

Machine Learning

CMPT 726

Mo Chen

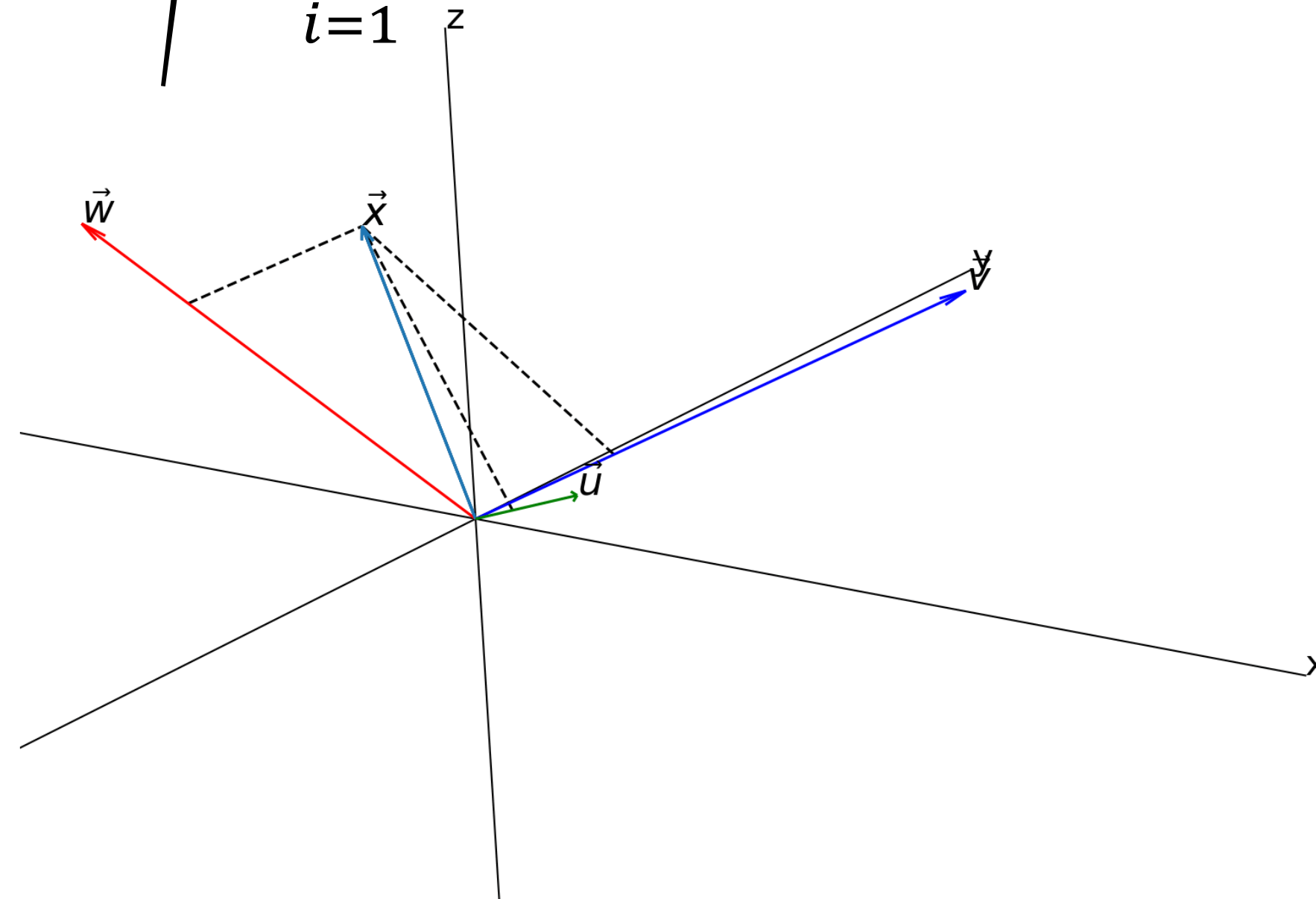
SFU School of Computing Science

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Orthogonal Basis

We like an orthogonal basis because it is easy to compute the coordinates with respect to the basis.

$$\langle \vec{x}, \vec{v}_j \rangle = \left\langle \sum_{i=1}^N \alpha_i \vec{v}_i, \vec{v}_j \right\rangle = \sum_{i=1}^n \alpha_i \langle \vec{v}_i, \vec{v}_j \rangle = \alpha_j \langle \vec{v}_j, \vec{v}_j \rangle = \alpha_j \|\vec{v}_j\|_2^2 \Rightarrow \alpha_j = \frac{\langle \vec{x}, \vec{v}_j \rangle}{\|\vec{v}_j\|_2^2}$$



\vec{x} is an arbitrary vector

Orthonormal Basis

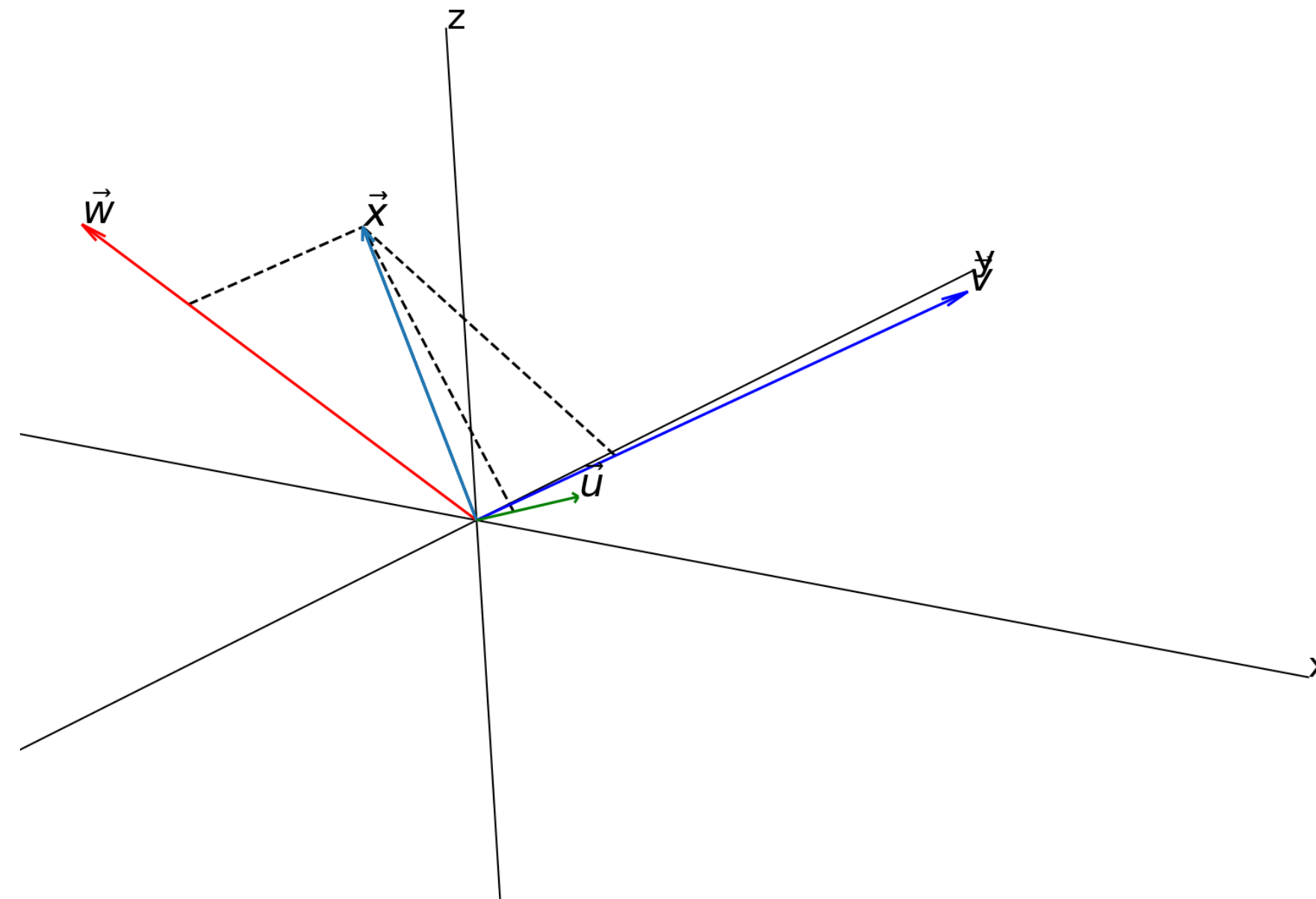
An orthonormal basis is a special case of an orthogonal basis with unit vectors.

$$\langle \vec{x}, \vec{v}_j \rangle = \left\langle \sum_{i=1}^n \alpha_i \vec{v}_i, \vec{v}_j \right\rangle = \sum_{i=1}^n \alpha_i \langle \vec{v}_i, \vec{v}_j \rangle = \alpha_j \langle \vec{v}_j, \vec{v}_j \rangle = \alpha_j \|\vec{v}_j\|_2^2 \Rightarrow \alpha_j = \frac{\langle \vec{x}, \vec{v}_j \rangle}{\|\vec{v}_j\|_2^2}$$

$$\|\vec{v}_j\|_2 = 1 \Rightarrow \alpha_j = \langle \vec{x}, \vec{v}_j \rangle$$

\vec{x} is an arbitrary vector

Finding the coordinates
gets even easier!



