GAMES103: Intro to Physics-Based Animation

Math Background:
Vector, Matrix and Tensor Calculus

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Vectors

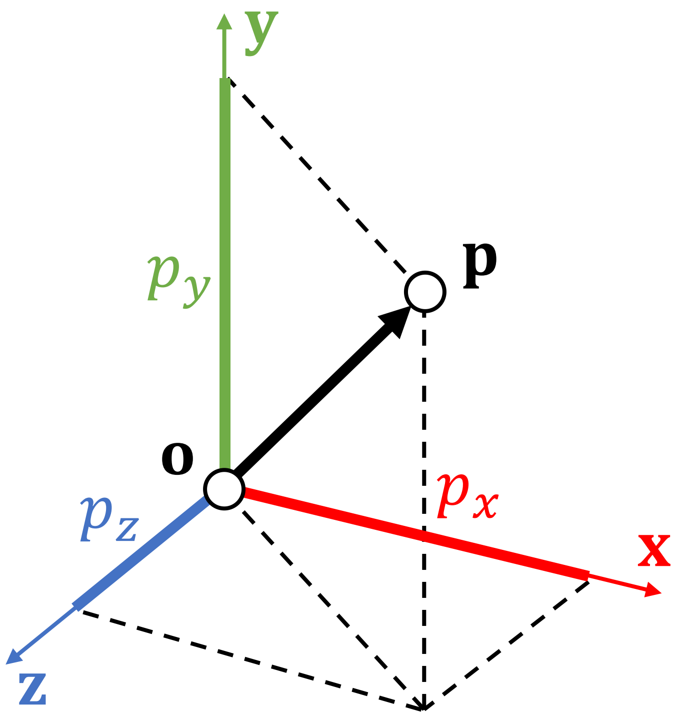
Vector: Definition

An (Euclidean) vector: *A geometric entity endowed with magnitude and direction*.

$$\mathbf{p} = \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} \in \mathbf{R}^3$$

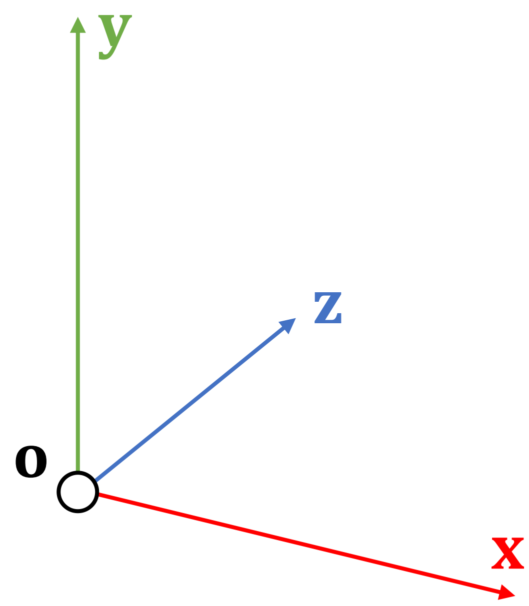
$$\mathbf{o} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

The vector $\mathbf{p}$ is defined with respect to the origin $\mathbf{o}$.



Right-Hand System

(OpenGL, Research, ...)



