

Singular Value Decomposition

Geometric Algorithms
Lecture 26

Introduction

Recap Problem (+ Course Evaluations)

Find an orthogonal diagonalization of $\begin{bmatrix} 1 & 3 \\ 3 & 1 \end{bmatrix}$.

$$\begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$$

<https://www.bu.edu/courseeval>

Answer

$$\begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$$

$$D = \begin{bmatrix} 4 & 0 \\ 0 & 2 \end{bmatrix}$$

$$A = P D P^T$$

① find eigenvalues

② find eigenvectors

③.0 Normalize eigenvectors
③ Create P out of the eigenvectors

$$\begin{bmatrix} 3-\lambda & 1 \\ 1 & 3-\lambda \end{bmatrix}$$

$$\textcircled{i} A - 4I = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$P = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$(3-\lambda)^2 - 1 = 0$$
$$\lambda^2 - 6\lambda + 8 = 0$$

$$(A - 4I)\vec{x} = \vec{0}$$

$$\vec{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$P^T = P$$

$$(\lambda - 4)(\lambda - 2) = 0$$

$$\textcircled{ii} A - 2I = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$A = P D P^T$$

$$\lambda = 4, 2$$

$$\vec{x}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$\langle \vec{x}_1, \vec{x}_2 \rangle = 1(1) + 1(-1) = 0$$

$$\|\vec{x}_1\| = \sqrt{1^2 + 1^2} = \sqrt{2}$$

Objectives

1. Finish up our discussion of quadratic forms.
2. Introduce the singular value decomposition (probably the most important matrix decomposition for computer science).
3. Talk very briefly about what to do after this course if you want (or have to) to see more linear algebra.

Quadratic Forms (Finishing Up)

Quadratic Forms

Definition. A quadratic form is an function of variables x_1, \dots, x_n in which every term has degree two.

Examples: $Q(x_1, x_2, x_3) = x_1^2 + 3x_2^2 + x_2x_3 - x_1x_3$

Non-examples:

$$Q(x_1, x_2) = x_1^3 + x_1x_2$$

$$Q(x_1, x_2) = x_1x_2 + x_1$$

Quadratic Forms and Symmetric Matrices

Fact. Every quadratic form can be represented as

$$\mathbf{x}^T \mathbf{A} \mathbf{x} \quad \langle \mathbf{x}, \mathbf{A} \mathbf{x} \rangle$$

where \mathbf{A} is symmetric.

Example:

$$\begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3x_1 \\ 2x_2 \end{bmatrix} = 3x_1^2 + 2x_2^2$$

Example: Computing the Quadratic Form for a Matrix

$$A = \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix}$$

This means, given a symmetric matrix A , we can compute its corresponding quadratic form:

$$\begin{aligned} \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} &= \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3x_1 - 2x_2 \\ -2x_1 + 7x_2 \end{bmatrix} \\ x_1(3x_1 - 2x_2) + x_2(-2x_1 + 7x_2) &= \\ 3x_1^2 - 2x_1x_2 - 2x_2x_1 + 7x_2^2 &= \boxed{3}x_1^2 - \boxed{4}x_1x_2 + \boxed{7}x_2^2 \end{aligned}$$

Quadratic forms and Symmetric Matrices (Again)

Furthermore, we can generally say

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \sum_{i=1}^n \sum_{j=1}^n A_{ij} x_i x_j = \sum_{i=1}^n A_{ii} x_i^2 + \sum_{i \neq j} (A_{ij} + A_{ji}) x_i x_j$$

Verify:

$$\begin{aligned} \vec{x}^T (\mathbf{A} \vec{x}) &= \sum_{i=1}^n x_i (A \vec{x})_i = \sum_{i=1}^n x_i \left(\sum_{j=1}^n A_{ij} x_j \right) \\ &= \sum_{i=1}^n \sum_{j=1}^n A_{ij} x_i x_j \end{aligned}$$

A Slightly more Complicated Example

$$A = \begin{bmatrix} \boxed{1} & \overset{A_{11}}{\circledast} 2 & \triangleleft -1 \\ \overset{A_{21}}{\circledast} 2 & \boxed{3} & 0 \\ \triangleleft -1 & 0 & \boxed{5} \end{bmatrix}$$

Let's expand $\mathbf{x}^T A \mathbf{x}$:

$$Q(x_1, x_2, x_3) = x_1^2 + 3x_2^2 + 5x_3^2 + \boxed{4x_1x_2} - 2x_1x_3$$

Matrices from Quadratic Forms

$$Q(\mathbf{x}) = 5x_1^2 + 3x_2^2 + 2x_3^2 - x_1x_2 + 8x_2x_3$$

We can also go in the other direction. Let's express this as $\mathbf{x}^T A \mathbf{x}$:

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

How To: Matrices of Quadratic Forms

Problem. Given a quadratic form $Q(\mathbf{x})$, find the symmetric matrix A such that $Q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$.

Solution.

» if $Q(\mathbf{x})$ has the term αx_i^2 then $A_{ii} = \alpha$

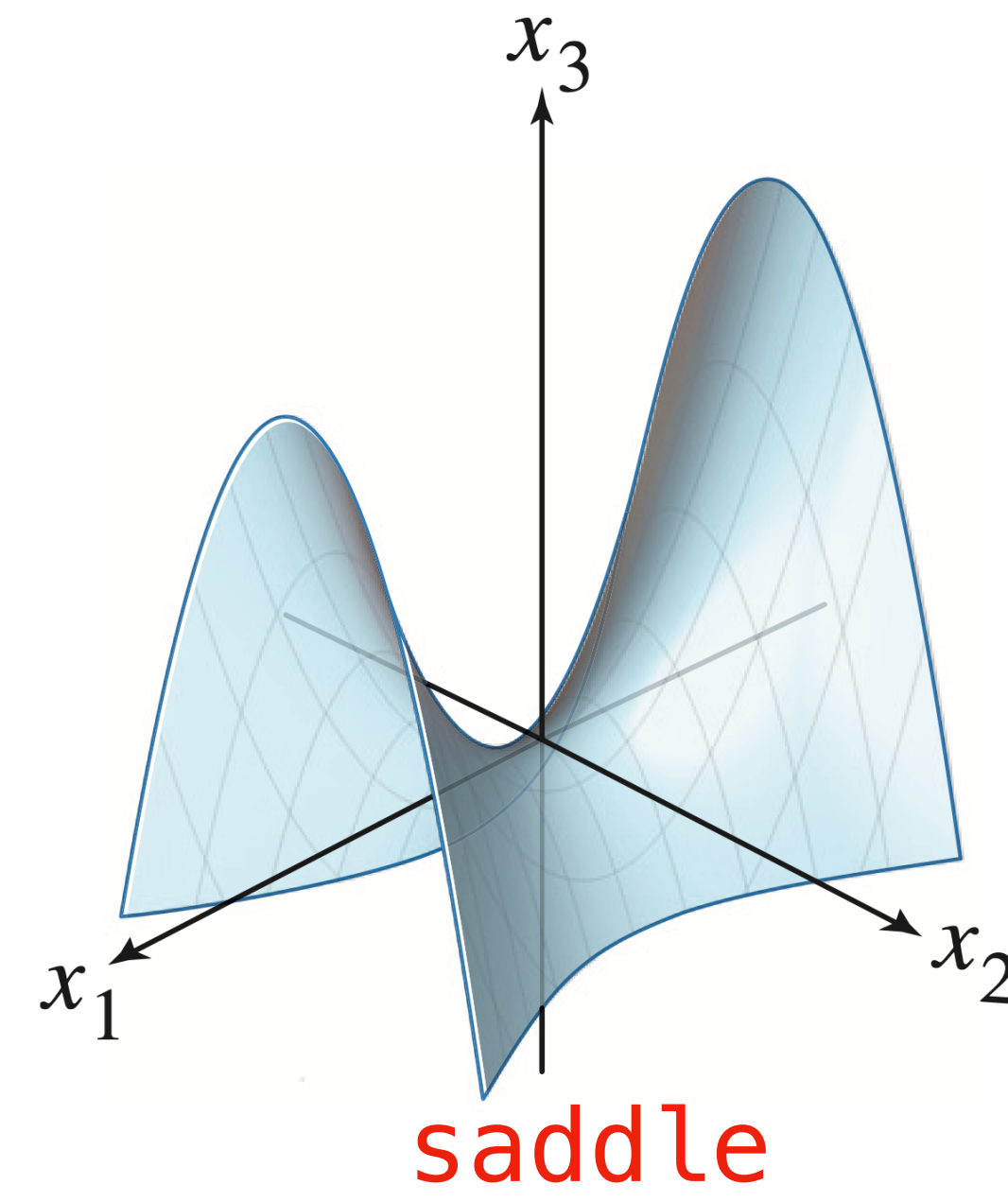
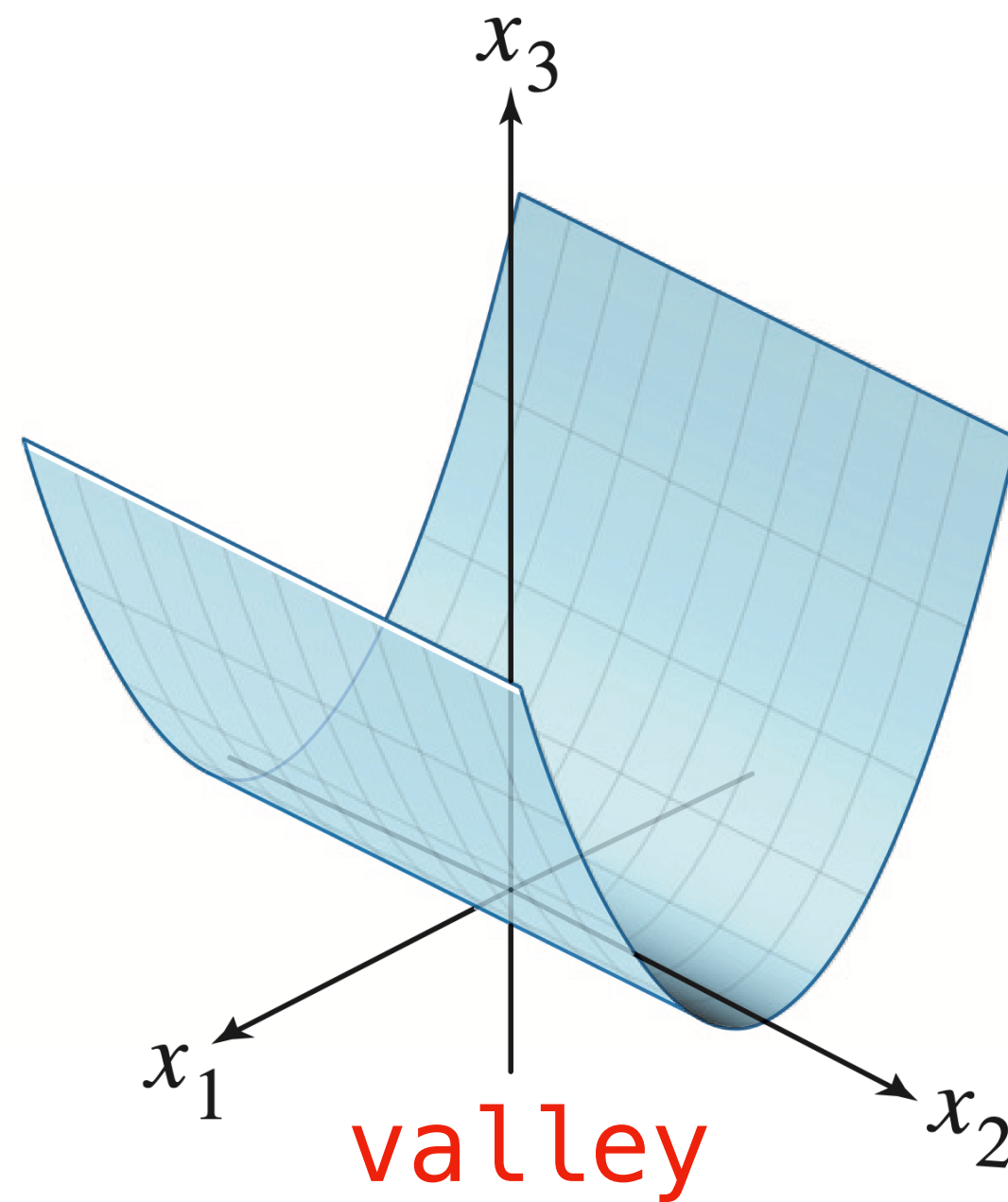
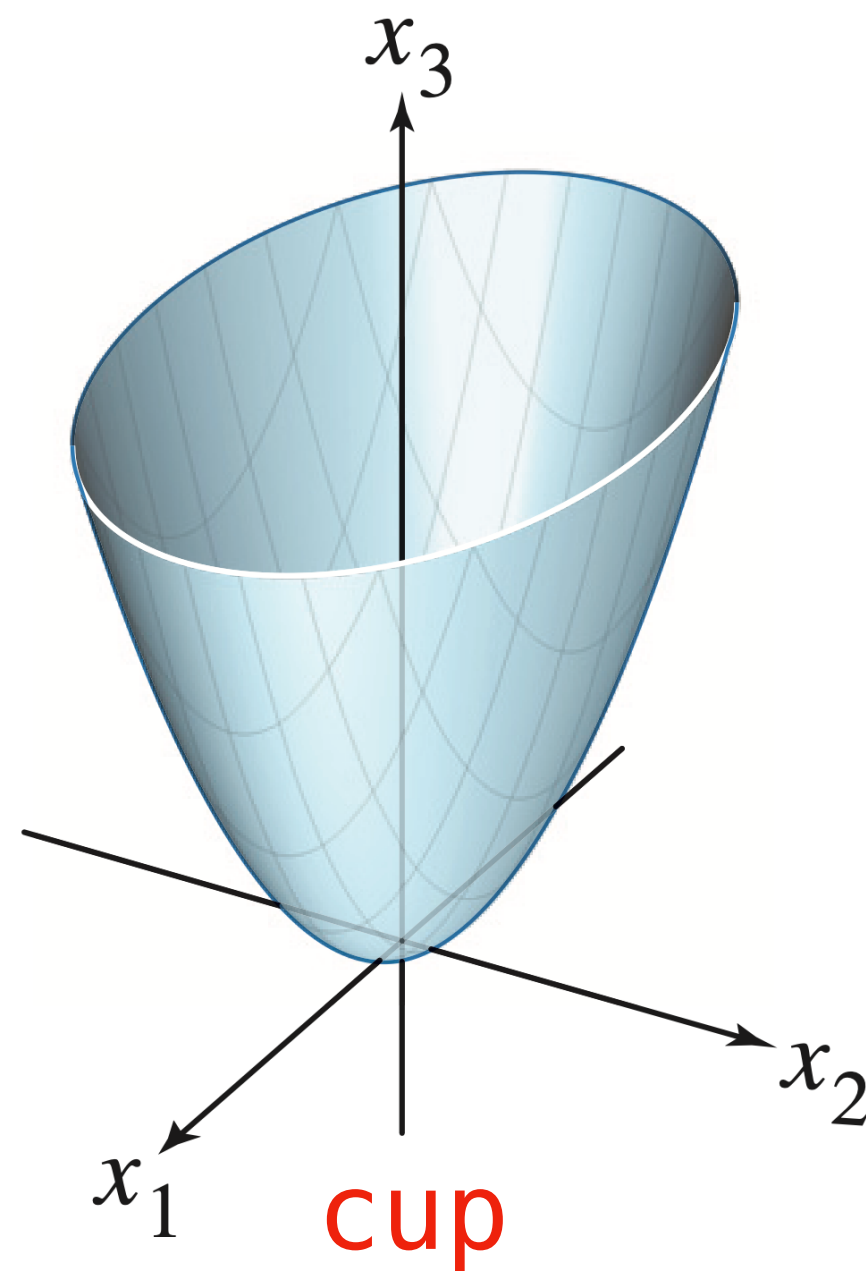
» if $Q(\mathbf{x})$ has the term $\alpha x_i x_j$, then $A_{ij} = A_{ji} = \frac{\alpha}{2}$

Example

$$Q(x_1, x_2, x_3, x_4) = x_1^2 + 3x_2^2 - 2x_3x_4 - 6x_4^2 + 7x_1x_3$$

Find the symmetric matrix A such that $Q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$.

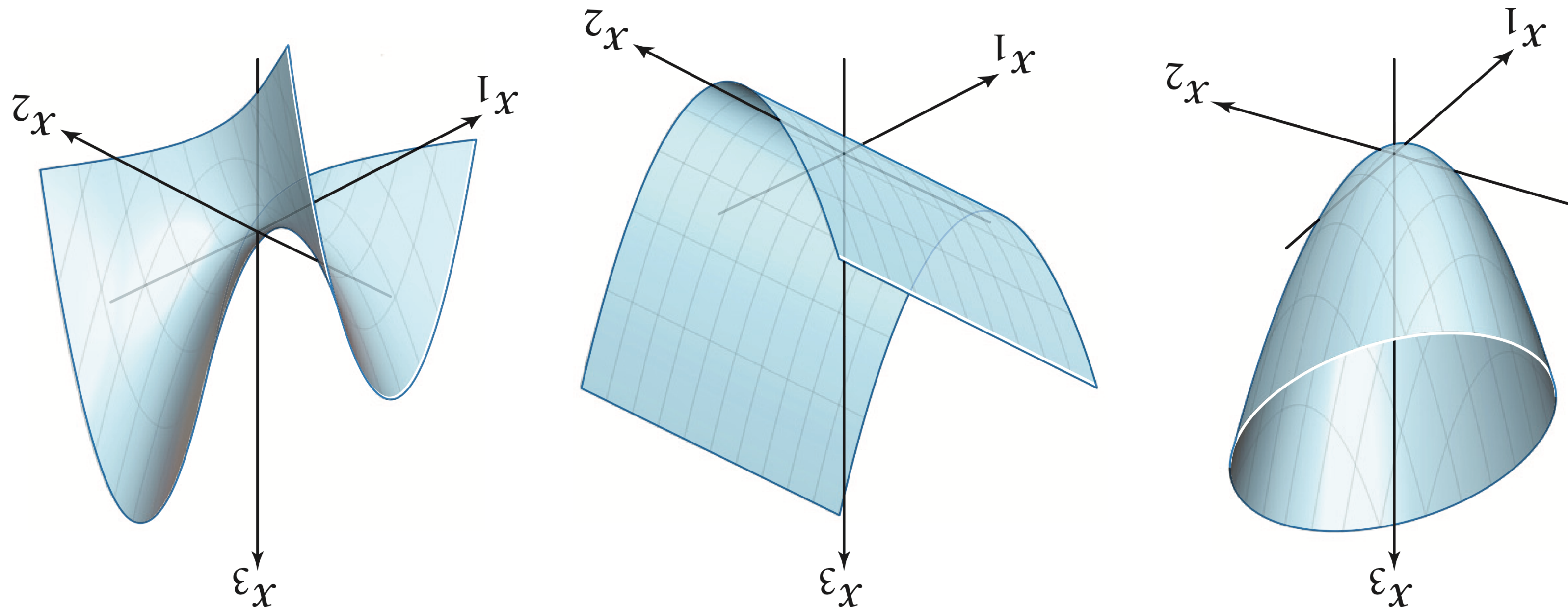
Shapes of of Quadratic Forms



There are essentially three possible shapes (six if you include the negations).

Can we determine what shape it will be mathematically?

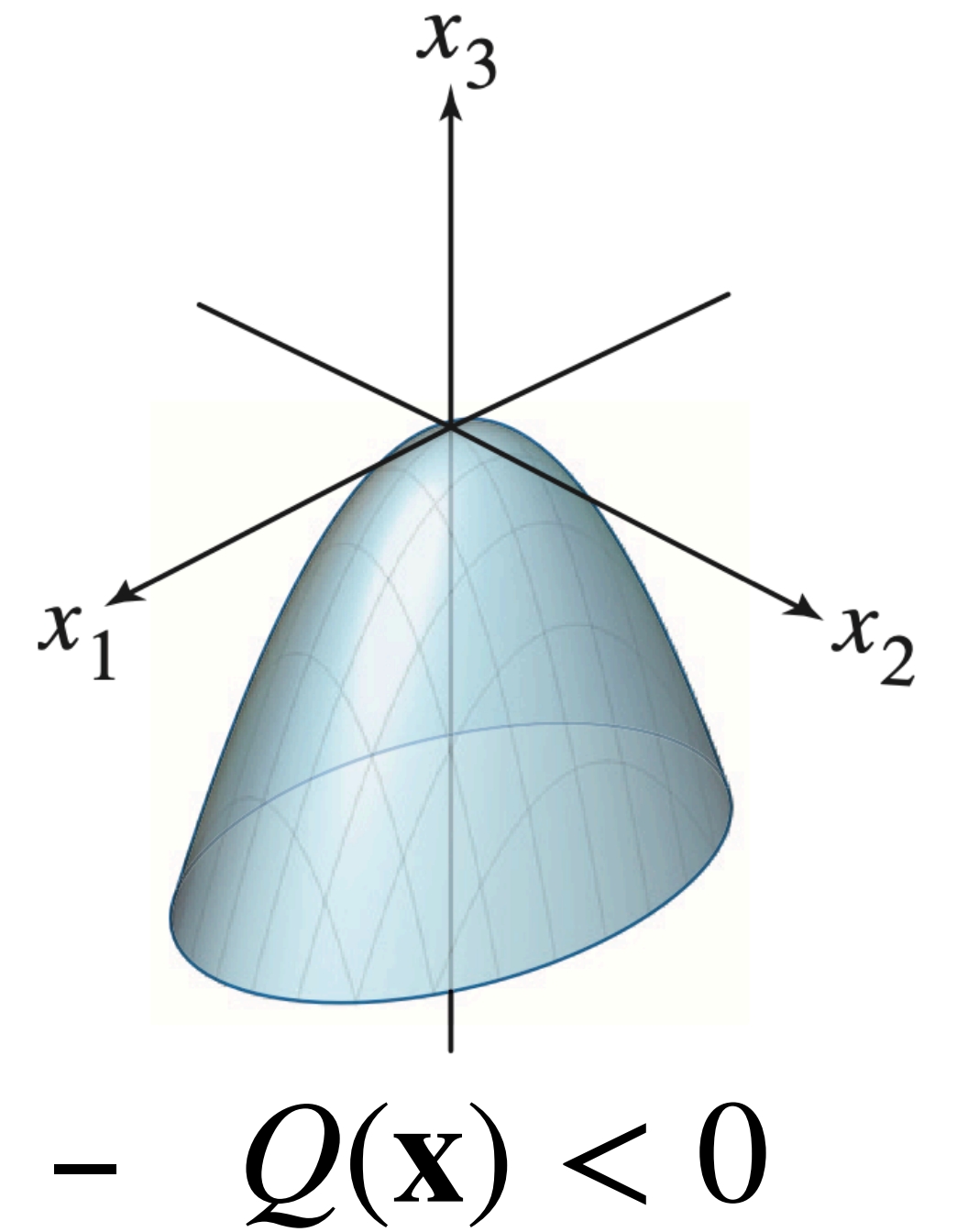
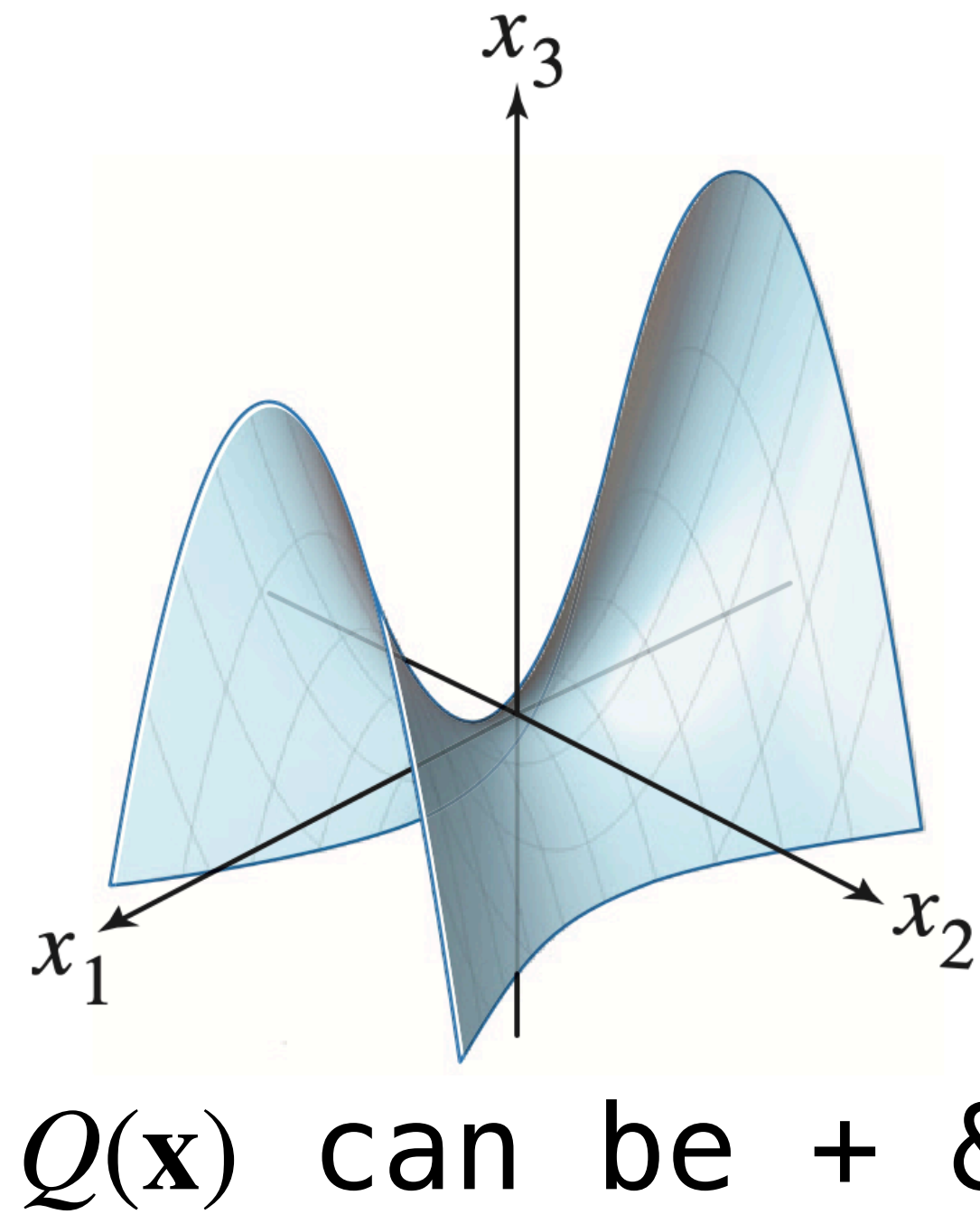
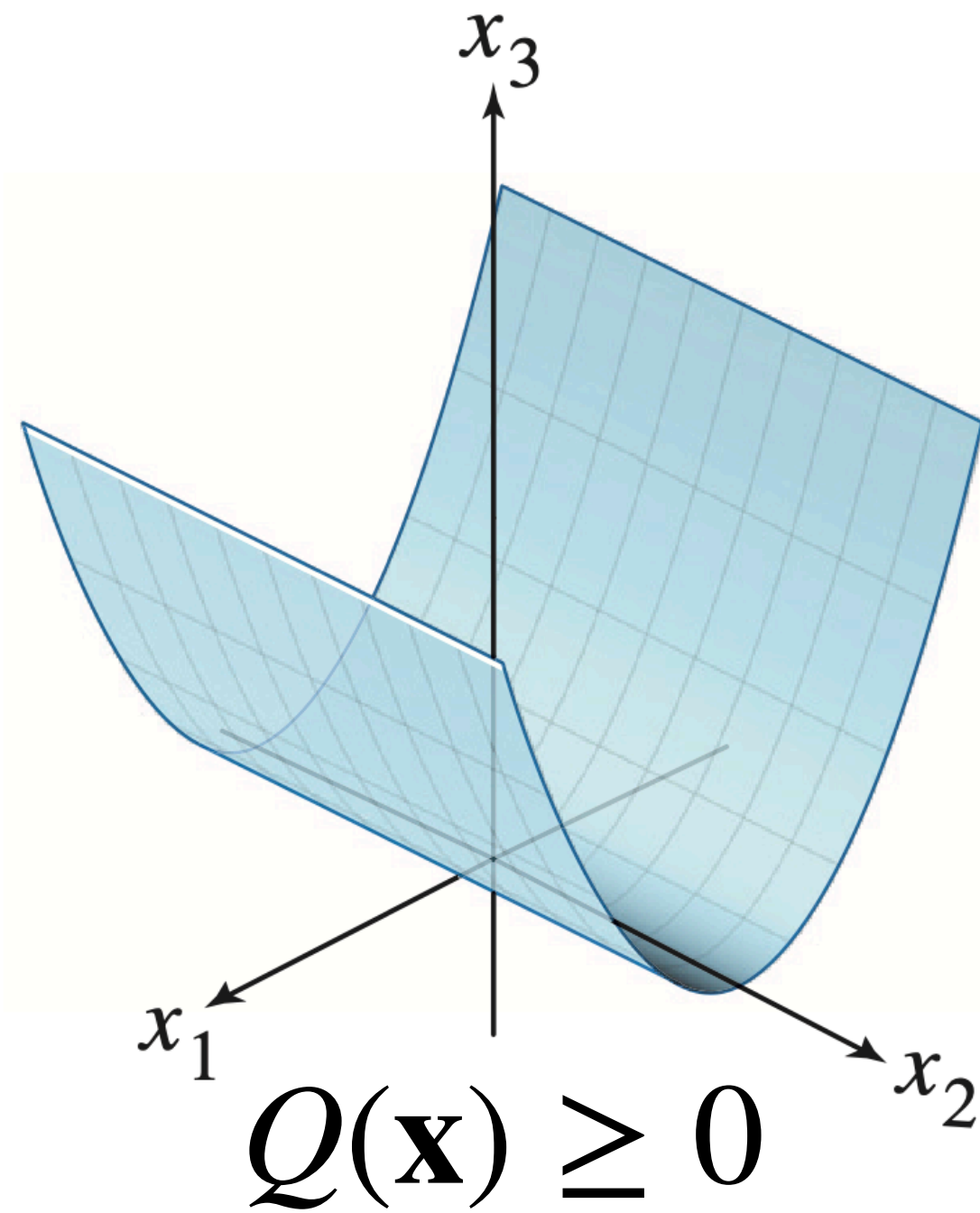
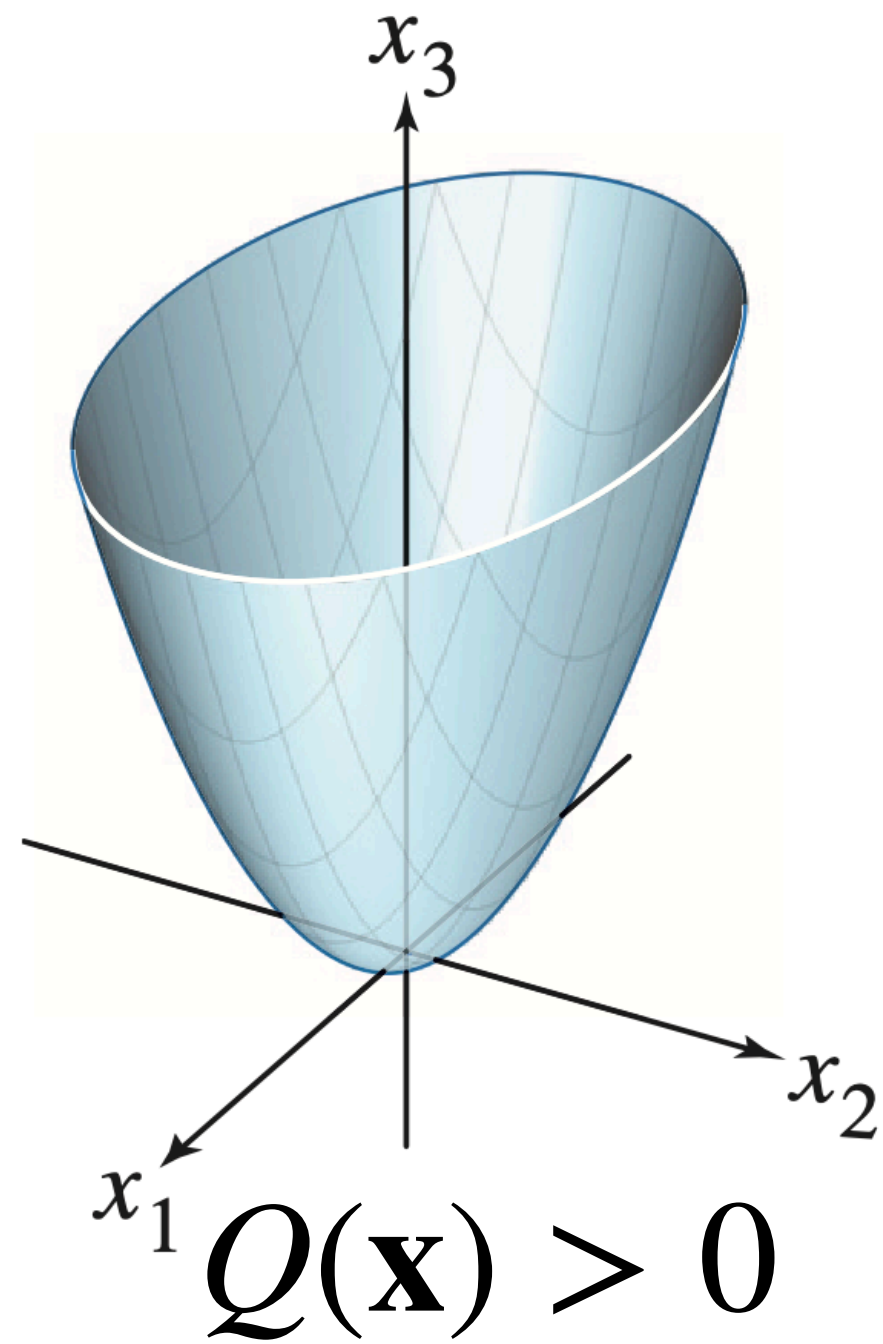
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Definiteness

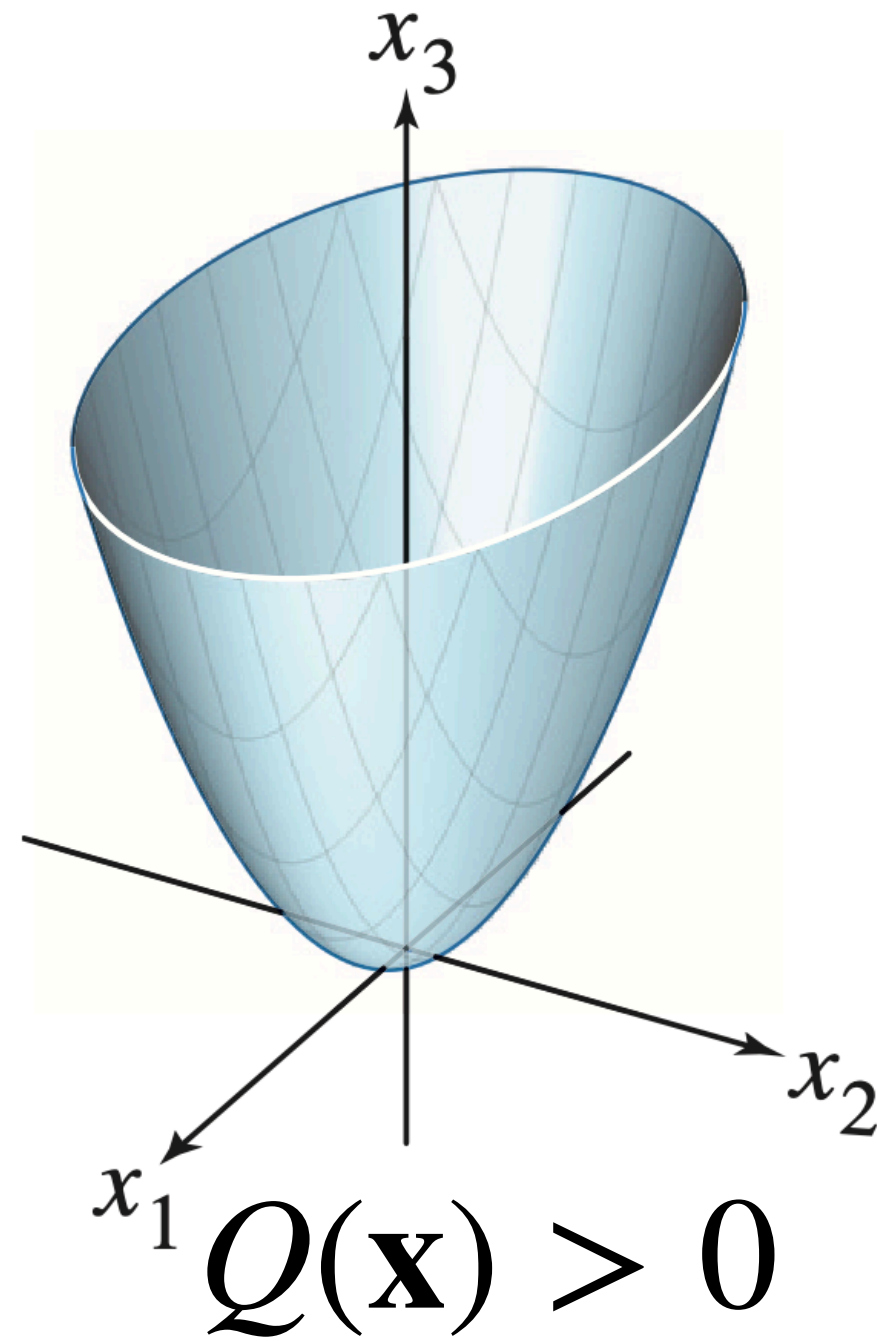


For $\mathbf{x} \neq \mathbf{0}$, each of the above graphs satisfy the associated properties.