Addendum (Coordinates for Non-Orthogonal Basis)

Suppose $\vec{x} = \sum_{i=1}^N \alpha_i \vec{v}_i$. Given \vec{x} and the basis $\{\vec{v}_i\}$, we'd like to determine the coordinates $\{\alpha_i\}$. The sum can be written as $\vec{x} = [\vec{v}_1 \quad \cdots \quad \vec{v}_N] \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{bmatrix}$

$$\text{(If we let } v_i = \begin{bmatrix} v_{i1} \\ \vdots \\ v_{iN} \end{bmatrix} \text{. Then, we can write } \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} v_{11} & \cdots & v_{N1} \\ \vdots & \ddots & \vdots \\ v_{1N} & \cdots & v_{NN} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{bmatrix} \text{)}$$

Next, we'd solve the above equation for the unknowns $\{\alpha_i\}$. There are many ways. One (potentially inefficient) way is by finding the inverse:

$$\begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{bmatrix} = [\vec{v}_1 \quad \cdots \quad \vec{v}_N]^{-1} \vec{x}$$

Eigenvectors vs. Right-Singular Vectors

Eigenvectors are the directions along which the vector retains its direction after being transformed by the matrix.

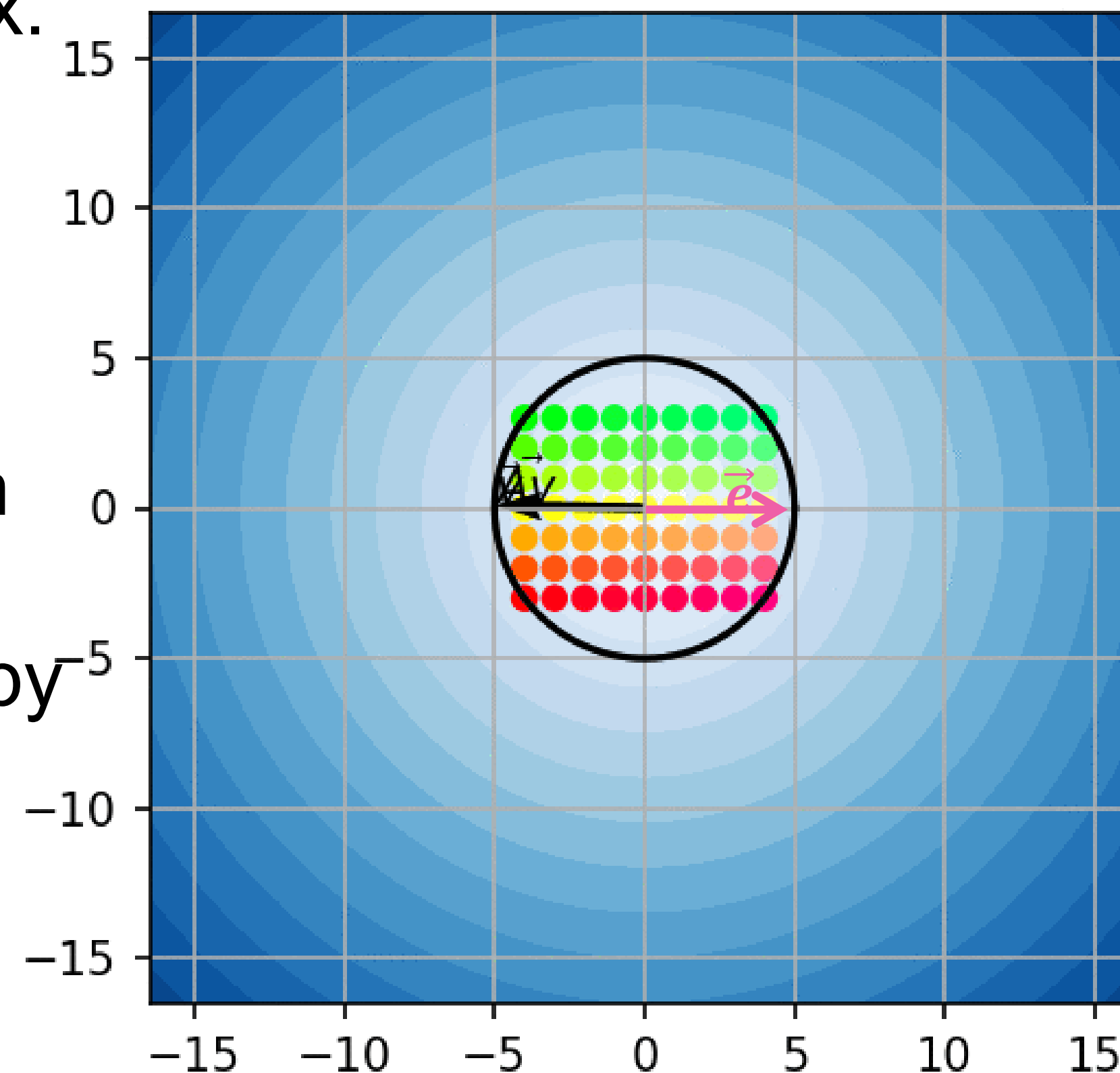
$$A\vec{u}_i = \lambda_{ii}\vec{u}_i$$

The right-singular vector with the largest singular value is the direction along which a unit vector becomes the longest after being transformed by the matrix.

$$\sigma_{1,1} = \max_{\vec{x}: \|\vec{x}\|_2=1} \|A\vec{x}\|_2$$

$$\vec{v}_1 = \arg \max_{\vec{x}: \|\vec{x}\|_2=1} \|A\vec{x}\|_2$$

For asymmetric matrices, eigenvectors are not necessarily orthogonal; in this case, they are coincident



\vec{v} - the right singular vector
 $A\vec{v}$ - after matrix transformation

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

Eigendecomposition More Generally

For asymmetric matrices, sometimes eigendecomposition is possible

- Only possible when the matrix is diagonalizable

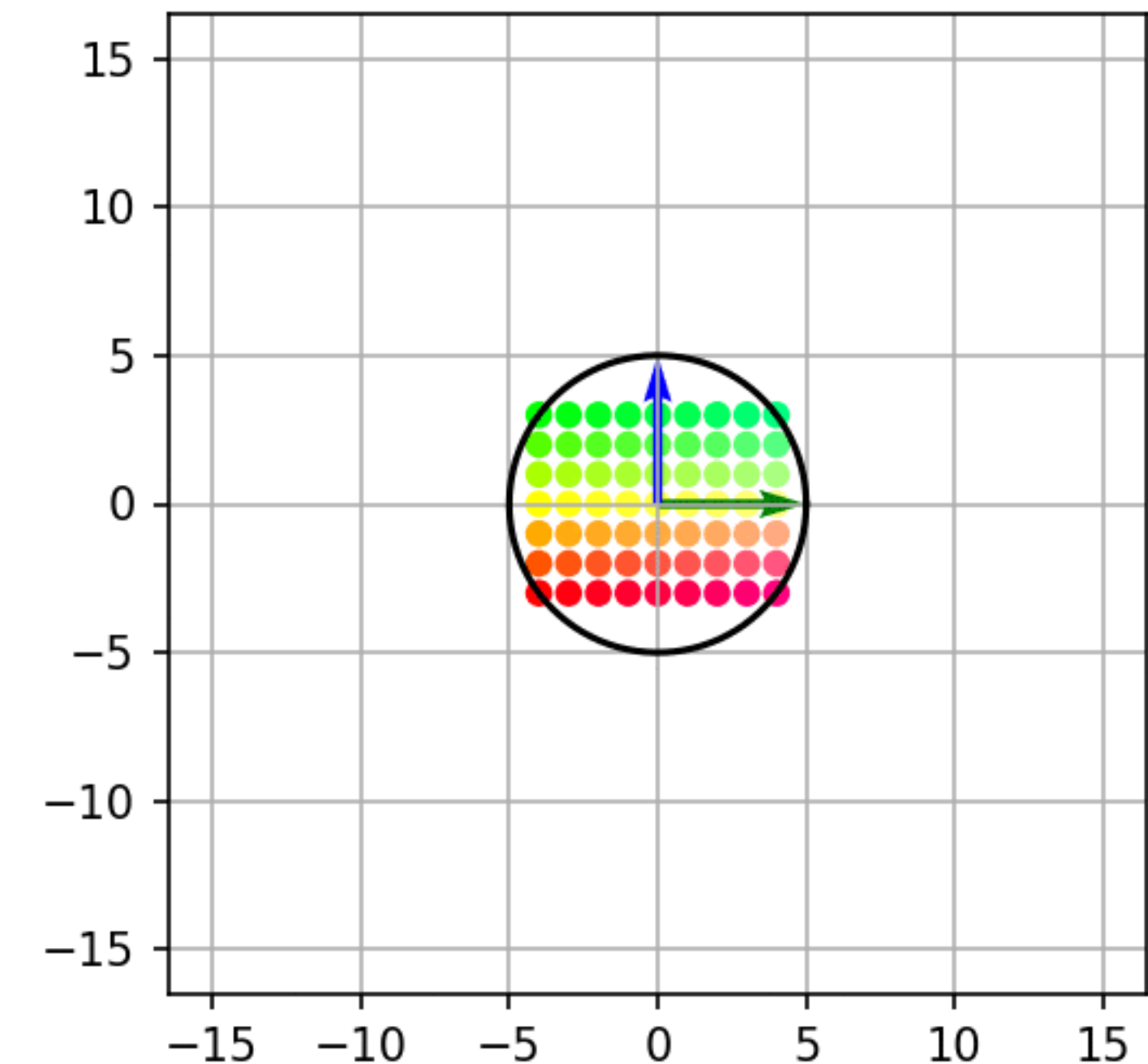
In such cases:

Eigenvectors are not necessarily orthogonal

Eigenvalues and eigenvectors are not necessarily real

No straightforward geometric interpretation

$$A = U\Lambda U^{-1} \neq U\Lambda U^T$$



$$A = \begin{pmatrix} 1 & 0 \\ 1 & 3 \end{pmatrix}$$

SVD and Eigendecomposition

SVD and eigendecomposition are closely related:

The right-singular vectors are eigenvectors of $A^T A$.