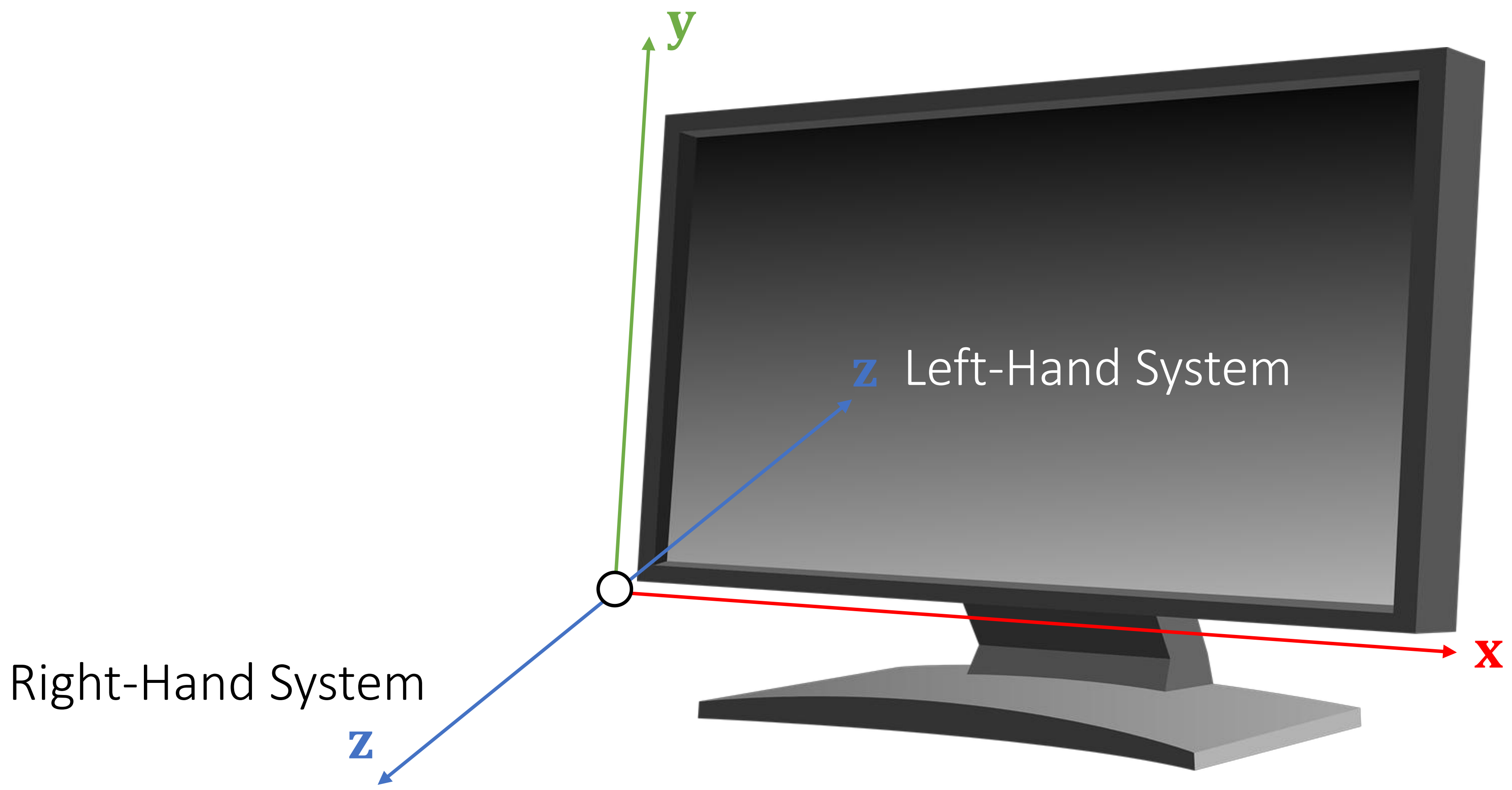
Left-Hand System

(Unity, DirectX, ...)

