

Singular Value Decomposition

**Geometric Algorithms
Lecture 26**

Introduction

Recap Problem (+ Course Evaluations)

Find an orthogonal diagonalization of

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

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

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

Answer

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

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

$$A = P D P^T$$

Normalized eigenvectors

1) find eigenvalues

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

$$(3-\lambda)^2 - 1$$

$$\lambda^2 - 6\lambda + 8 = 0$$

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

$$\lambda = 1, 2$$

2) find eigenvectors

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

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

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

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

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

$$P^T = P$$

$$A = P D P^T$$

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

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

$$\|\vec{x}_2\| = \sqrt{1^2 + 1^2} = \sqrt{2}$$

3.0
3

Create P out

of the eigenvectors

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 a 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

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

where 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:

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

Quadratic forms and Symmetric Matrices (Again)

Furthermore, we can generally say

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

Verify:

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

A Slightly more Complicated Example

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 3 & 0 \\ -1 & 0 & 5 \end{bmatrix}$$

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

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

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

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

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.

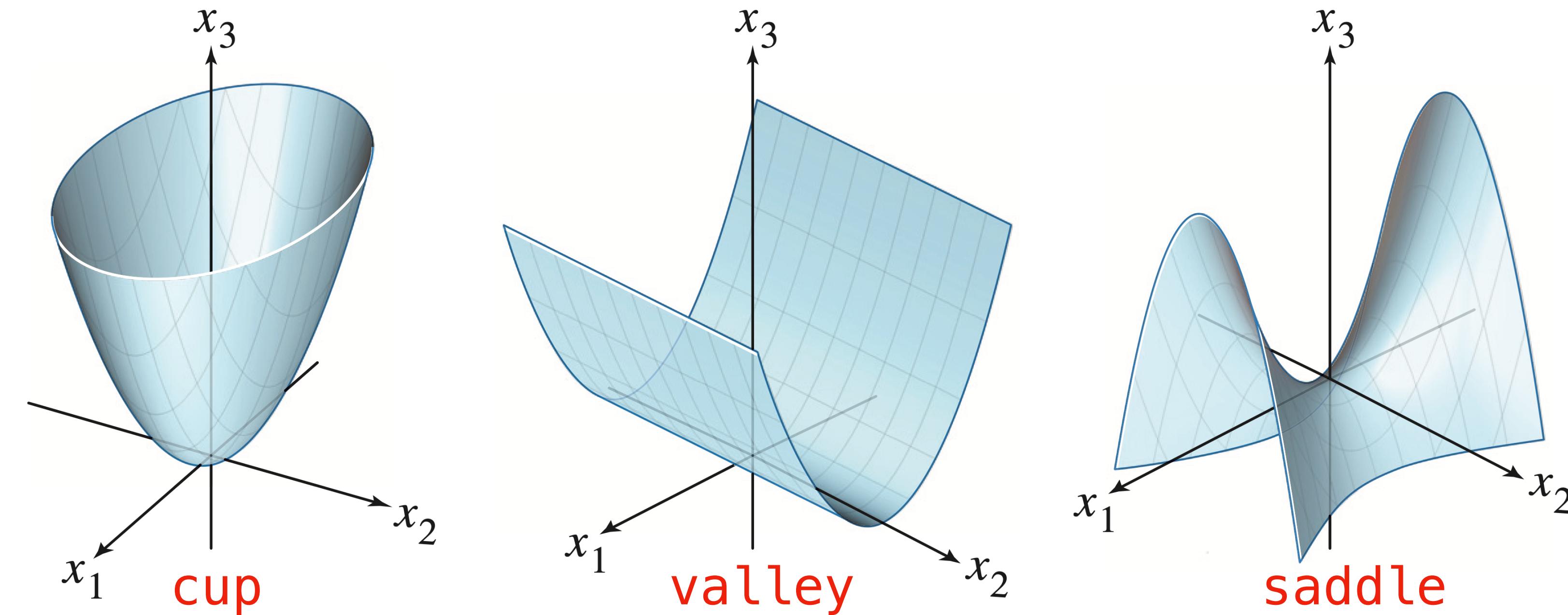
- » if $Q(\mathbf{x})$ has the term αx_i^2 then $A_{ii} = \alpha$
- » if $Q(\mathbf{x})$ has the term $\alpha x_i x_j$, then $A_{ij} = A_{ji} = \frac{\alpha}{2}$

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

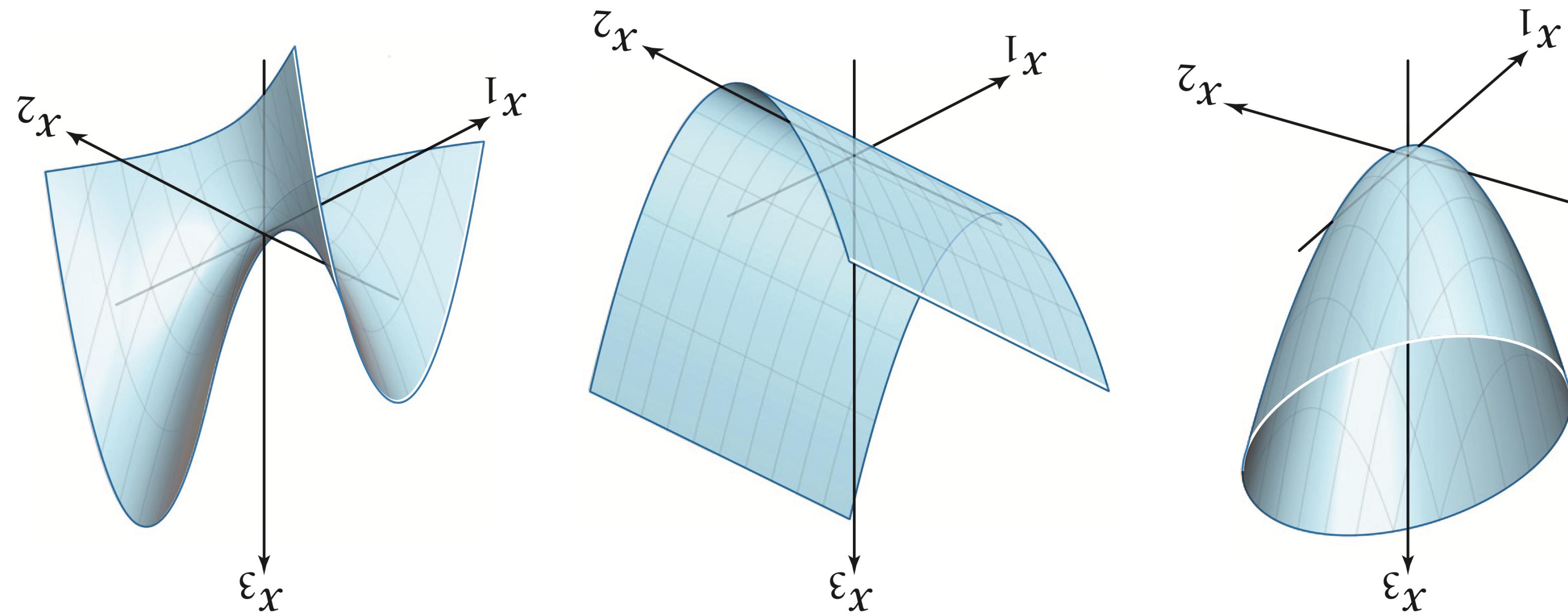
Shapes of Quadratic Forms



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

Can we determine what shape it will be mathematically?

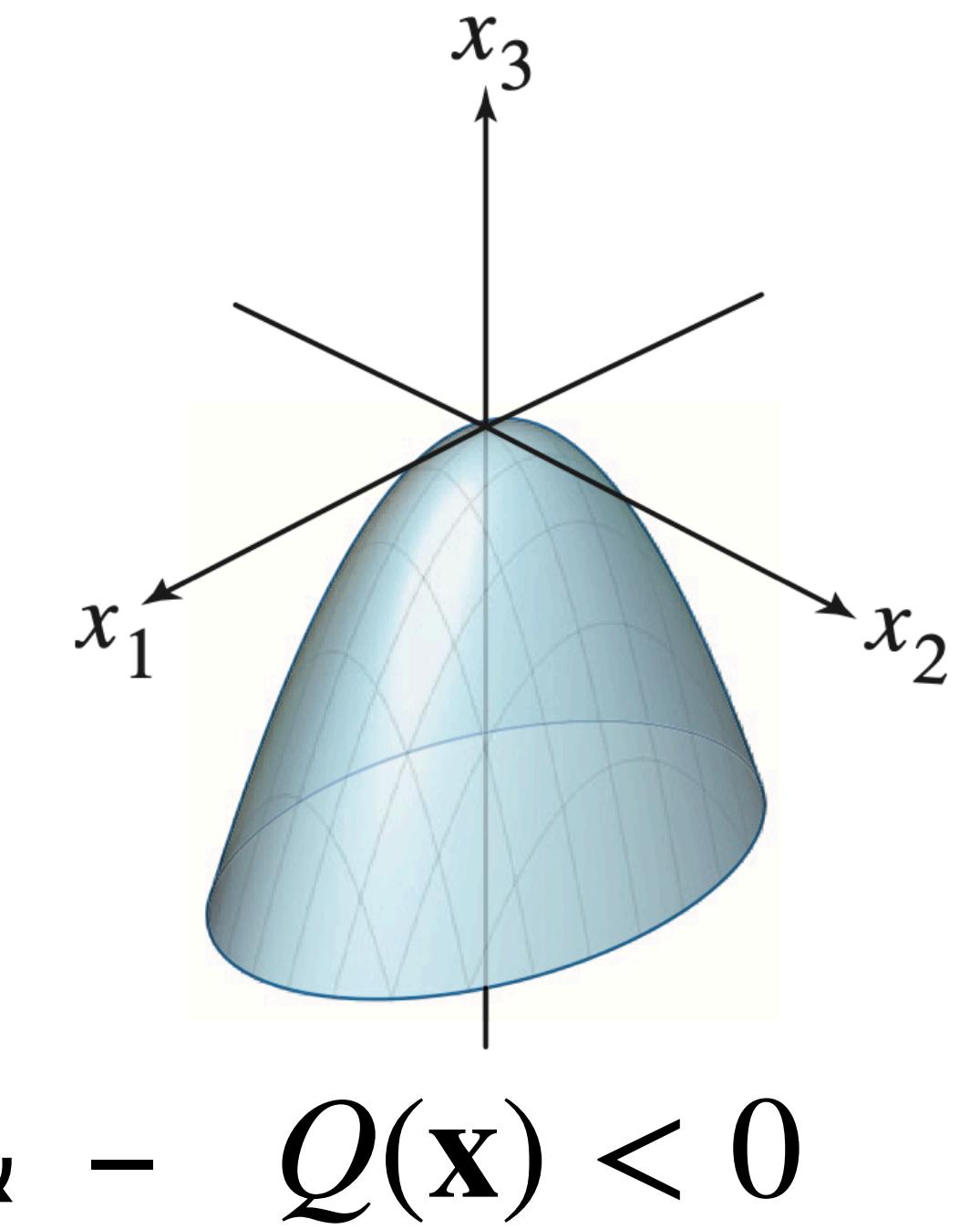
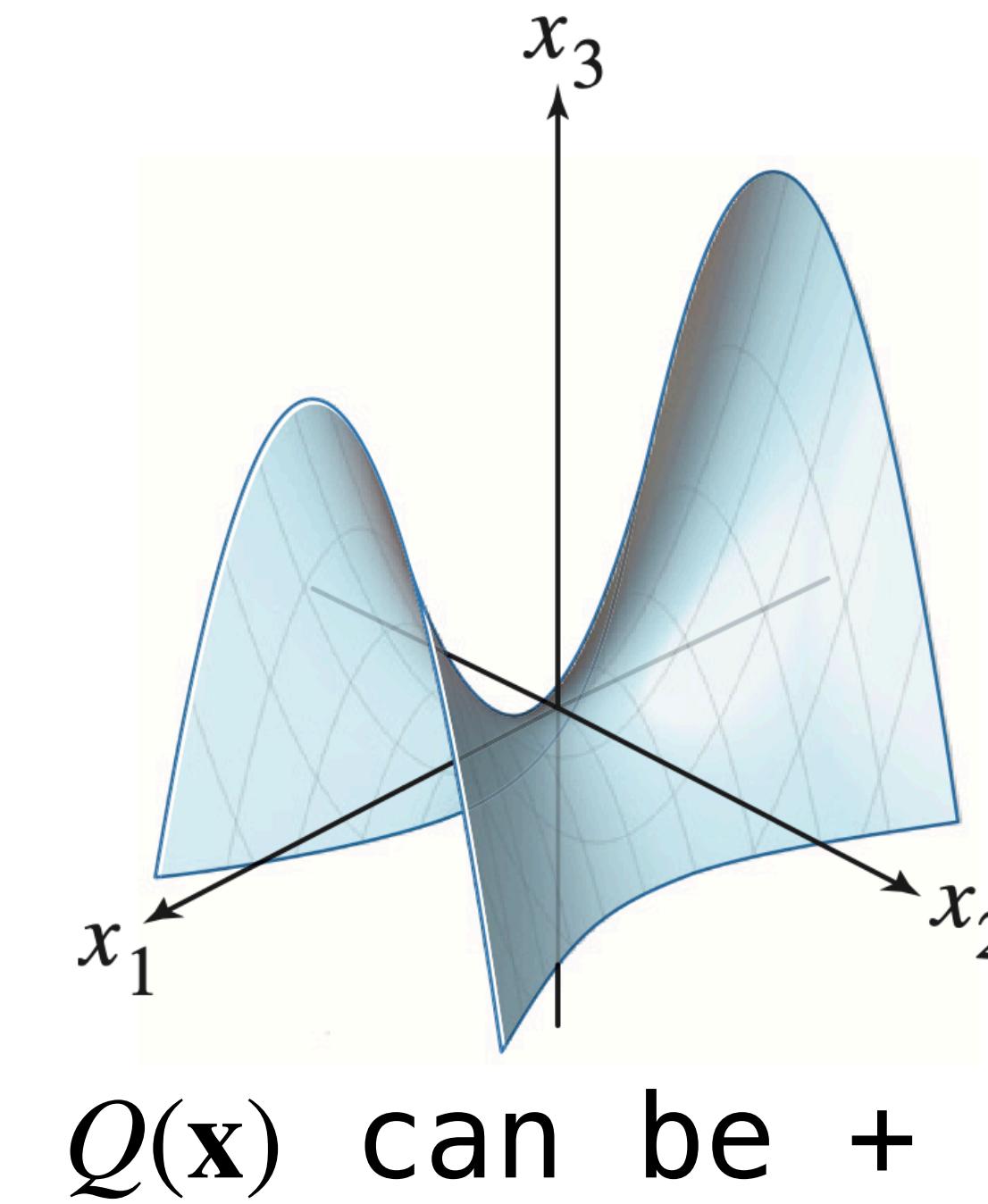
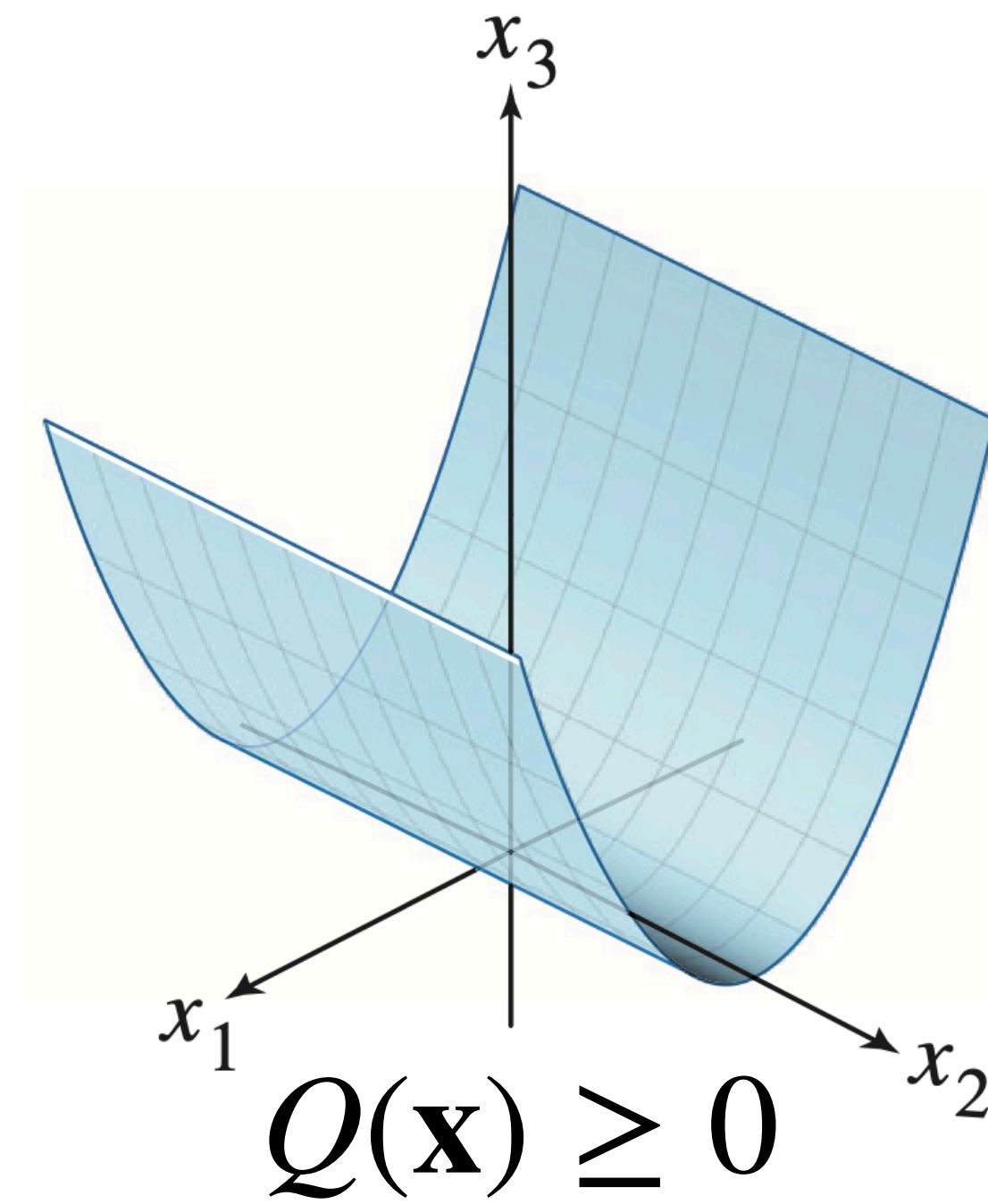
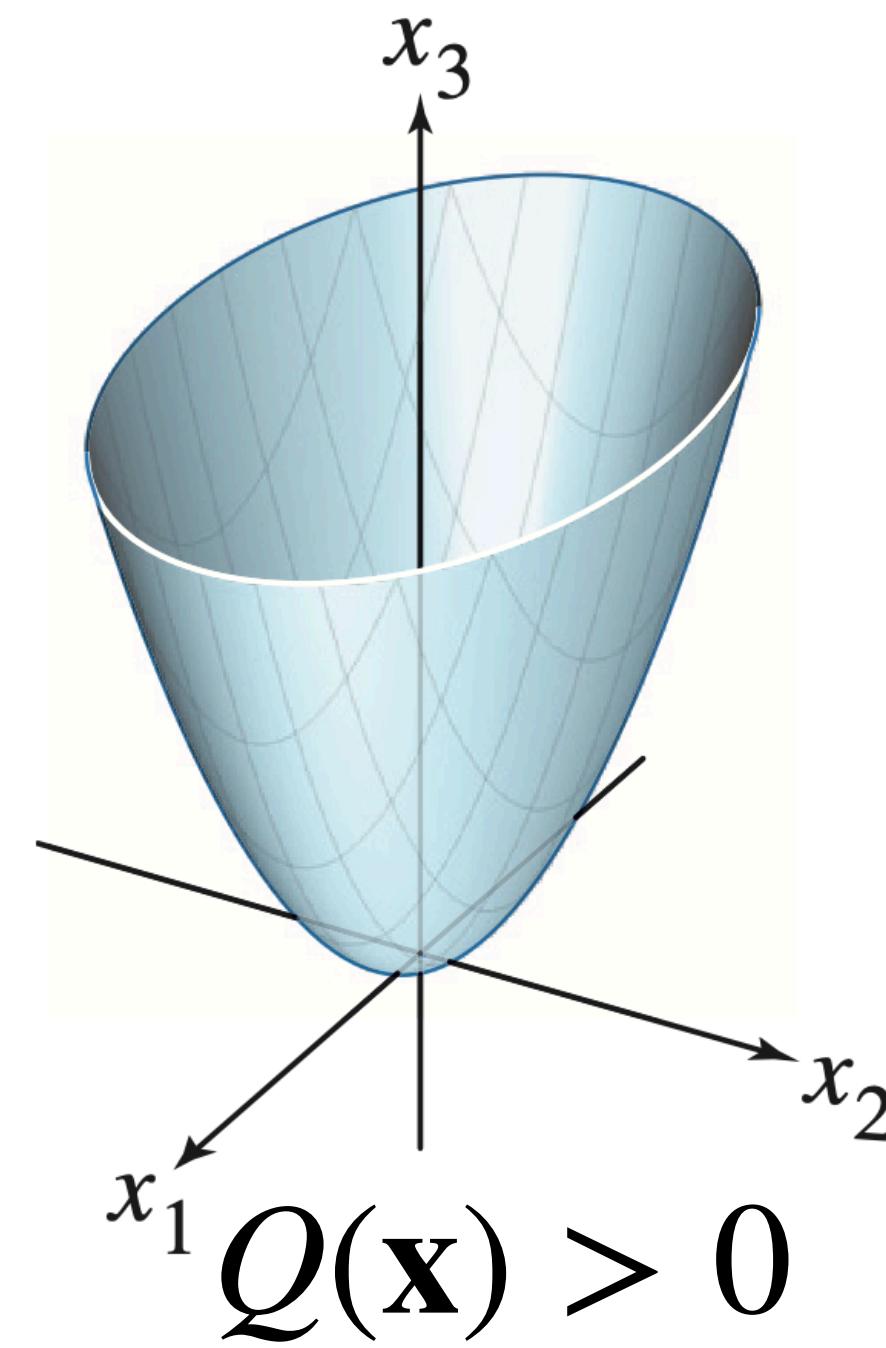
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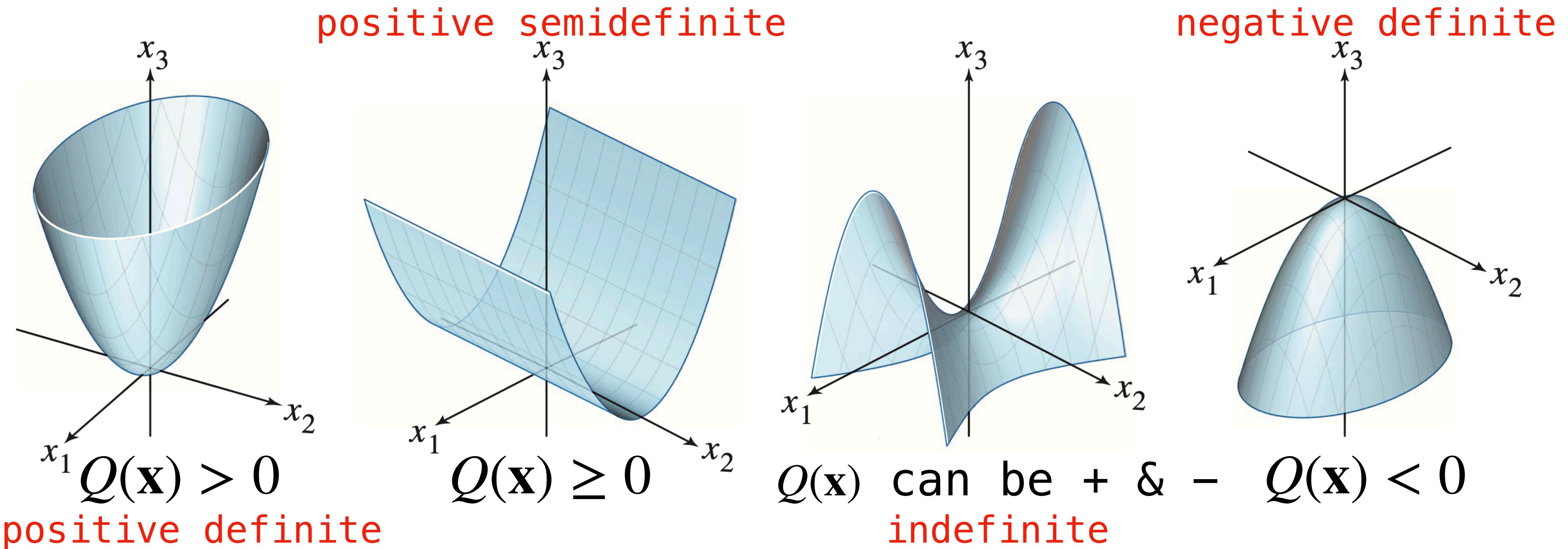
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Definiteness



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

Definiteness



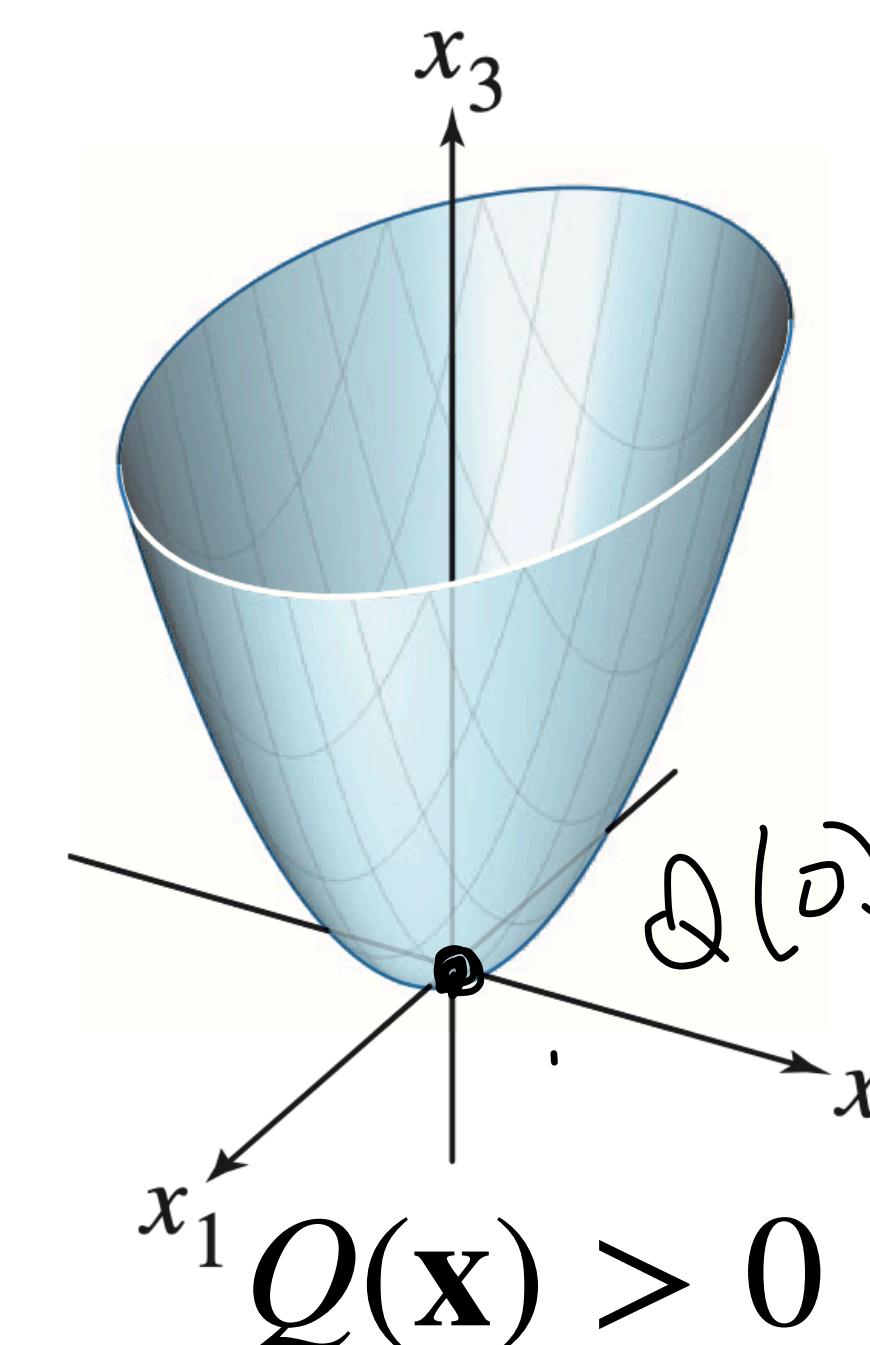
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Definiteness and Eigenvectors