The left-singular vectors are eigenvectors of AA^T .

The non-zero singular values are the square roots of non-zero eigenvalues of $A^T A$
(or equivalently the square roots of non-zero eigenvalues of AA^T)

Application of Eigendecomposition

Finding the inverse of a symmetric matrix:

$$A = U\Lambda U^T$$

$$A^{-1} = (U\Lambda U^T)^{-1} = (U^T)^{-1}\Lambda^{-1}U^{-1} = U\Lambda^{-1}U^T$$

Since Λ is diagonal

$$\Lambda^{-1} = \begin{pmatrix} \frac{1}{\lambda_{11}} & 0 & \dots & 0 \\ 0 & \frac{1}{\lambda_{22}} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{\lambda_{nn}} \end{pmatrix}$$

Why?

Linear Algebra and Calculus Review (cont'd)

p -Norms

Also known as ℓ_p norms.

These are norms of **vectors**. In general, the p -norm of a vector \vec{x} is

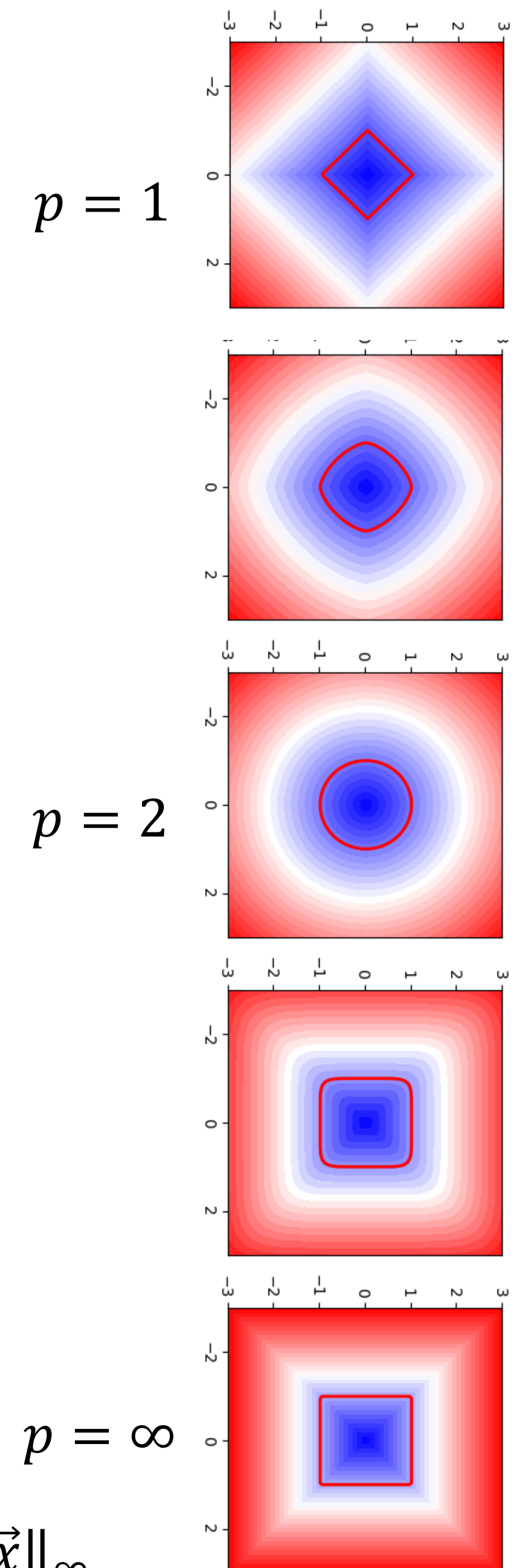
$$\|\vec{x}\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{\frac{1}{p}}$$

Common norms:

$$\ell_1 \text{ norm ("Manhattan norm")}: \|\vec{x}\|_1 = \sum_{i=1}^n |x_i|$$

$$\ell_2 \text{ norm ("Euclidean norm")}: \|\vec{x}\|_2 = \sqrt{\sum_{i=1}^n x_i^2}$$

$$\ell_\infty \text{ norm ("Max norm")}: \|\vec{x}\|_\infty = \max\{|x_1|, \dots, |x_n|\}$$



$$\|\vec{x}\|_1 \geq \|\vec{x}\|_2 \geq \|\vec{x}\|_\infty$$

Matrix Norms

Frobenius norm:

$$\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}$$

Induced/operator norms:

$$\|A\|_p = \sup_{\|\vec{x}\|_p=1} \{\|A\vec{x}\|_p\}$$

Special case ($p = 2$): known as “spectral norm”:

$$\|A\|_2 = \sup_{\|\vec{x}\|_2=1} \{\|A\vec{x}\|_2\} = \sigma_{1,1}(A)$$

- $\sigma_{1,1}(A)$ denotes the largest singular value of A

Positive/Negative (Semi-)Definite Matrices

- A symmetric matrix A is
 - positive definite if all of its eigenvalues are positive
 - negative definite if all of its eigenvalues are negative
 - positive semi-definite if all of its eigenvalues are non-negative (≥ 0)
 - negative semi-definite if all of its eigenvalues are non-positive (≤ 0)
 - indefinite if some of its eigenvalues are positive and others are negative

Positive/Negative (Semi-)Definite Matrices

- A symmetric matrix A is
 - positive definite if all of its eigenvalues are positive $A \succ 0$
 - negative definite if all of its eigenvalues are negative $A \prec 0$
 - positive semi-definite if all of its eigenvalues are non-negative $A \succcurlyeq 0$
 - negative semi-definite if all of its eigenvalues are non-positive $A \preceq 0$
 - indefinite if some of its eigenvalues are positive and others are negative

Taylor Expansion

Polynomial: $g(x) = \sum_{i=1}^d \alpha_i x^i$, where d , the highest power, is known as the **degree**

How to approximate an arbitrary function $f: \mathbb{R} \rightarrow \mathbb{R}$ with a polynomial g ?

We can try to match the function value at a certain point, the first derivative, the second derivative, etc.

$$\begin{aligned} f(x_0) &= g(x_0) \\ f'(x_0) &= g'(x_0) \\ f''(x_0) &= g''(x_0) \end{aligned}$$

⋮

A polynomial g that satisfies these conditions is known as a **Taylor polynomial**

Taylor Expansion

Consider a function $f: \mathbb{R} \rightarrow \mathbb{R}$ and its approximations with Taylor polynomials of various degrees.

The 0th order Taylor expansion at x_0 is:

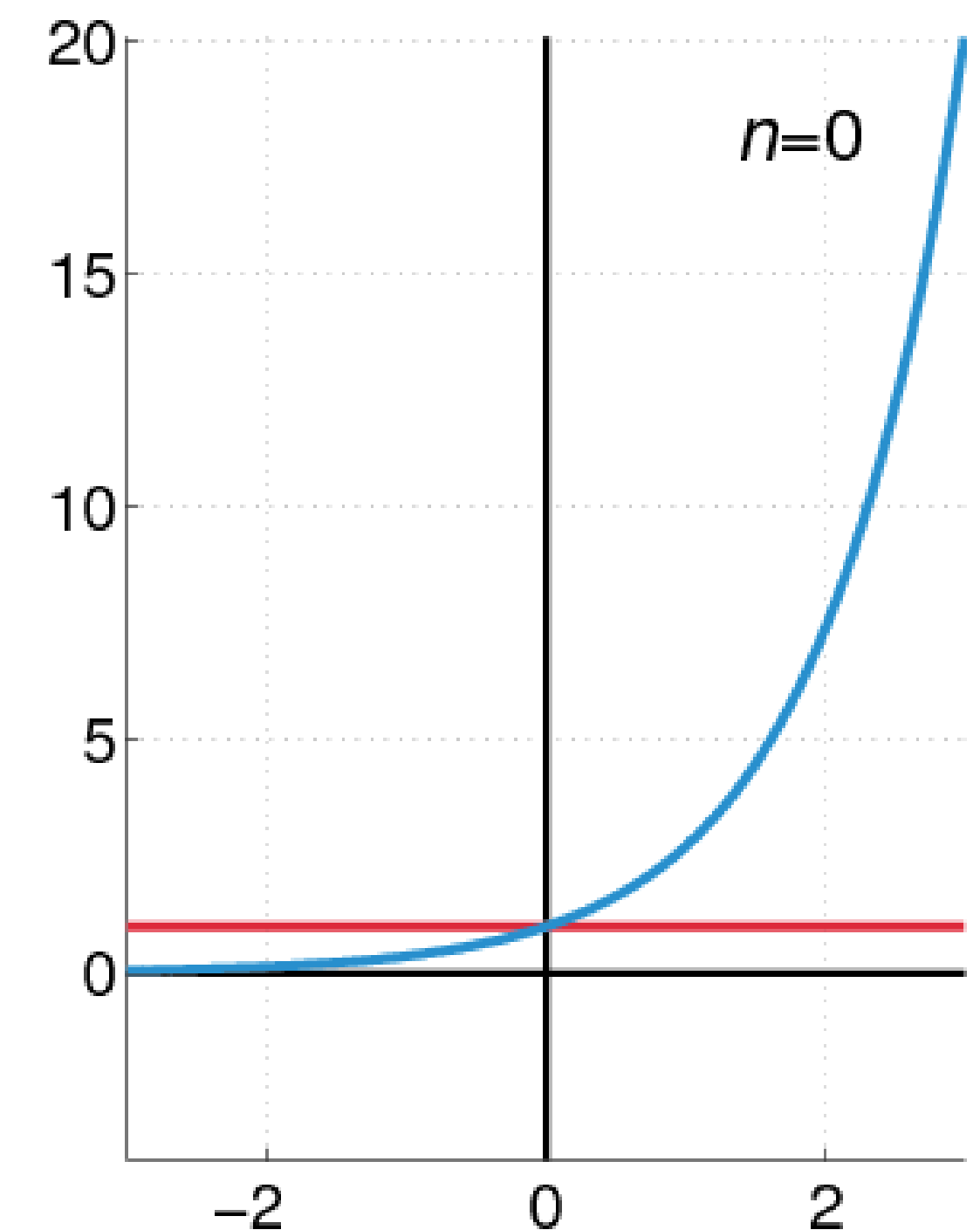
$$g(x) = f(x_0)$$

The 1st order Taylor expansion at x_0 is:

$$g(x) = f(x_0) + \frac{1}{1!} (x - x_0) f'(x_0)$$

The 2nd order Taylor expansion at x_0 is:

$$g(x) = f(x_0) + \frac{1}{1!} (x - x_0) f'(x_0) + \frac{1}{2!} (x - x_0)^2 f''(x_0)$$