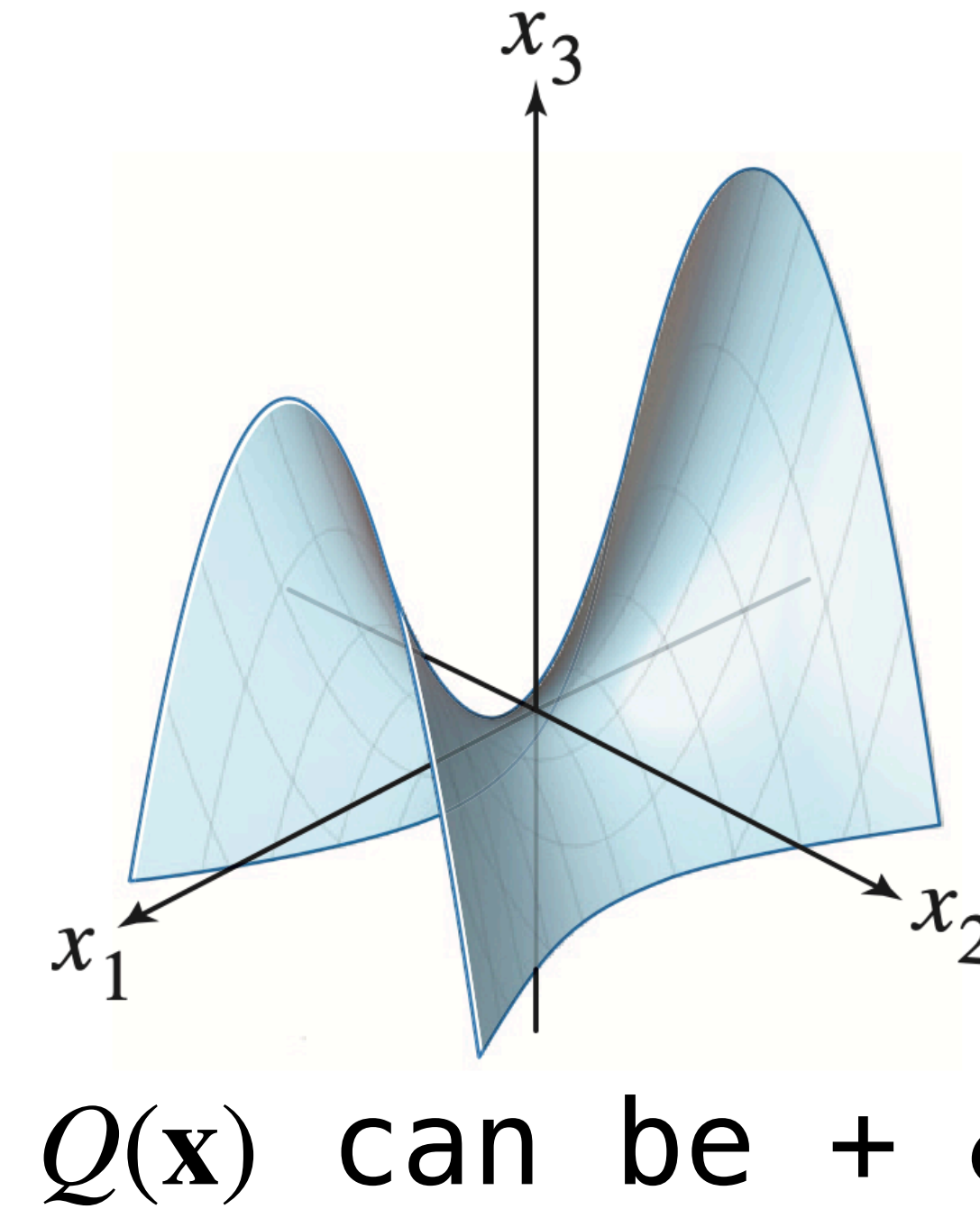
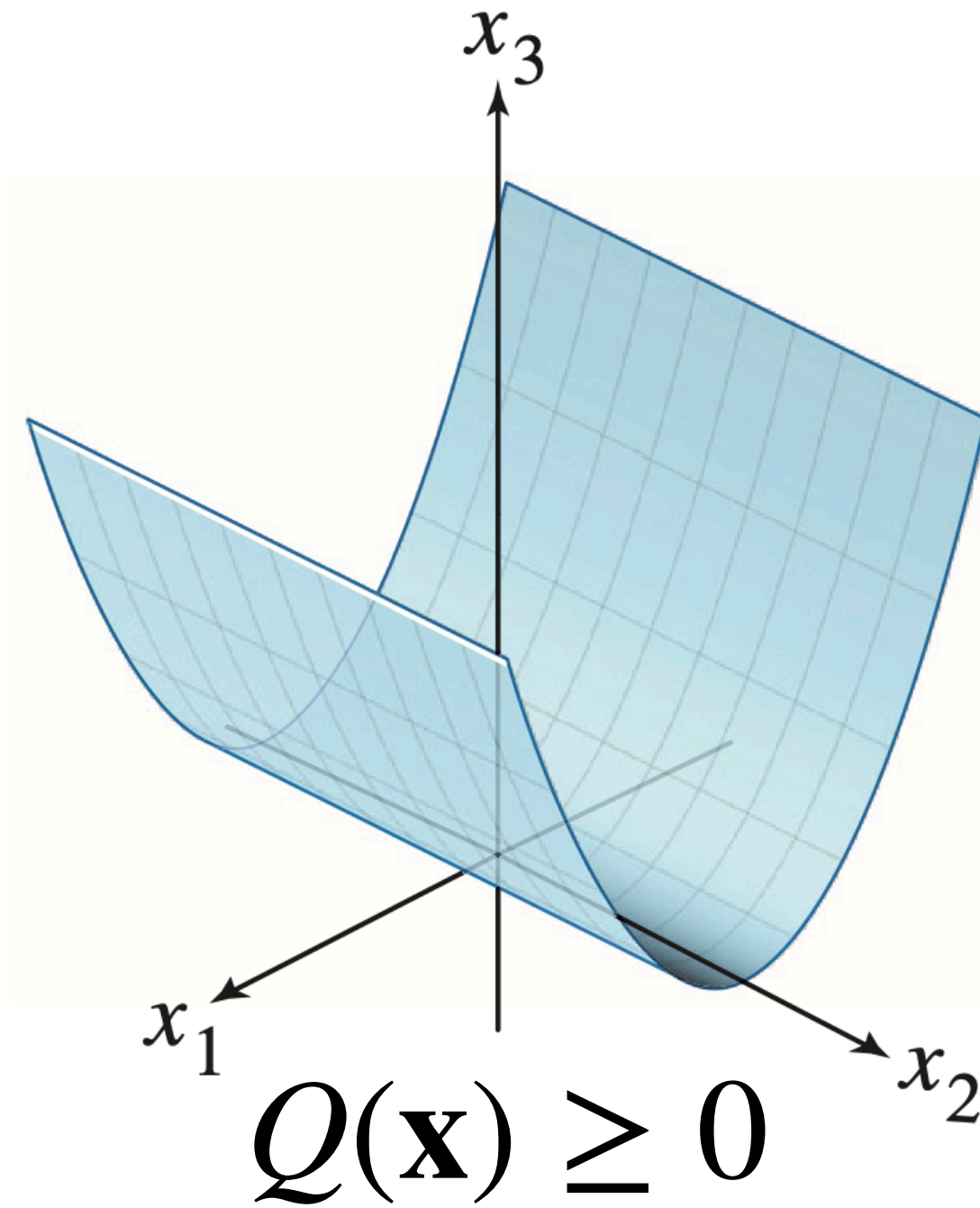
Definiteness

positive semidefinite

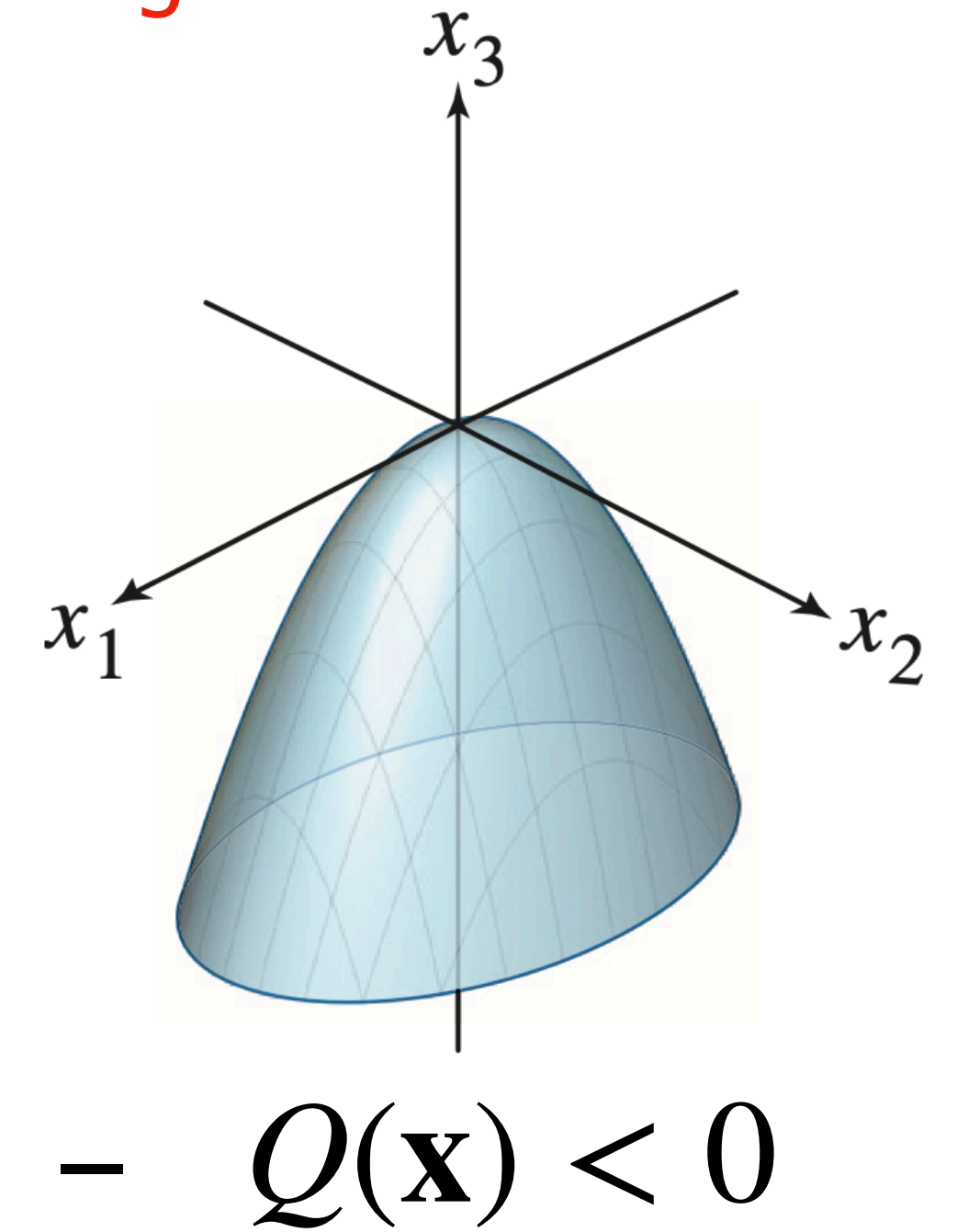
negative definite



positive definite



indefinite



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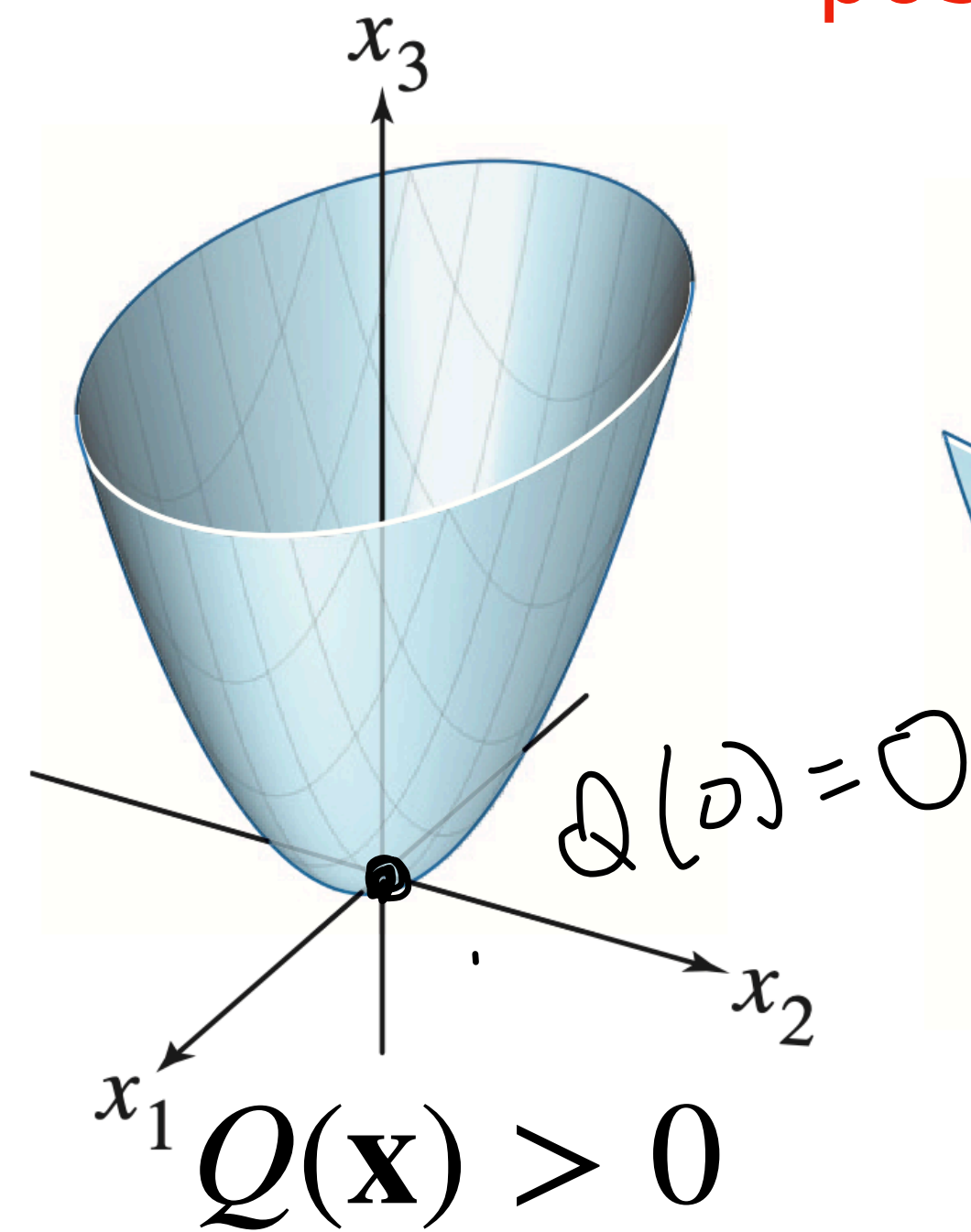
Definiteness and Eigenvectors

Theorem. For a symmetric matrix A , the quadratic form $\mathbf{x}^T A \mathbf{x}$

- » **positive definite** \equiv all positive eigenvalues
- » **positive semidefinite** \equiv all nonnegative eigenvalues
- » **indefinite** \equiv positive and negative eigenvalues
- » **negative definite** \equiv all negative eigenvalues

Definiteness

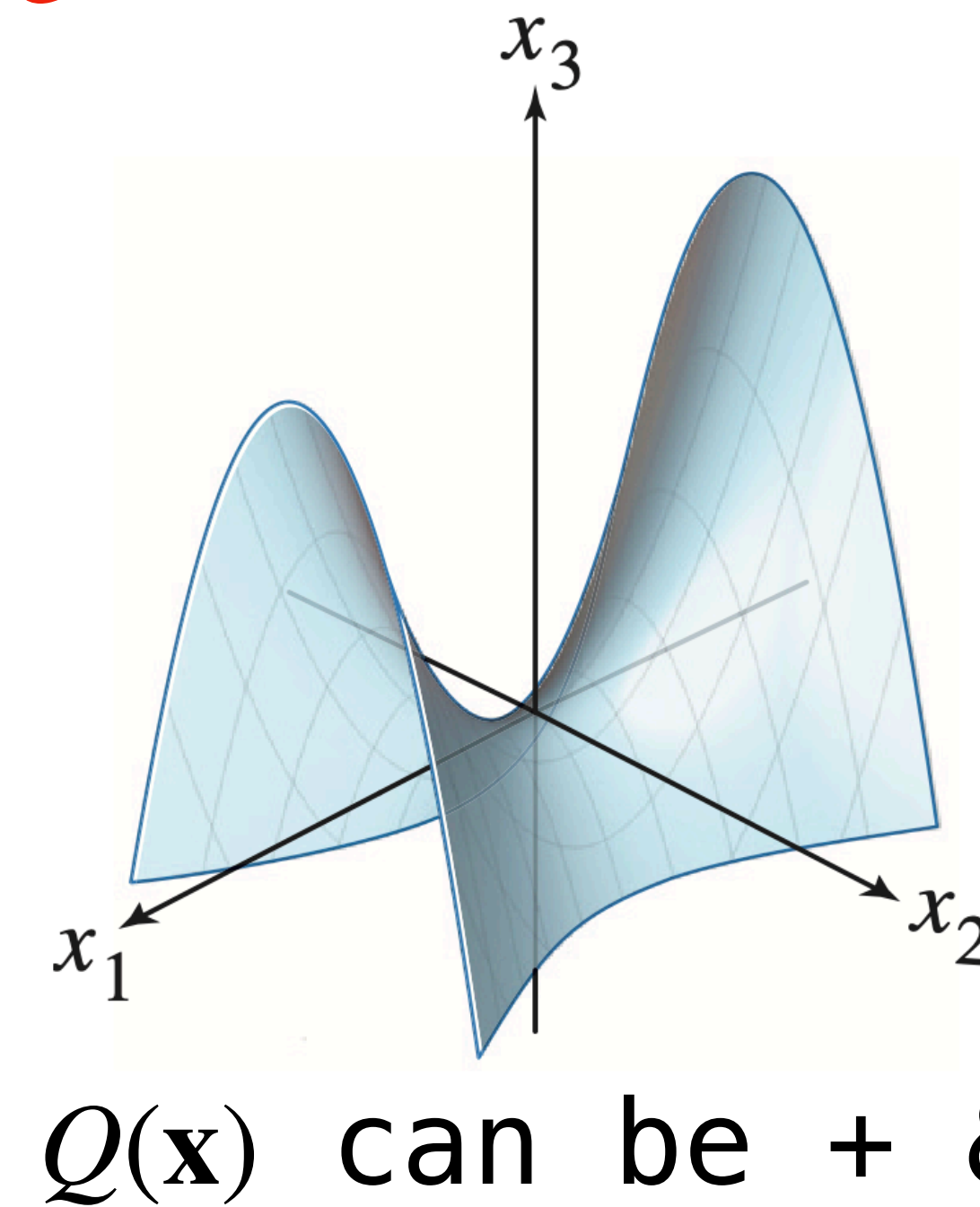
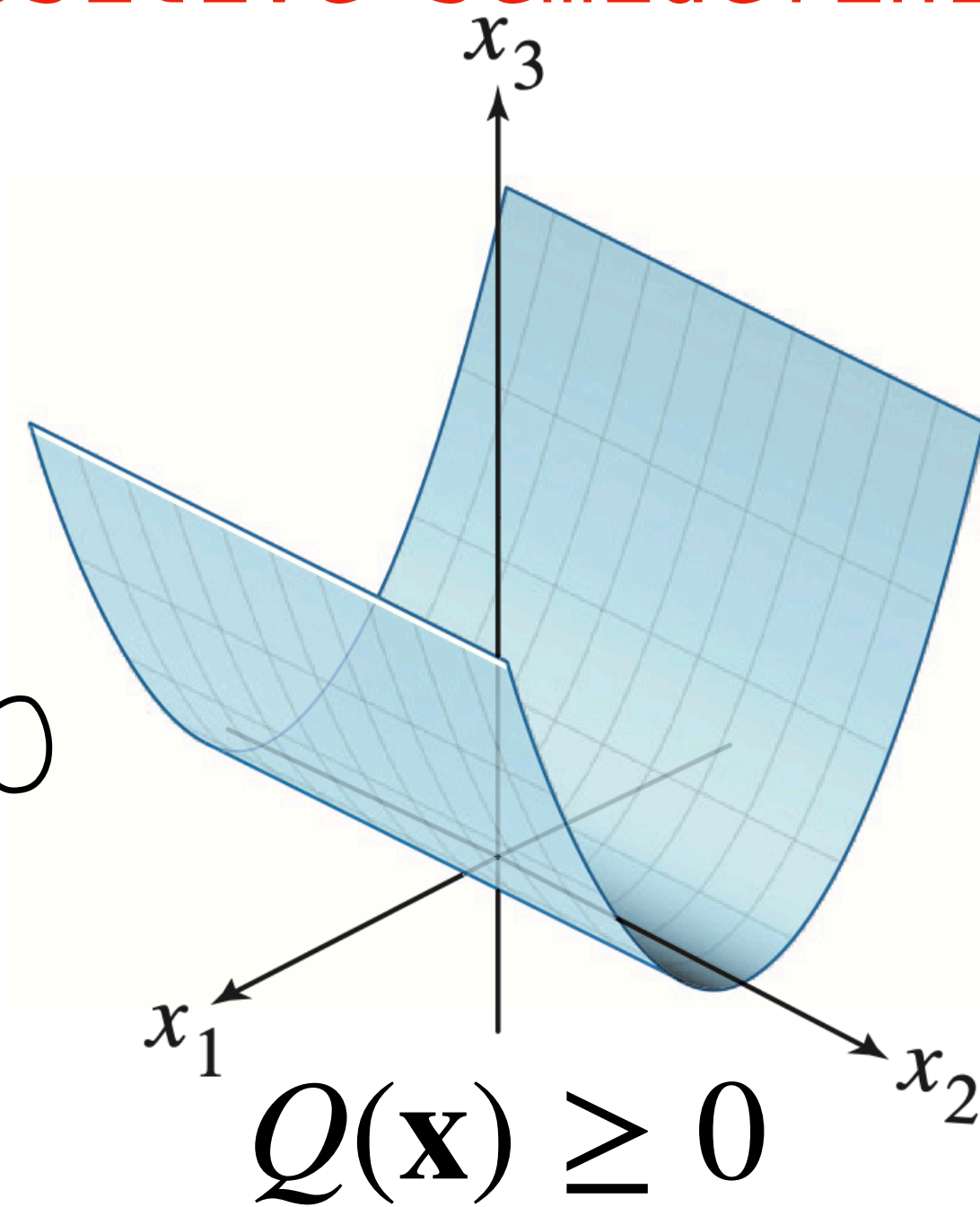
all nonneg. eigenvals
positive semidefinite



positive definite

all pos. eigenvals

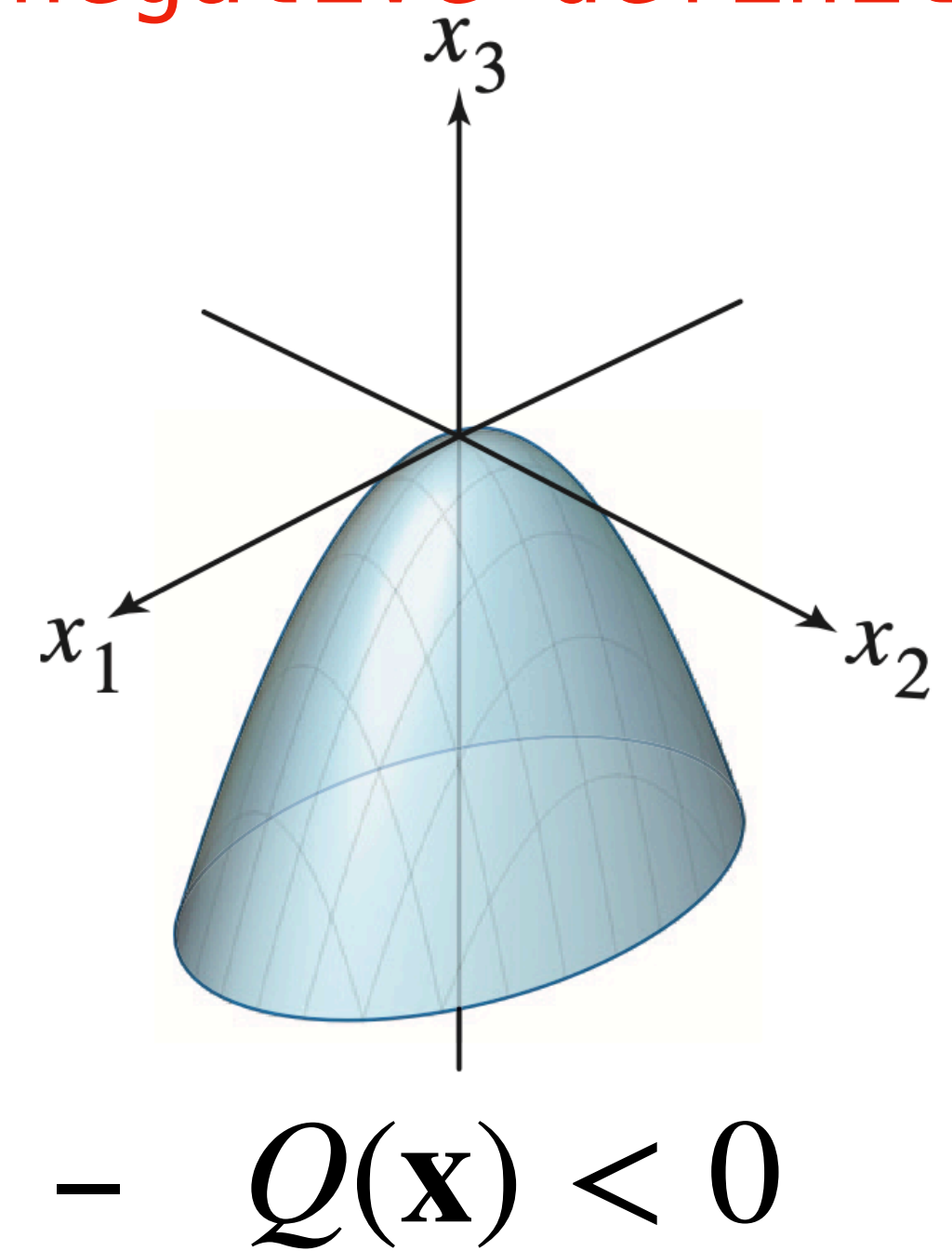
$$Q(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x}$$



indefinite

pos. and neg. eigenvals

all neg. eigenvals
negative definite



Example

$$\lambda = 3, -1$$

$$x_2, x_3 = -1, x_1 = 0$$

$$Q(x_1, x_2, x_3) = 3x_1^2 + x_2^2 + 4x_2x_3 + x_3^2$$

Let's determine which case this is:

$$A = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 2 & 1 \end{bmatrix} \quad \begin{bmatrix} 3-\lambda & 0 & 0 \\ 0 & 1-\lambda & 2 \\ 0 & 2 & 1-\lambda \end{bmatrix} \sim \begin{bmatrix} 3-\lambda & 0 & 0 \\ 0 & 1-\lambda & 2 \\ 0 & 2(1-\lambda) & (1-\lambda)^2 \end{bmatrix}$$

$$\det(A - \lambda I) = \frac{1}{1-\lambda} (3-\lambda) \cancel{(1-\lambda)} ((1-\lambda)^2 - 4) \sim \begin{bmatrix} 3-\lambda & 0 & 0 \\ 0 & 1-\lambda & 2 \\ 0 & 0 & (1-\lambda)^2 - 4 \end{bmatrix}$$
$$(3-\lambda)(\lambda^2 - 2\lambda - 3) = \boxed{(3-\lambda)(\lambda-3)(\lambda+1)}$$

Constrained Optimization

In General

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Given a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ and a set of vectors X from \mathbb{R}^n the **constrained minimization problem** for f over X is the problem of determining

$$\min_{\mathbf{v} \in X} f(\mathbf{v})$$

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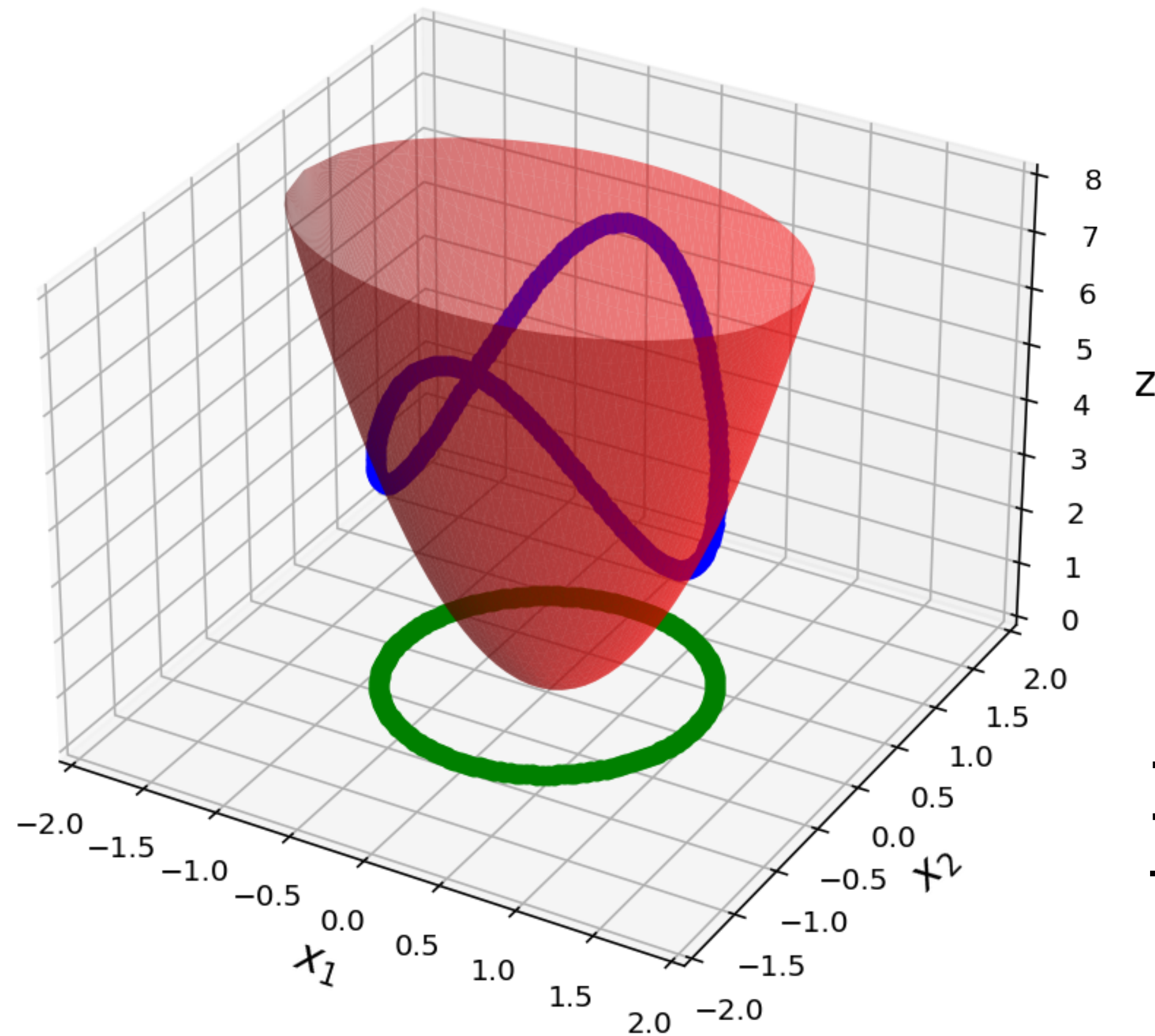
$$\min_{\mathbf{v} \in X} f(\mathbf{v})$$

(analogously for maximization)

Find the smallest value of $f(\mathbf{v})$ subject to choosing a vector in X

Constrained Optimization for Quadratic Forms and Unit Vectors

mini/maximize $\mathbf{x}^T A \mathbf{x}$ subject to $\|\mathbf{x}\| = 1$



It's common to constraint to unit vectors.