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

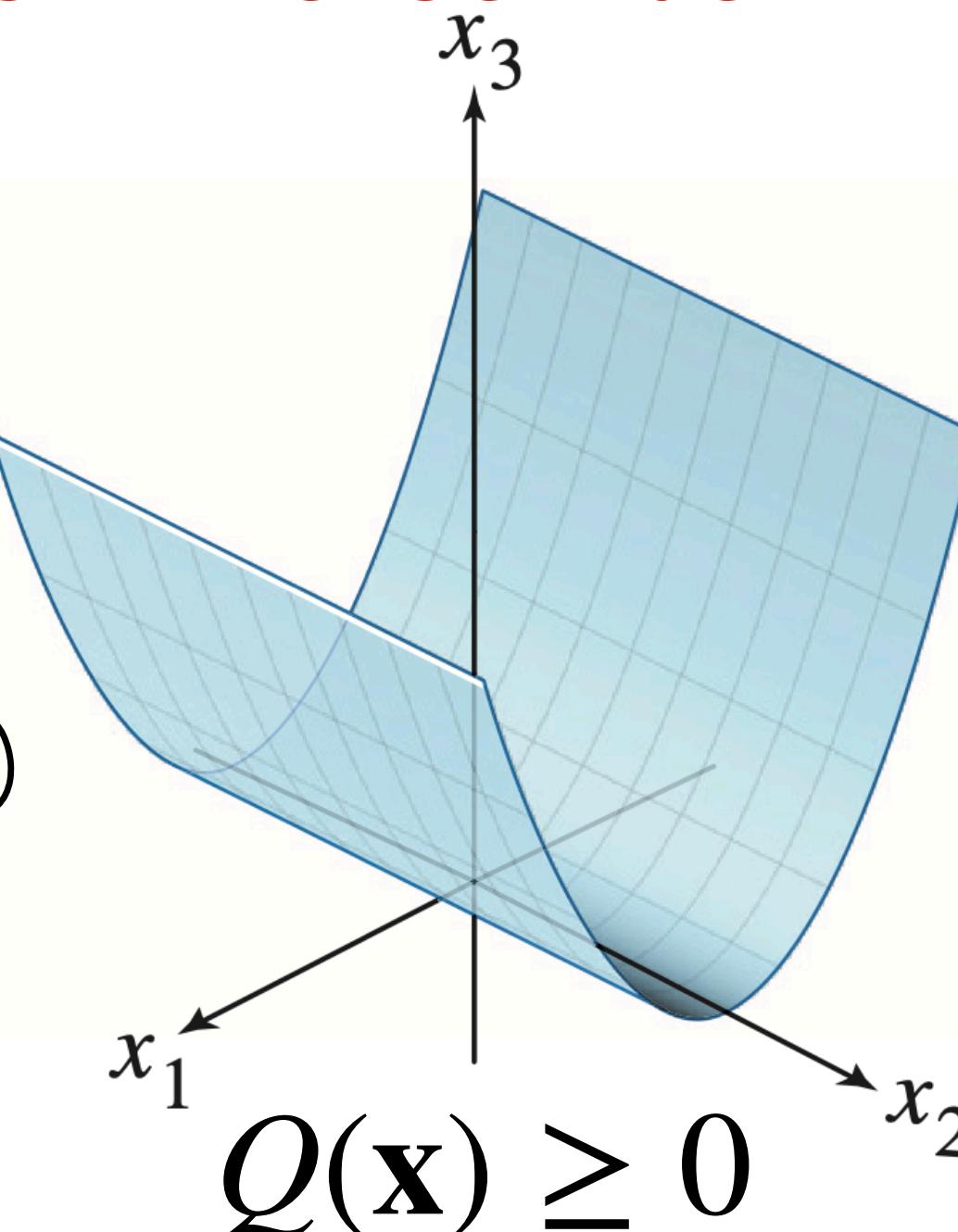
Definiteness



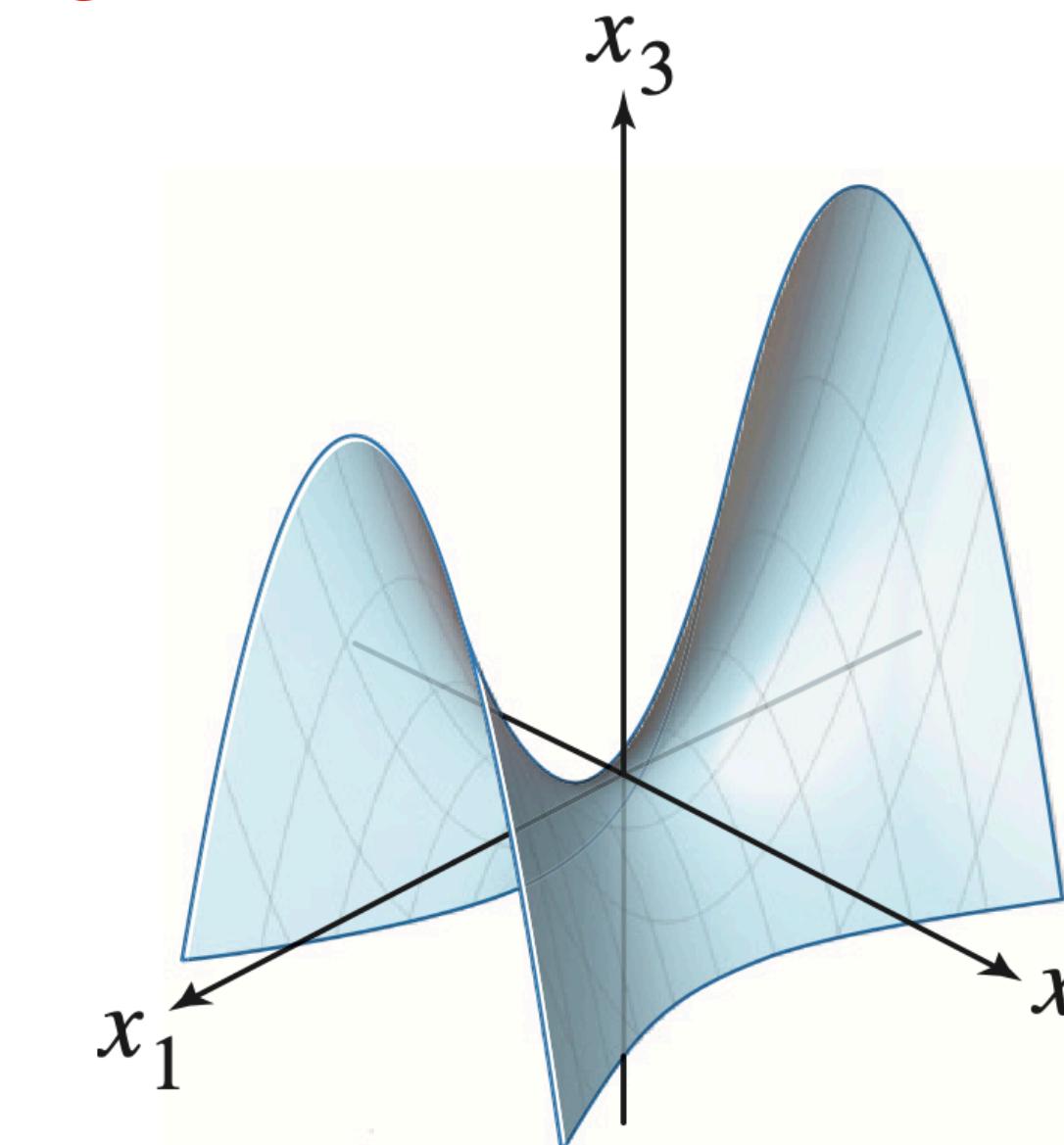
positive definite
all pos. eigenvals

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

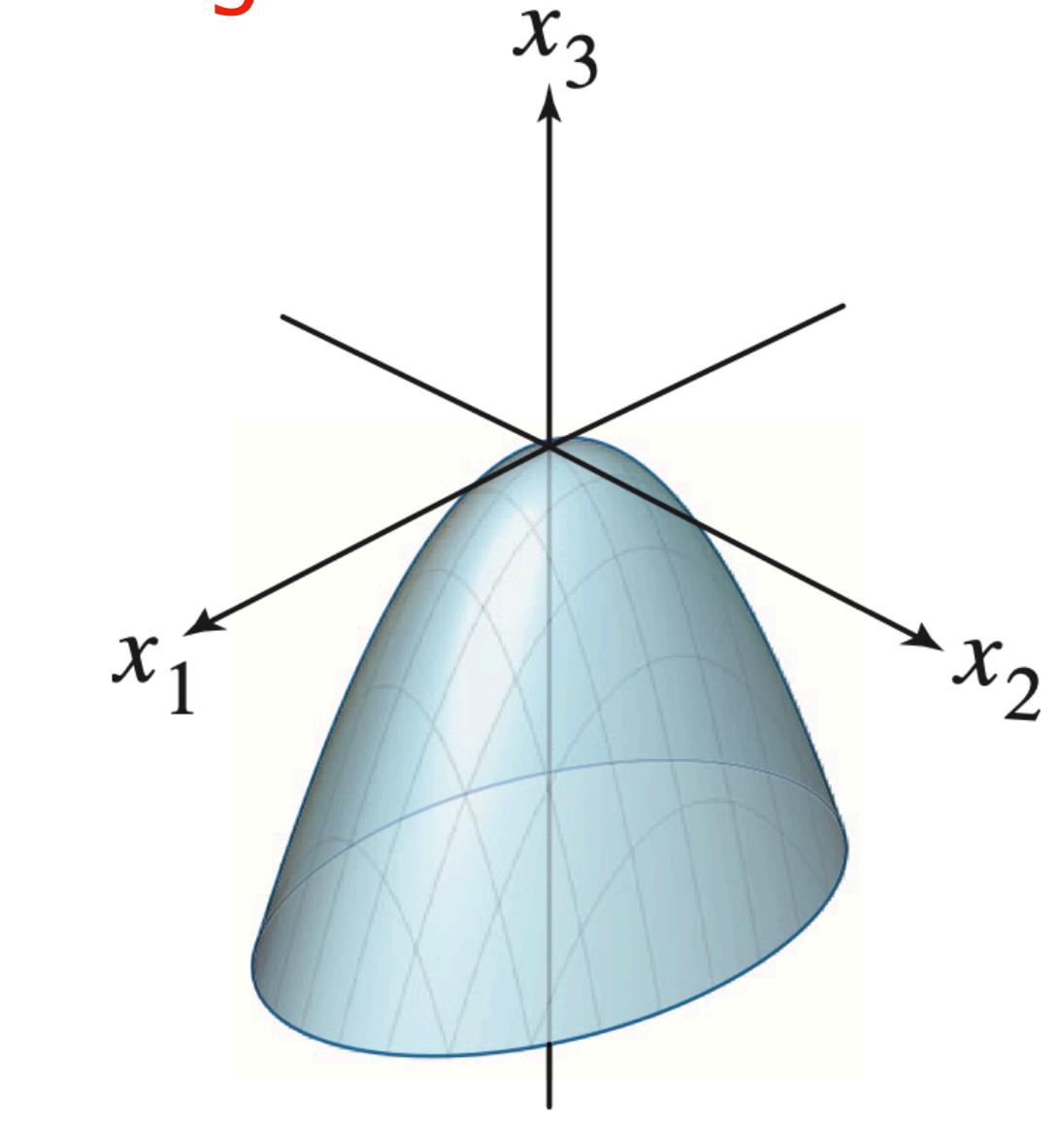
all nonneg. eigenvals
positive semidefinite



$Q(\mathbf{x})$ can be + & -
indefinite
pos. and neg. eigenvals



all neg. eigenvals
negative definite



Example

$$\lambda = 3, -1$$

$$x_1, x_3 = -1$$

$$x_2 = 0$$

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

Let's determine which case this is:

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

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

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

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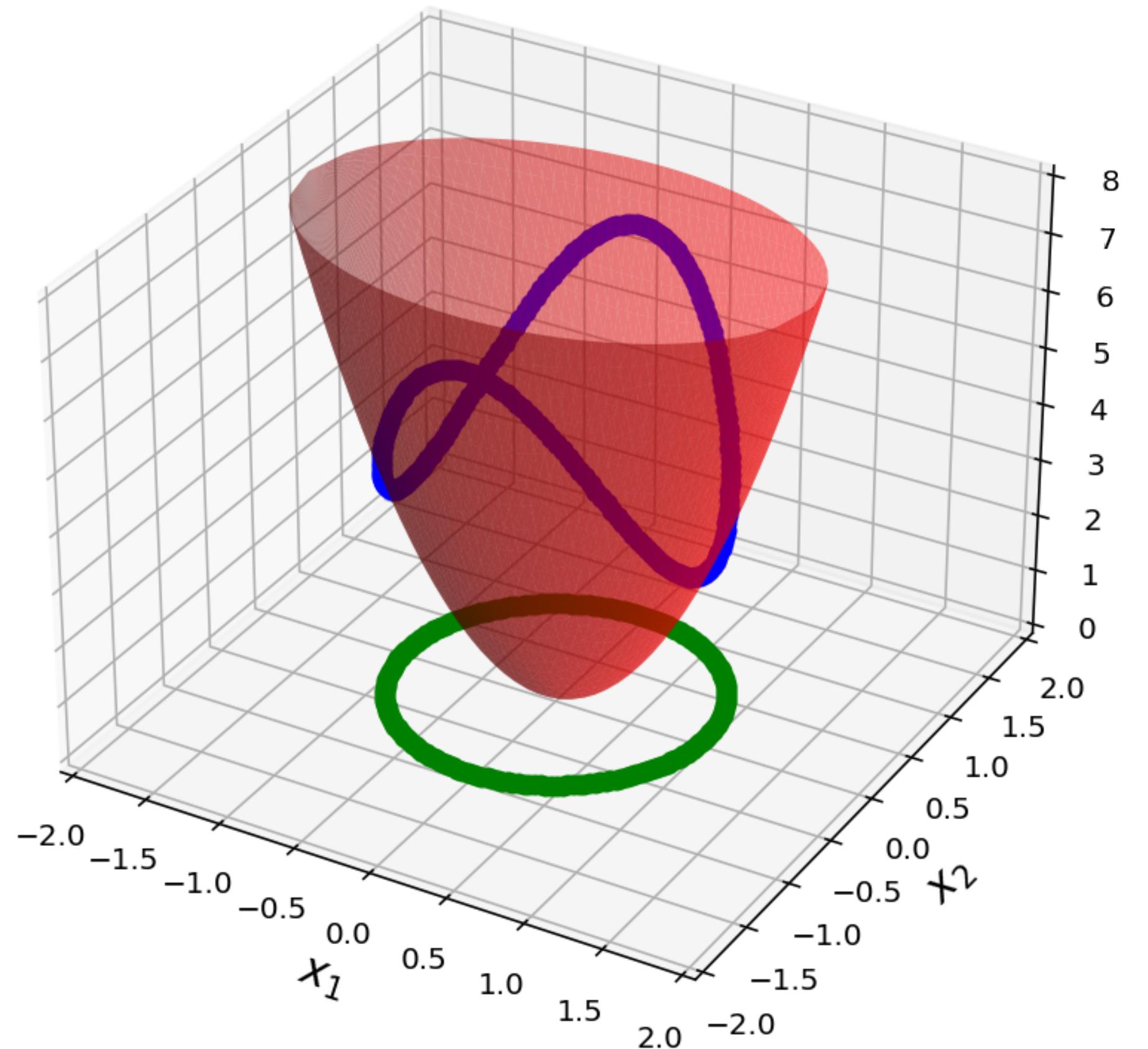
$$\min_{\mathbf{v} \in X} f(\mathbf{v})$$

(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 $\mathbf{x}^T \mathbf{A} \mathbf{x}$ subject to $\|\mathbf{x}\| = 1$



It's common to constraint
to unit vectors.

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

$$3(0) + 7(1) = 7 \quad (\text{max value})$$

$$3(1) + 7(0) = 3 \quad (\text{min value})$$

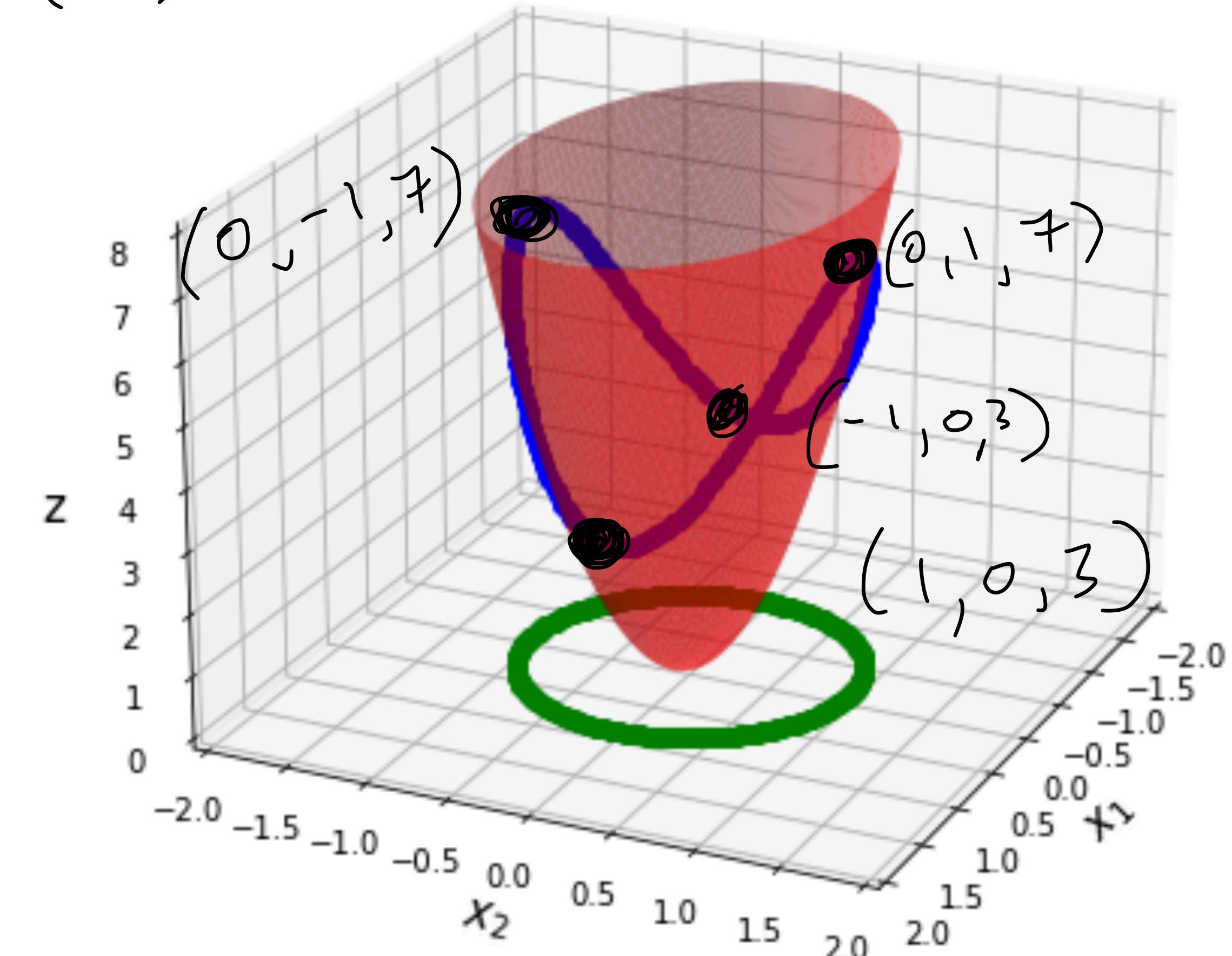
What are the min/max values?:

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

$$7x_1^2 + 7x_2^2$$

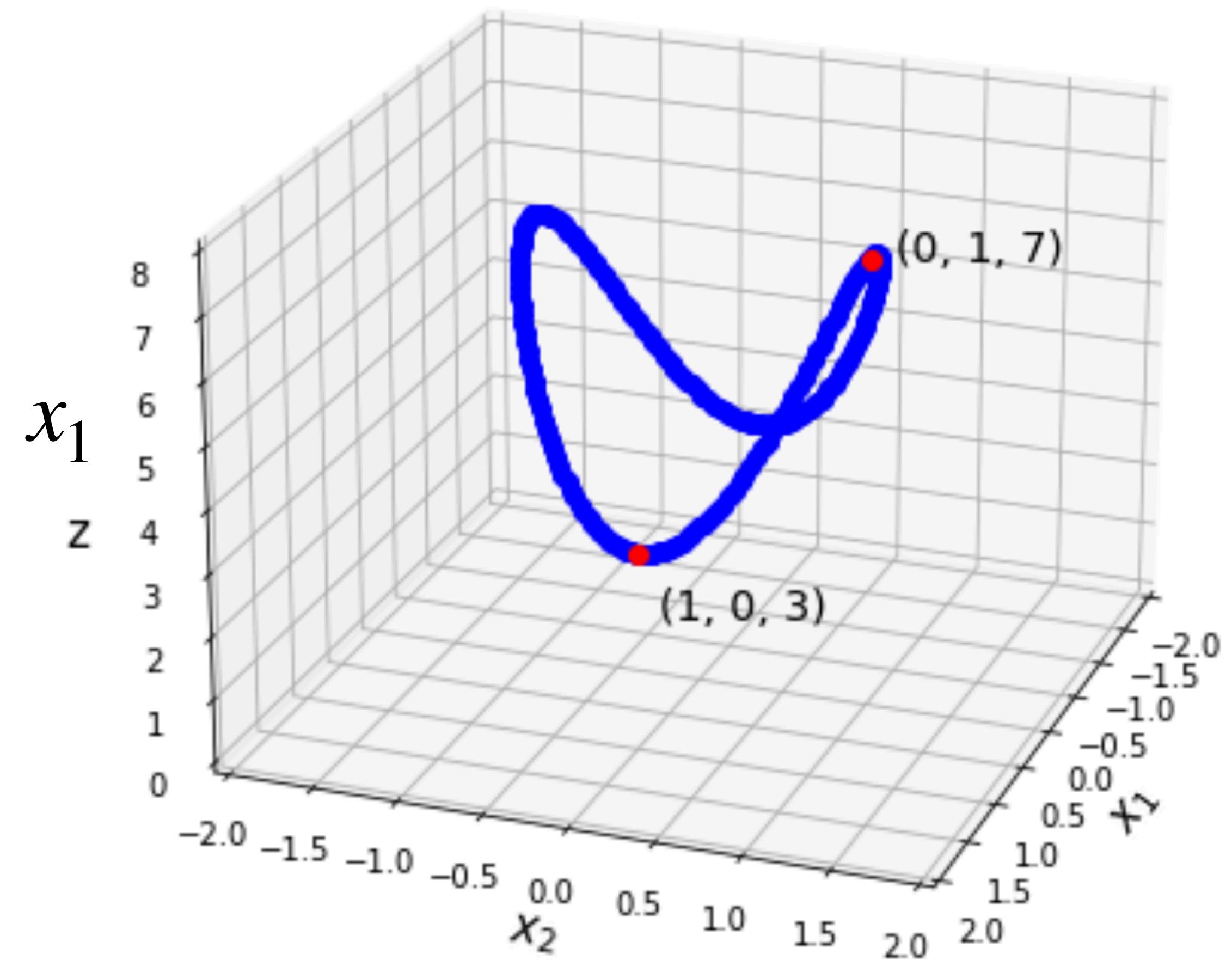
$$7(x_1^2 + x_2^2) = 7$$

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



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 .

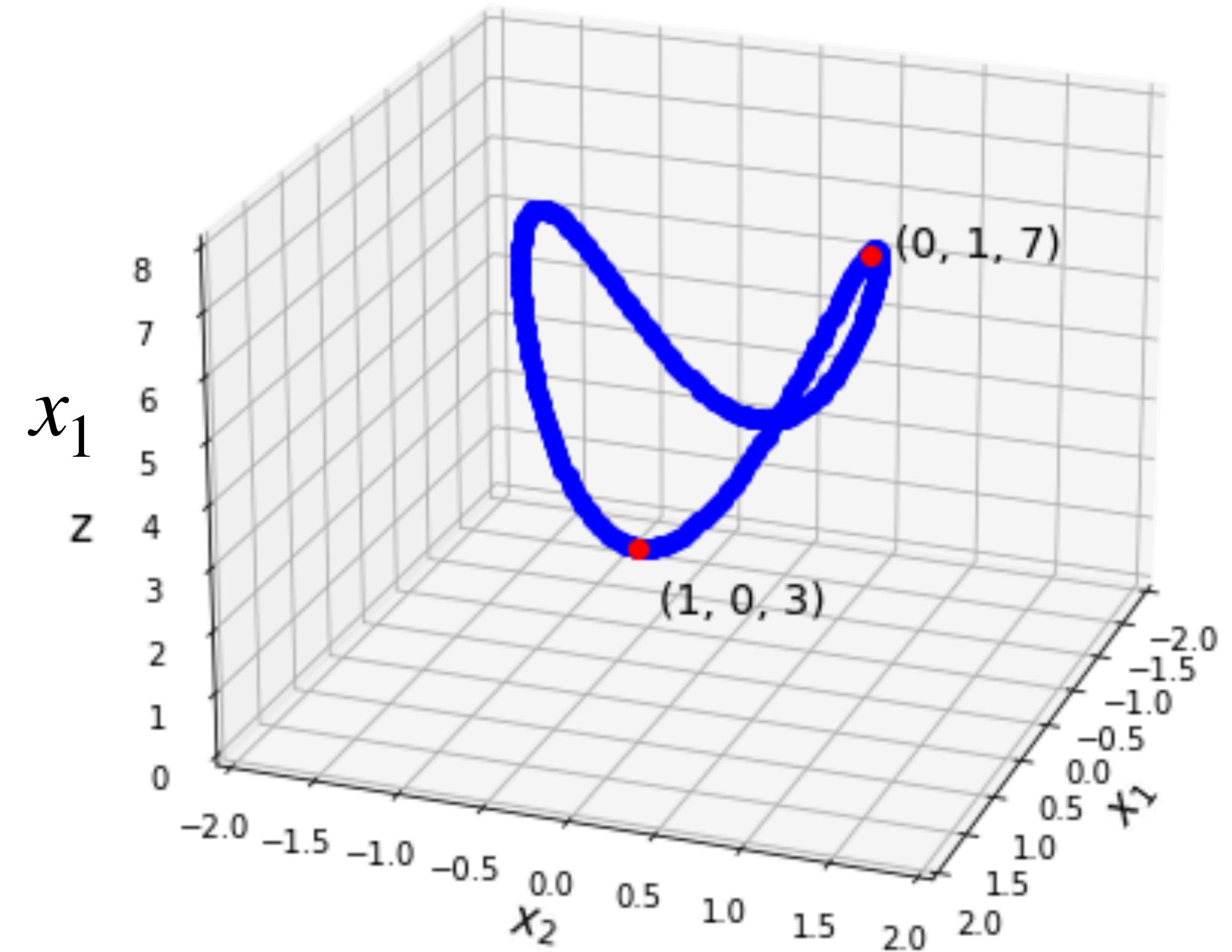


Example: $3x_1^2 + 7x_2^2$

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

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

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

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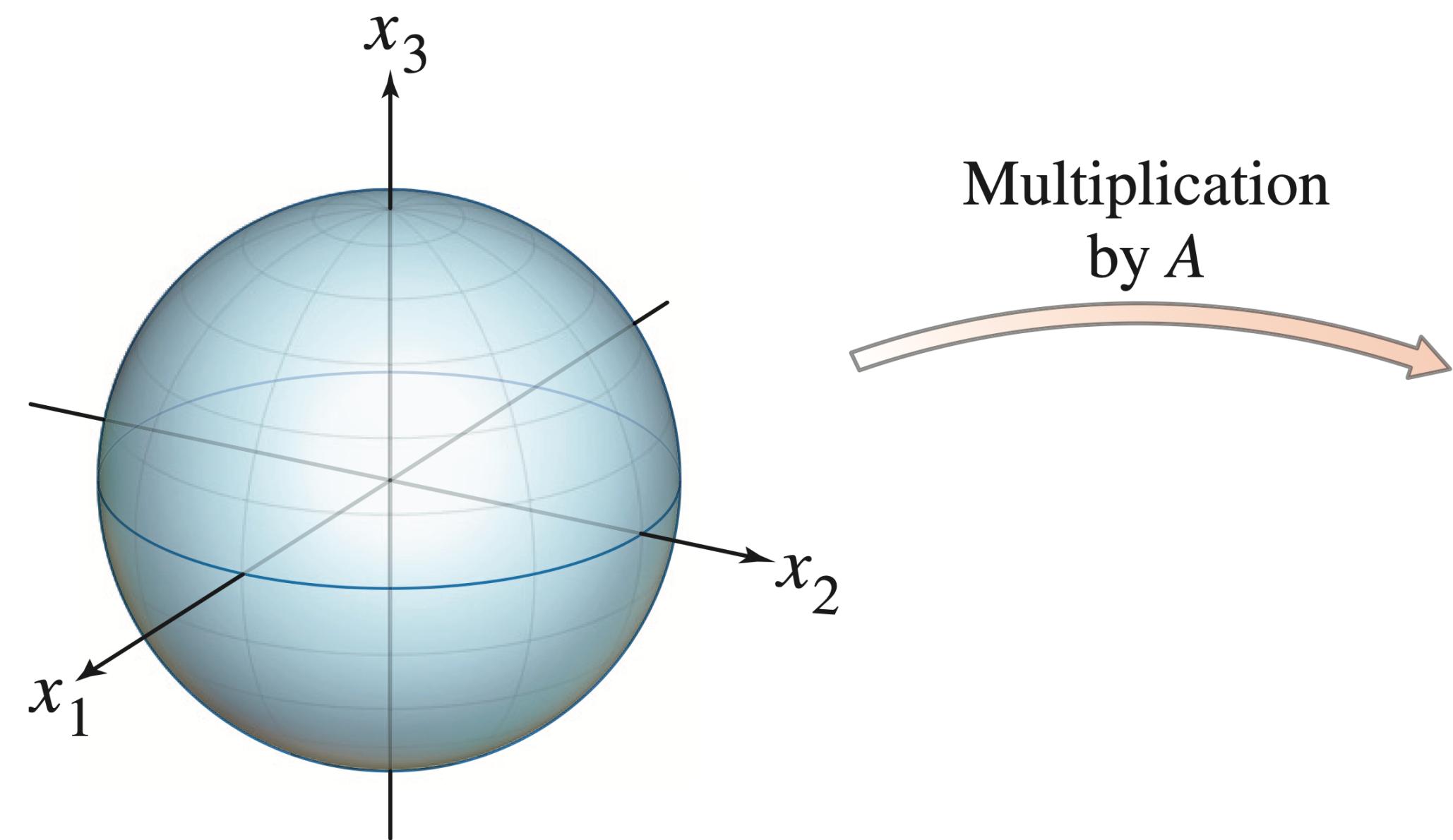
Solution. Find the largest eigenvalue of A , this will be the maximum value.