Vector: Definition

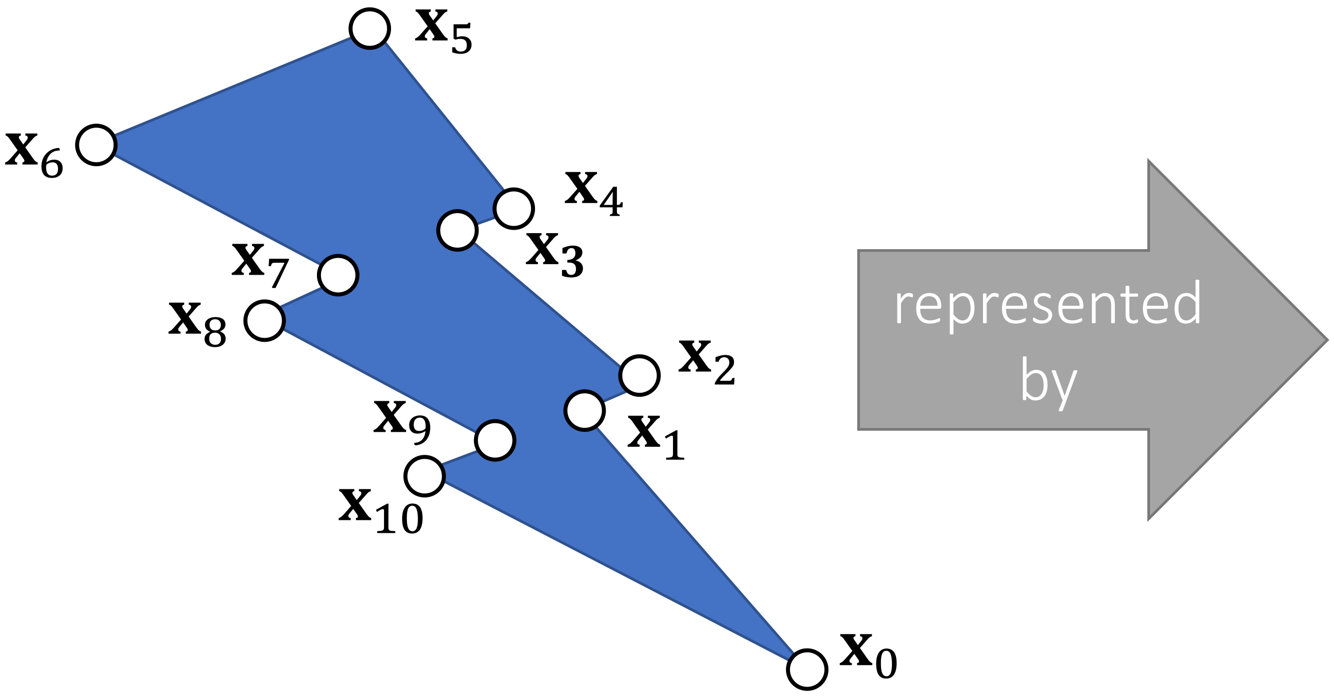
The choice of a right-hand or left-hand system is largely due to:

the convention of the screen space.



Vector: Definition

Vectors can be stacked up to form a high-dimensional vector, commonly used for describing the state of an object.



$$\mathbf{p} = \begin{bmatrix} \mathbf{x}_0 \\ \vdots \\ \mathbf{x}_i \\ \vdots \\ \mathbf{x}_{10} \end{bmatrix} \in \mathbf{R}^{33}$$

for every $\mathbf{x}_i \in \mathbf{R}^3$

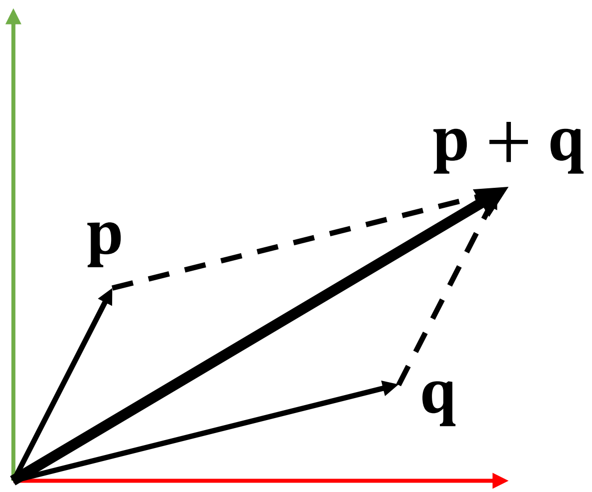
Not a geometric vector, but a stacked vector.

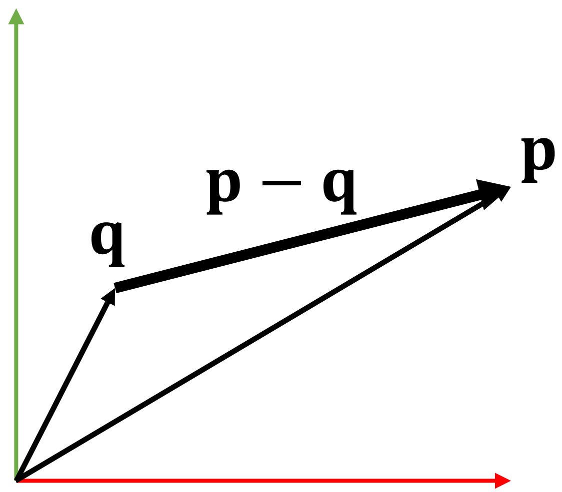
Vector Arithematic: Addition and Subtraction

$$\mathbf{p} \pm \mathbf{q} = \begin{bmatrix} p_x \pm q_x \\ p_y \pm q_y \\ p_z \pm q_z \end{bmatrix}$$

$$\mathbf{p} + \mathbf{q} = \mathbf{q} + \mathbf{p}$$

Addition is commutative.