Example: $3x_1^2 + 7x_2^2$

$3(0) + 7(1) = 7$ (max value)

$3(1) + 7(0) = 3$ (min value)

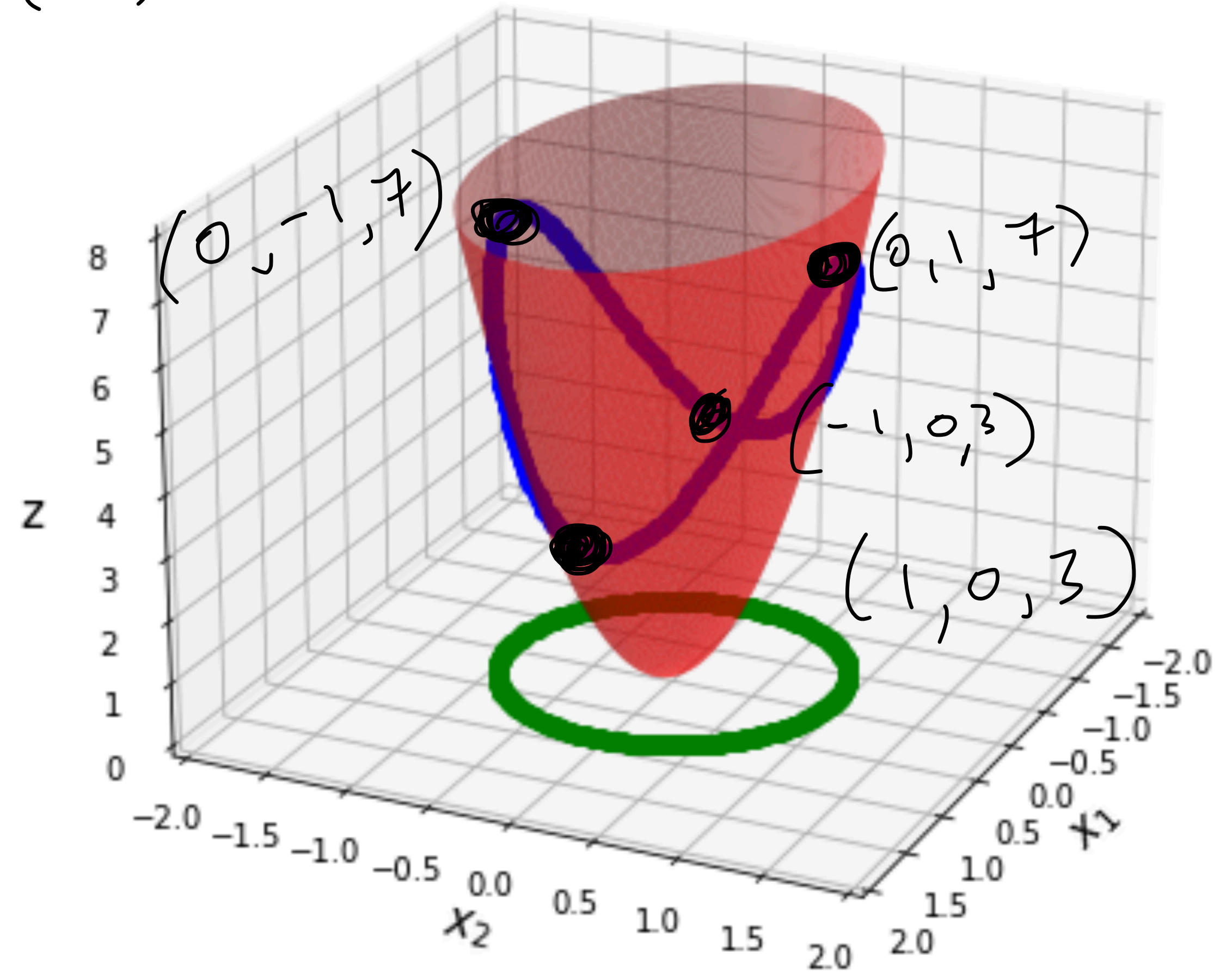
What are the min/max values?:

$3x_1^2 + 7x_2^2 \leq$

$7x_1^2 + 7x_2^2$

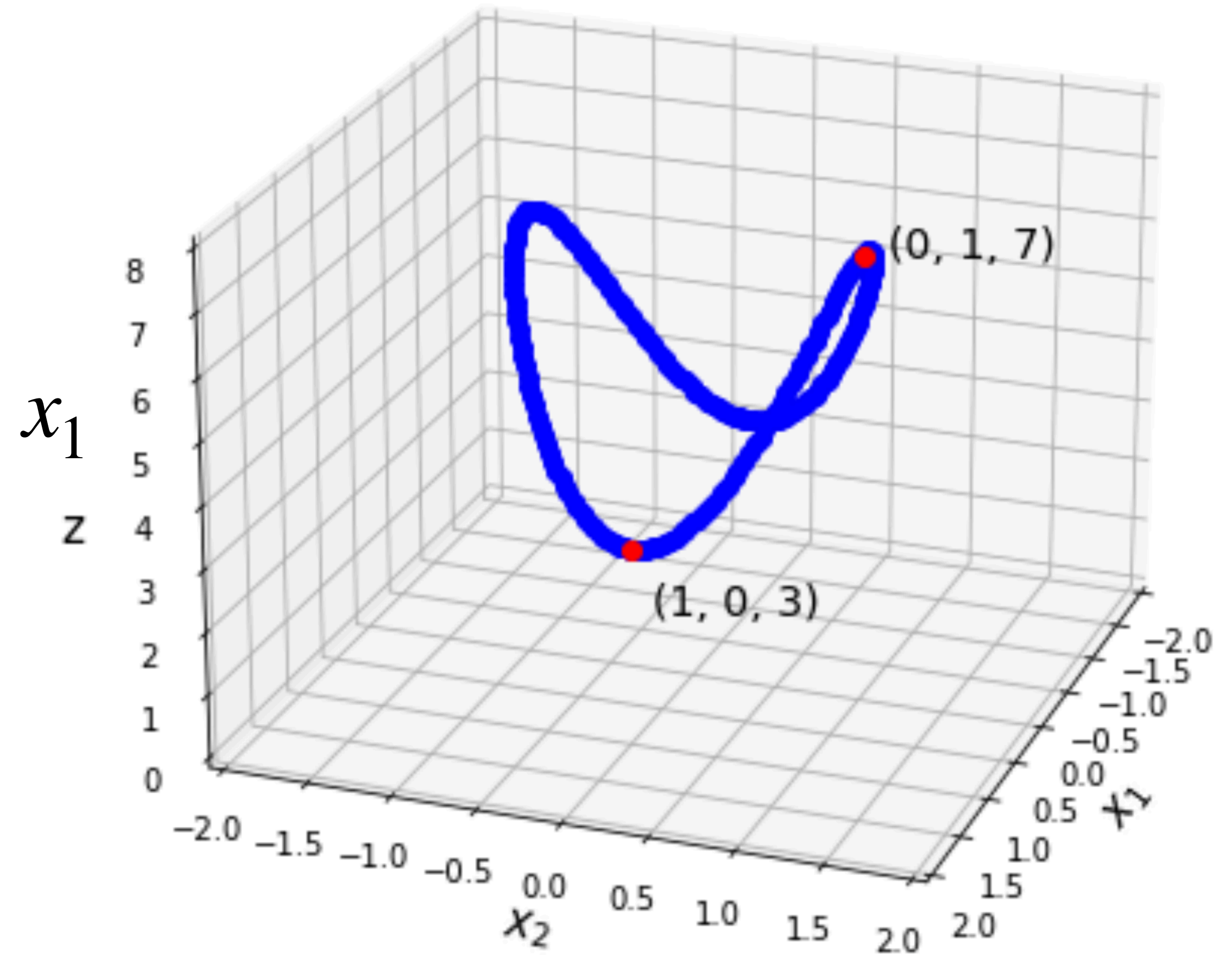
$7(x_1^2 + x_2^2) = 7$

$3x_1^2 + 7x_2^2 \geq 3$



Example: $3x_1^2 + 7x_2^2$

The minimum and maximum values are attained when the "weight" of the vector is distributed all on x_1 or x_2 .

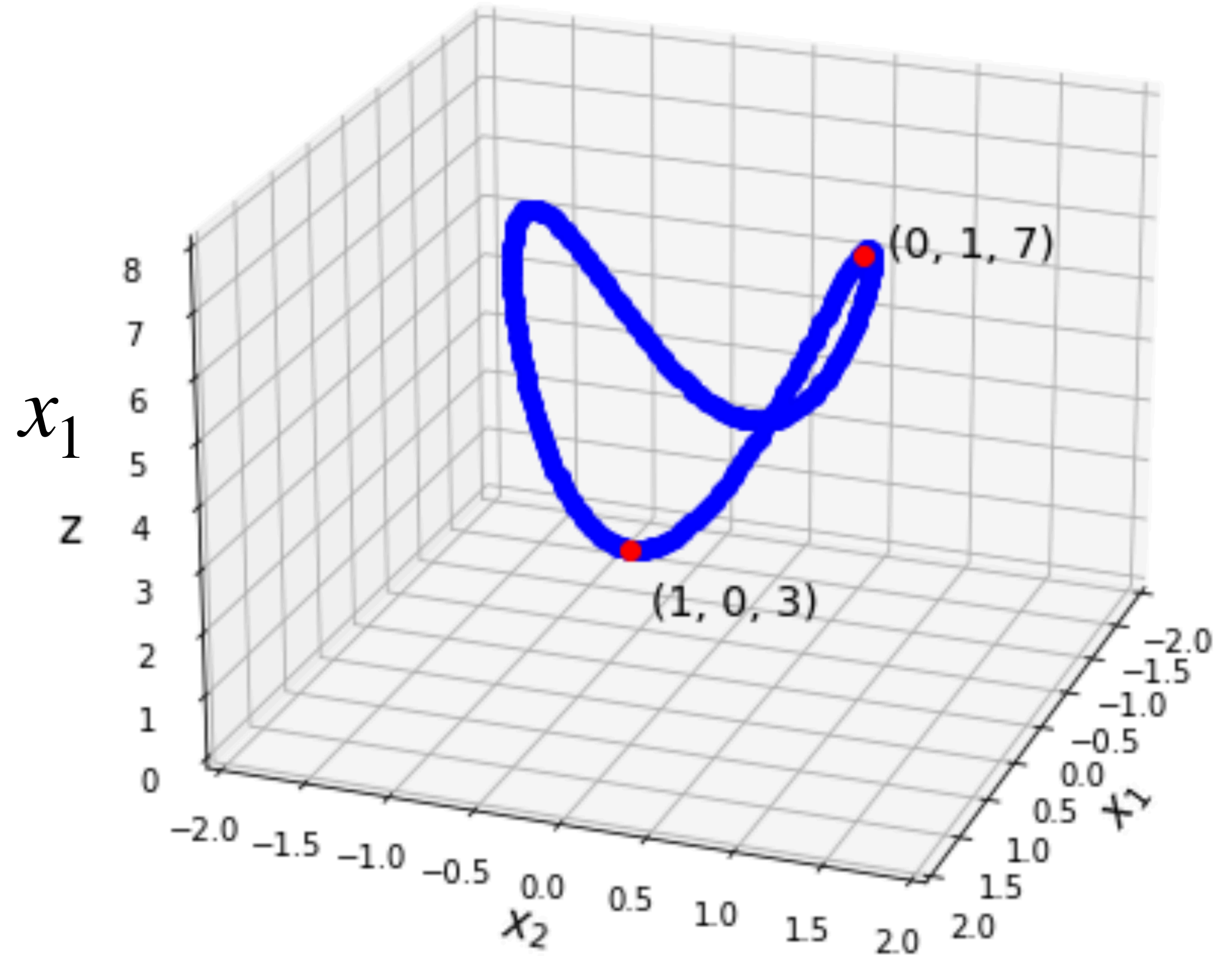


Example: $3x_1^2 + 7x_2^2$

What is the matrix?:

$$\begin{bmatrix} 3 & 0 \\ 0 & 7 \end{bmatrix}$$

eigenvalues are 3, 7



Constrained Optimization and Eigenvalues

Theorem. For a symmetric matrix A , with *largest* eigenvalue λ_1 and *smallest* eigenvalue λ_n

$$\max_{\|\mathbf{x}\|=1} \mathbf{x}^T A \mathbf{x} = \lambda_1 \qquad \min_{\|\mathbf{x}\|=1} \mathbf{x}^T A \mathbf{x} = \lambda_n$$

No matter the shape of A , this will hold.

How To: Constrained Optimization

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Problem. Find the maximum value of $\mathbf{x}^T A \mathbf{x}$ subject to $\|\mathbf{x}\| = 1$.

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Solution. Find the largest eigenvalue of A , this will be the maximum value.

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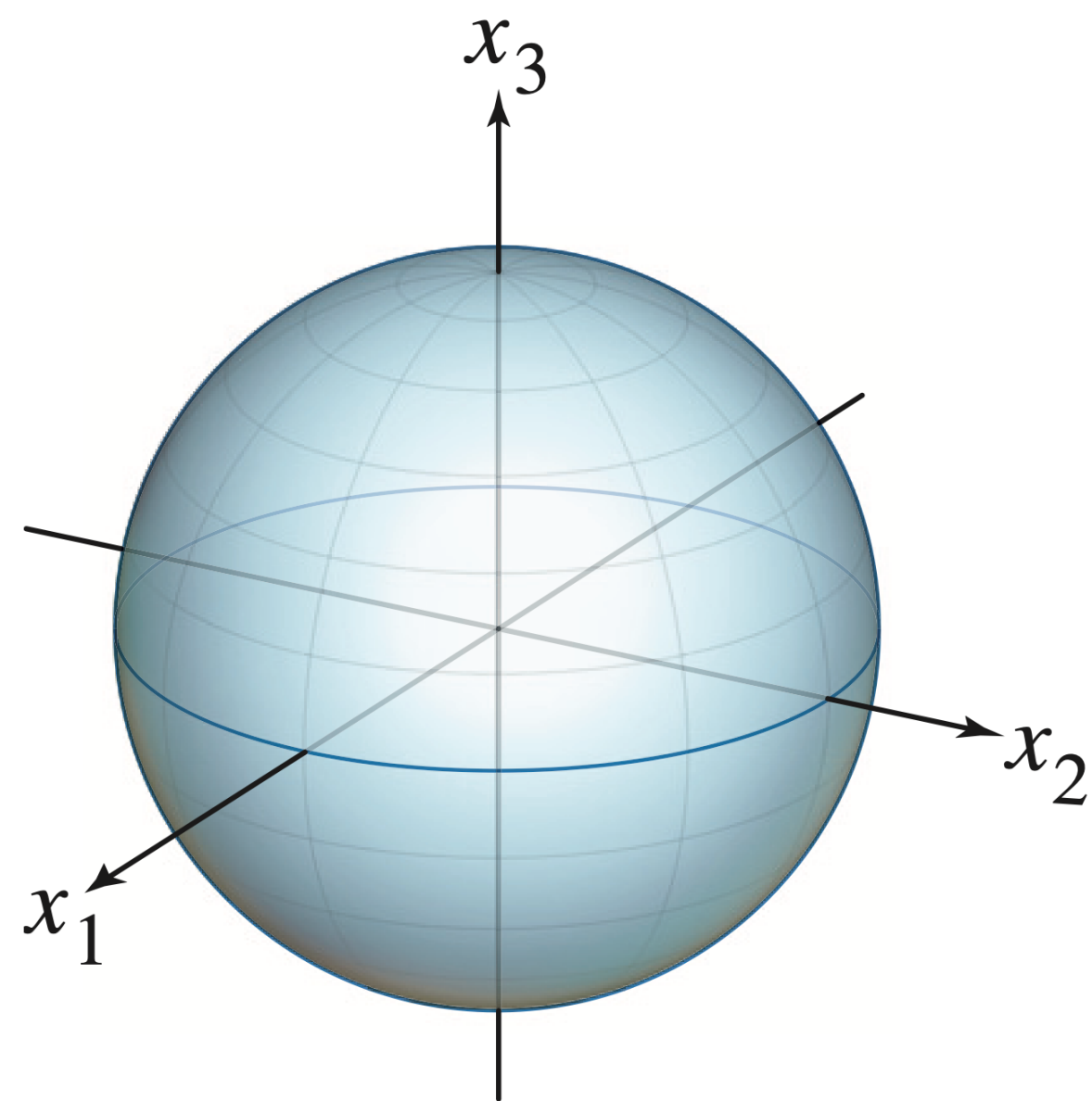
Solution. Find the largest eigenvalue of A , this will be the maximum value.

(Use NumPy)

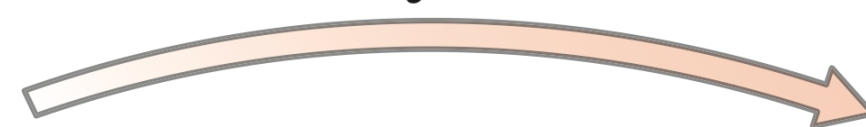
Singular Value Decomposition

Question

What shape is a the unit sphere after a linear transformation?



Multiplication
by A

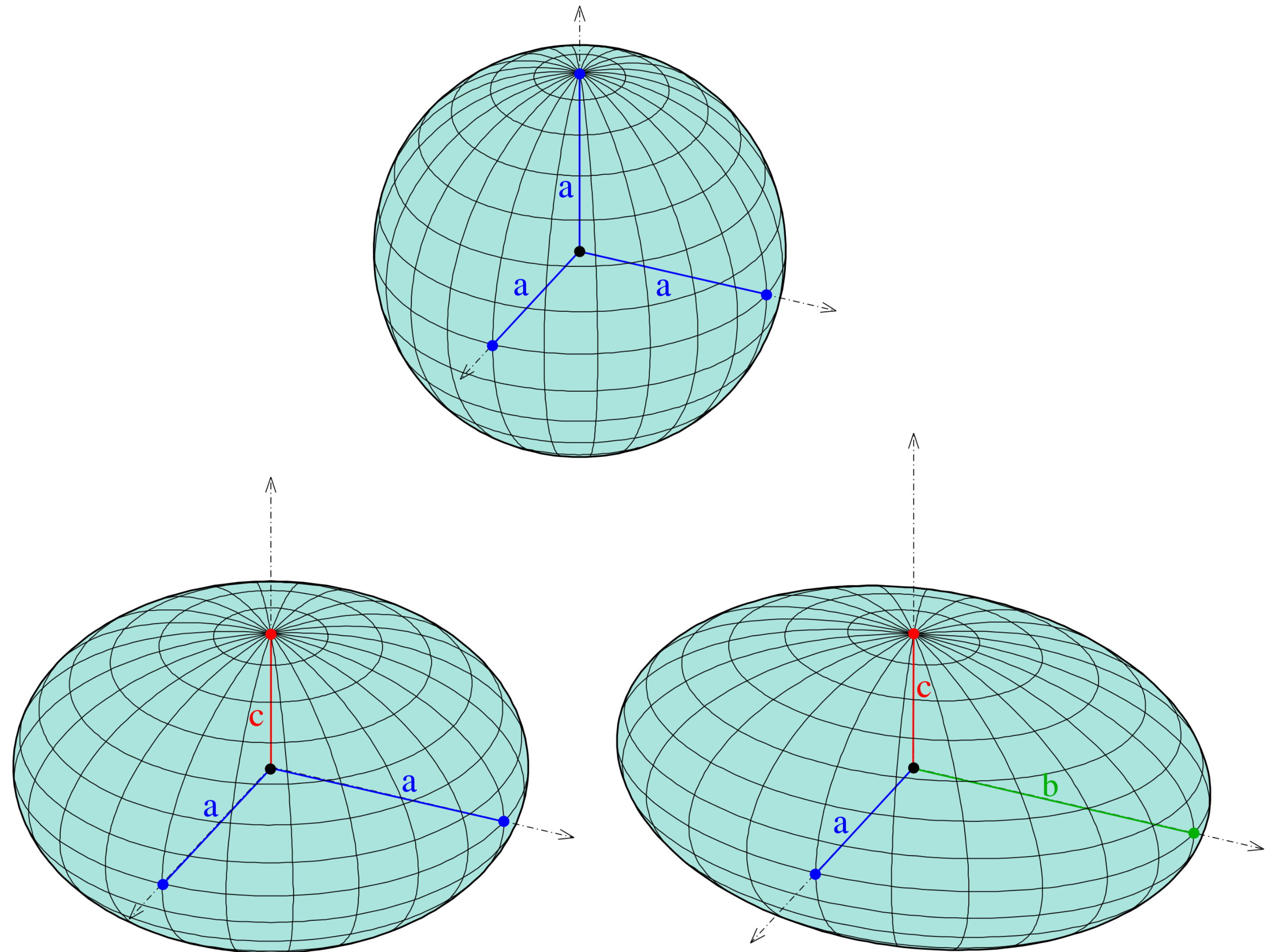


???

Ellipsoids

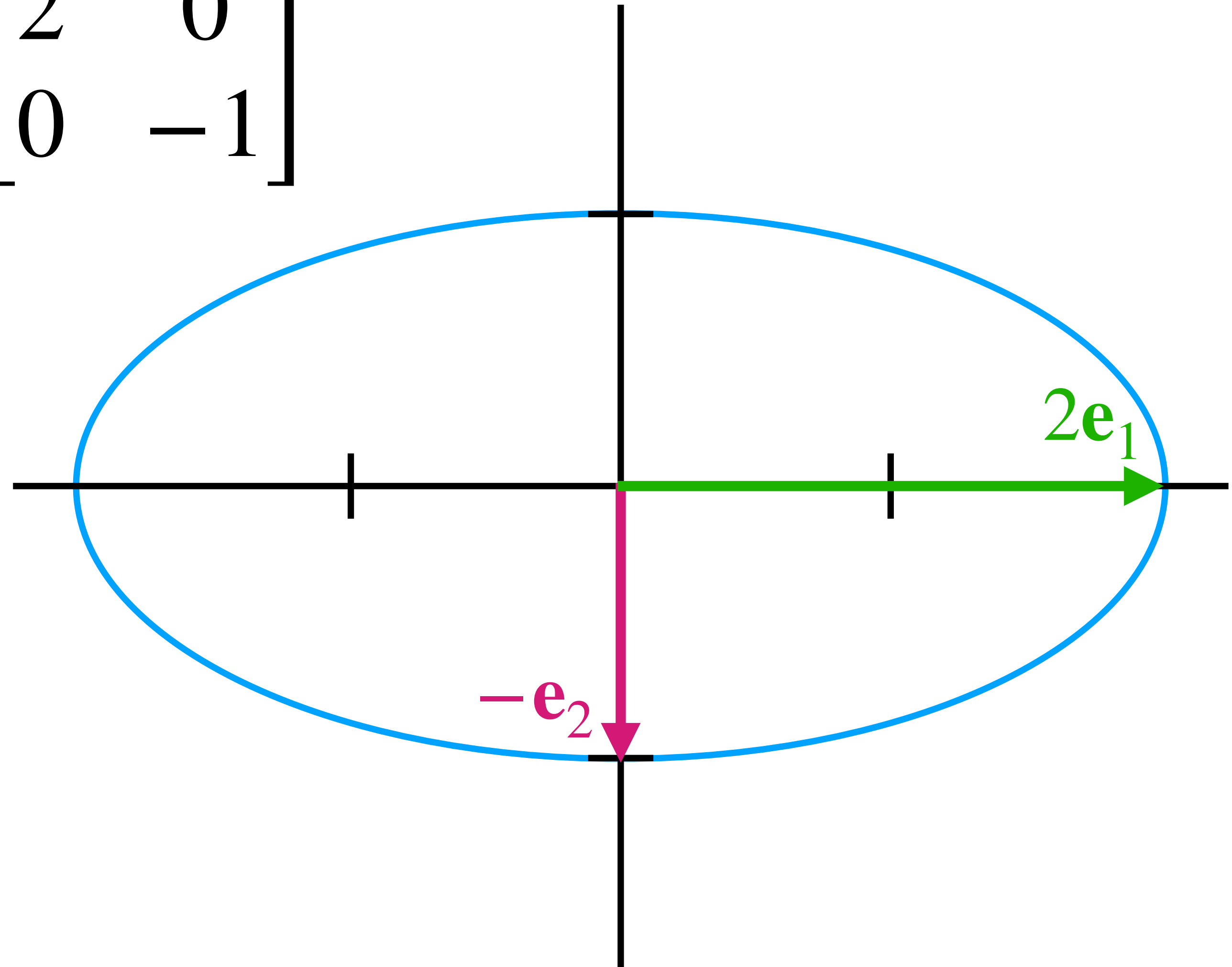
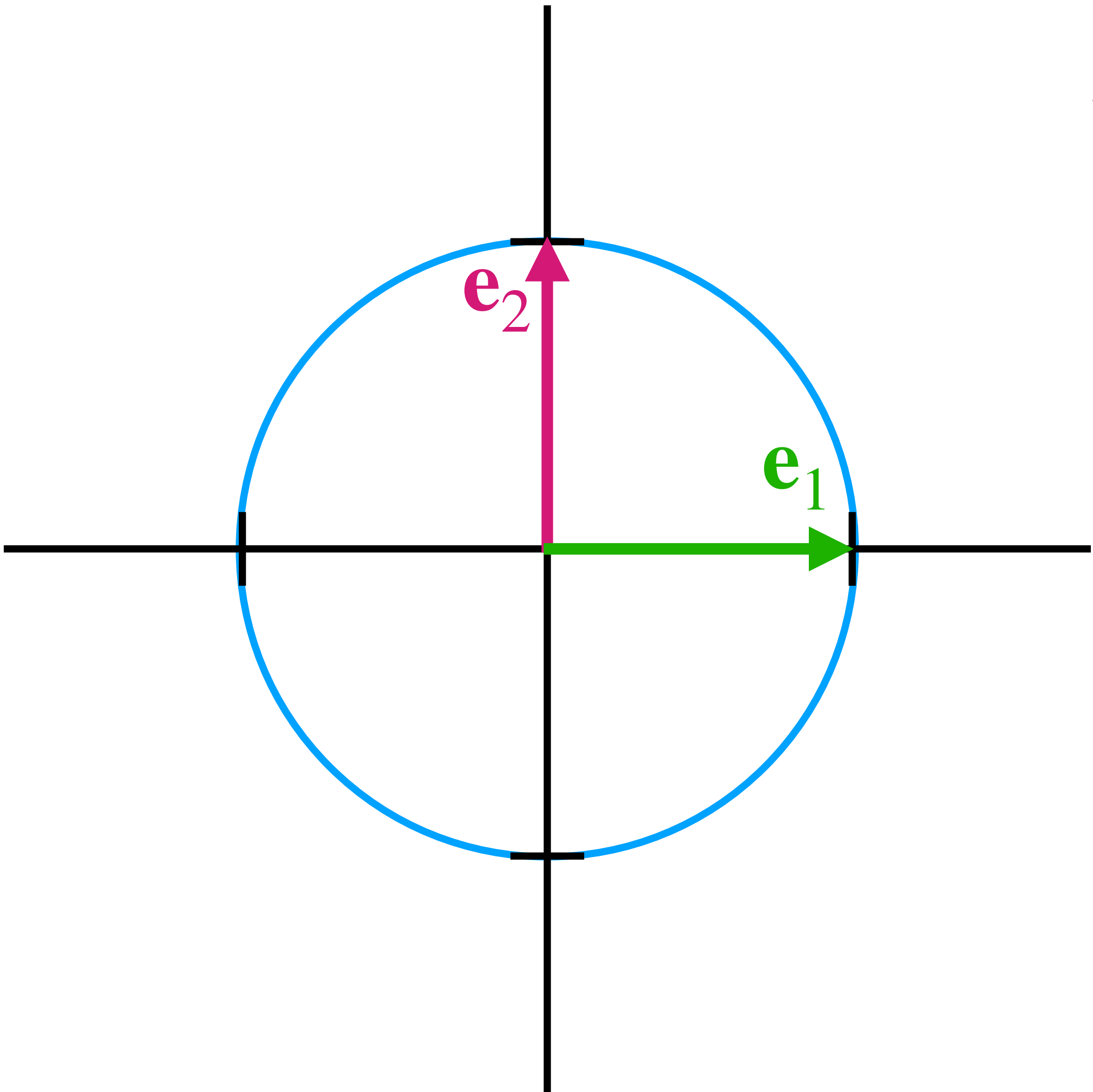
Ellipsoids are spheres "stretched" in orthogonal directions called the **axes of symmetry** or the **principle axes**.

Linear transformations maps spheres to ellipsoids.

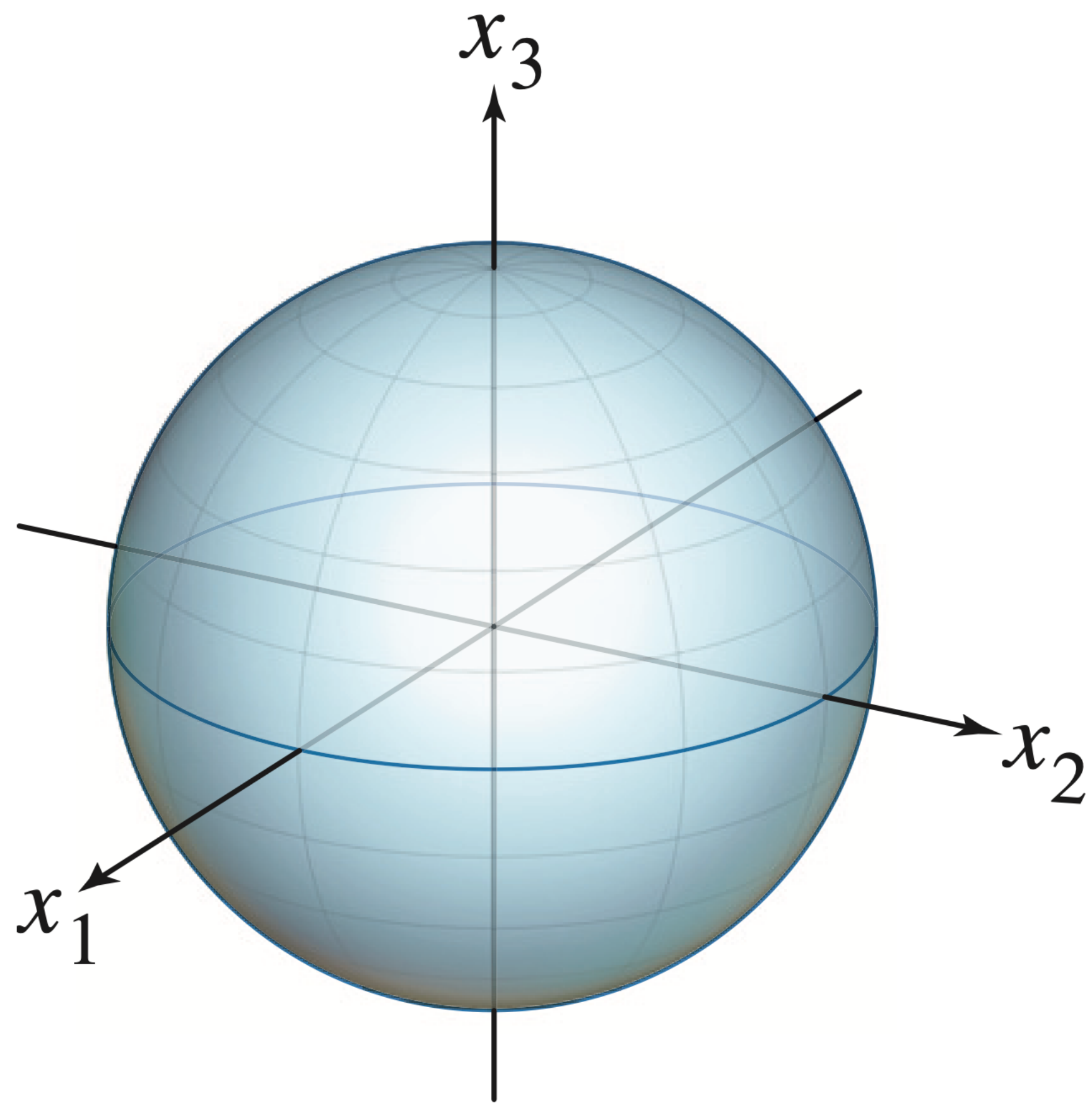


Simple Example : Scaling Matrices

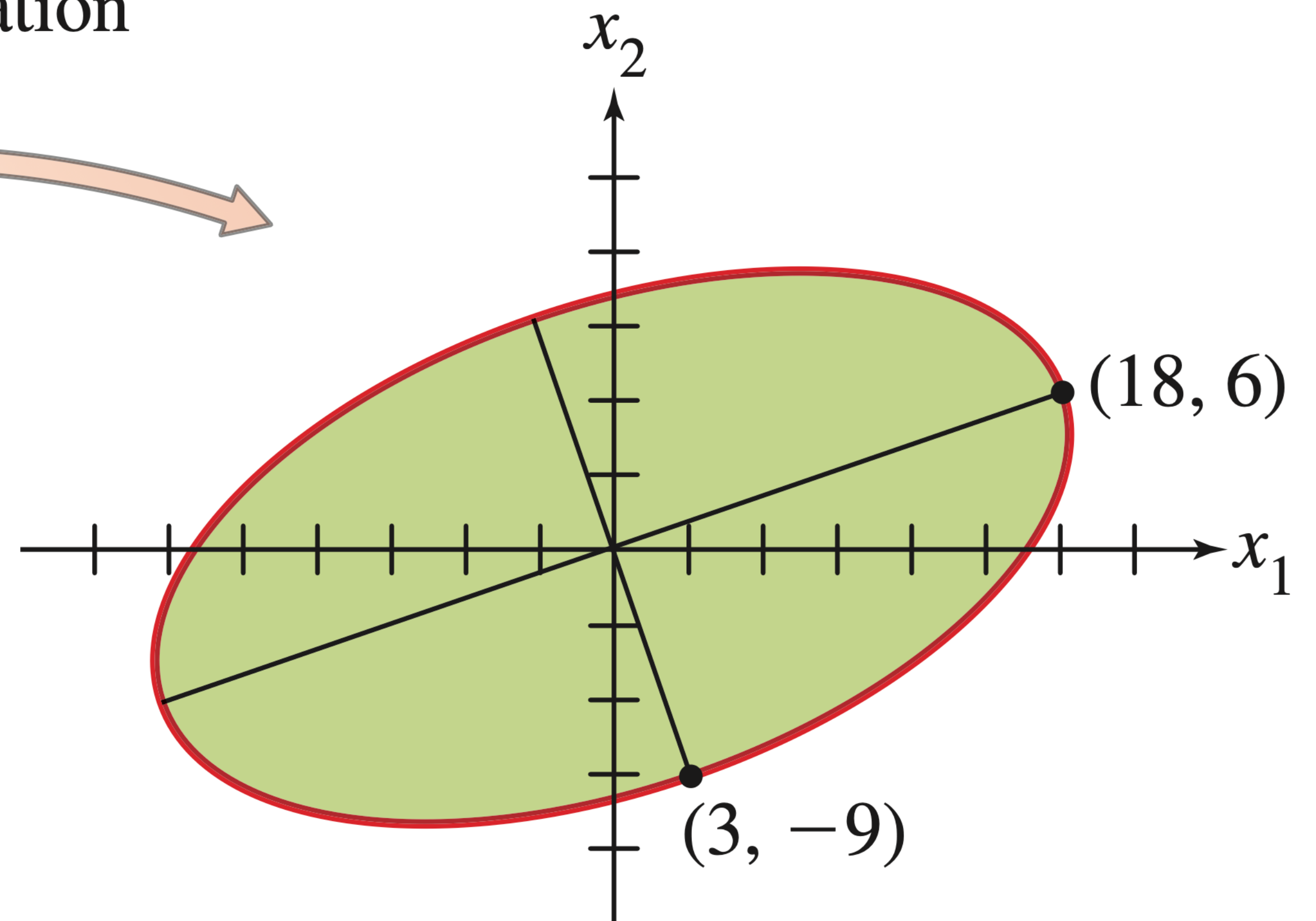
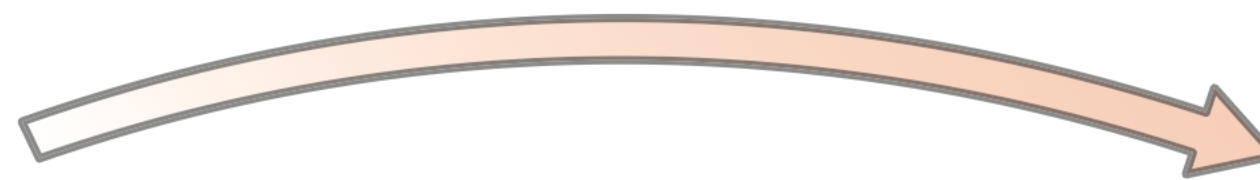
$$A = \begin{bmatrix} 2 & 0 \\ 0 & -1 \end{bmatrix}$$