Taylor Expansion

Polynomials in multiple variables:

$$g(x_1, x_2) = \alpha + \beta_1 x_1 + \beta_2 x_2 + \gamma_{11} x_1^2 + 2\gamma_{12} x_1 x_2 + \gamma_{22} x_2^2 \text{ (degree 2 polynomial)}$$

In matrix notation:

$$\text{Let } \vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$g(\vec{x}) = \alpha + \vec{x}^\top \vec{\beta} + \vec{x}^\top \Gamma \vec{x}, \text{ where } \vec{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}, \Gamma = \begin{pmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{12} & \gamma_{22} \end{pmatrix}$$

Note that Γ is symmetric

Taylor Expansion

Consider a function $f: \mathbb{R}^n \rightarrow \mathbb{R}$.

The 0th order Taylor expansion at \vec{x}_0 is

$$f(\vec{x}_0)$$

The 1st order Taylor expansion at \vec{x}_0 is

$$f(\vec{x}_0) + (\vec{x} - \vec{x}_0)^\top \frac{\partial f}{\partial \vec{x}}(\vec{x}_0)$$

The 2nd order Taylor expansion at \vec{x}_0 is

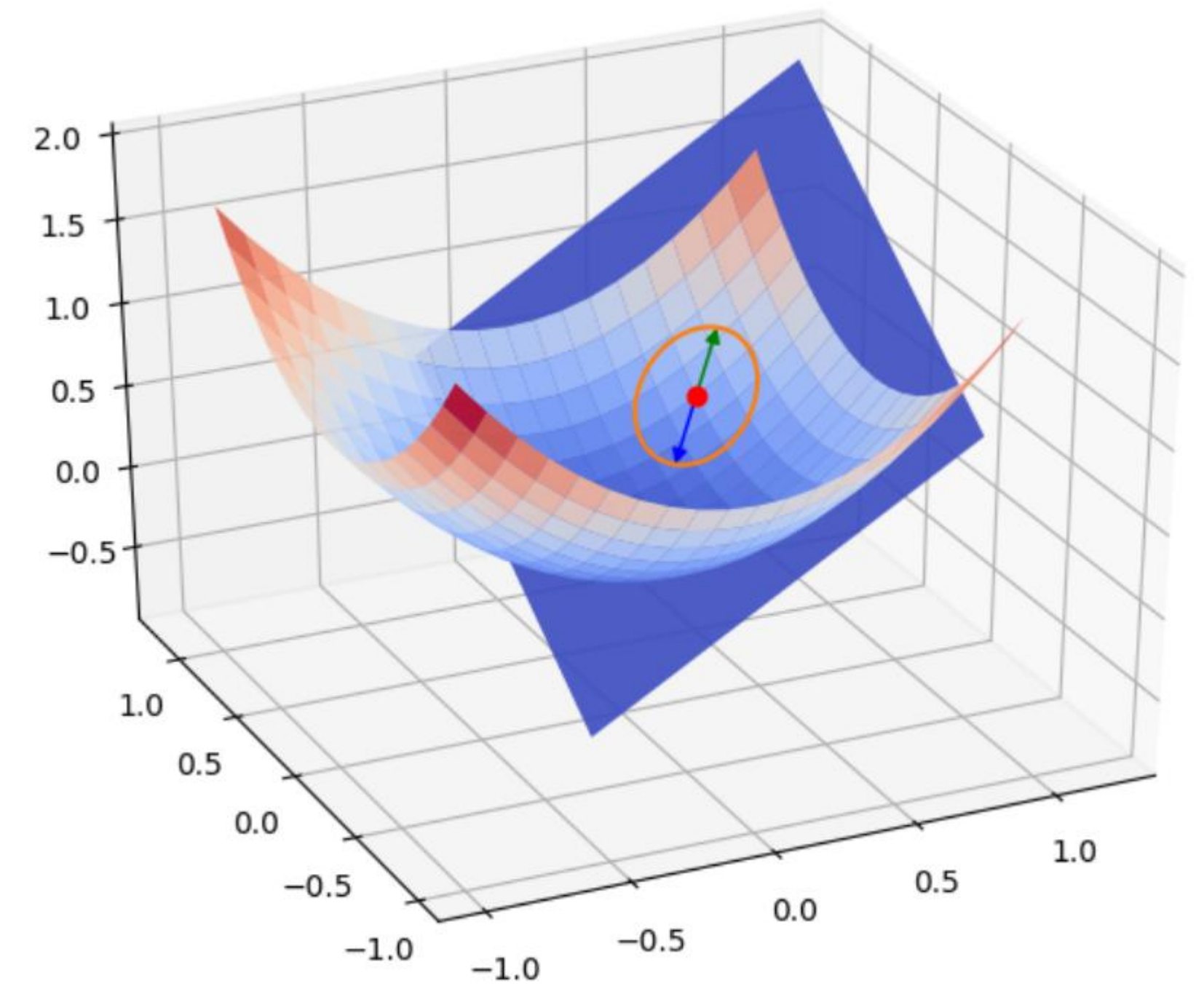
$$f(\vec{x}_0) + (\vec{x} - \vec{x}_0)^\top \frac{\partial f}{\partial \vec{x}}(\vec{x}_0) + \frac{1}{2} (\vec{x} - \vec{x}_0)^\top \frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top} (\vec{x} - \vec{x}_0)$$

Taylor Expansion

The 2nd order Taylor expansion at \vec{x}_0 is:

$$f(\vec{x}_0) + (\vec{x} - \vec{x}_0)^\top \frac{\partial f}{\partial \vec{x}}(\vec{x}_0) + \frac{1}{2} (\vec{x} - \vec{x}_0)^\top \frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top} (\vec{x} - \vec{x}_0)$$

$$\frac{\partial f}{\partial \vec{x}}(\vec{x}_0) := \begin{pmatrix} \frac{\partial f}{\partial x_1}(\vec{x}_0) \\ \frac{\partial f}{\partial x_2}(\vec{x}_0) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\vec{x}_0) \end{pmatrix}$$



Gradient, Direction of steepest ascent

Taylor Expansion

The 2nd order Taylor expansion at \vec{x}_0 is:

$$f(\vec{x}_0) + (\vec{x} - \vec{x}_0)^\top \frac{\partial f}{\partial \vec{x}}(\vec{x}_0) + \frac{1}{2} (\vec{x} - \vec{x}_0)^\top \frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top} (\vec{x} - \vec{x}_0)$$

$$\frac{\partial f}{\partial \vec{x}}(\vec{x}_0) := \begin{pmatrix} \frac{\partial f}{\partial x_1}(\vec{x}_0) \\ \frac{\partial f}{\partial x_2}(\vec{x}_0) \\ \vdots \\ \frac{\partial f}{\partial x_n}(\vec{x}_0) \end{pmatrix}, \quad \frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top} = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1}(\vec{x}_0) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(\vec{x}_0) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n}(\vec{x}_0) \\ \frac{\partial^2 f}{\partial x_2 \partial x_1}(\vec{x}_0) & \frac{\partial^2 f}{\partial x_2 \partial x_2}(\vec{x}_0) & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n}(\vec{x}_0) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1}(\vec{x}_0) & \frac{\partial^2 f}{\partial x_n \partial x_2}(\vec{x}_0) & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n}(\vec{x}_0) \end{pmatrix}$$

Gradient, Direction of steepest ascent, and **Hessian**

Order of differentiation doesn't matter, so the Hessian is symmetric.

Quadratic Forms

A function $g(\vec{x}) = \vec{x}^\top A \vec{x}$ is known as a quadratic form.

Alternative definition of positive/negative (semi-)definiteness of A :

- Positive definite: $\vec{x}^\top A \vec{x} > 0 \ \forall \vec{x} \neq \vec{0}$
- Negative definite: $\vec{x}^\top A \vec{x} < 0 \ \forall \vec{x} \neq \vec{0}$
- Positive semi-definite: $\vec{x}^\top A \vec{x} \geq 0 \ \forall \vec{x}$
- Negative semi-definite: $\vec{x}^\top A \vec{x} \leq 0 \ \forall \vec{x}$
- Indefinite: $\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} > 0$ and $\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} < 0$

Quadratic Forms

Let's check if the two definitions agree.