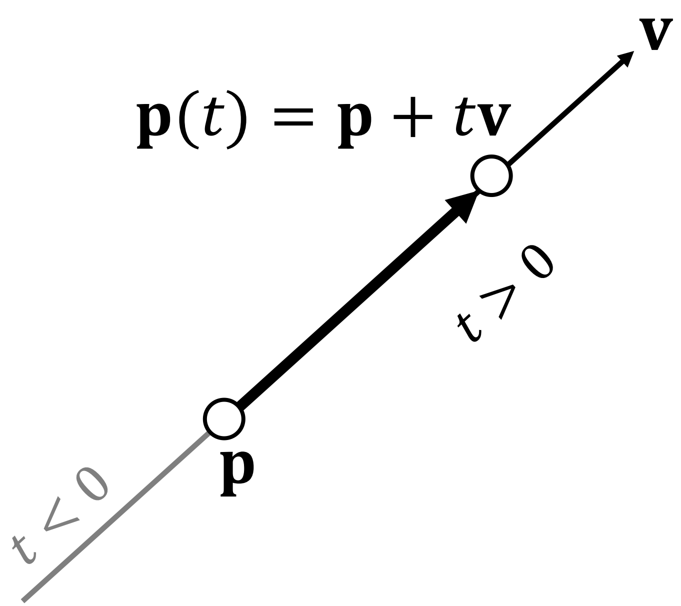
Relative position of $\mathbf{p}$ with respect to $\mathbf{q}$, a.k.a., a displacement

Geometric Meanings

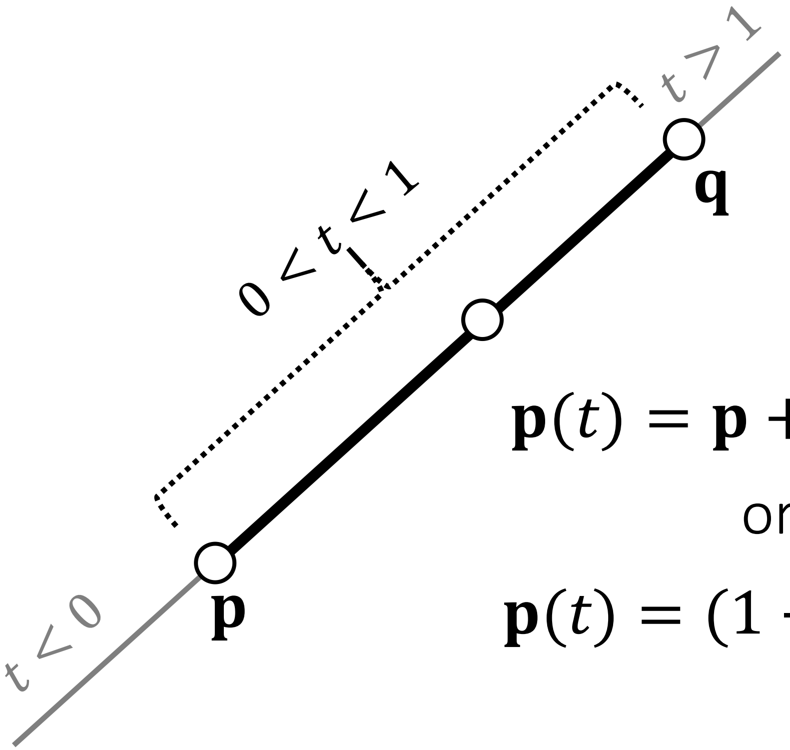
Example 1: Linear Representation

A (geometric) vector can represent a position, a velocity, a force, or a line/ray/segment.

$$\mathbf{p}(t) = \mathbf{p} + t\mathbf{v}$$



t stands for time.



