Machine Learning CMPT 726

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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

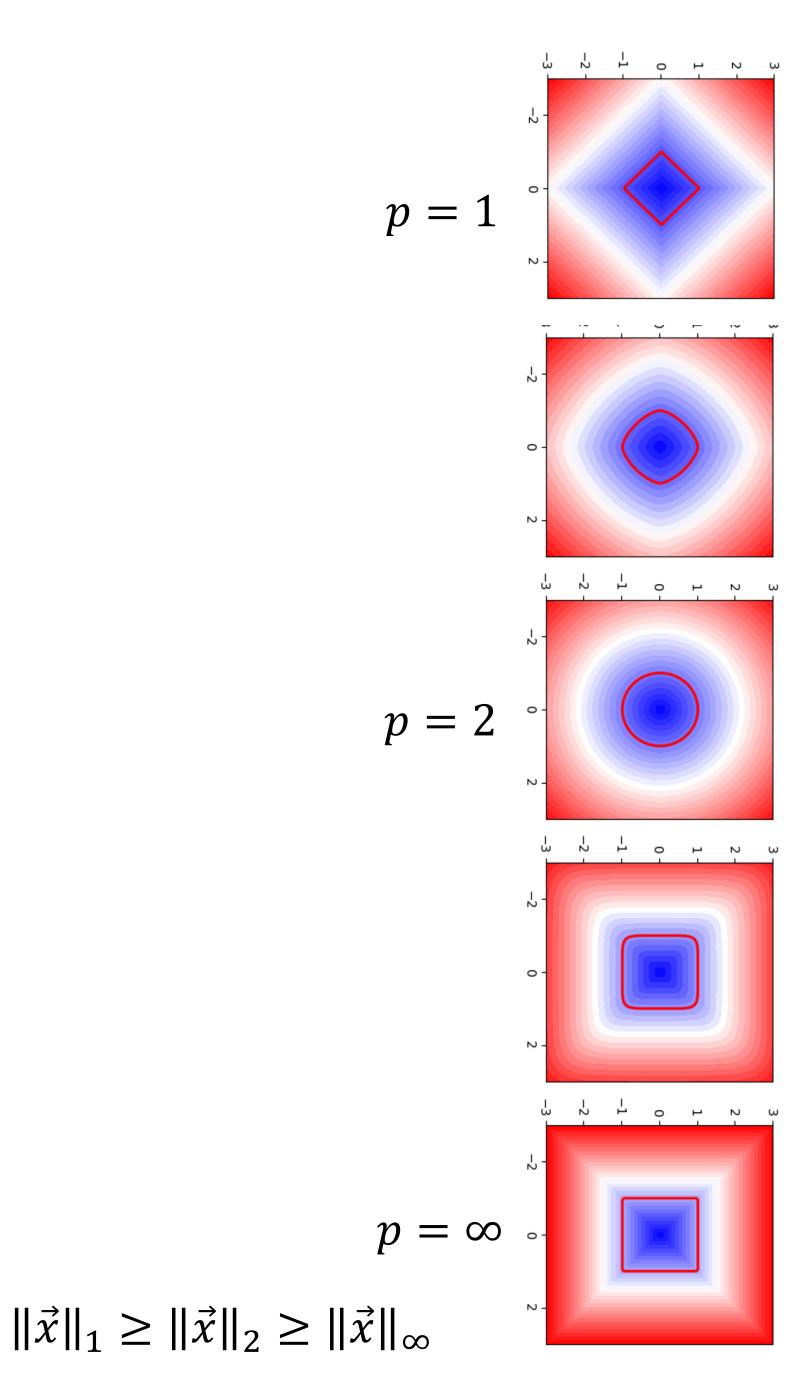
$$\|\vec{x}\|_{p} = \left(\sum_{i=1}^{n} |x_{i}|^{p}\right)^{\frac{1}{p}}$$

Common norms:

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

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

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



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

- ullet A symmetric matrix A is
 - positive definite if all of its eigenvalues are positive
 - negative definite if all of its eigenvalues are negative
 - ullet 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

- ullet A symmetric matrix A is
 - ullet positive definite if all of its eigenvalues are positive A>0
 - negative definite if all of its eigenvalues are negative A < 0
 - positive semi-definite if all of its eigenvalues are non-negative $A \geqslant 0$
 - negative semi-definite if all of its eigenvalues are non-positive $A\leqslant 0$
 - indefinite if some of its eigenvalues are positive and others are negative

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 $f: \mathbb{R} \to \mathbb{R}$ with a polynomial g?