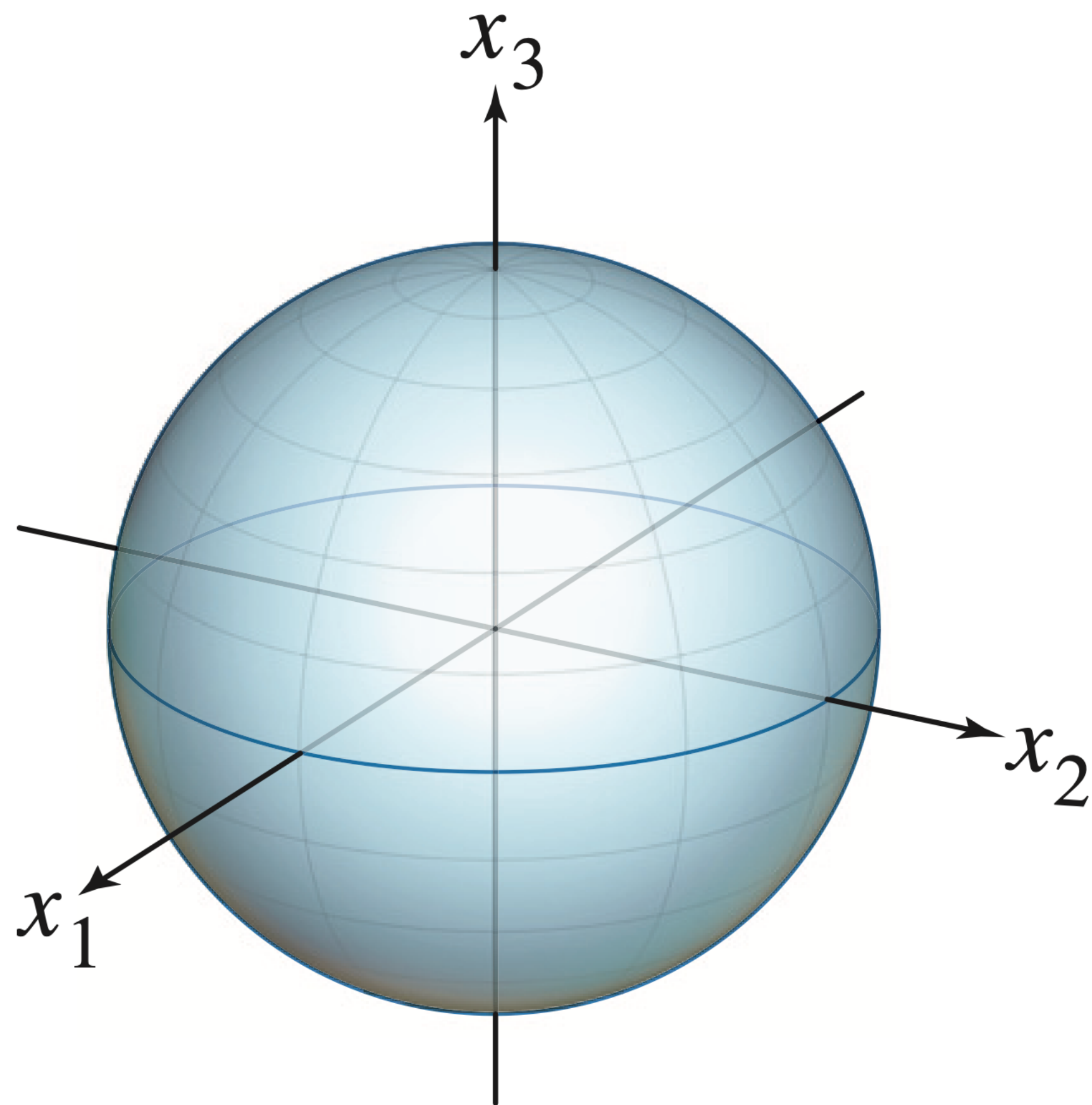
The Picture



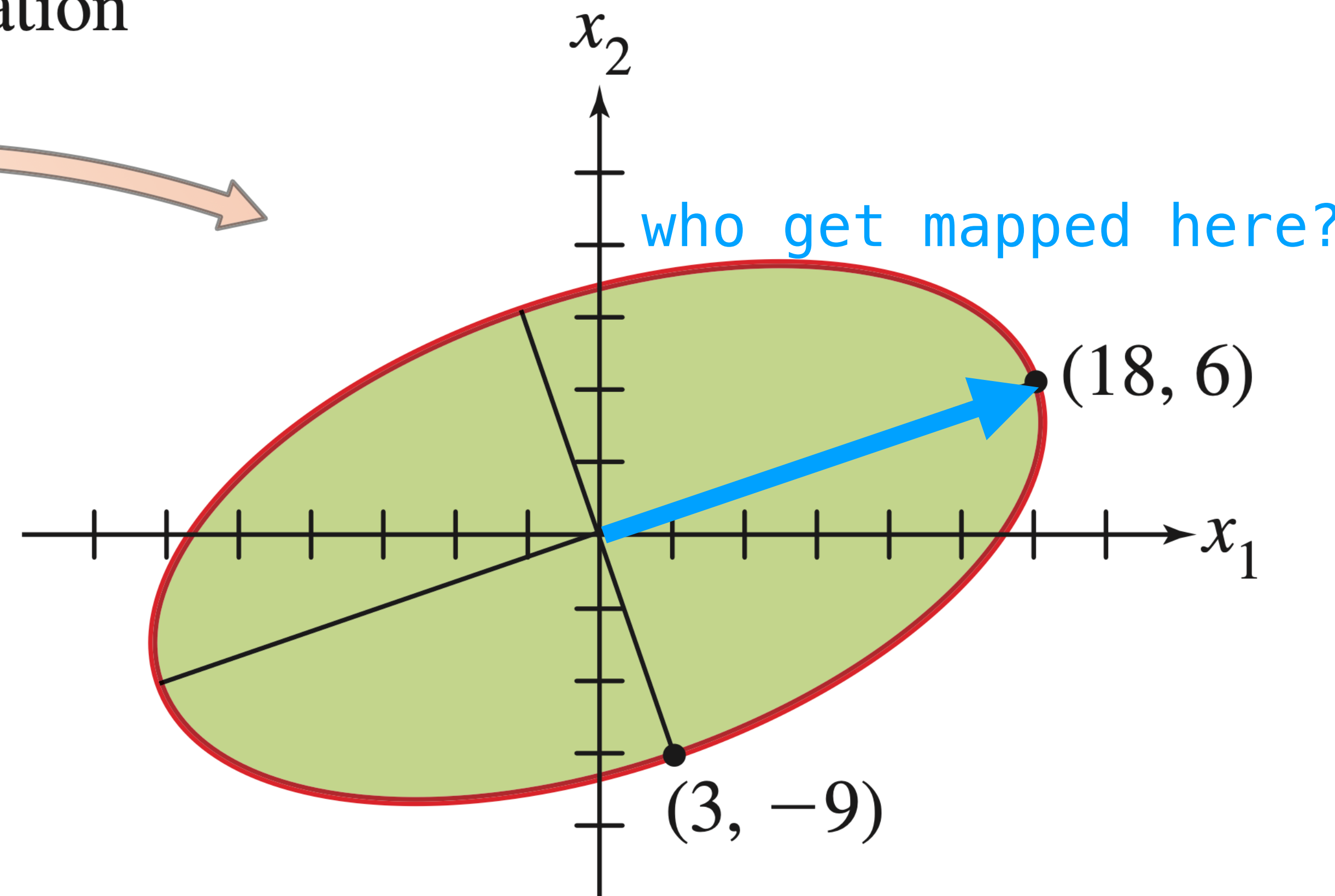
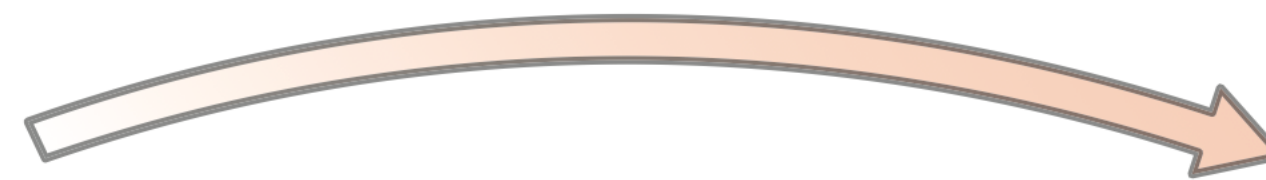
Multiplication
by A



The Picture

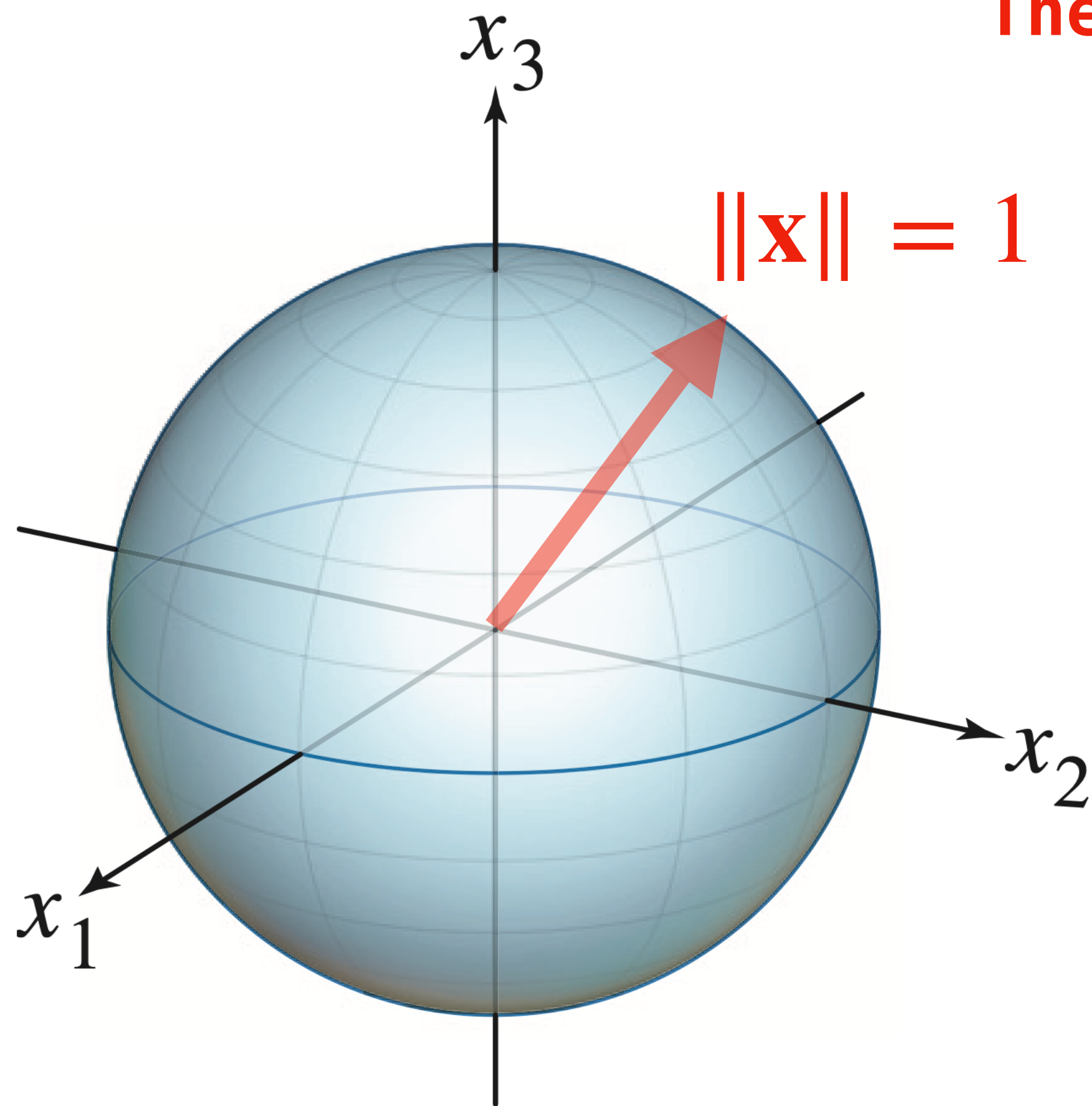


Multiplication
by A

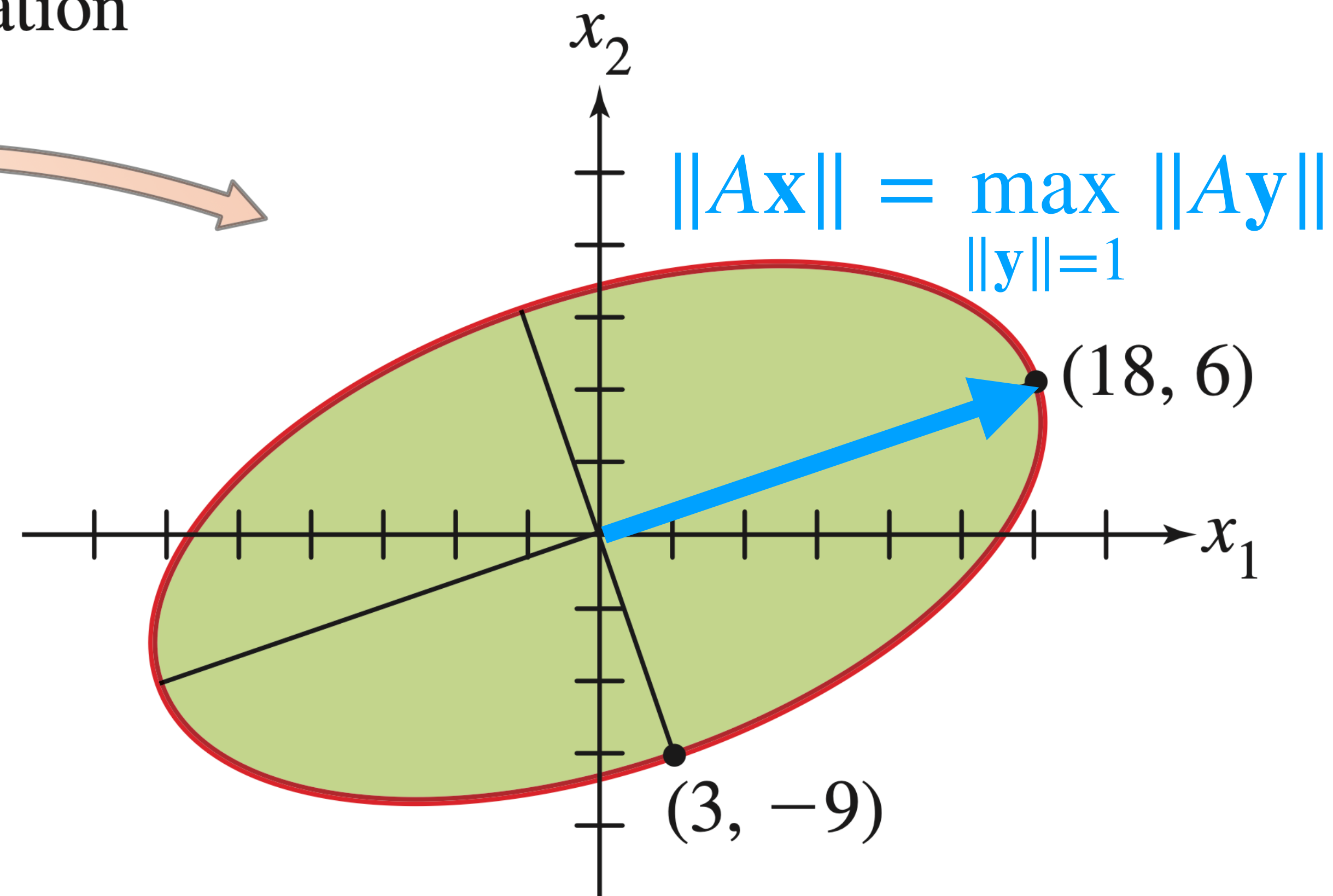
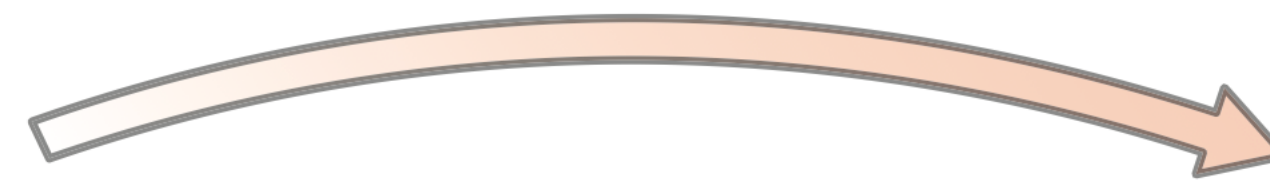


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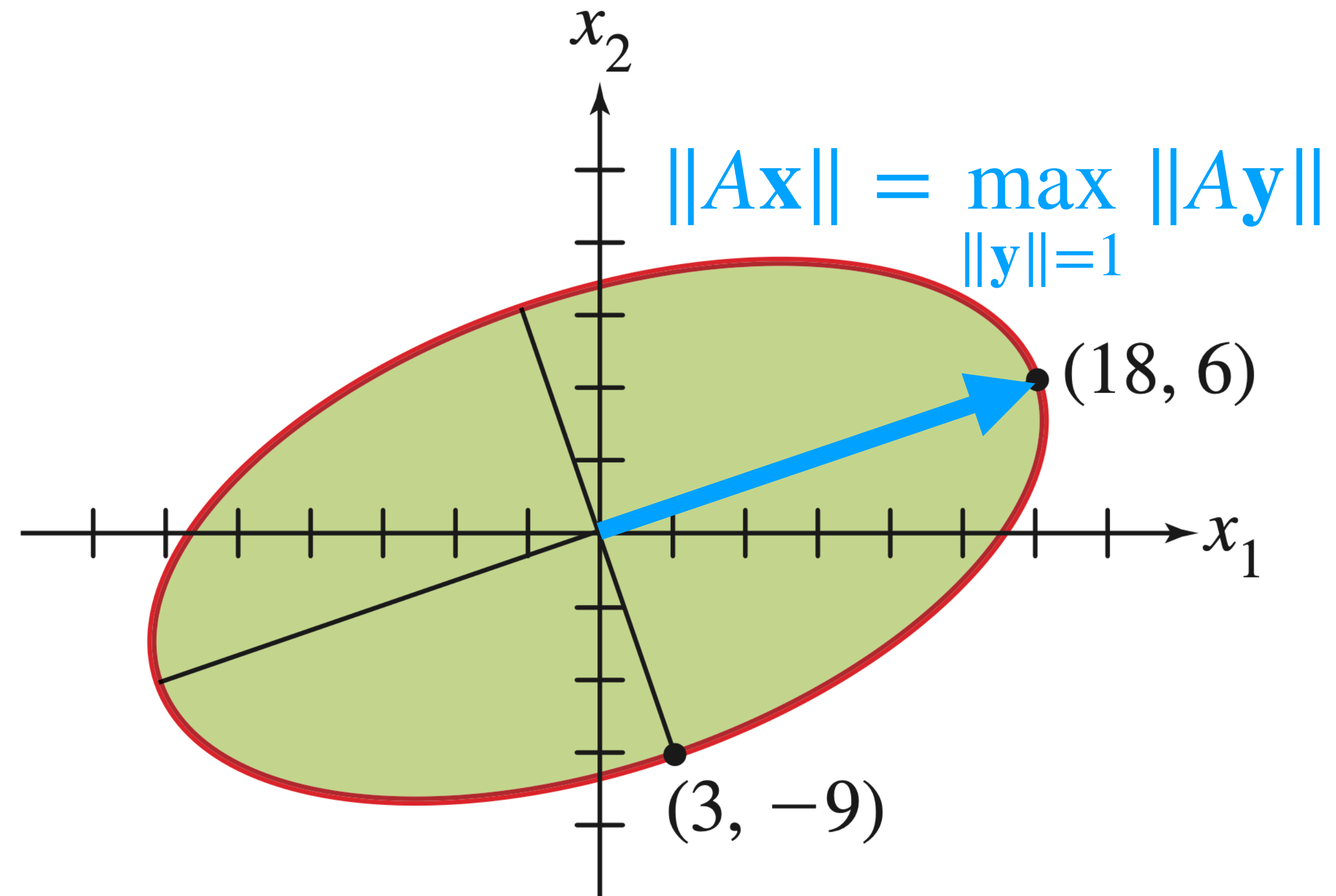
The longest end of the ellipse is the solution to a constrained optimization problem



Multiplication
by A

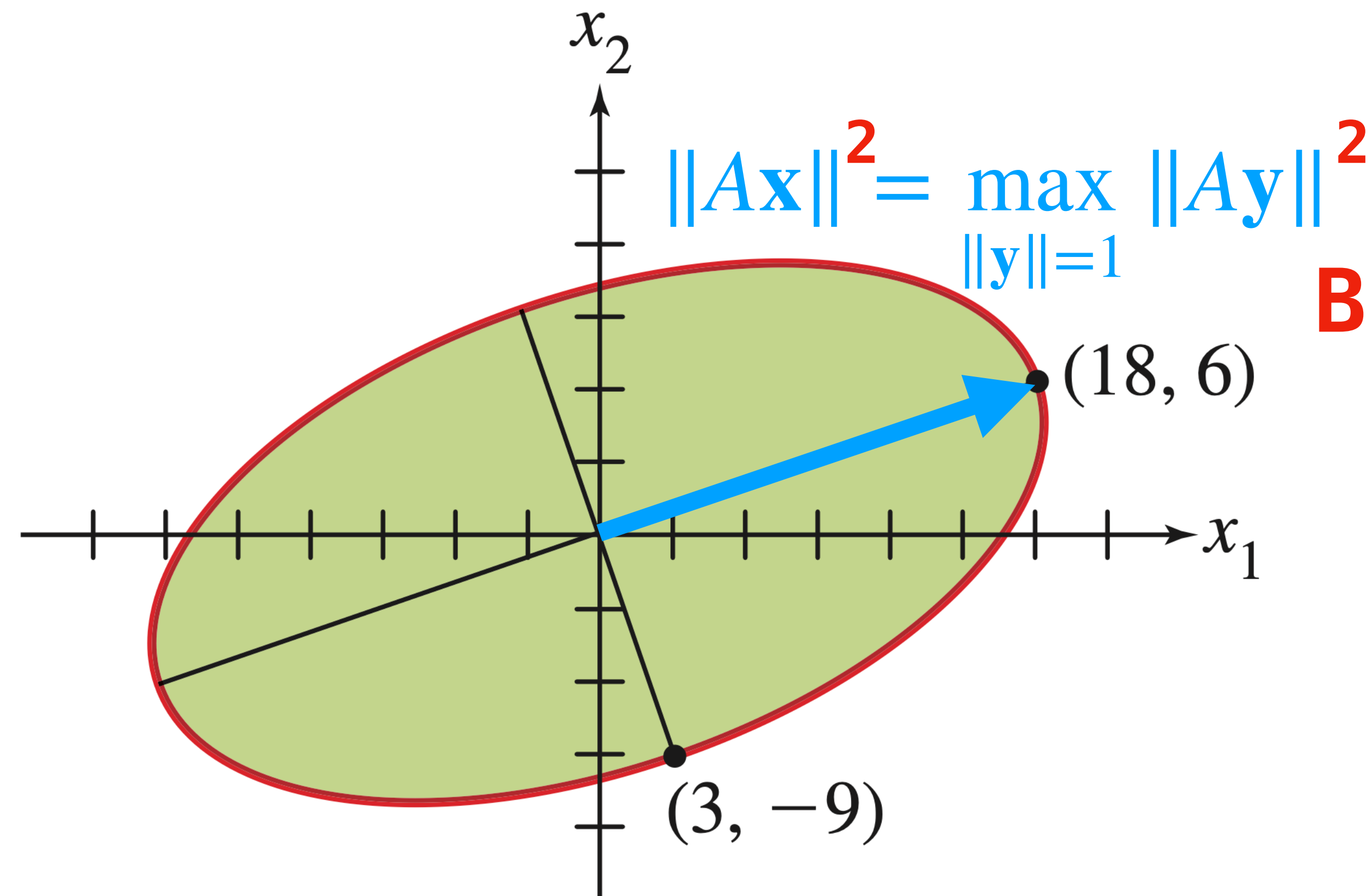


The Picture



This is not a quadratic form...

The Picture



But this is.

This is not a quadratic form...

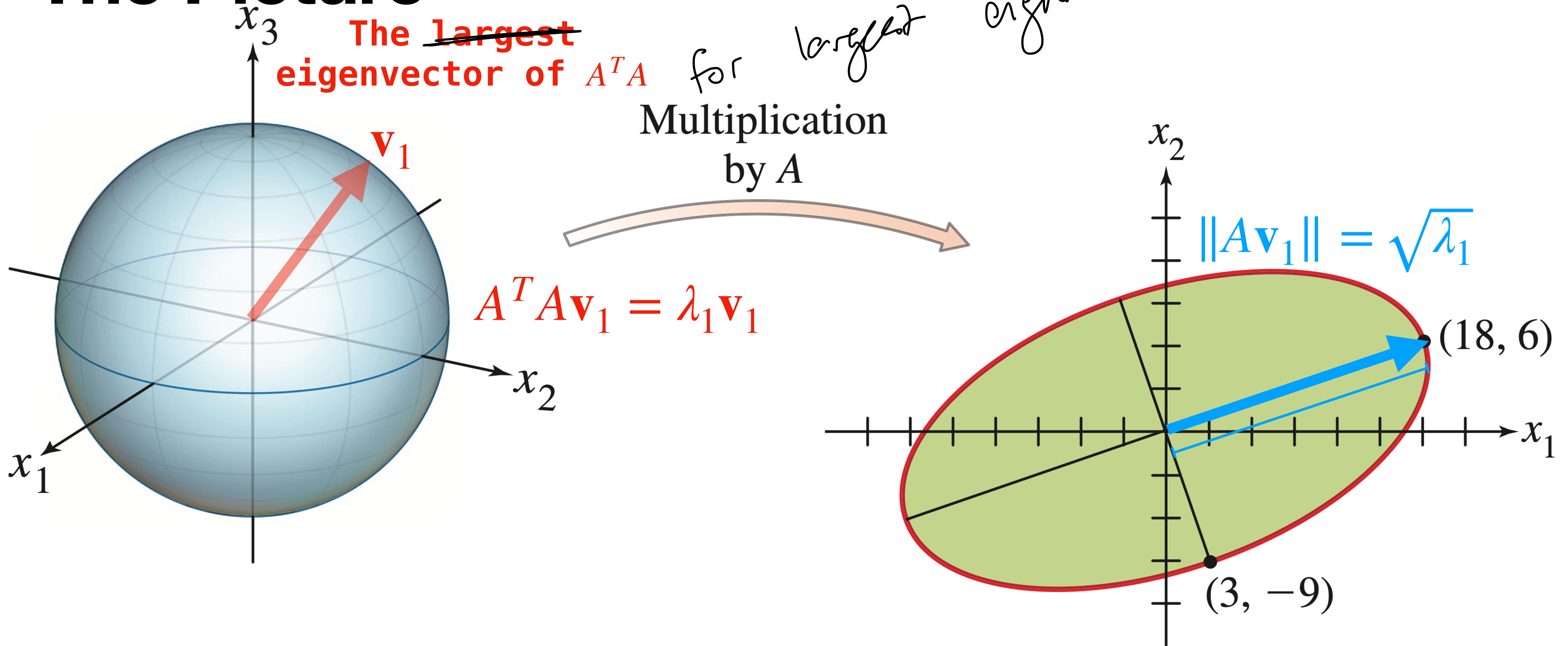
A Quadratic Form

What does $\|A\mathbf{x}\|^2$ look like?:

$$\langle A\vec{x}, A\vec{x} \rangle = (A\vec{x})^T A\vec{x}$$

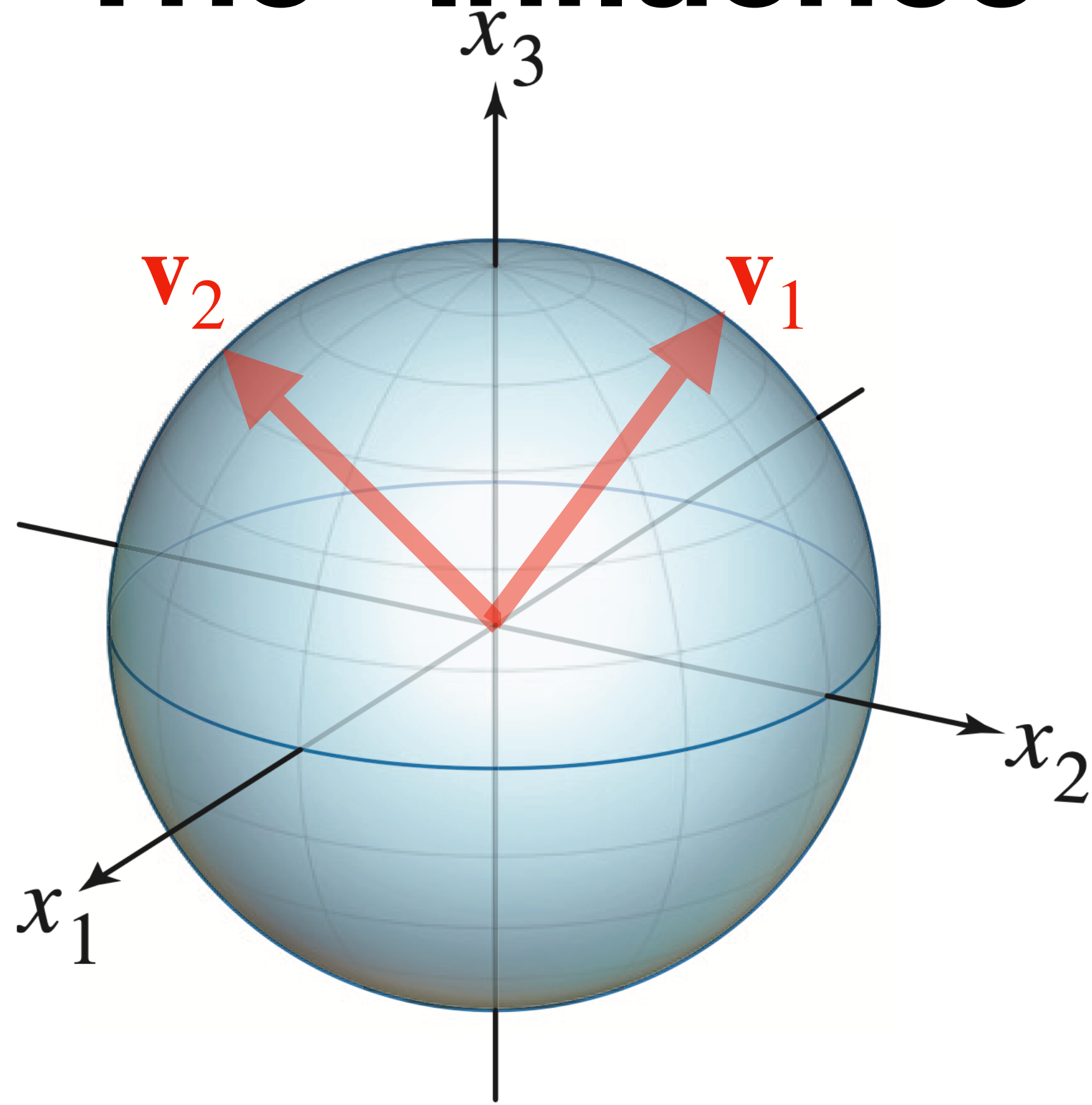
$$\vec{x}^T \boxed{A^T A} \vec{x}$$

The Picture

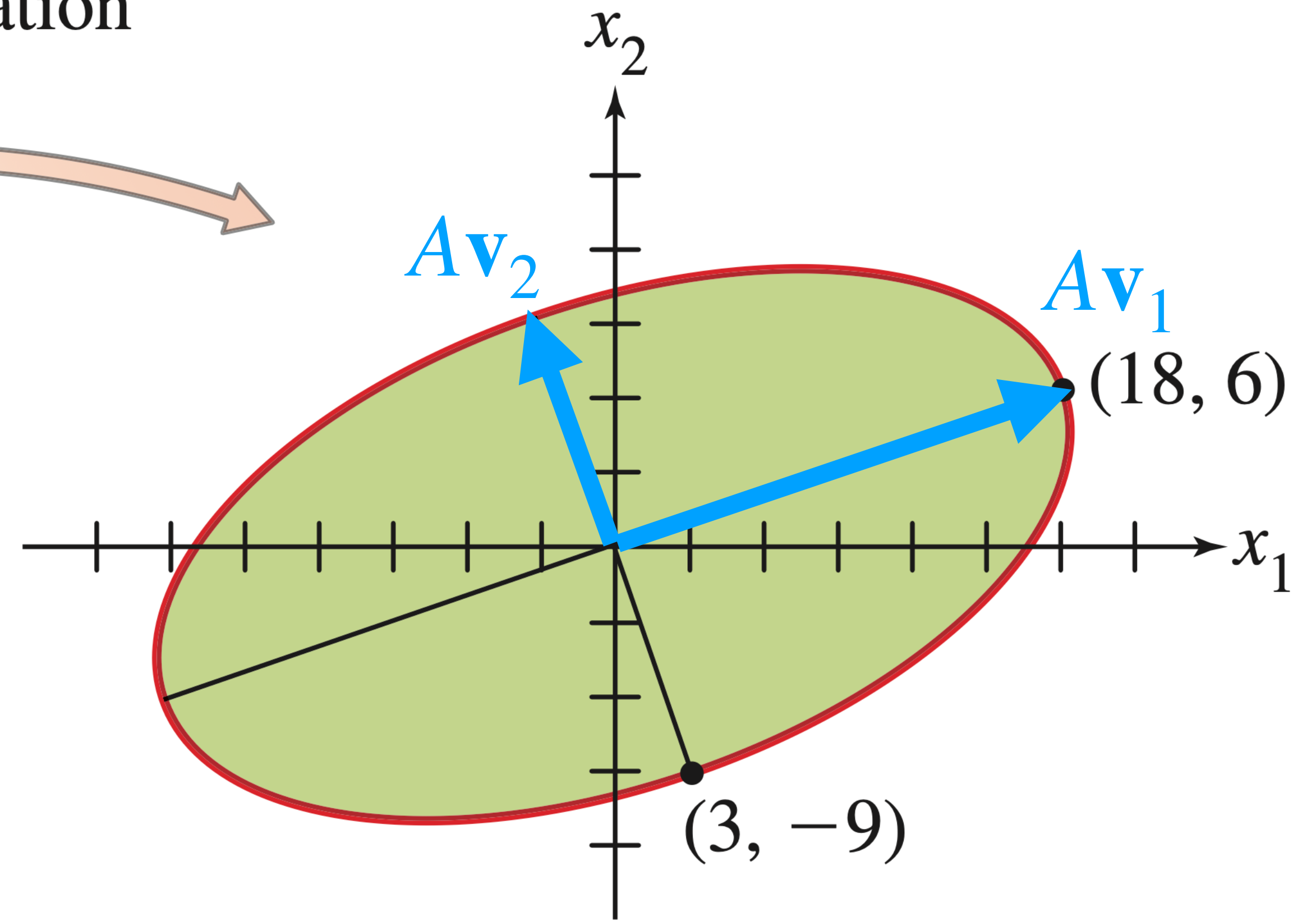
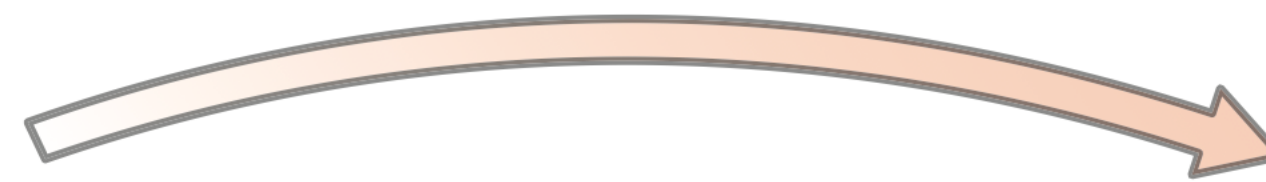


\mathbf{v}_1 solves the constrained optimization problem.