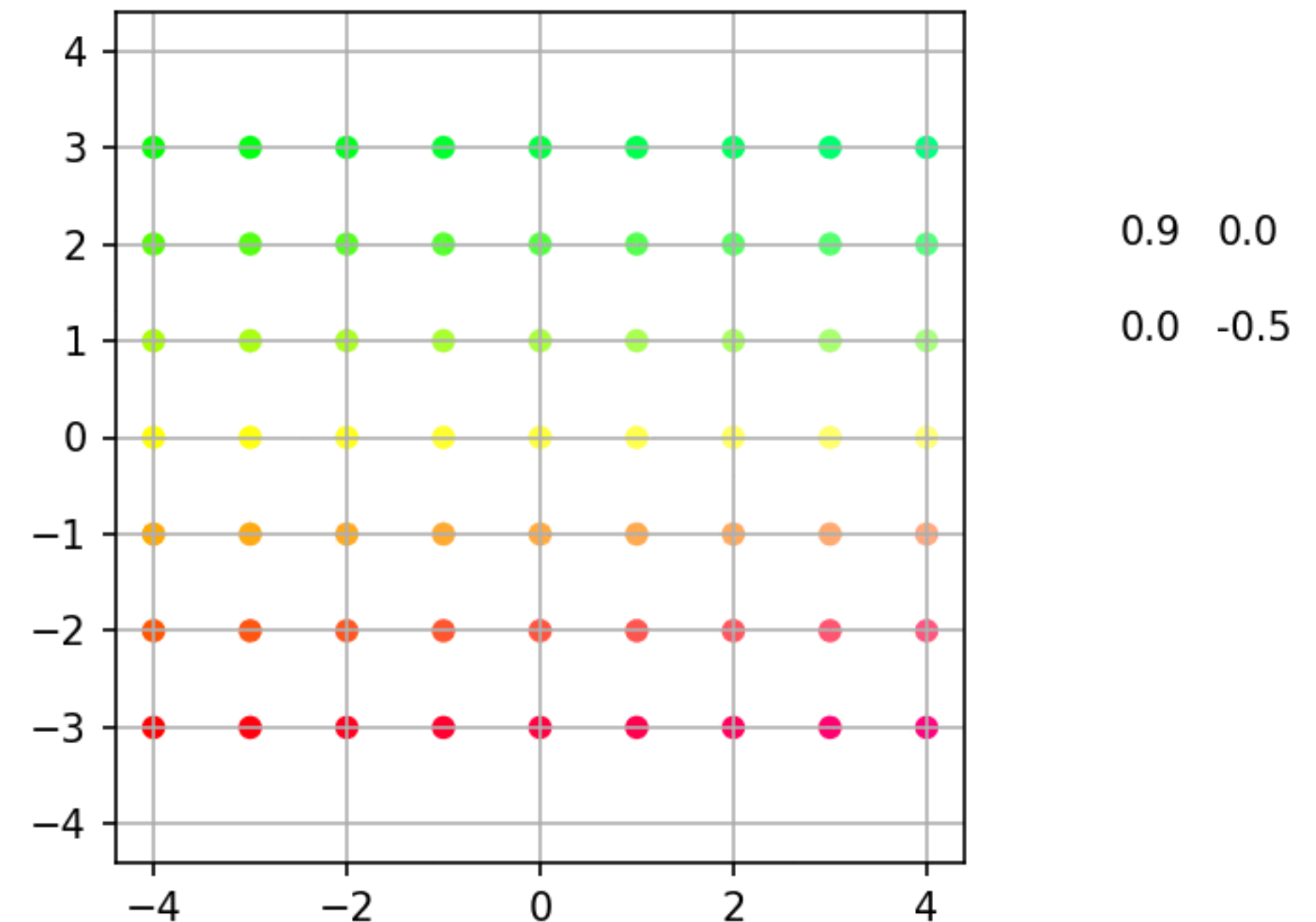
- Indefinite: $\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} > 0$ and $\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} < 0$

$$A = \begin{pmatrix} 0.9 & 0 \\ 0 & -0.5 \end{pmatrix} = I \begin{pmatrix} 0.9 & 0 \\ 0 & -0.5 \end{pmatrix} I^\top$$

Eigenvalues are 0.9 and -0.5 , according to earlier definition, matrix is indefinite.

$$\vec{x}^\top A \vec{x} = \langle \vec{x}, A \vec{x} \rangle$$

Recall: Positive if original and transformed vectors are less than 90 degrees apart, and negative otherwise.



Quadratic Forms

Let's check if the two definitions agree.

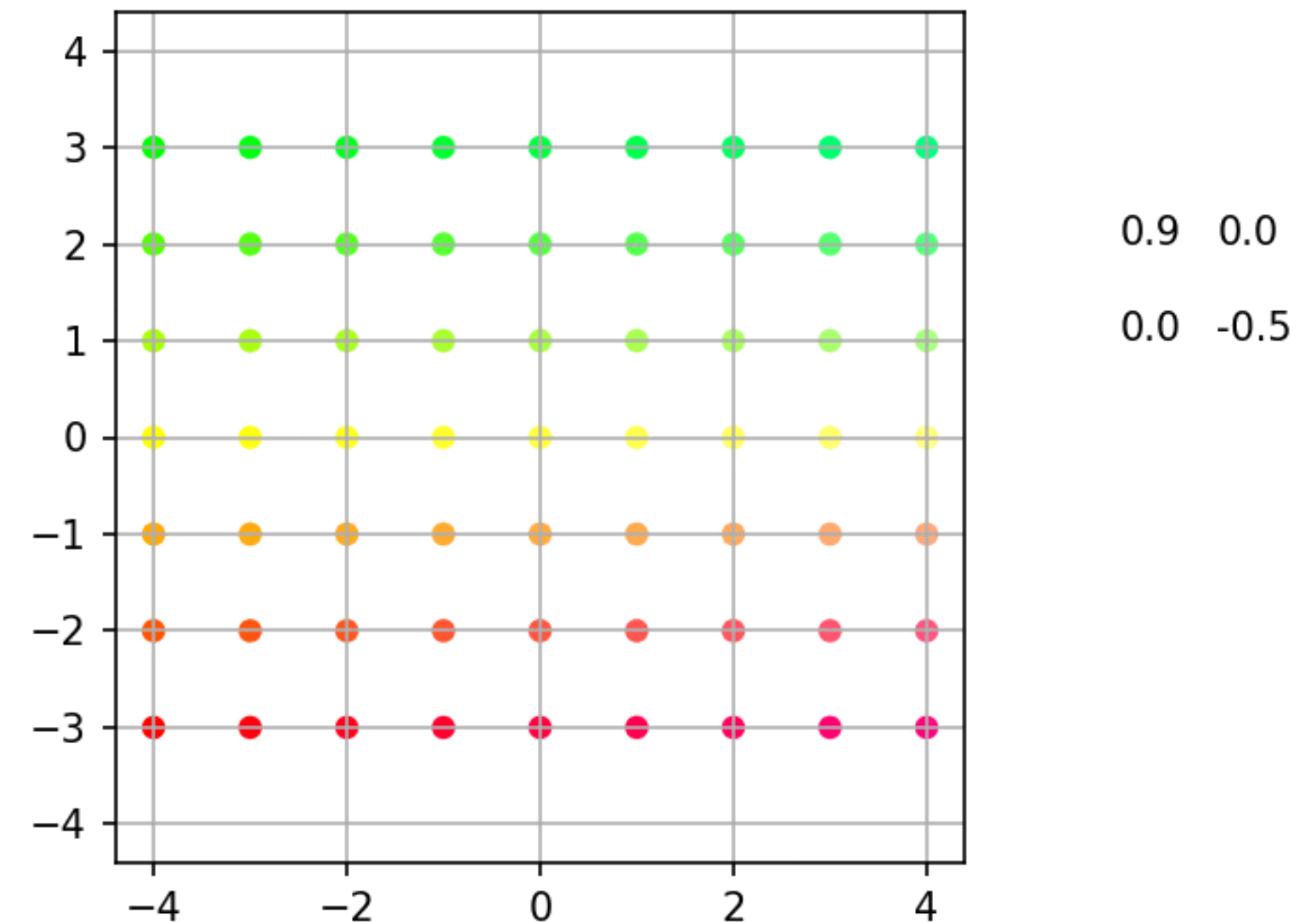
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$$\vec{x}^\top A \vec{x} = \langle \vec{x}, A \vec{x} \rangle$$

Recall: Positive if original and transformed vectors are less than 90 degrees apart, and negative otherwise. Consider the two eigenvectors



