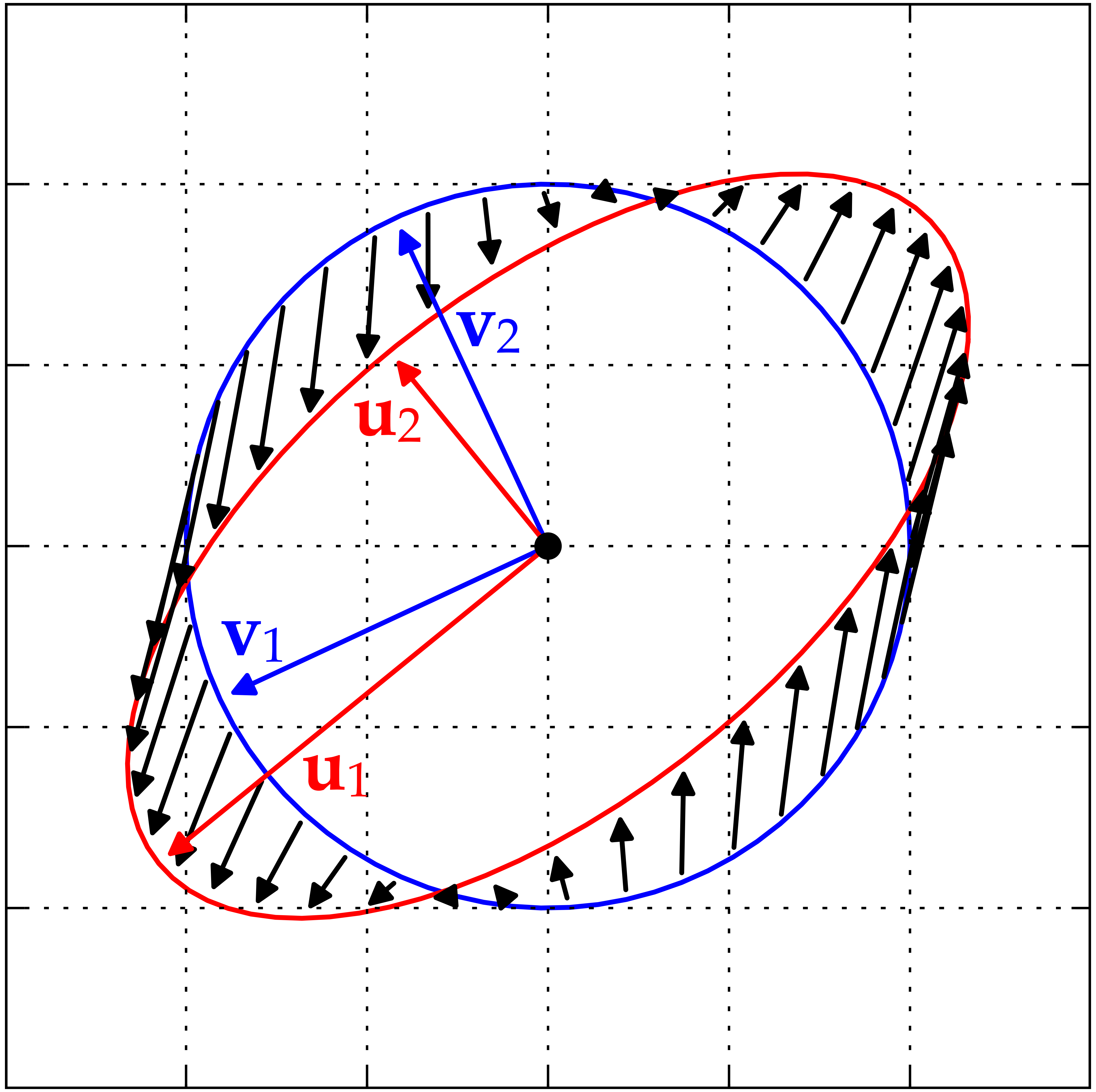
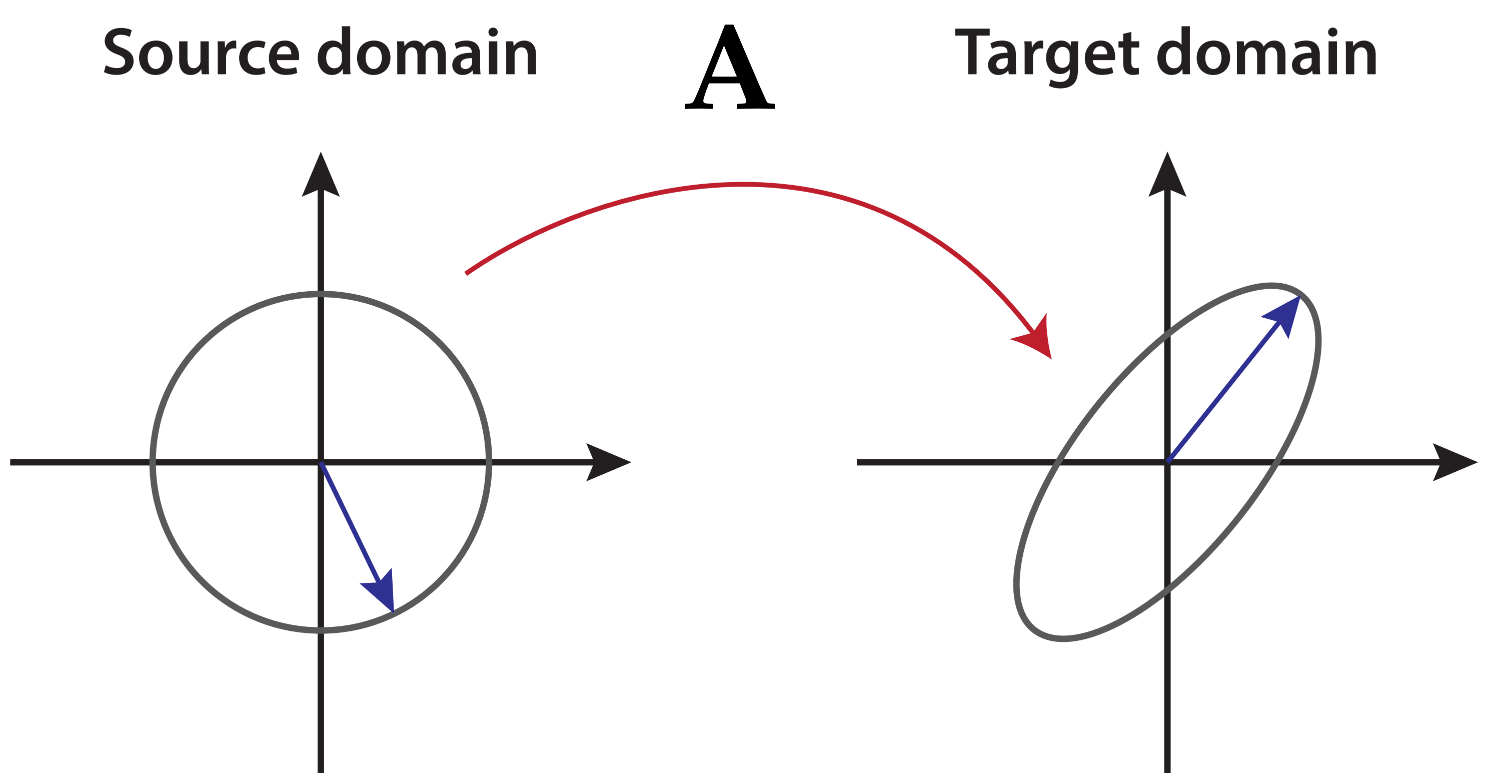
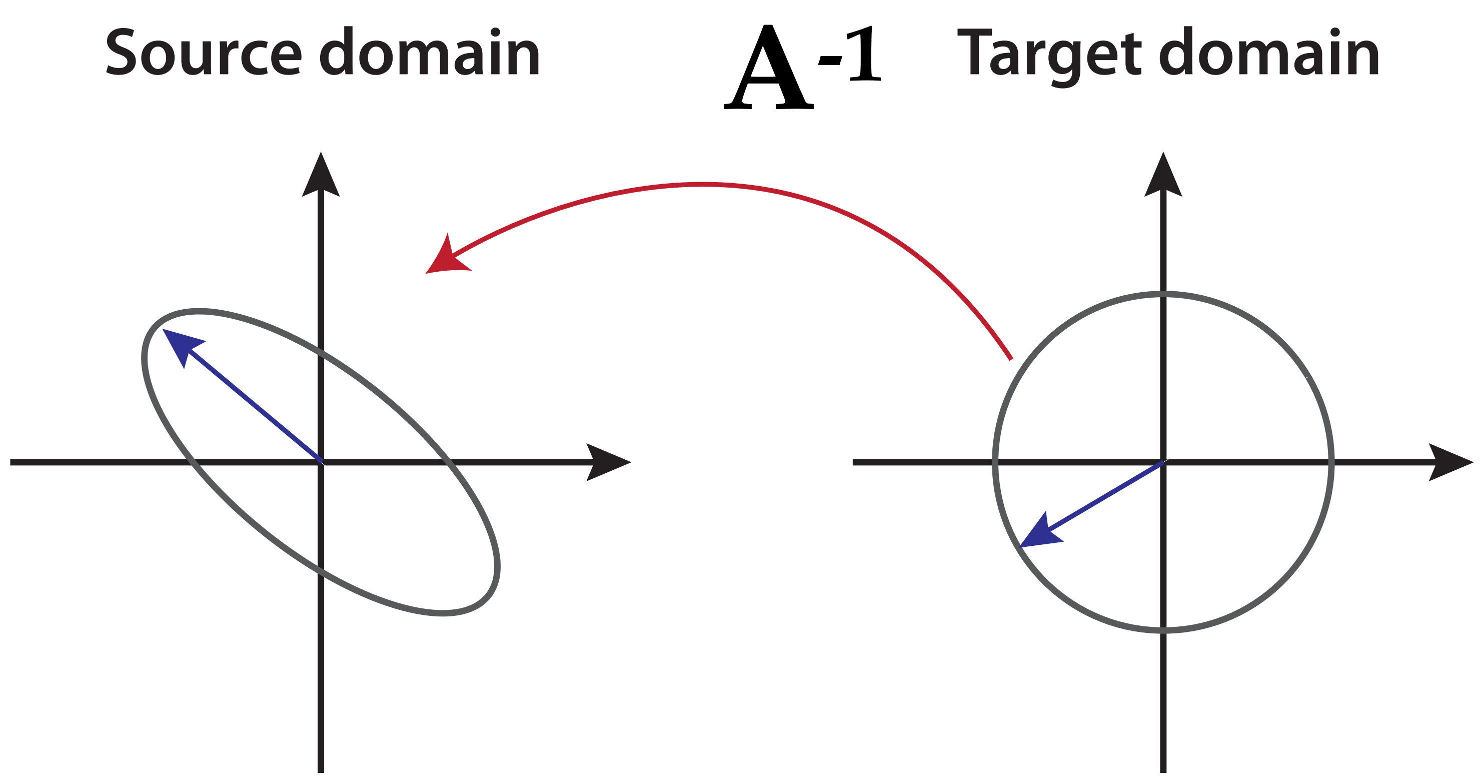


Revisiting the condition number

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





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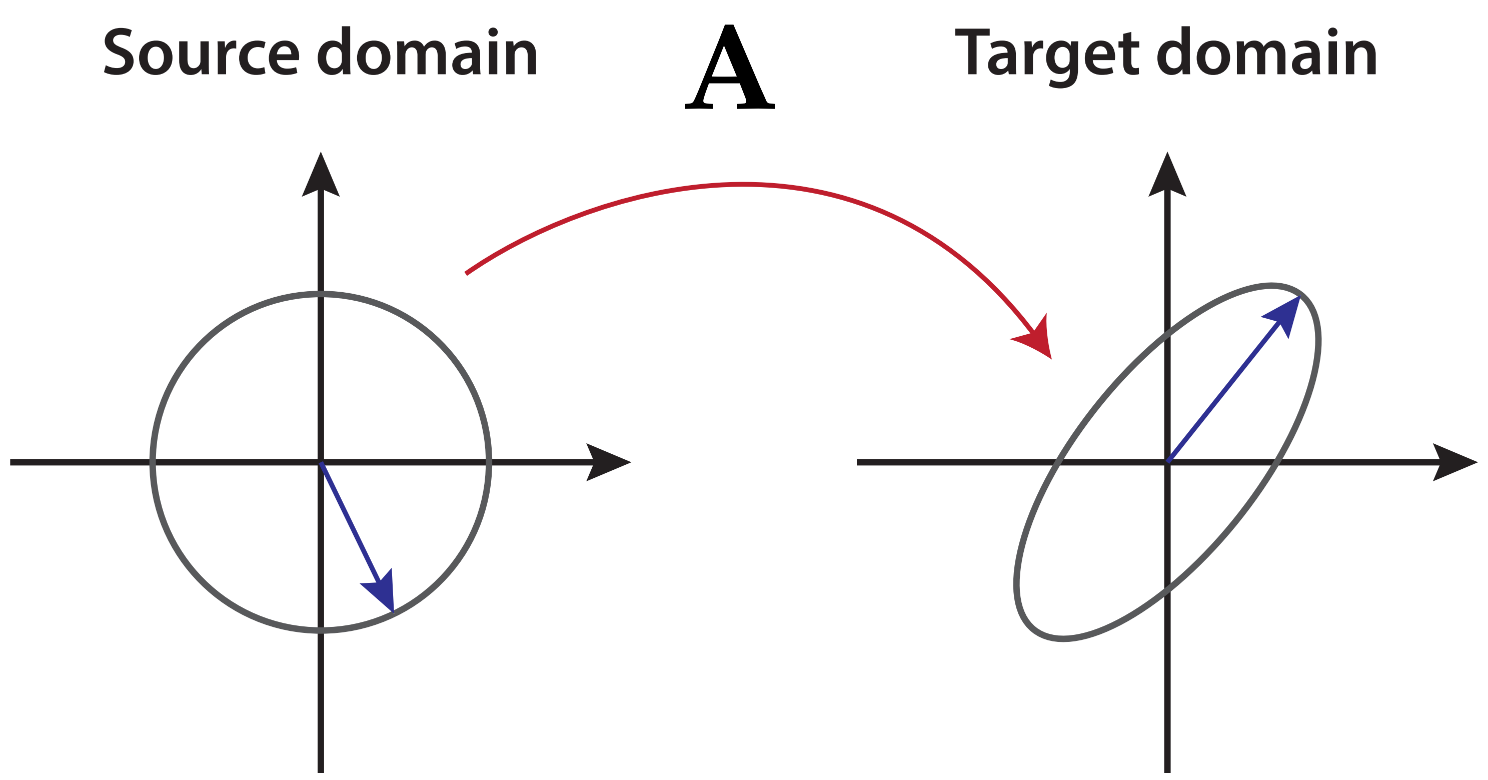
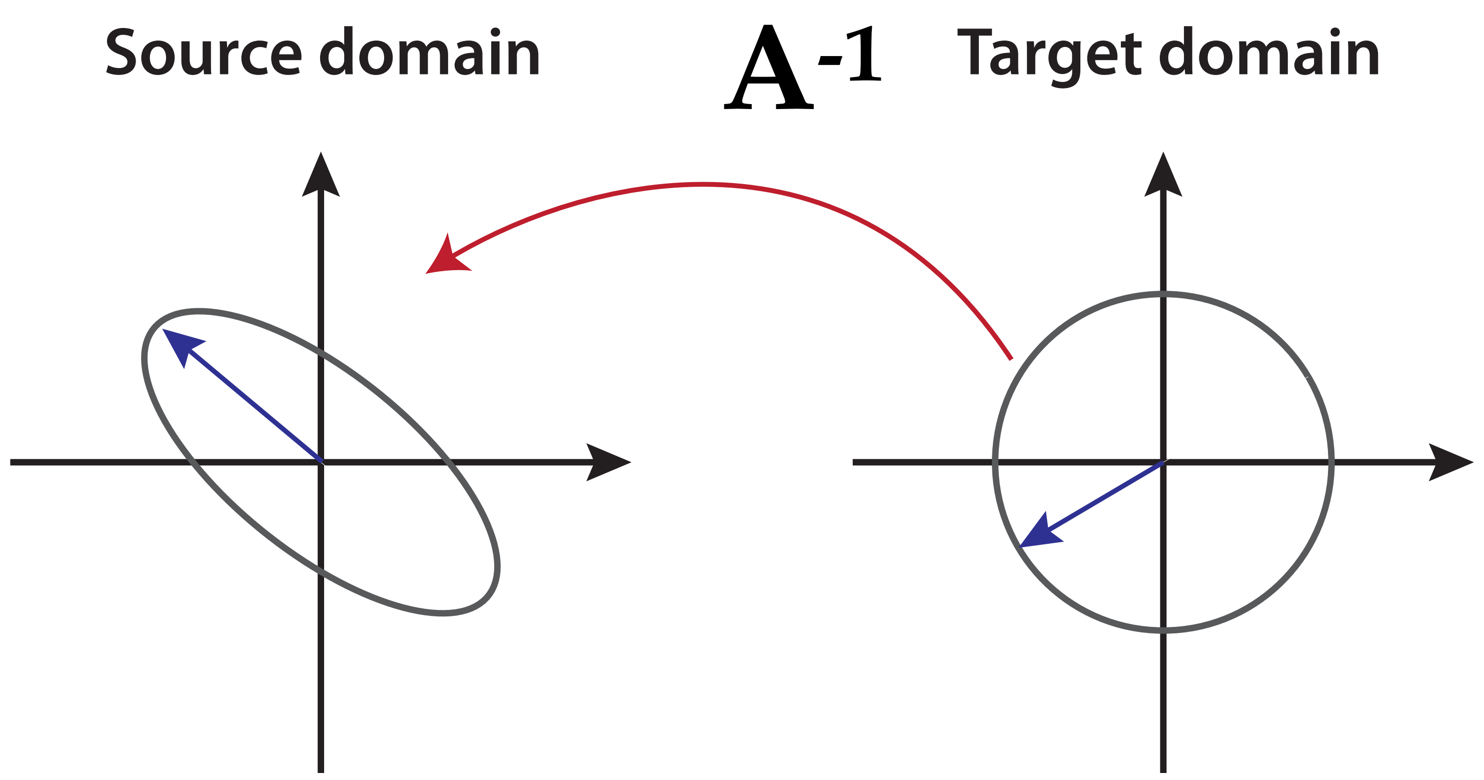
$$\operatorname{cond}(\mathbf{A}) = \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\|$$
$$= \frac{\sigma_1}{\sigma_n}.$$





Another view of the SVD

$$\begin{bmatrix} \mathbf{A} \end{bmatrix} = \begin{bmatrix} \mathbf{U} \end{bmatrix} \begin{bmatrix} \diagdown \mathbf{\Sigma} \diagdown \end{bmatrix} \begin{bmatrix} \mathbf{V}^T \end{bmatrix}$$

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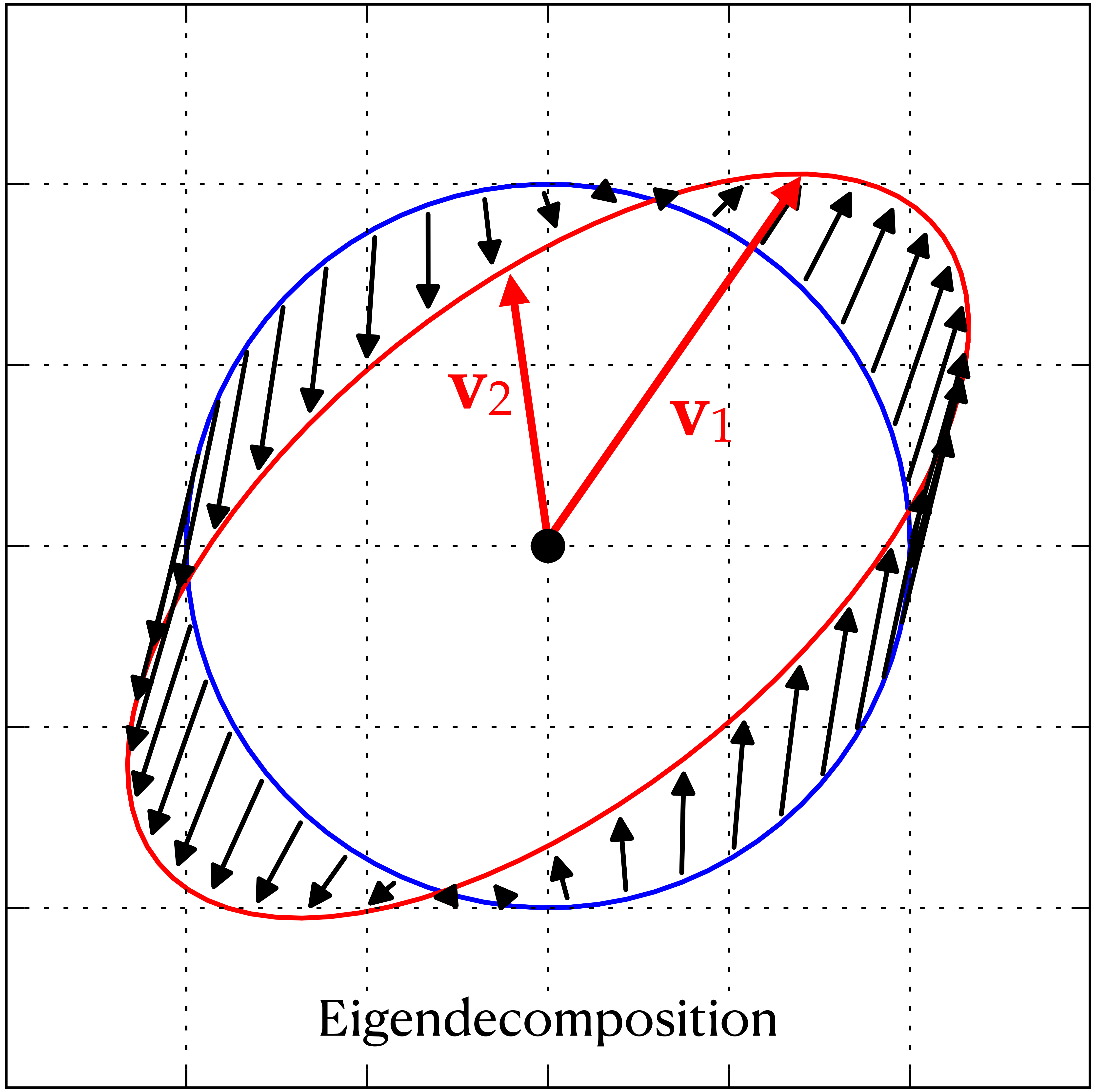
Then $\mathbf{A} = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$

Eigendecomposition vs. SVD



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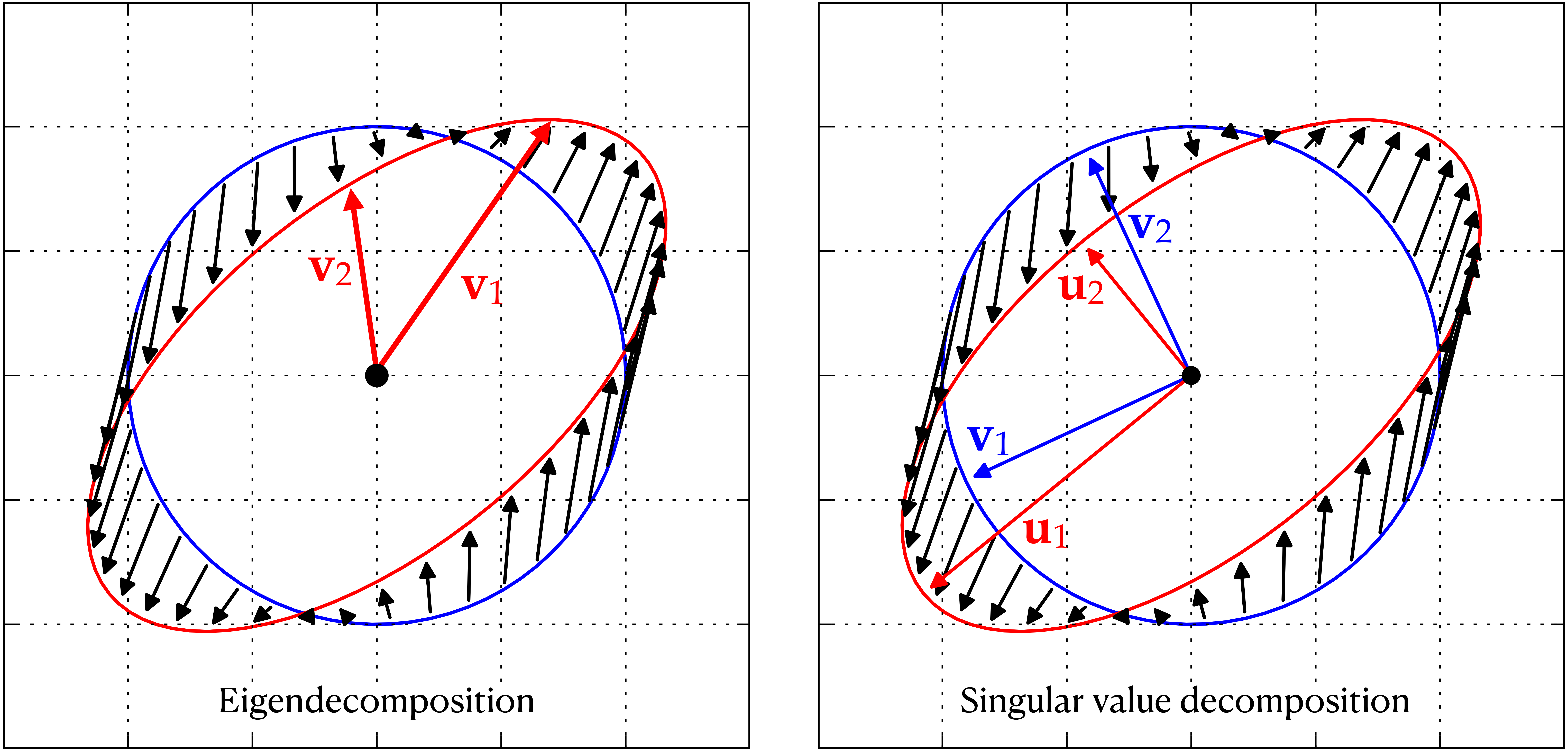

MATH-232 Review: The Normal Distribution

Univariate (1D) case. Also known as "*Gaussian distribution*"

$$X \sim \mathcal{N}(\mu, \sigma^2)$$

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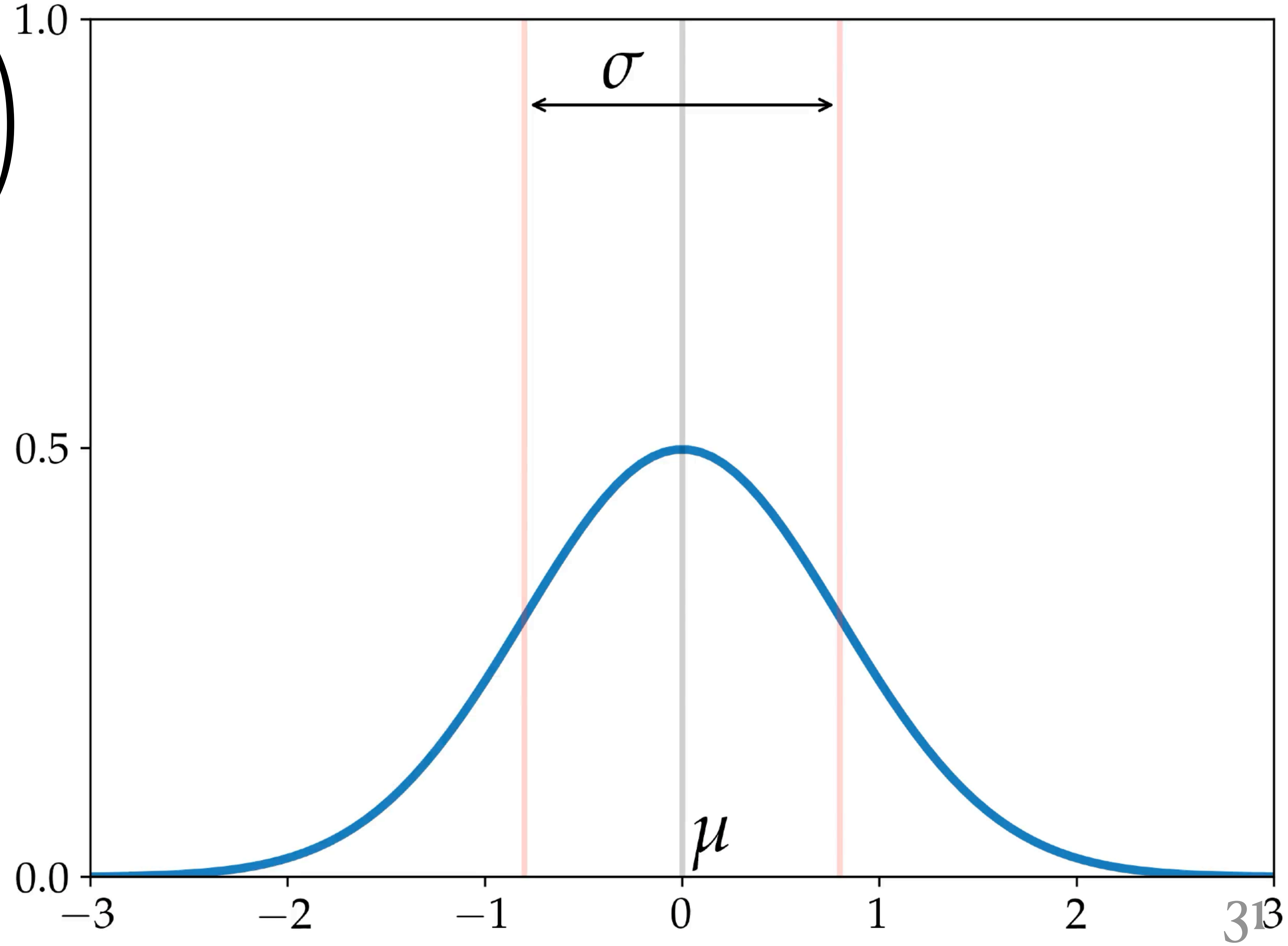