The "Influence" of A



Multiplication
by A



v_1 is "most affected" by A and v_2 is "least affected"

Properties of $A^T A$

Properties of $A^T A$

» It's symmetric. $(A^T A)^T = A^T A^{TT} = A^T A$

Properties of $A^T A$

- » It's symmetric.
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Properties of $A^T A$

- » It's symmetric.
- » So its orthogonally diagonalizable.
- » **There is an orthogonal basis of eigenvectors.**
- » It's eigenvalues are nonnegative.
- » **It's positive semidefinite.**

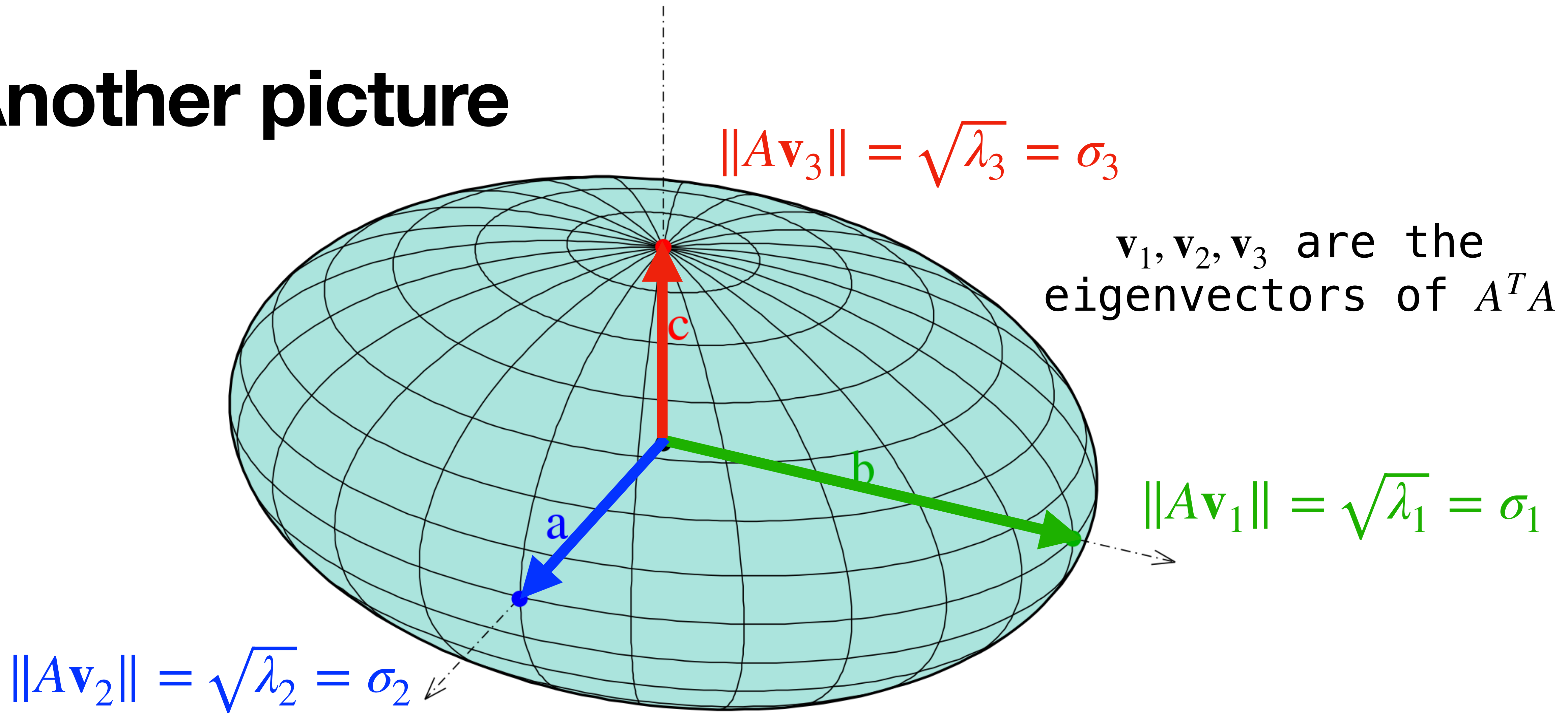
Singular Values

Definition. For an $m \times n$ matrix A , the **singular values** of A are the n values

$$\sigma_1 \geq \sigma_2 \dots \geq \sigma_n \geq 0$$

where $\sigma_i = \sqrt{\lambda_i}$ and λ_i is an eigenvalue of $A^T A$.

Another picture



The **singular values** are the lengths of the *axes of symmetry* of the ellipsoid after transforming the unit sphere.

Every $m \times n$ matrix transforms the unit m -sphere into an n -ellipsoid.

So every $m \times n$ matrix has
 n singular values.

What else can we say?

Let $\mathbf{v}_1, \dots, \mathbf{v}_n$ be an **orthogonal** eigenbasis of \mathbb{R}^n for $A^T A$ and suppose A has r nonzero singular values.

Theorem. $A\mathbf{v}_1, \dots, A\mathbf{v}_r$ is an orthogonal basis of $\text{Col}(A)$.

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Let $\mathbf{v}_1, \dots, \mathbf{v}_n$ be an **orthogonal** eigenbasis of \mathbb{R}^n for $A^T A$ and suppose A has r nonzero singular values.

Theorem. $A\mathbf{v}_1, \dots, A\mathbf{v}_r$ is an orthogonal basis of $\text{Col}(A)$.

This is the most important theorem for SVD.

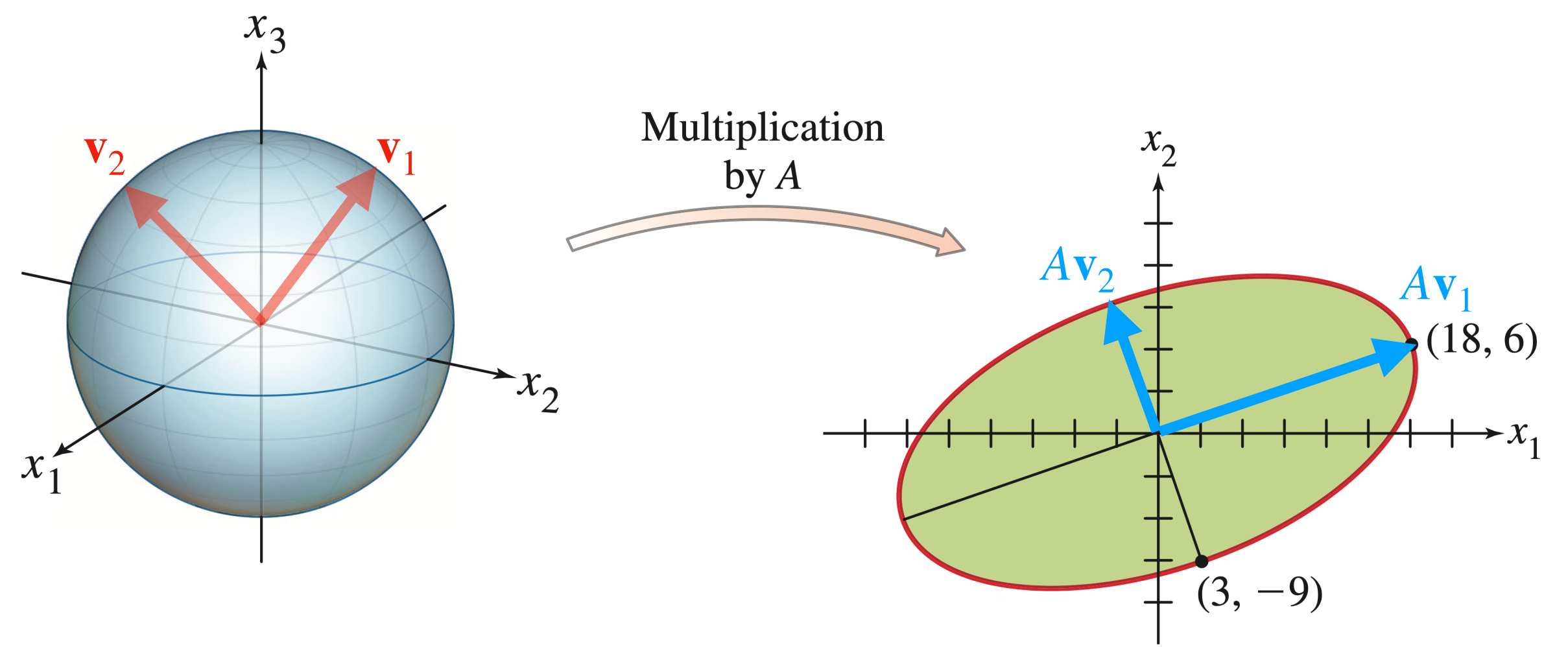
Verifying it

Let's show $A\mathbf{v}_1, \dots, A\mathbf{v}_r$ are linearly independent:

Verifying it

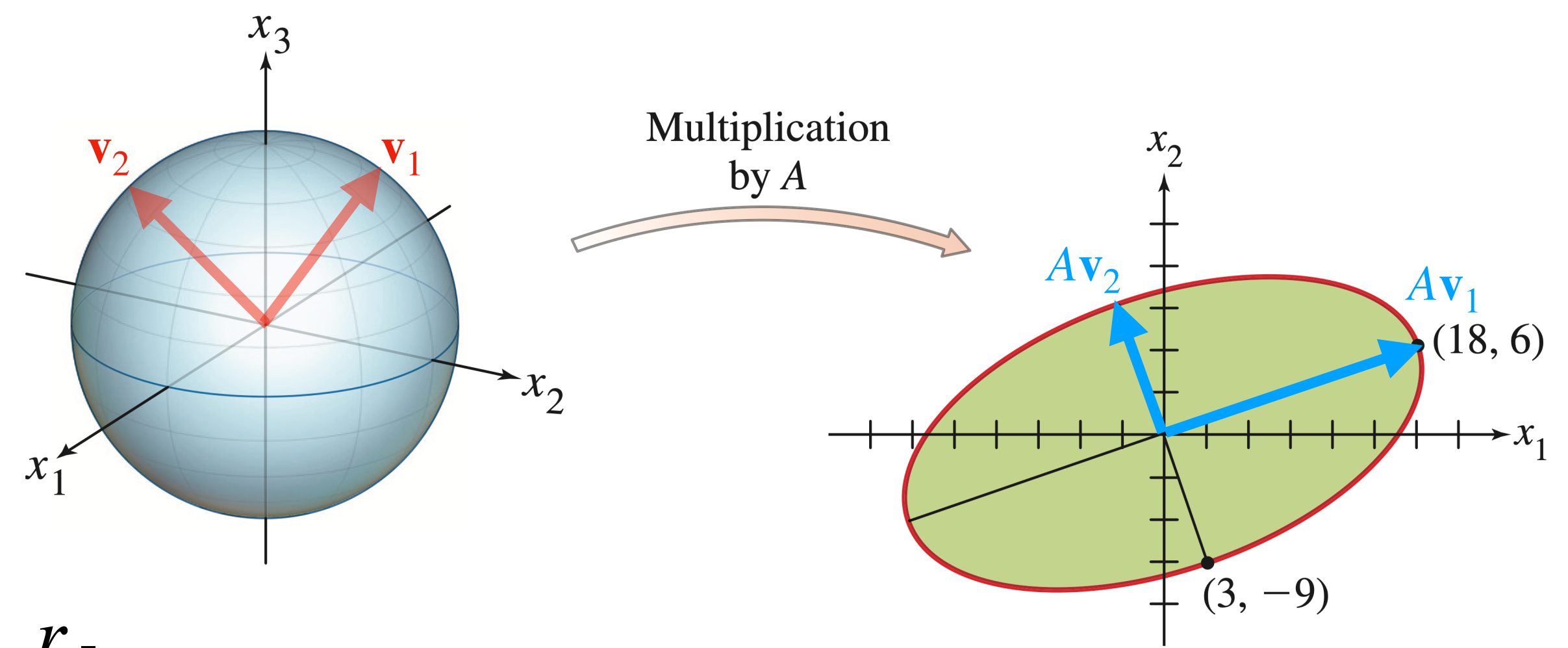
Let's show $A\mathbf{v}_1, \dots, A\mathbf{v}_r$ span $\text{Col}(A)$:

Putting it all together



Putting it all together

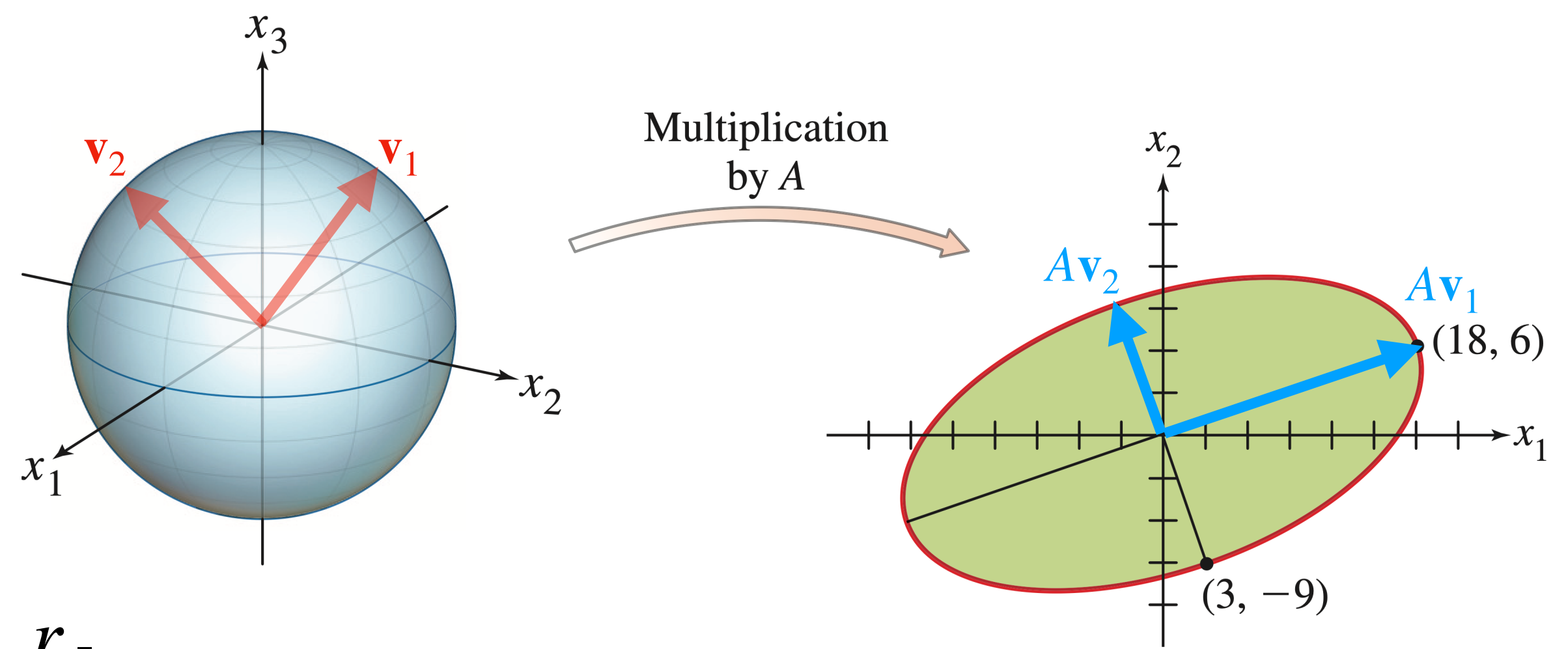
Let A be an $m \times n$ matrix of rank r .



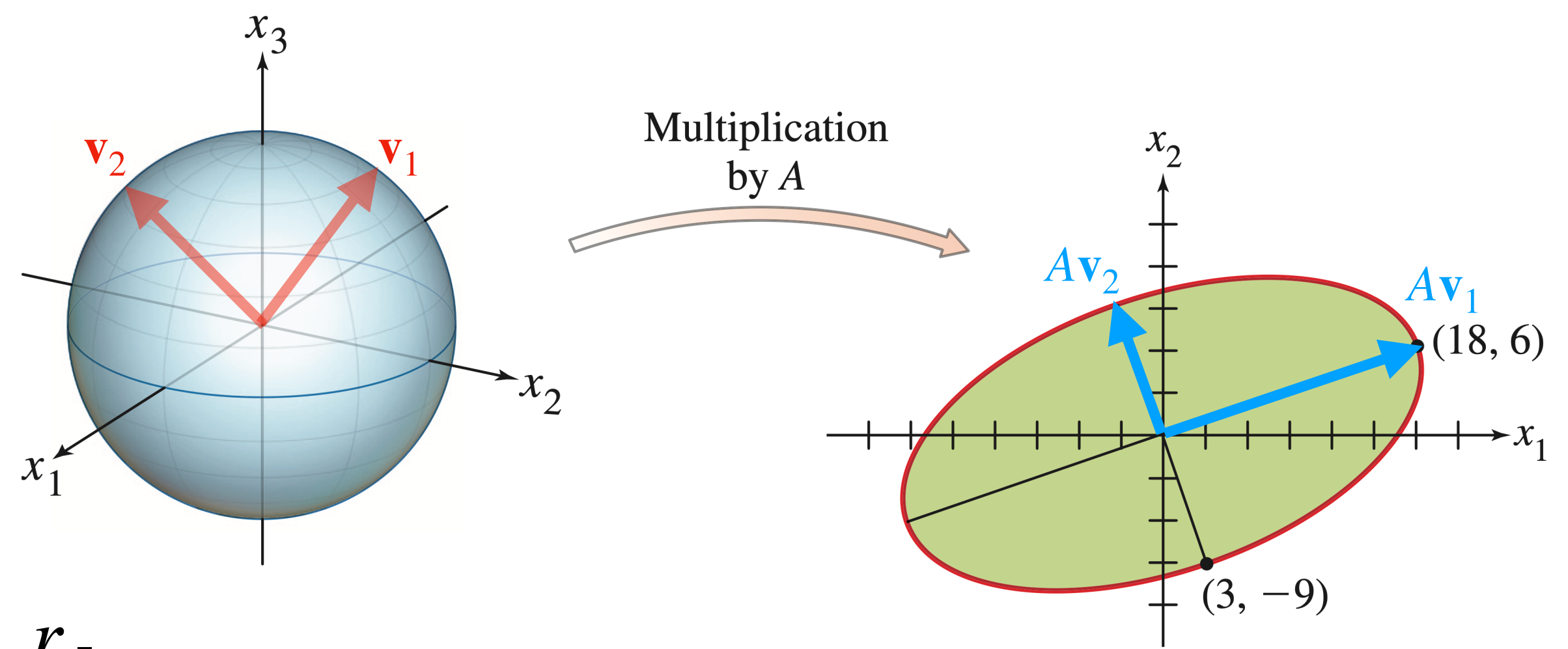
Putting it all together

Let A be an $m \times n$ matrix of rank r .

What we know:



Putting it all together

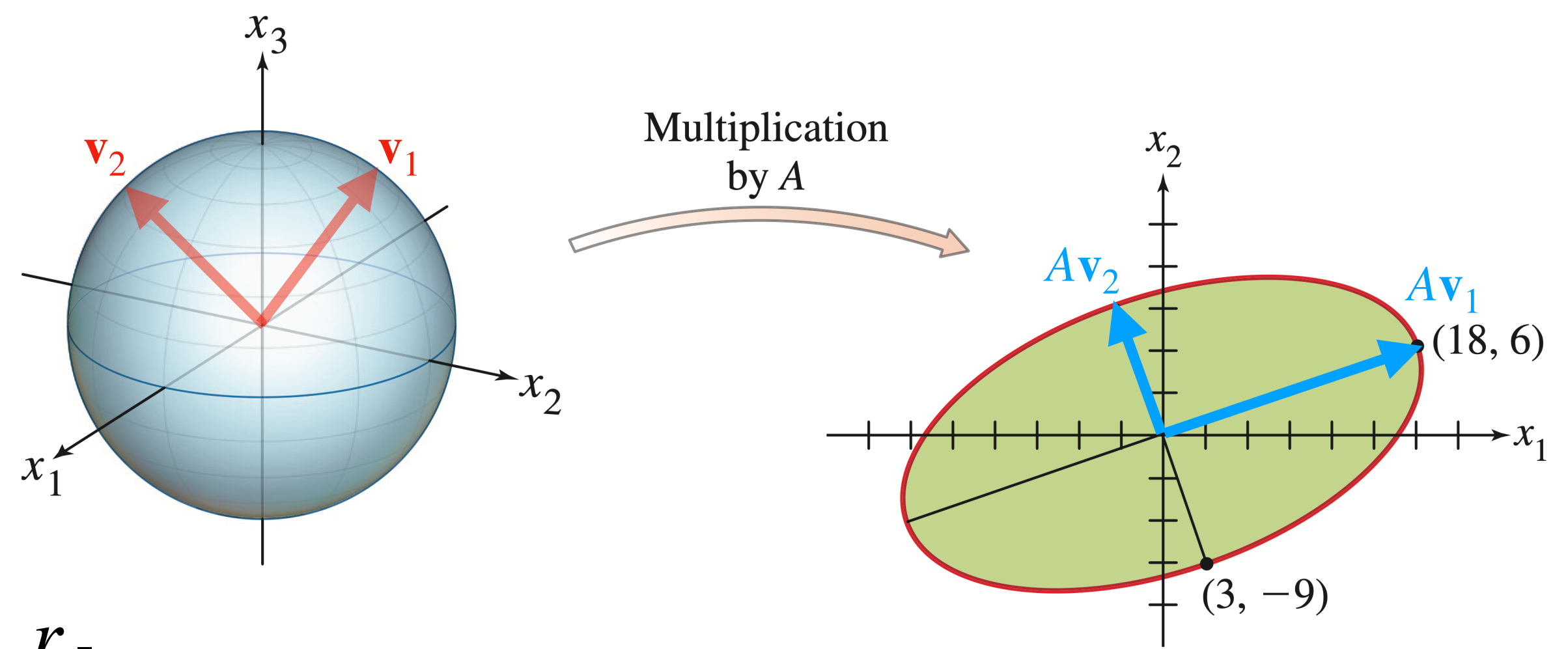


Let A be an $m \times n$ matrix of rank r .

What we know:

» We can find orthonormal vectors $\mathbf{v}_1, \dots, \mathbf{v}_r$ in \mathbb{R}^n such that $A\mathbf{v}_1, \dots, A\mathbf{v}_r$ in \mathbb{R}^m form an orthogonal basis for $\text{Col}(A)$.

Putting it all together



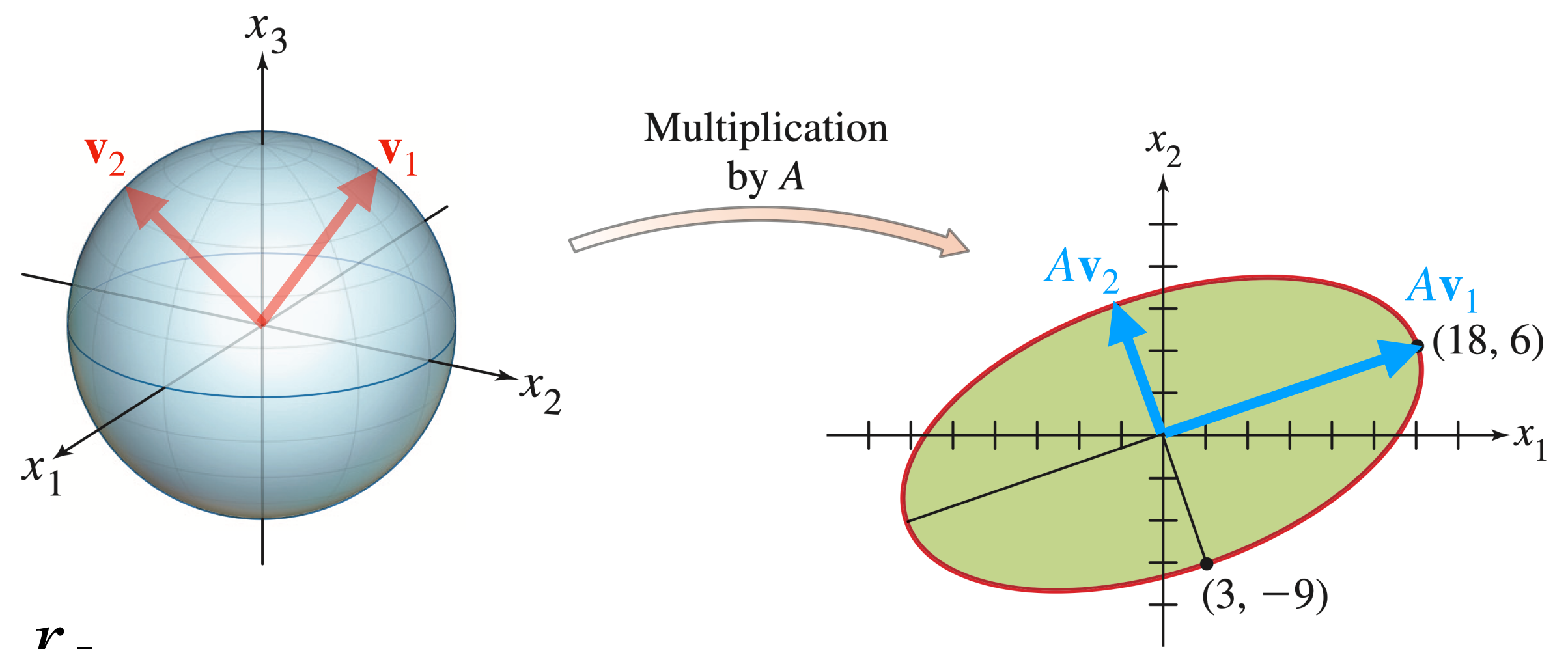
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Putting it all together



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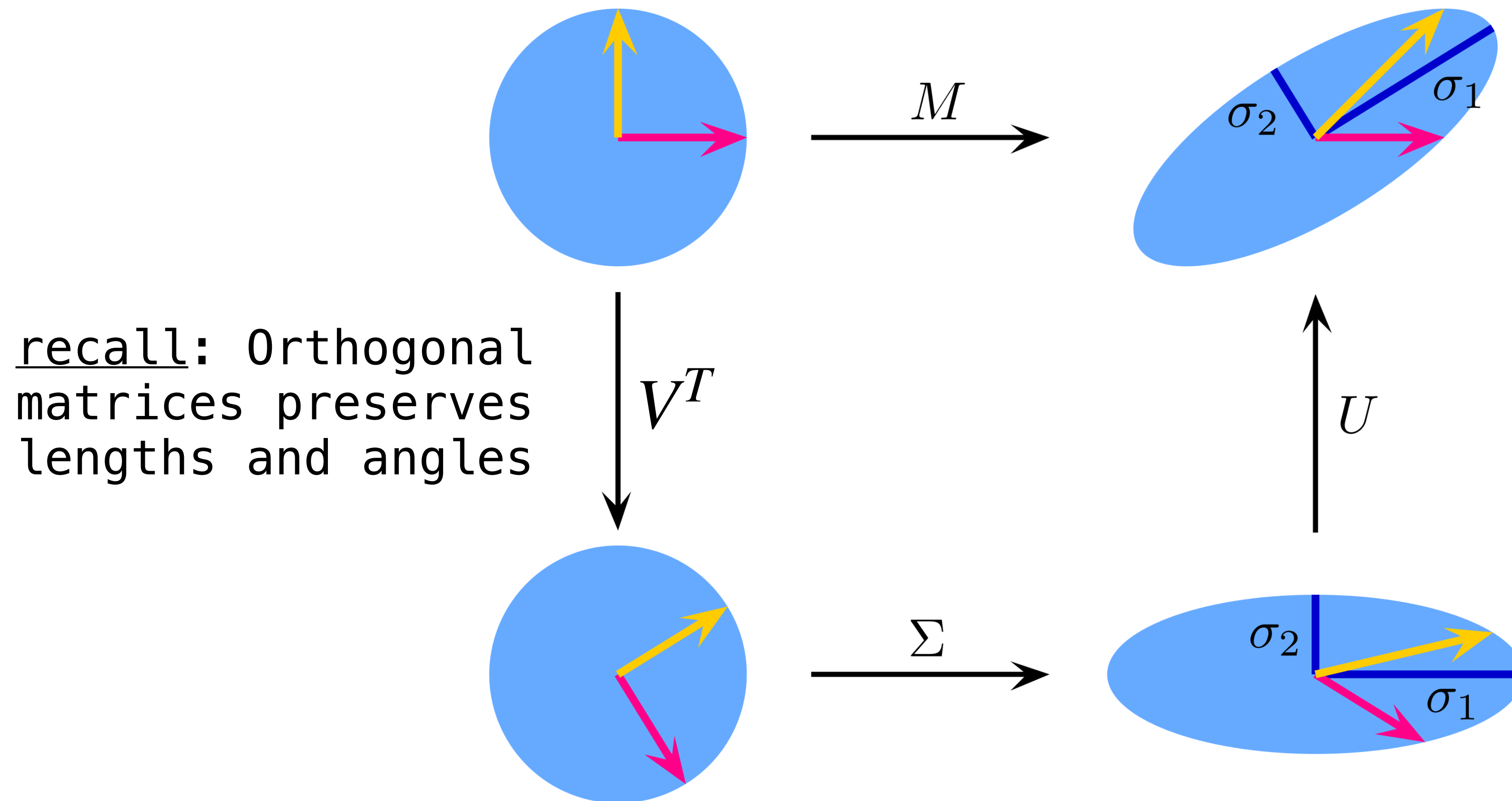
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» So if we take $\mathbf{u}_i = \frac{A\mathbf{v}_i}{\|A\mathbf{v}_i\|}$, we get an **orthonormal** basis of $\text{Col}(A)$

» And we can extend this to $\mathbf{u}_1, \dots, \mathbf{u}_m$ an orthonormal basis of \mathbb{R}^m (via Gram-Schmidt).

High Level View of the Decomposition



$$M = U \cdot \Sigma \cdot V^T$$

The Important Equality

$$\mathbf{u}_i = \frac{A\mathbf{v}_i}{\|A\mathbf{v}_i\|}$$

$$A\mathbf{v}_i = \|A\mathbf{v}_i\|\mathbf{u}_i = \sigma_i\mathbf{u}_i$$

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Remember that $\sigma_i = \sqrt{\lambda_i}$ is the singular value, which is the length $\|A\mathbf{v}_i\|$.

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What happens when we write this in matrix form?

The Important Equality

$$A[\mathbf{v}_1 \ \dots \ \mathbf{v}_n] = [\sigma_1 \mathbf{u}_1 \ \dots \ \sigma_n \mathbf{u}_n]$$

Remember that $\sigma_i = \sqrt{\lambda_i}$ is the singular value, which is the length $\|A\mathbf{v}_i\|$.

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$$A[\mathbf{v}_1 \ \dots \ \mathbf{v}_n] = [\sigma_1 \mathbf{u}_1 \ \dots \ \sigma_n \mathbf{u}_n]$$

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The Important Equality

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$$\Sigma = \begin{matrix} m > n \\ \begin{bmatrix} \sigma_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_n \\ 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix} \end{matrix} \text{ or } \Sigma = \begin{matrix} m < n \\ \begin{bmatrix} \sigma_1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_m & 0 & \dots & 0 \end{bmatrix} \end{matrix} \text{ or } \Sigma = \begin{matrix} m = n \\ \begin{bmatrix} \sigma_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_n \end{bmatrix} \end{matrix}$$

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The Important Equality

$$AV = U\Sigma$$

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The Important Equality

$$\begin{matrix} m \times n & & m \times m \\ A & V & = & U & \Sigma \\ n \times n & & & m \times n \end{matrix}$$

Remember that $\sigma_i = \sqrt{\lambda_i}$ is the singular value, which is the length $\|A\mathbf{v}_i\|$.

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

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

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singular value decomposition

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Singular Value Decomposition

Theorem. For a $m \times n$ matrix A , there are *orthogonal* matrices $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ such that

$$A = \overset{m \times m}{U} \underset{m \times n}{\Sigma} \overset{n \times n}{V^T}$$

where diagonal entries* of Σ are $\sigma_1, \dots, \sigma_n$ the singular values of A .

* these are diagonal entries in a non-square matrix.

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Theorem. For a $m \times n$ matrix A , there are *orthogonal* matrices $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ such that
left singular vectors *right singular vectors*

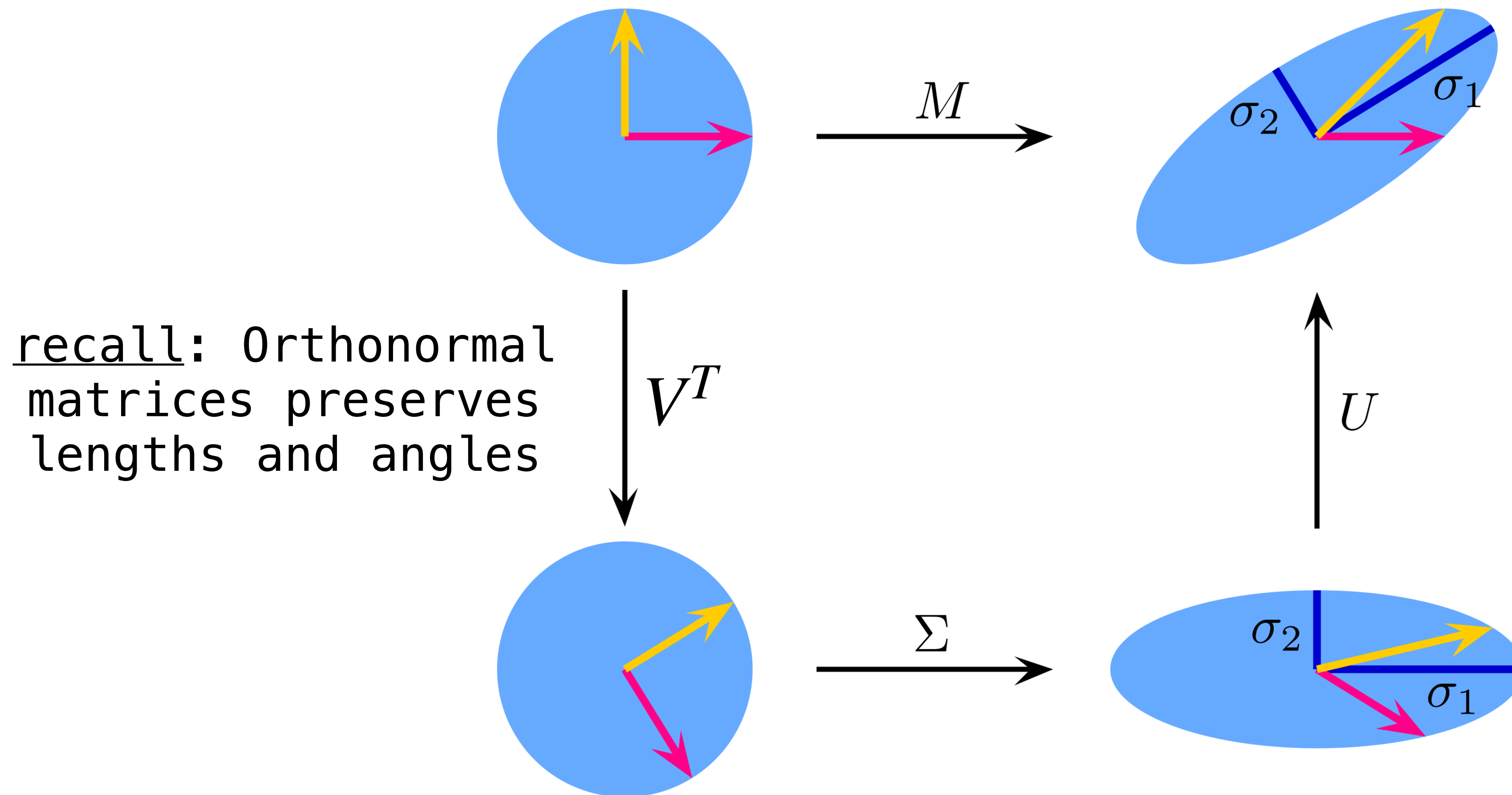
$$A = U \Sigma V^T$$

$m \times m$ $n \times n$
 $m \times n$

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The Picture (Again)



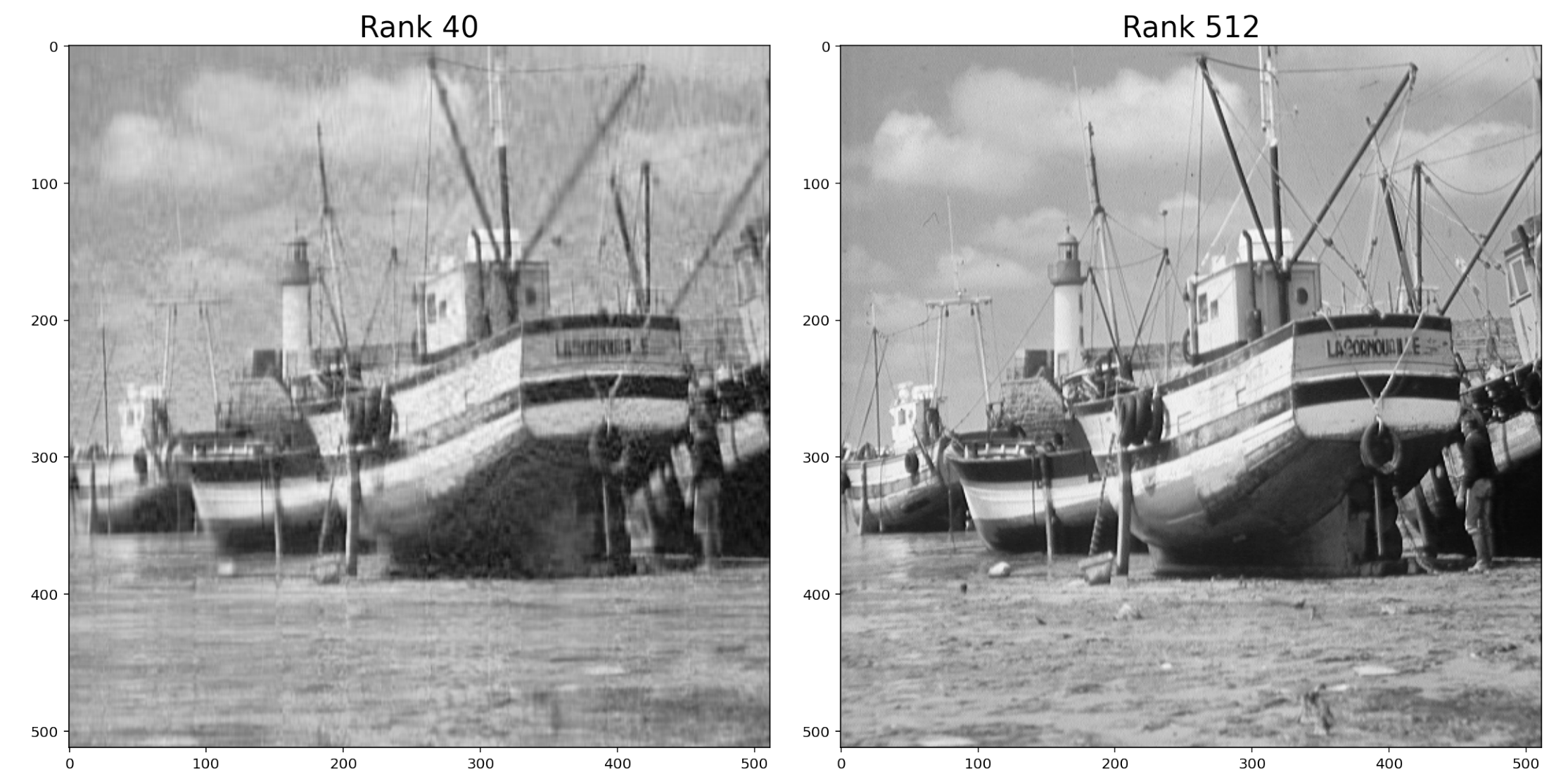
$$M = U \cdot \Sigma \cdot V^T$$

What's next?