A segment: $0 < t < 1$
A ray: $0 < t$
A line: $t \in \mathbf{R}$

$$\mathbf{p}(t) = \mathbf{p} + t(\mathbf{q} - \mathbf{p})$$

or

$$\mathbf{p}(t) = (1 - t)\mathbf{p} + t\mathbf{q}$$

t is an interpolant.

Vector Norm

A vector norm measures the magnitude of a vector: its length.

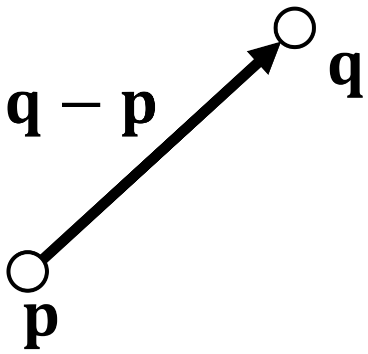
$$\|\mathbf{p}\|_2 = \left(p_x^2 + p_y^2 + p_z^2\right)^{1/2}$$ Euclidean norm (2-norm)

$$\|\mathbf{p}\|_p = \left(|p_x|^p + |p_y|^p + |p_z|^p\right)^{1/p}$$ p-norm

$$\|\mathbf{p}\|_1 = |p_x| + |p_y| + |p_z|$$ 1-norm

$$\|\mathbf{p}\|_\infty = \max(|p_x|, |p_y|, |p_z|)$$ Infinity norm

Vector Norm: Usage



$\|\mathbf{q} - \mathbf{p}\|$

Distance between $\mathbf{q}$ and $\mathbf{p}$

$\|\mathbf{p}\| = 1$

A unit vector

$\bar{\mathbf{p}} = \mathbf{p}/\|\mathbf{p}\|$

Normalization

as

$\|\bar{\mathbf{p}}\| = \|\mathbf{p}\|/\|\mathbf{p}\| = 1$

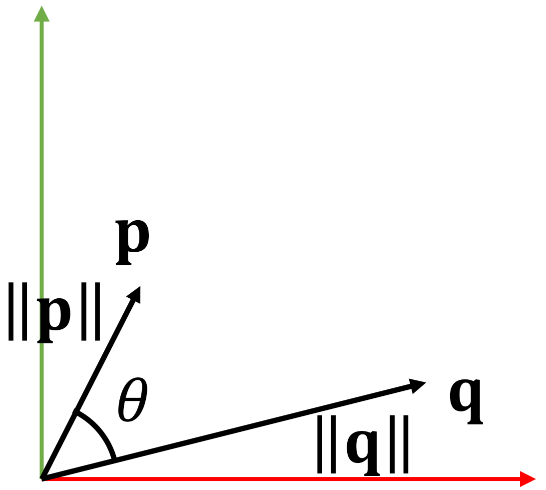
Vector Arithematic: Dot Product

A dot product, also called inner product, is:

$\langle p, q \rangle$

$$\mathbf{p} \cdot \mathbf{q} = p_x q_x + p_y q_y + p_z q_z = \mathbf{p}^{\mathrm{T}} \mathbf{q}$$

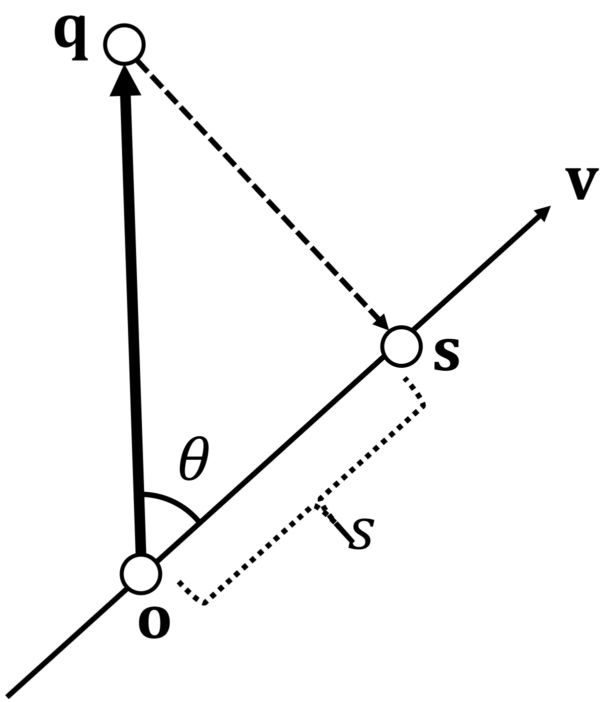
$$= \|\mathbf{p}\| \|\mathbf{q}\| \cos\theta$$