(Use NumPy)

Singular Value Decomposition

Question

What shape is the unit sphere after a linear transformation?

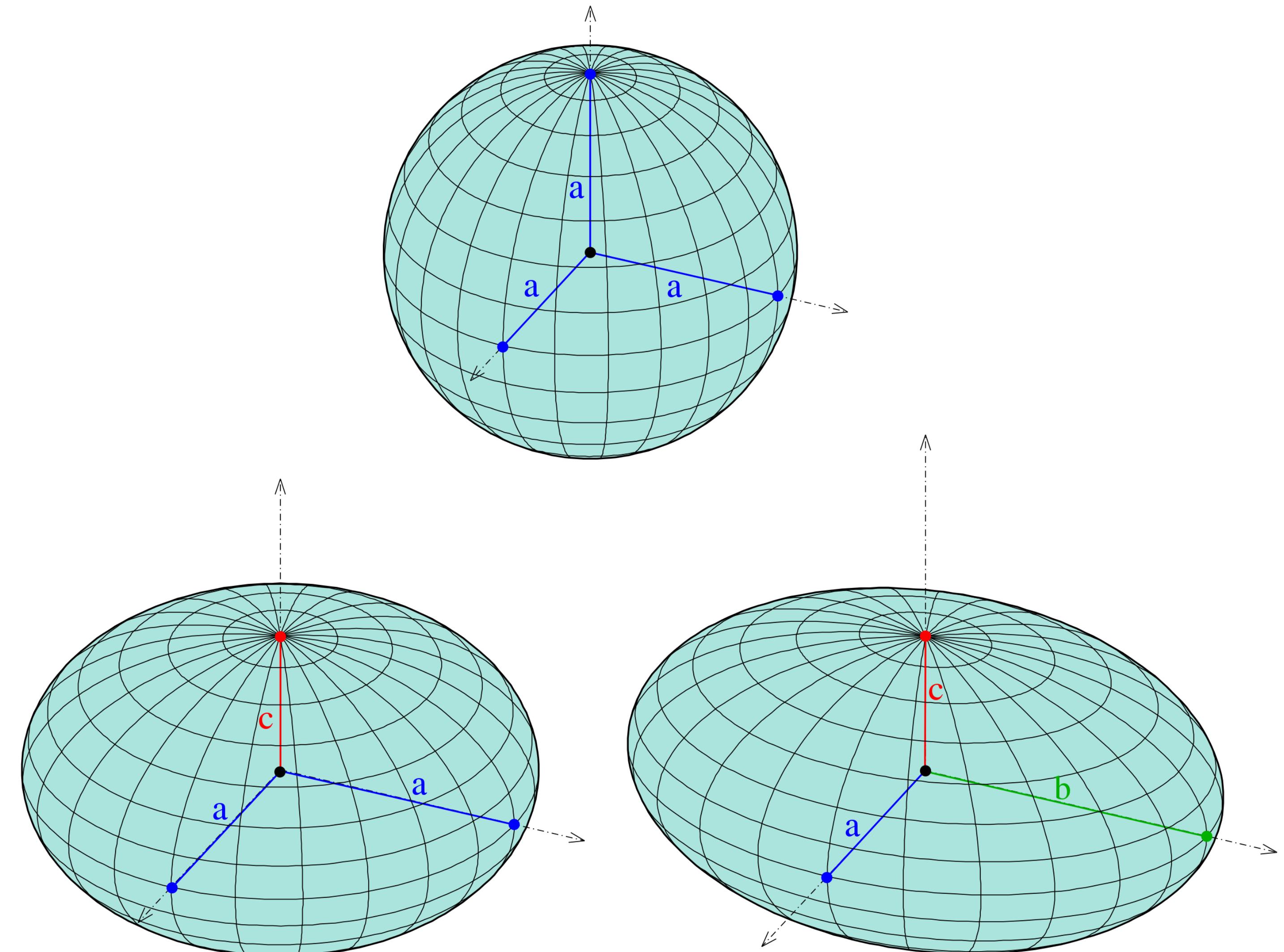


???

Ellipsoids

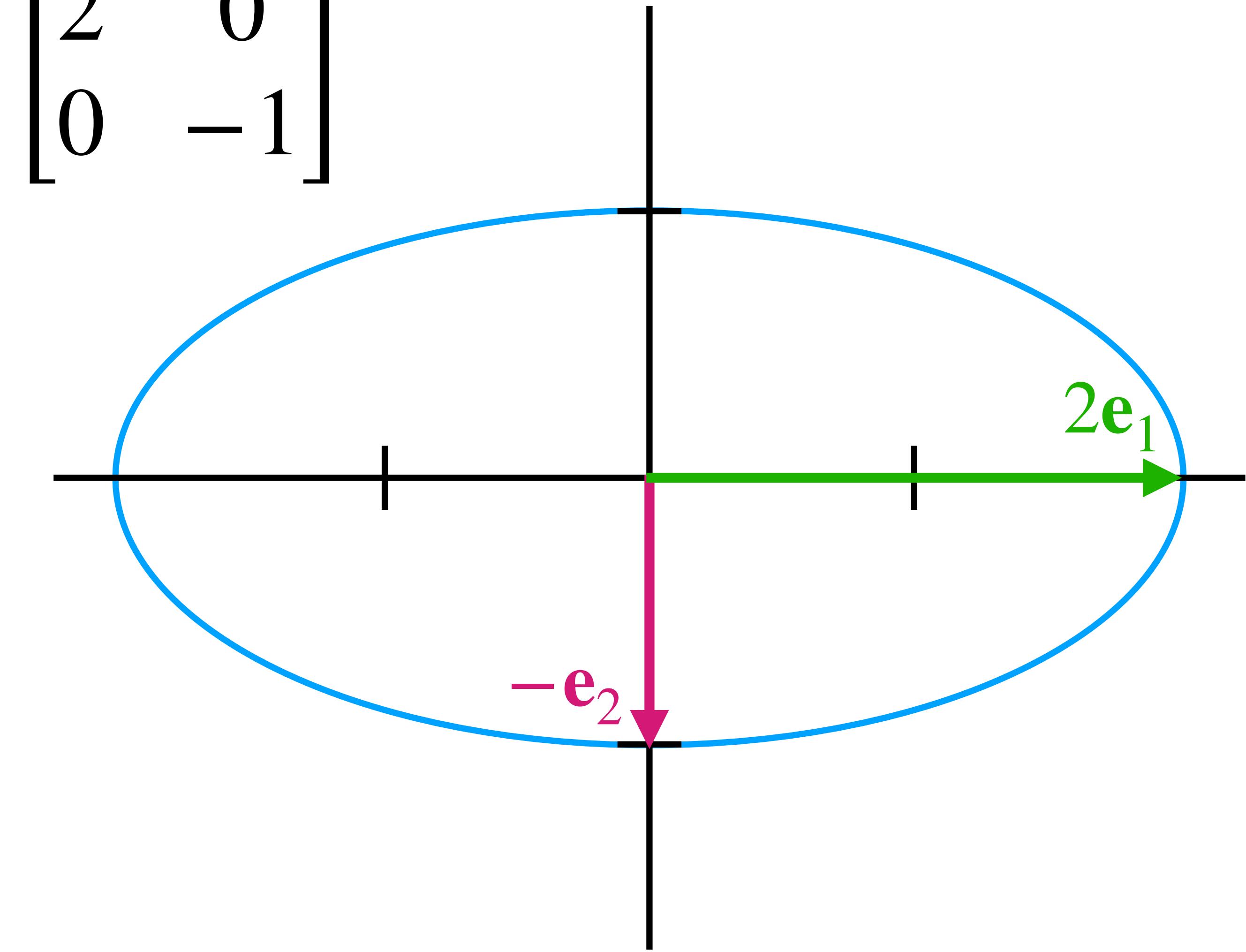
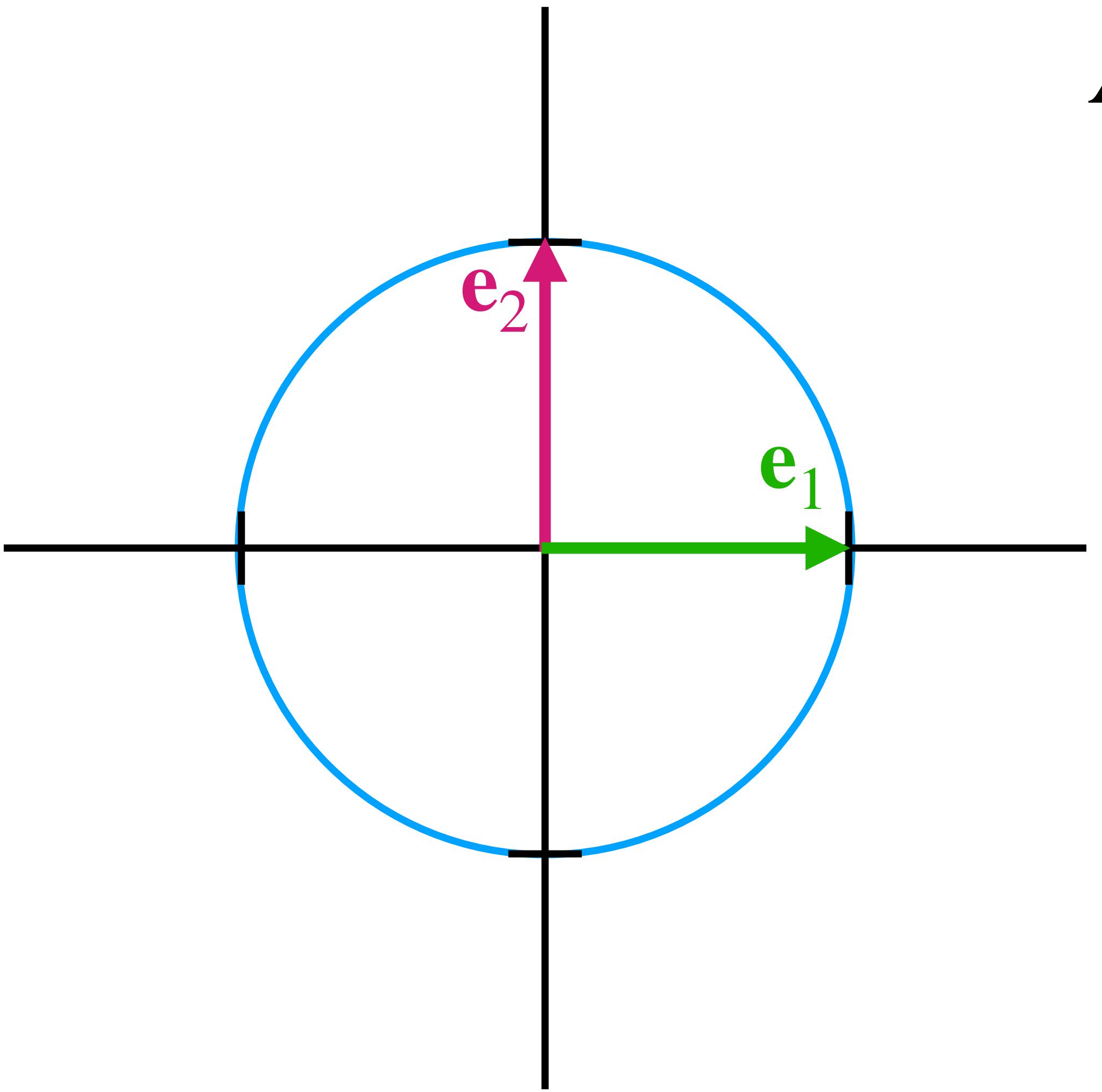
Ellipsoids are spheres "stretched" in orthogonal directions called the **axes of symmetry** or the **principle axes**.

Linear transformations maps spheres to ellipsoids.

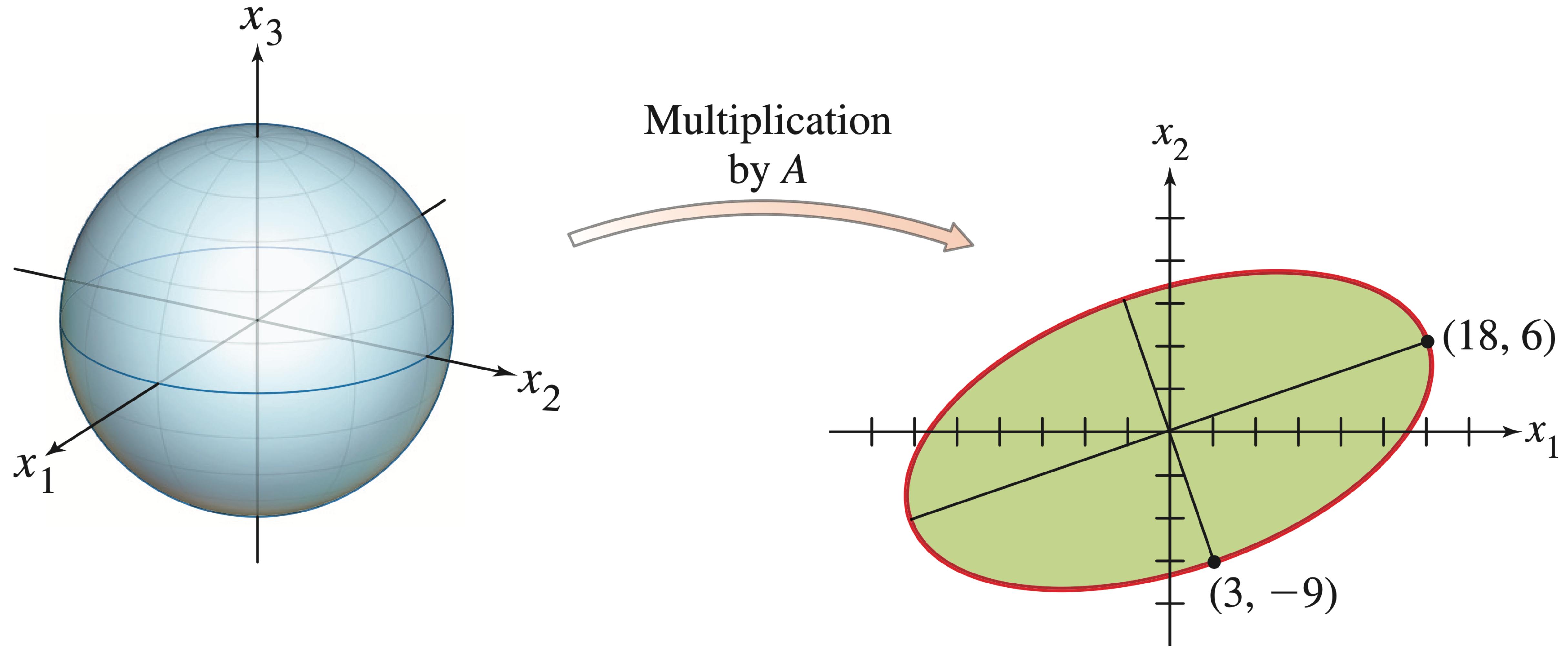


Simple Example : Scaling Matrices

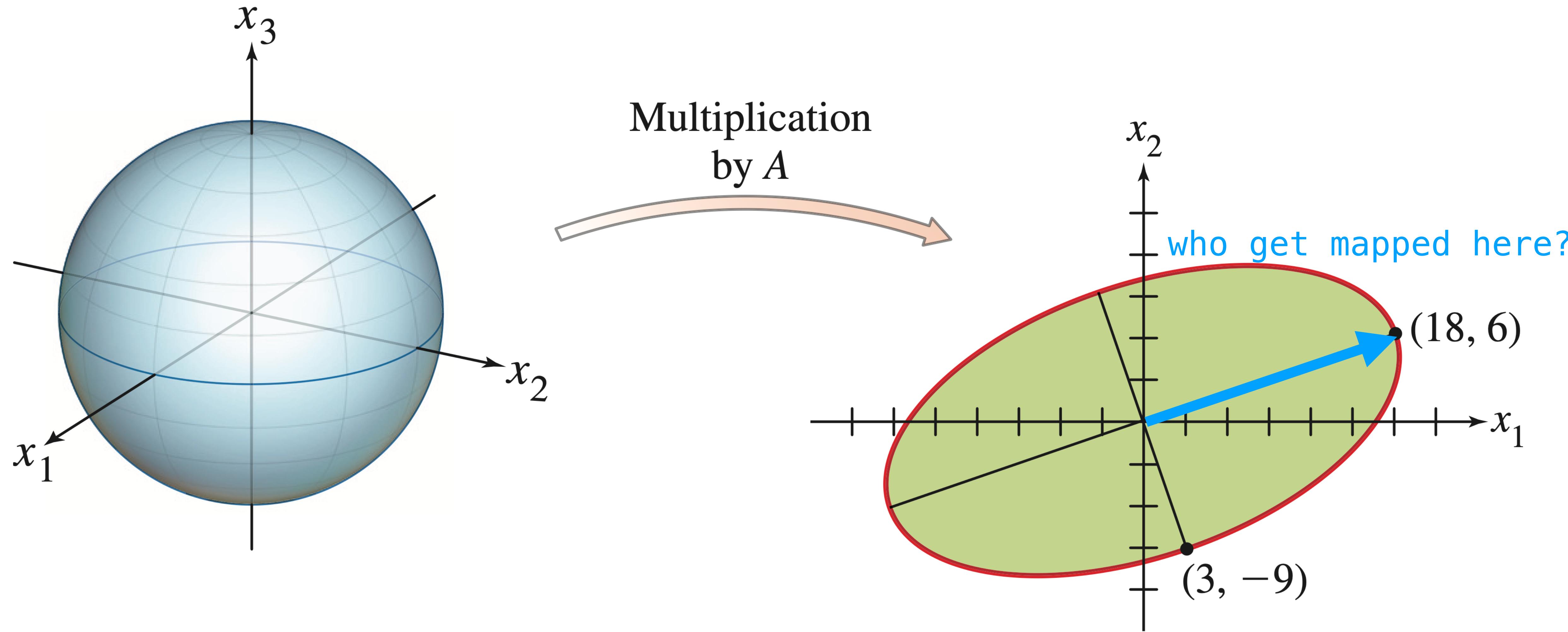
$$A = \begin{bmatrix} 2 & 0 \\ 0 & -1 \end{bmatrix}$$



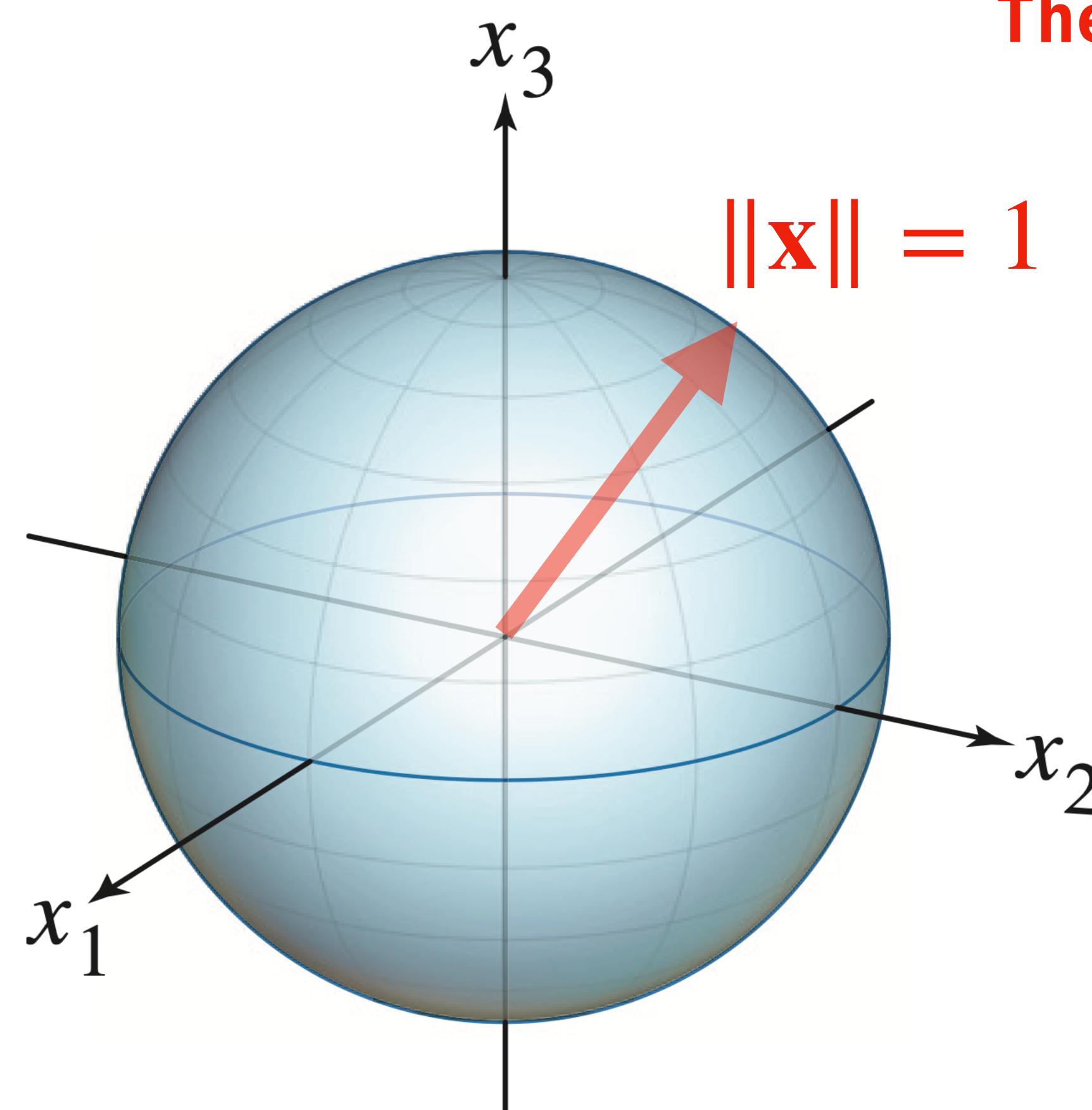
The Picture



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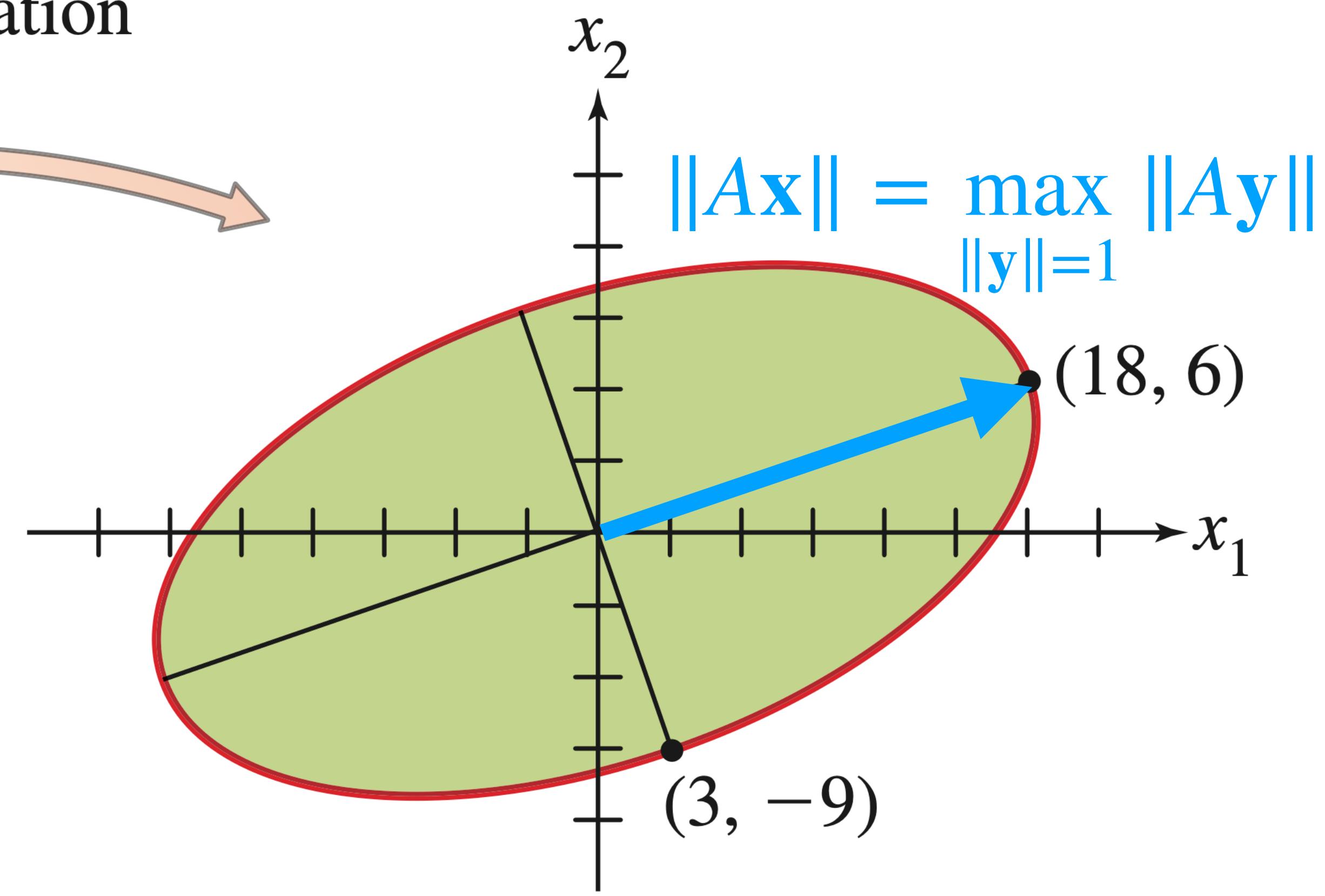


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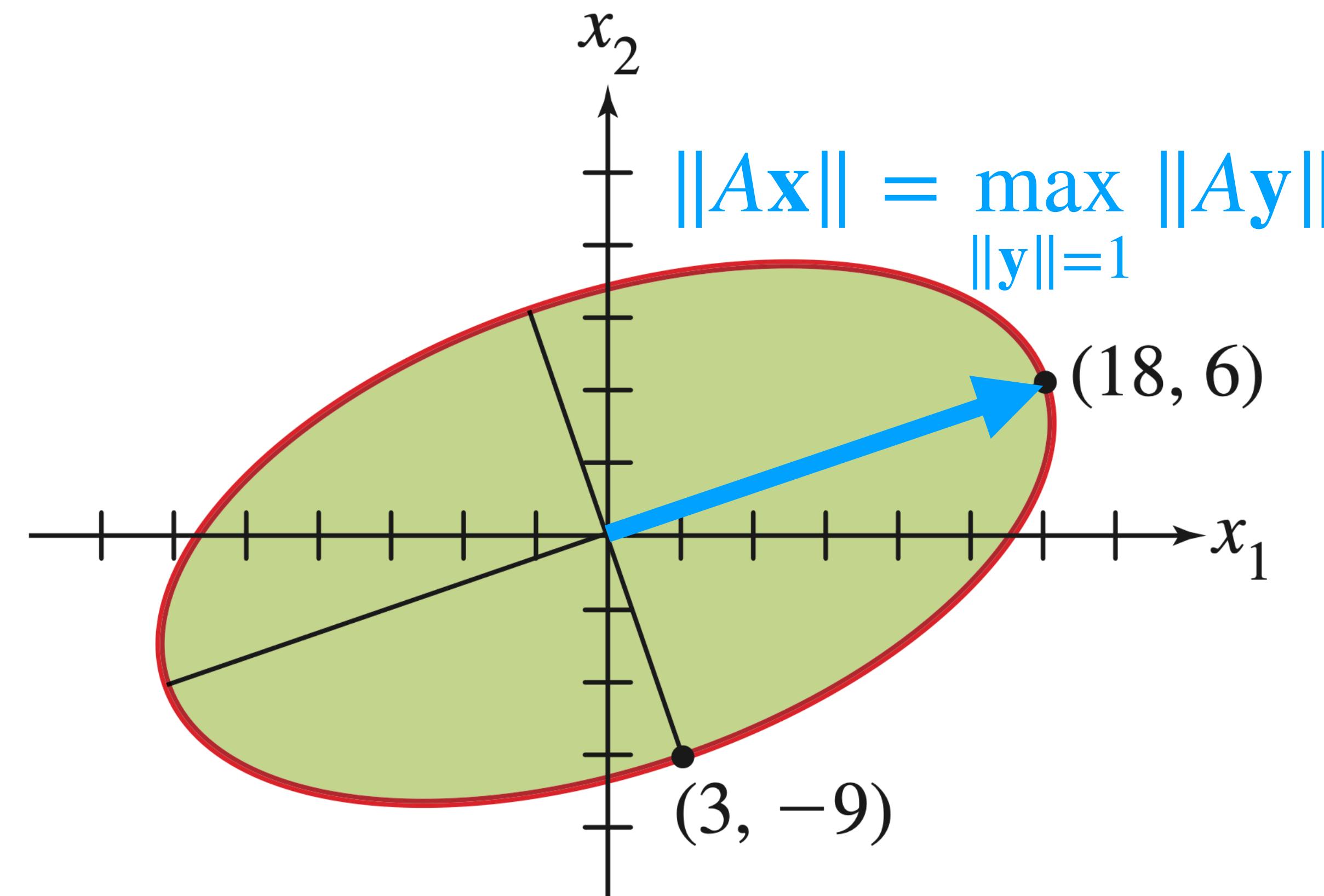


The longest end of the ellipse is the solution to a constrained optimization problem

Multiplication
by A

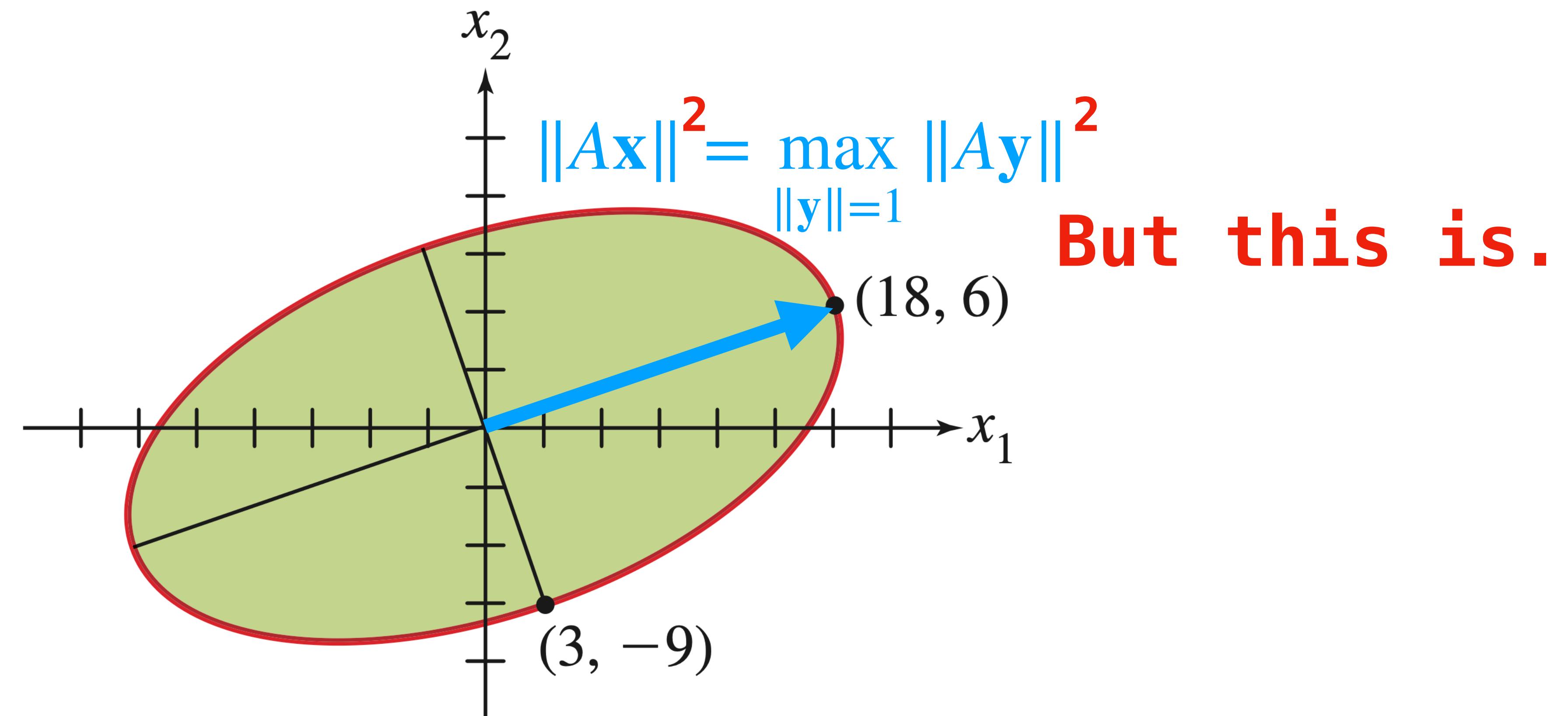


The Picture



This is not a quadratic form...