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

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

$$f'(x_0) = g'(x_0)$$

$$f''(x_0) = g''(x_0)$$

•

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

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

The 0th order Taylor expansion at x_0 is:

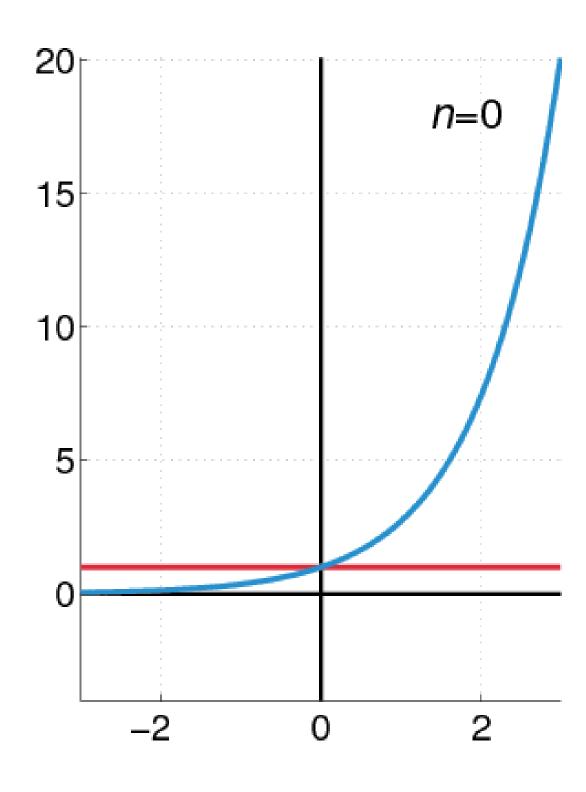
$$g(x) = f(x_0)$$

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:

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



Polynomials in multiple variables:

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

In matrix notation:

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

$$g(\vec{x}) = \alpha + \vec{x}^{\mathsf{T}} \vec{\beta} + \vec{x}^{\mathsf{T}} \Gamma \vec{x}$$
, 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

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

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

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

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

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

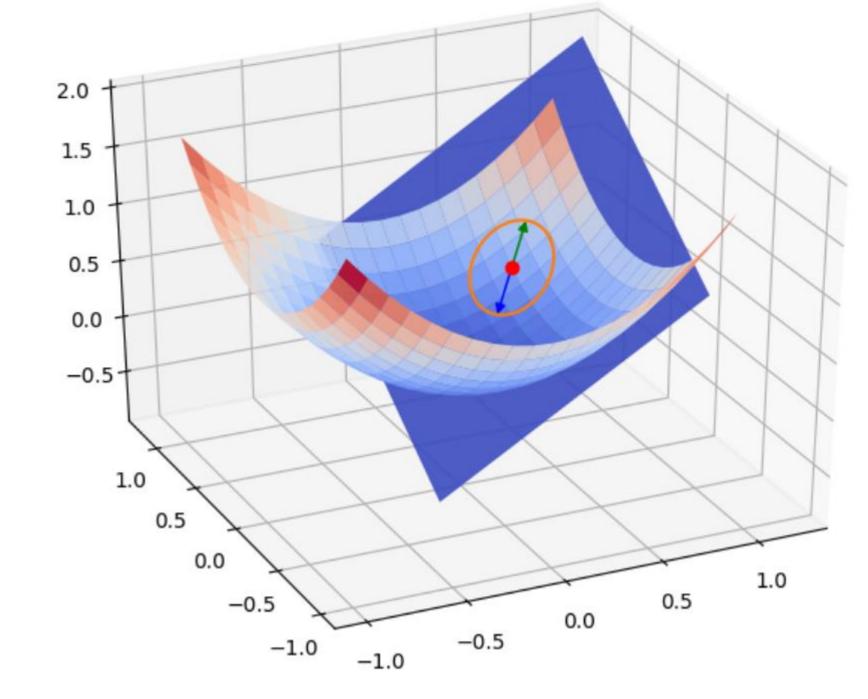
The 2nd order Taylor expansion at \vec{x}_0 is

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

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

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

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



Gradient, Direction of steepest ascent

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

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

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

Gradient, Direction of steepest ascent, and Hessian

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

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

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

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

Let's check if the two definitions agree.