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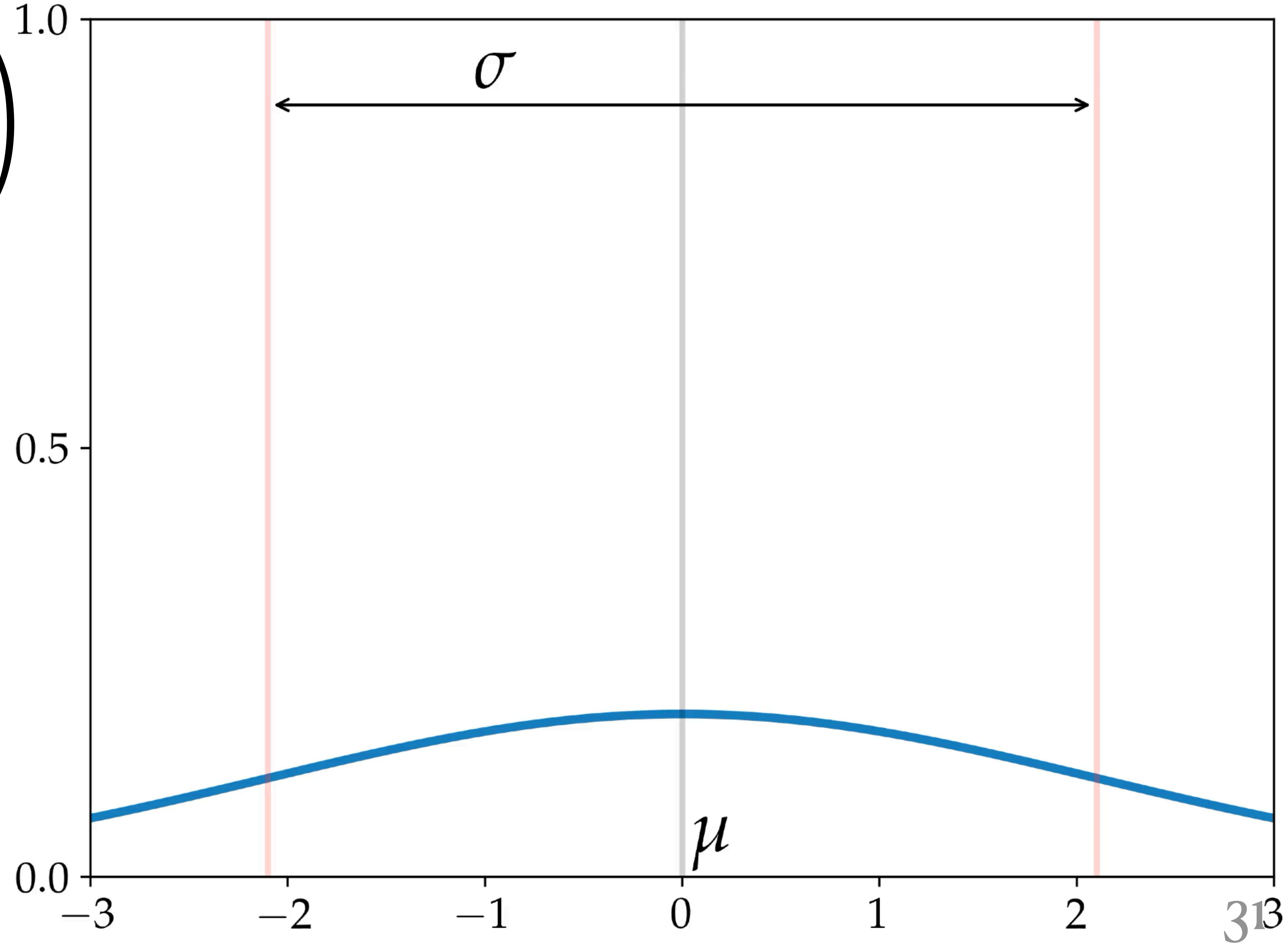

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Variance (square of std. deviation)

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Standard deviation

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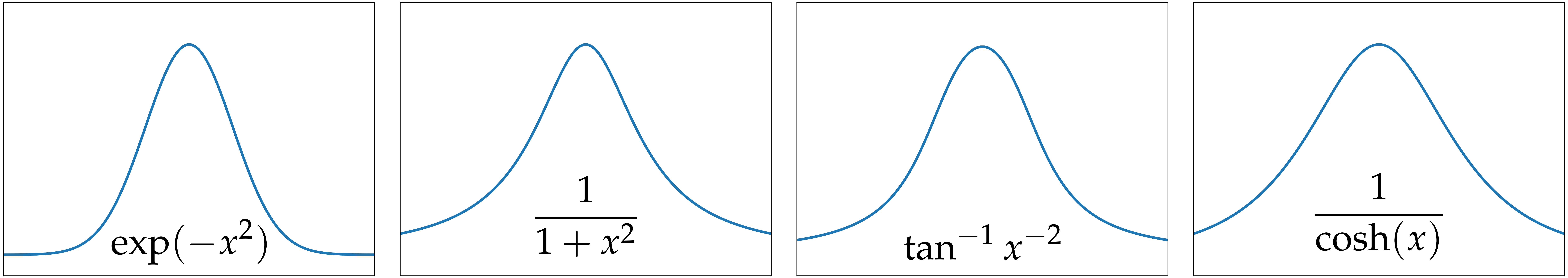

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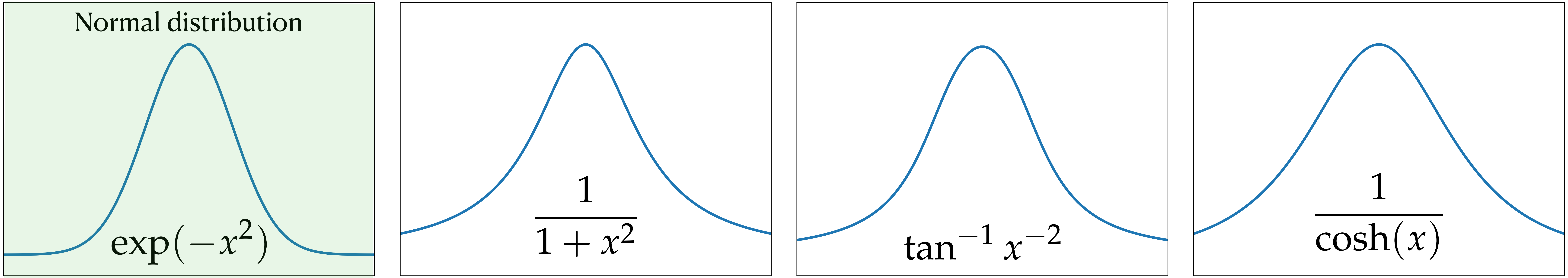

The Normal Distribution

Why is *this particular* function interesting?

$$X_1, X_2, \ldots \quad \text{iid. random variables with } E[X_i] = \mu \text{ and } \mathrm{Var}[X_i] = \sigma^2$$

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$X_1, X_2, \ldots$ iid. random variables with $E[X_i] = \mu$ and $\mathrm{Var}[X_i] = \sigma^2$

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The Normal Distribution

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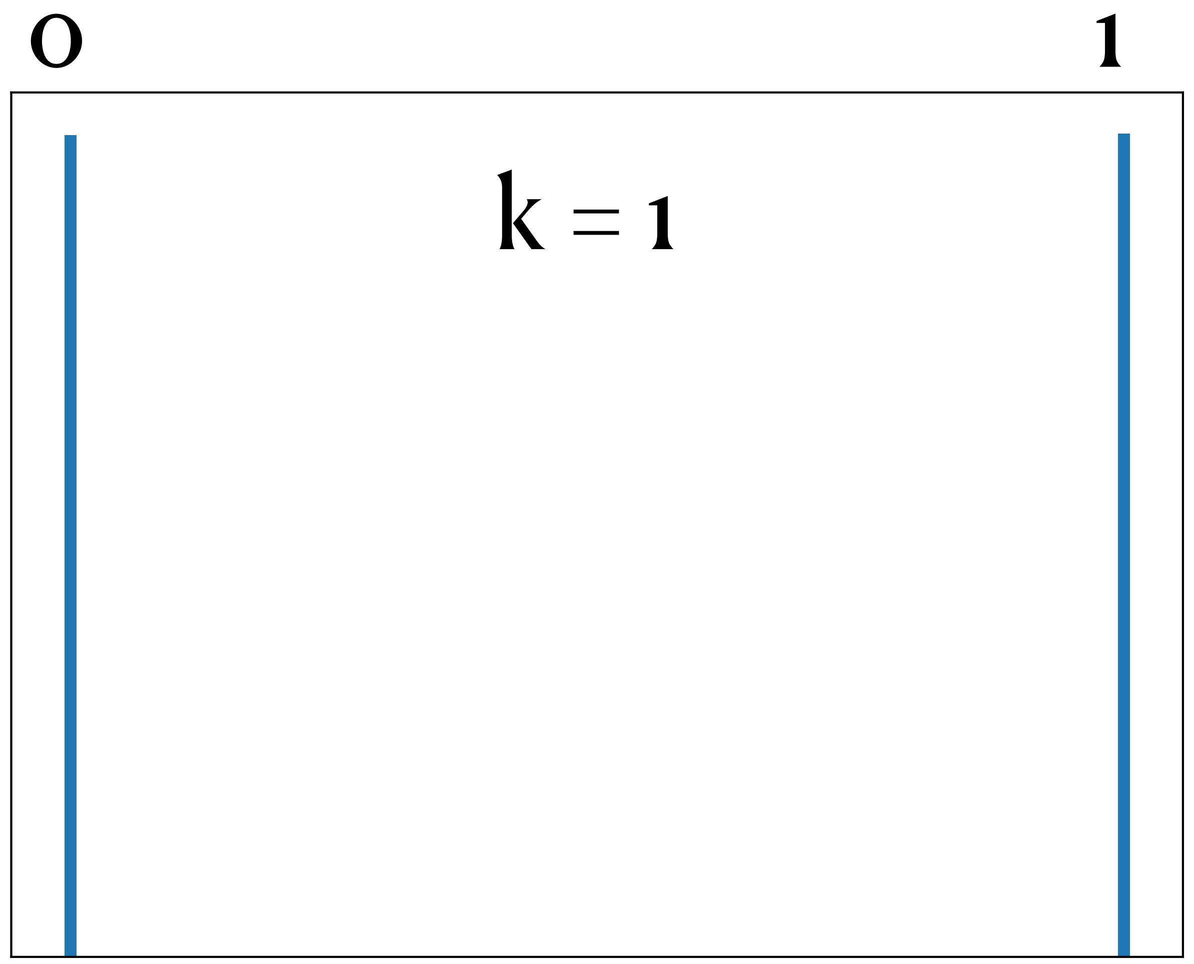

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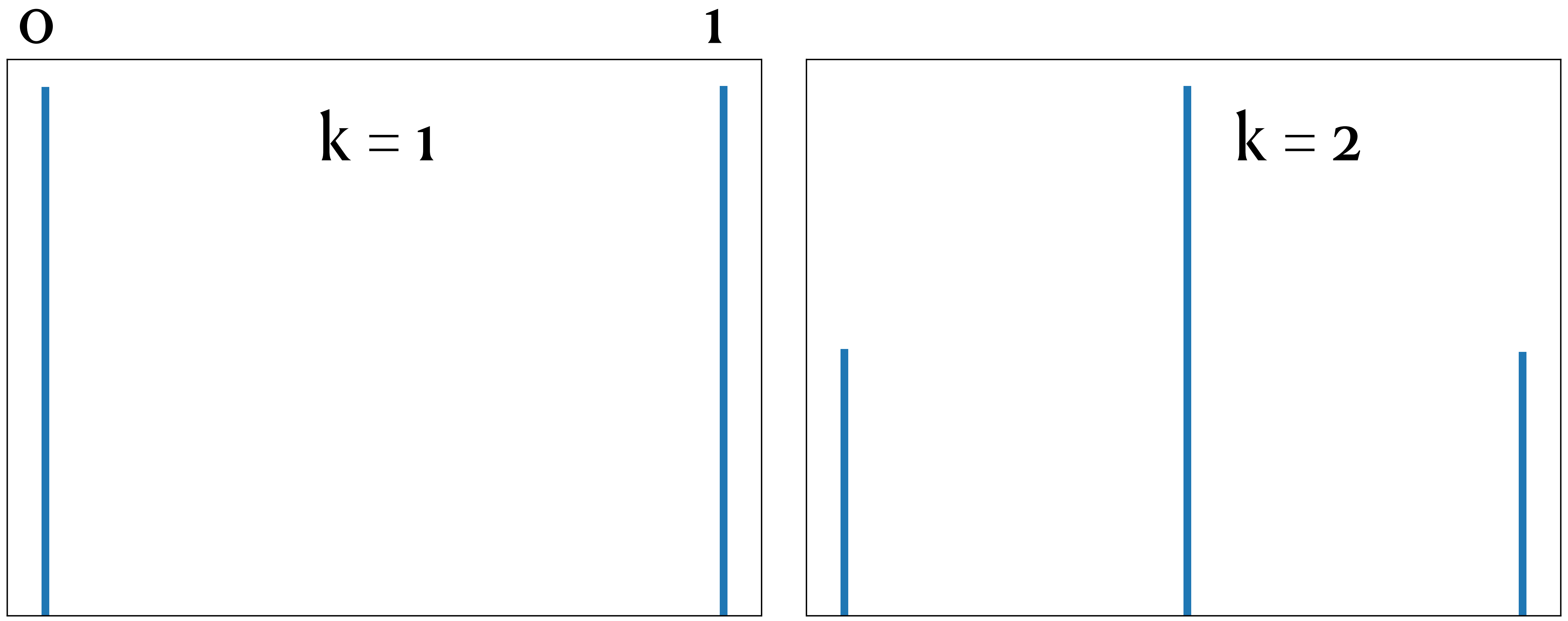

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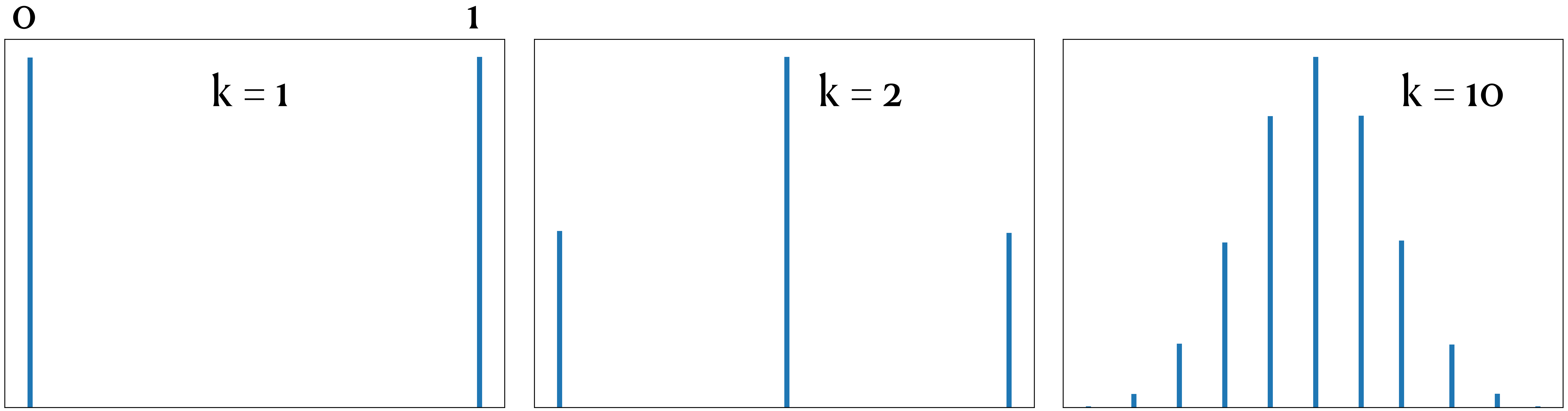

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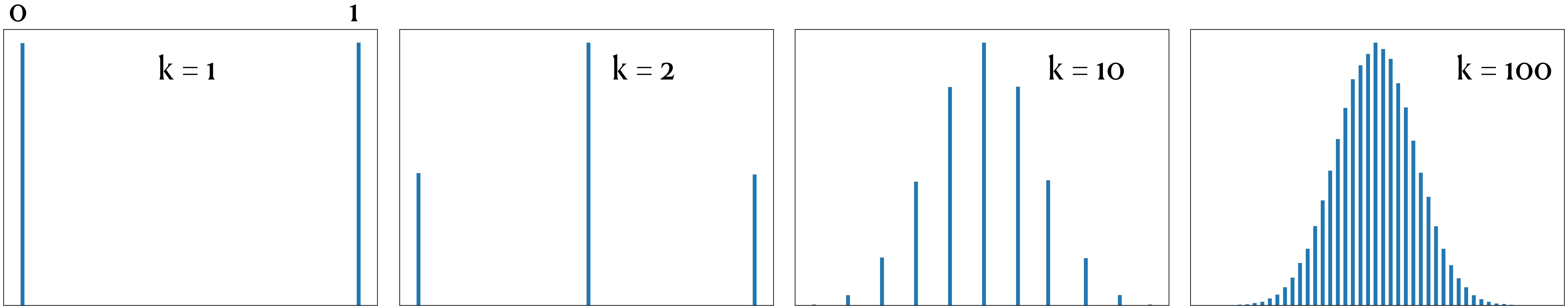

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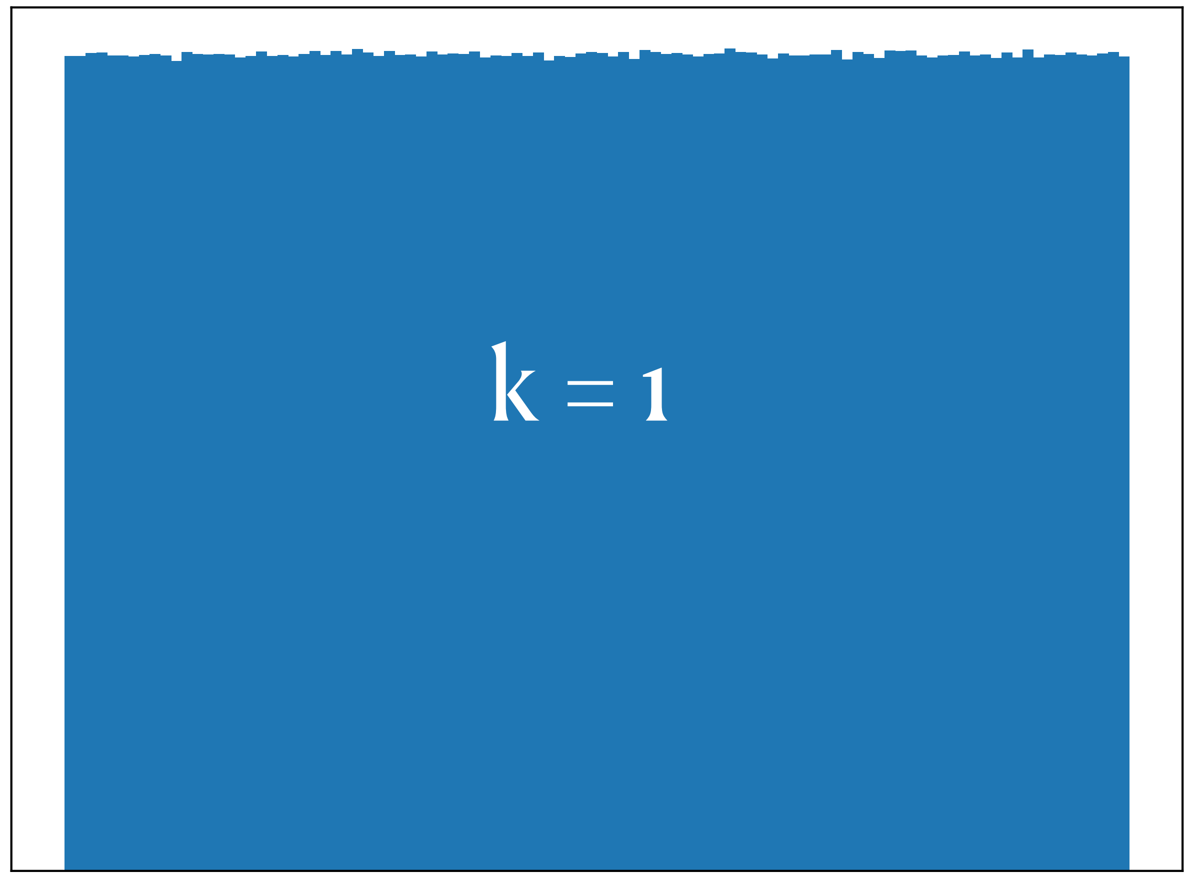

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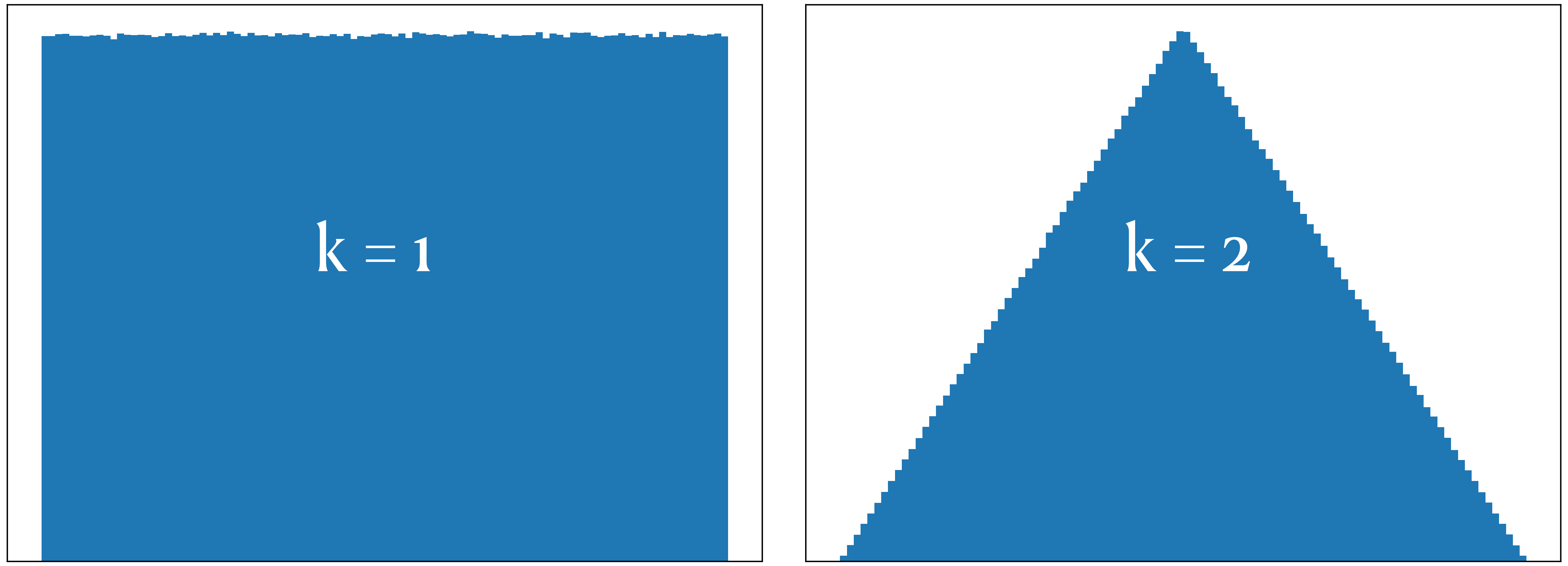

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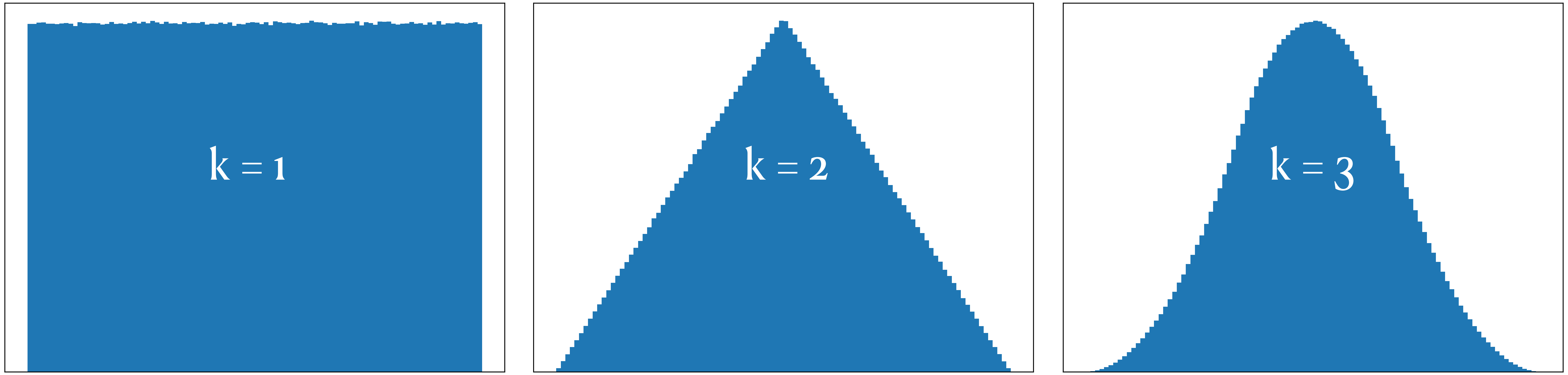

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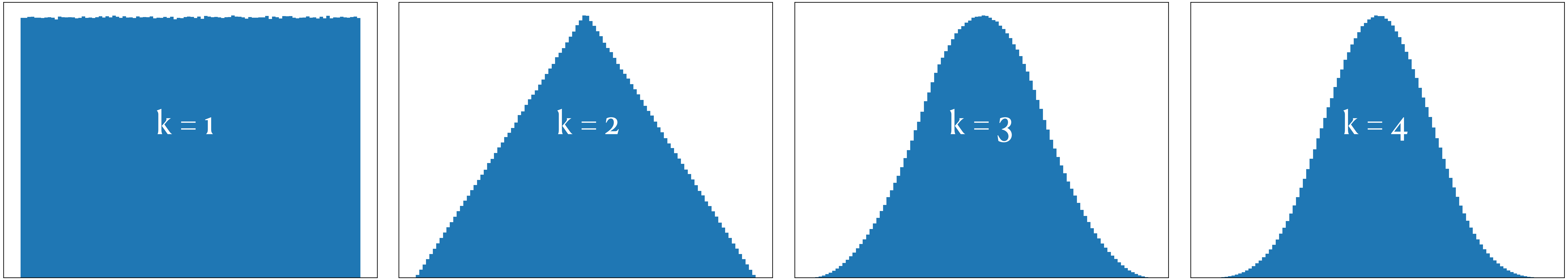