The Picture



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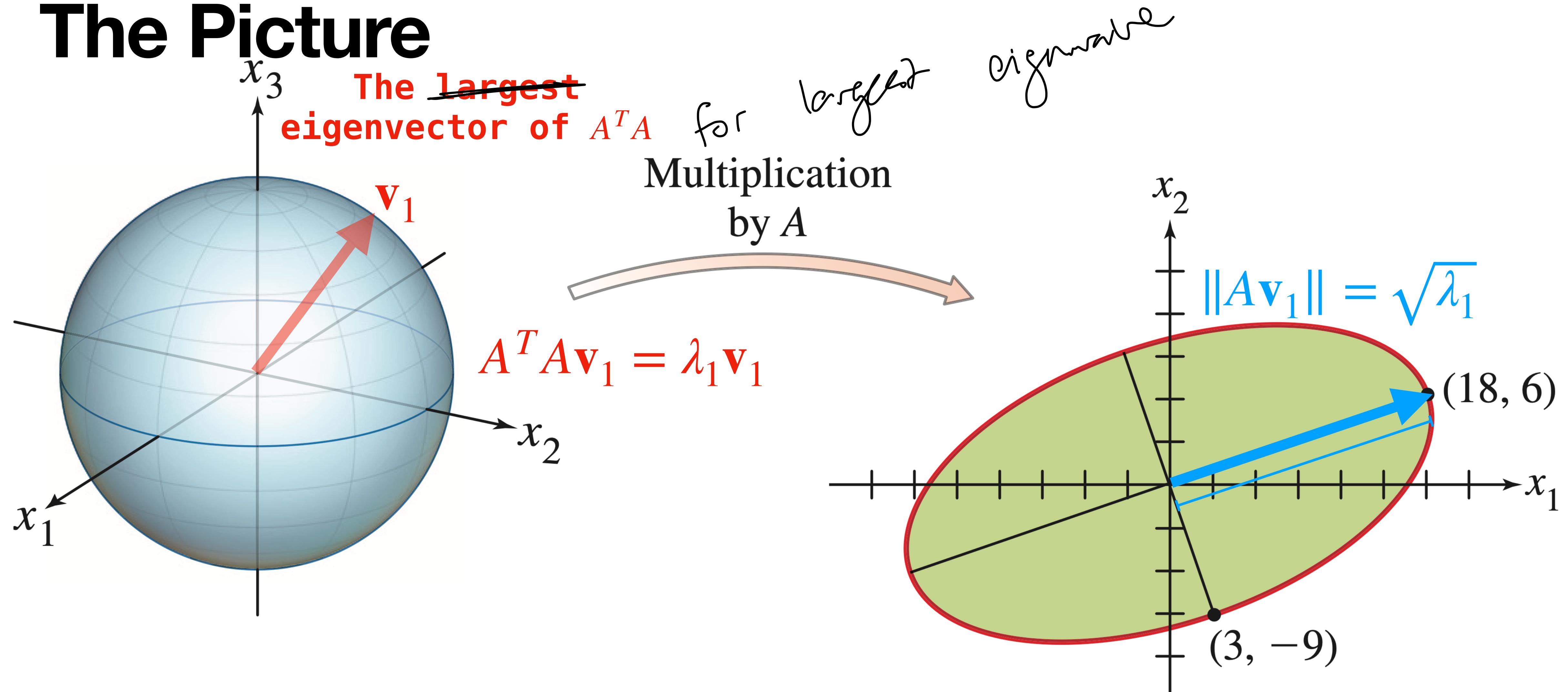
A Quadratic Form

What does $\|Ax\|^2$ look like?:

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

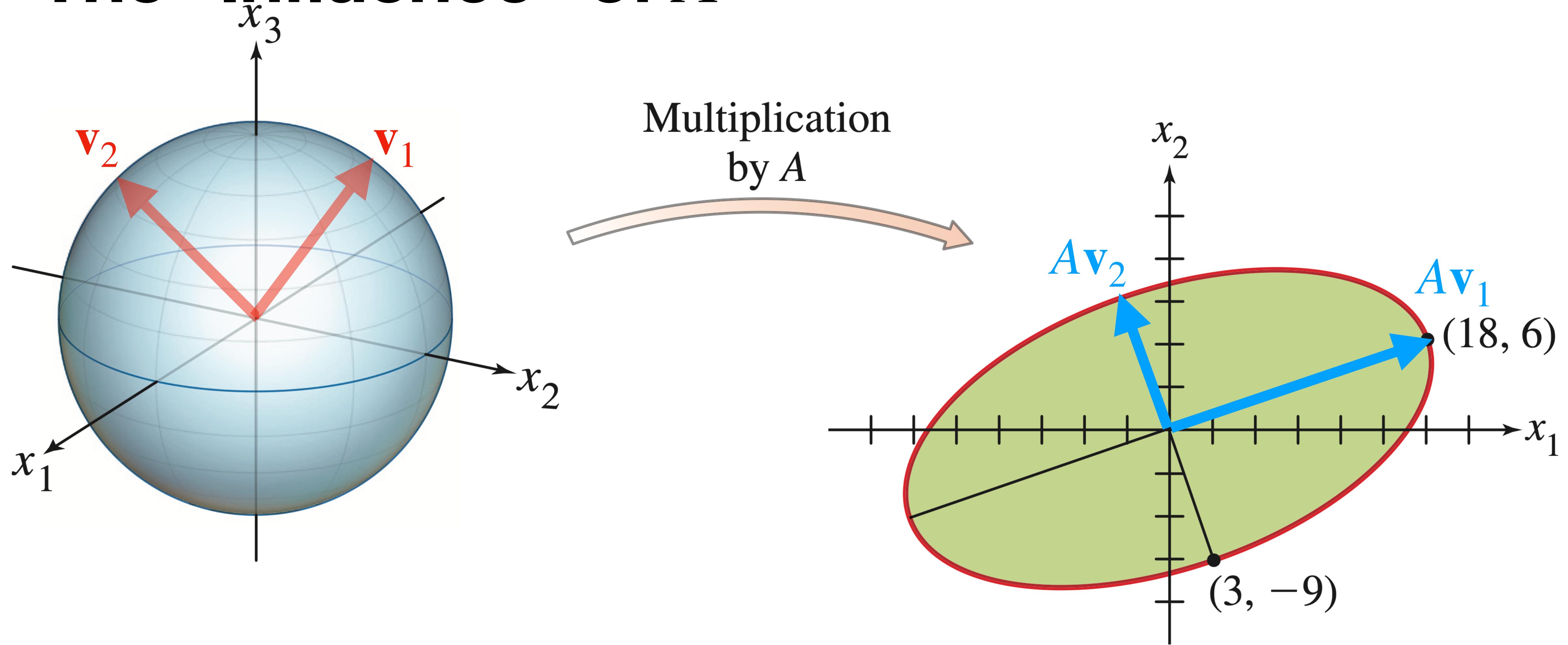
$$\vec{x}^T \boxed{A^T A} \vec{x}$$

The Picture



v_1 solves the constrained optimization problem.

The "Influence" of 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. $(A^T A)^T = A^T A^T T = A^T A$

Properties of $A^T A$

- » It's symmetric.
- » So its orthogonally diagonalizable.

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- » Its eigenvalues are nonnegative. $x^T A^T A x = \|A x\|_2^2$

Properties of $A^T A$

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

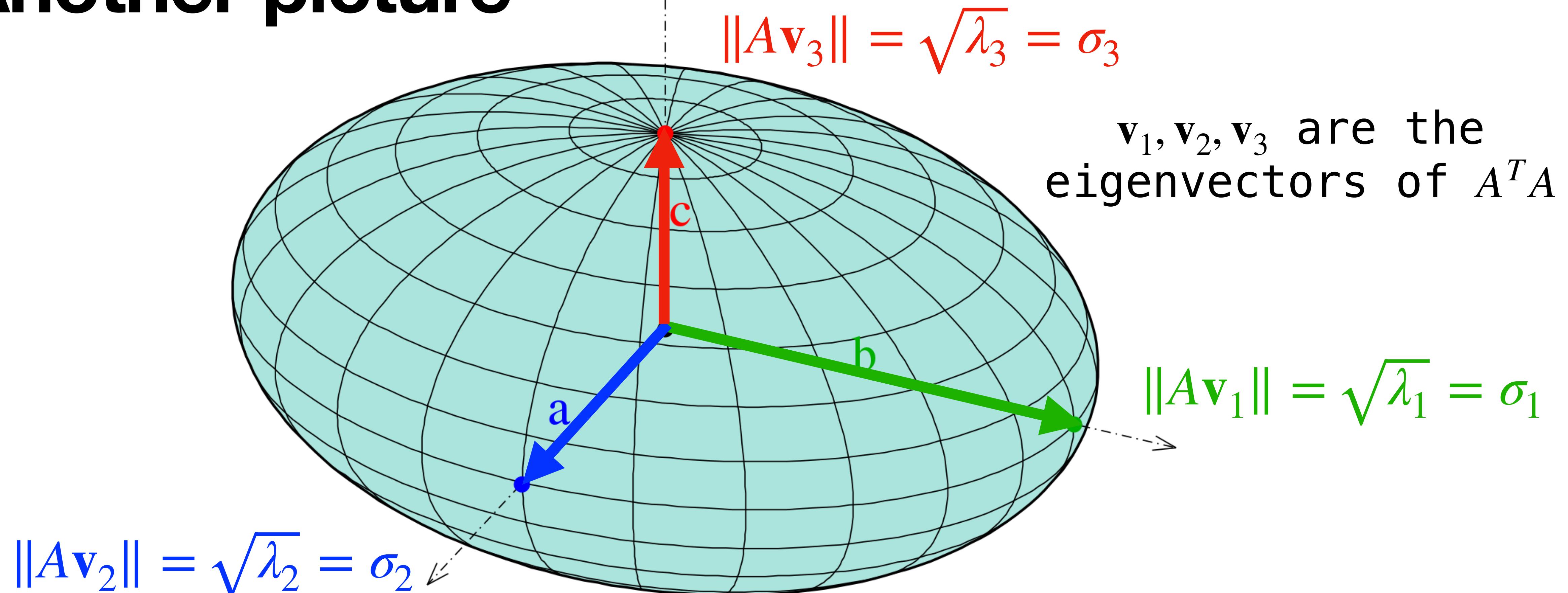
Singular Values

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 v_1, \dots, v_n be an **orthogonal** eigenbasis of \mathbb{R}^n for $A^T A$ and suppose A has r nonzero singular values.

Theorem. Av_1, \dots, Av_r is an orthogonal basis of $\text{Col}(A)$.

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This is the most important theorem for SVD.

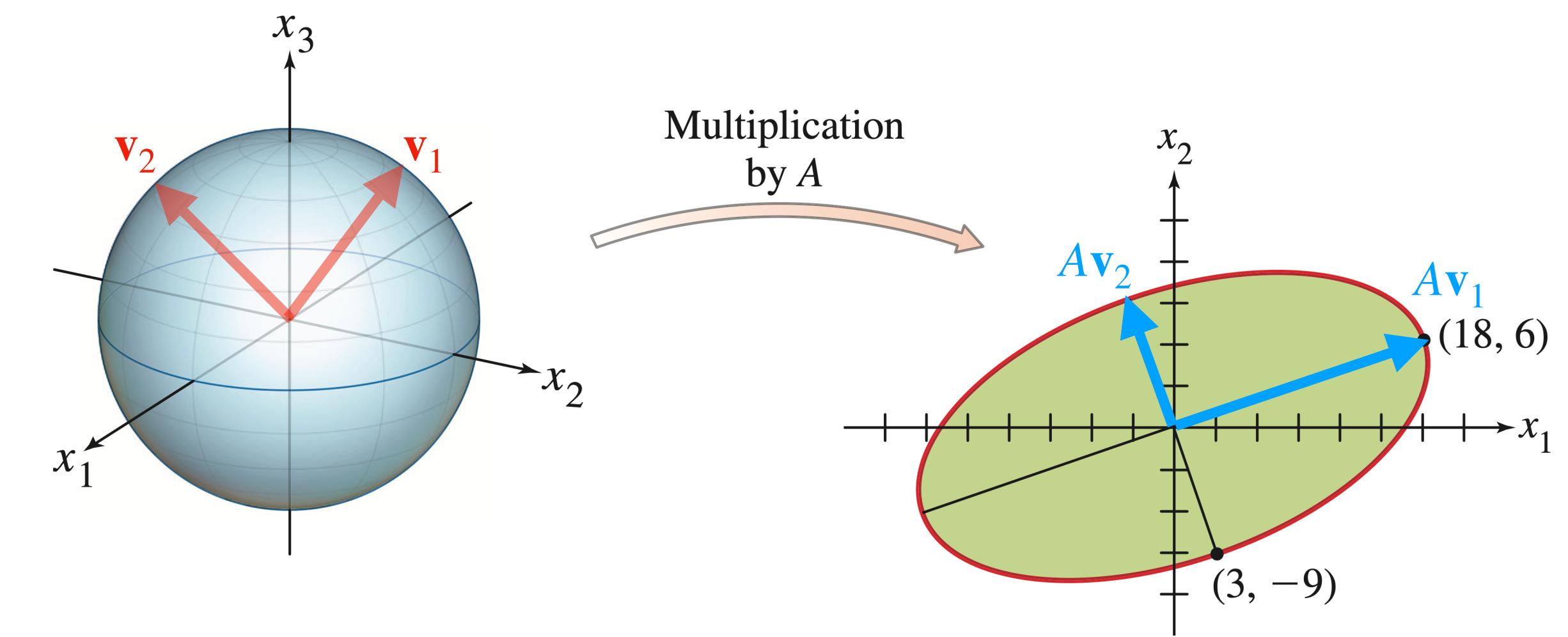
Verifying it

Let's show Av_1, \dots, Av_r are linearly independent:

Verifying it

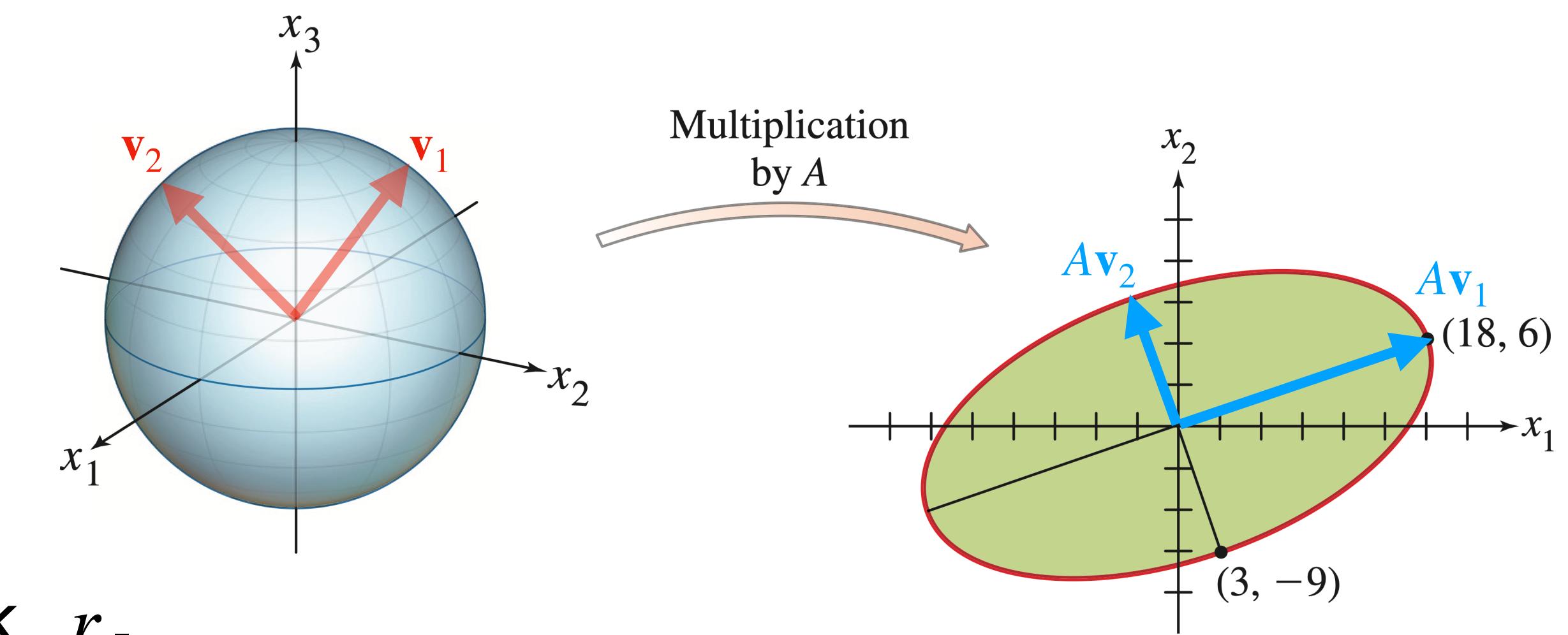
Let's show $A\mathbf{v}_1, \dots, A\mathbf{v}_r$ span $\text{Col}(A)$:

Putting it all together



Putting it all together

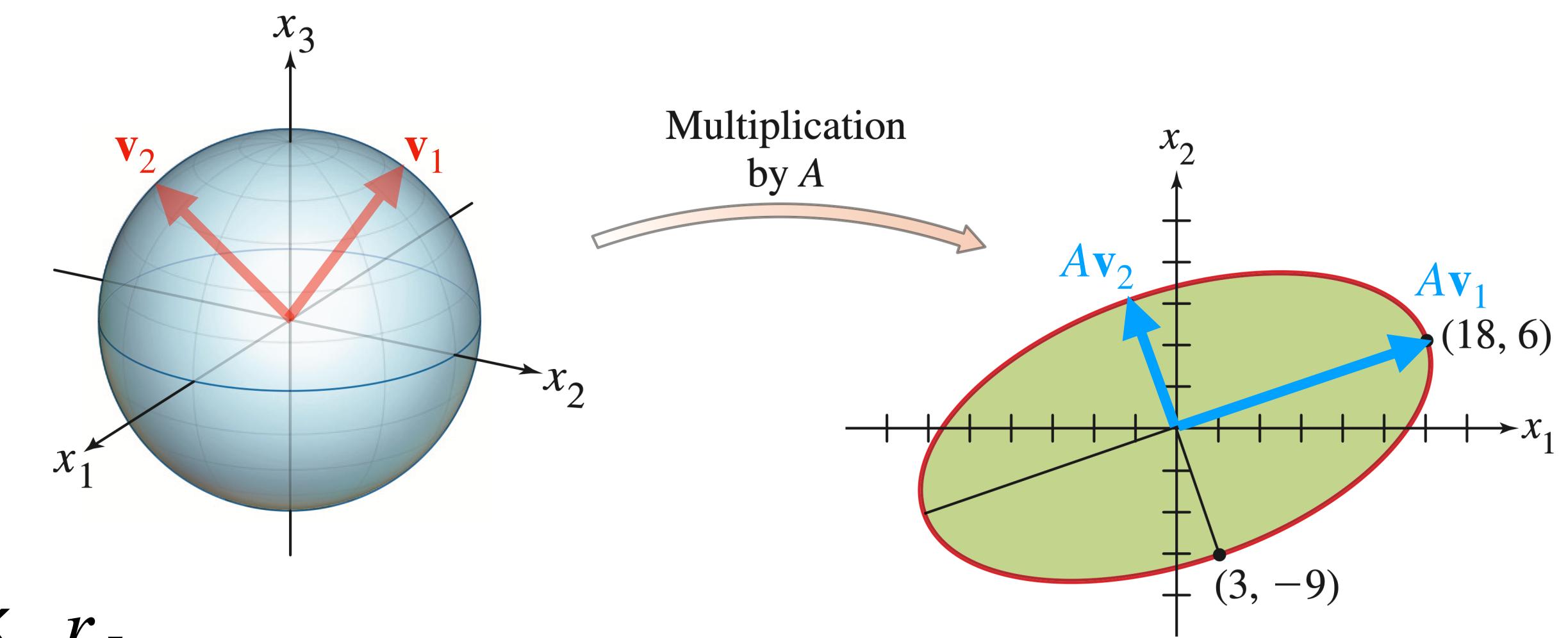
Let A be an $m \times n$ matrix of rank r .



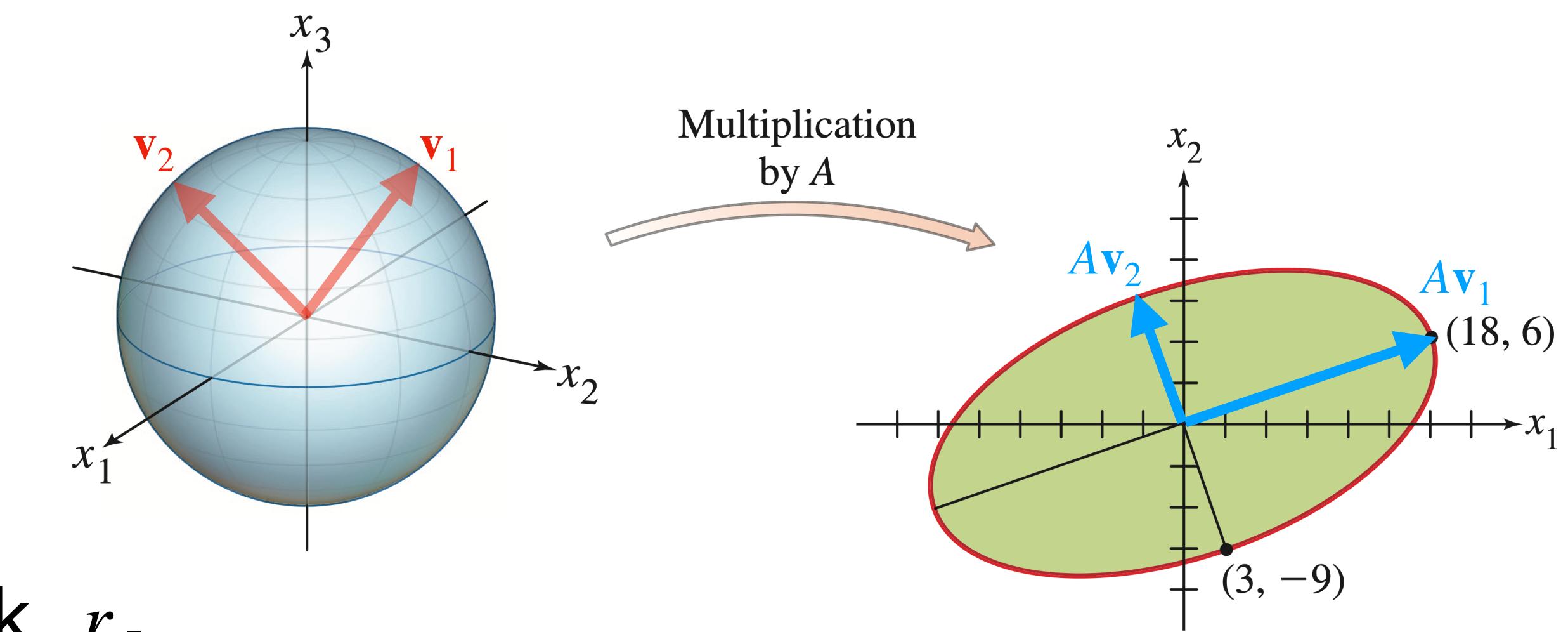
Putting it all together

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What we know:



Putting it all together

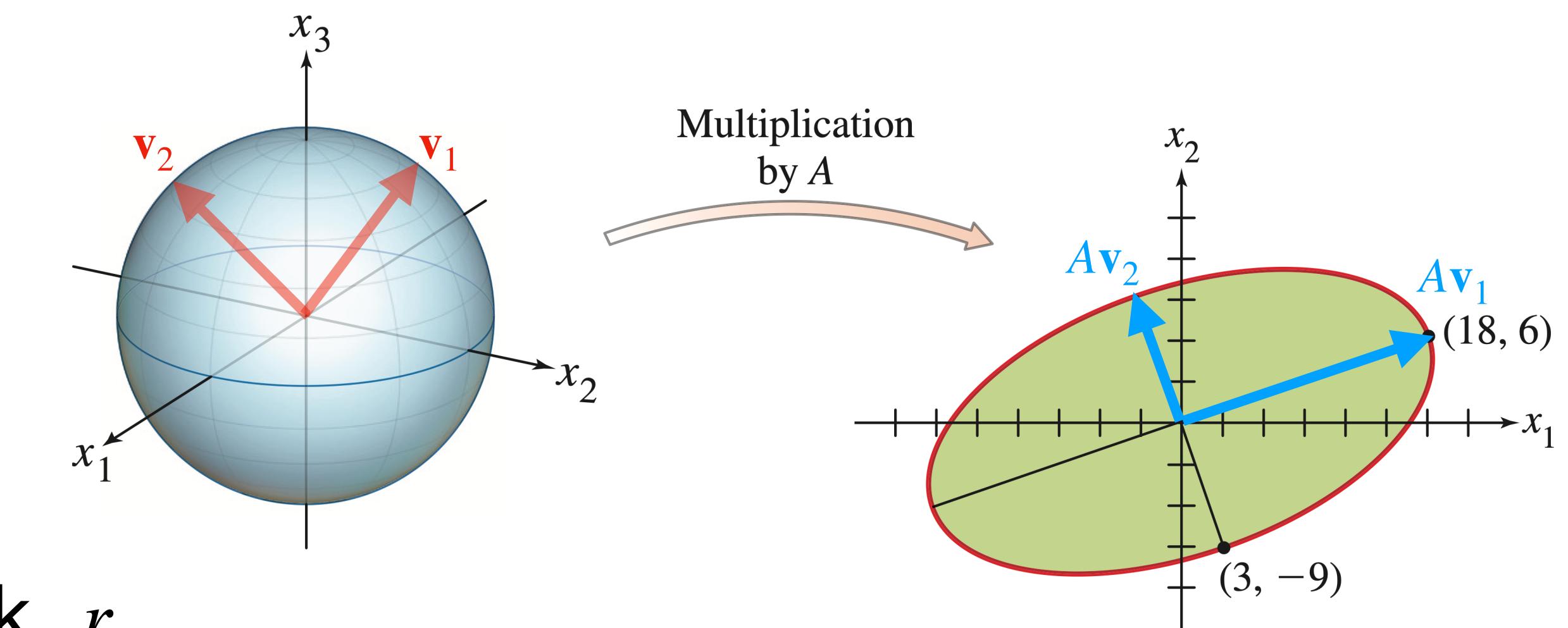


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What we know:

- » We can find orthonormal vectors v_1, \dots, v_r in \mathbb{R}^n such that Av_1, \dots, Av_r in \mathbb{R}^m form an orthogonal basis for $\text{Col}(A)$.