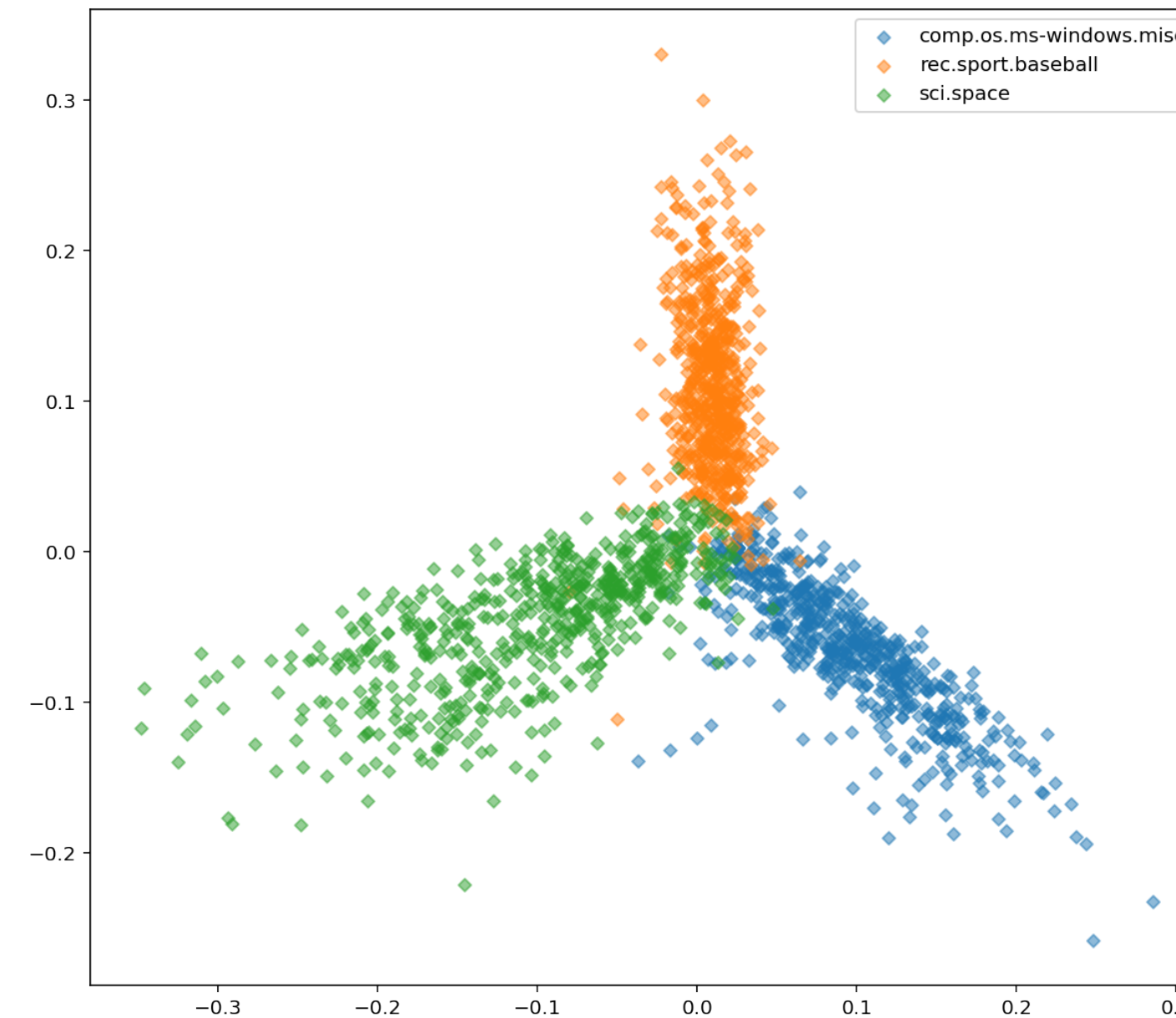
A couple final thoughts

Applications of SVD

image compression



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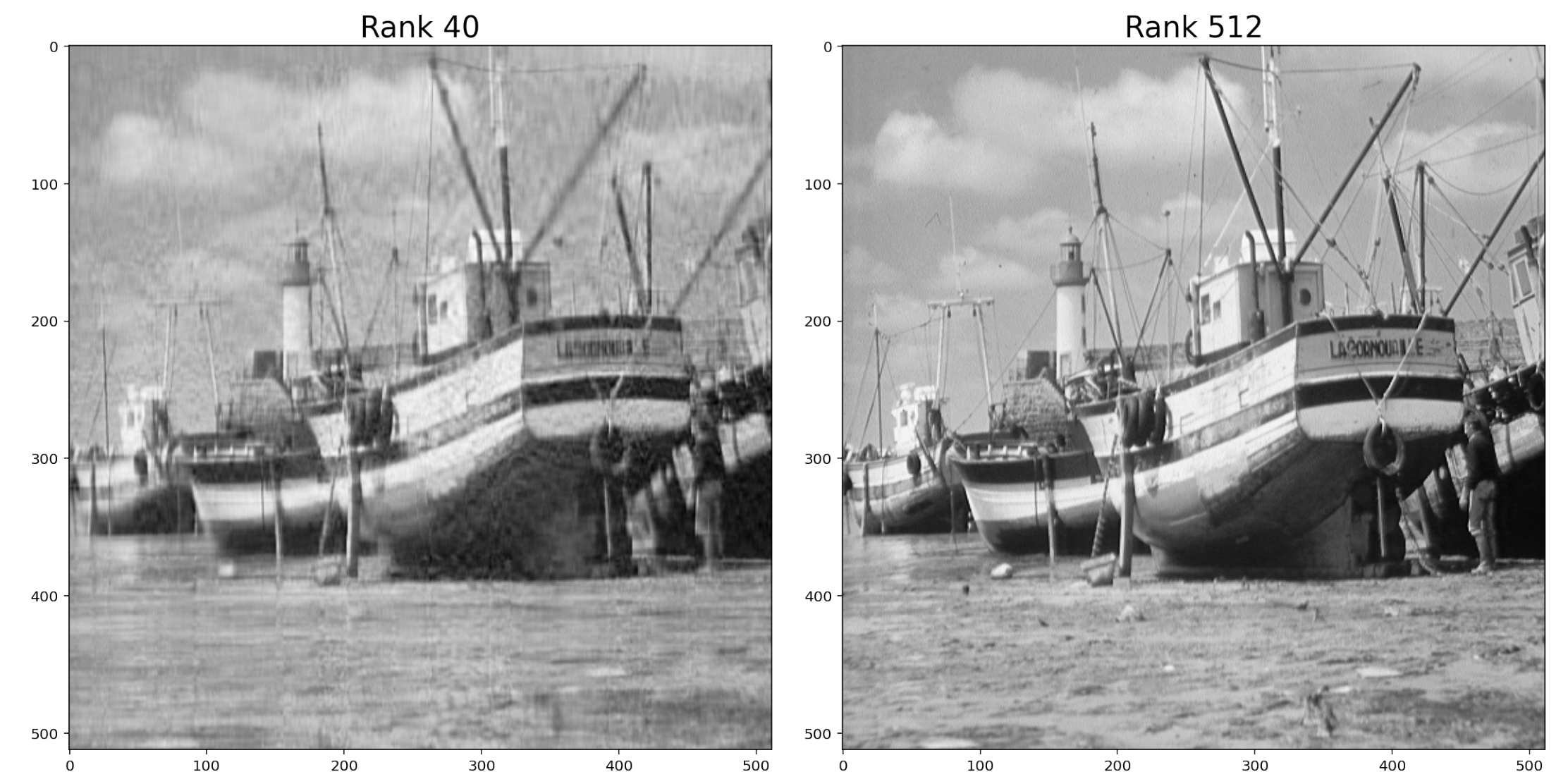


document
classification

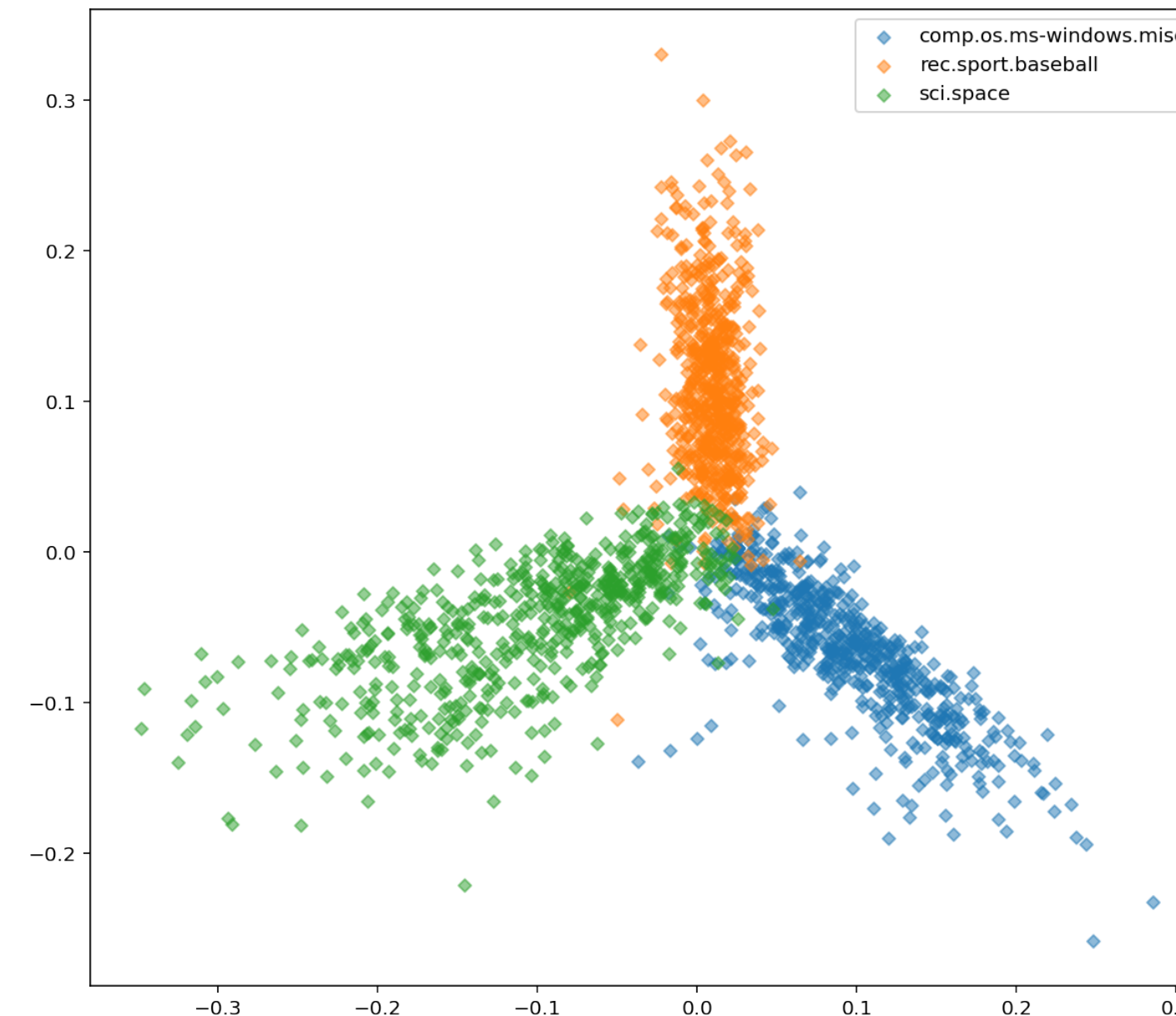
Applications of SVD

- Reduced SVD, pseudoinverses and least squares

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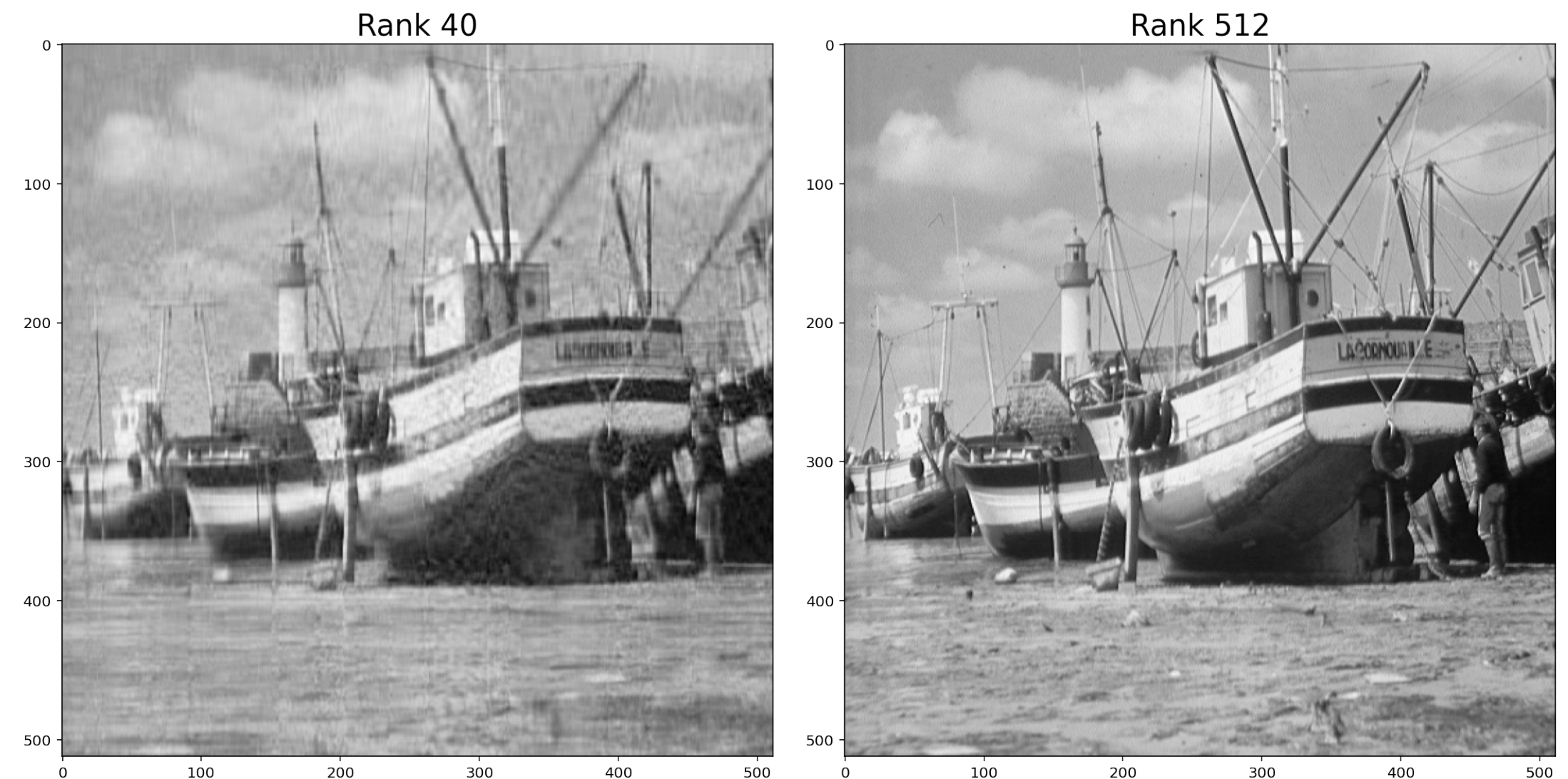


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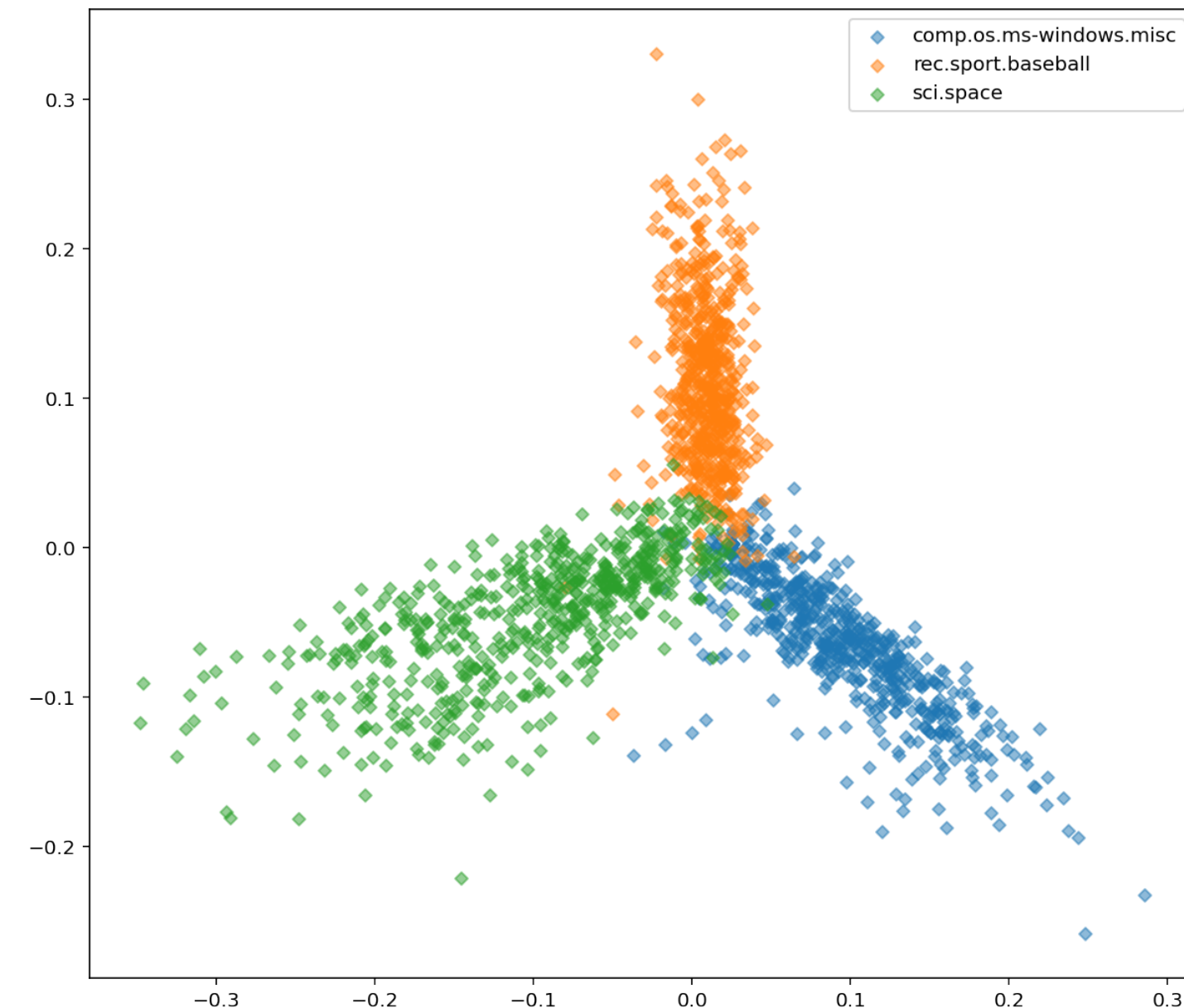
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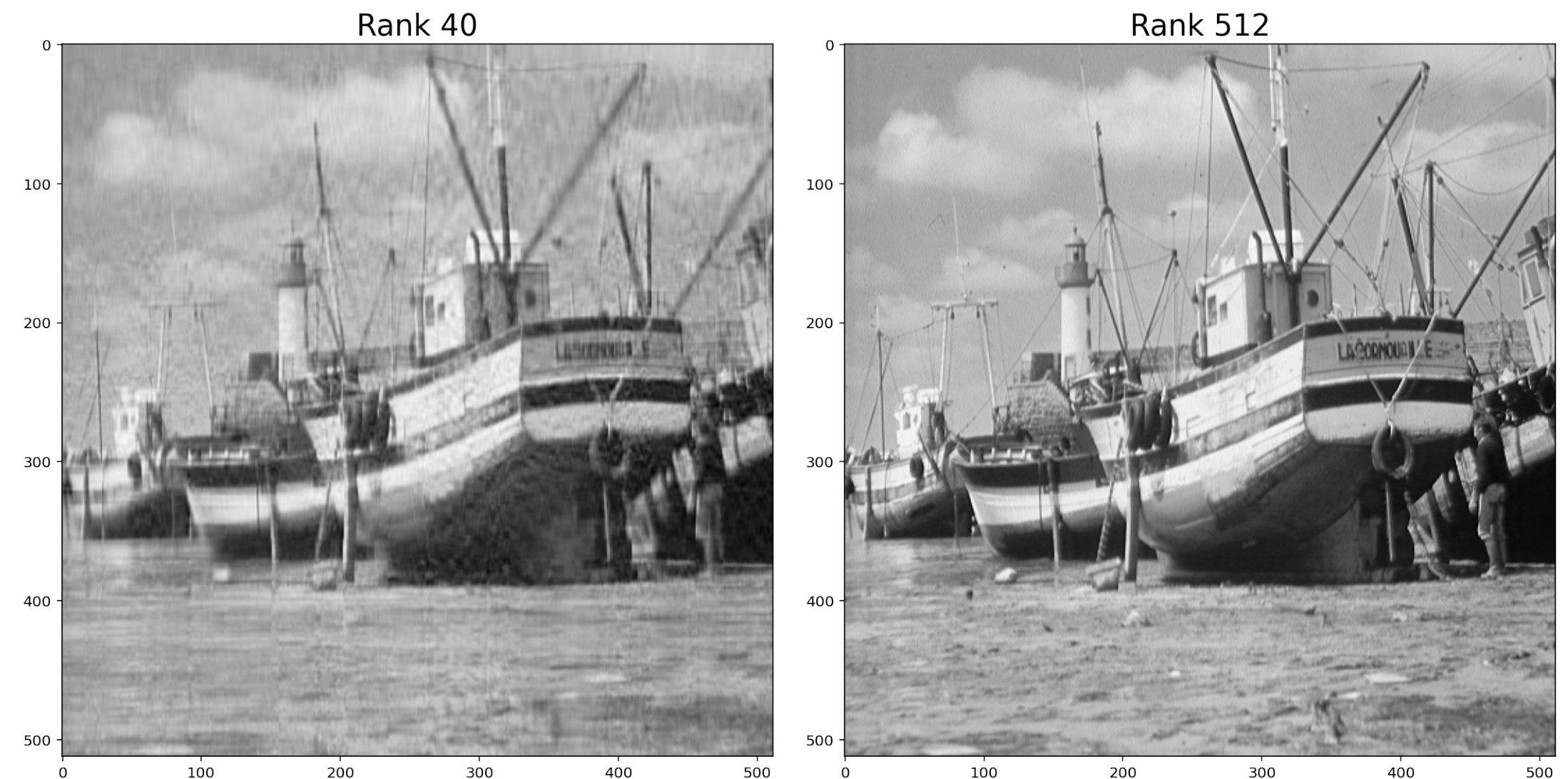


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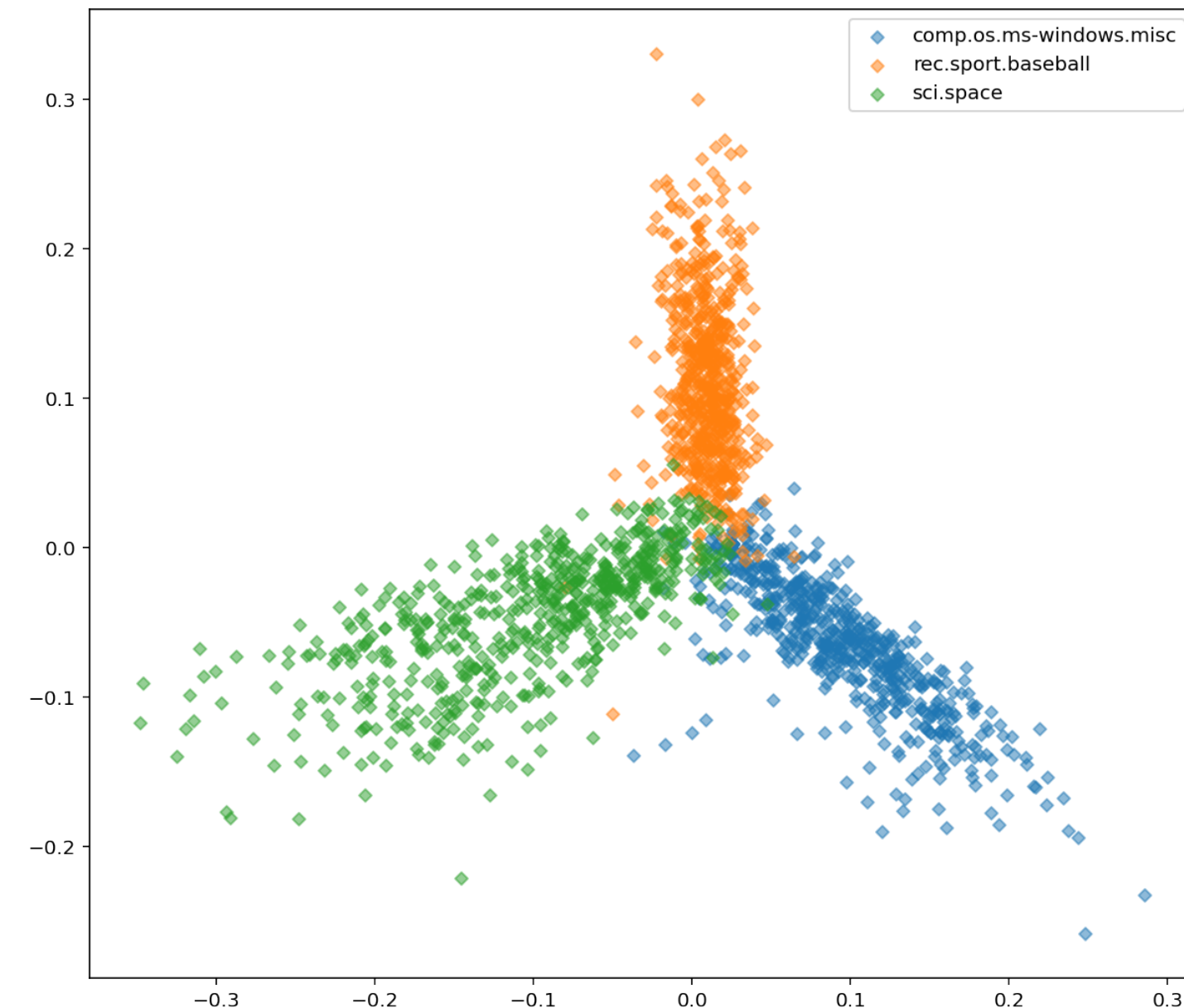
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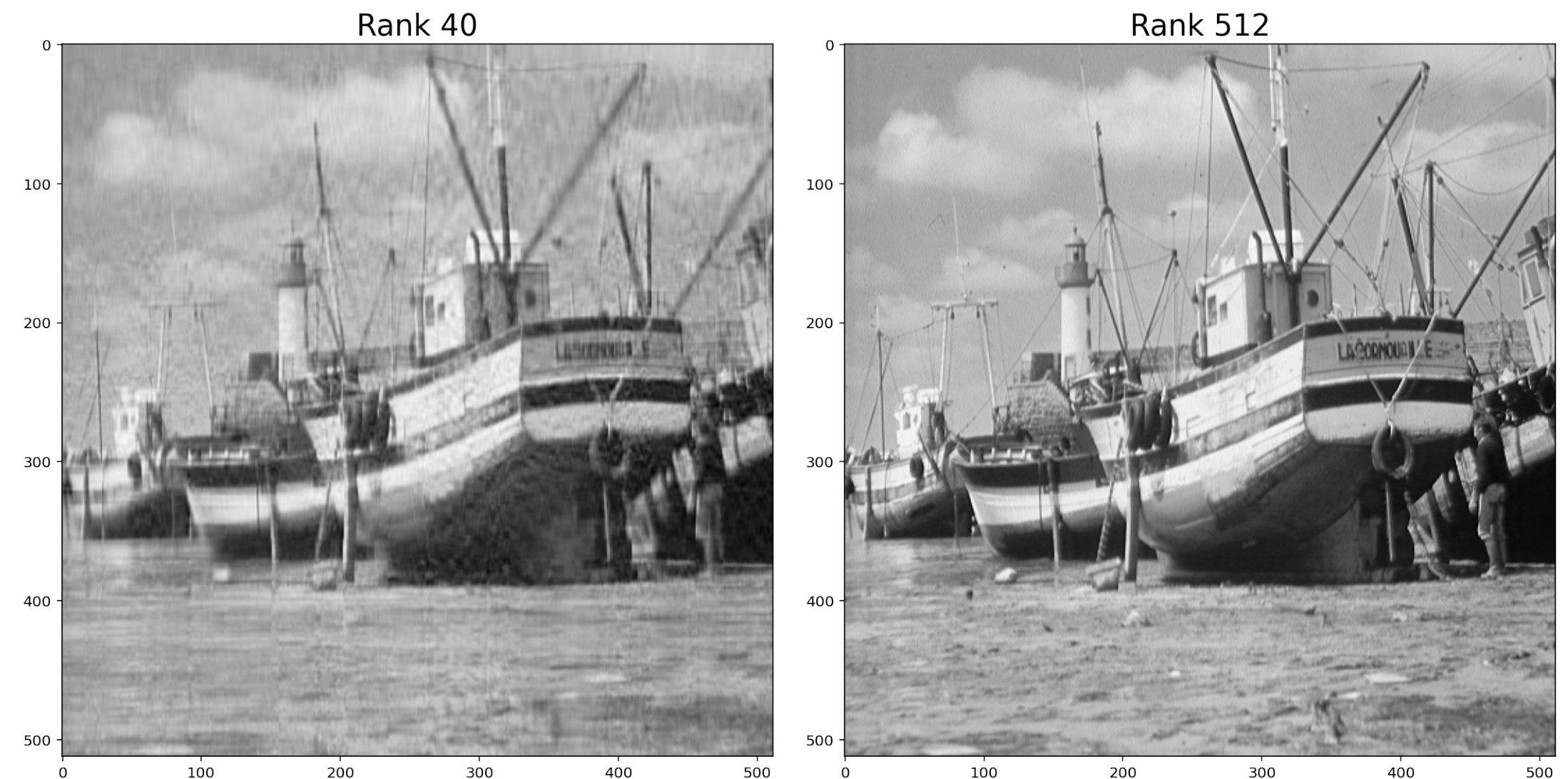


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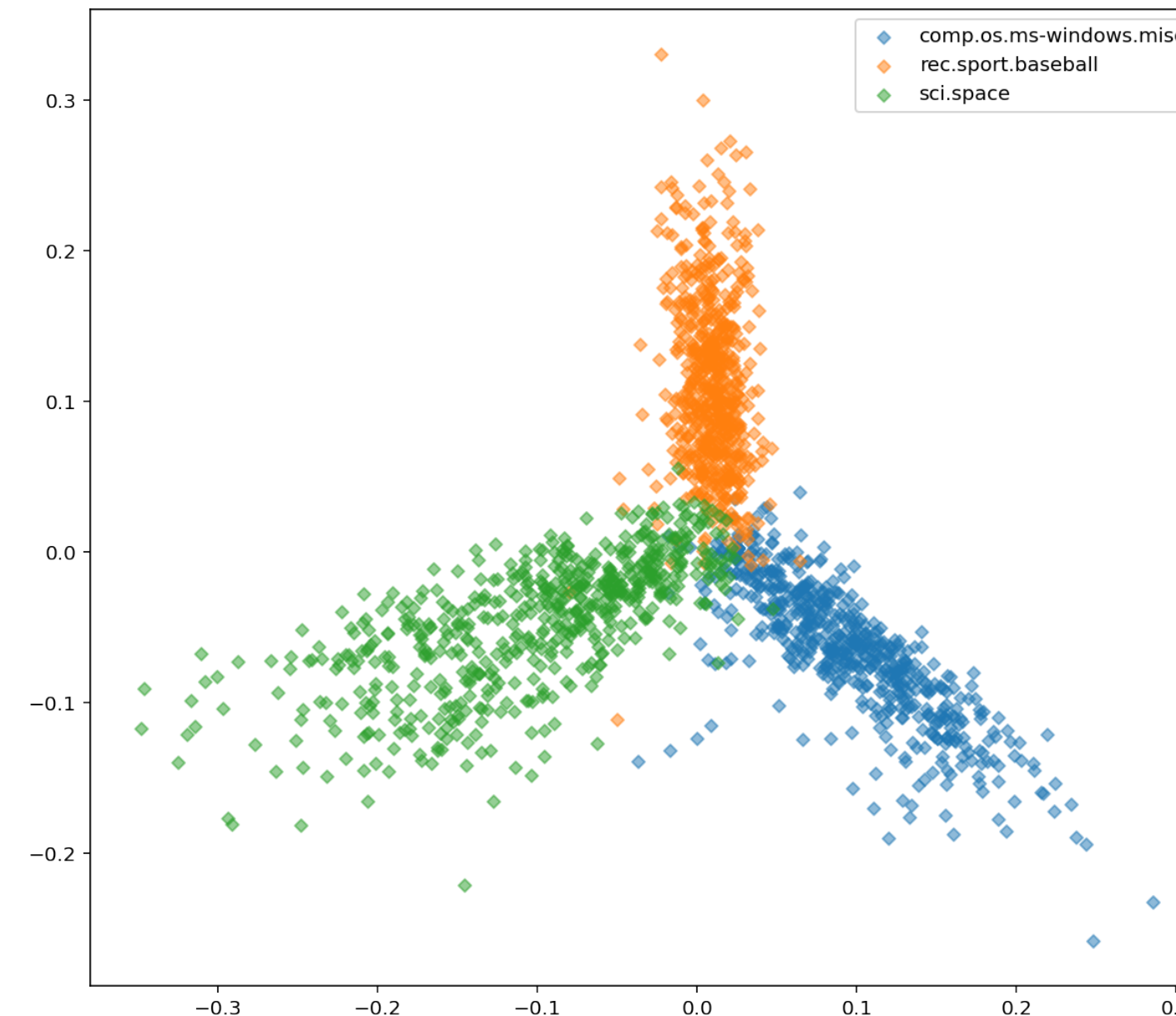
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image compression