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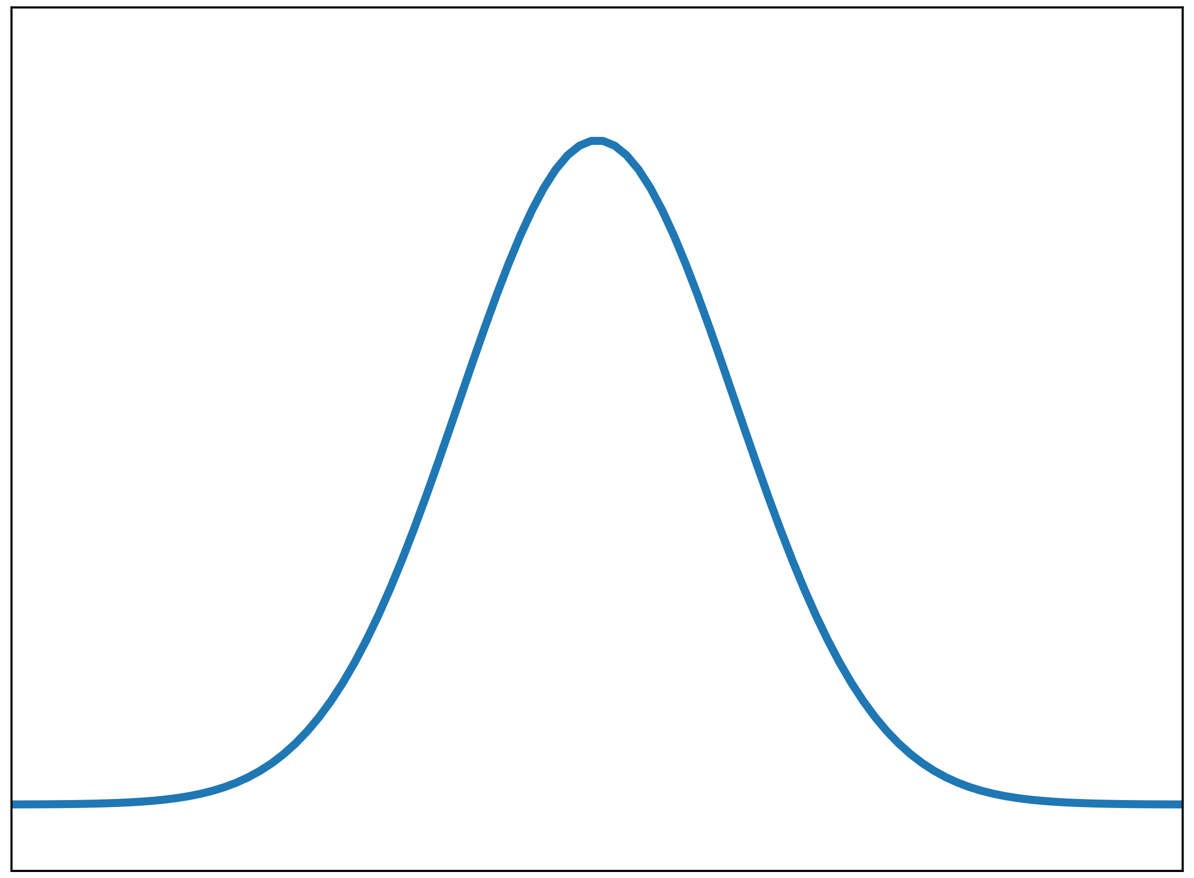

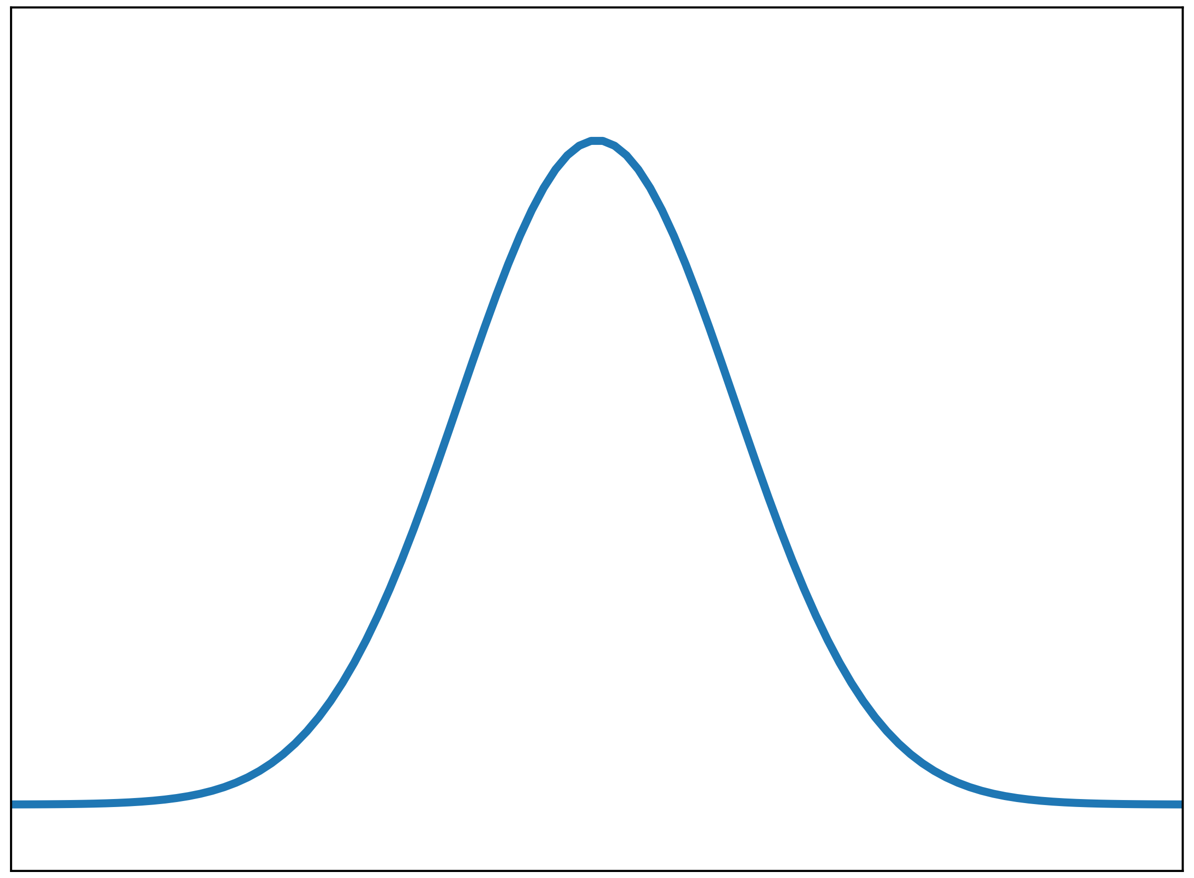

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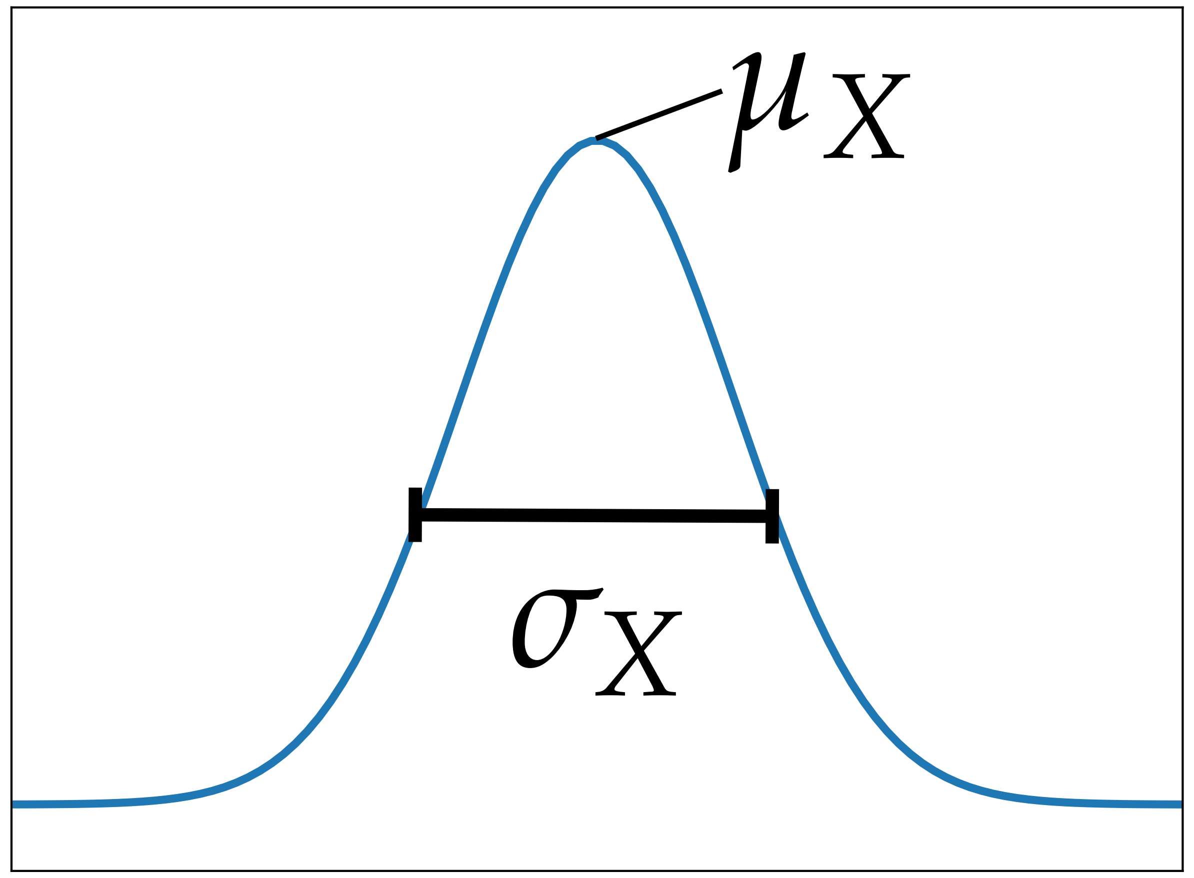

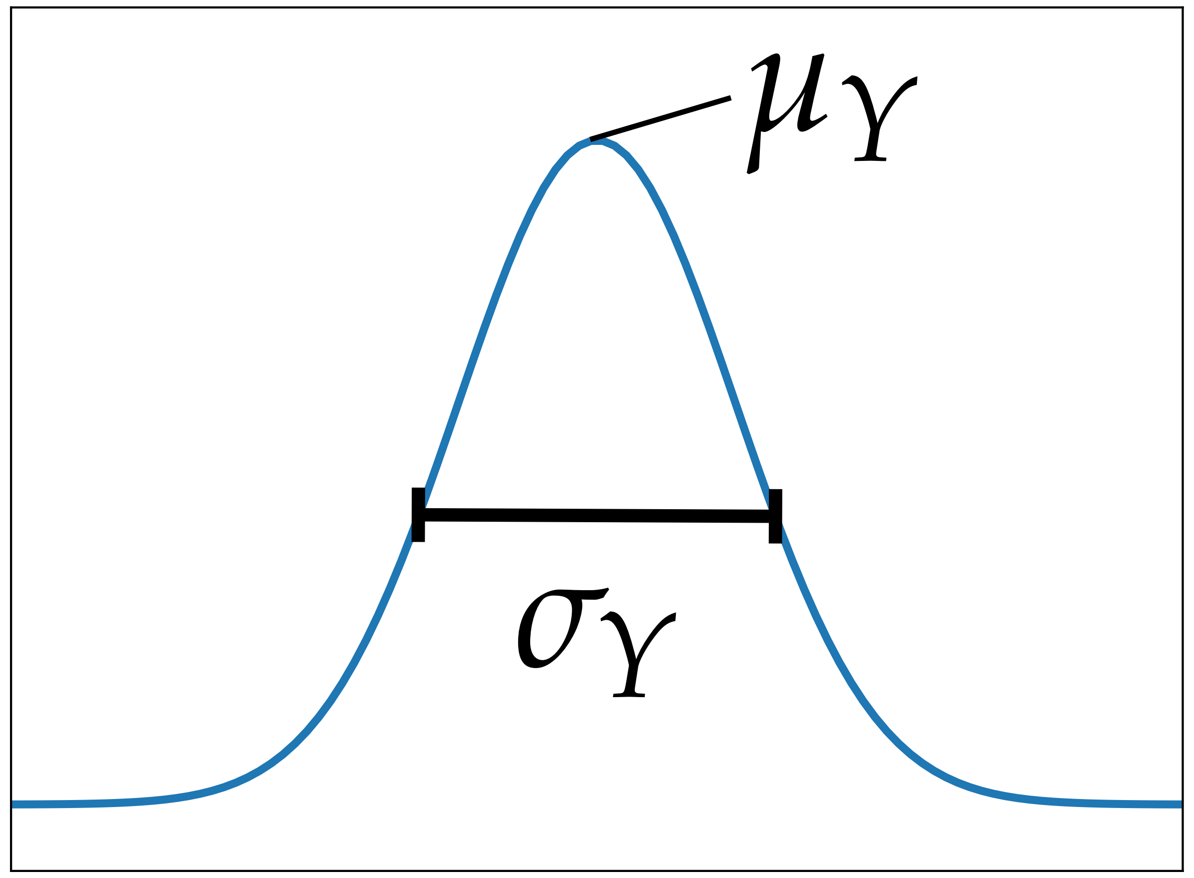

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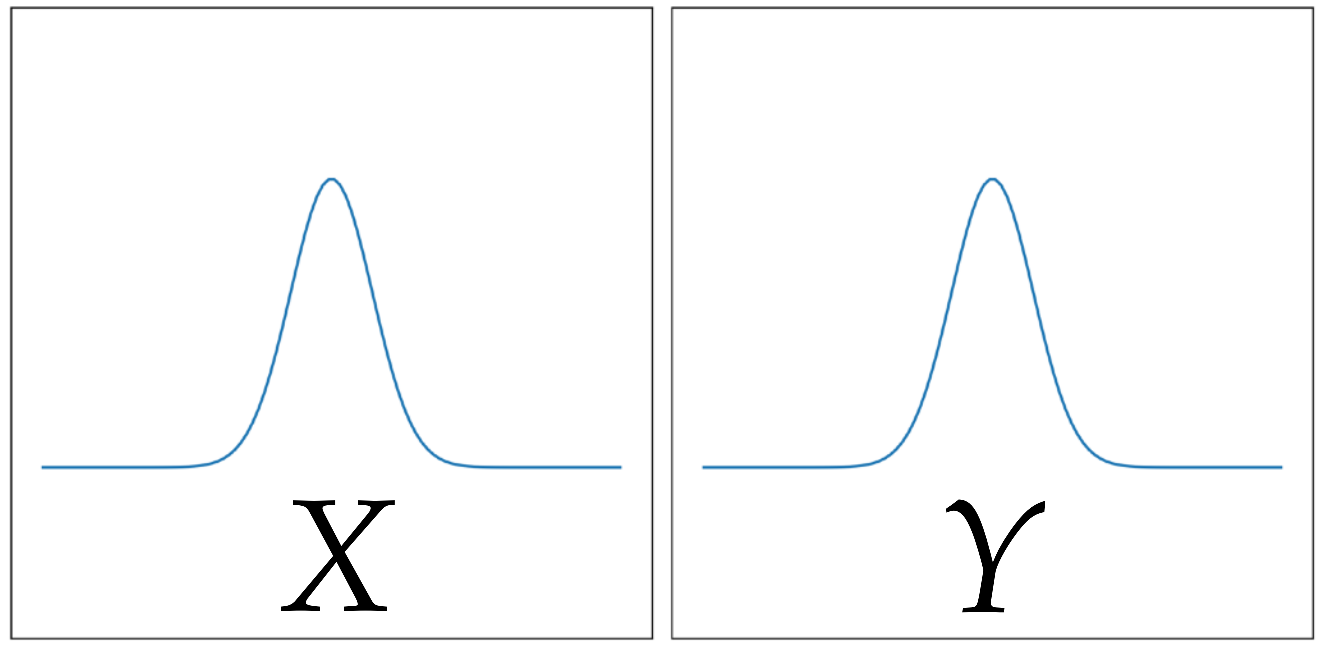

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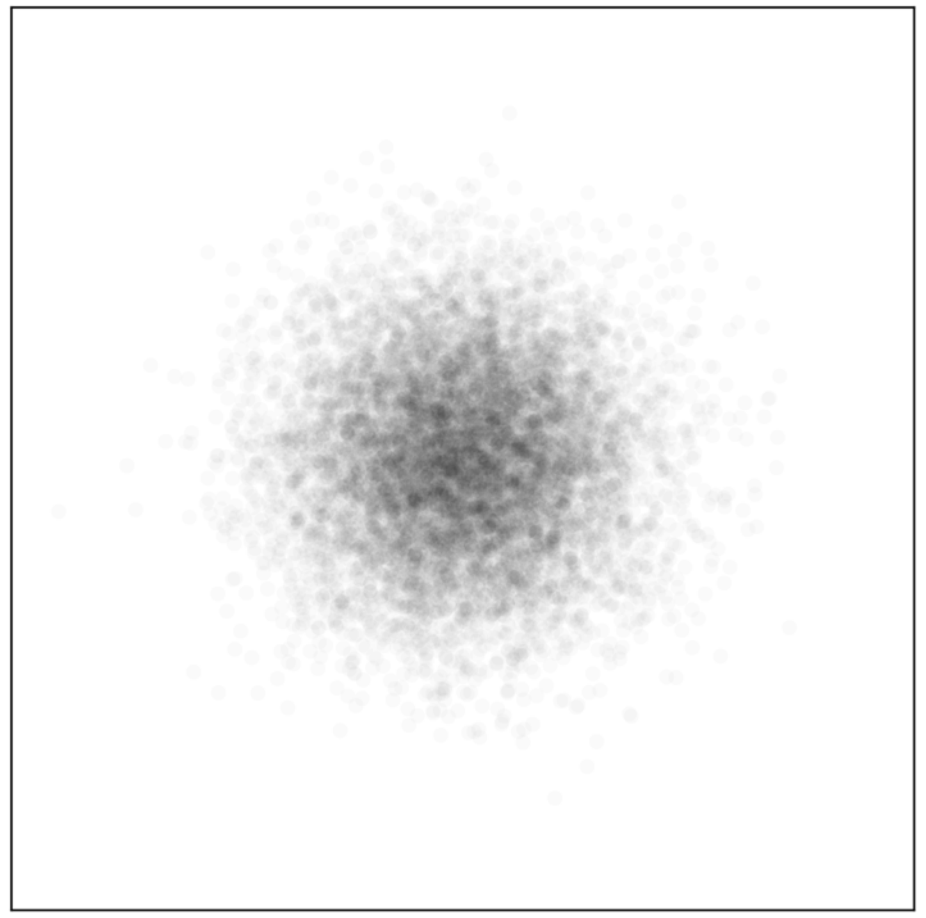

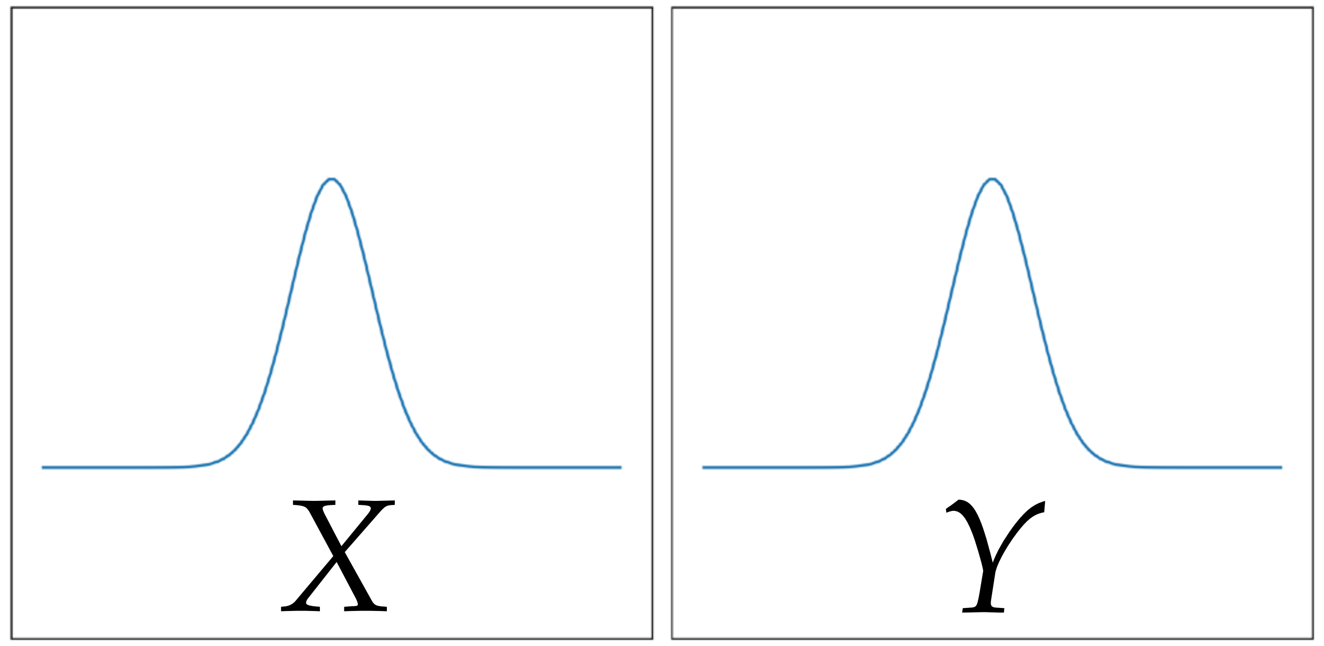

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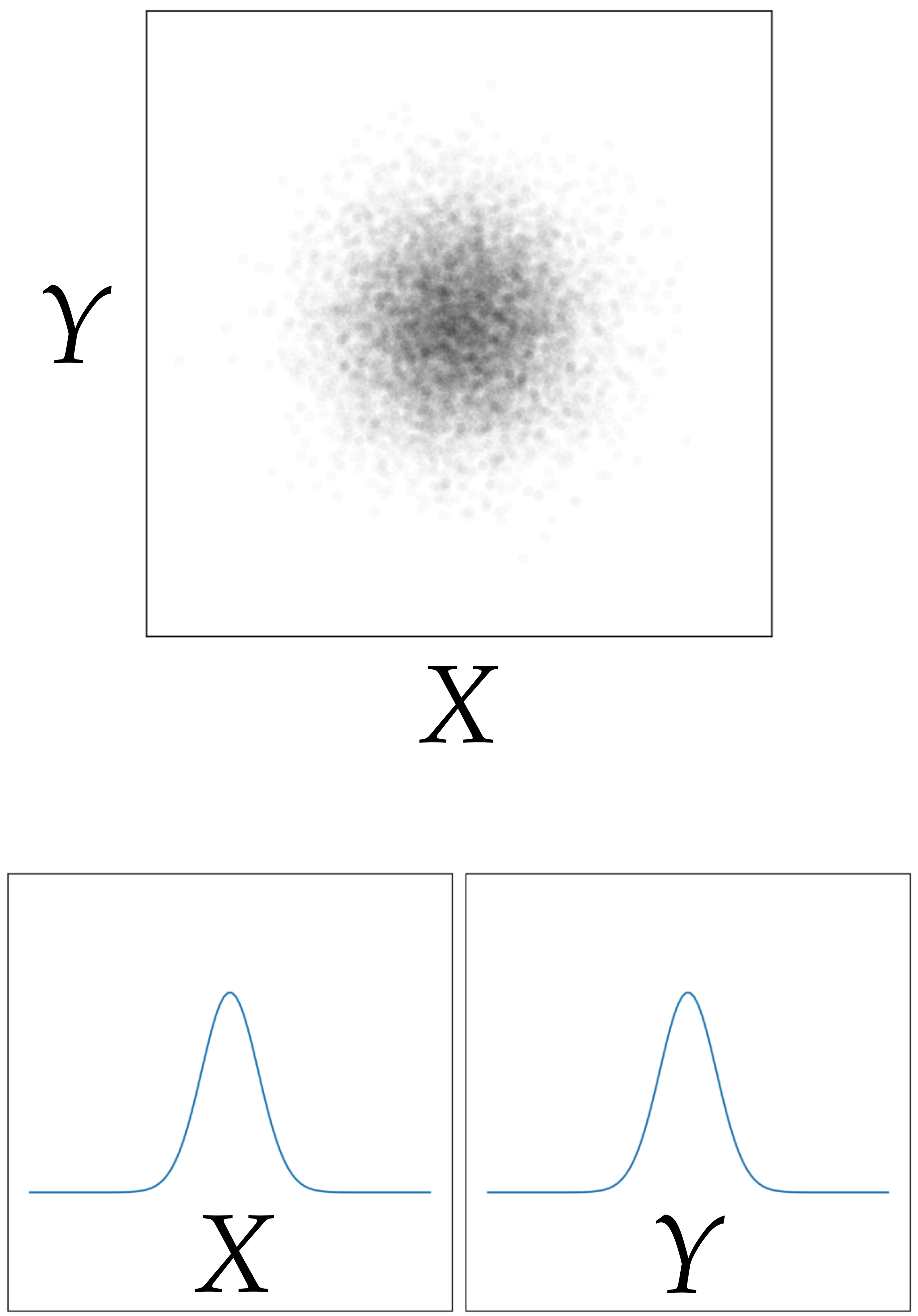

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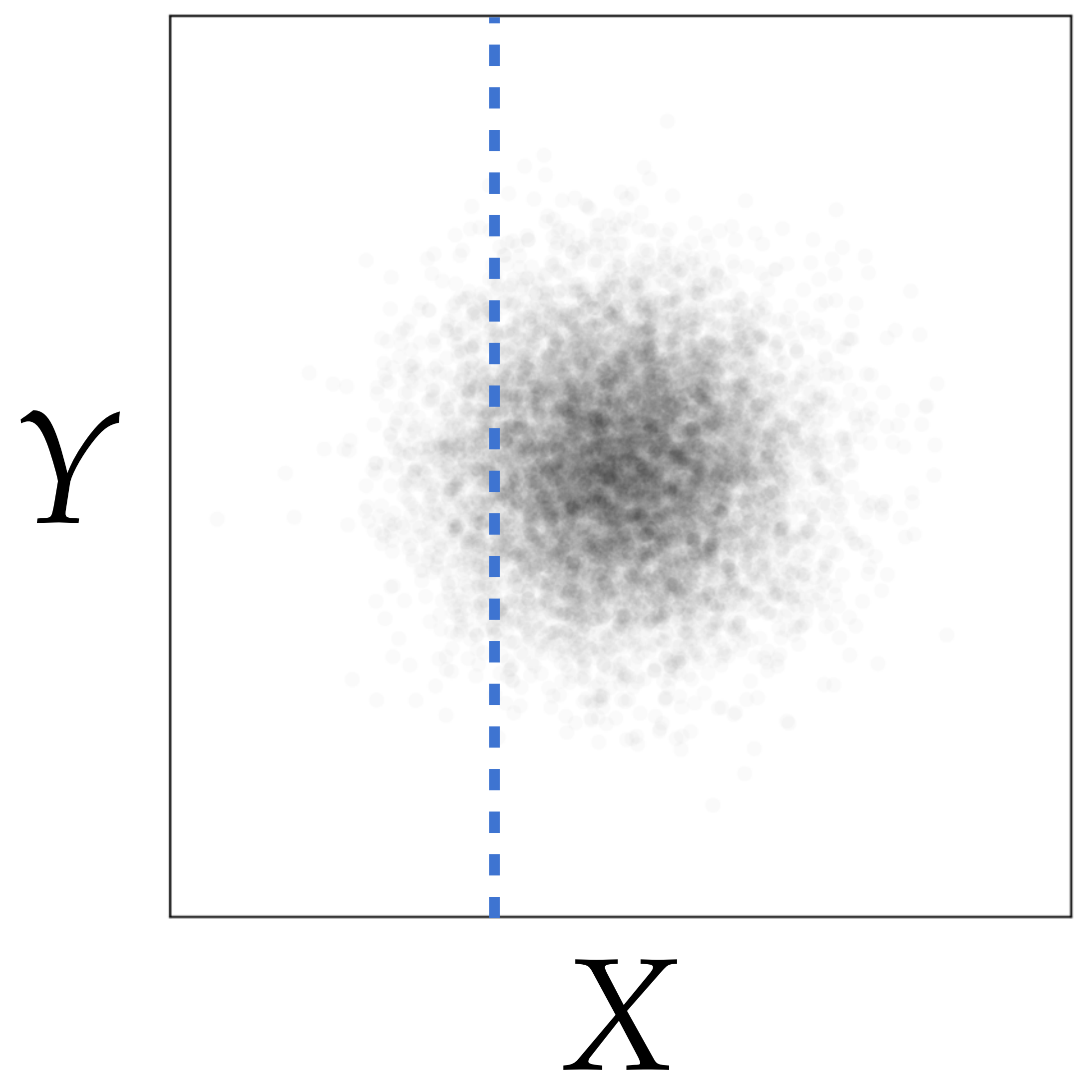