Putting it all together

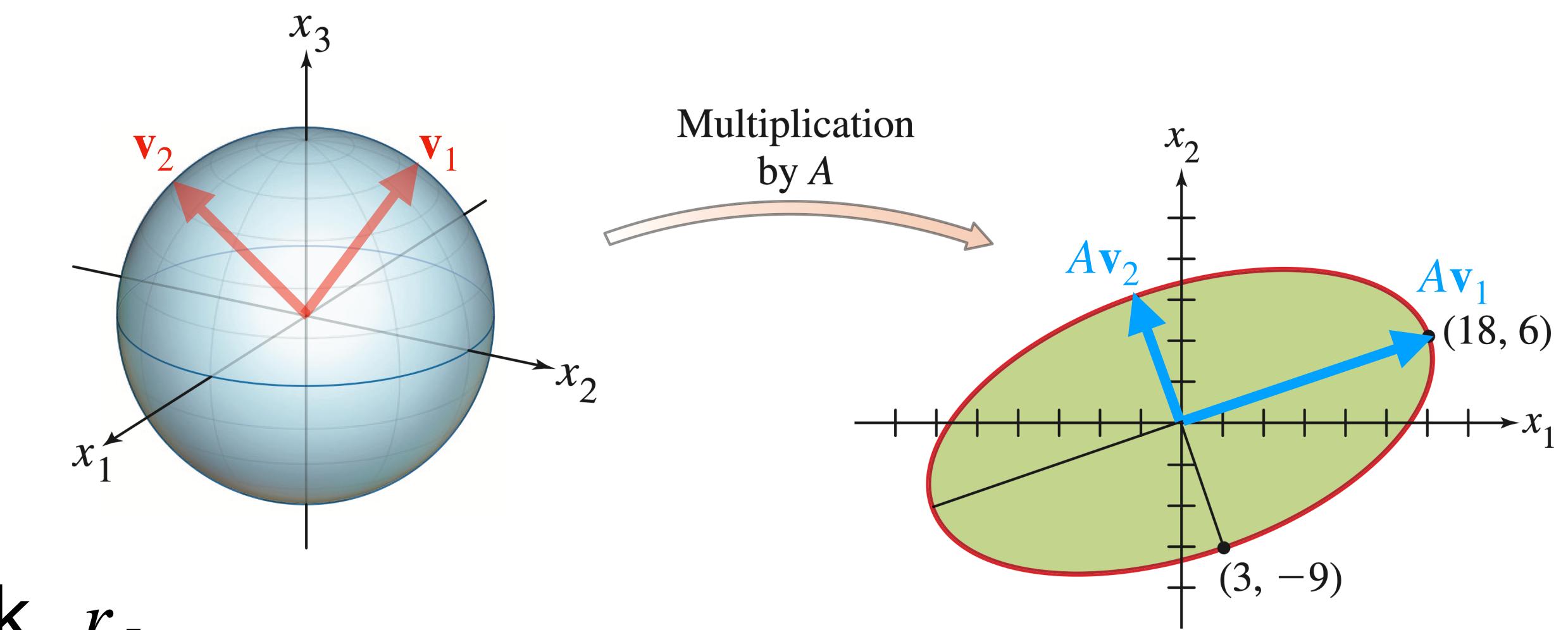


Let A be an $m \times n$ matrix of rank r .

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- » We can find orthonormal vectors v_1, \dots, v_r in \mathbb{R}^n such that Av_1, \dots, Av_r in \mathbb{R}^m form an orthogonal basis for $\text{Col}(A)$.
- » So if we take $u_i = \frac{Av_i}{\|Av_i\|}$, we get an **orthonormal** basis of $\text{Col}(A)$

Putting it all together

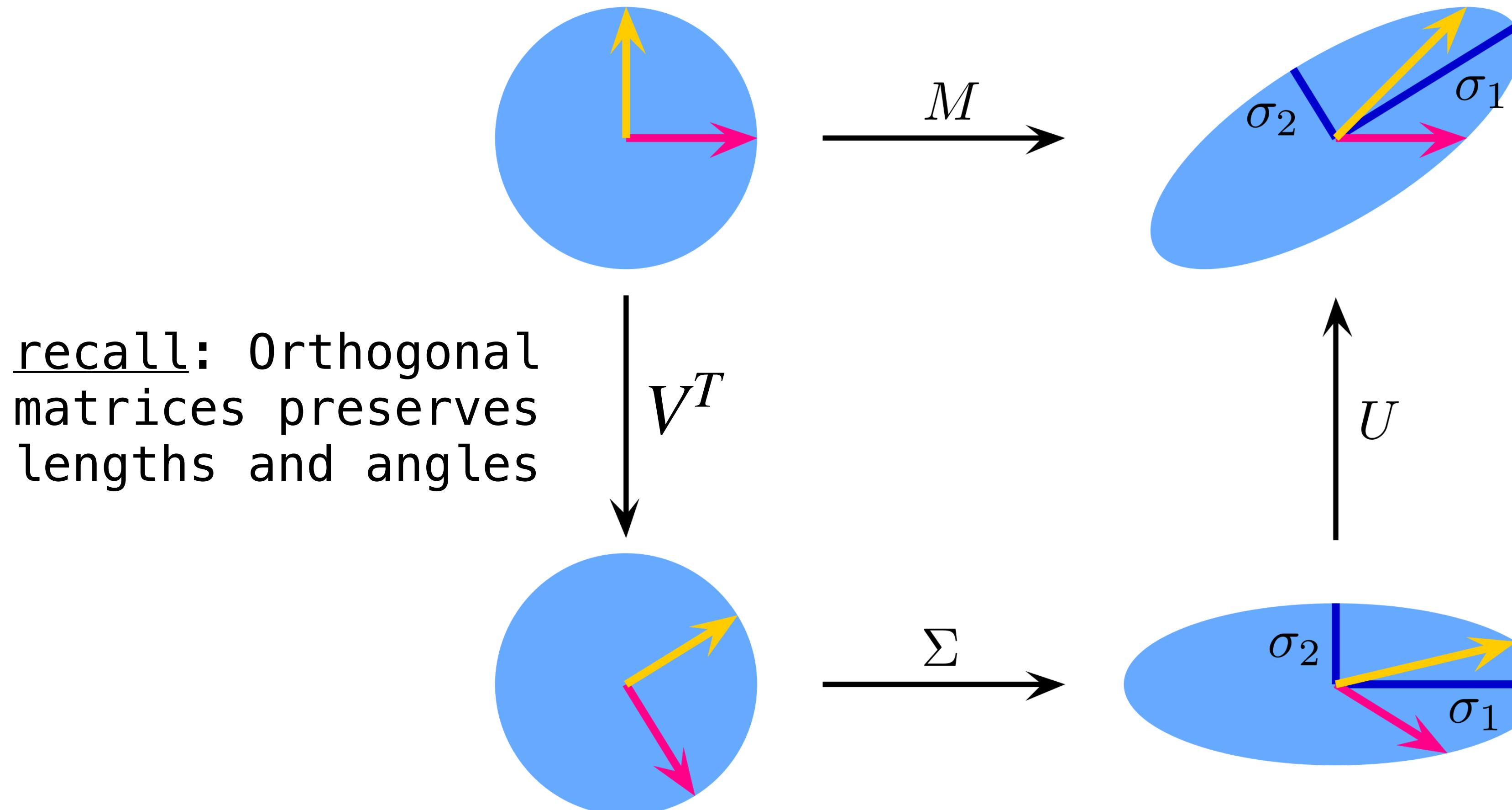


Let A be an $m \times n$ matrix of rank r .

What we know:

- » We can find orthonormal vectors v_1, \dots, v_r in \mathbb{R}^n such that Av_1, \dots, Av_r in \mathbb{R}^m form an orthogonal basis for $\text{Col}(A)$.
- » So if we take $u_i = \frac{Av_i}{\|Av_i\|}$, we get an **orthonormal** basis of $\text{Col}(A)$
- » And we can extend this to u_1, \dots, 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

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

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

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

Let's take $V = [\mathbf{v}_1 \dots \mathbf{v}_n]$ and $U = [\mathbf{u}_1 \dots \mathbf{u}_m]$ and

The Important Equality

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$$\Sigma = \begin{bmatrix} \sigma_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_n \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix} \quad \text{or} \quad \Sigma = \begin{bmatrix} \sigma_1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_m & 0 & \dots & 0 \end{bmatrix} \quad \text{or} \quad \Sigma = \begin{bmatrix} \sigma_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_n \end{bmatrix}$$

$m > n$

$m < n$

$m = n$

The Important Equality

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

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The Important Equality

$$AV = U\Sigma$$

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

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$m > n$ $m < n$ $m = n$

The Important Equality

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

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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The Important Equality

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

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The Important Equality

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

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

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.

Singular Value Decomposition

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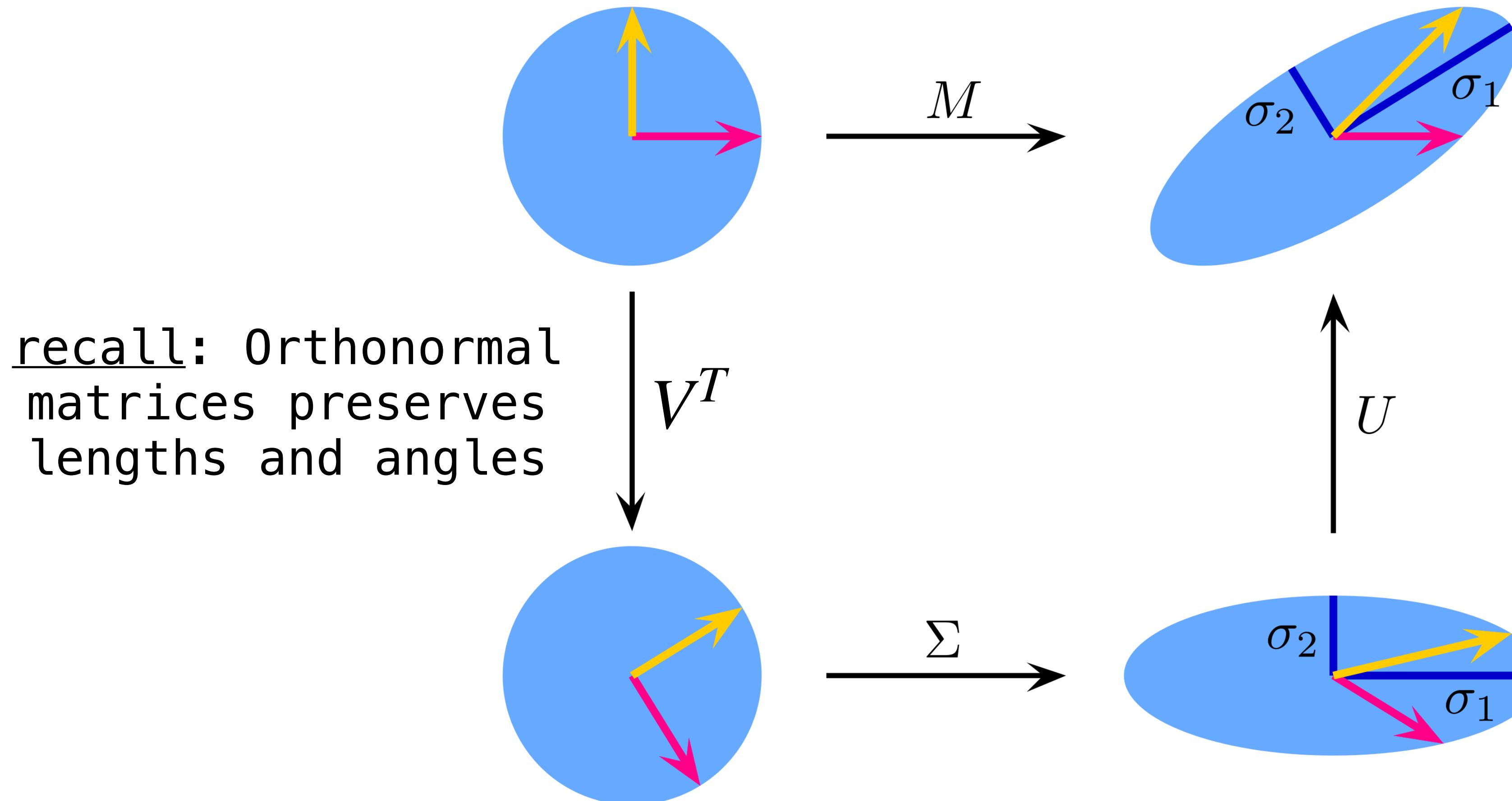
left singular vectors **right singular vectors**

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

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

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The Picture (Again)

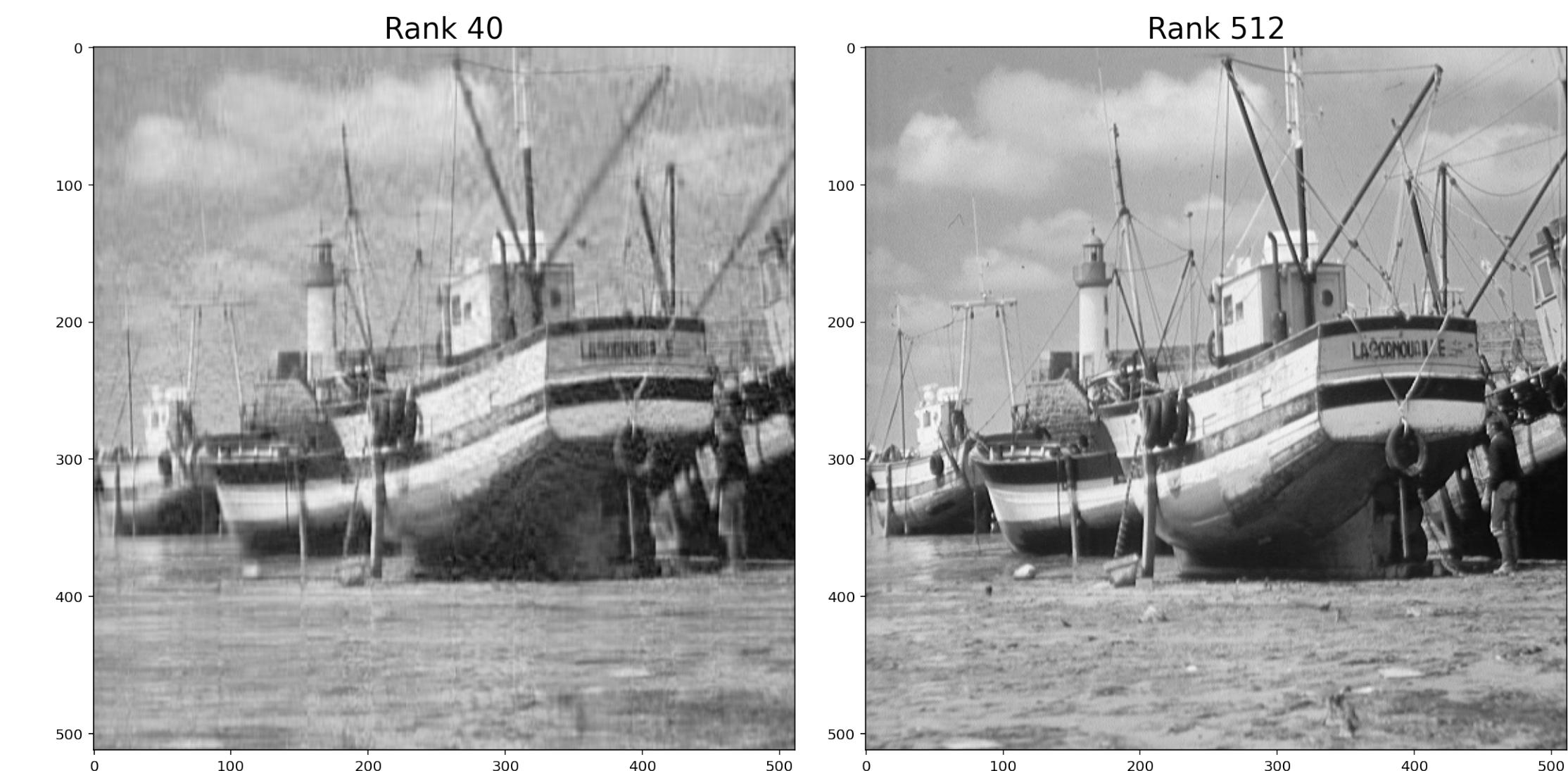


$$M = U \cdot \Sigma \cdot V^T$$

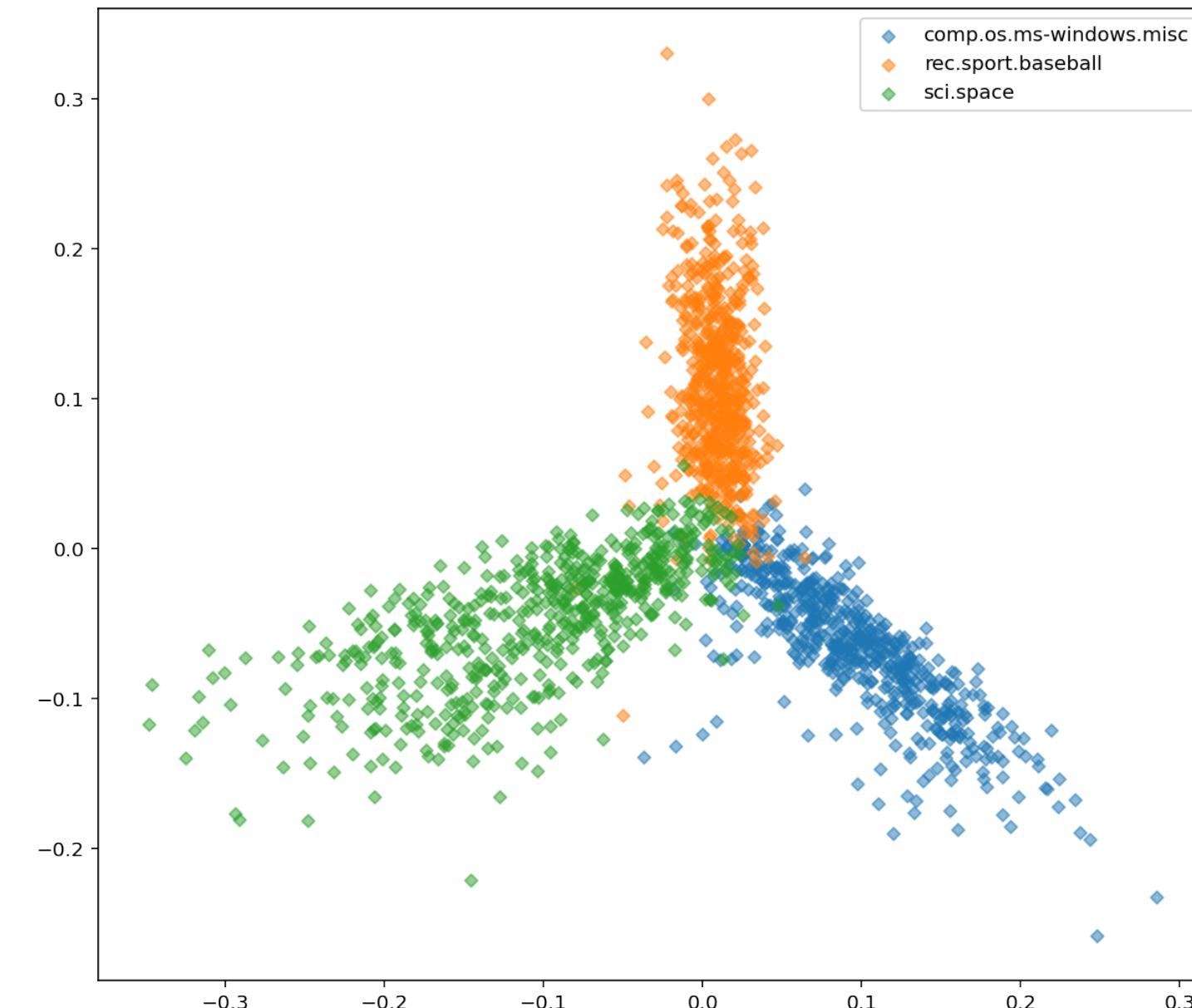
**What's next?
A couple final thoughts**

Applications of SVD

image compression



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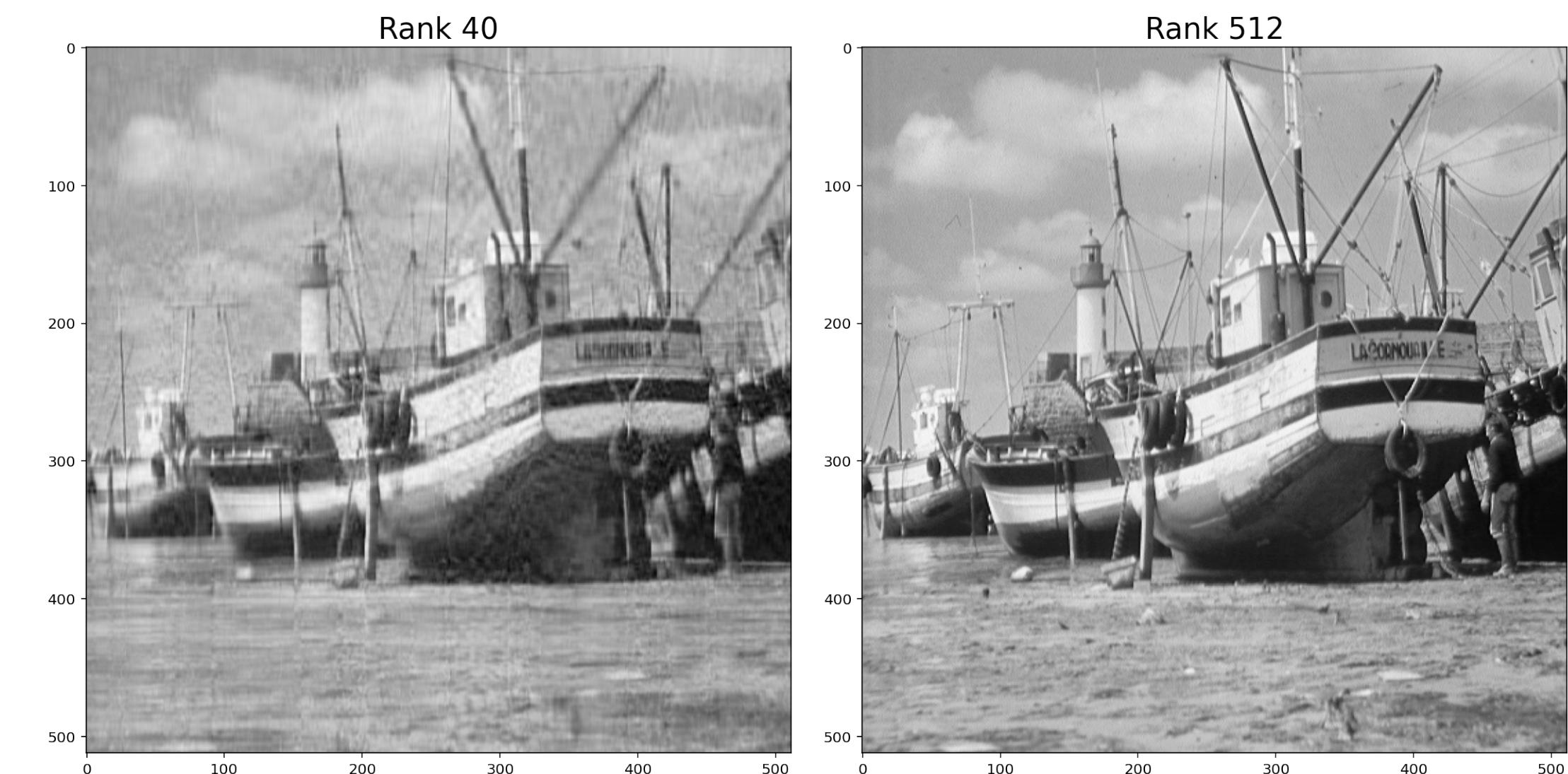


document
classification

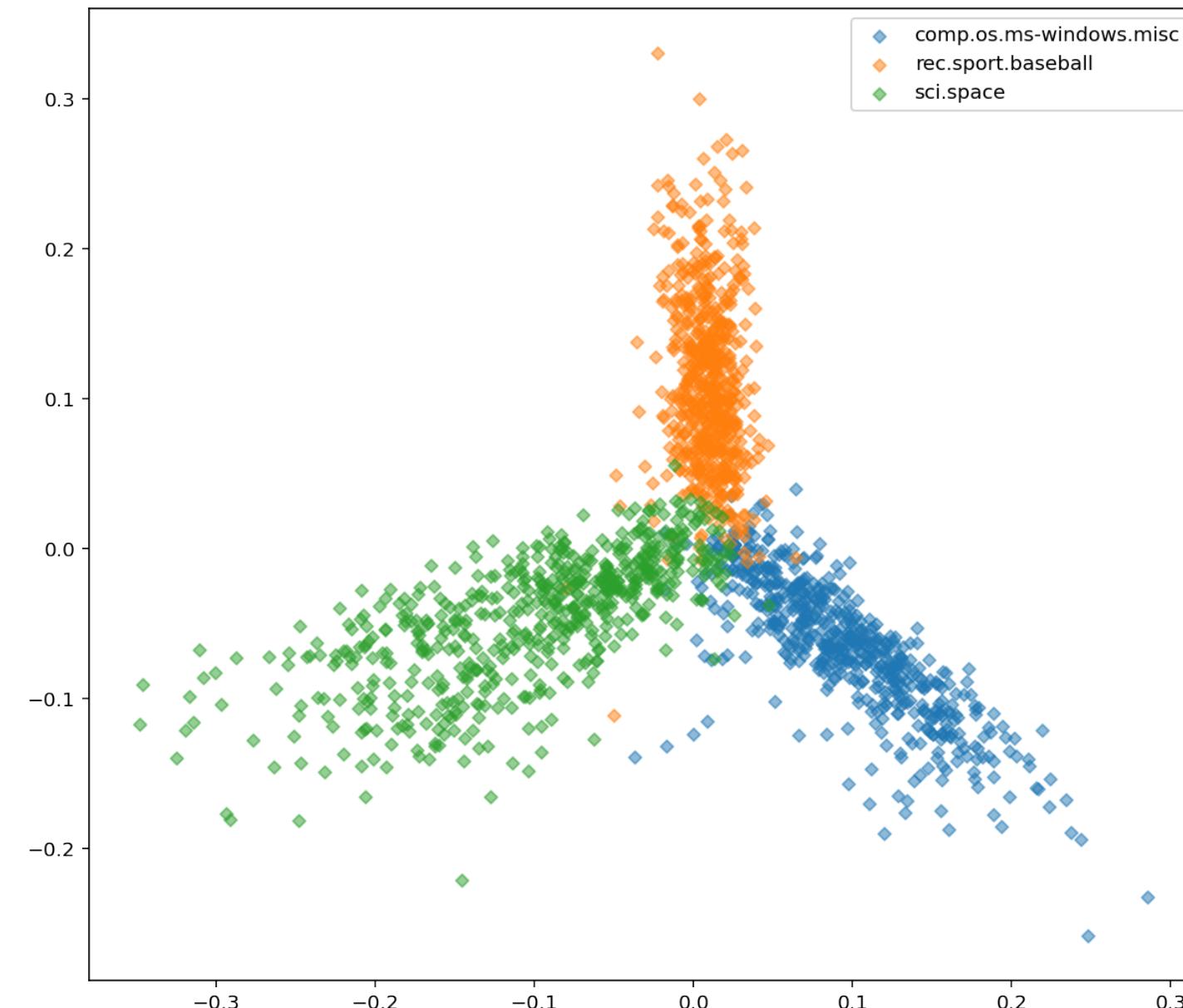
Applications of SVD

- Reduced SVD, pseudoinverses and least squares

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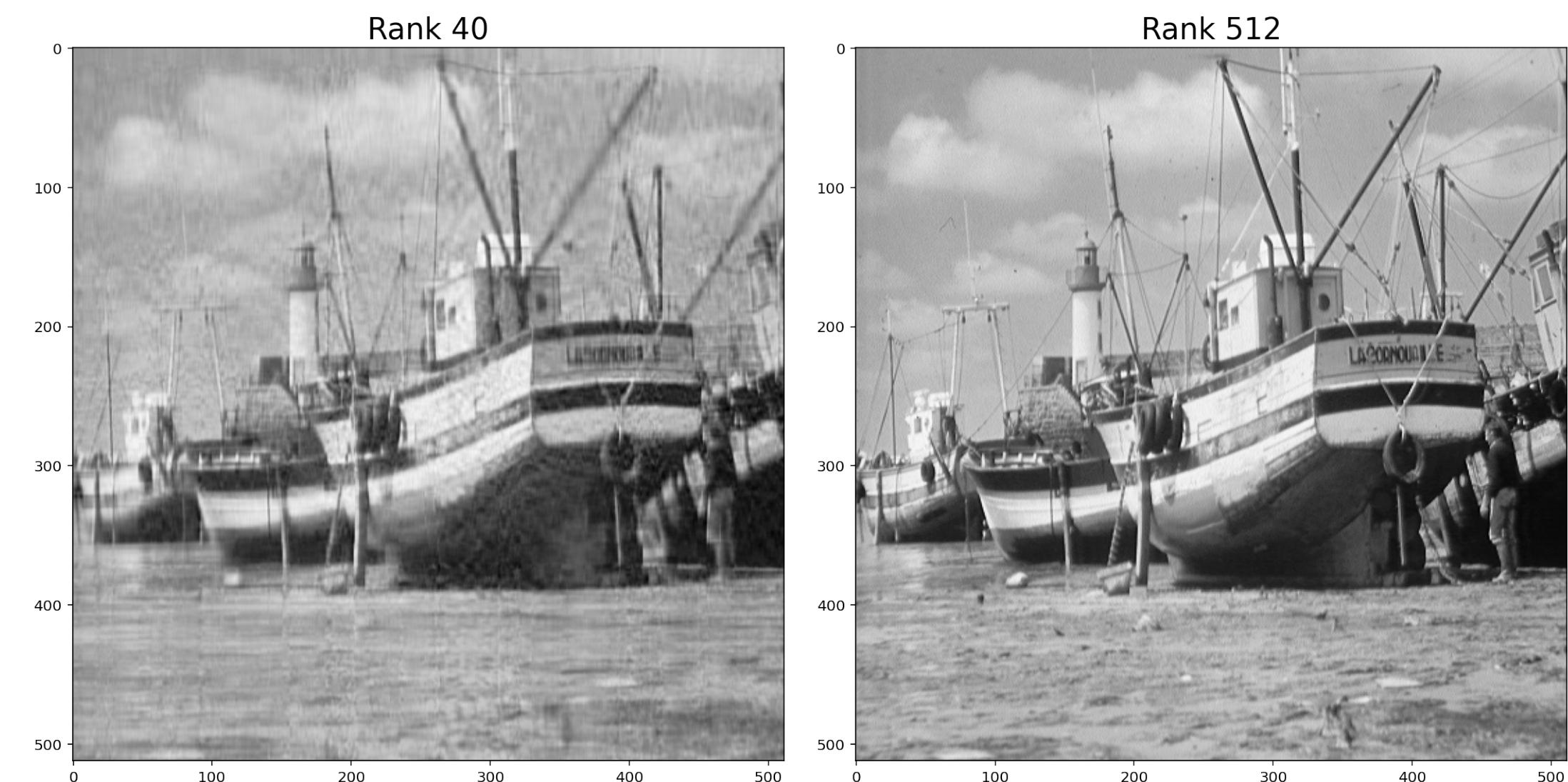