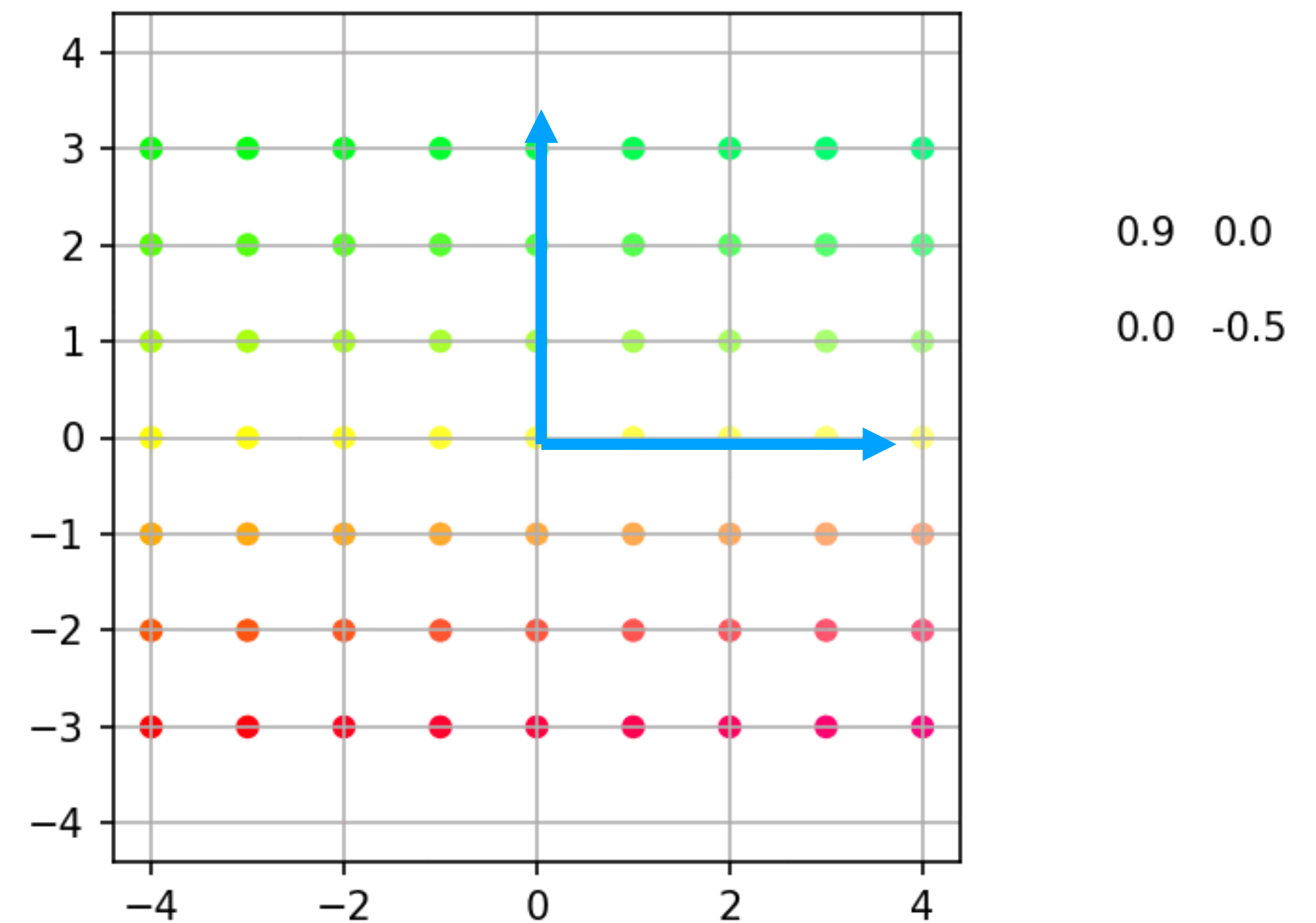
Quadratic Forms

Let's check if the two definitions agree.

- Indefinite: $\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} > 0$ and $\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} < 0$

$$\vec{e}_1^\top A \vec{e}_1 = \begin{pmatrix} 0.9 & 0 \\ 0 & -0.5 \end{pmatrix} = 0.9$$

$$\vec{e}_2^\top A \vec{e}_2 = \begin{pmatrix} 0.9 & 0 \\ 0 & -0.5 \end{pmatrix} = -0.5$$



Quadratic Forms

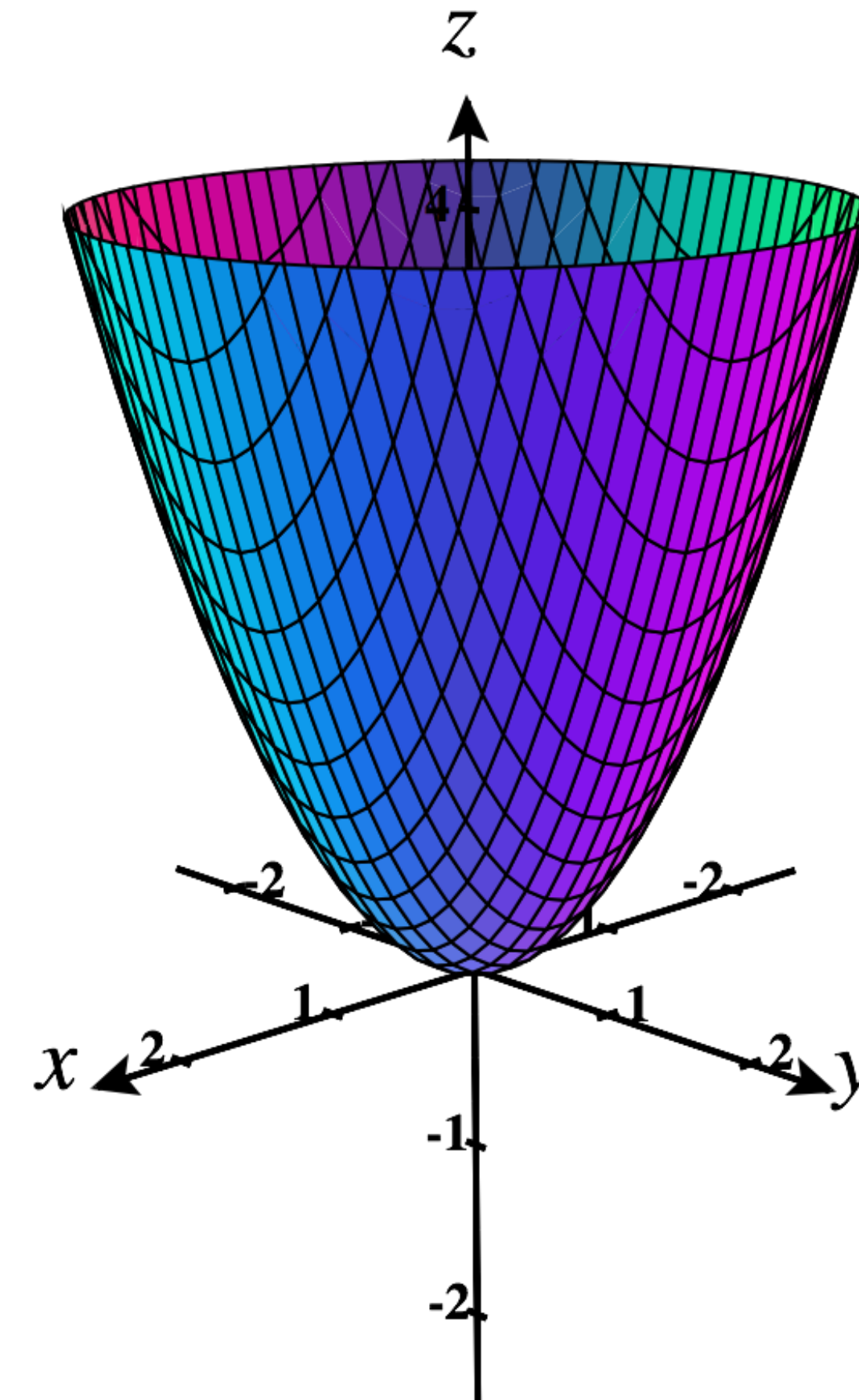
What does $\vec{x}^T A \vec{x}$ look like when:

- A is positive definite?
- A is negative definite?
- A is positive semi-definite?
- A is negative semi-definite?
- A is indefinite?

Quadratic Forms

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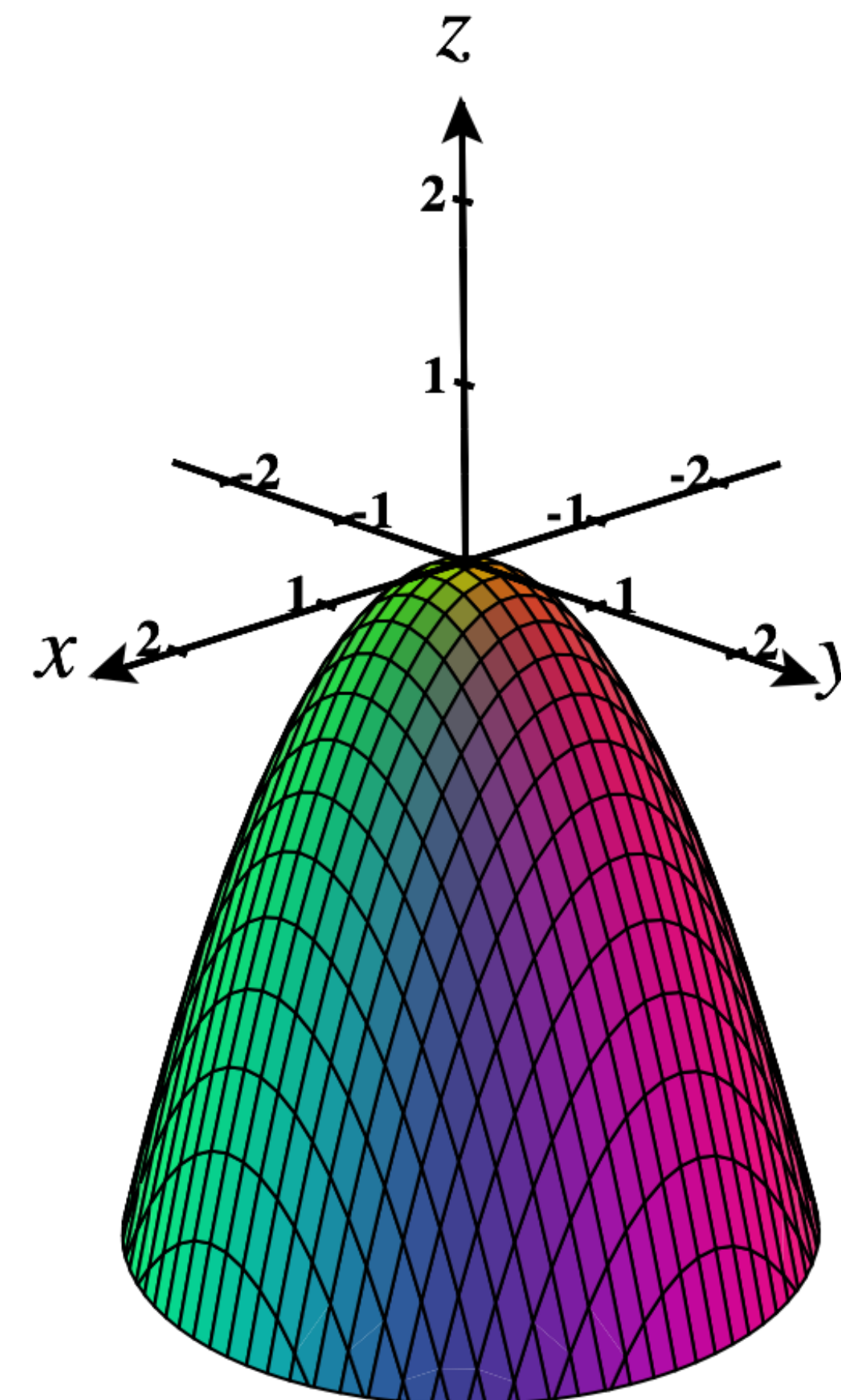
$$\vec{x}^T A \vec{x} > 0 \quad \forall \vec{x} \neq \vec{0}$$