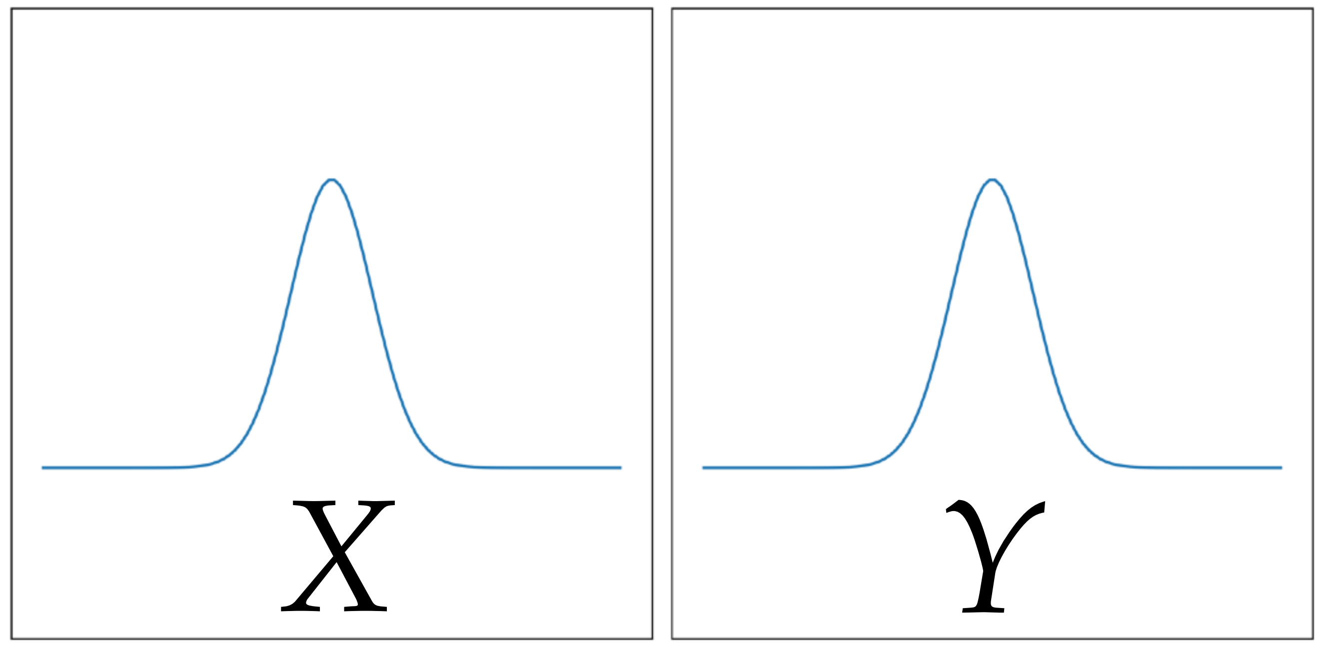

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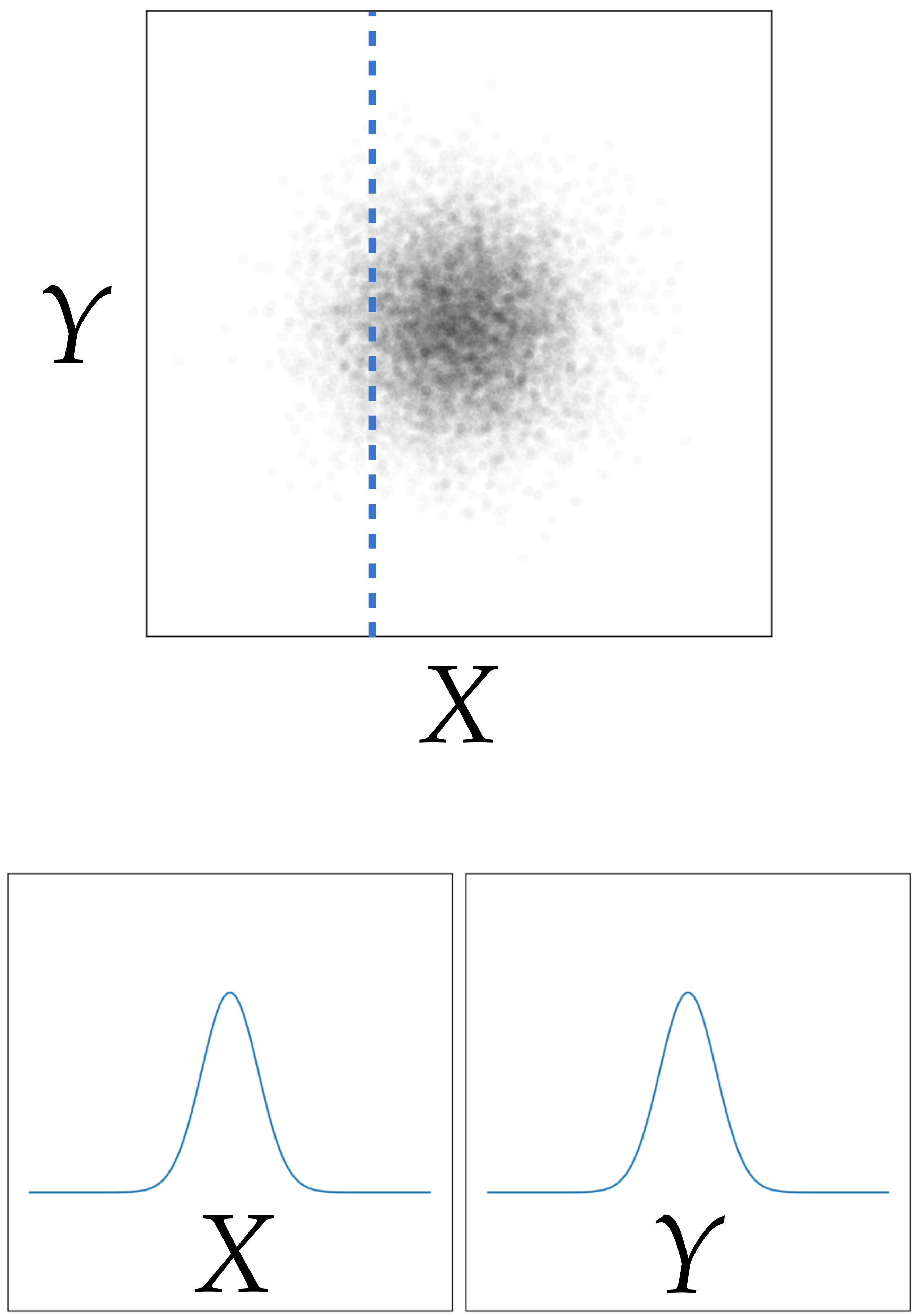

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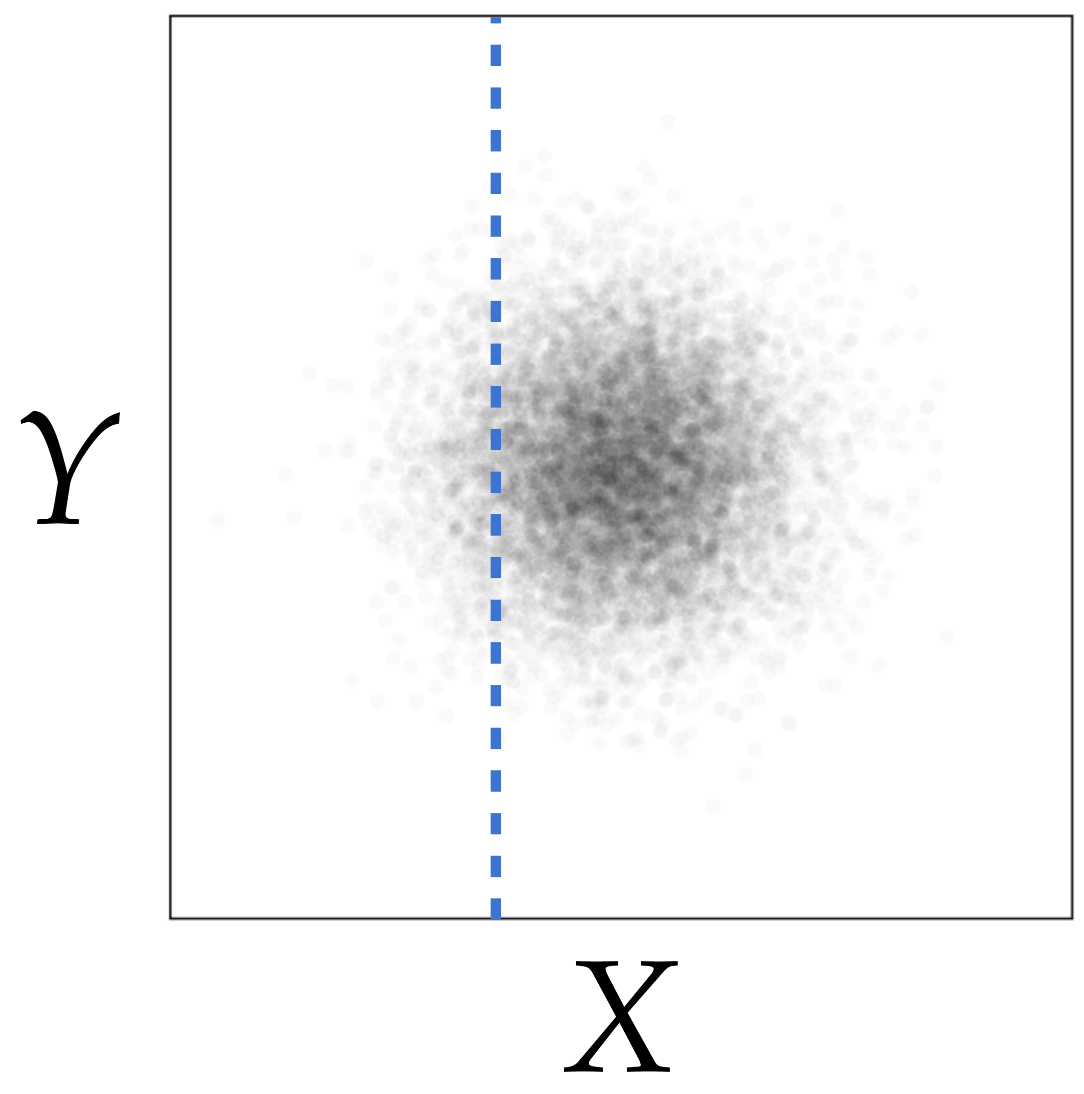

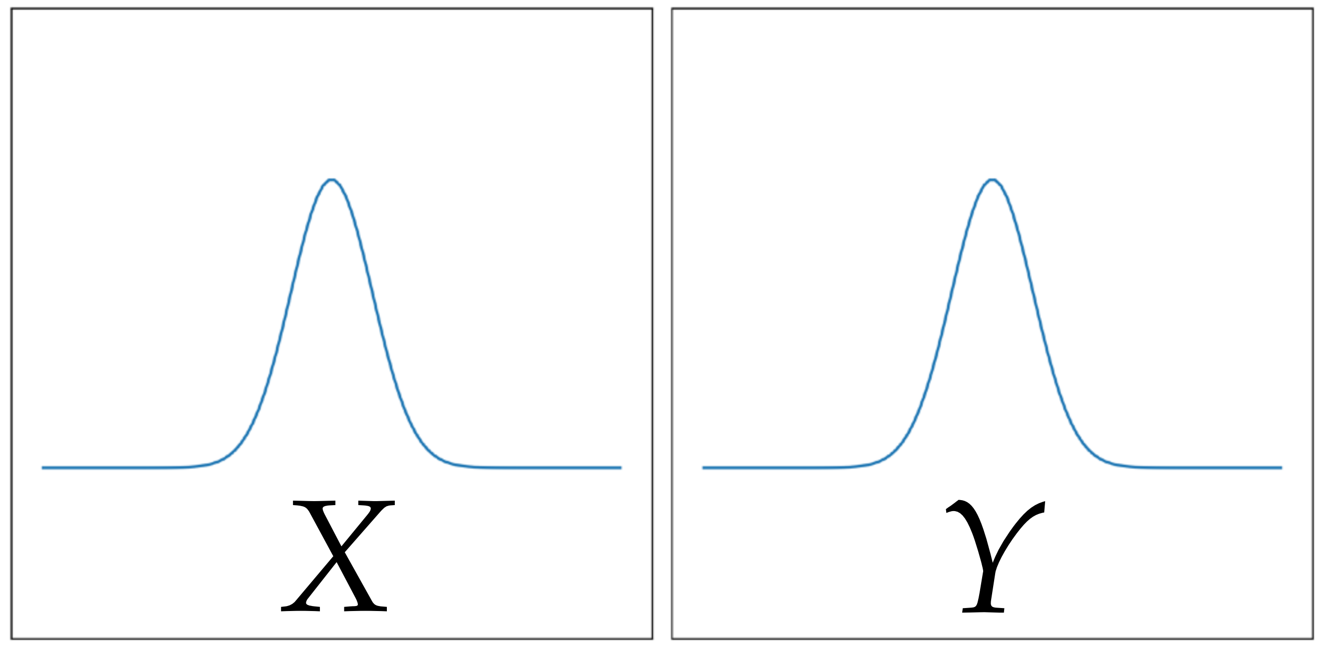

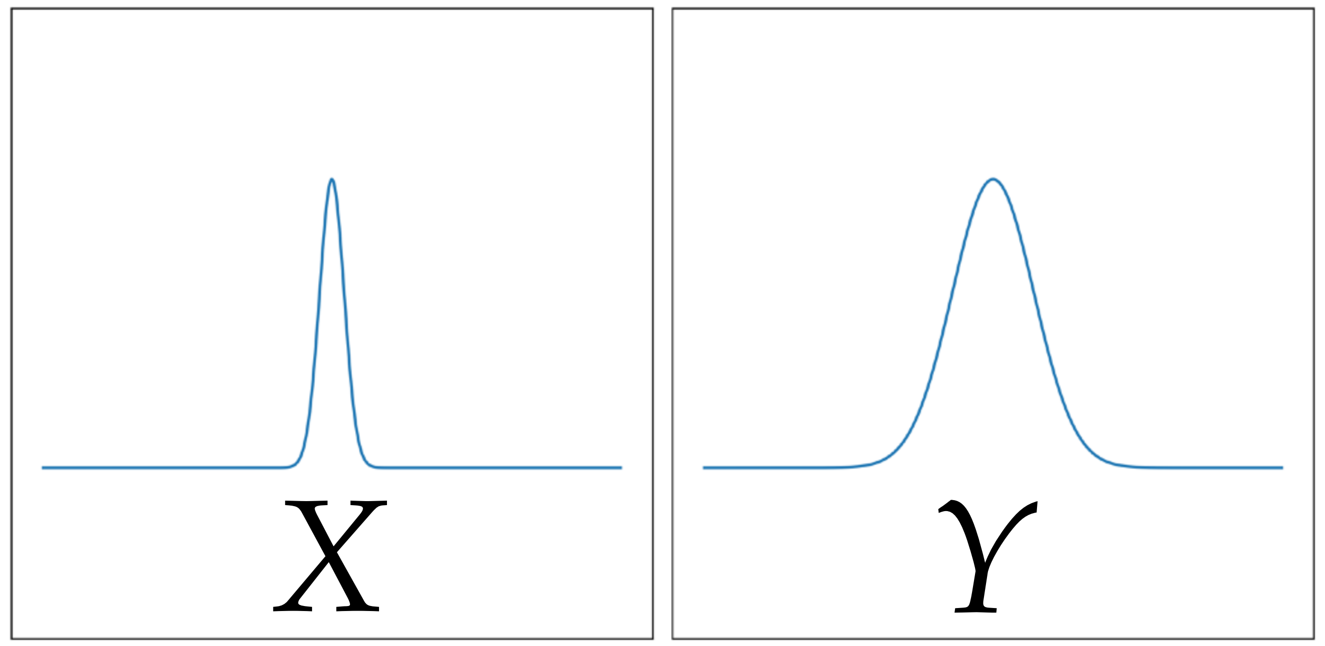

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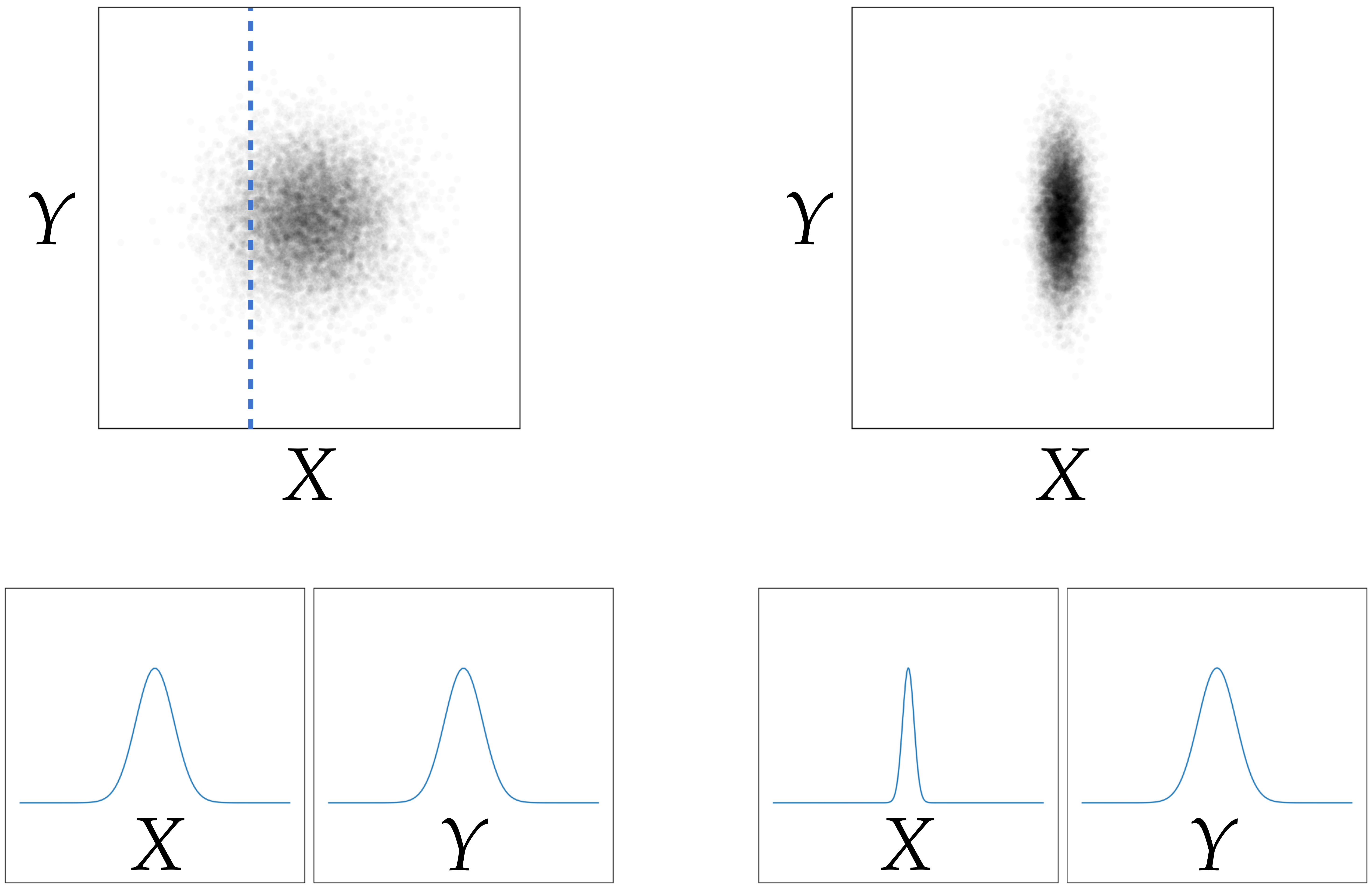

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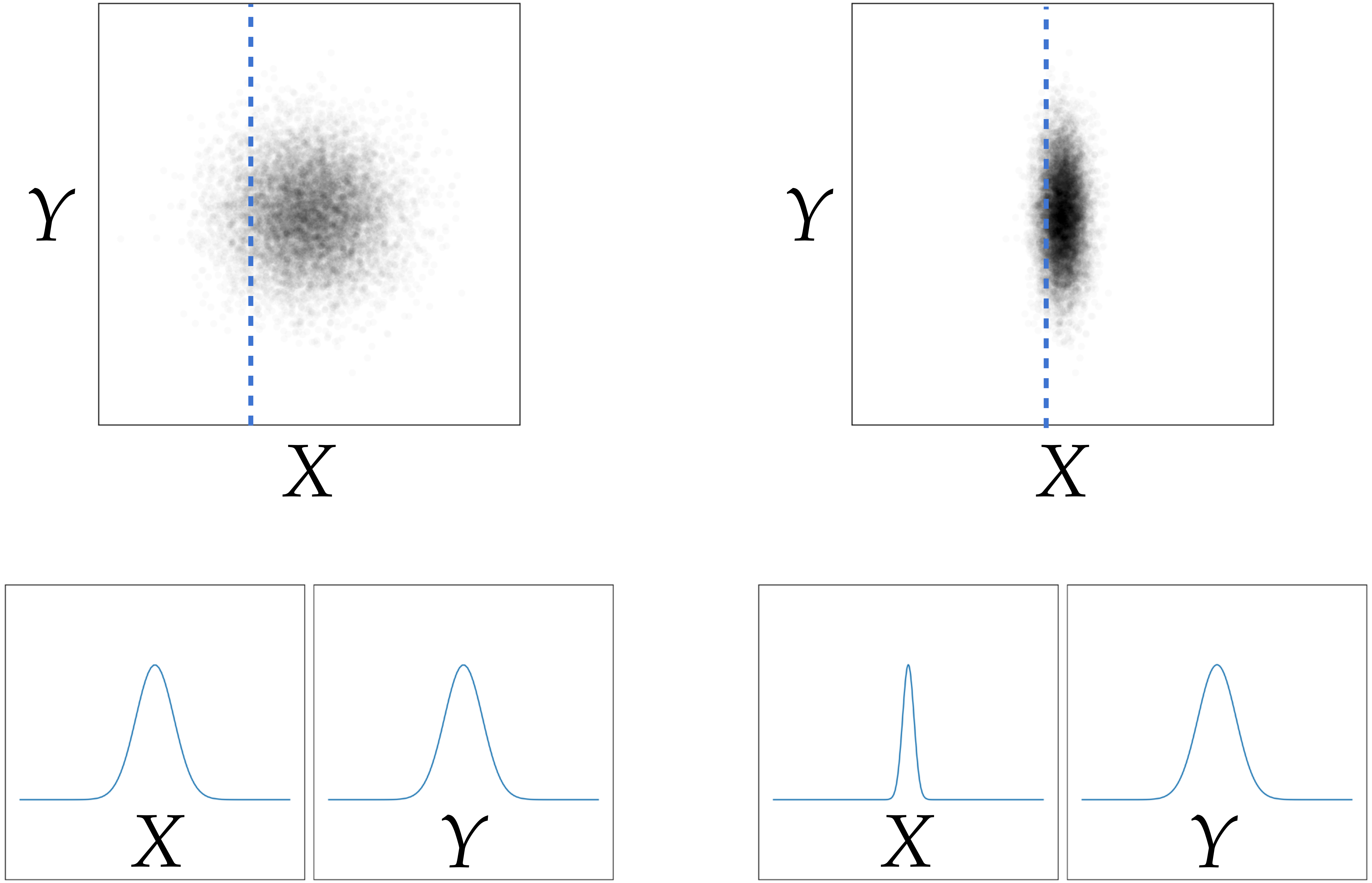

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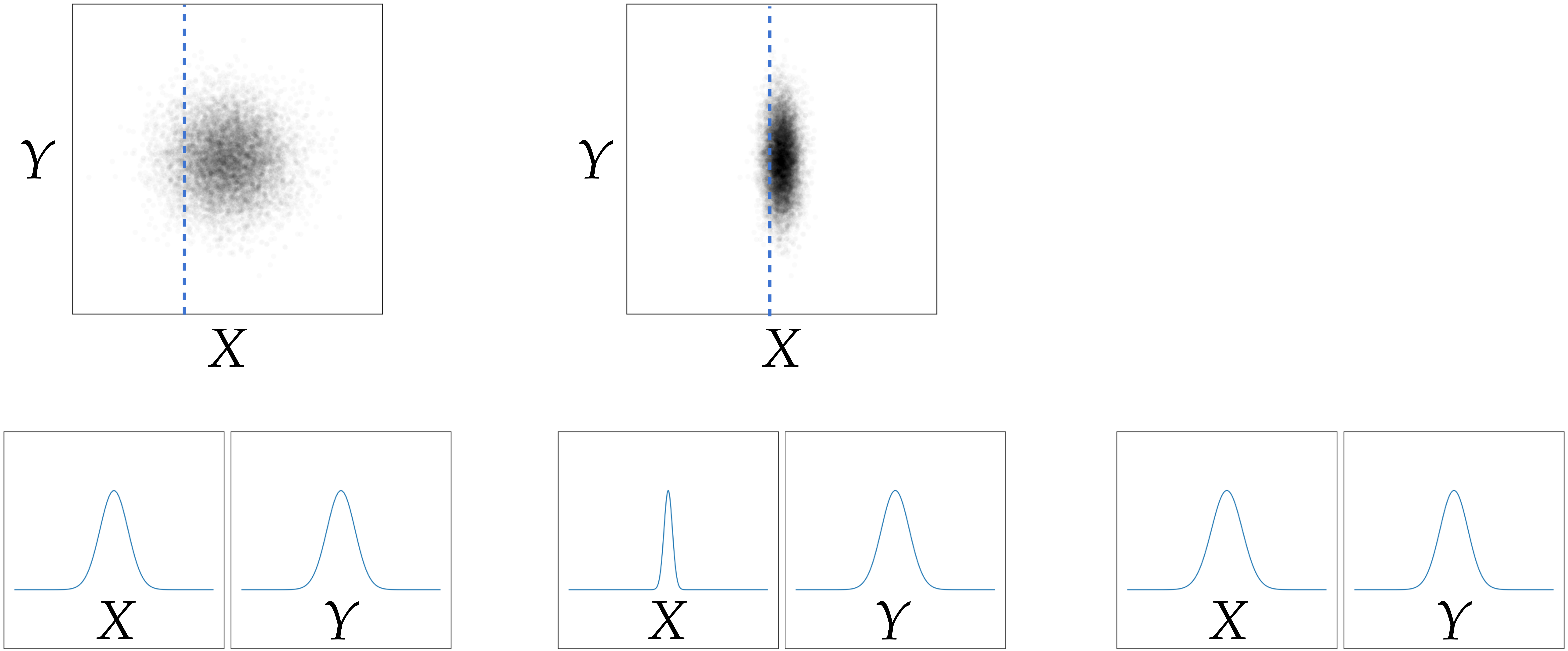

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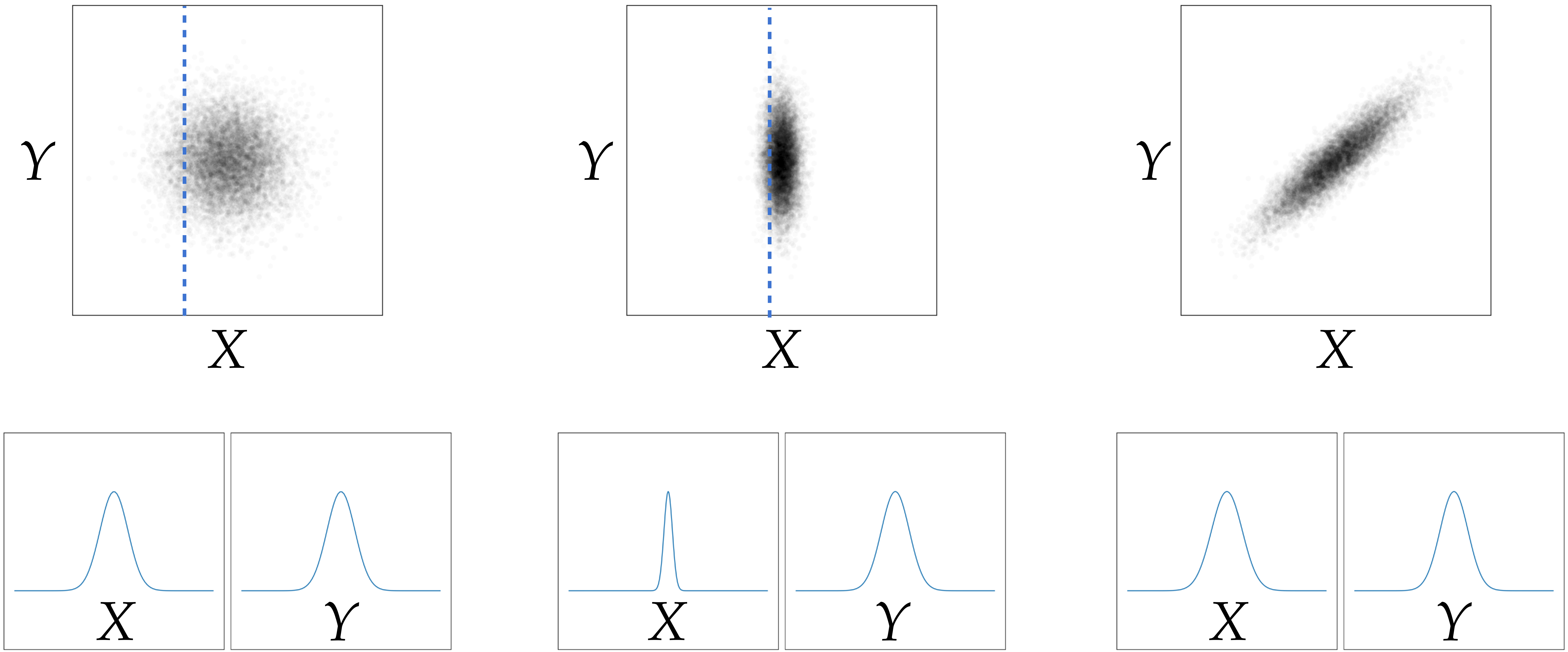