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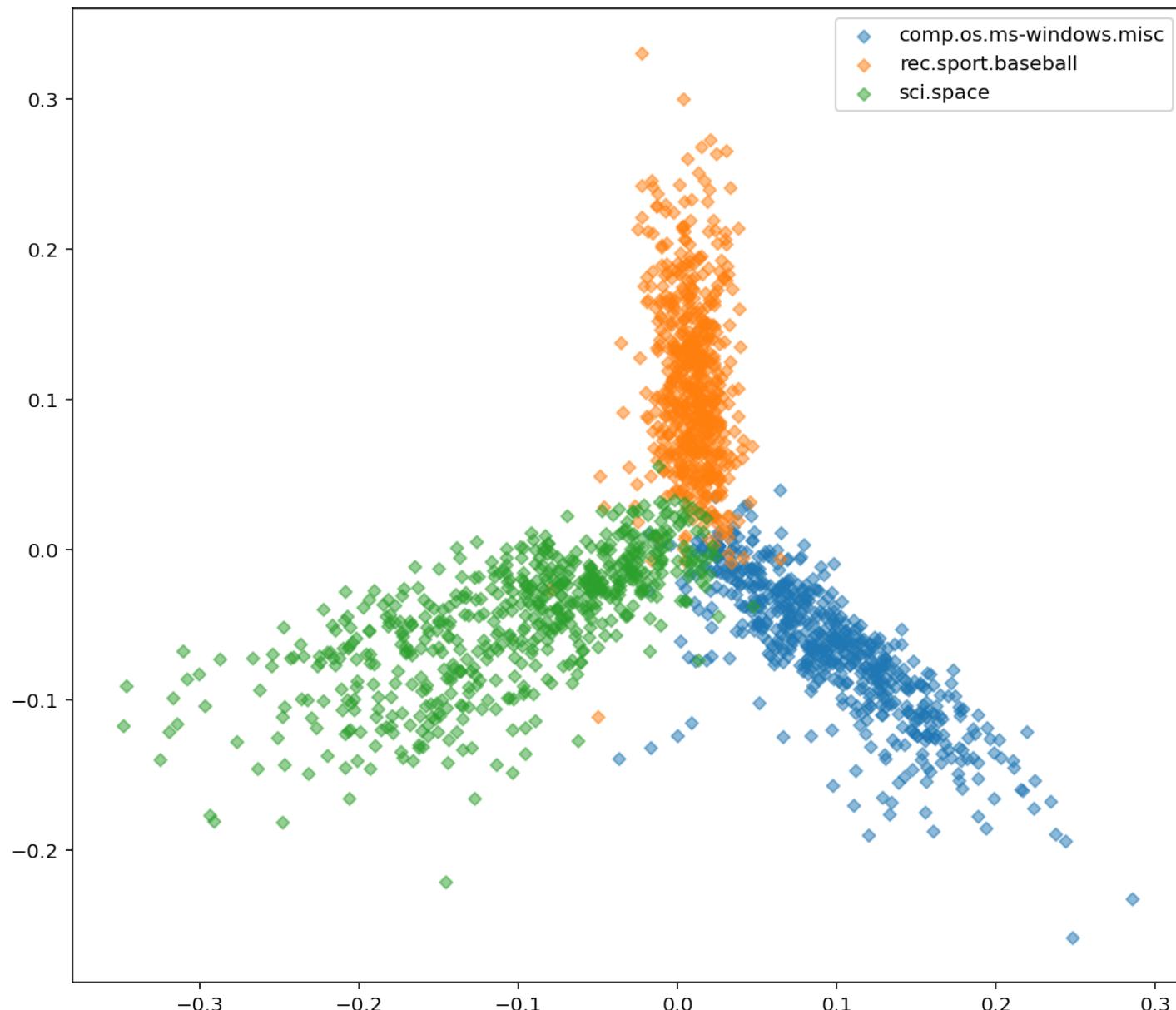
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- Reduced SVD, pseudoinverses and least squares
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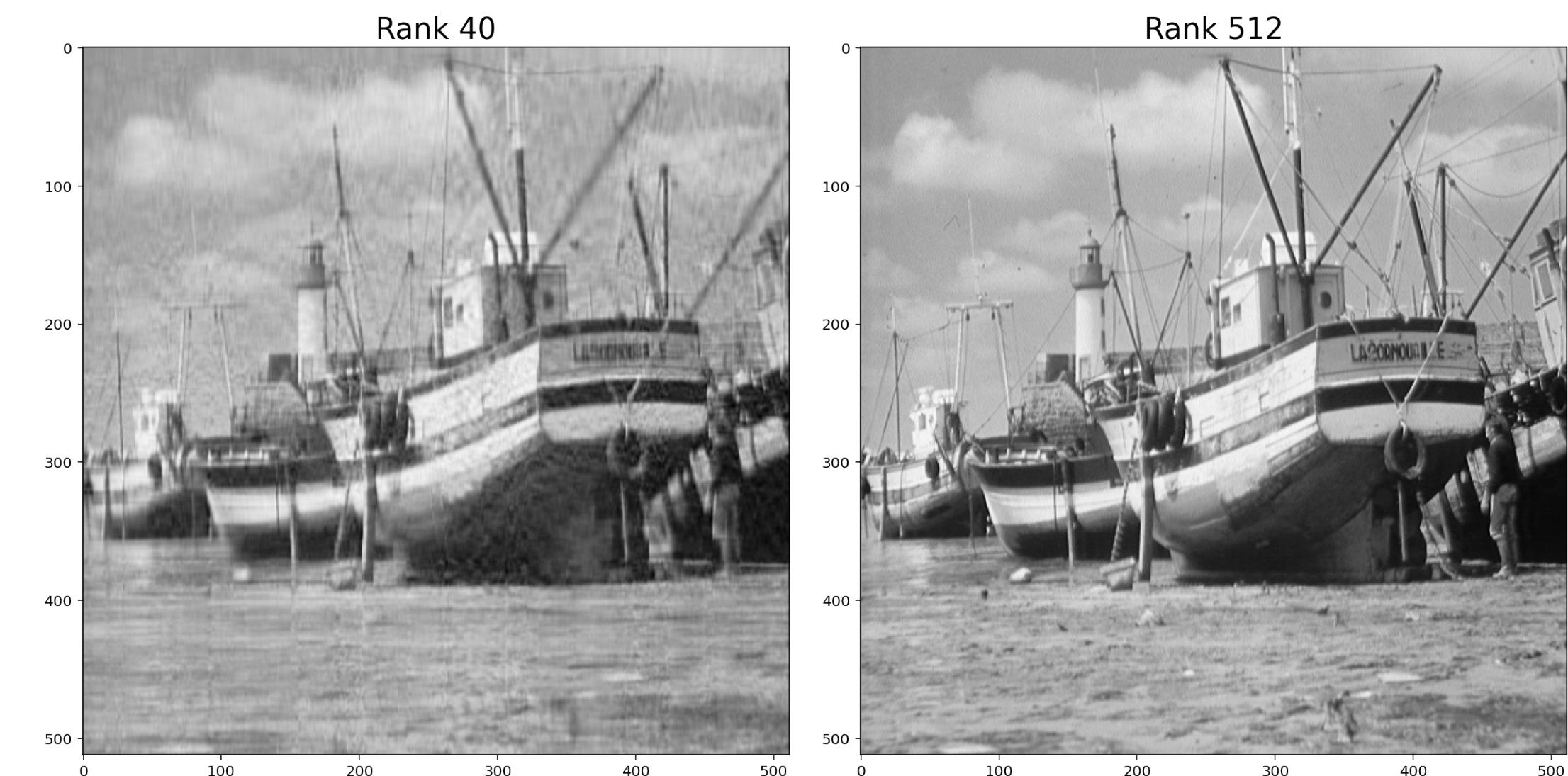


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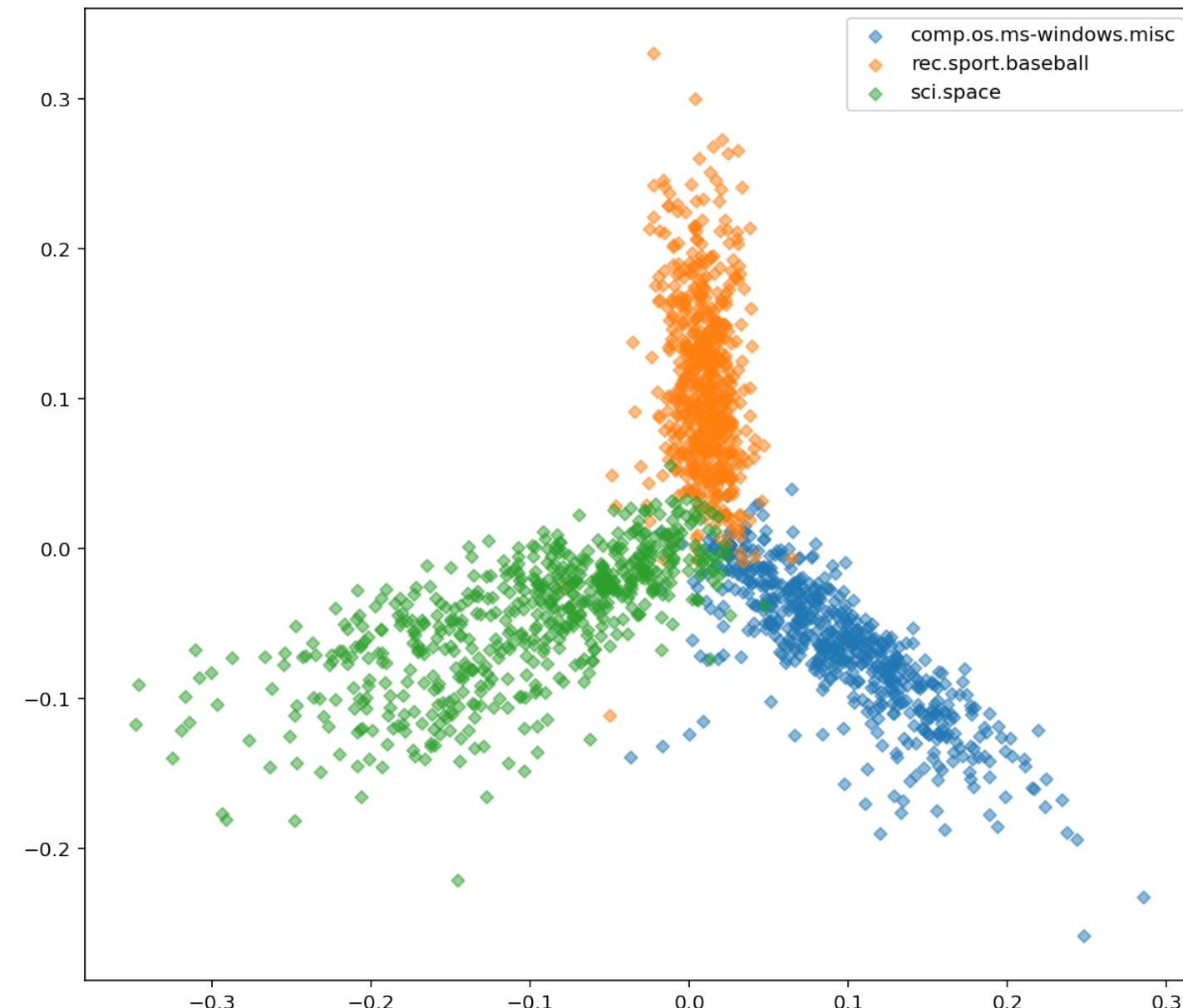
Applications of SVD

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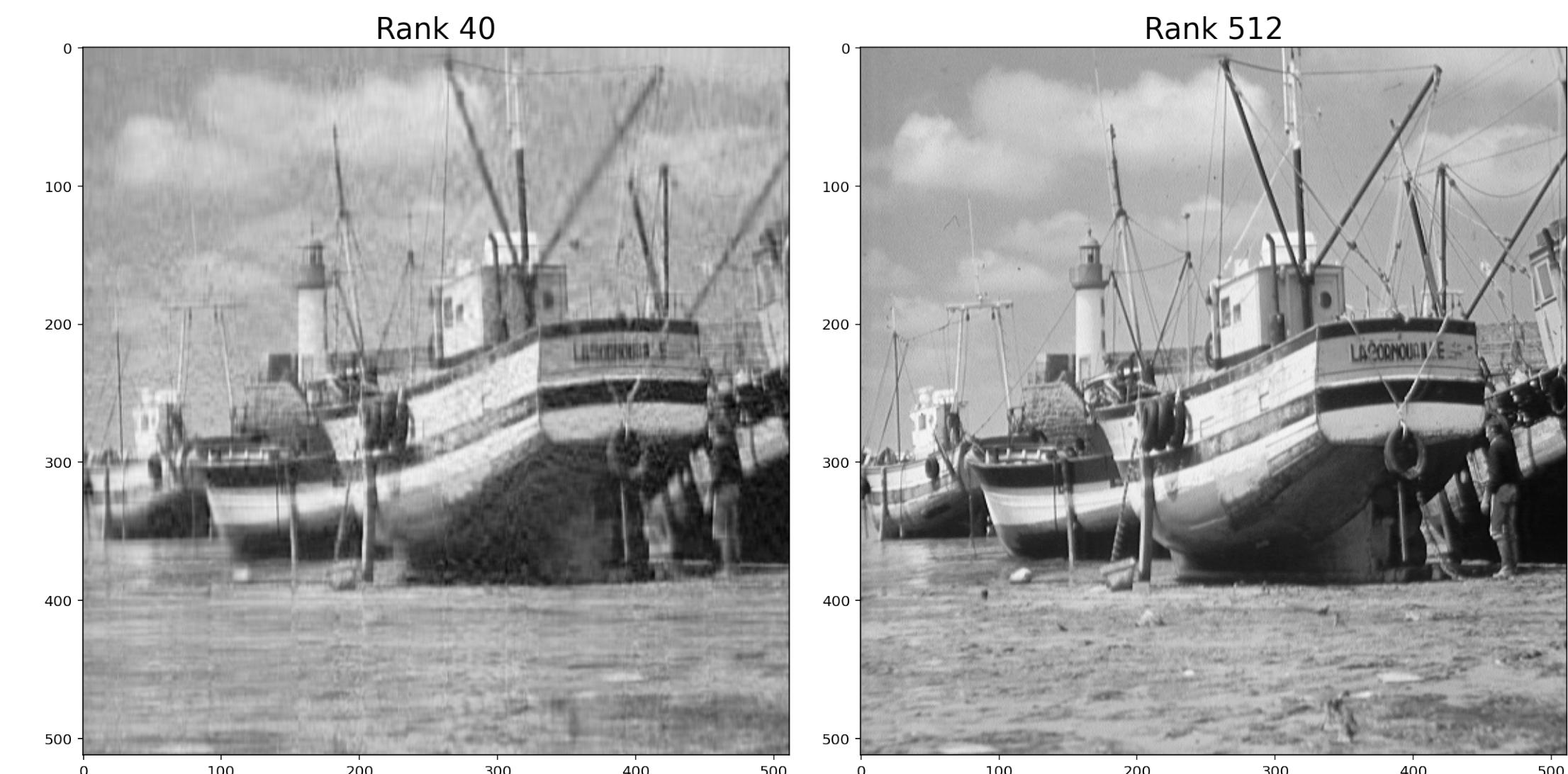


document classification

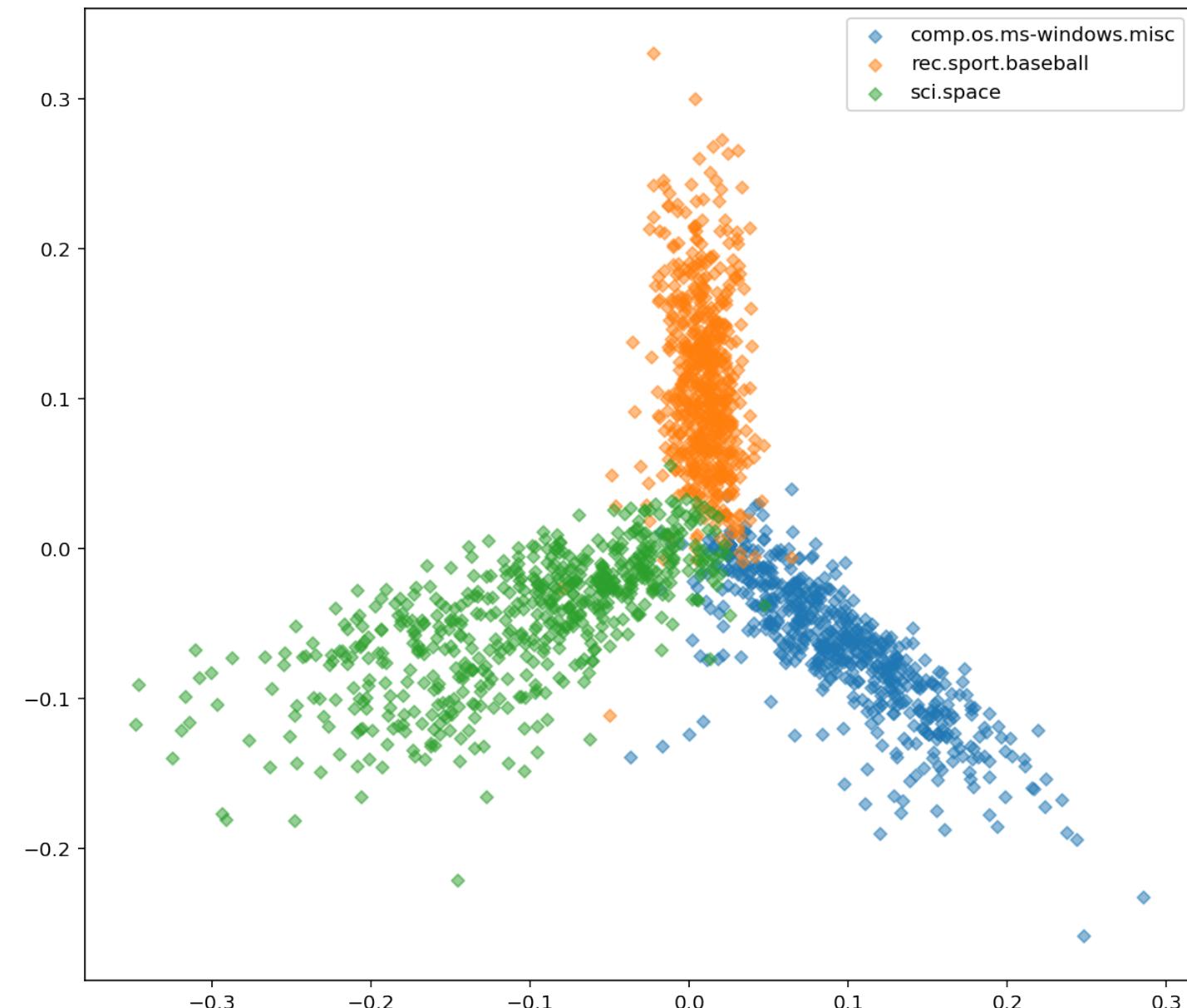
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image compression



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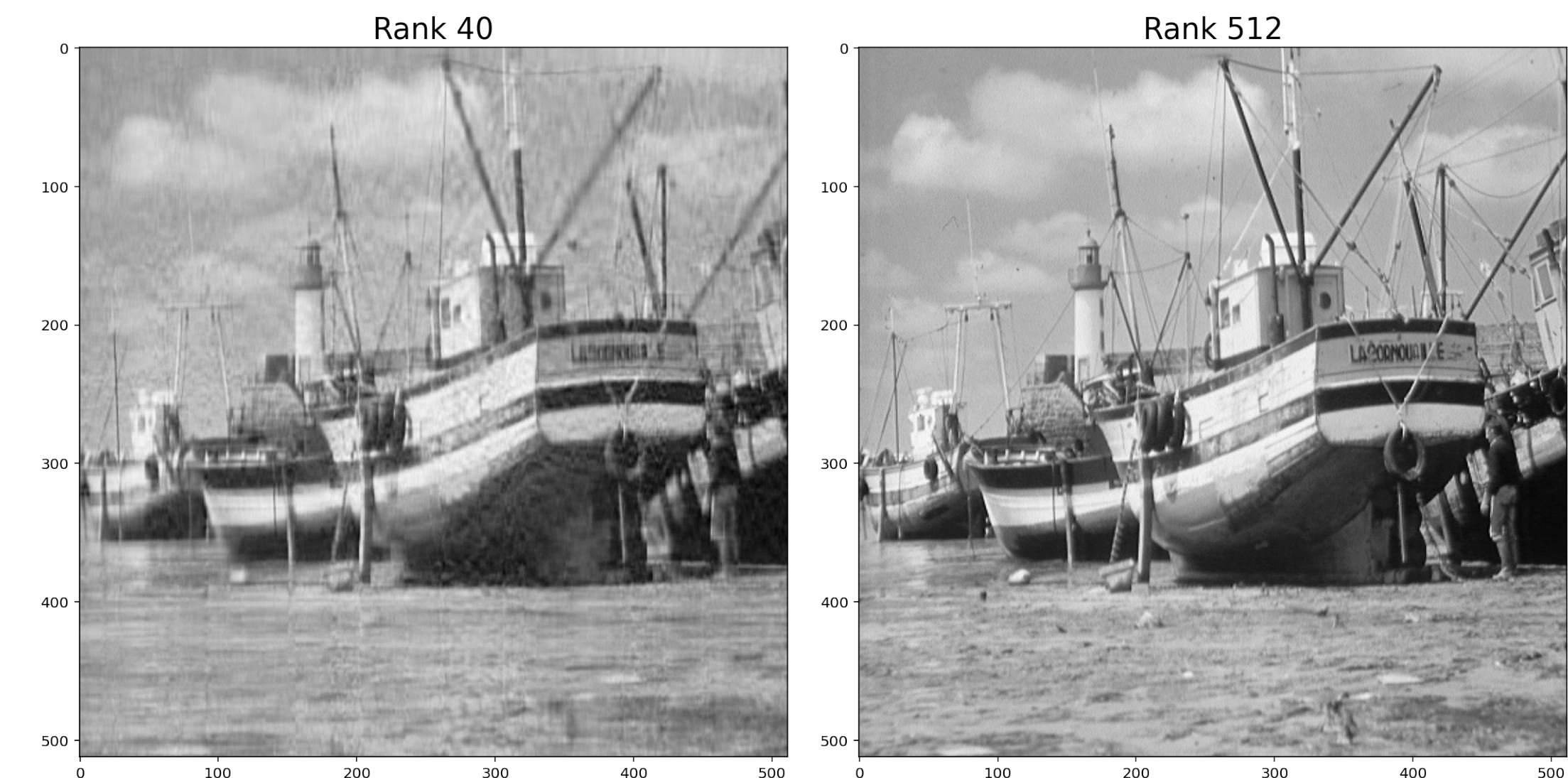


document classification

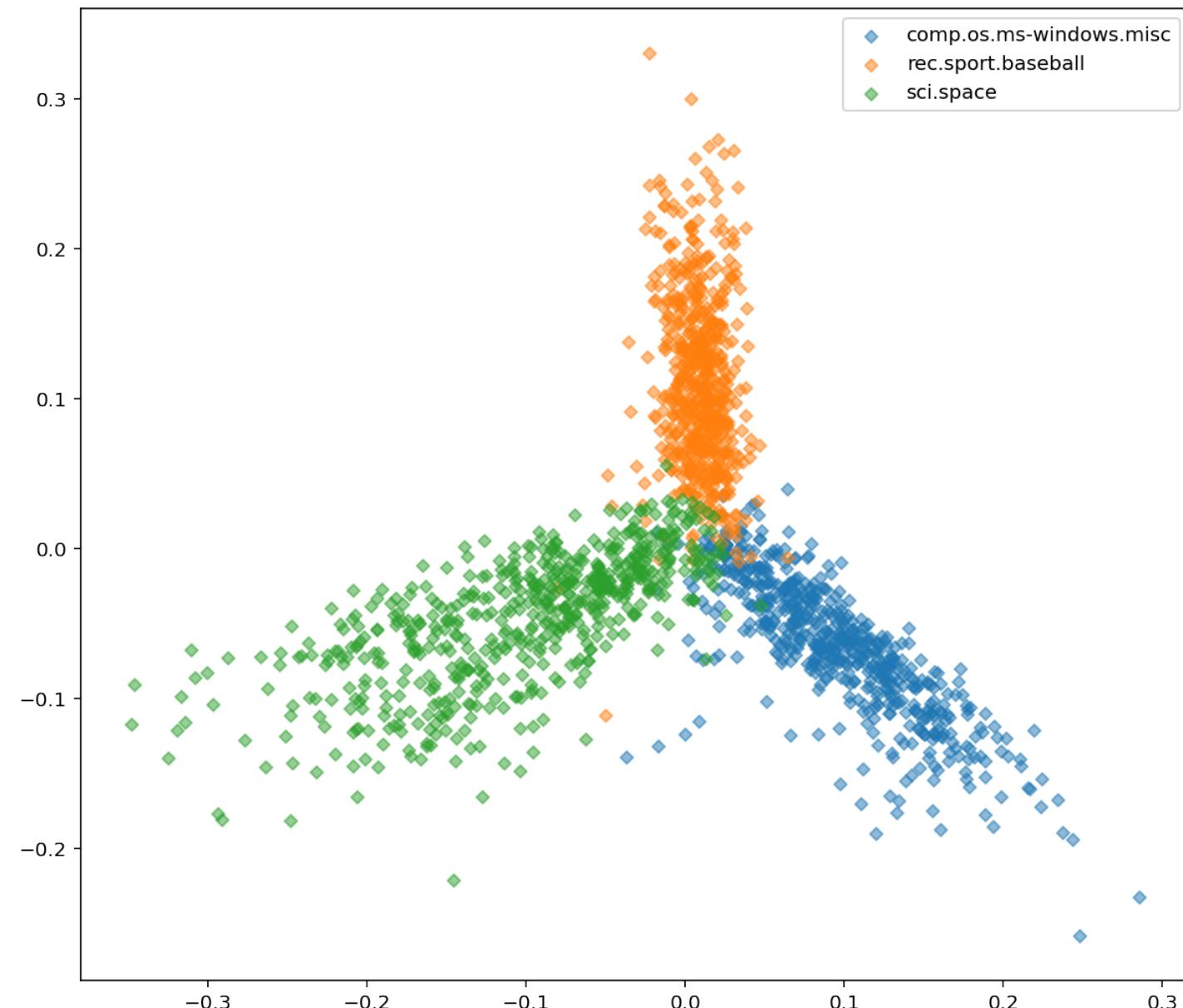
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image compression