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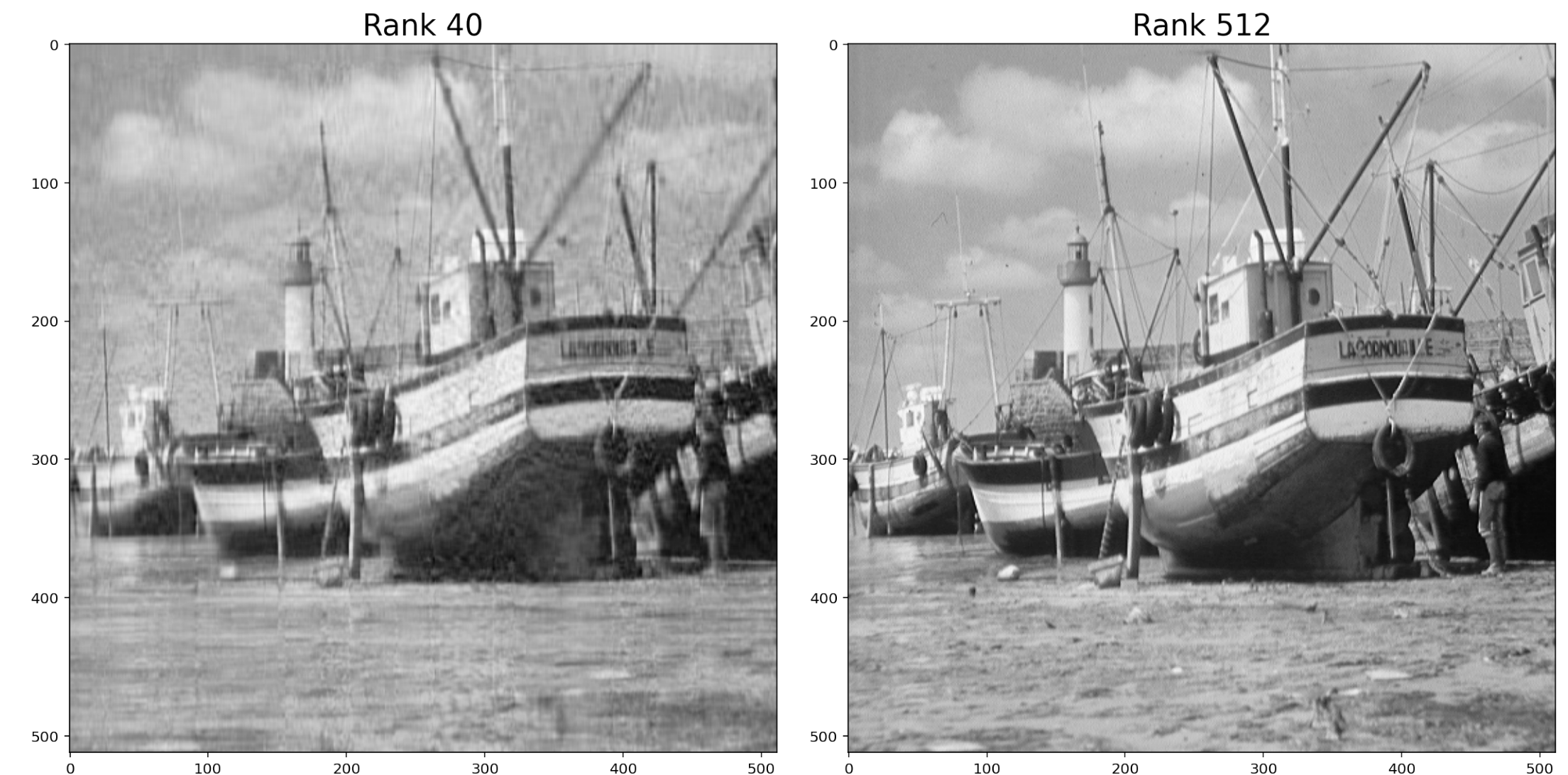


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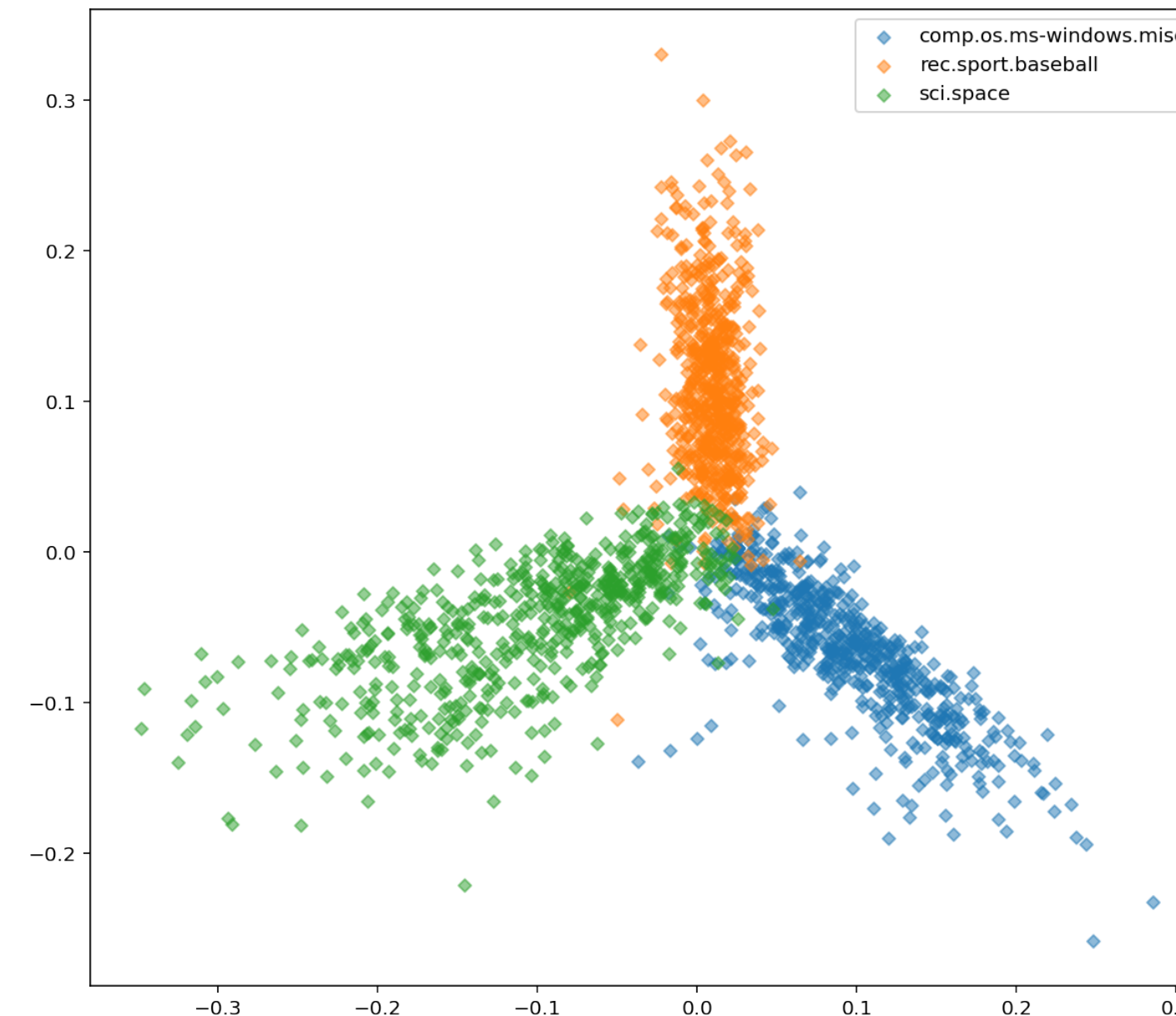
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image compression



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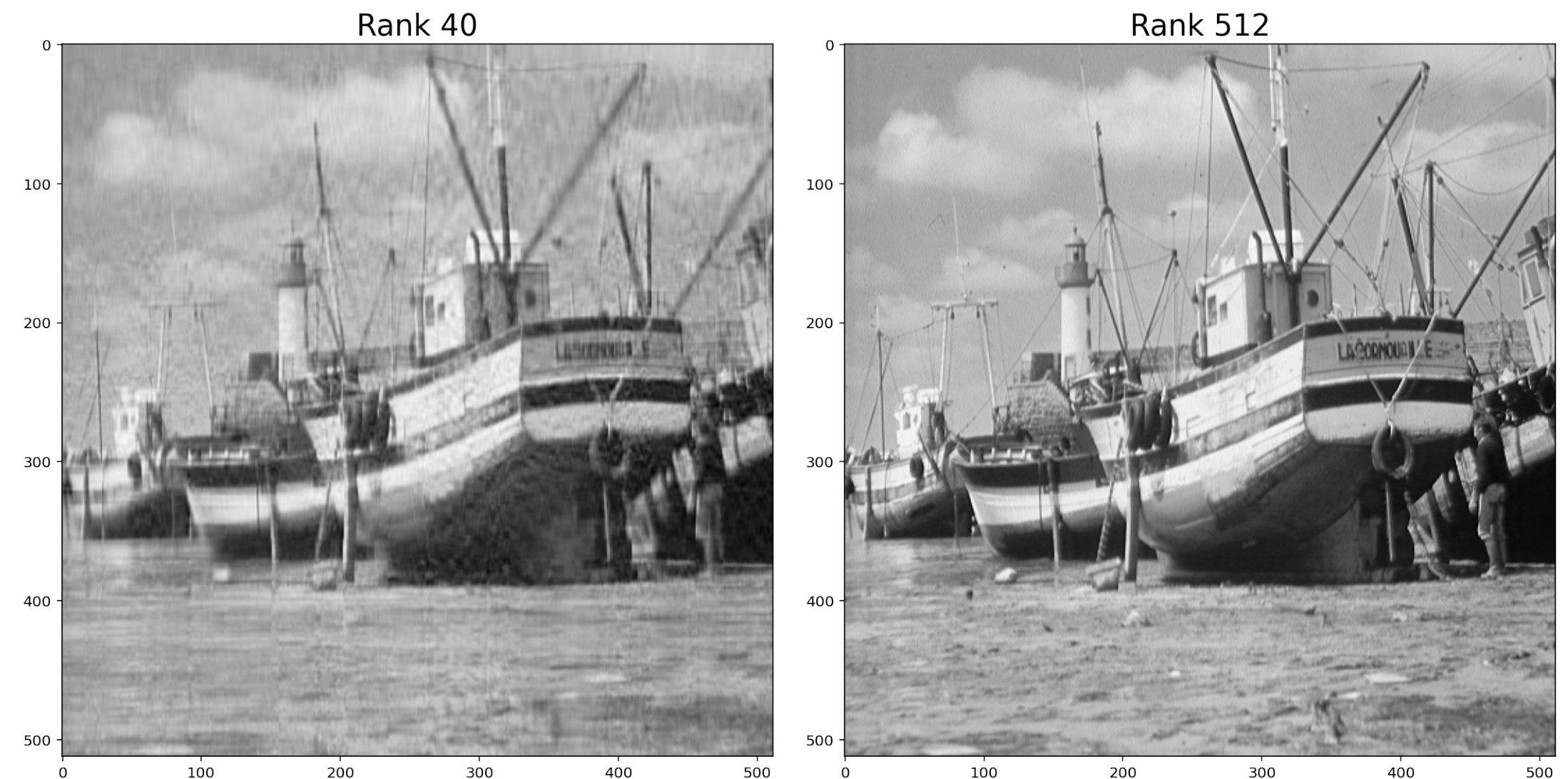


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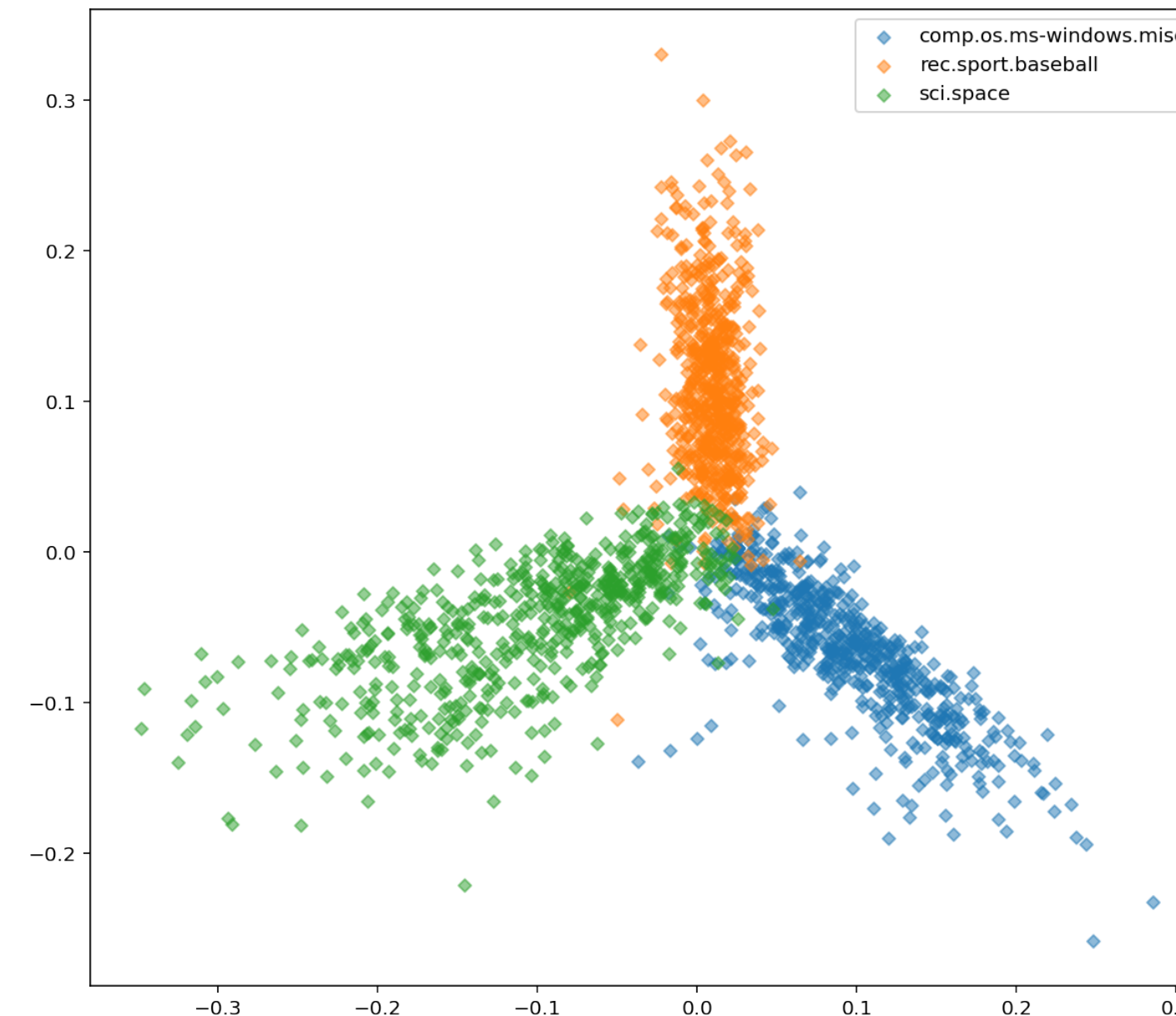
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image compression



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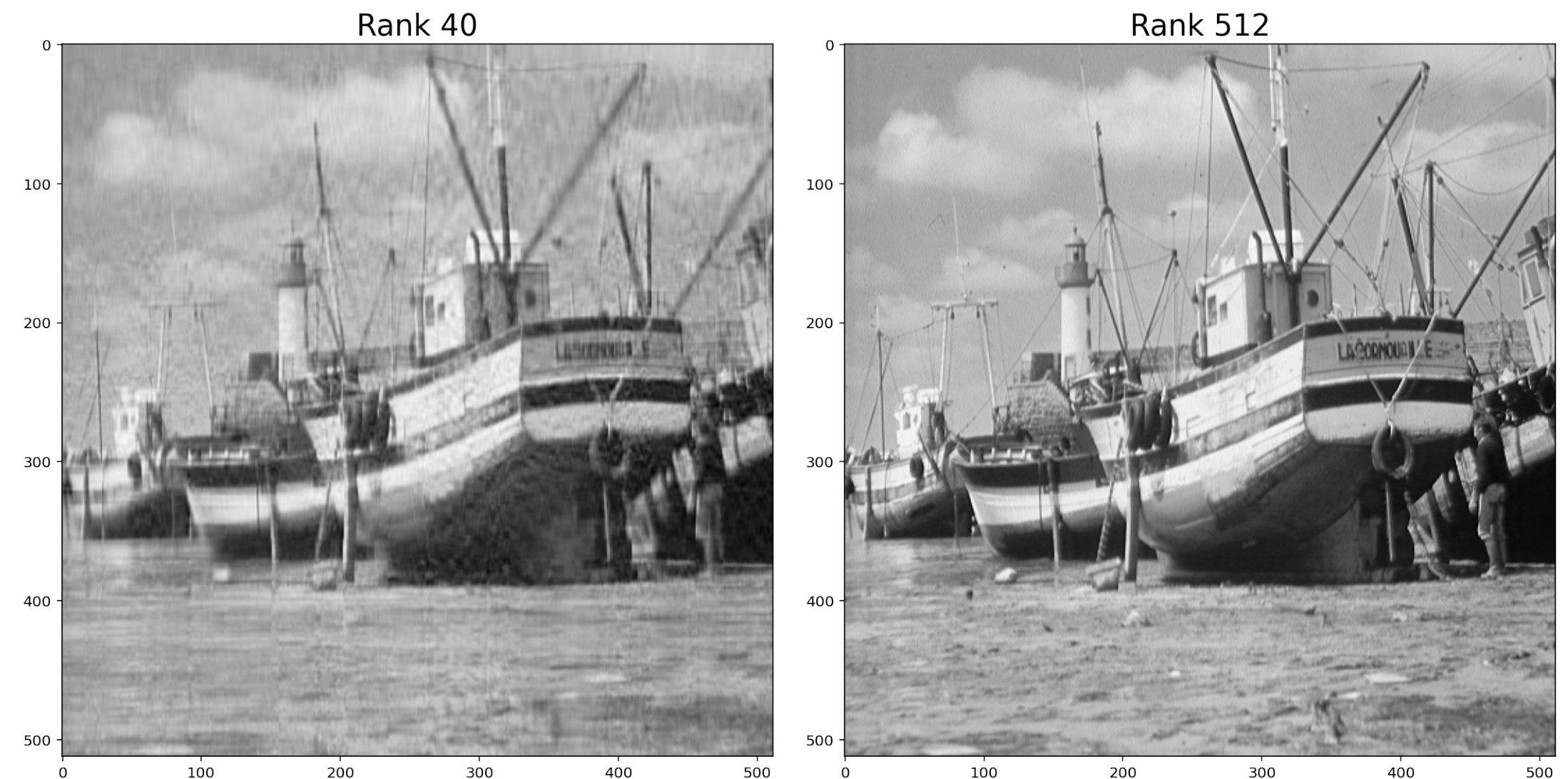


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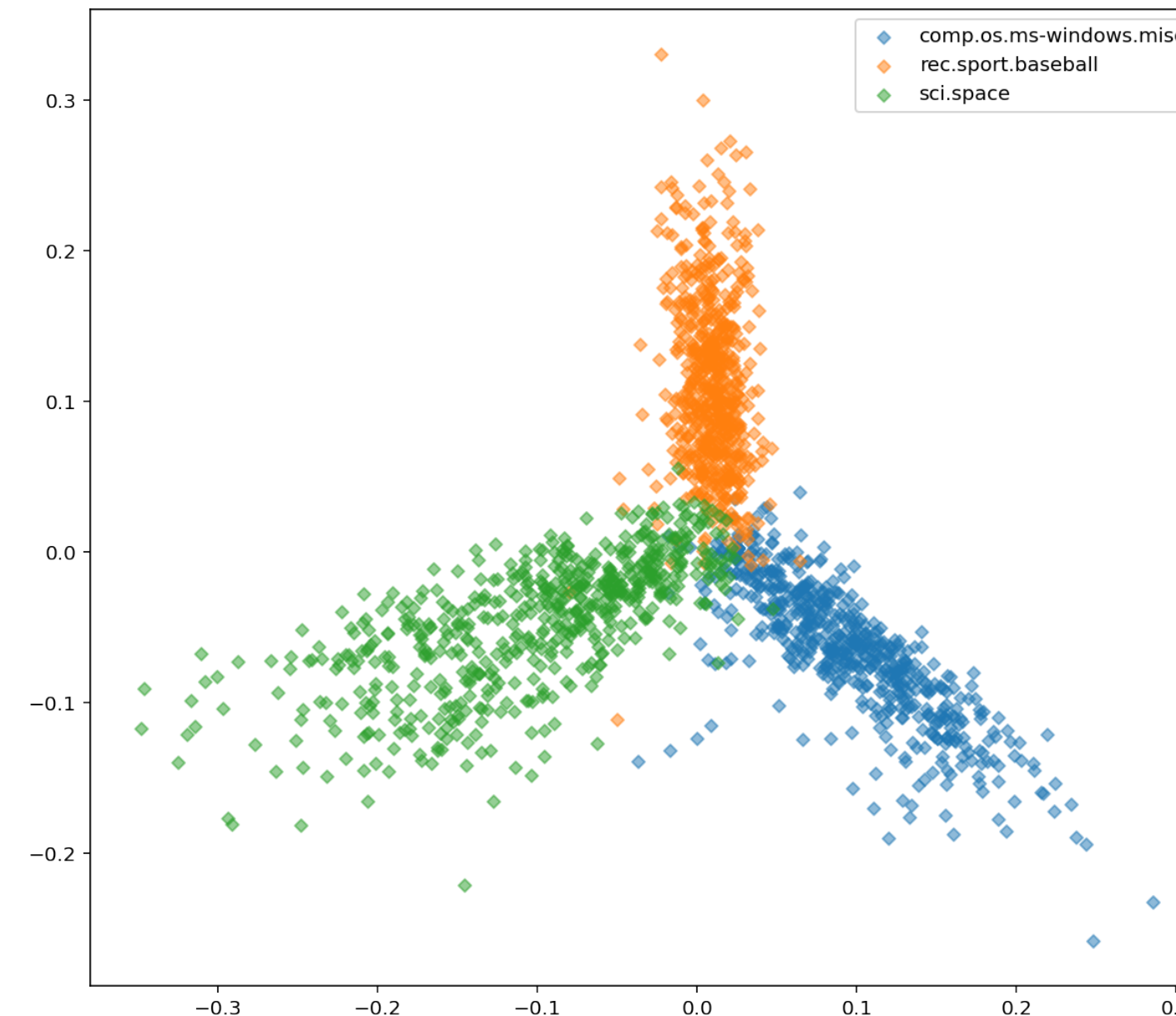
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- Principle Component Analysis
 - Large singular vectors are "most affected."

image compression



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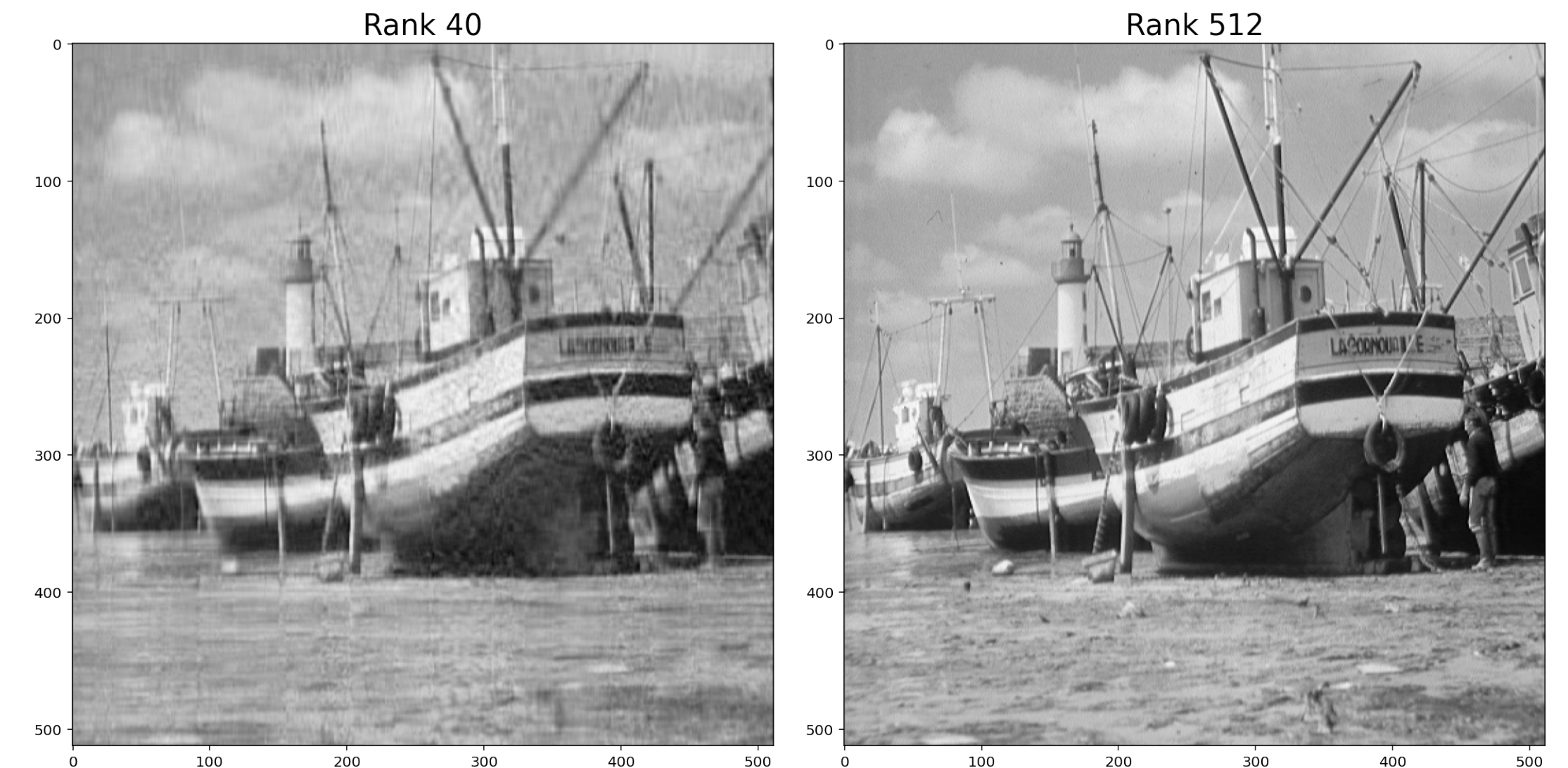


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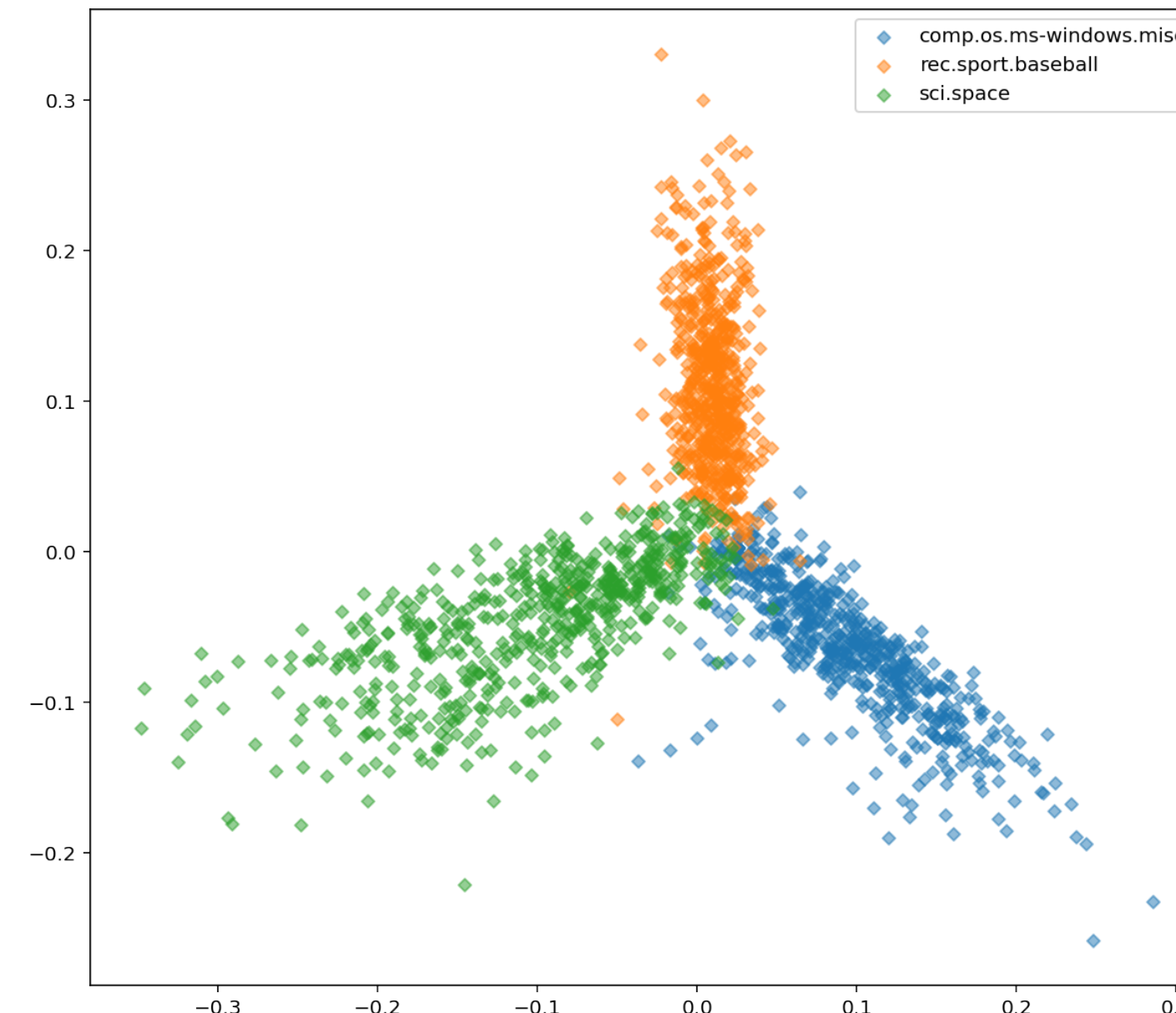
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 - Large singular vectors are "most affected."
 - These are good vectors to look at for classifying data

image compression

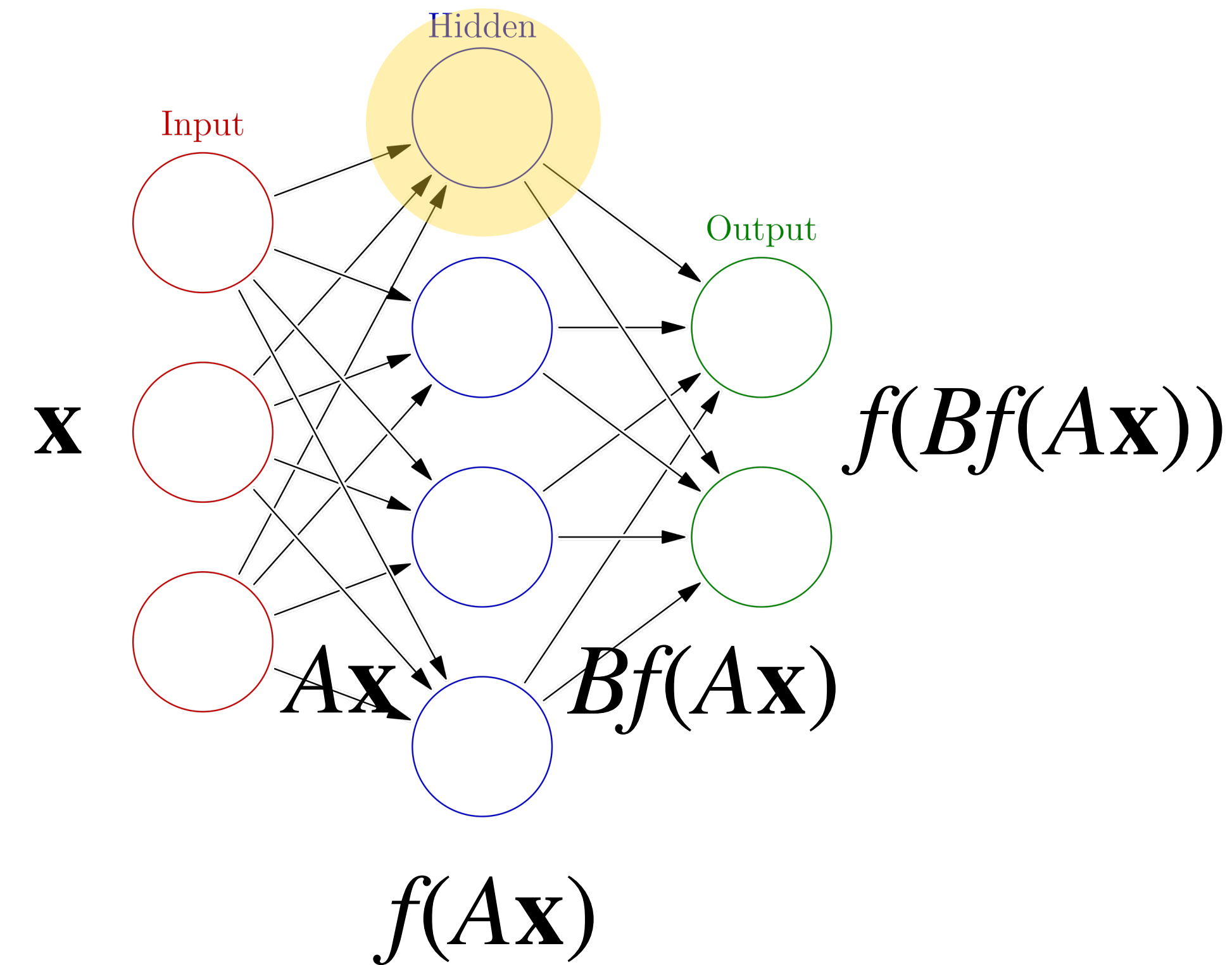
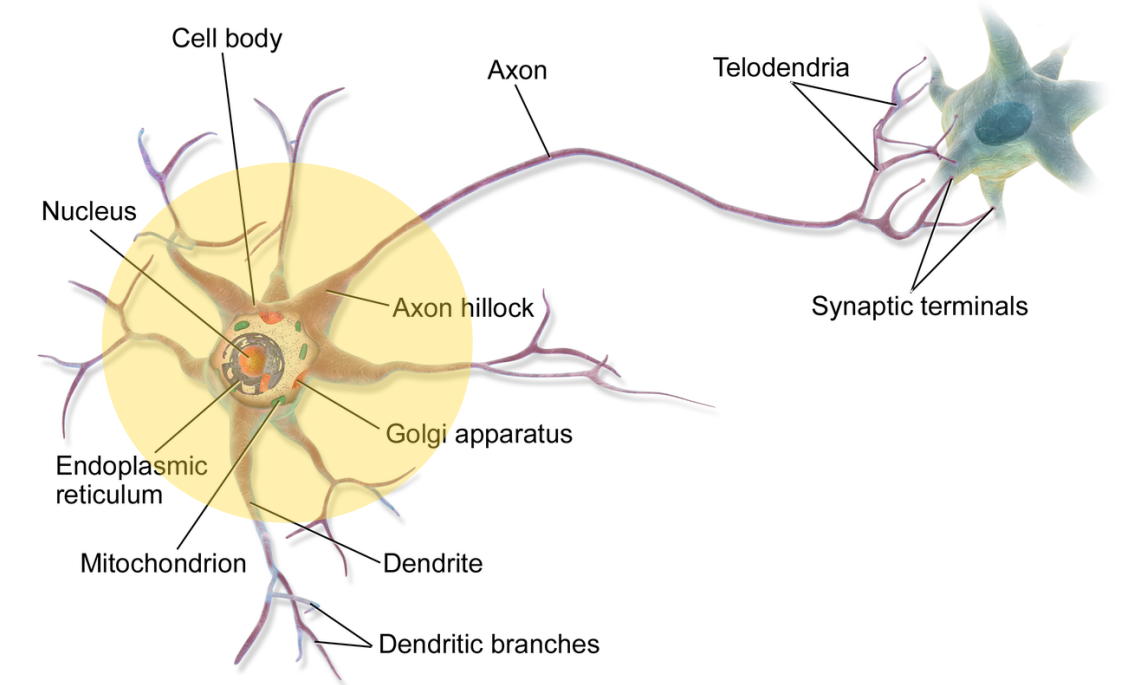