Quadratic Forms

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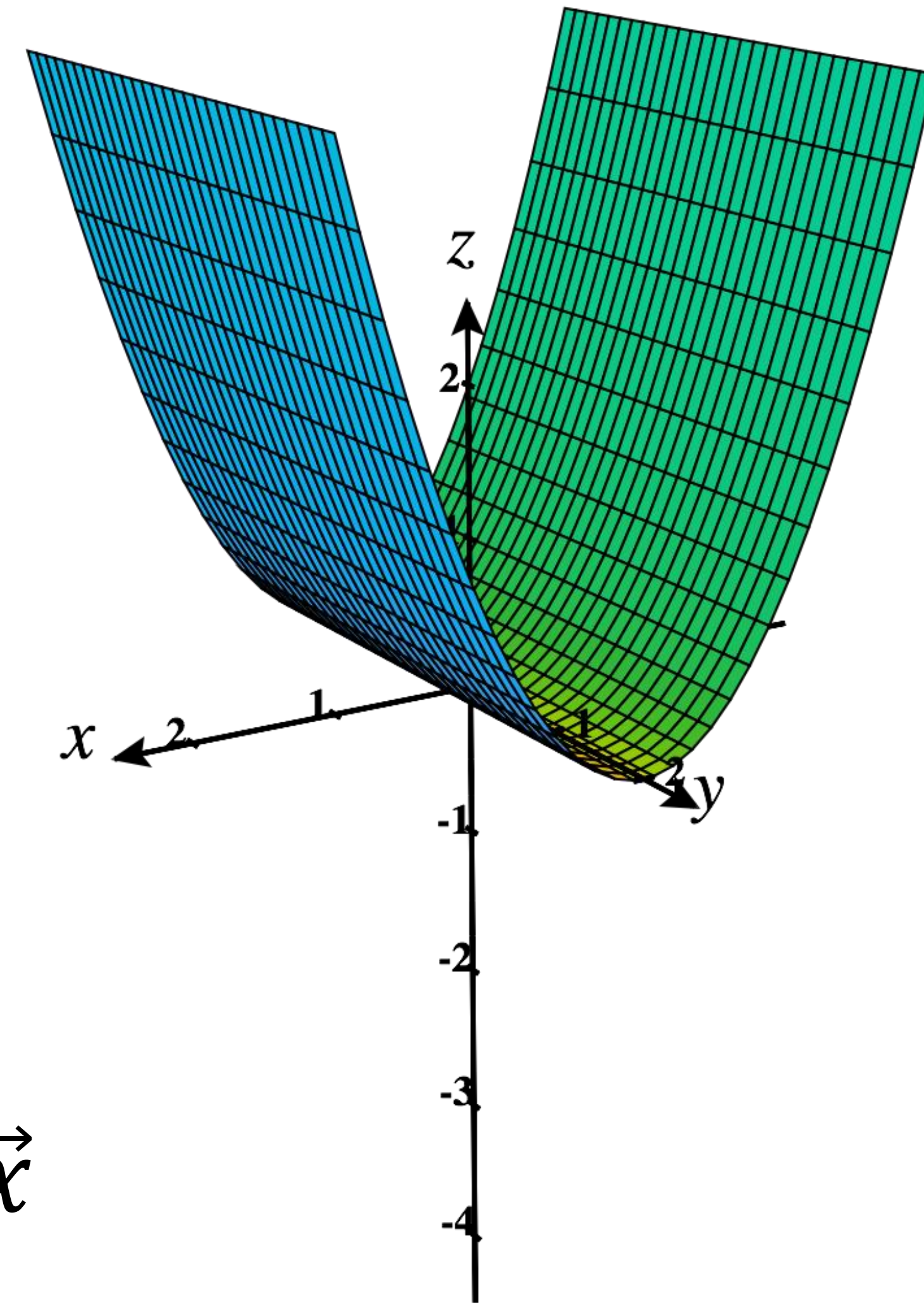
$$\vec{x}^T A \vec{x} < 0 \quad \forall \vec{x} \neq \vec{0}$$



Quadratic Forms

What does $\vec{x}^T A \vec{x}$ look like when:

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- A is **positive semi-definite?**
- A is negative semi-definite?
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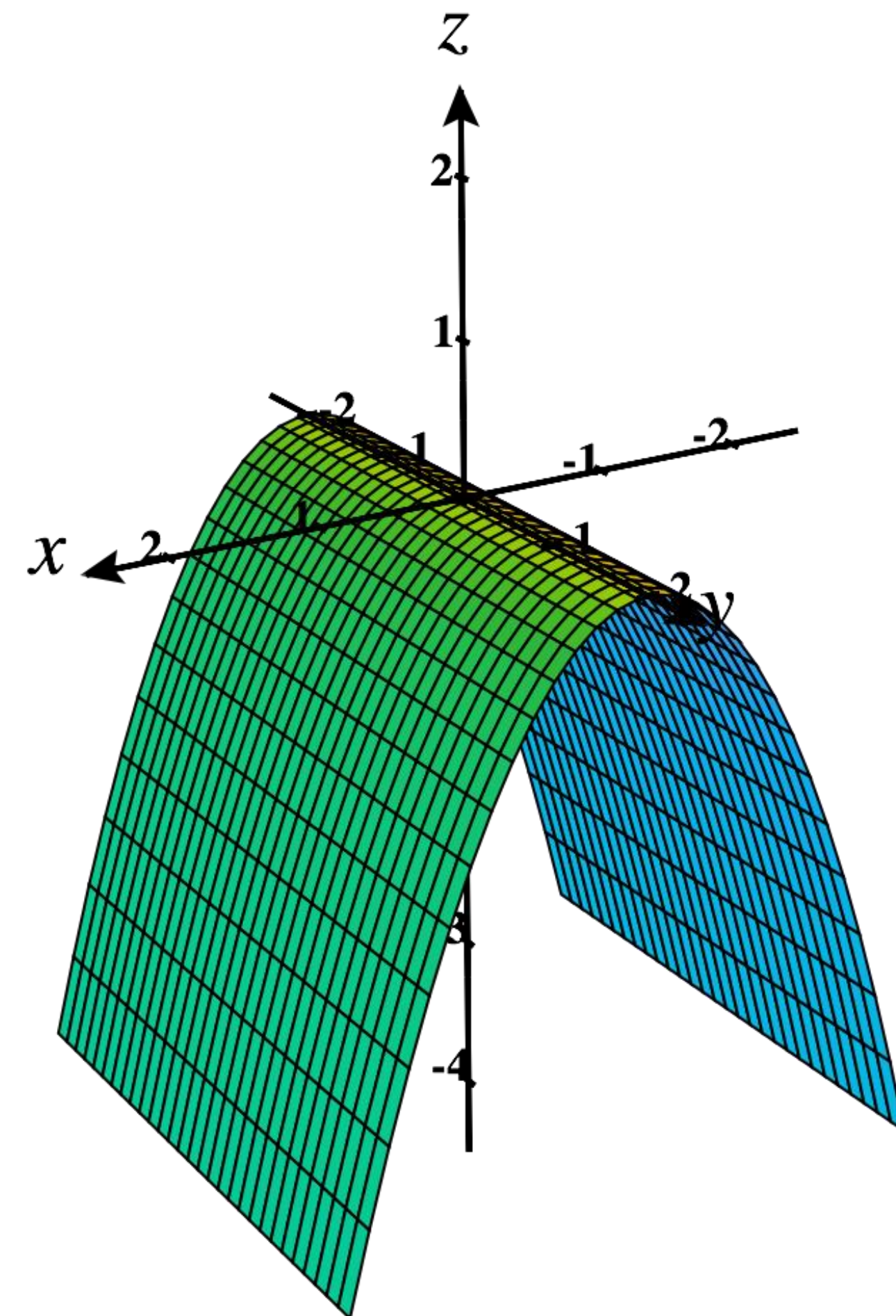
$$\vec{x}^T A \vec{x} \geq 0 \quad \forall \vec{x}$$

Quadratic Forms

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- A is positive semi-definite?
- A is **negative semi-definite**?
- A is indefinite?