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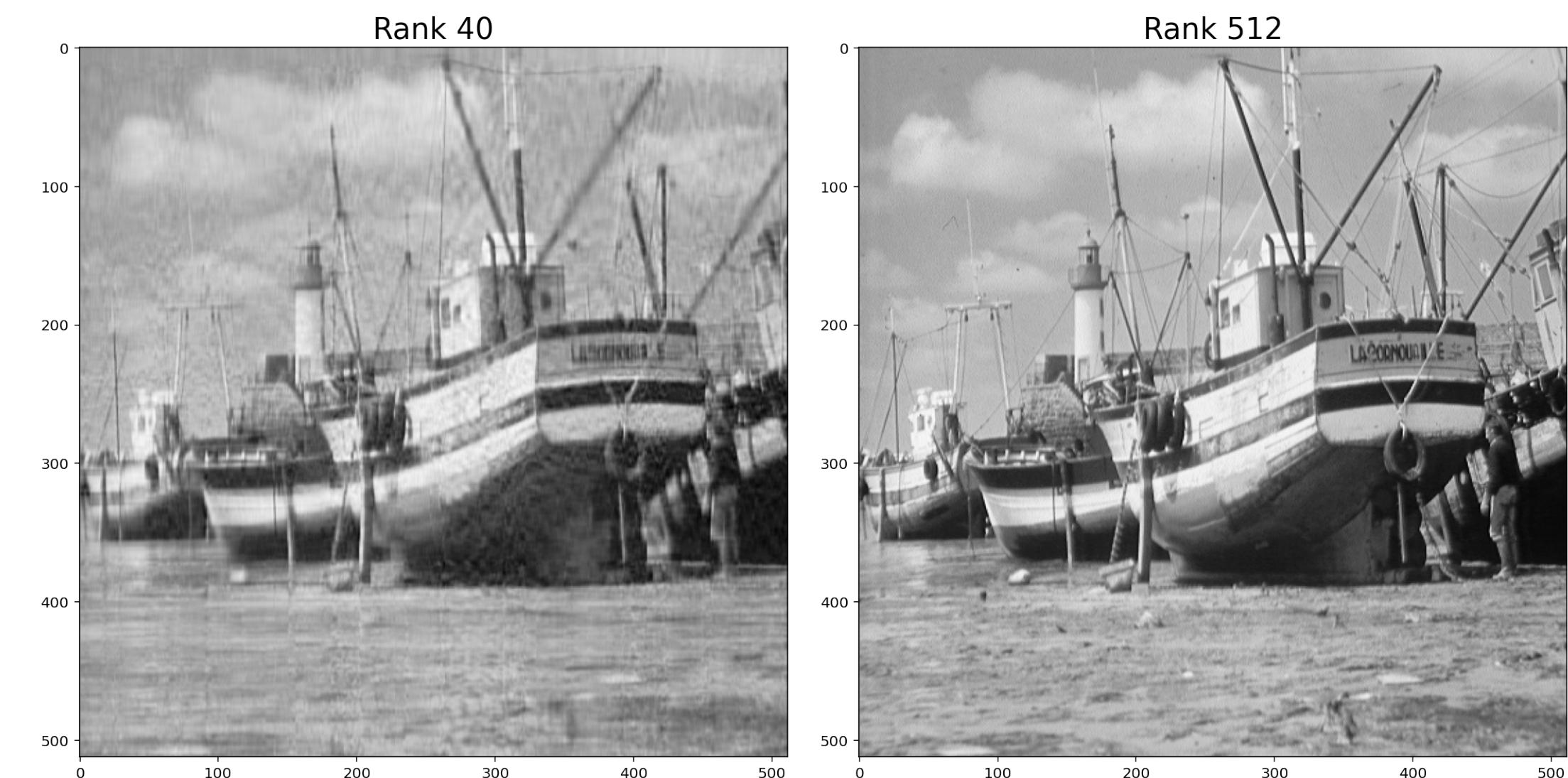


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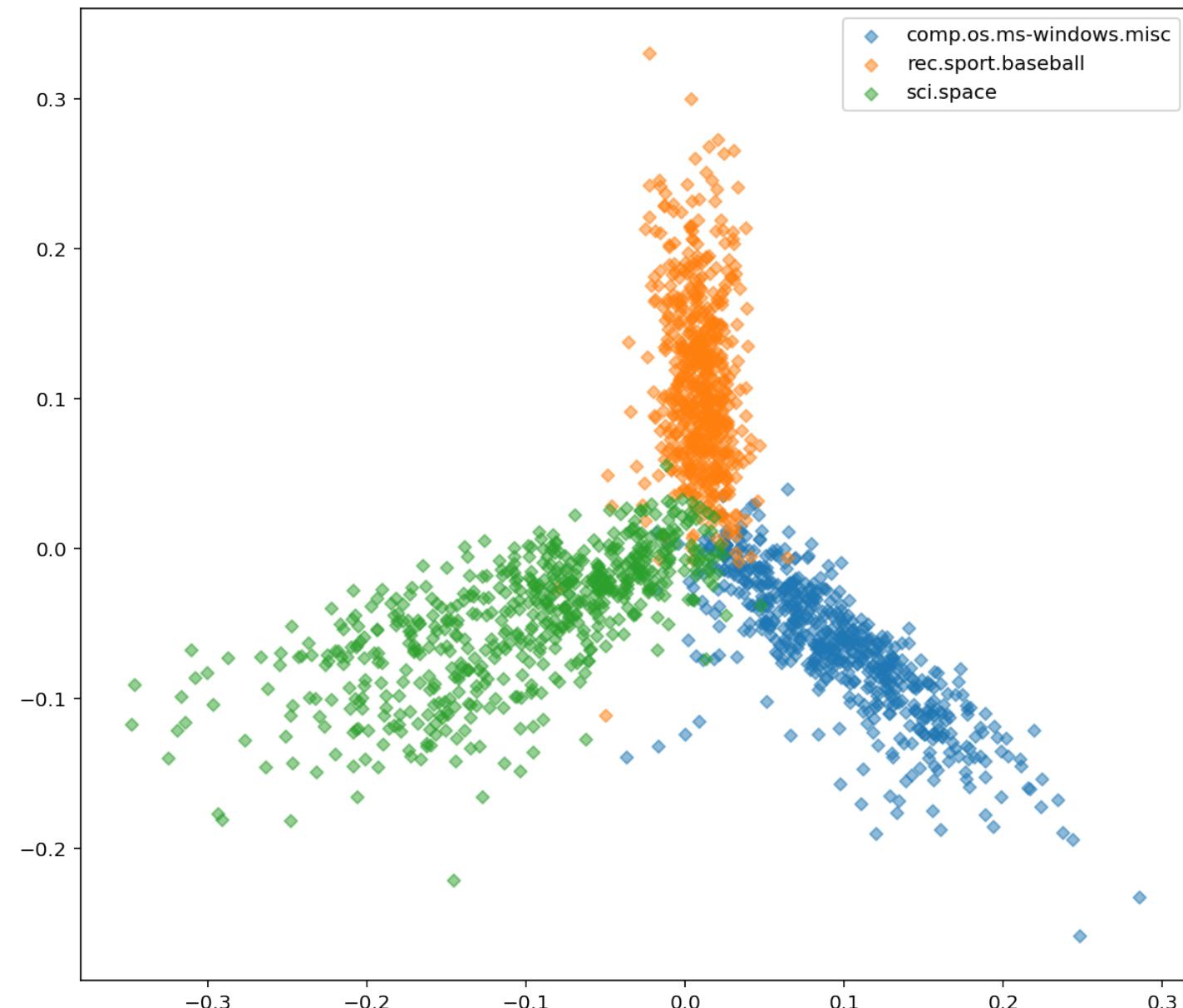
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image compression



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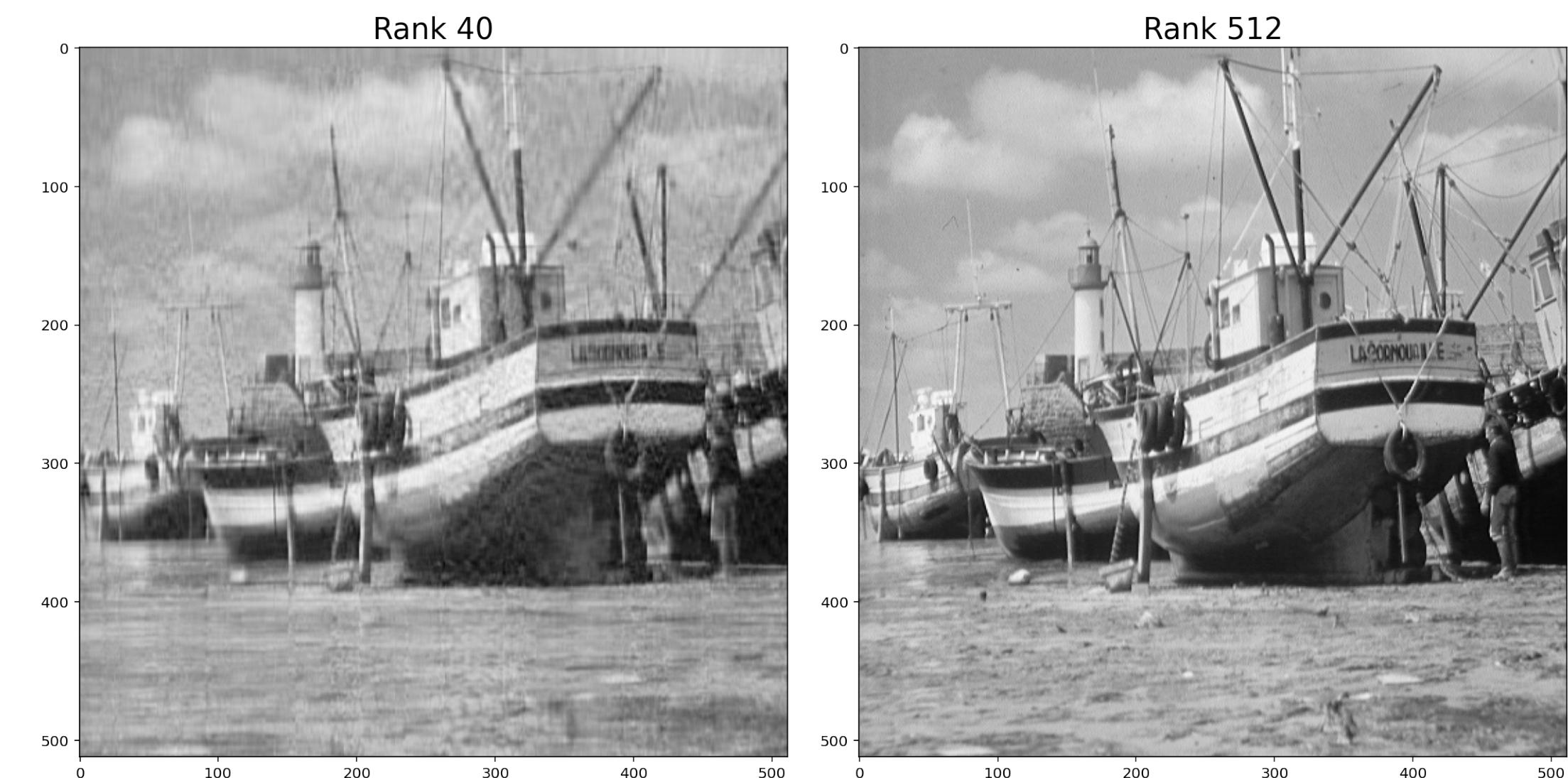


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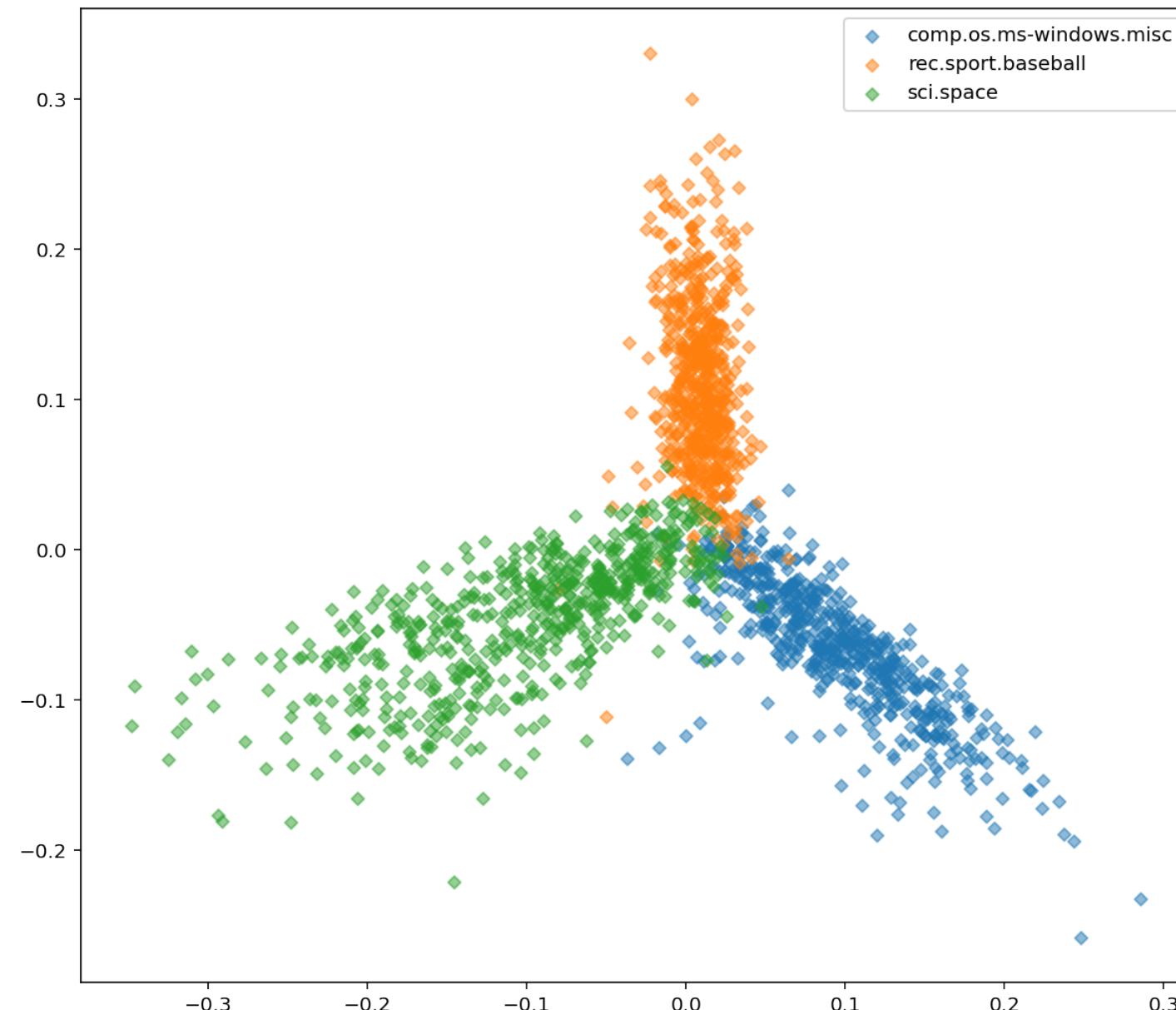
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 - Large singular vectors are "most affected."

image compression



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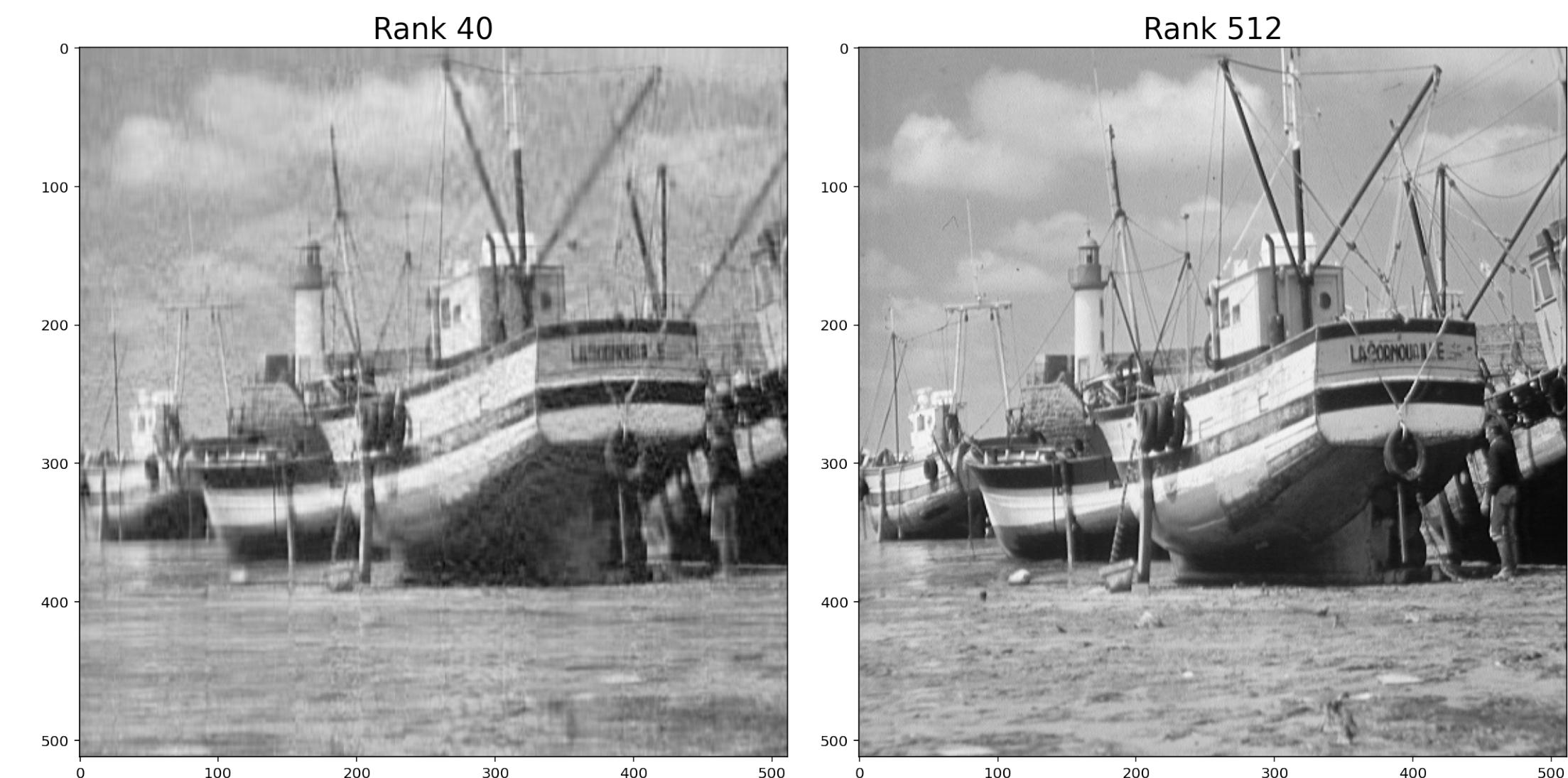


document classification

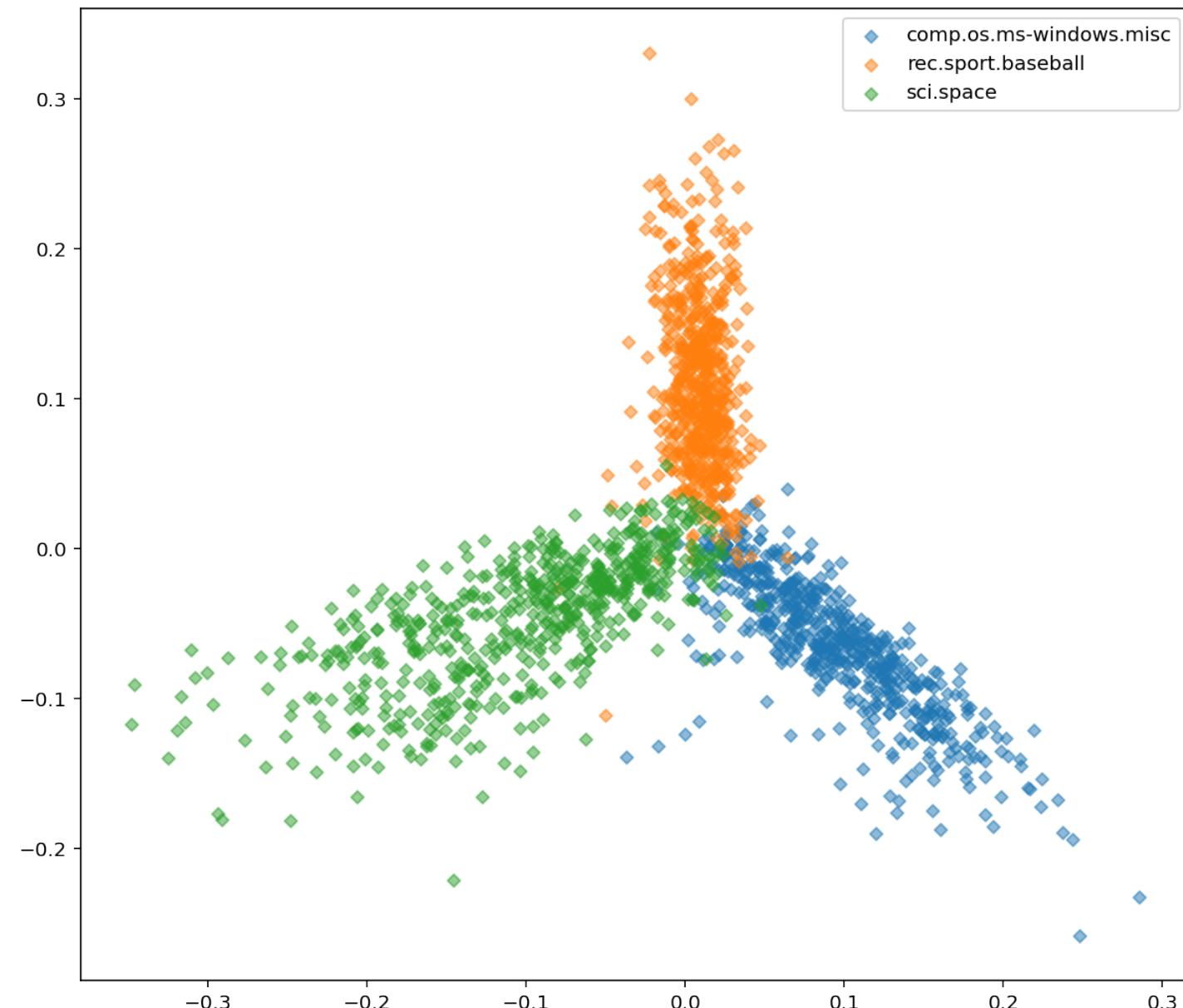
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 - This is used for image compression
- Principle Component Analysis
 - Large singular vectors are "most affected."
 - These are good vectors to look at for classifying data

image compression

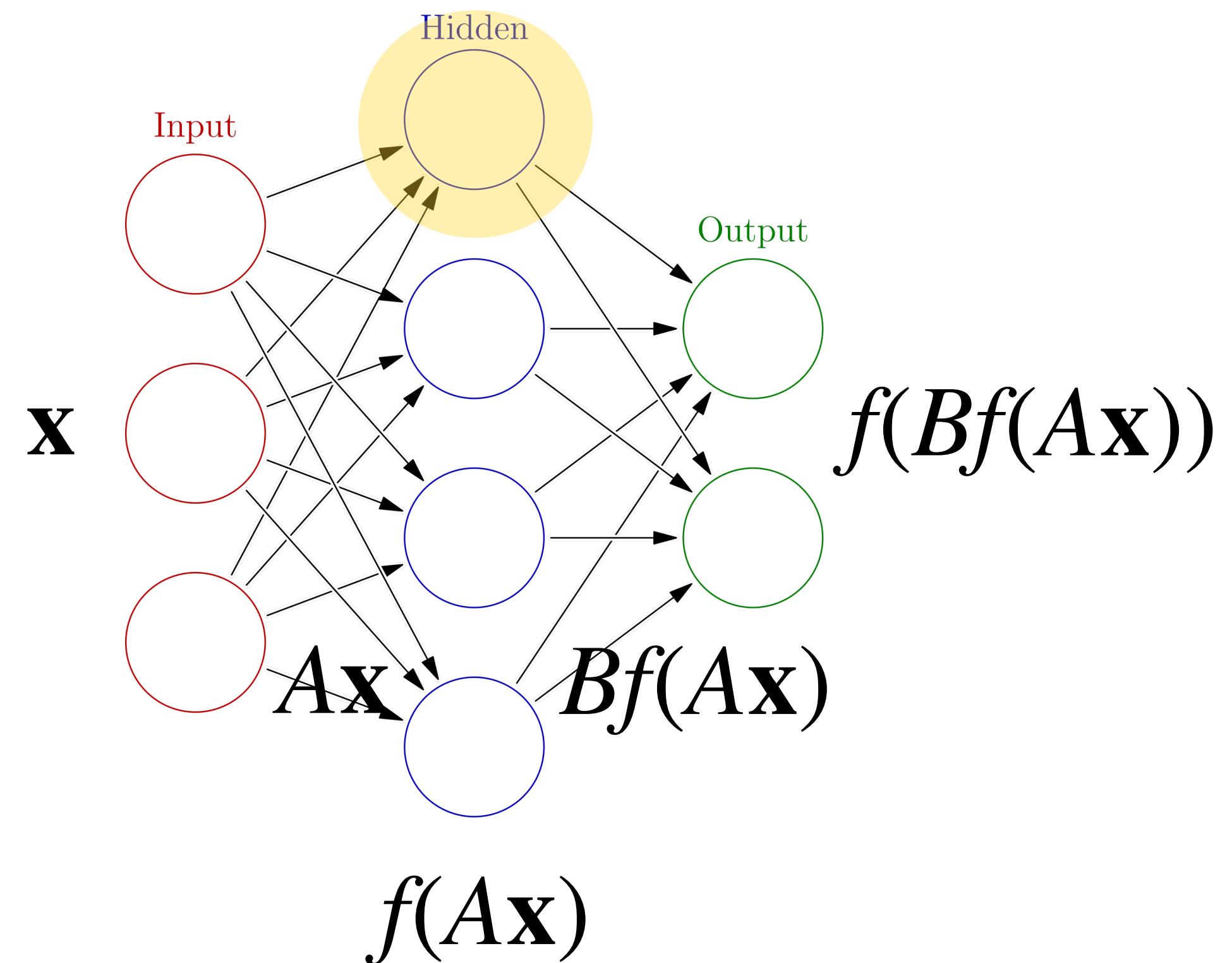
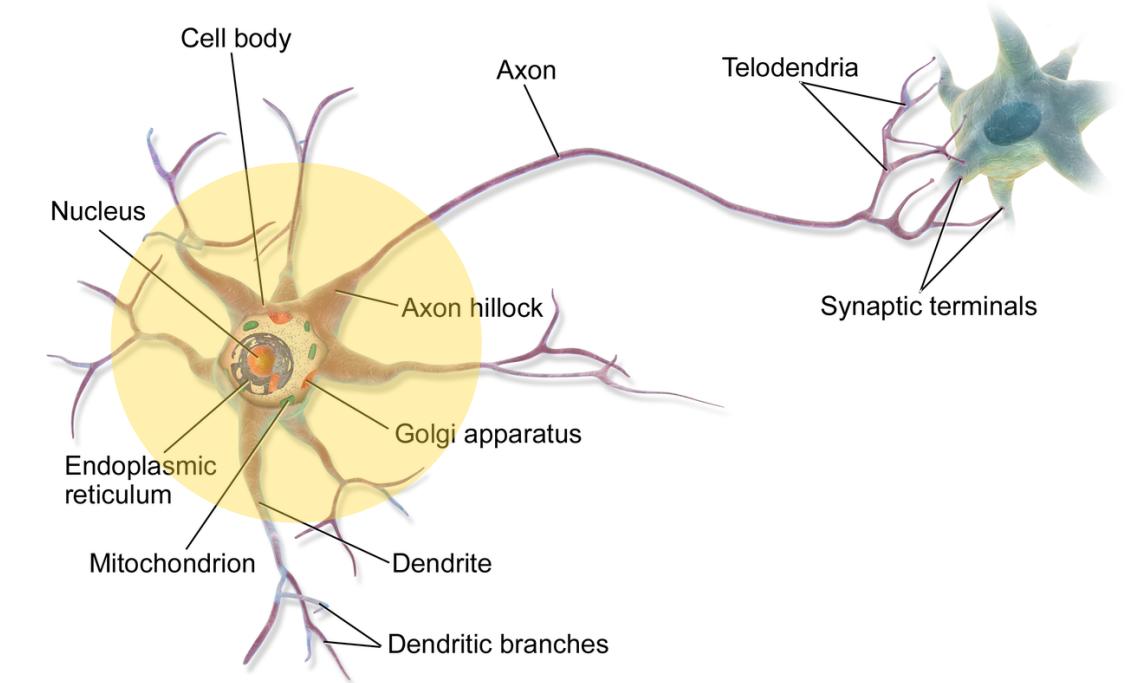


2D PCA Visualization Labeled with Document Source



document
classification

Neural Networks (Non-Linearity)