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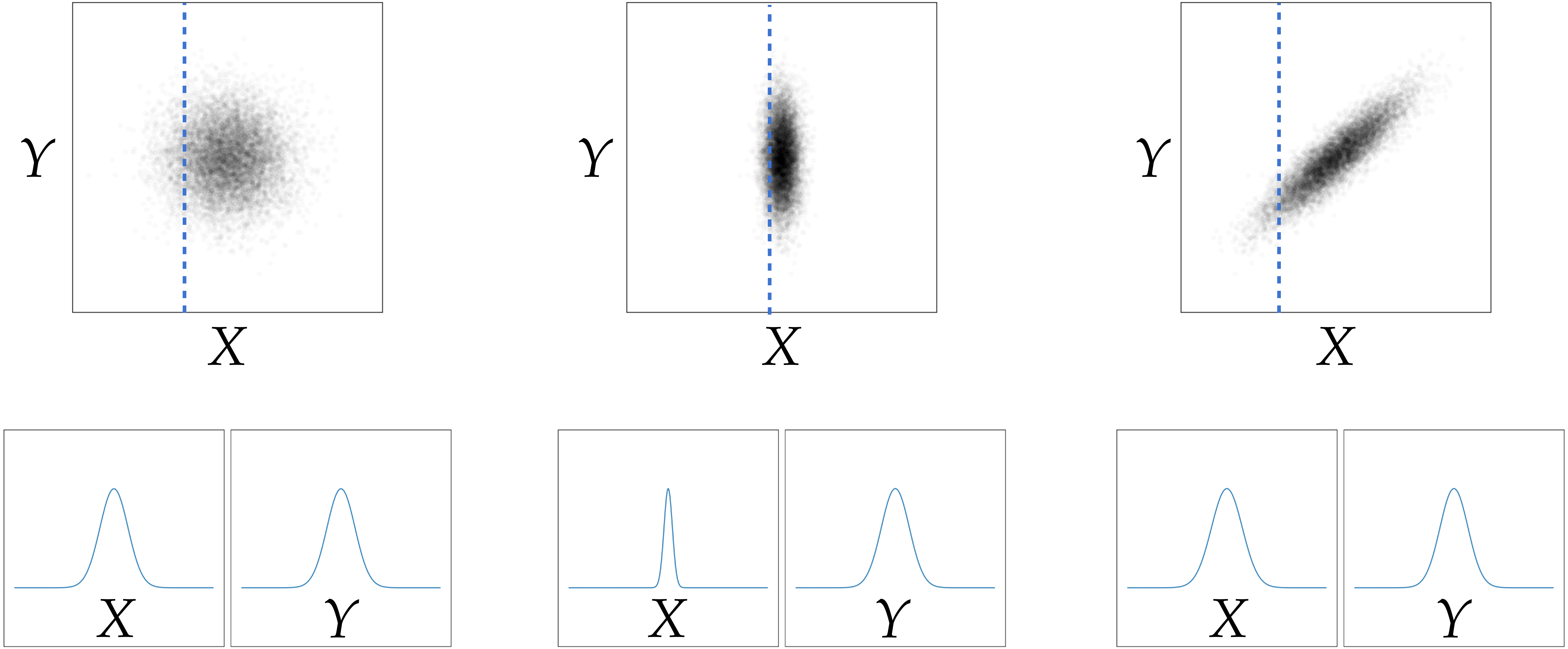

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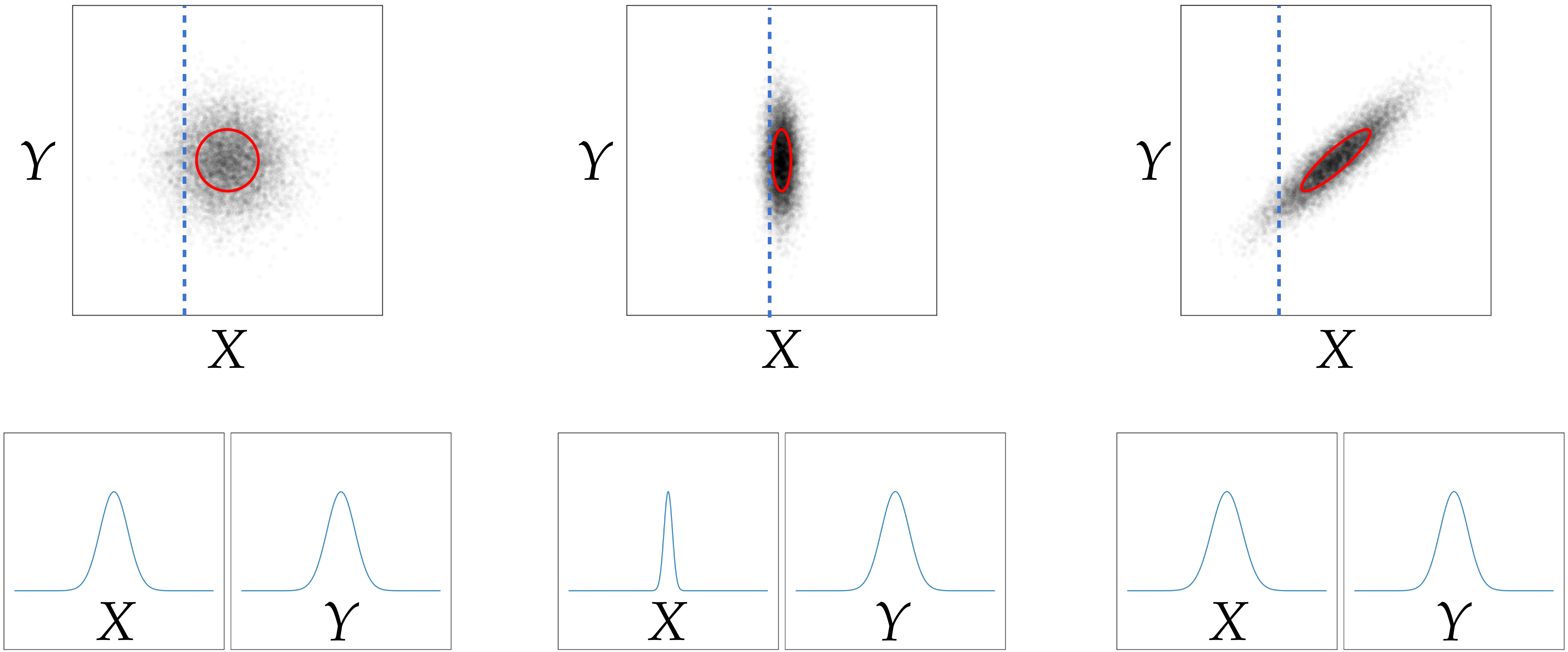

Correlations in multidimensional data

1. Age
2. Hardness
3. Smell intensity
4. Taste intensity
5. Amount of mold
6. Average color (RGB)

MidJourney: *Board with cheese selection, white background.*

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Intuitively, collecting data will reveal that some fields have an approximately linear relationship (they are **correlated**), e.g.:

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- Blue cheeses are generally blue because of mold.

Other axes will show **no correlation** in plots.

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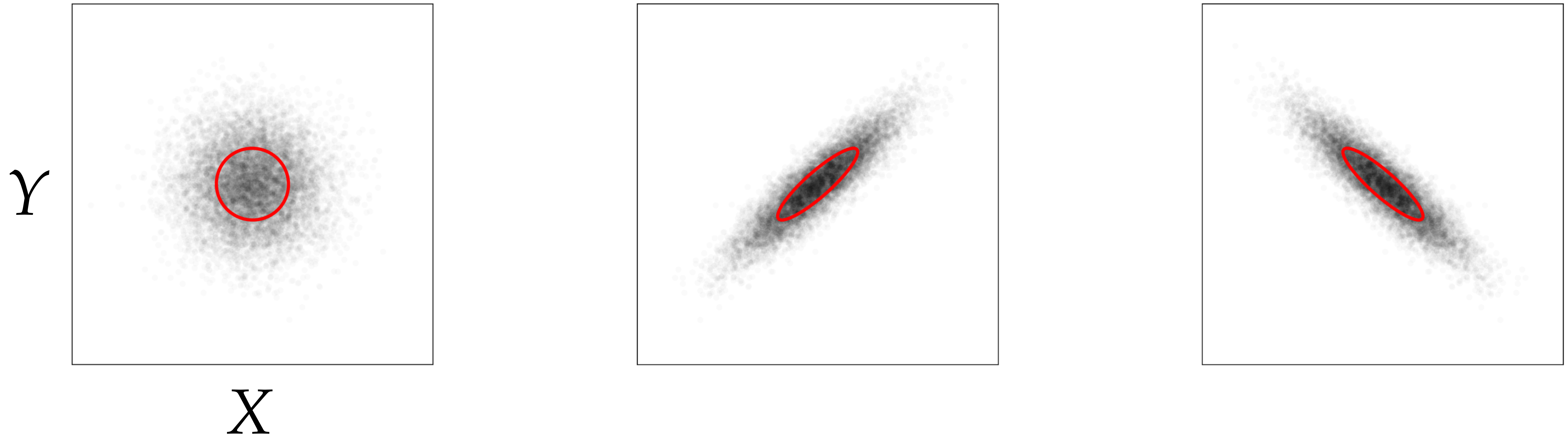

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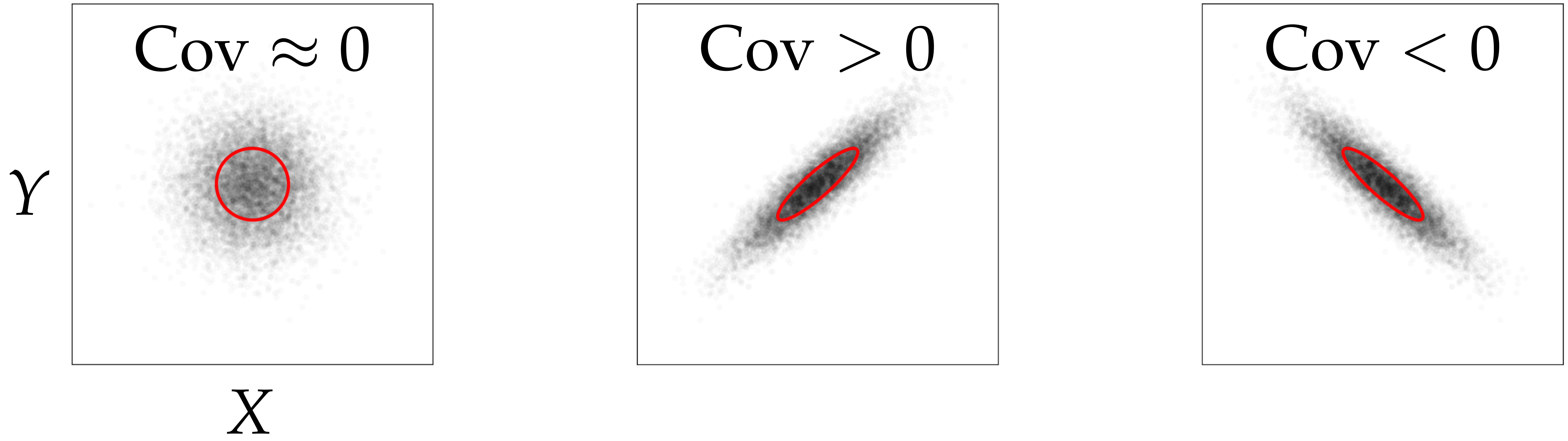

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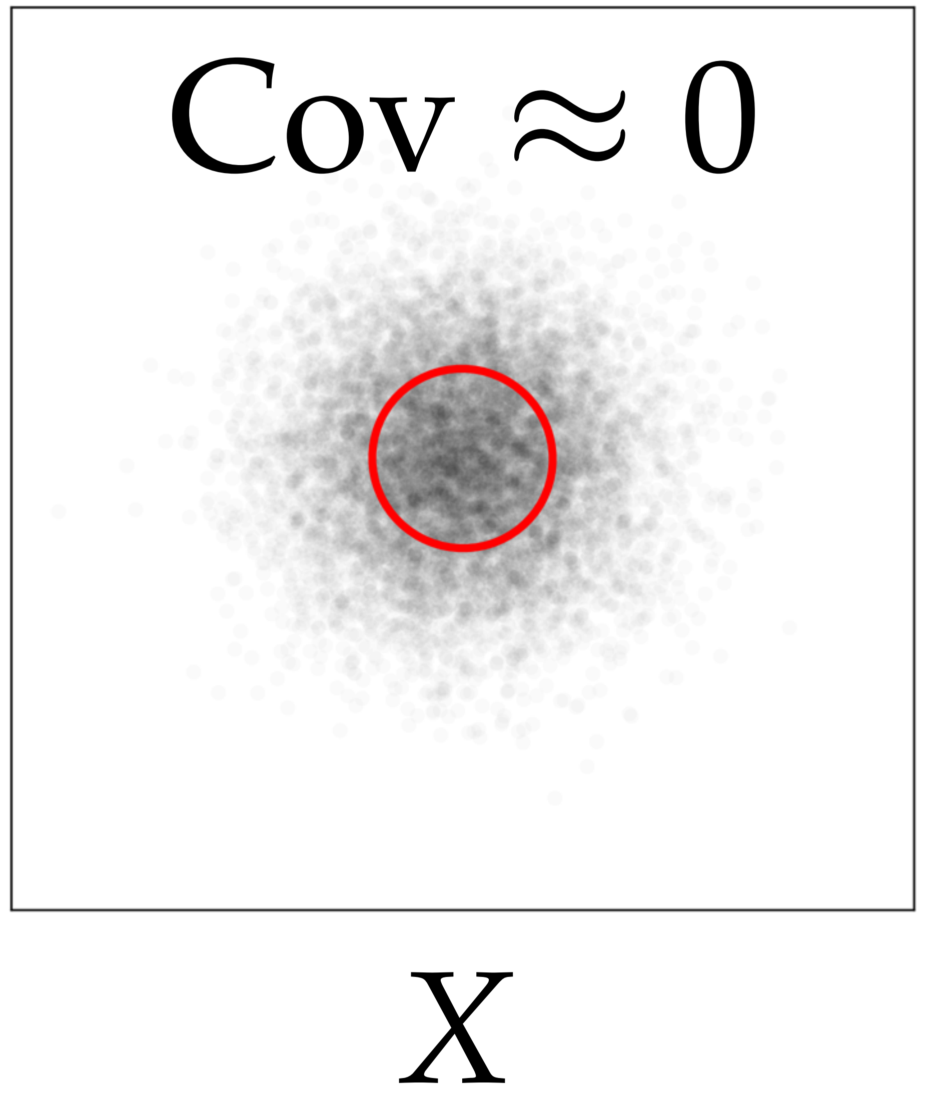

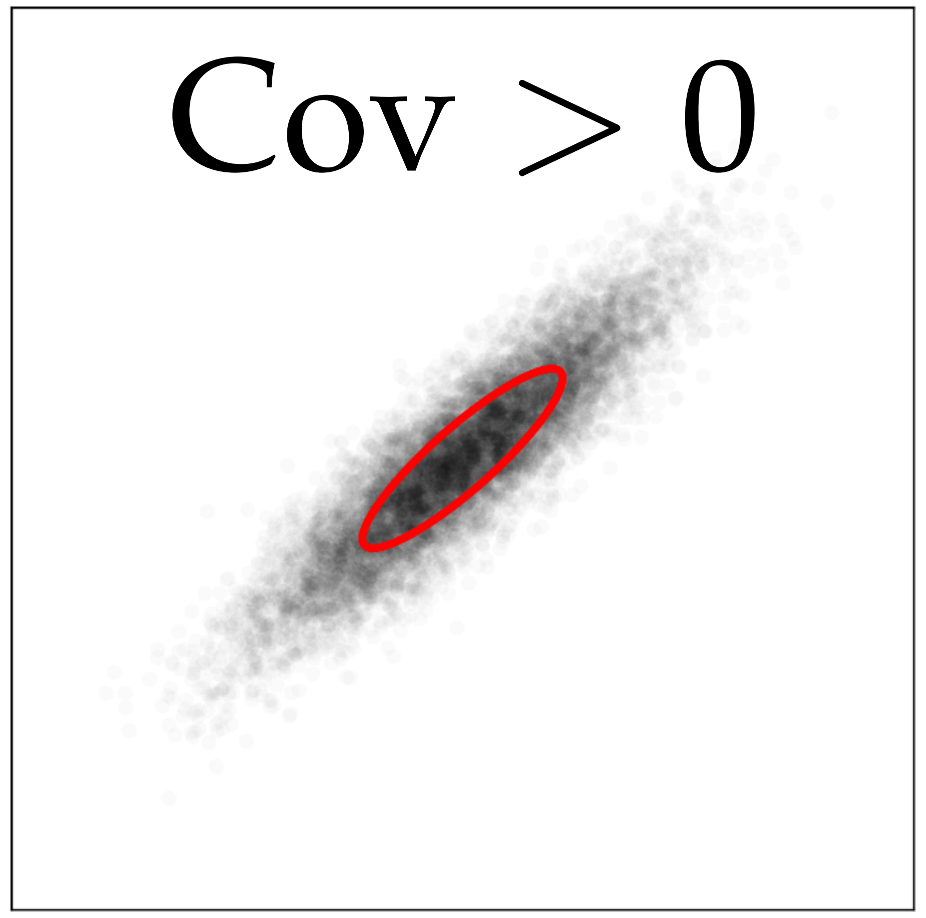

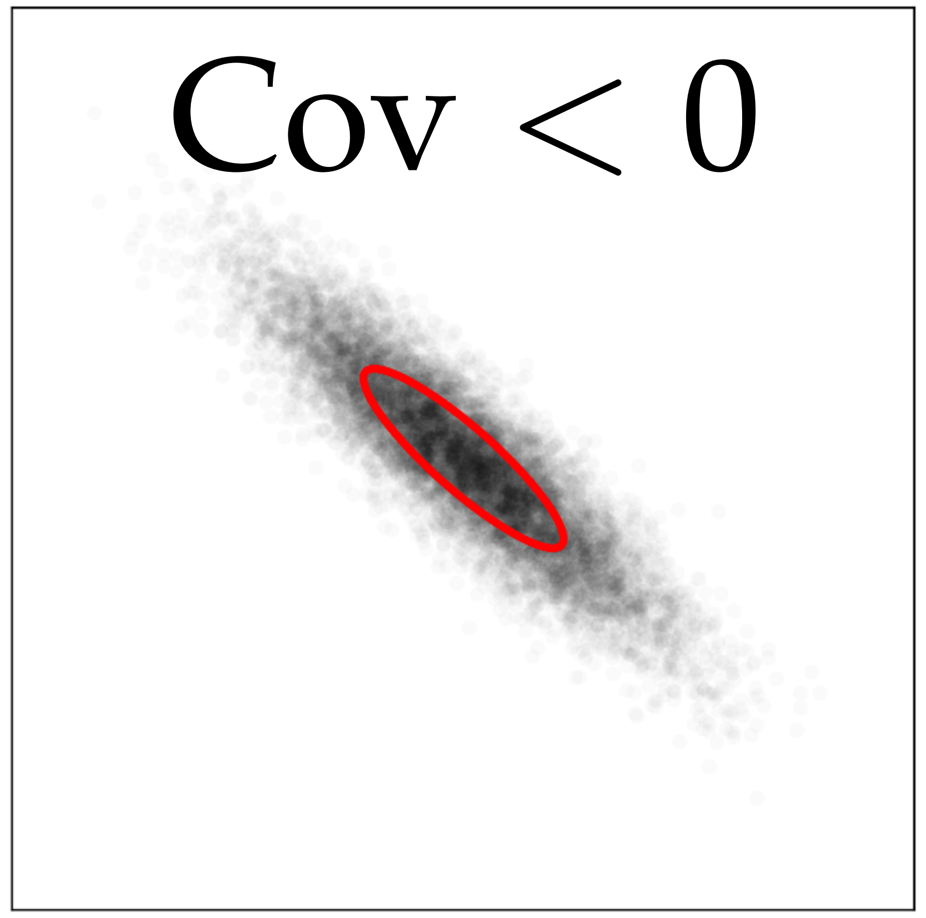

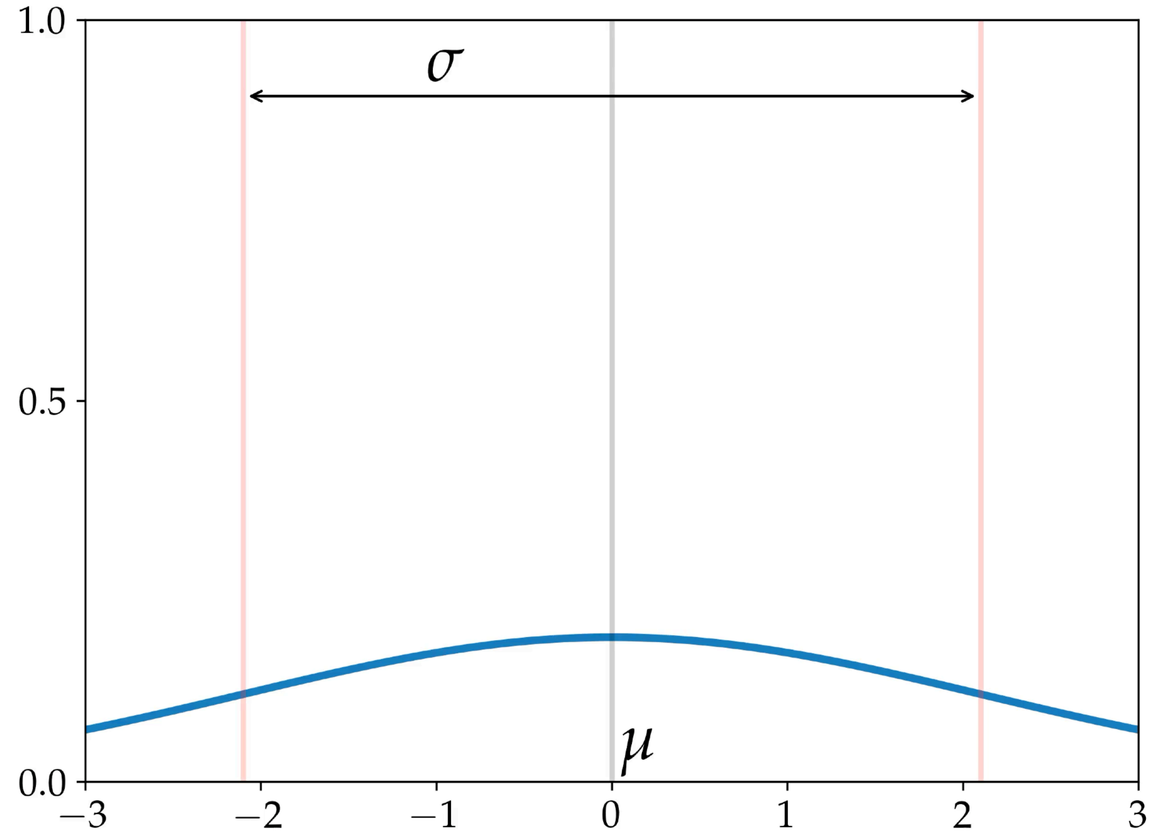

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n observations

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Sometimes *N-1* is used here instead. It depends on the setup (beyond the scope of CS328).