- $\mathbf{p} \cdot \mathbf{q} = \mathbf{q} \cdot \mathbf{p}$
- $\mathbf{p} \cdot (\mathbf{q} + \mathbf{r}) = \mathbf{p} \cdot \mathbf{q} + \mathbf{p} \cdot \mathbf{r}$
- $\mathbf{p} \cdot \mathbf{p} = \|\mathbf{p}\|_2^2$, a different way to write norm.
- If $\mathbf{p} \cdot \mathbf{q} = 0$ and $\mathbf{p}, \mathbf{q} \neq 0$ then $\cos\theta = 0$, then $\mathbf{p}$ and $\mathbf{q}$ are orthogonal.

Geometric Meanings

Example 2: Particle-Line Projection



By definition,

$$s = \|\mathbf{q} - \mathbf{o}\| \cos\theta$$

So,

$$s = \|\mathbf{q} - \mathbf{o}\| \, \|\mathbf{v}\| \cos\theta / \|\mathbf{v}\|$$

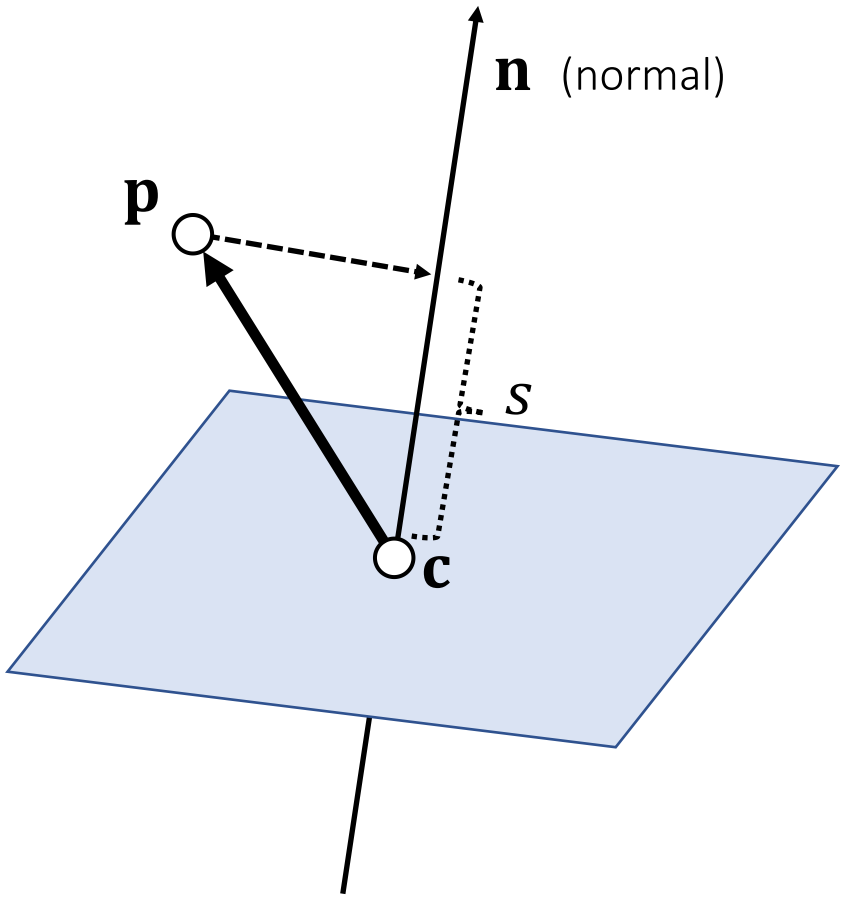
$$s = (\mathbf{q} - \mathbf{o})^{\mathrm{T}} \boxed{\mathbf{v}/\|\mathbf{v}\|}$$ normalization