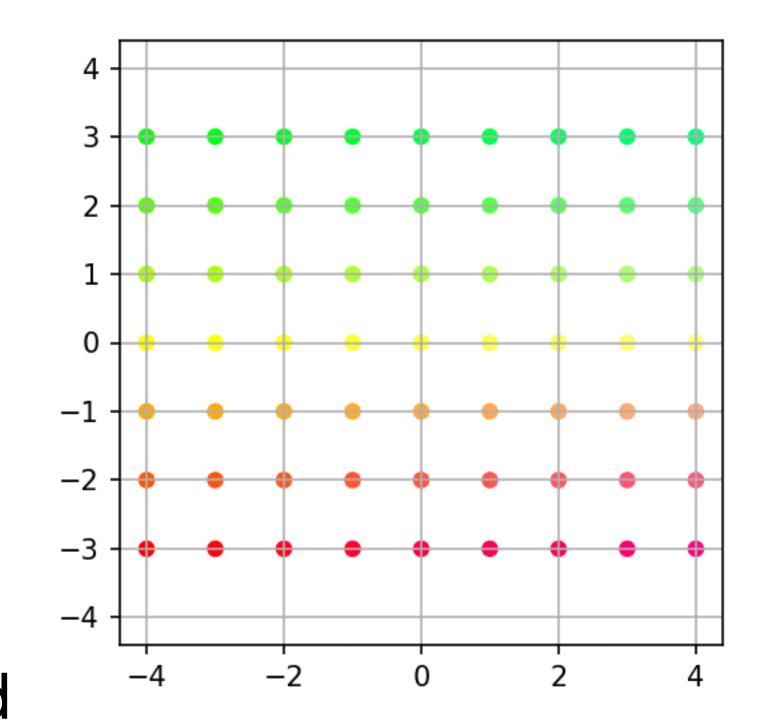
• Indefinite: $\exists \vec{x}$ such that $\vec{x}^{T}A\vec{x} > 0$ and $\exists \vec{x}$ such that $\vec{x}^{T}A\vec{x} < 0$

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

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

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

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



0.9 0.0

0.0 -0.5

Let's check if the two definitions agree.

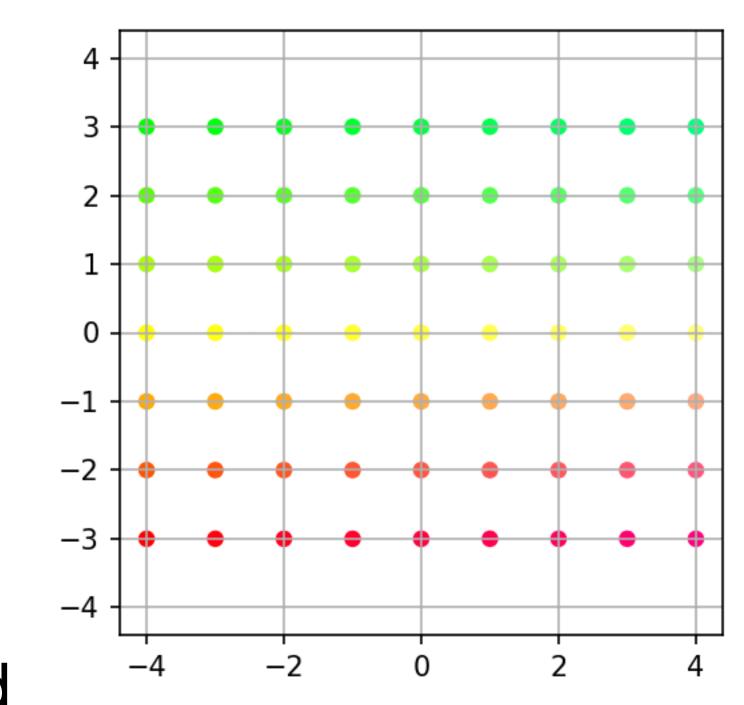
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$$\vec{x}^{\mathsf{T}} A \vec{x} = \langle \vec{x}, A \vec{x} \rangle$$