Multivariate Normal Distribution

$$\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$$

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Covariance matrix

Multivariate Normal Distribution

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Mean $\in \mathbb{R}^n$

Covariance matrix $\in \mathbb{R}^{n \times n}$

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Mean $\in \mathbb{R}^n$

Covariance matrix $\in \mathbb{R}^{n \times n}$

Density function:

$$f_{\mathbf{x}}(\mathbf{x}) = (2\pi)^{-\frac{n}{2}} \det(\boldsymbol{\Sigma})^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu})\right)$$

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Creating Normal Variates

Creating general normal variates (a.k.a. "simulating" or "sampling" them)

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NumPy recipe:

```
sqrt_sigma @ np.random.randn(n) + mu
```

Demo time

The Outer Product

Also often called a rank-1 matrix.

$$\mathbf{uv}^T = \begin{bmatrix} u_1v_1 & u_1v_2 & \dots & u_1v_n \\ u_2v_1 & u_2v_2 & \dots & u_2v_n \\ \vdots & \vdots & \ddots & \vdots \\ u_mv_1 & u_mv_2 & \dots & u_mv_n \end{bmatrix}$$

Another view of the SVD

$$\begin{bmatrix} \mathbf{A} \end{bmatrix} = \begin{bmatrix} \mathbf{U} \end{bmatrix} \begin{bmatrix} \ddots \boldsymbol{\Sigma} \ddots \end{bmatrix} \begin{bmatrix} \mathbf{V}^T \end{bmatrix}$$

Another view of the SVD

$$\left[\mathbf{A}\right] = \left[\mathbf{U}\right]\left[\boldsymbol{\Sigma}\right]\left[\mathbf{V}^T\right]$$

where

$$\mathbf{V} = \begin{pmatrix} | & & | \\ \mathbf{v}_1 & \cdots & \mathbf{v}_n \\ | & & | \end{pmatrix} \mathbf{U} = \begin{pmatrix} | & & | \\ \mathbf{u}_1 & \cdots & \mathbf{u}_n \\ | & & | \end{pmatrix} \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{pmatrix}$$

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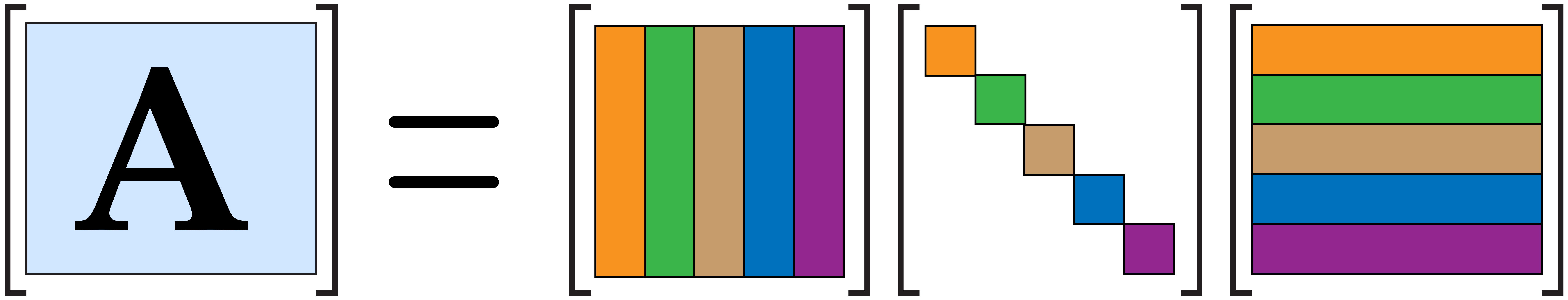
Then $\mathbf{A} = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$

Another view of the SVD

Coloring each combination of left/right singular vector & value reveals outer product structure



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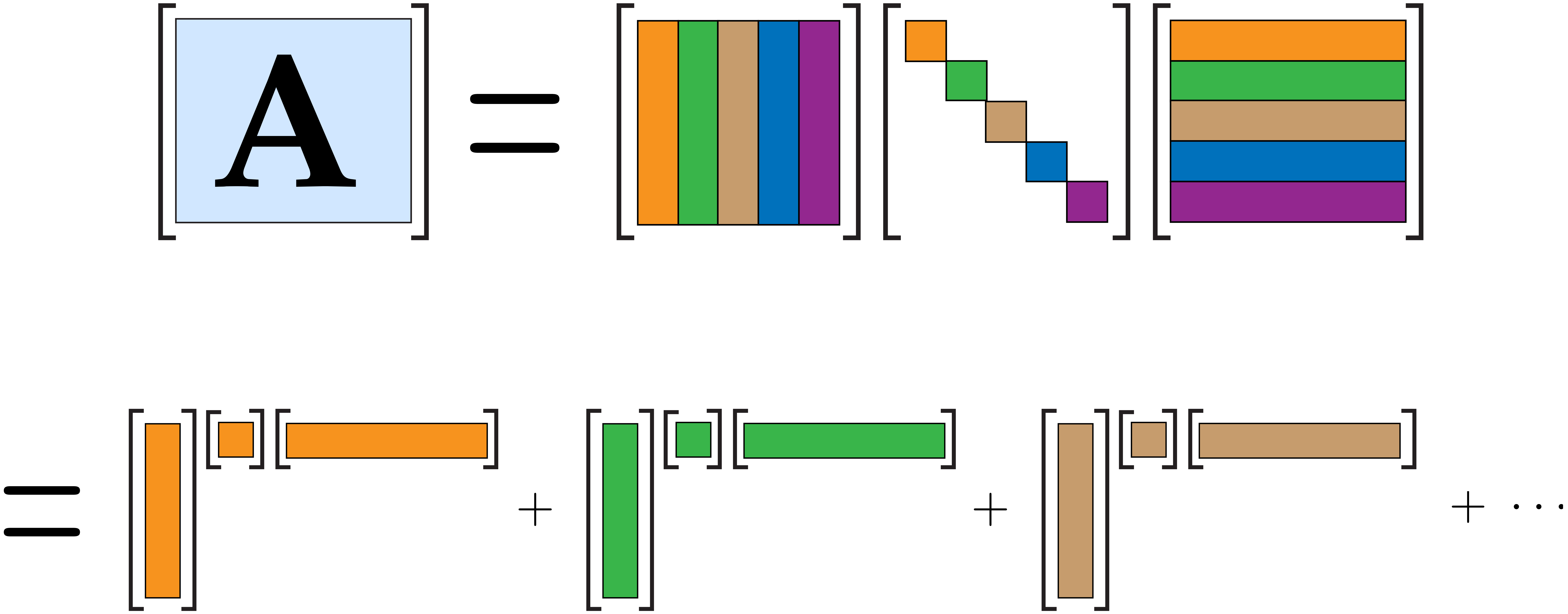
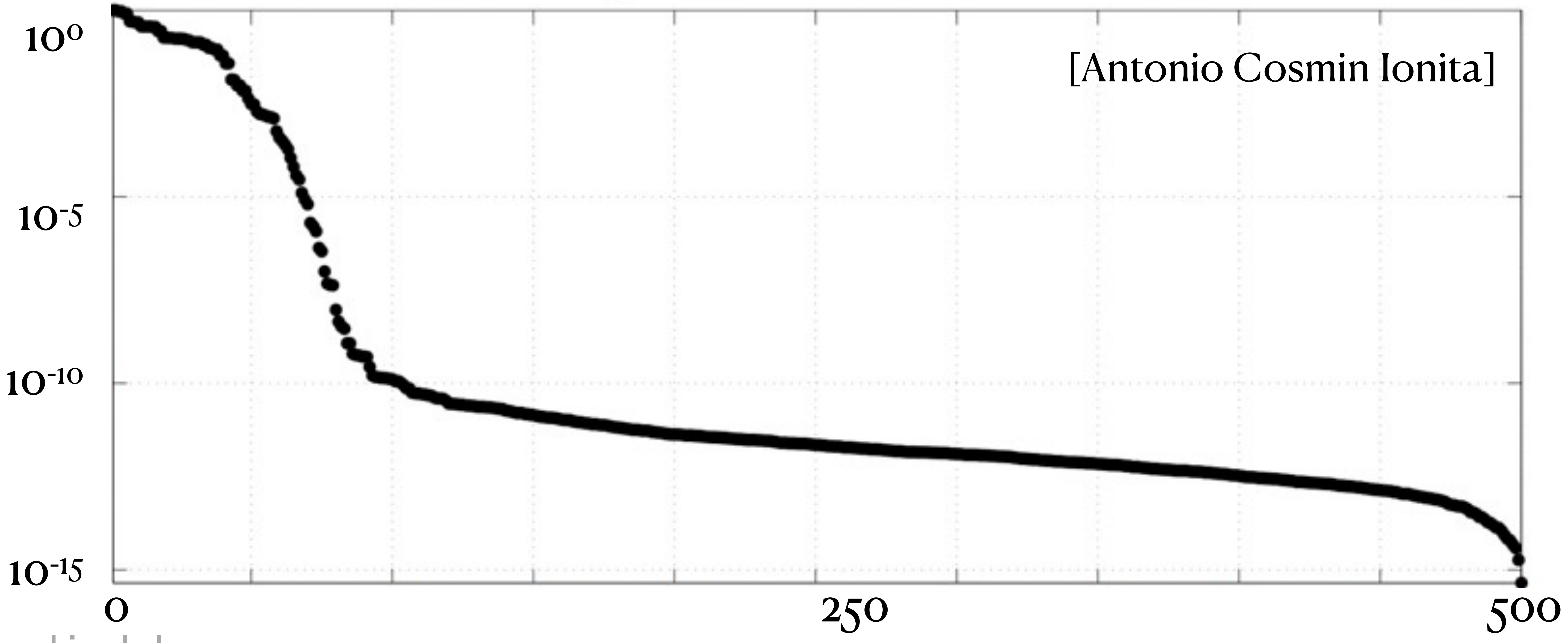


Matrix approximation

$$\mathbf{A} = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

Plot of singular values (in decreasing magnitude)



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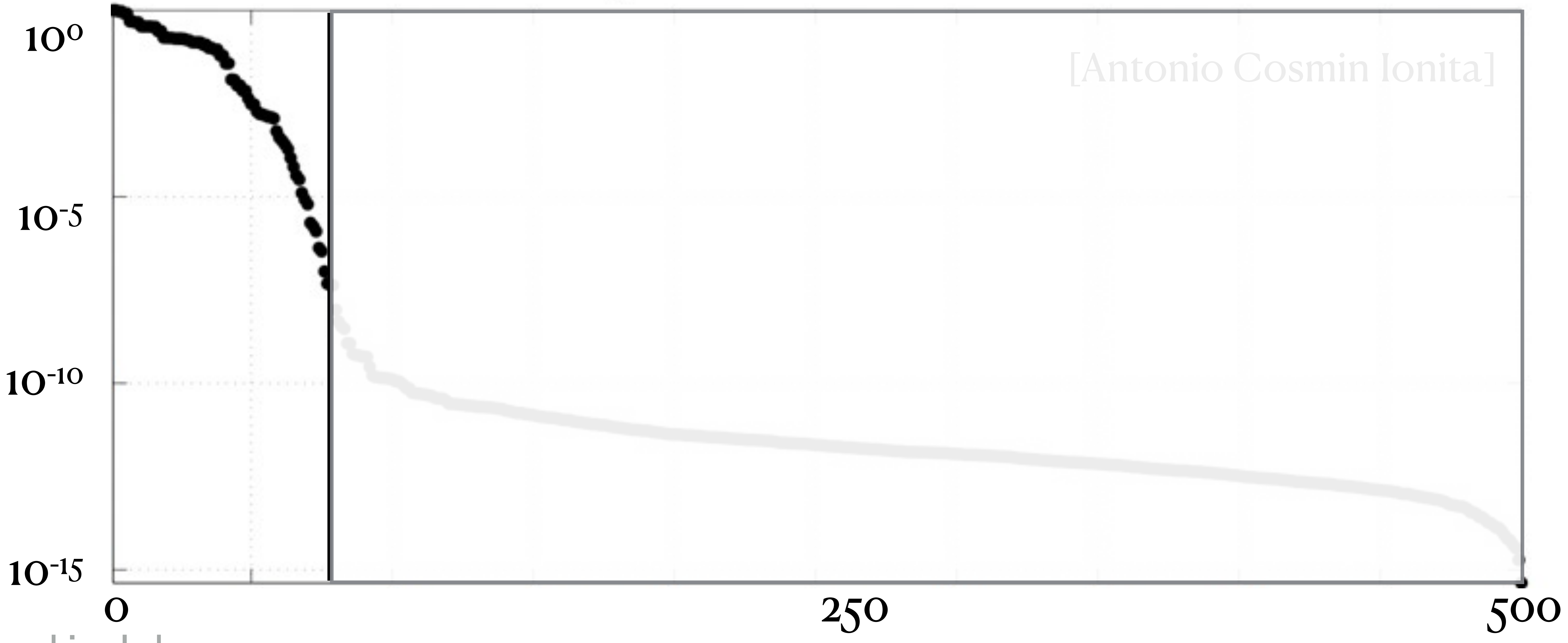

Matrix approximation

$$\mathbf{A} = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T \longrightarrow \mathbf{A} \approx \sum_{i=1}^{n_{\max}} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

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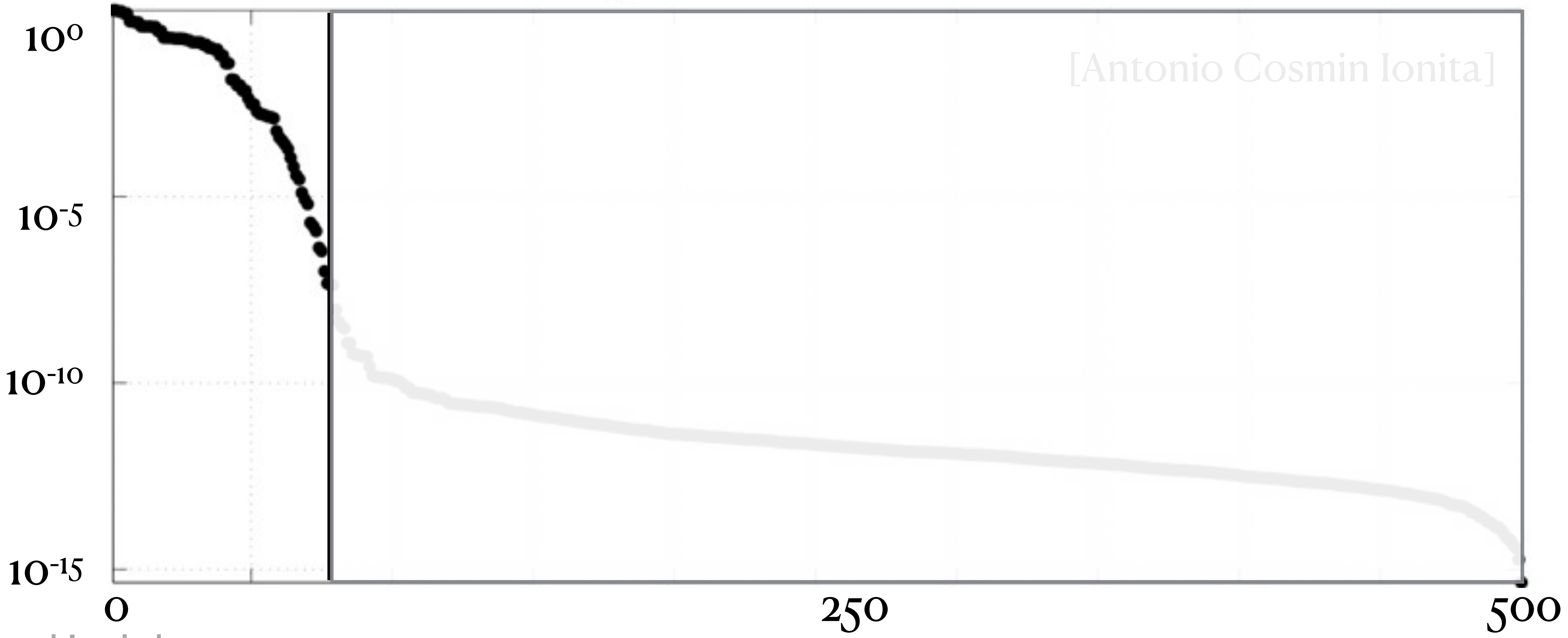

Eckart-Young Theorem

Stated without proof.

Suppose that **A'** is obtained from **A** by truncating all but the largest *k* singular values from its singular value decomposition.

Then **A'** minimizes both

$$\text{(i)} \quad \|\mathbf{A} - \mathbf{A}'\|_F \quad \textit{and}$$

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among all matrices **A'** with rank *k*.

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$$||\mathbf{A}||_F^2 := \sum_{ij} A_{ij}^2$$

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("Frobenius norm")

Demo time

Computing inverses via the SVD

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \sum_{i=1}^{n} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

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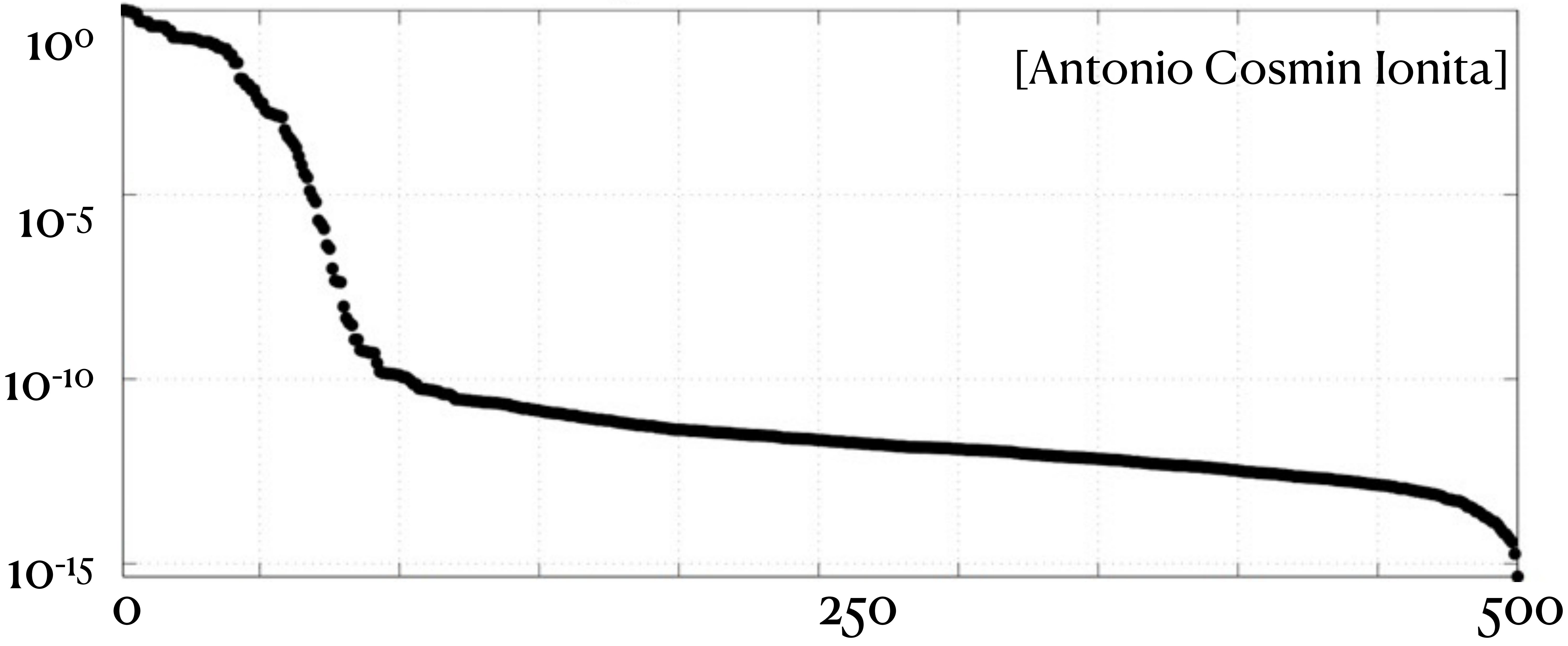

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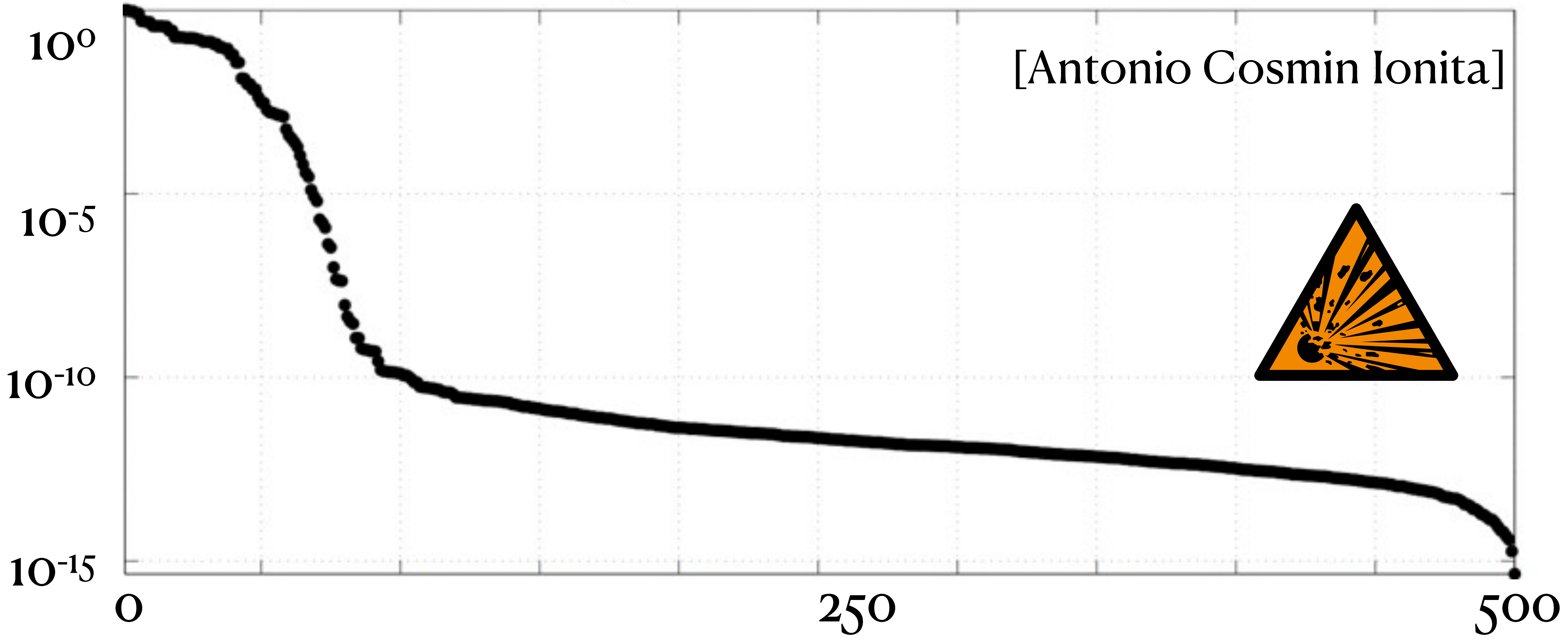

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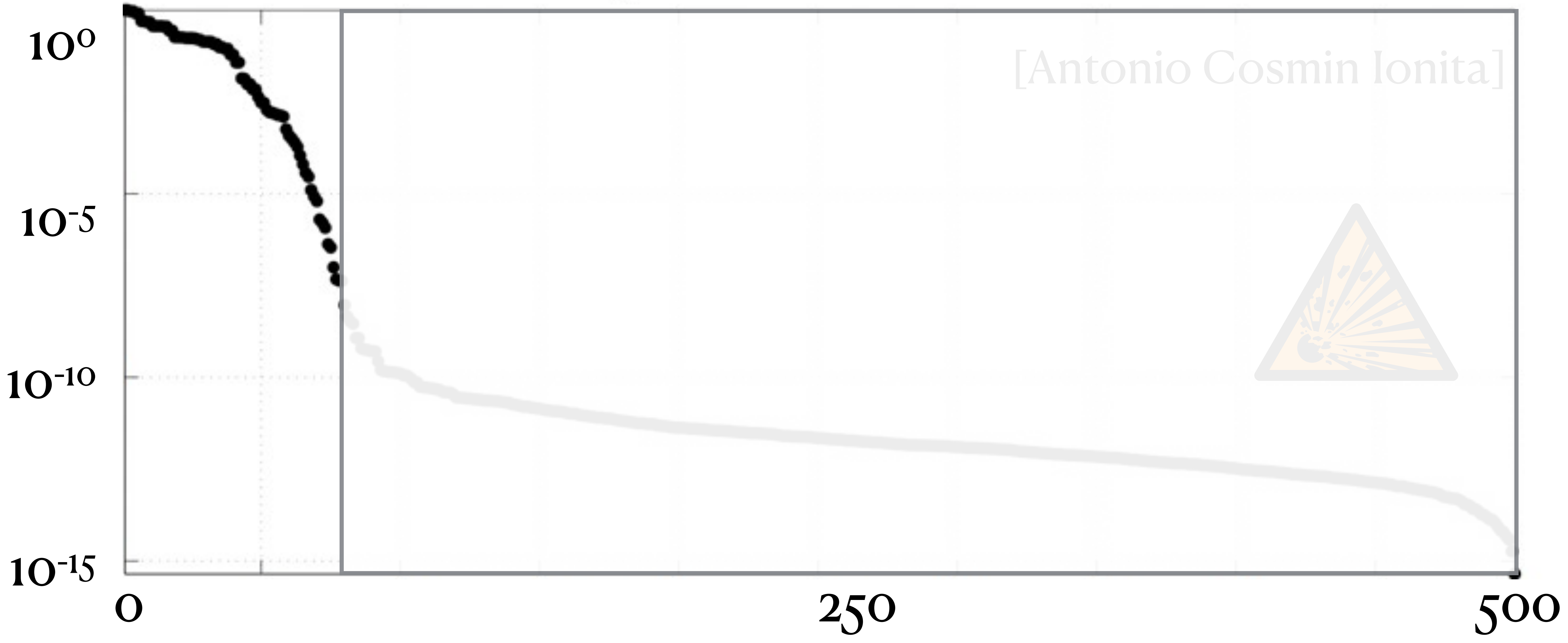

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$$\mathbf{A}^{-1} = \mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^T = \sum_{i=1}^{n} \frac{1}{\sigma_i}\mathbf{v}_i\mathbf{u}_i^T \approx \sum_{i=1}^{n_{\max}} \frac{1}{\sigma_i}\mathbf{v}_i\mathbf{u}_i^T$$

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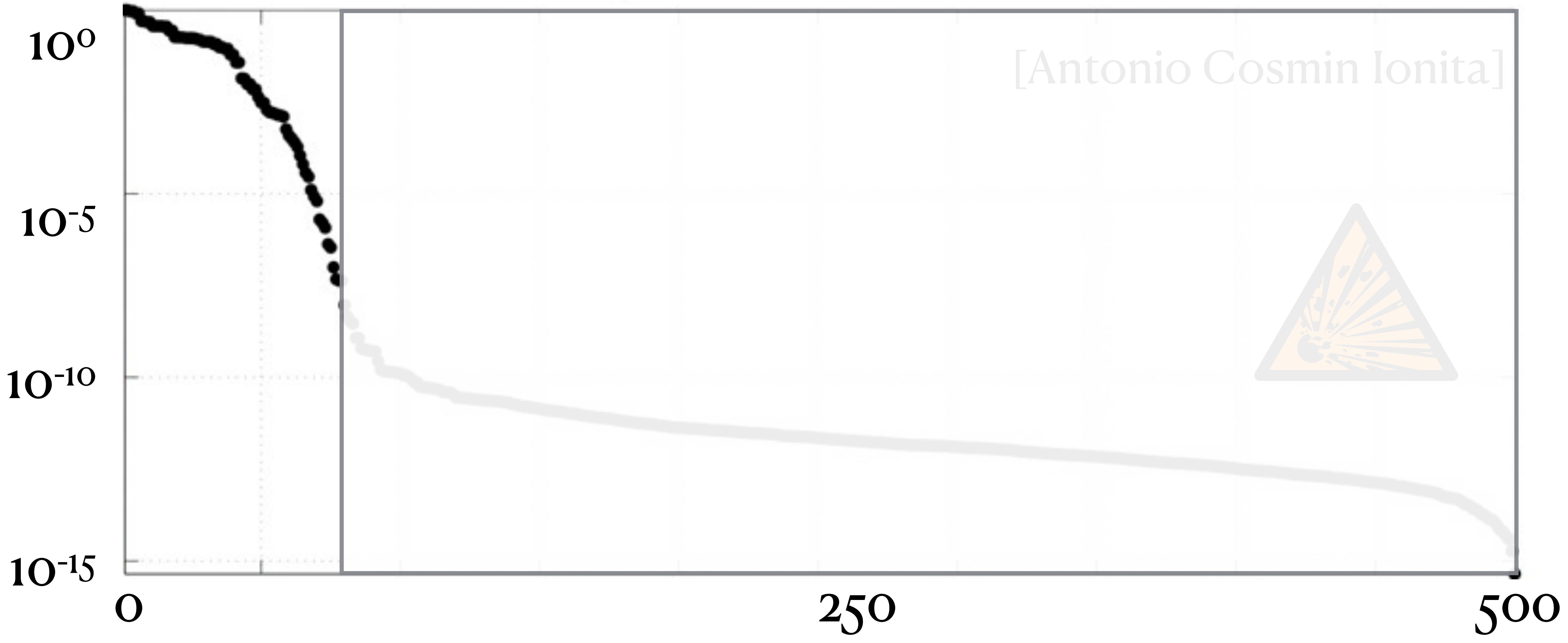
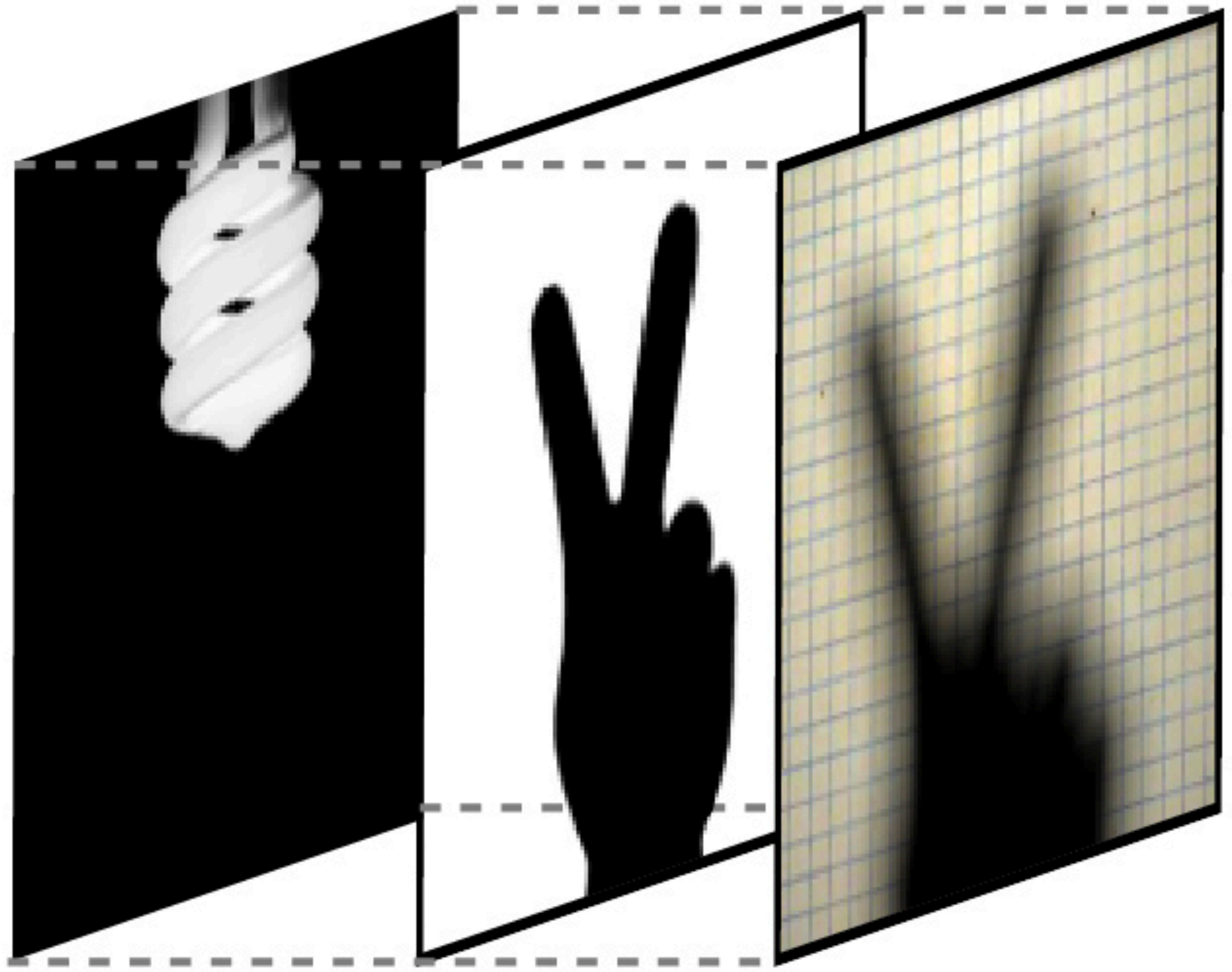
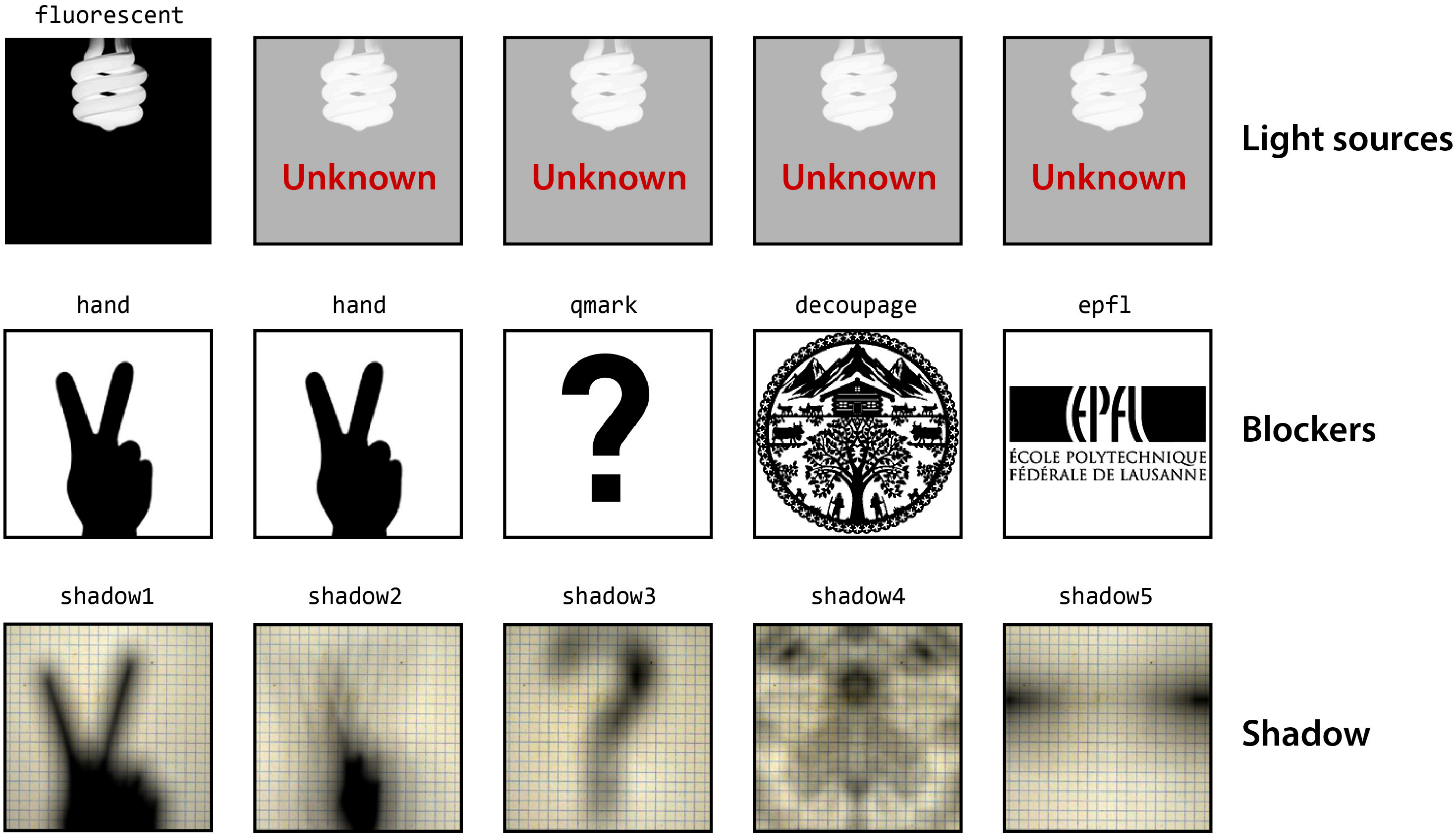