$$s = (\mathbf{q} - \mathbf{o})^{\mathrm{T}} \bar{\mathbf{v}}$$

And,

$$\mathbf{s} = \mathbf{o} + s\bar{\mathbf{v}}$$

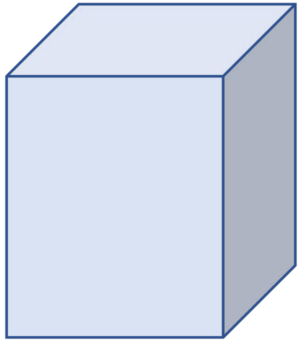
Example 3: Plane Representation



$$s = (\mathbf{p} - \mathbf{c})^{\mathrm{T}}\mathbf{n} \quad \begin{cases} > 0 & \text{Above the plane} \\ = 0 & \text{On the plane} \\ < 0 & \text{Below the plane} \end{cases}$$

The signed distance to the plane

Quiz: How to test if a point is within a box?



Example 4: Particle-Sphere Collision

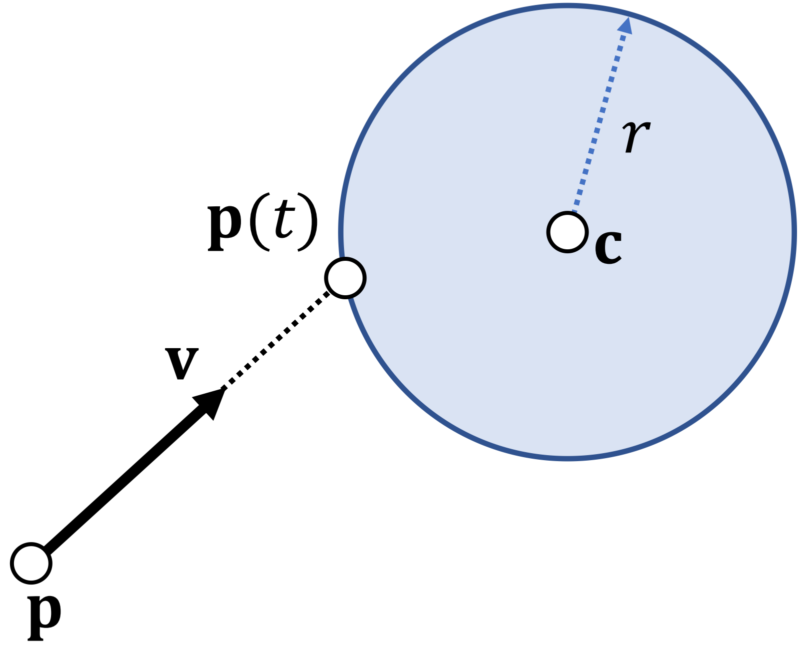
If collision does happen, then:

$$\|\mathbf{p}(t) - \mathbf{c}\|^2 = r^2$$

$$(\mathbf{p} - \mathbf{c} + t\mathbf{v}) \cdot (\mathbf{p} - \mathbf{c} + t\mathbf{v}) = r^2$$

$$(\mathbf{v} \cdot \mathbf{v})t^2 + 2(\mathbf{p} - \mathbf{c}) \cdot \mathbf{v}t + (\mathbf{p} - \mathbf{c}) \cdot (\mathbf{p} - \mathbf{c}) - r^2 = 0$$

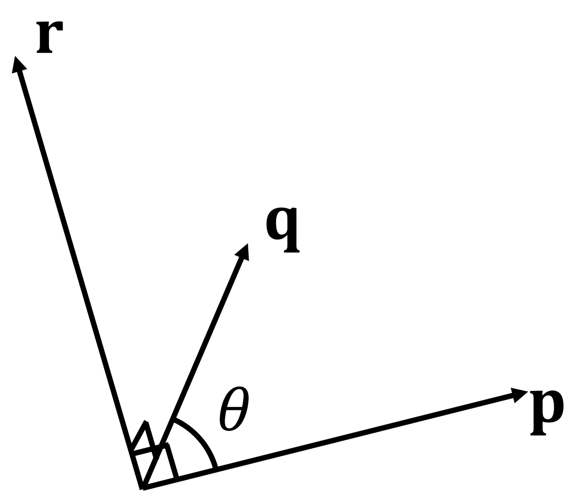
- Three possiblities:
  - No root
  - One root
  - Two roots