Recall: Positive if original and transformed -4 to vectors are less than 90 degrees apart, and negative otherwise. Consider the two eigenvectors



0.9 0.0

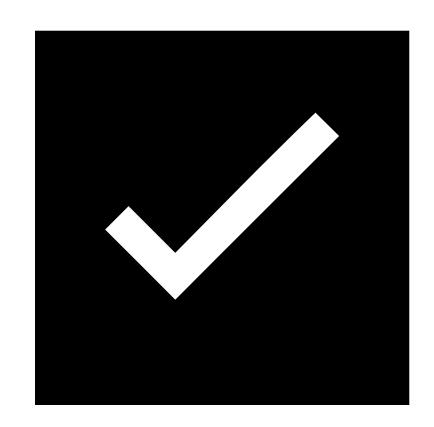
0.0 -0.5

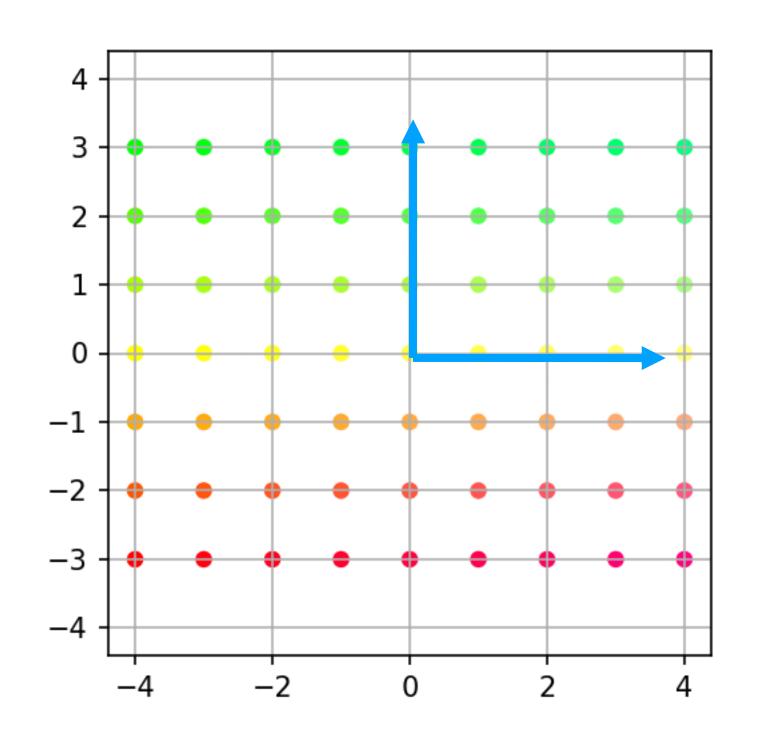
Let's check if the two definitions agree.

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

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

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



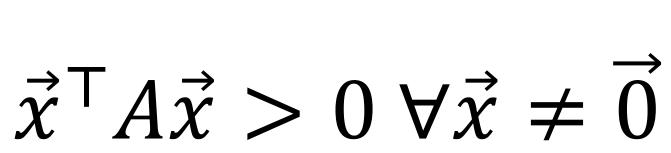


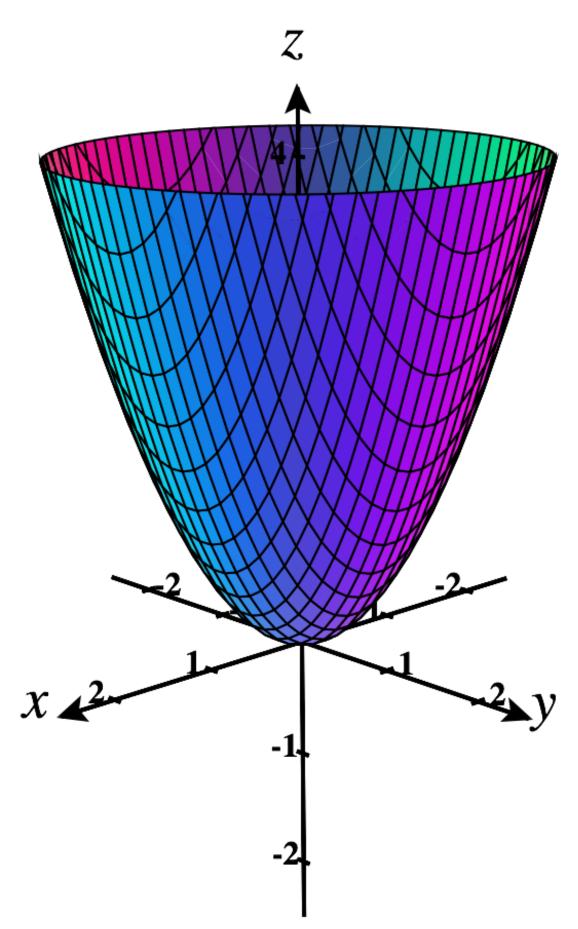
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- A is positive definite?
- A is negative definite?
- \bullet A is positive semi-definite?
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- A is indefinite?