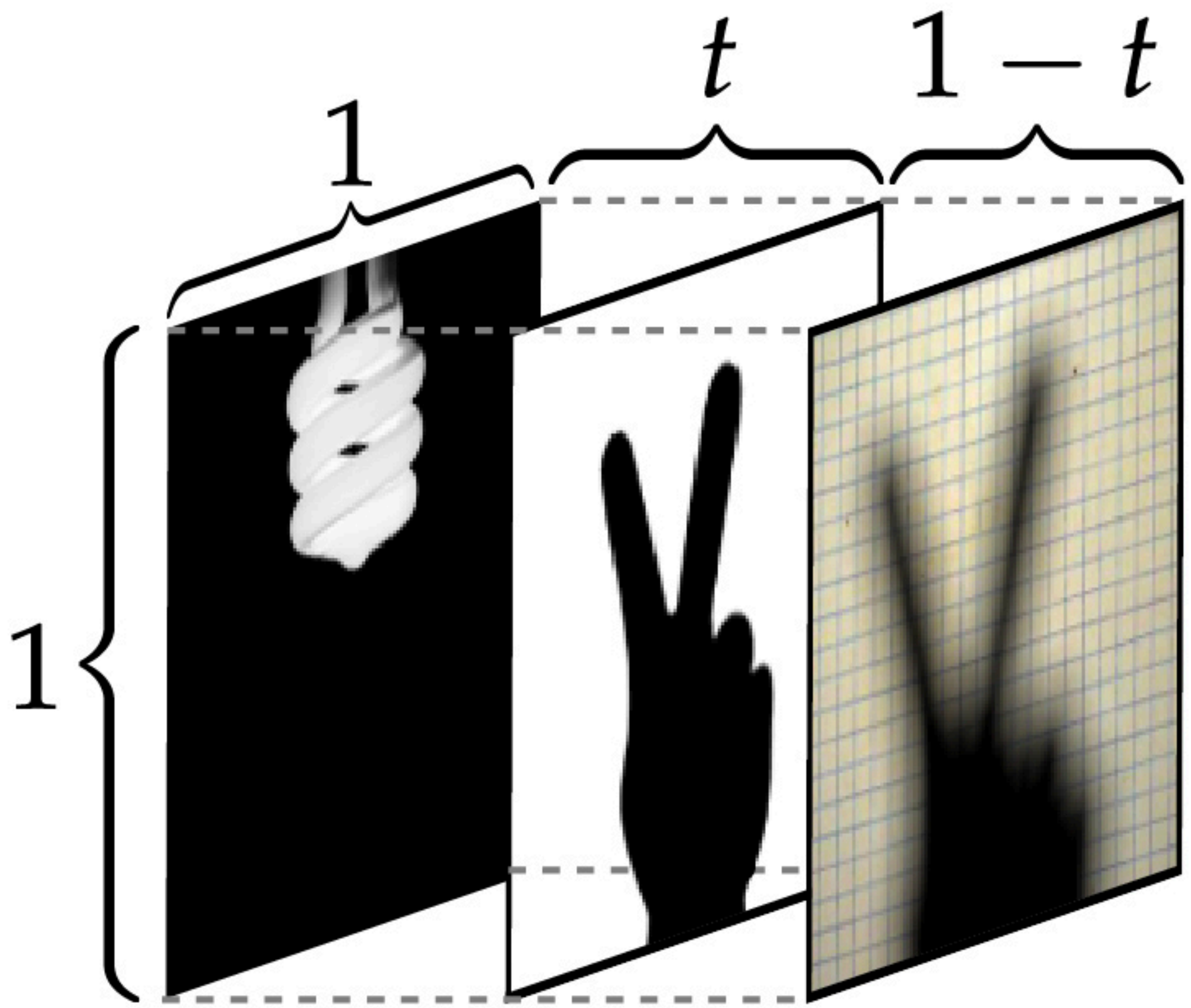
SVD as a regularization strategy



The *SVD-powered X-ray glasses*
(originally by Doug James @ Stanford U.)


fluorescent
Unknown
Unknown
Unknown
Unknown
Light sources
hand
hand
qmark
decoupage
epfl
ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE
Blockers
shadow1
shadow2
shadow3
shadow4
shadow5
Shadow

Problem setup



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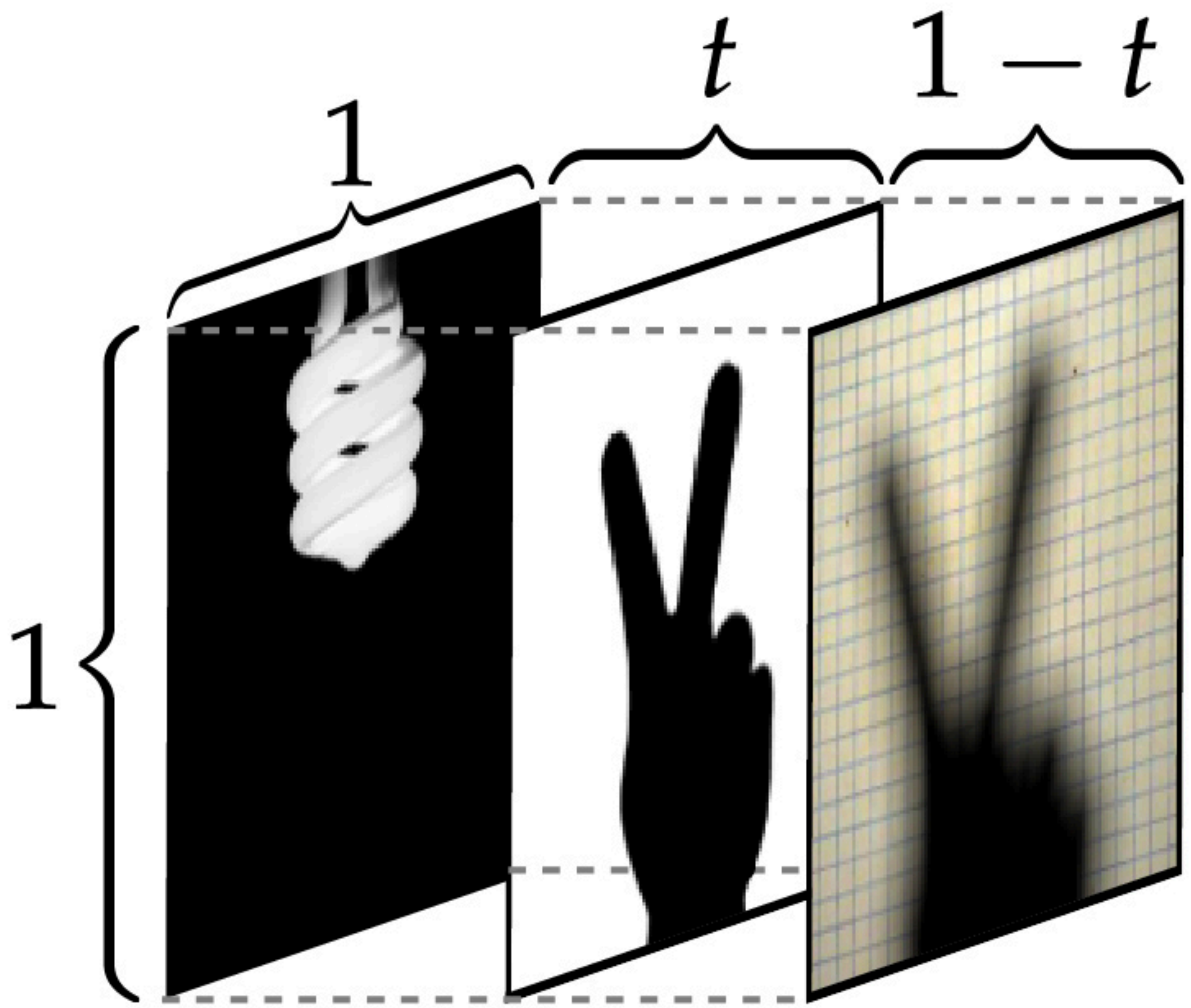

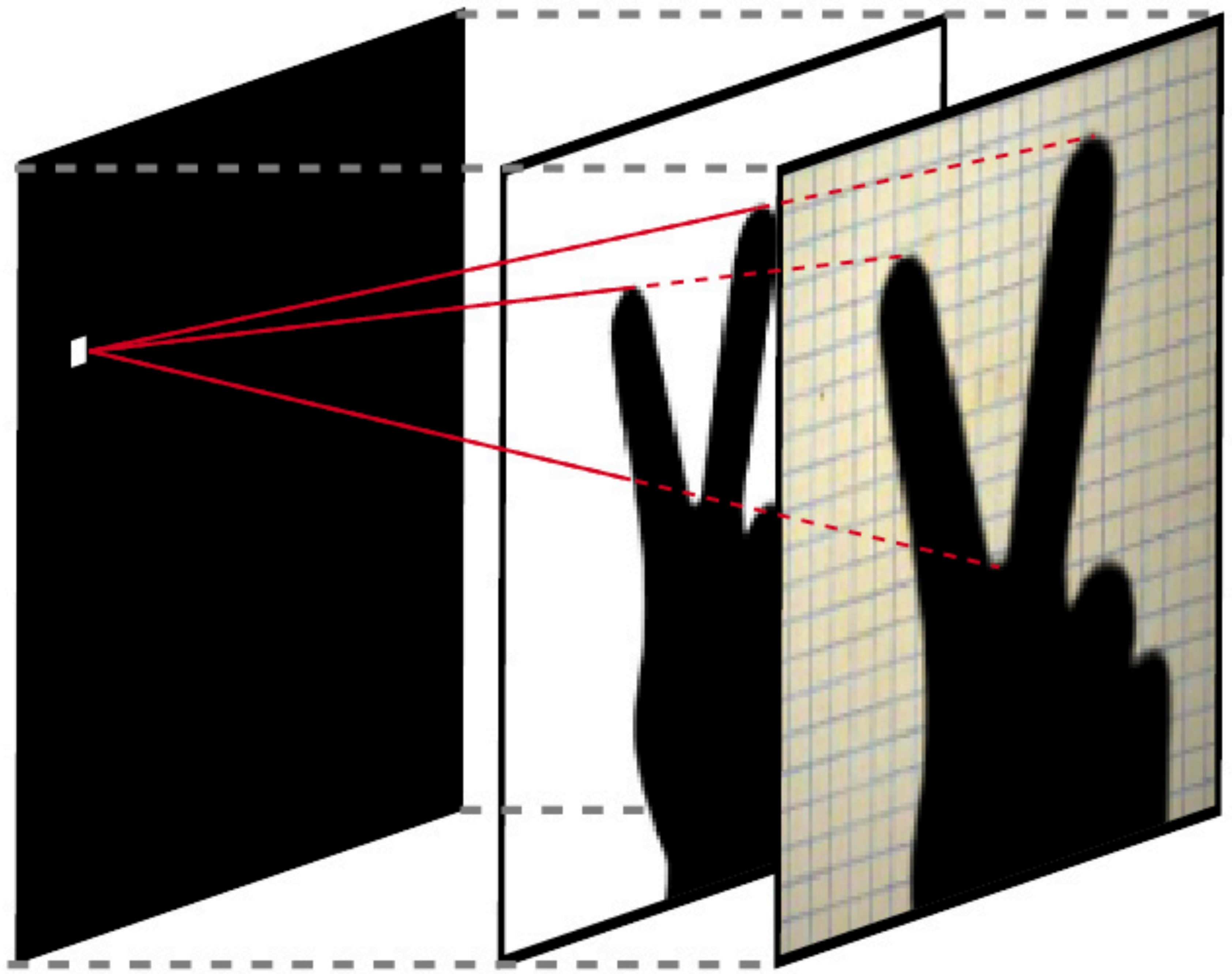

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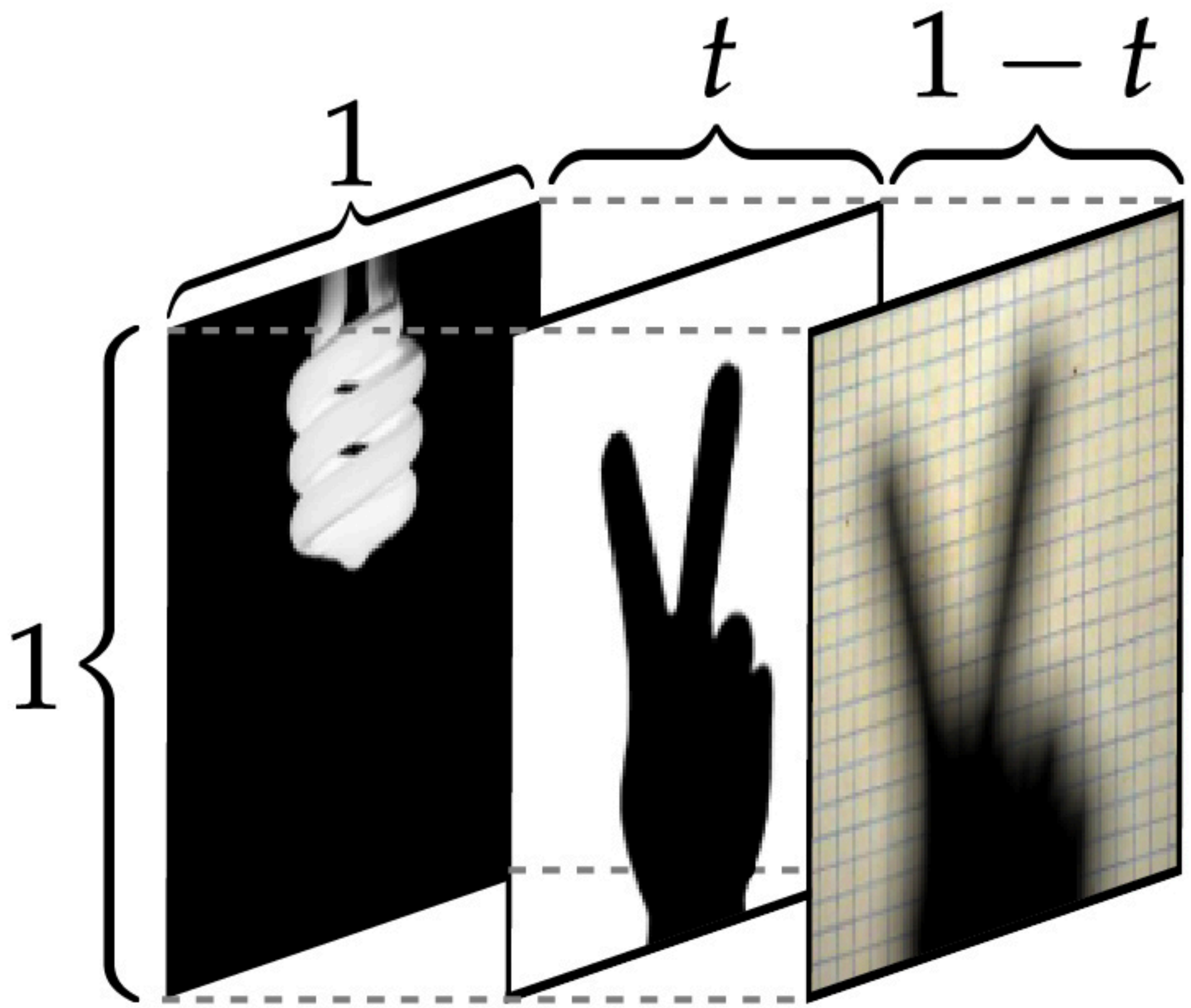

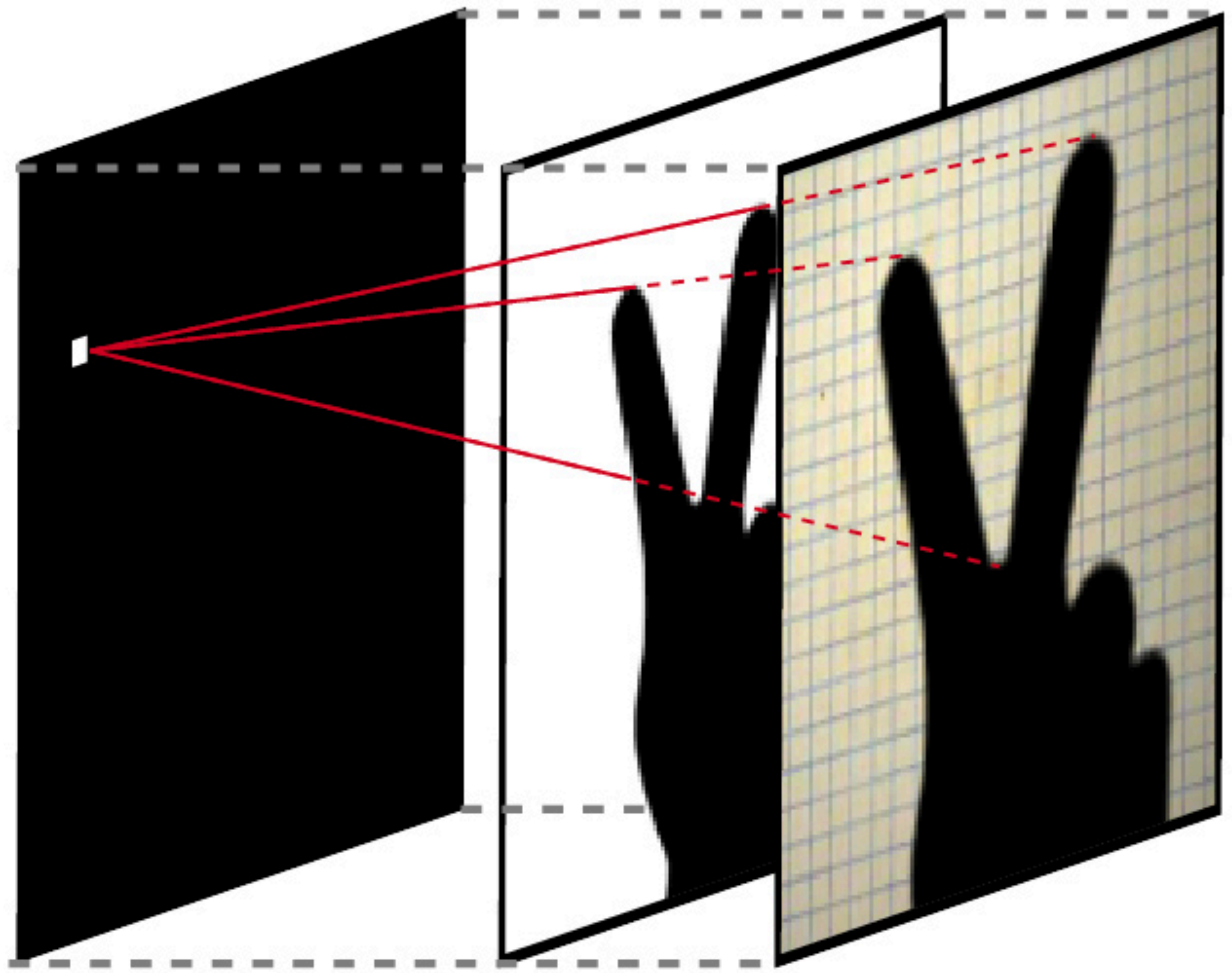

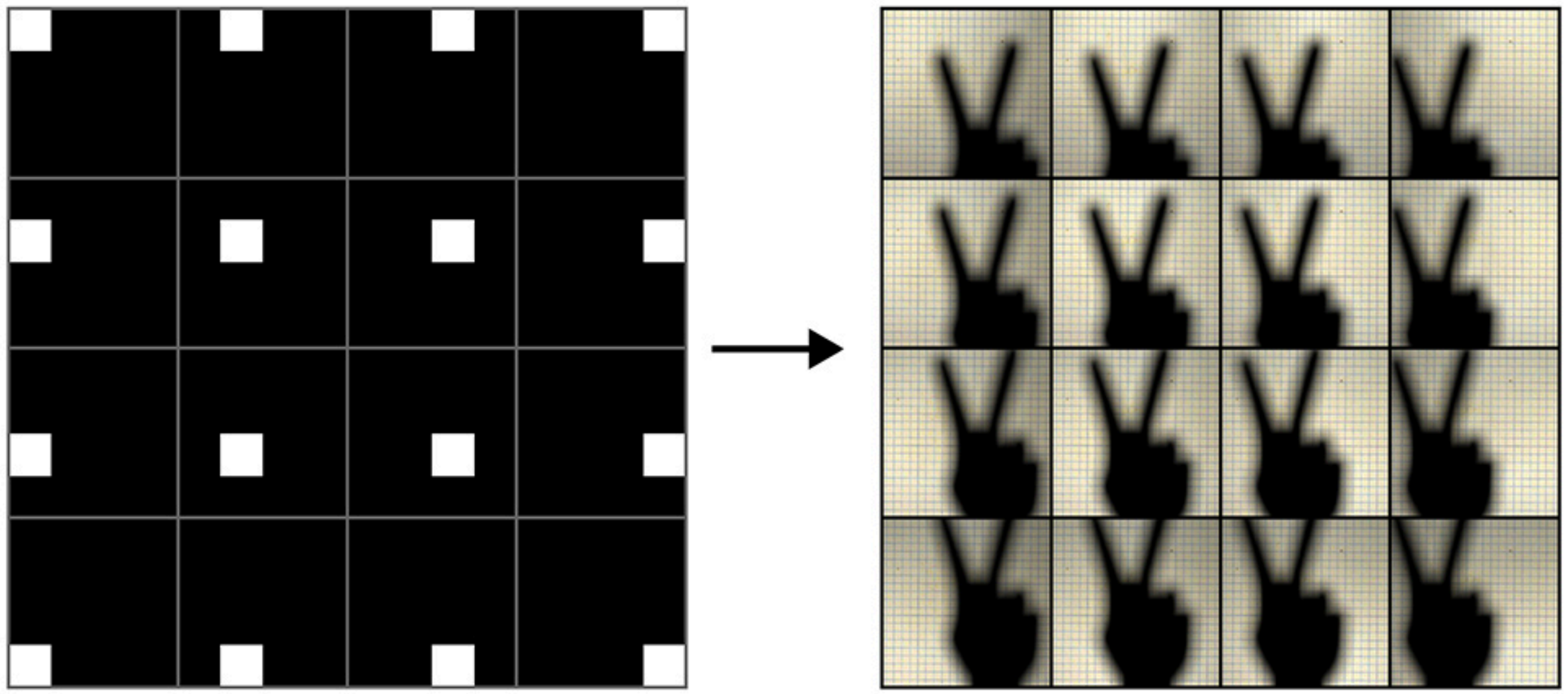

Demo time

Revisiting the condition number

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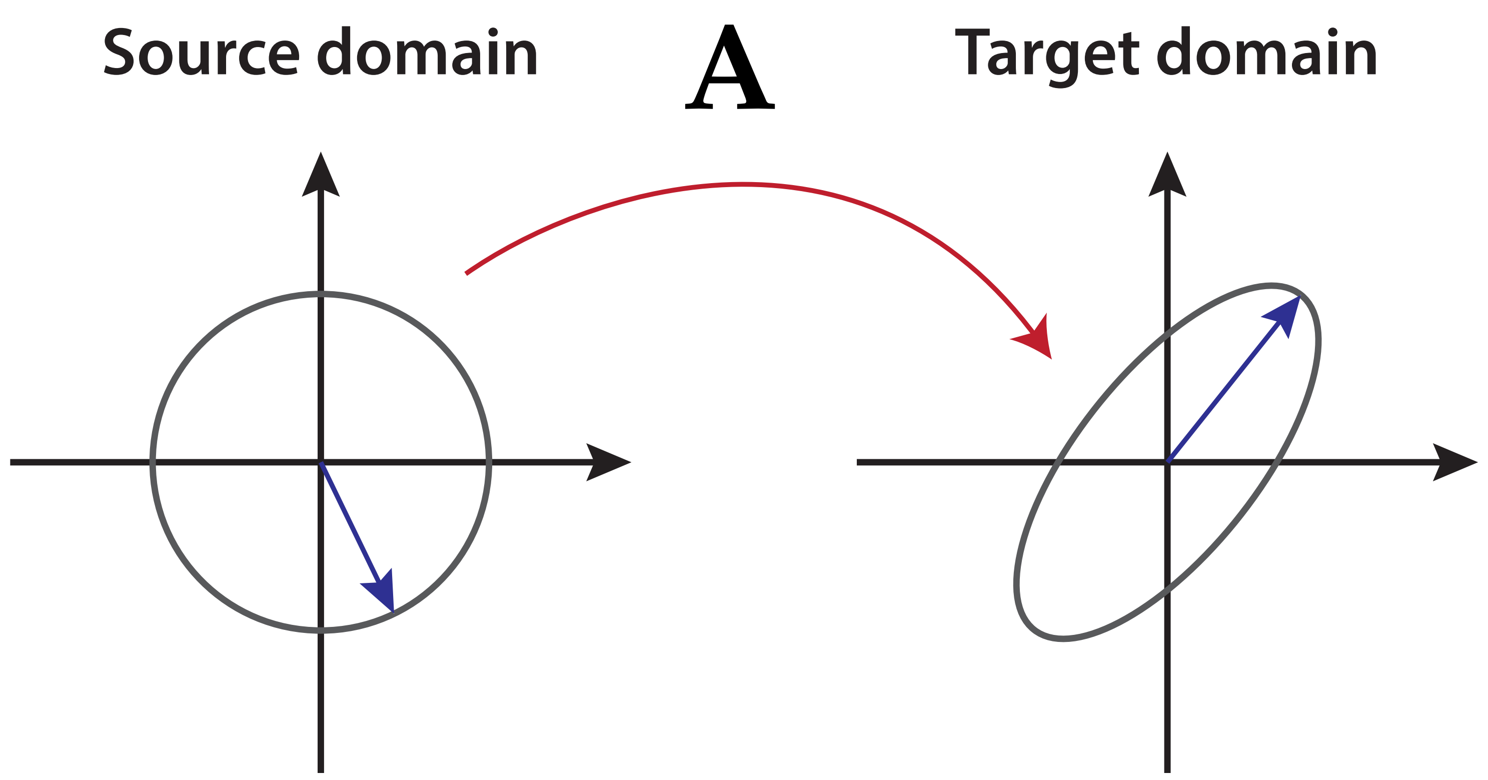