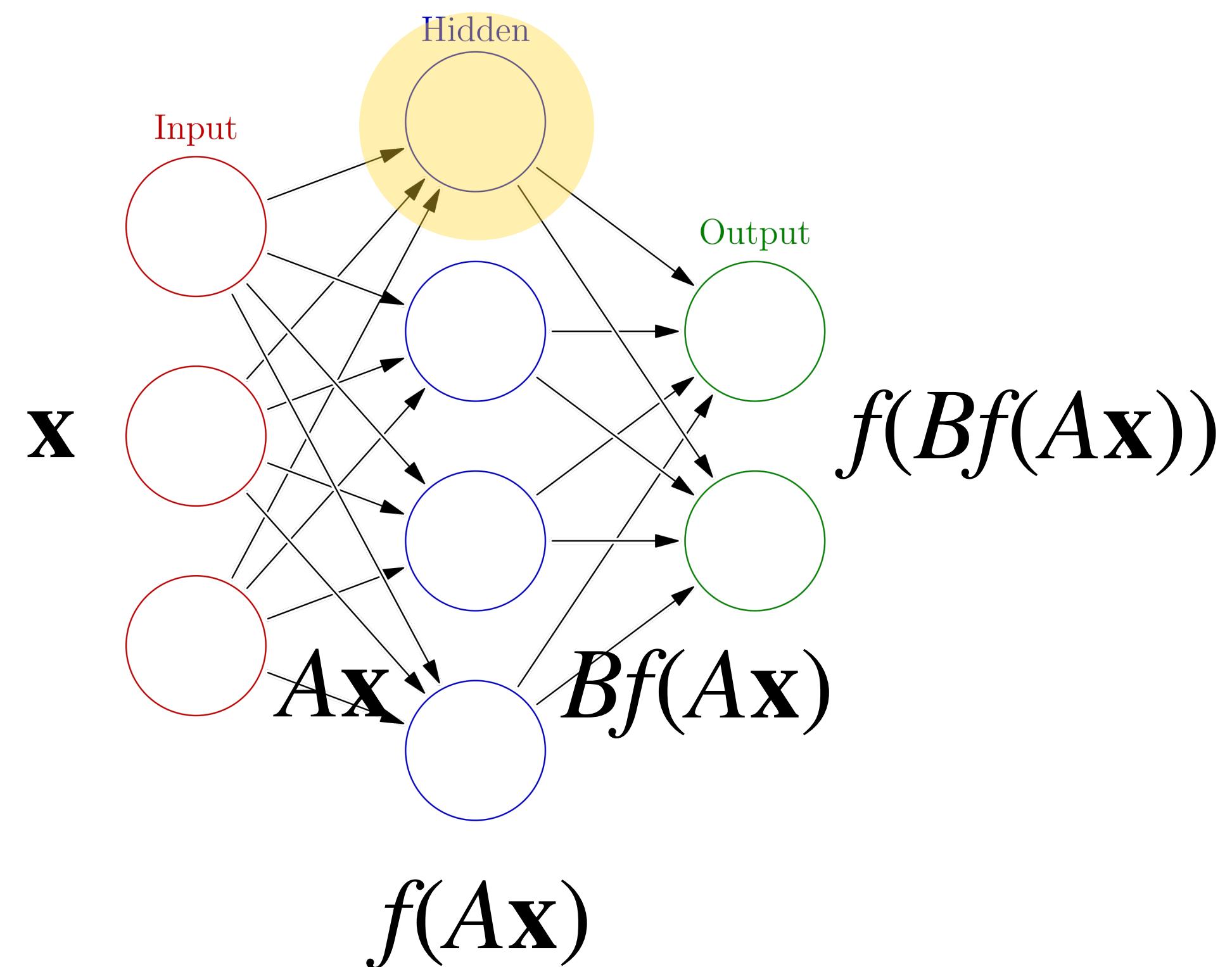
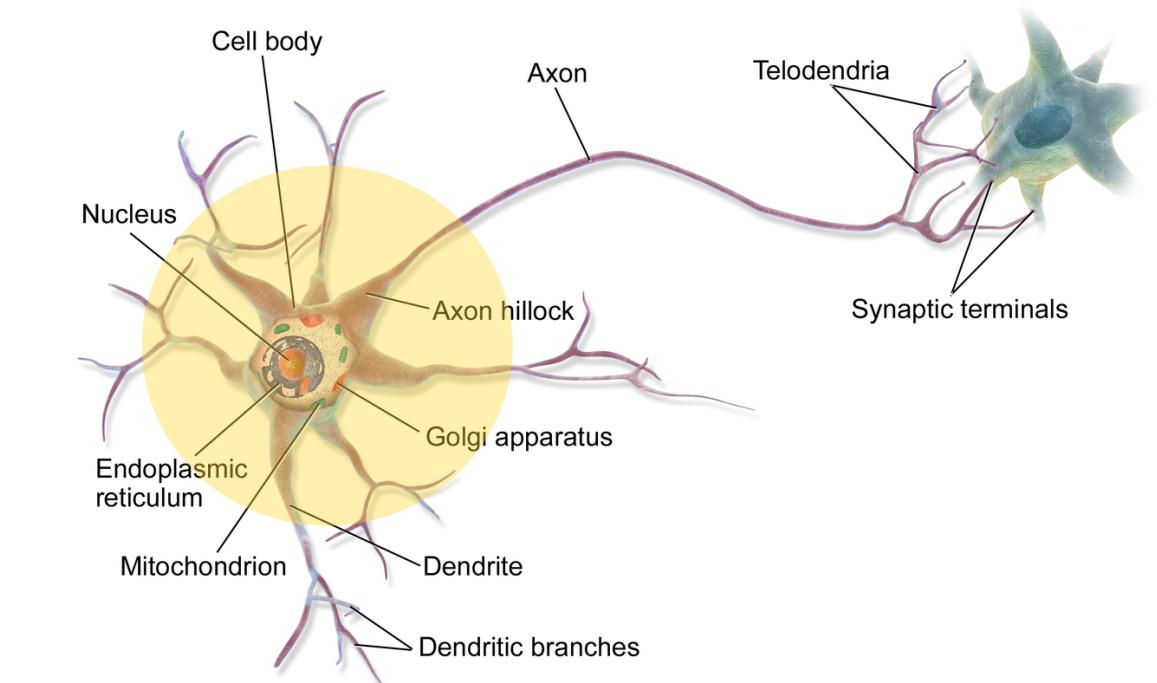


https://commons.wikimedia.org/wiki/File:Blausen_0657_MultipolarNeuron.png

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

Neural Networks (Non-Linearity)

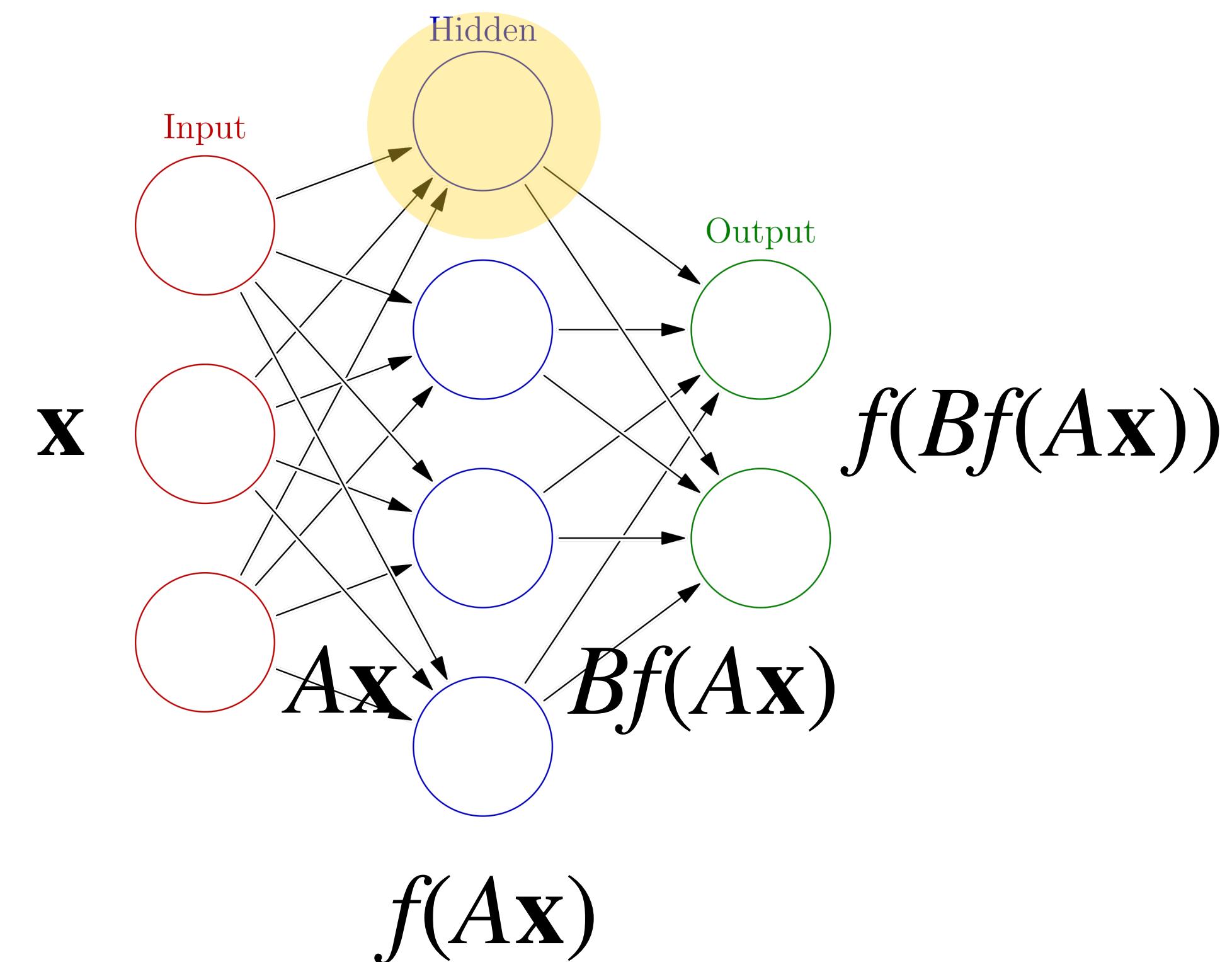
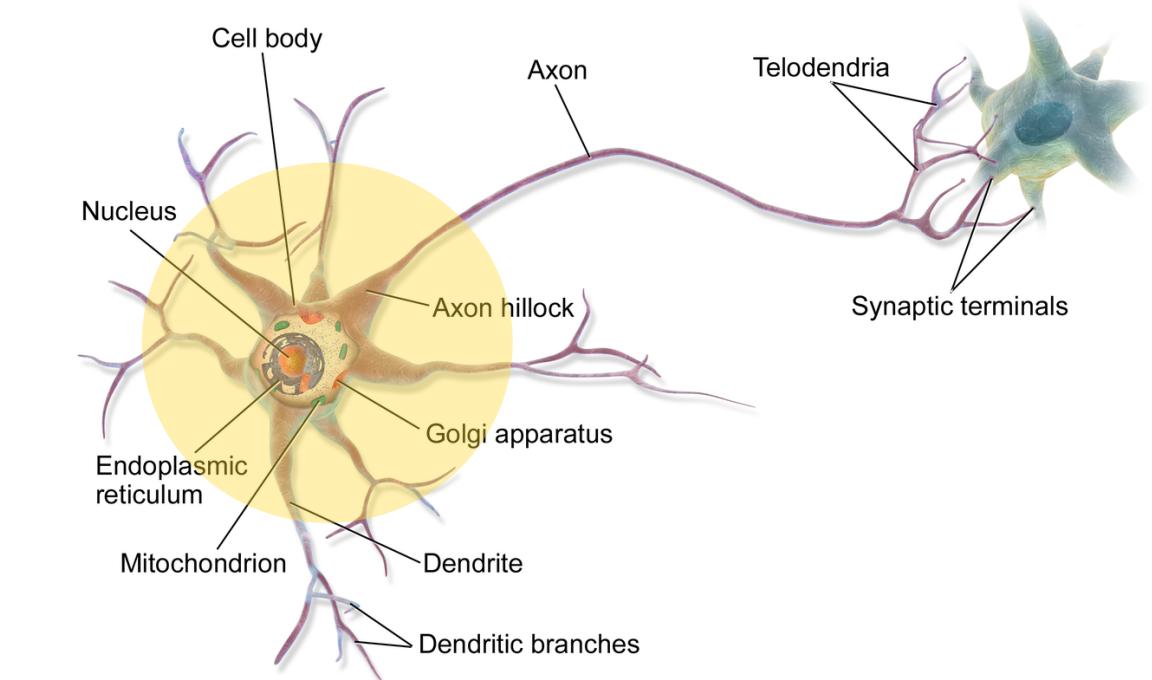
Neural networks are models of artificial neurons bundles.



Neural Networks (Non-Linearity)

Neural networks are models of artificial neurons bundles.

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.

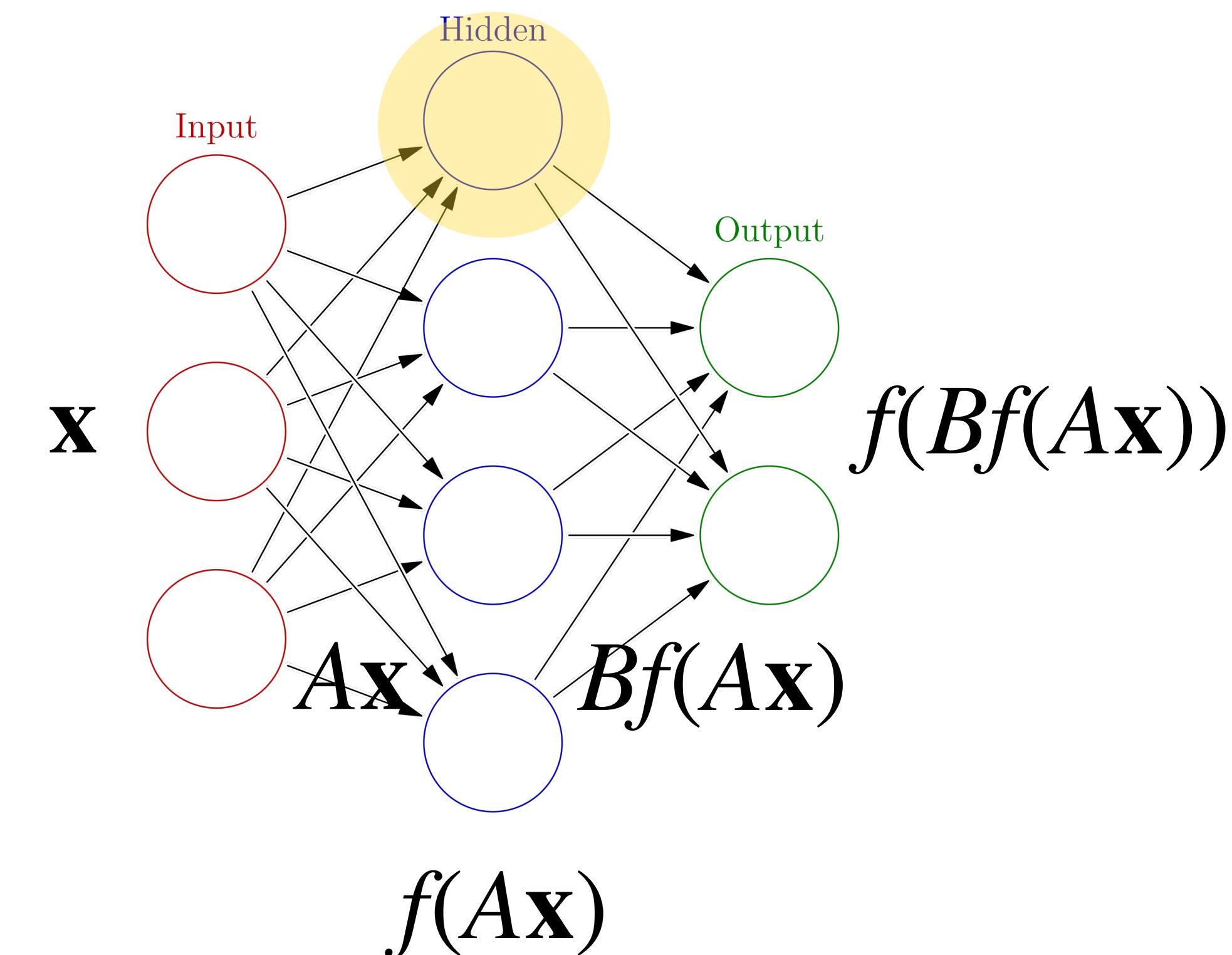
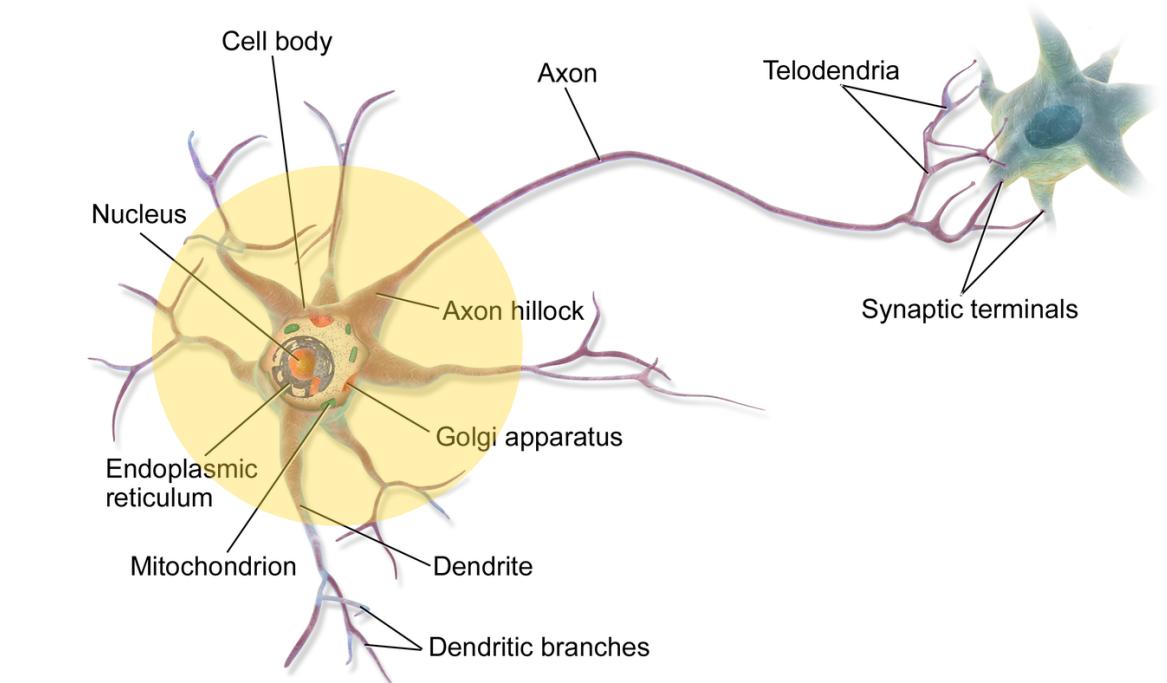


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Neural networks are just matrix multiplications with intermediate calls to a nonlinear function f .



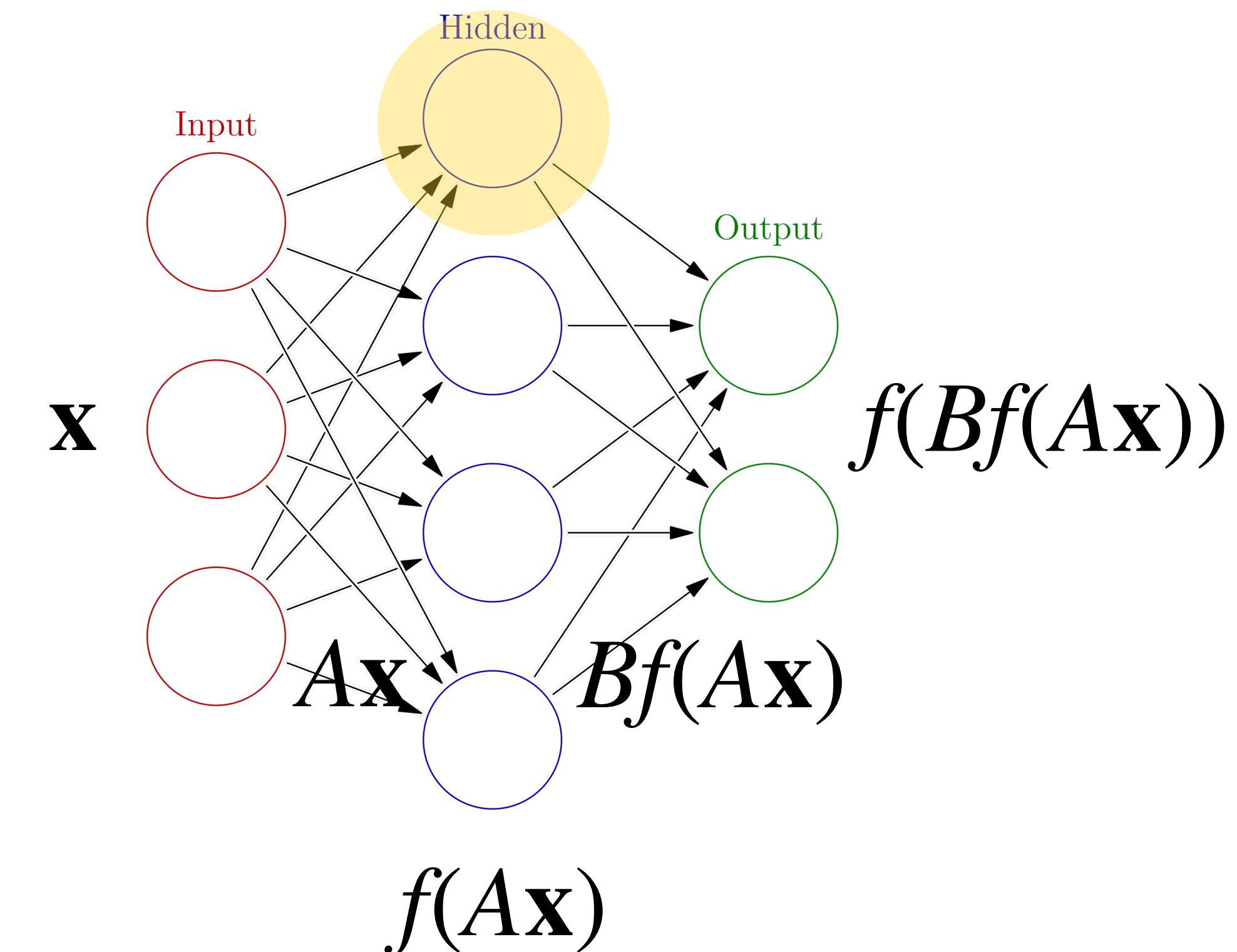
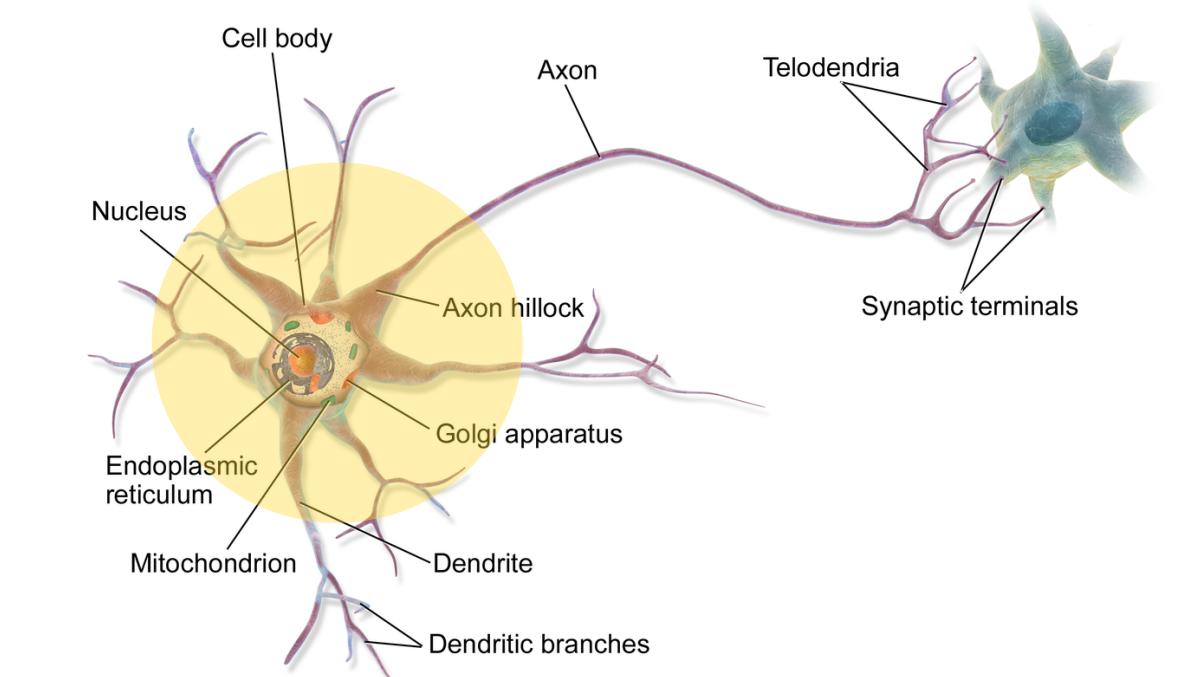
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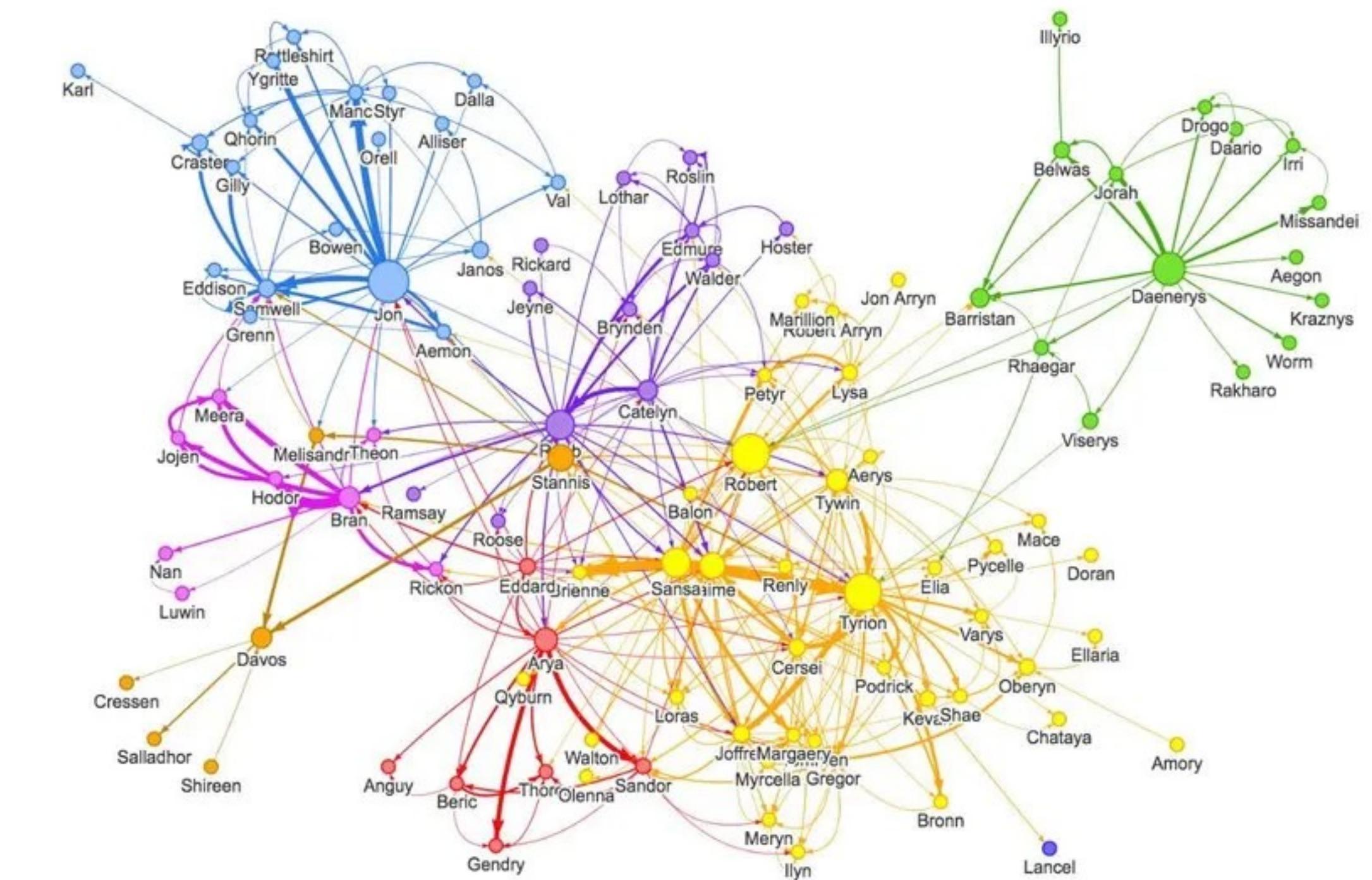
$$\text{NN}(x) = f(A_k(f(A_{k-1} \dots f(A_1 x)))$$



Spectral/Algebraic Graph Theory

Graphs can be viewed as matrices.

The finding eigenvalues in graphs can gives user better clustering and cutting algorithms.



Abstract Algebra

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

$$\begin{array}{ccc} U & \xrightarrow{f} & V \\ \downarrow & & \searrow \\ & & U/\text{Nul}(f) \end{array}$$

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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