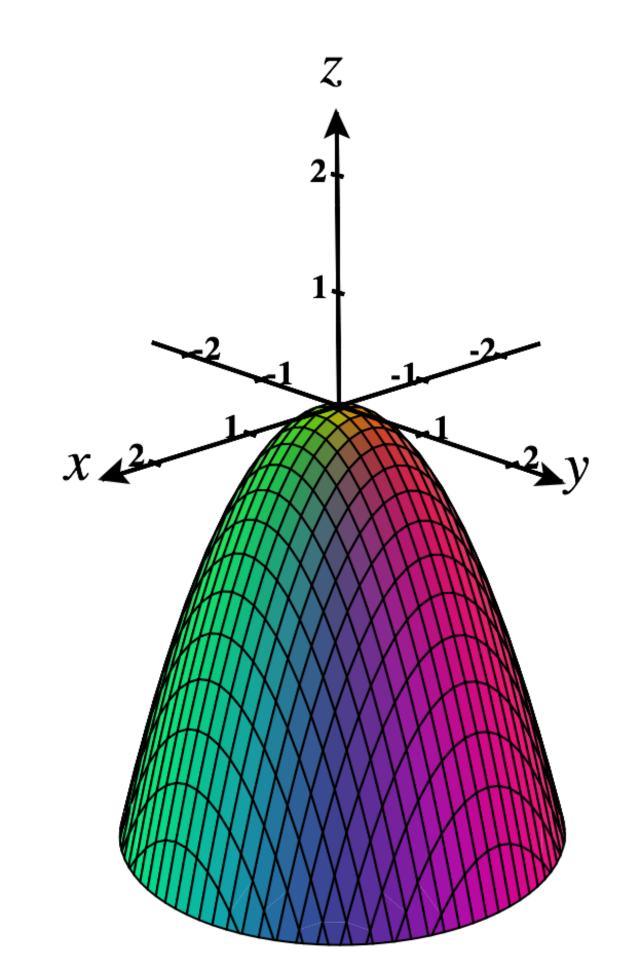
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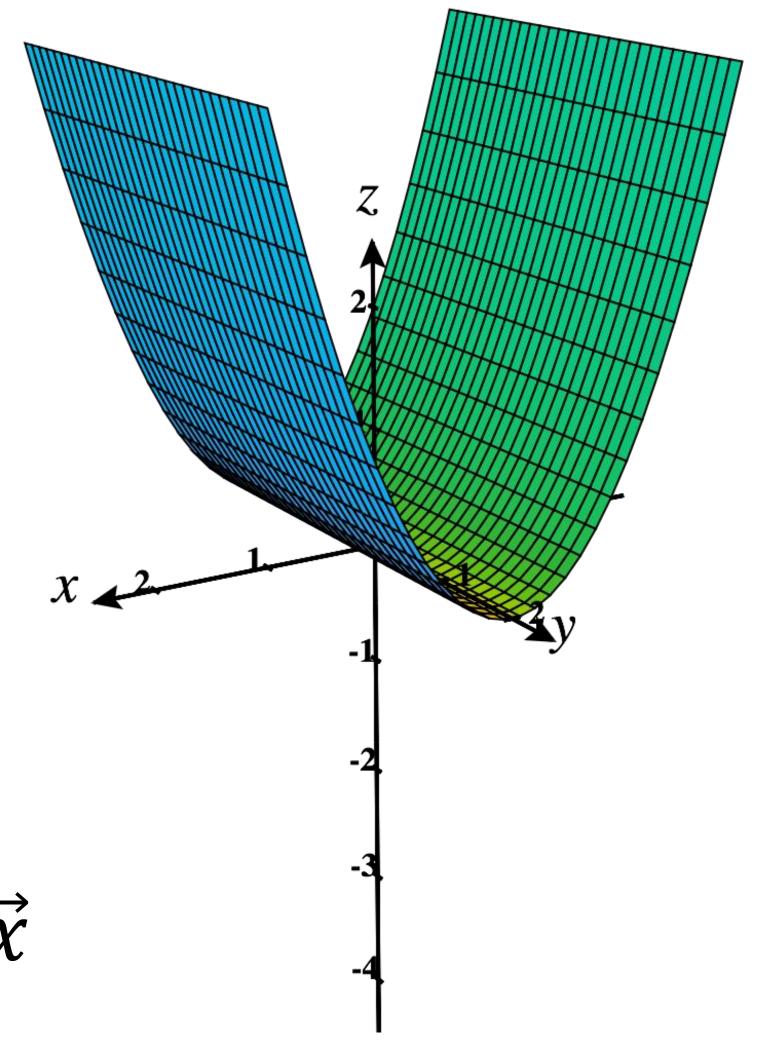
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$$\vec{x}^{\mathsf{T}} A \vec{x} < 0 \ \forall \vec{x} \neq \vec{0}$$