$$\vec{x}^T A \vec{x} \leq 0 \forall \vec{x}$$

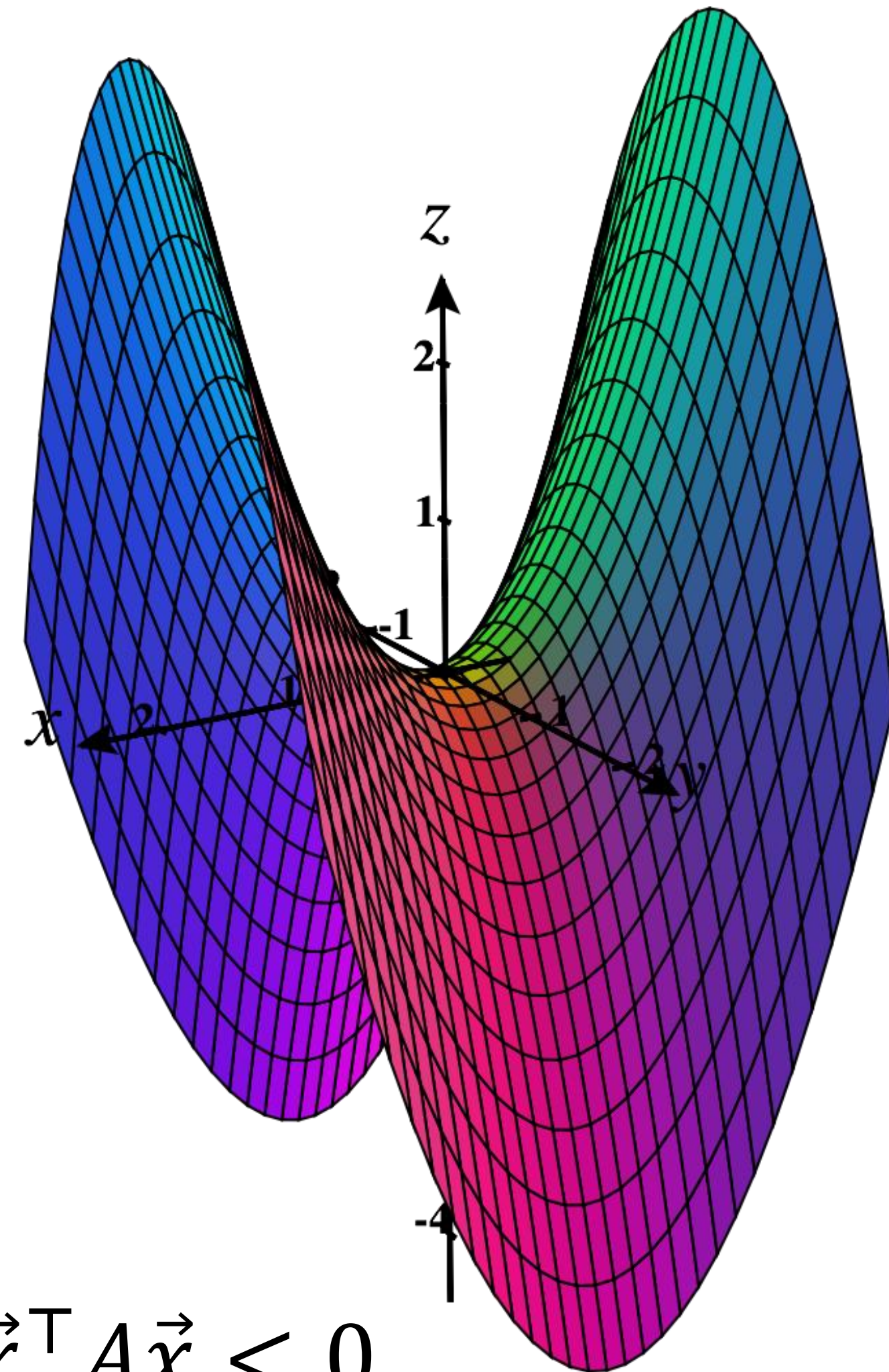


Quadratic Forms

What does $\vec{x}^\top A \vec{x}$ look like when:

- A is positive definite?
- A is negative definite?
- A is positive semi-definite?
- A is negative semi-definite?
- **A is indefinite?**

$\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} > 0$ and $\exists \vec{x}$ such that $\vec{x}^\top A \vec{x} < 0$



Quadratic Forms

What if A is non-symmetric?

Recall that the eigenvectors are not necessarily orthogonal - would weird things happen?

Quadratic Forms

What if A is non-symmetric?

Recall that the eigenvectors are not necessarily orthogonal - would weird things happen? No.

$$\begin{aligned} A &= \frac{A + A^T}{2} + \frac{A - A^T}{2} \\ \vec{x}^T A \vec{x} &= \vec{x}^T \left(\frac{A + A^T}{2} + \frac{A - A^T}{2} \right) \vec{x} \\ &= \vec{x}^T \left(\frac{A + A^T}{2} \right) \vec{x} + \vec{x}^T \left(\frac{A - A^T}{2} \right) \vec{x} \end{aligned}$$

$$\begin{aligned} \vec{x}^T \left(\frac{A - A^T}{2} \right) \vec{x} &= \frac{1}{2} \vec{x}^T A \vec{x} - \frac{1}{2} \vec{x}^T A^T \vec{x} \\ &= \frac{1}{2} \vec{x}^T A \vec{x} - \frac{1}{2} (A \vec{x})^T \vec{x} \\ &= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle A \vec{x}, \vec{x} \rangle \\ &= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle = 0 \end{aligned}$$

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$$\text{Hence } \vec{x}^T A \vec{x} = \vec{x}^T \left(\frac{A + A^T}{2} \right) \vec{x}$$

$$\begin{aligned} \vec{x}^T \left(\frac{A - A^T}{2} \right) \vec{x} &= \frac{1}{2} \vec{x}^T A \vec{x} - \frac{1}{2} \vec{x}^T A^T \vec{x} \\ &= \frac{1}{2} \vec{x}^T A \vec{x} - \frac{1}{2} (A \vec{x})^T \vec{x} \\ &= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle A \vec{x}, \vec{x} \rangle \\ &= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle = 0 \end{aligned}$$

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$$\begin{aligned} A &= \frac{A + A^T}{2} + \frac{A - A^T}{2} \\ \vec{x}^T A \vec{x} &= \vec{x}^T \left(\frac{A + A^T}{2} + \frac{A - A^T}{2} \right) \vec{x} \\ &= \vec{x}^T \left(\frac{A + A^T}{2} \right) \vec{x} + \vec{x}^T \left(\frac{A - A^T}{2} \right) \vec{x} \end{aligned}$$

$$\begin{aligned} \vec{x}^T \left(\frac{A - A^T}{2} \right) \vec{x} &= \frac{1}{2} \vec{x}^T A \vec{x} - \frac{1}{2} \vec{x}^T A^T \vec{x} \\ &= \frac{1}{2} \vec{x}^T A \vec{x} - \frac{1}{2} (A \vec{x})^T \vec{x} \\ &= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle A \vec{x}, \vec{x} \rangle \\ &= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle = 0 \end{aligned}$$

$$\text{Hence } \vec{x}^T A \vec{x} = \vec{x}^T \left(\frac{A + A^T}{2} \right) \vec{x}$$

$\left(\frac{A + A^T}{2} \right)$ is always a symmetric matrix

Quadratic Forms

For any matrix A :

$$A^T A \succcurlyeq 0 \quad (\text{i.e.: } A^T A \text{ is positive semi-definite})$$

Show this.

Quadratic Forms

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$$A^T A \succcurlyeq 0 \quad (\text{i.e.: } A^T A \text{ is positive semi-definite})$$

Show this.

$$\vec{x}^T (A^T A) \vec{x}$$

Quadratic Forms

For **any matrix** A :

$$A^T A \succcurlyeq 0 \quad (\text{i.e.: } A^T A \text{ is positive semi-definite})$$

Show this.

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

$$(AB)C = A(BC), \text{ but } AB \neq BA$$

Quadratic Forms

For **any matrix** A :

$$A^T A \succcurlyeq 0 \quad (\text{i.e.: } A^T A \text{ is positive semi-definite})$$

Show this.

$$\begin{aligned} \vec{x}^T (A^T A) \vec{x} &= (\vec{x}^T A^T) (A \vec{x}) \\ &= (A \vec{x})^T (A \vec{x}) \end{aligned}$$

$$(AB)^T = B^T A^T$$

Quadratic Forms

For **any matrix** A :

$$A^T A \succcurlyeq 0 \quad (\text{i.e.: } A^T A \text{ is positive semi-definite})$$

Show this.

$$\begin{aligned} \vec{x}^T (A^T A) \vec{x} &= (\vec{x}^T A^T) (A \vec{x}) \\ &= (A \vec{x})^T (A \vec{x}) \\ &= \langle A \vec{x}, A \vec{x} \rangle \end{aligned}$$

Alternative inner product notation:

$$\begin{aligned} \vec{x}^T \vec{y} &= (x_1 \quad \cdots \quad x_n) \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \\ &= \sum_{i=1}^n x_i y_i = \langle \vec{x}, \vec{y} \rangle \end{aligned}$$

Quadratic Forms

For any matrix A :

$$A^T A \succcurlyeq 0 \quad (\text{i.e.: } A^T A \text{ is positive semi-definite})$$

Show this.

$$\begin{aligned} \vec{x}^T (A^T A) \vec{x} &= (\vec{x}^T A^T) (A \vec{x}) \\ &= (A \vec{x})^T (A \vec{x}) \\ &= \langle A \vec{x}, A \vec{x} \rangle \\ &= \|A \vec{x}\|_2^2 \end{aligned}$$

Euclidean norm:

$$\begin{aligned} \|\vec{x}\|_2 &= \sqrt{\langle \vec{x}, \vec{x} \rangle} = \sqrt{\sum_{i=1}^n x_i^2} \\ \|\vec{x}\|_2 &\geq 0 \quad \forall \vec{x} \end{aligned}$$

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