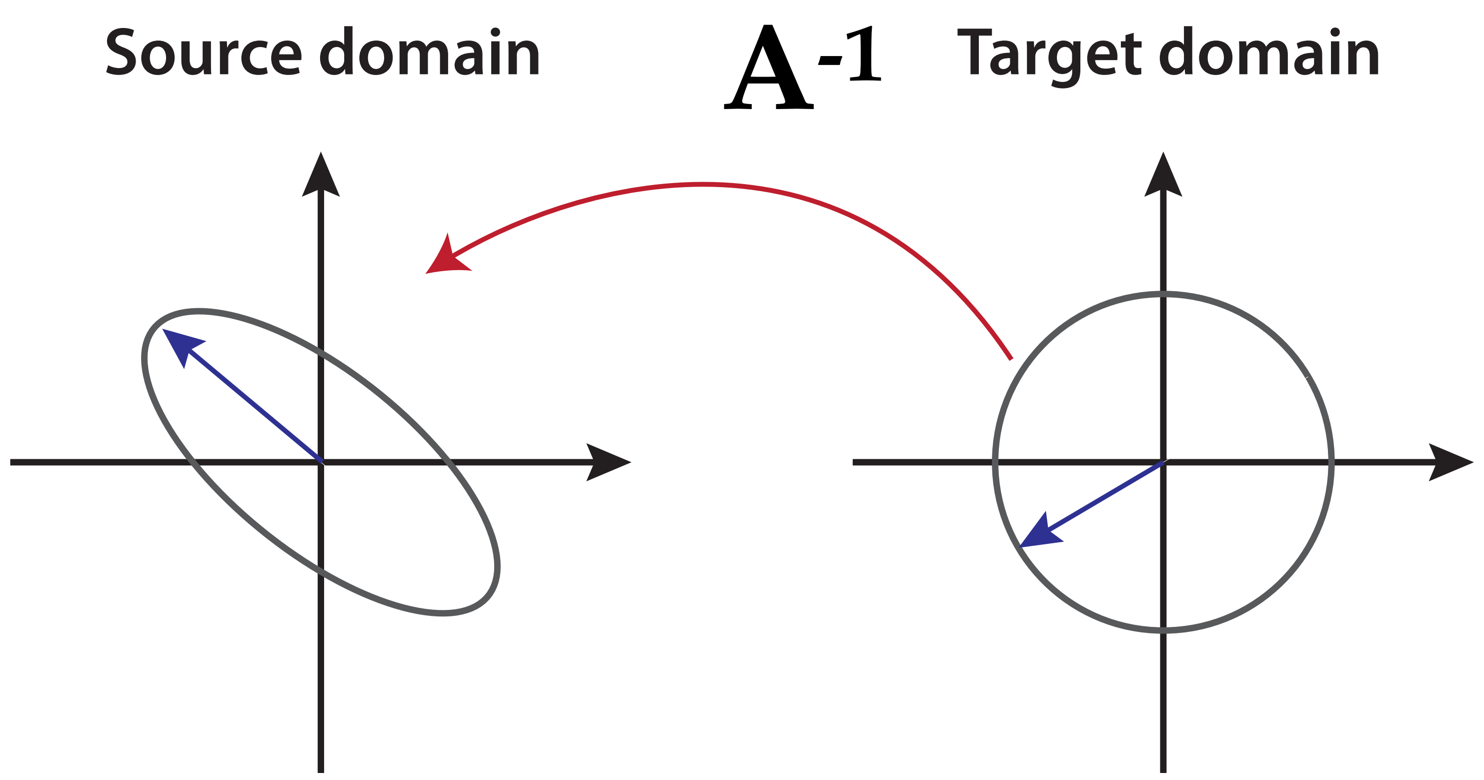

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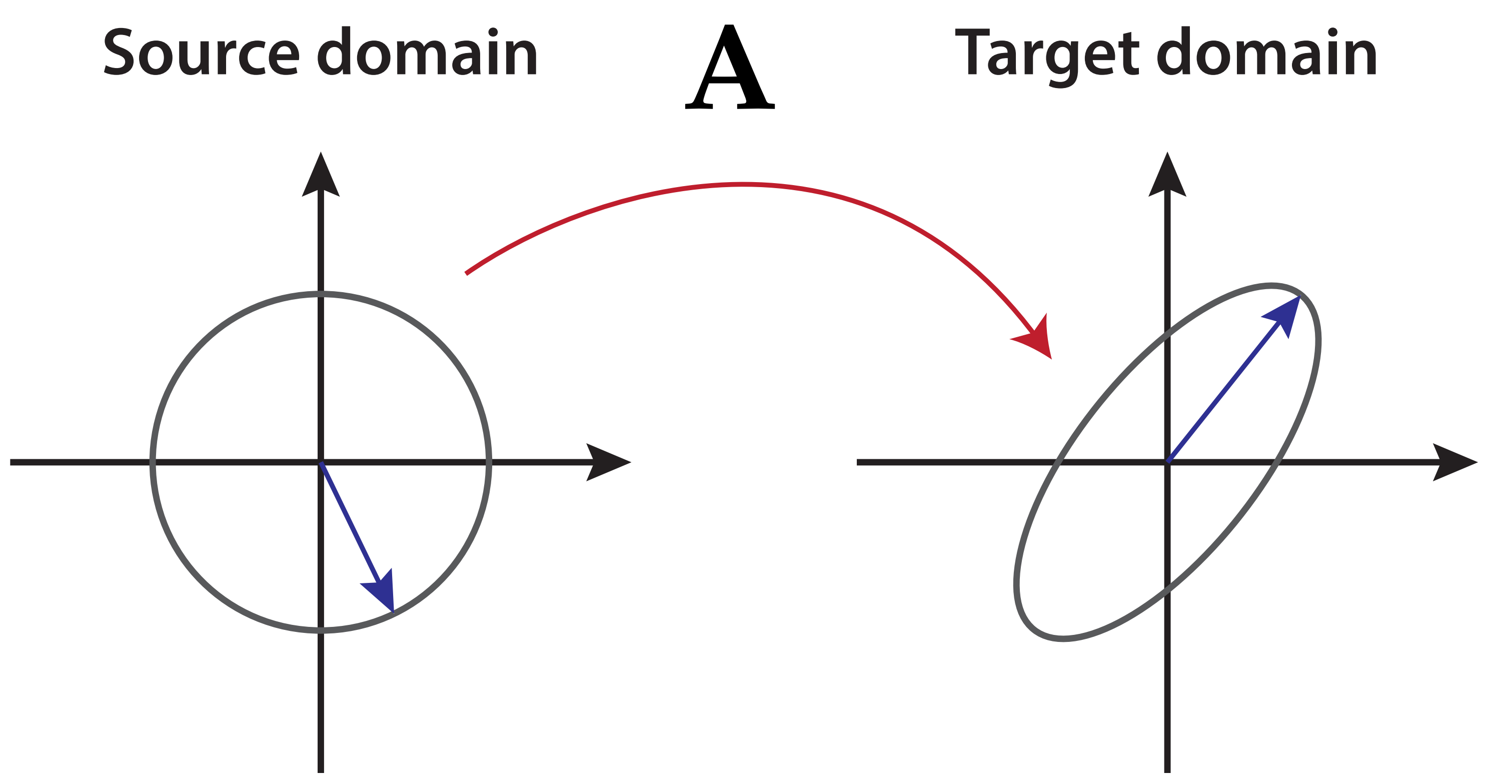
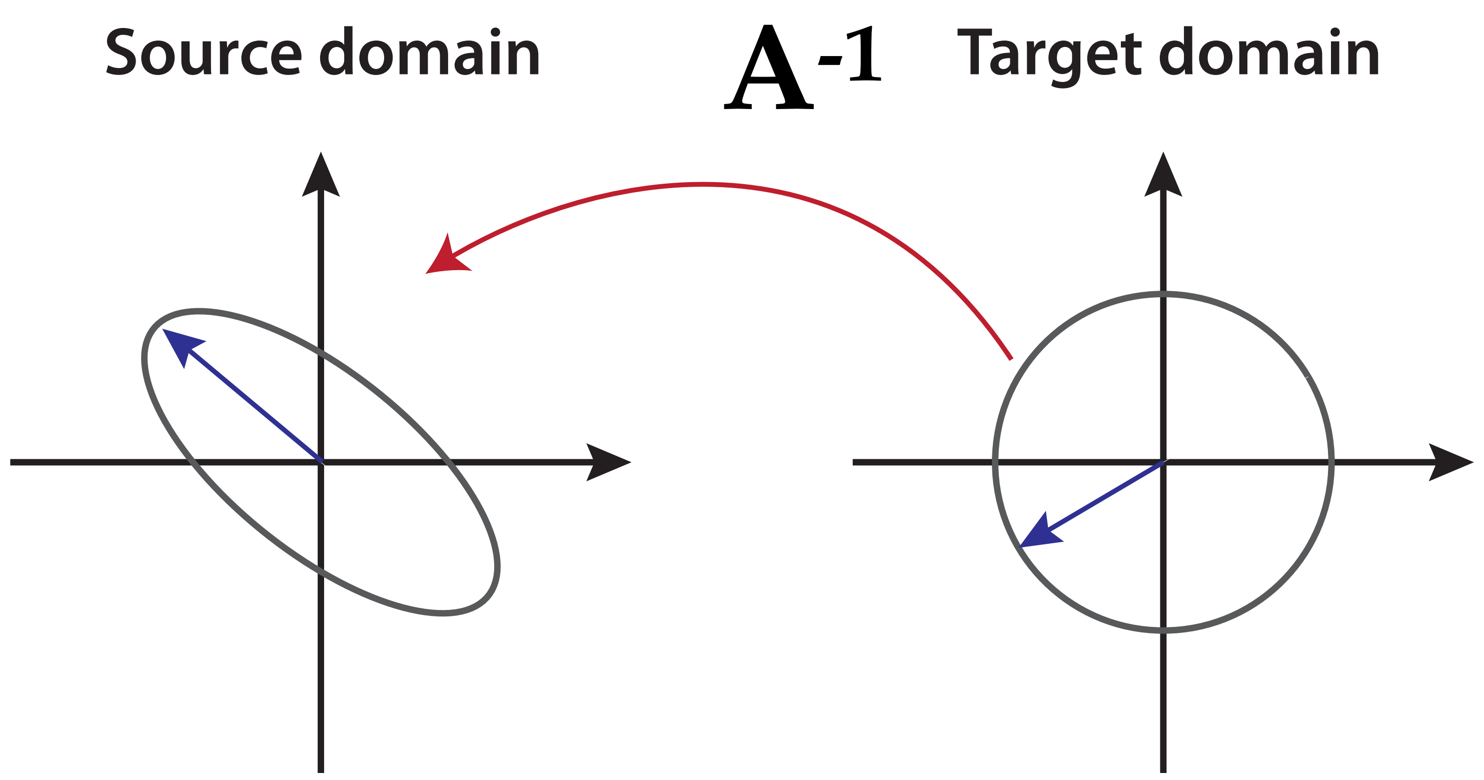
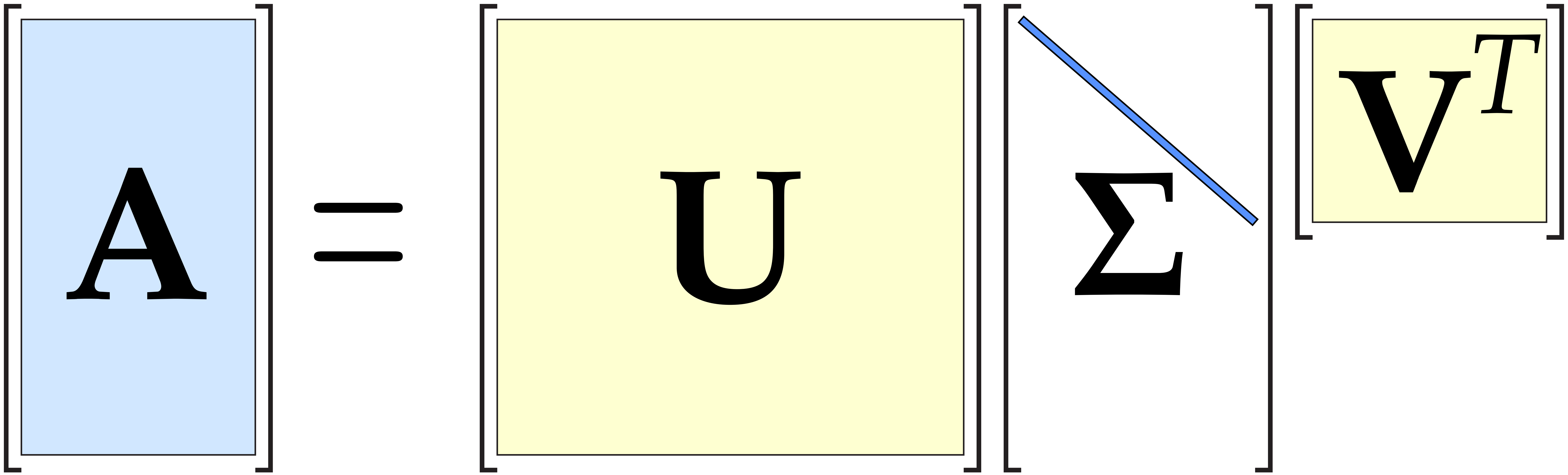




SVD shape (tall & wide case)



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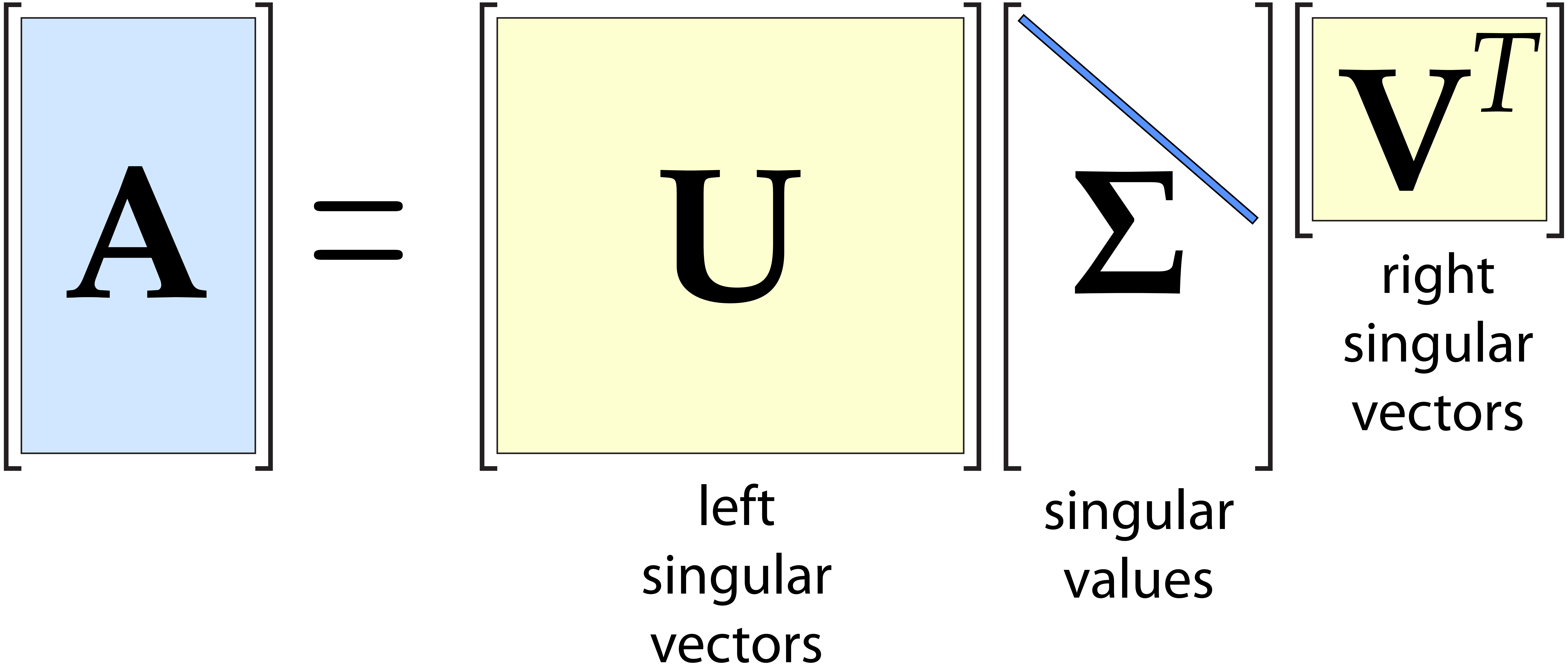

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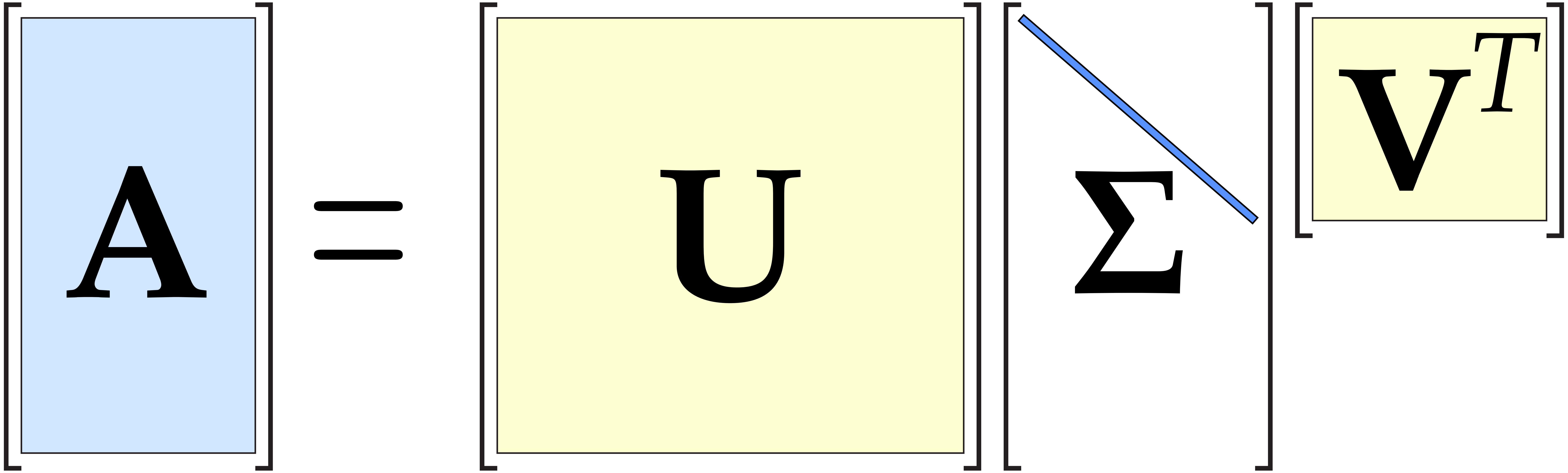

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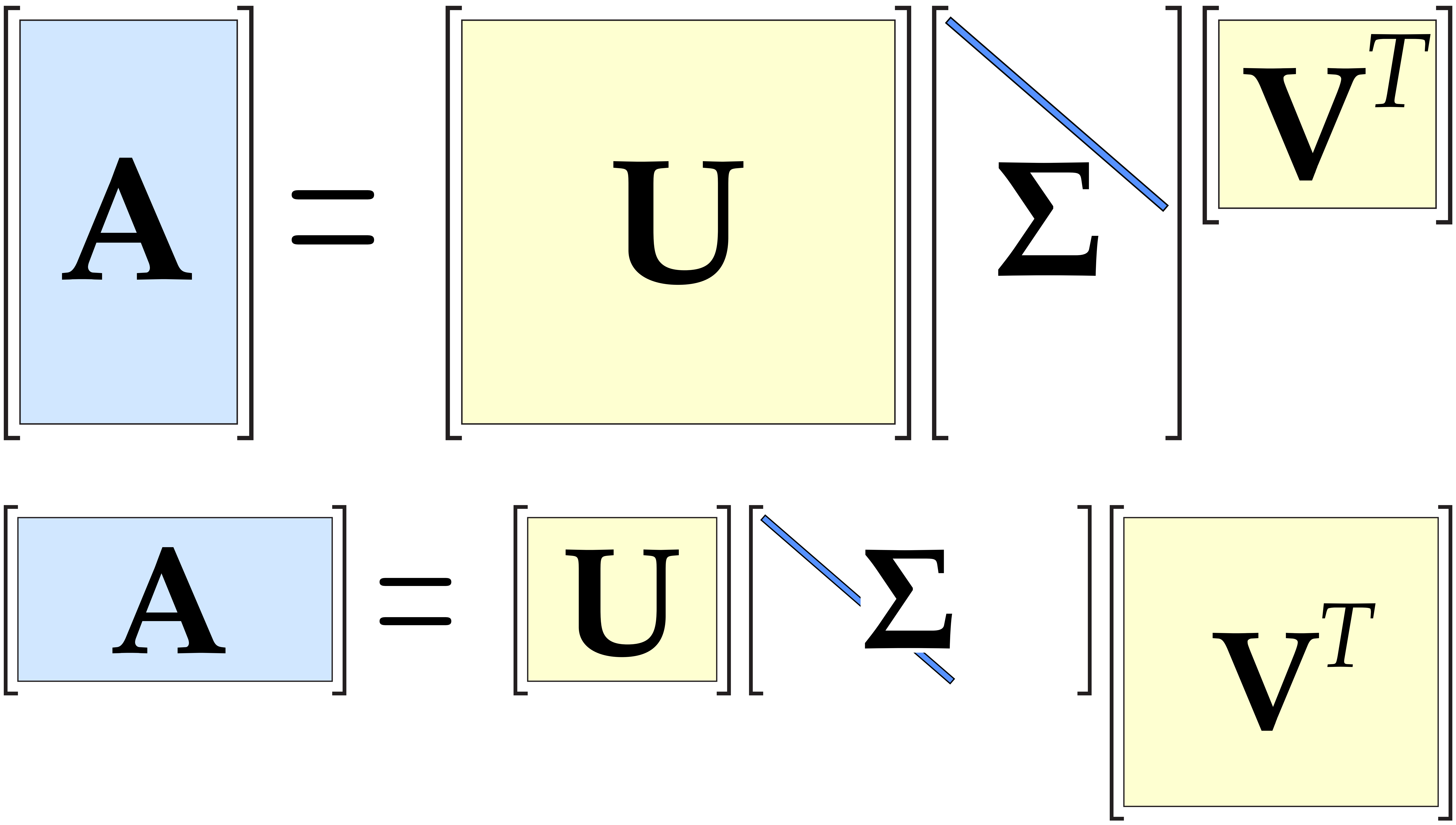

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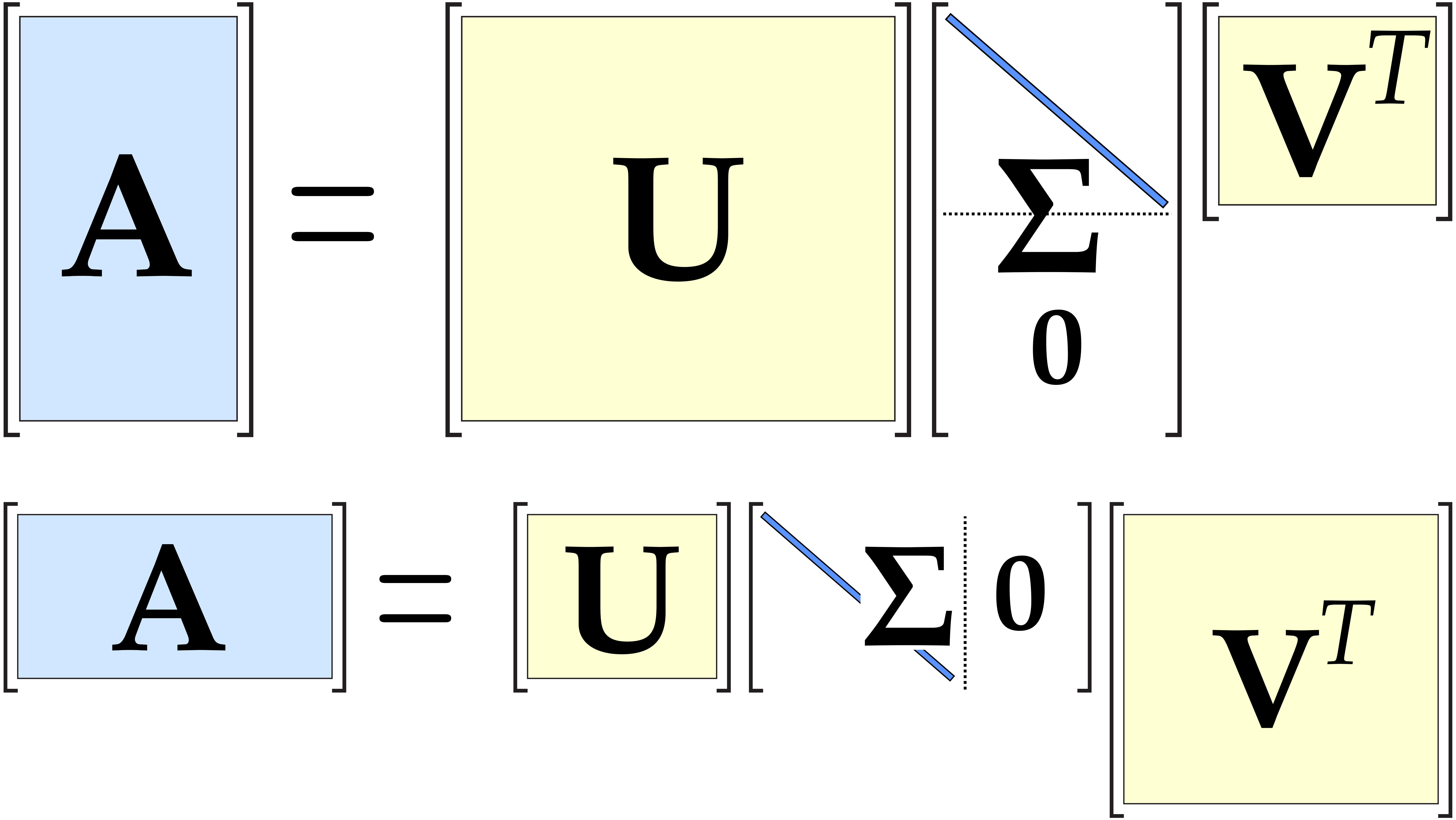

The Pseudoinverse

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3. Gives minimum-norm solution for underconstrained /wide linear systems