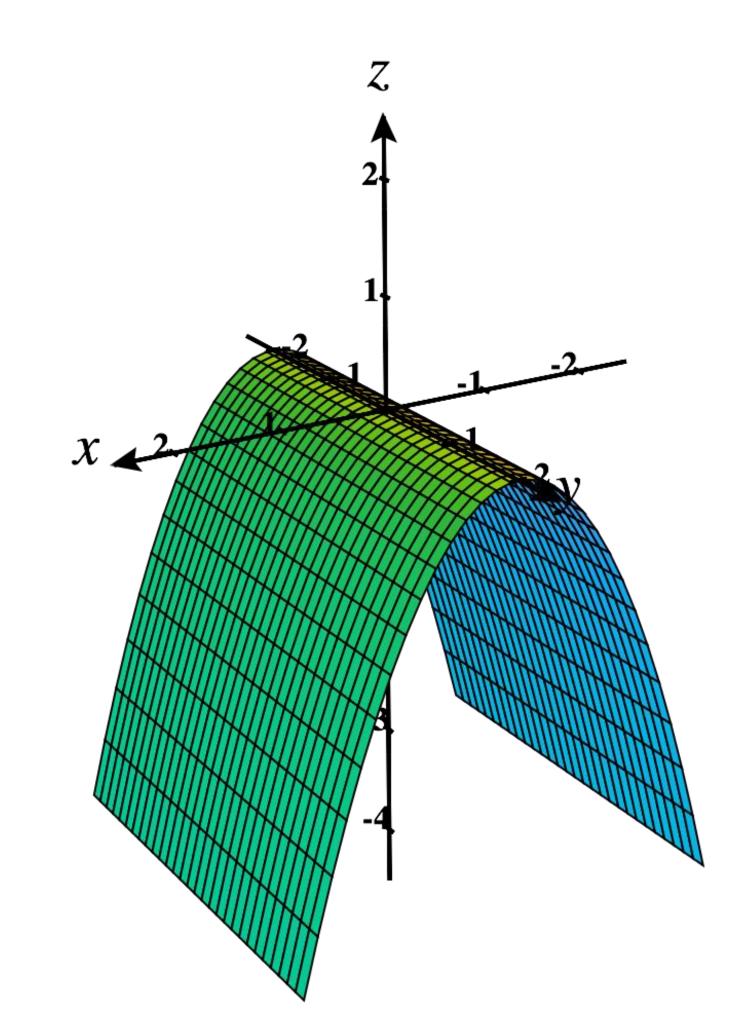
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$$\vec{x}^{\mathsf{T}} A \vec{x} \ge 0 \ \forall \vec{x}$$