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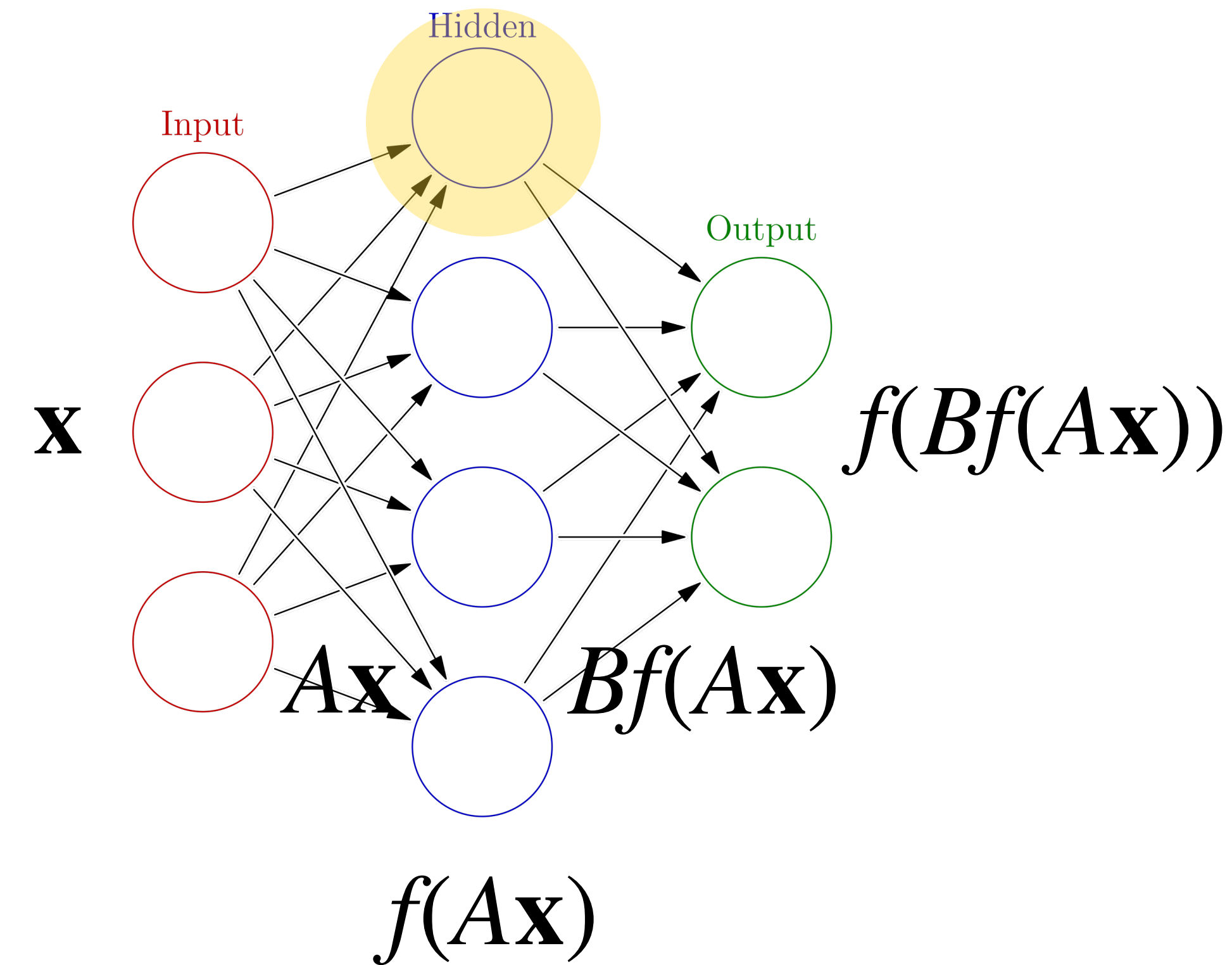
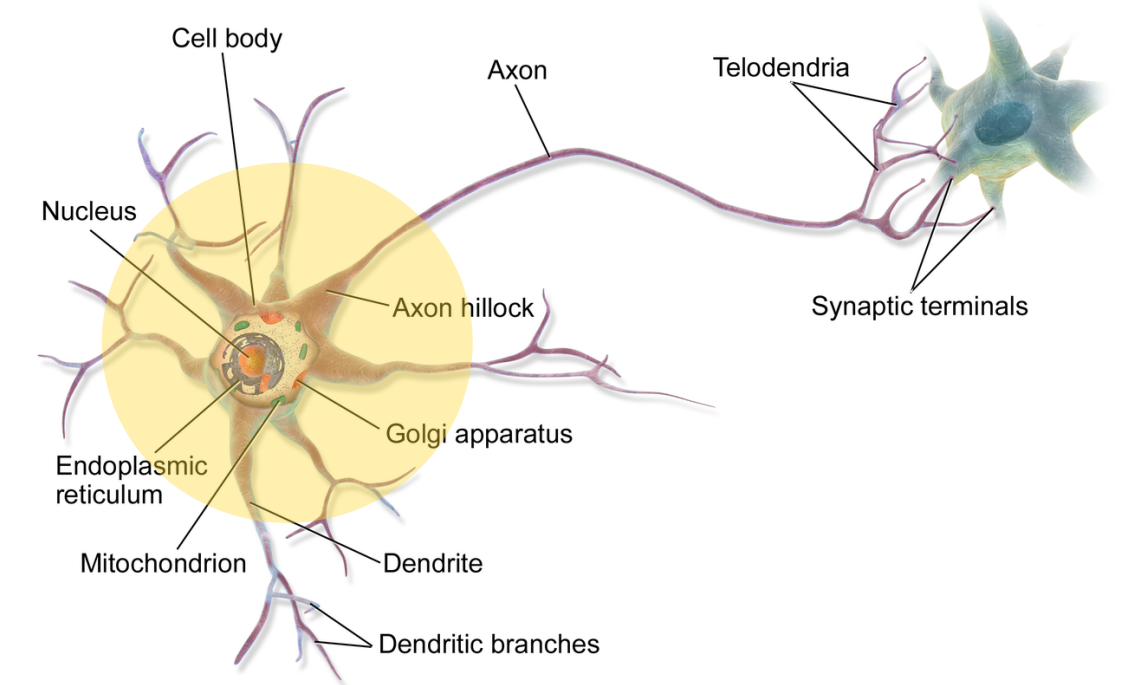
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Neural Networks (Non-Linearity)



Neural Networks (Non-Linearity)

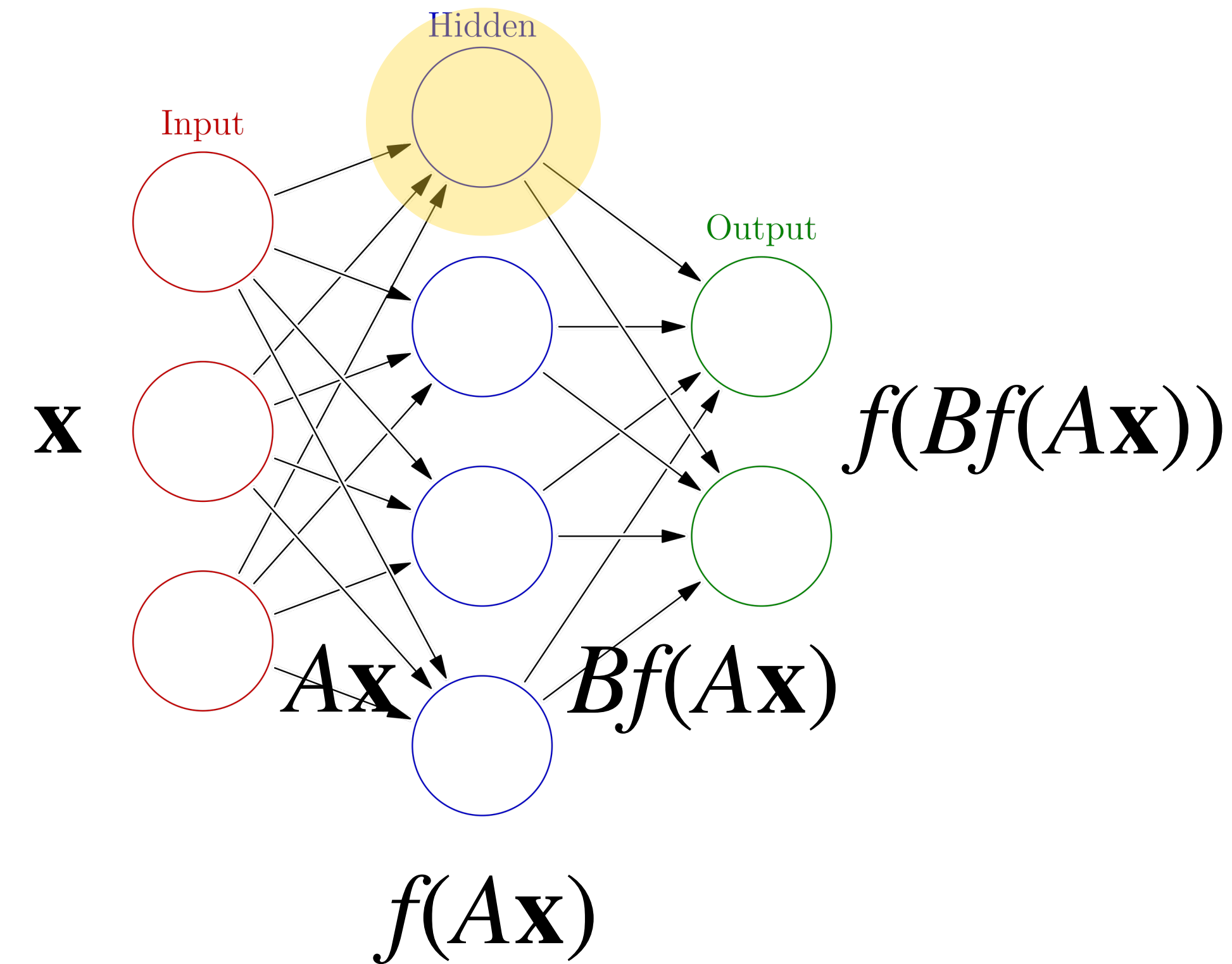
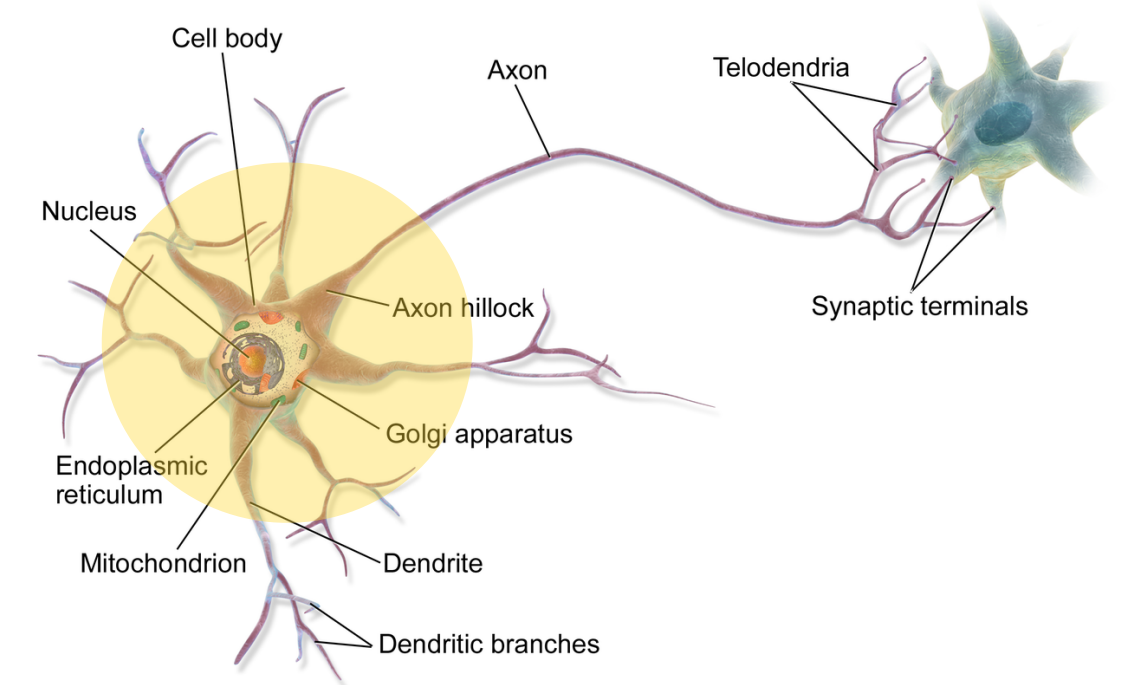
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Neural Networks (Non-Linearity)

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Given an input vector \mathbf{x} , it is transformed into a *hidden* vector $A\mathbf{x}$ by a linear transformation, and then an *activation function* f is applied to the result.

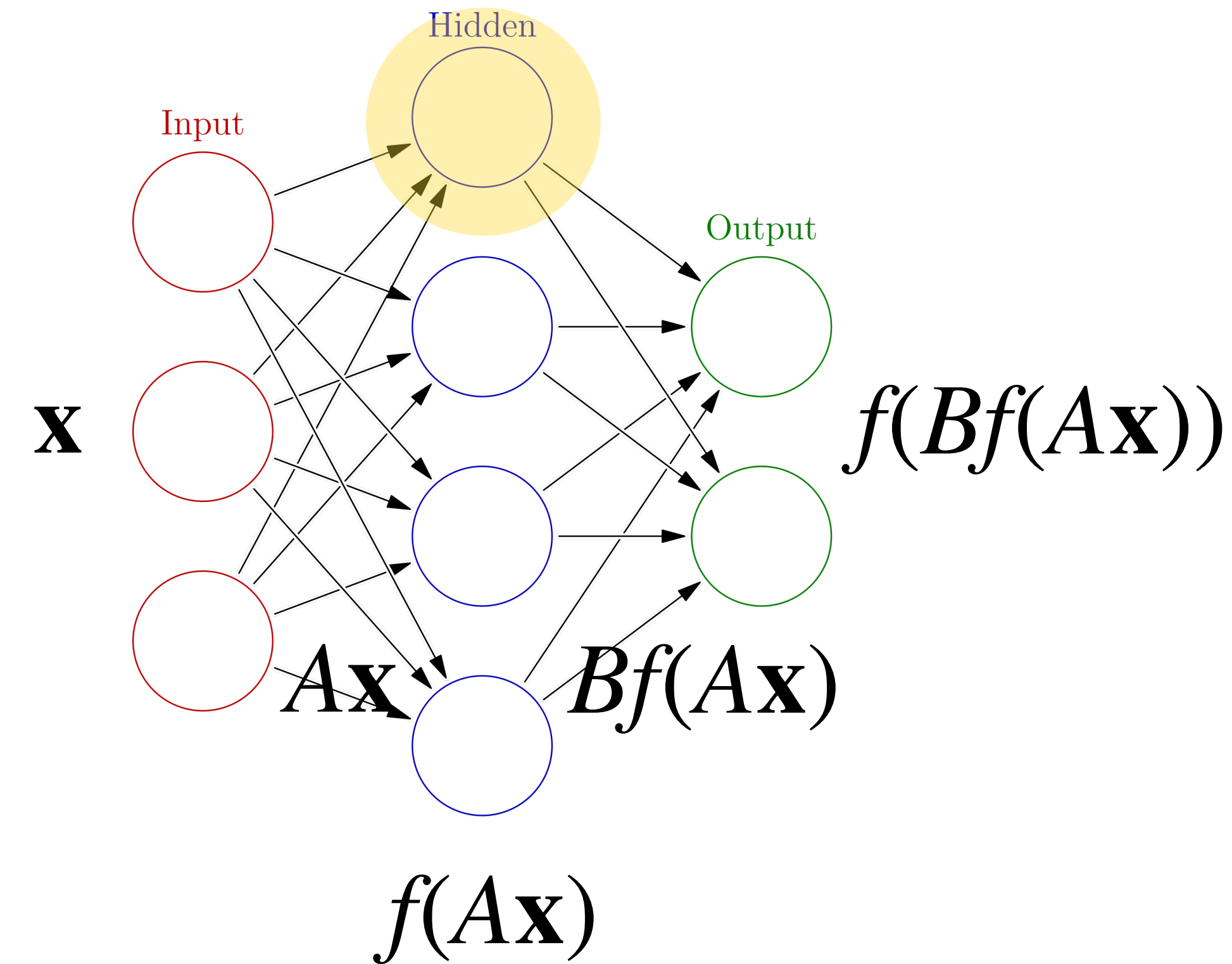
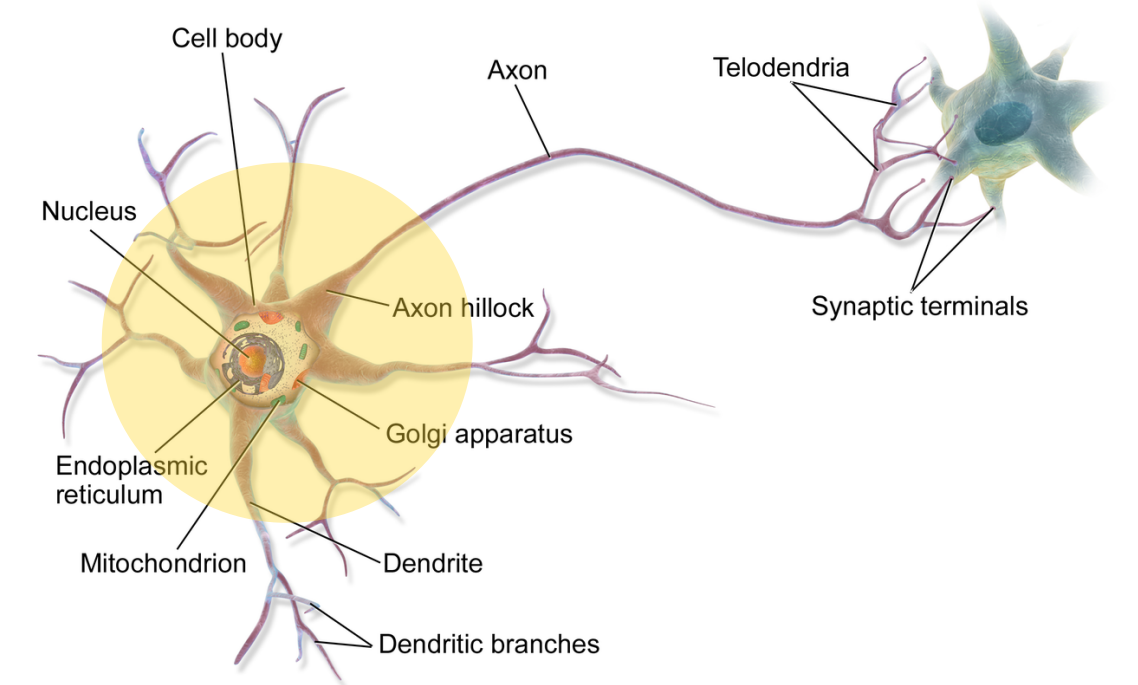


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Neural networks are just matrix multiplications with intermediate calls to a nonlinear function f .



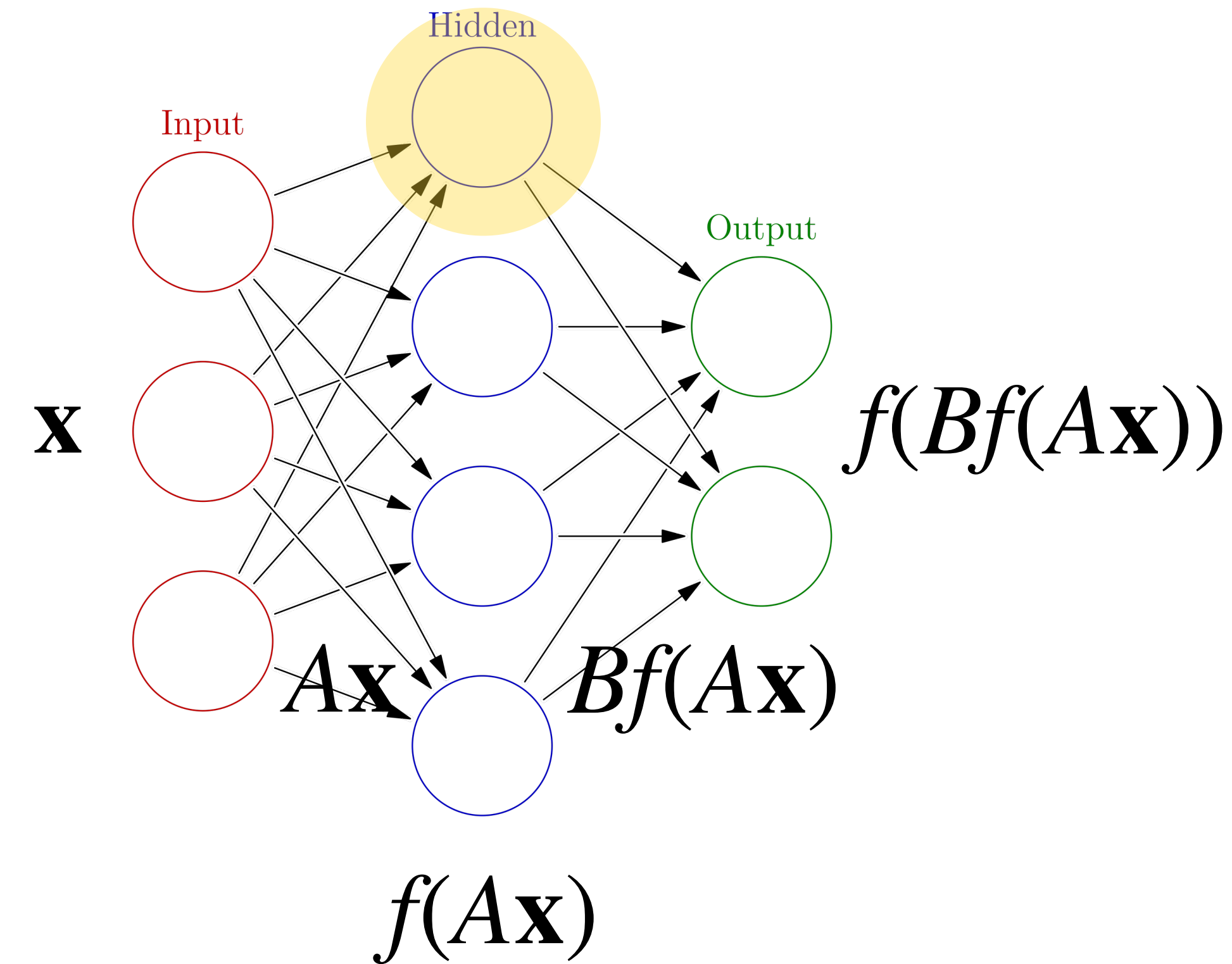
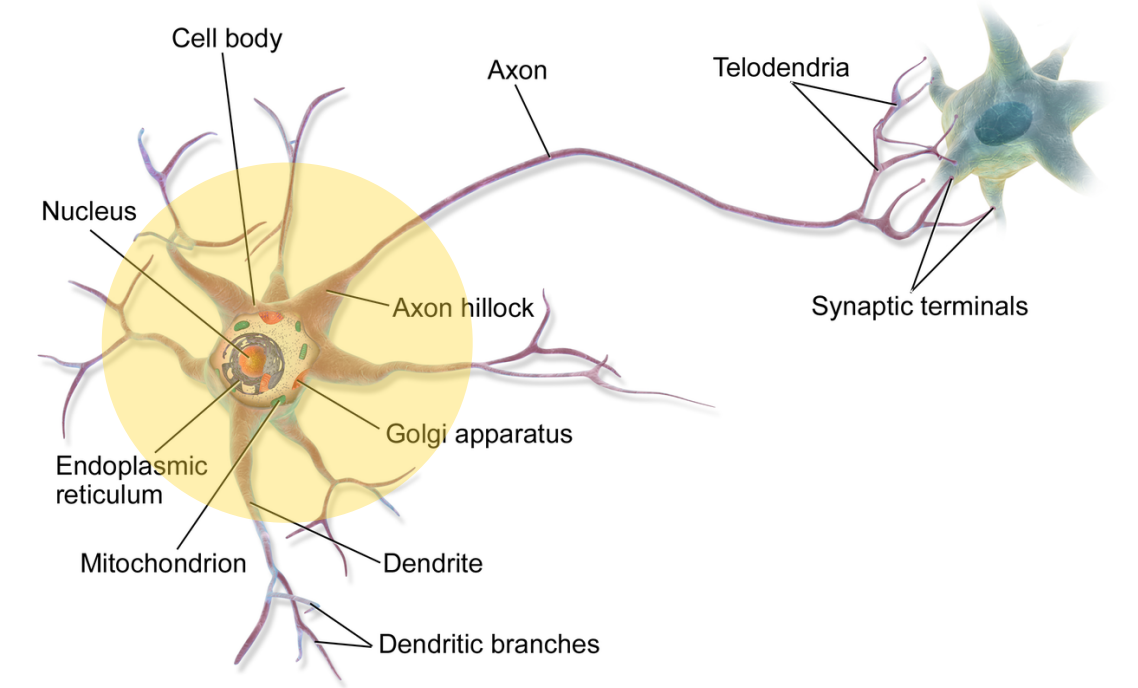
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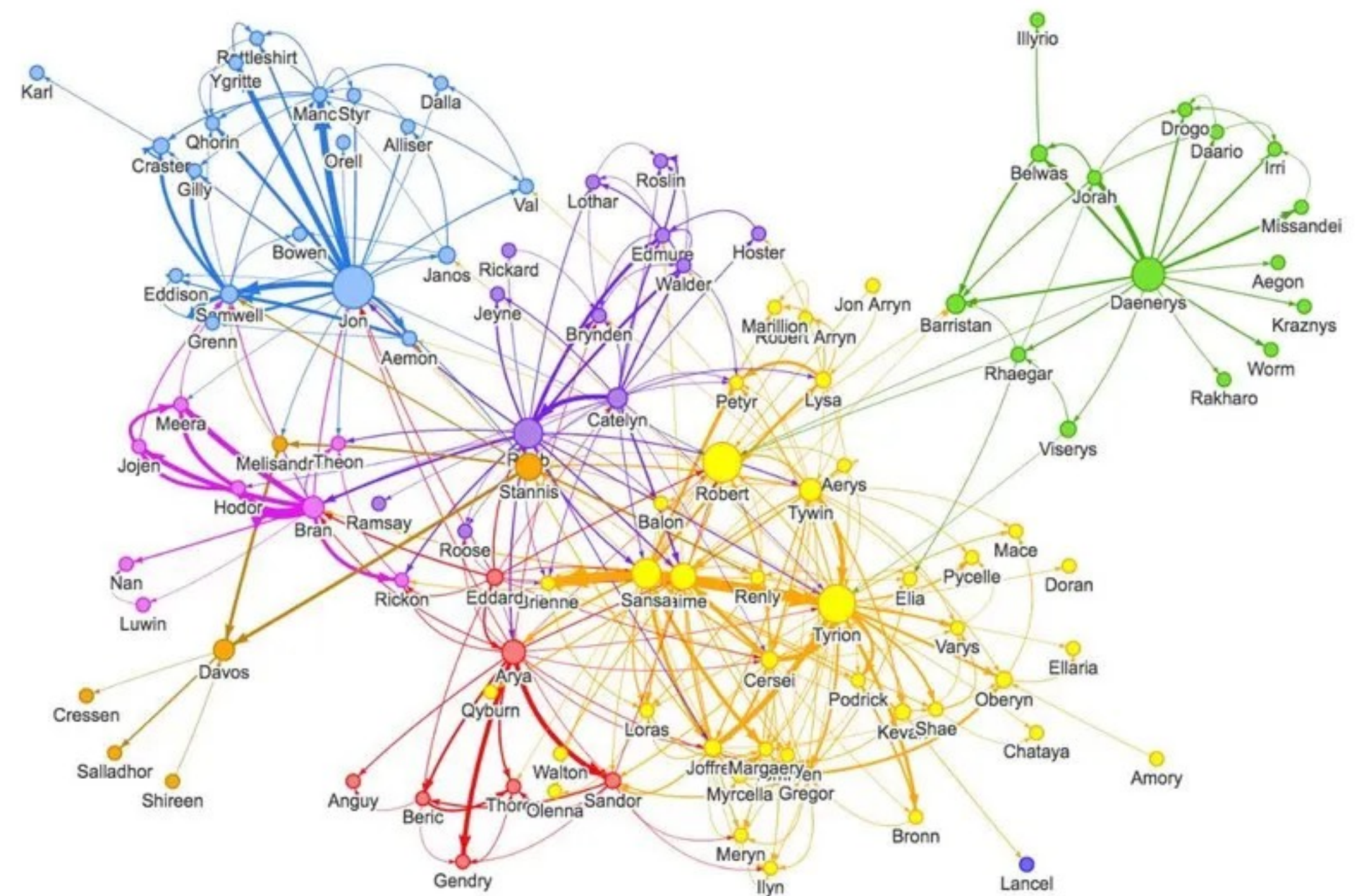
$$\text{NN}(\mathbf{x}) = f(A_k(f(A_{k-1} \dots f(A_1 \mathbf{x})))$$



Spectral/Algebraic Graph Theory

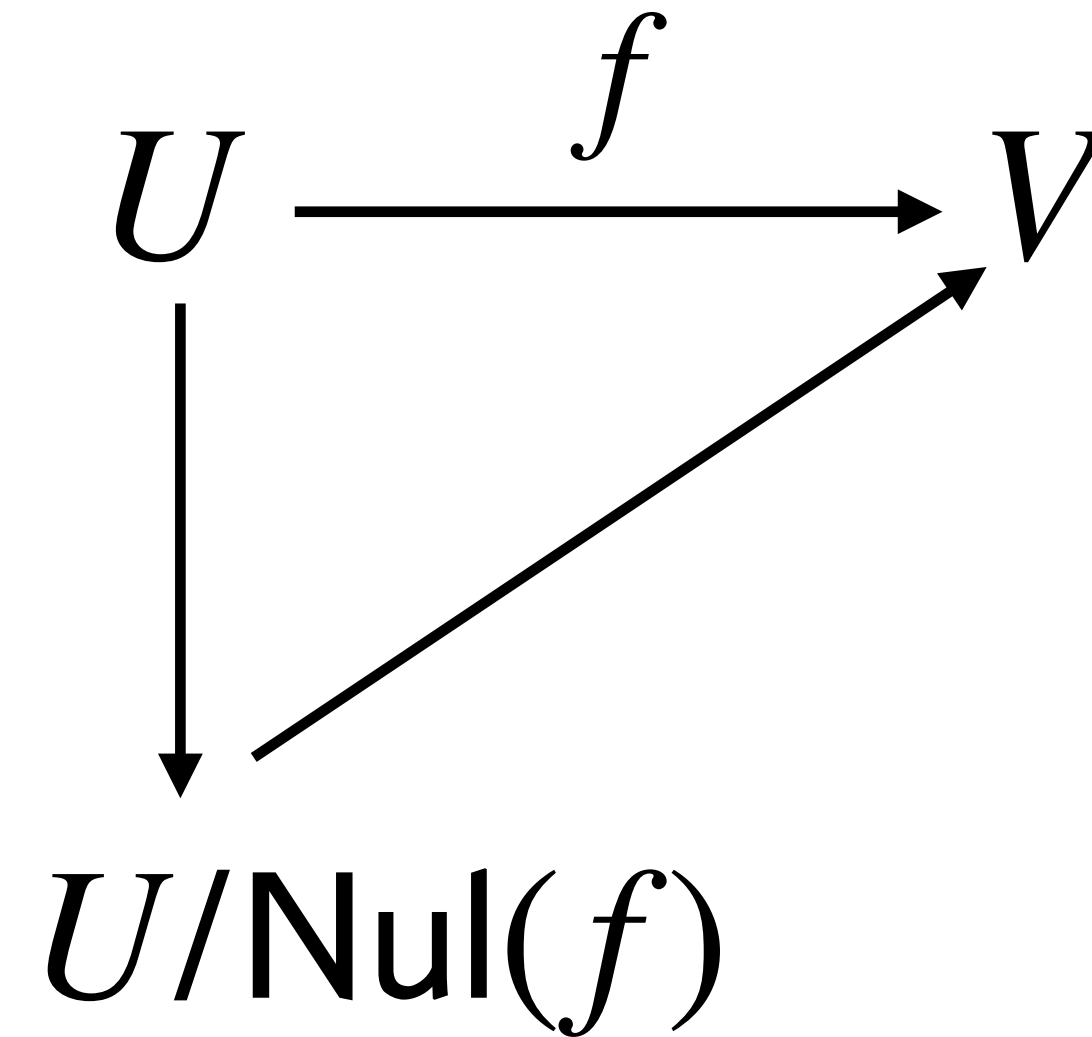
Graphs can be viewed as matrices.

The finding eigenvalues in graphs can give us better clustering and cutting algorithms.



Abstract Algebra

$$\frac{U}{\text{Nul}(f)} \cong \text{Range}(f)$$



There's a lot of beautiful structure in the algebra we've done in this course.

And there are lots of directions to go from here (infinite dimensional spaces, less restrictive settings like groups and modules,...)

Course List

- CS 365 Foundations of Data Science
- CS 440 Intro to Artificial Intelligence
- CS 480 Intro to Computer Graphics
- CS 505 Intro to Natural Language Processing
- CS 506 Tools for Data Science
- CS 507 Intro to Optimization in ML
- CS 523 Deep Learning
- CS 530 Advanced Algorithms
- CS 531 Advanced Optimization Algorithms
- CS 542 Machine Learning
- CS 565 Algorithmic Data Mining
- CS 581 Computational Fabrication
- CS 583 Audio Computation

Some of these may not exist anymore...

Appreciations

The Course Staff

I'd like to thank:

Rahul Mitra, Ryan Yu, Vishesh Jain, Jincheng Zhang, Reshab Chhabra, Rachel Du, Yi Du, Eugene Jung, Chris Min, Ieva Sagaitis, Aparna Singh, Kevin Wrenn

If you see them around you should thank them as well.

The CS Department Staff

If you're ever in the CS Department office, be kind to the people who work there. They work very hard to keep all our courses running.

The Students of CS132

Thanks for sticking with it.

For giving feedback.

For adjusting and re-adjusting.

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