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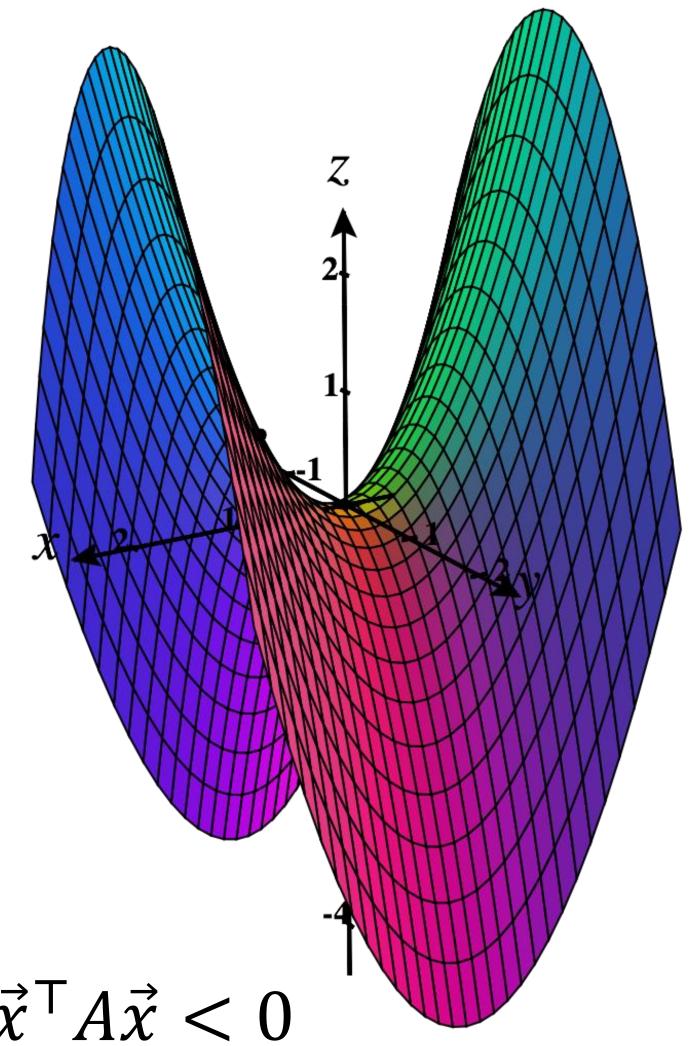
$$\vec{x}^{\mathsf{T}} A \vec{x} \leq 0 \forall \vec{x}$$



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

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

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



What if *A* is non-symmetric?

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

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

$$A = \frac{A + A^{\mathsf{T}}}{2} + \frac{A - A^{\mathsf{T}}}{2}$$

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

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

$$\vec{x}^{\mathsf{T}} \left(\frac{A - A^{\mathsf{T}}}{2} \right) \vec{x} = \frac{1}{2} \vec{x}^{\mathsf{T}} A \vec{x} - \frac{1}{2} \vec{x}^{\mathsf{T}} A^{\mathsf{T}} \vec{x}$$

$$= \frac{1}{2} \vec{x}^{\mathsf{T}} A \vec{x} - \frac{1}{2} (A \vec{x})^{\mathsf{T}} \vec{x}$$

$$= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle A \vec{x}, \vec{x} \rangle$$

$$= \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle - \frac{1}{2} \langle \vec{x}, A \vec{x} \rangle = 0$$

What if A is non-symmetric?

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

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

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

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

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

For any matrix A:

 $A^{\mathsf{T}}A \geqslant 0$ (i.e.: $A^{\mathsf{T}}A$ is positive semi-definite)

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

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

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

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

$$(AB)^{\mathsf{T}} = B^{\mathsf{T}}A^{\mathsf{T}}$$

For any matrix A:

$$A^{\mathsf{T}}A \geqslant 0$$

(i.e.: A^TA is positive semi-definite)

Show this.

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

Alternative inner product notation:

$$\vec{x}^{\mathsf{T}} \vec{y} = (x_1 \quad \cdots \quad x_n) \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$= \sum_{i=1}^n x_i y_i = \langle \vec{x}, \vec{y} \rangle$$

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Show this.

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

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

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

$$= ||A\vec{x}||_2^2$$

Euclidean norm:

$$\|\vec{x}\|_{2} = \sqrt{\langle \vec{x}, \vec{x} \rangle} = \sqrt{\sum_{i=1}^{n} x_{i}^{2}}$$

$$\|\vec{x}\|_{2} \ge 0 \ \forall \vec{x}$$

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

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

$$= ||A\vec{x}||_2^2$$

$$\geq 0 \ \forall A, \vec{x}$$

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