Vector Arithematic: Cross Product

The result of a cross product is a vector:

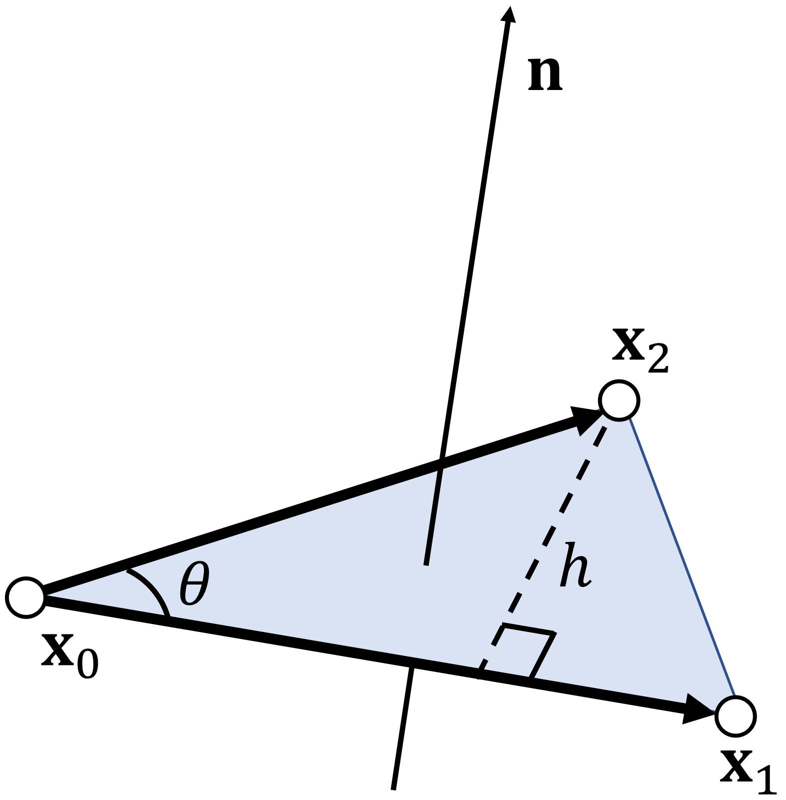
$$\mathbf{r} = \mathbf{p} \times \mathbf{q} = \begin{bmatrix} p_y q_z - p_z q_y \\ p_z q_x - p_x q_z \\ p_x q_y - p_y q_x \end{bmatrix}$$



Geometric Meanings

- $\mathbf{r} \cdot \mathbf{p} = 0$; $\mathbf{r} \cdot \mathbf{q} = 0$; $\|\mathbf{r}\| = \|\mathbf{p}\|\|\mathbf{q}\| \sin\theta$
- $\mathbf{p} \times \mathbf{q} = - \ \mathbf{q} \times \mathbf{p}$
- $\mathbf{p} \times (\mathbf{q} + \mathbf{r}) = \mathbf{p} \times \mathbf{q} + \mathbf{p} \times \mathbf{r}$
- If $\mathbf{p} \times \mathbf{q} = \mathbf{0}$ and $\mathbf{p}, \mathbf{q} \neq 0$ then $\sin\theta = 0$, then $\mathbf{p}$ and $\mathbf{q}$ are parallel (in the same or opposite direction).

Example 5: Triangle Normal and Area



Edge vectors:

$$\mathbf{x}_{10} = \mathbf{x}_1 - \mathbf{x}_0 \qquad \mathbf{x}_{20} = \mathbf{x}_2 - \mathbf{x}_0$$

Normal:

$$\mathbf{n} = (\mathbf{x}_{10} \times \mathbf{x}_{20}) / \|\mathbf{x}_{10} \times \mathbf{x}_{20}\|$$

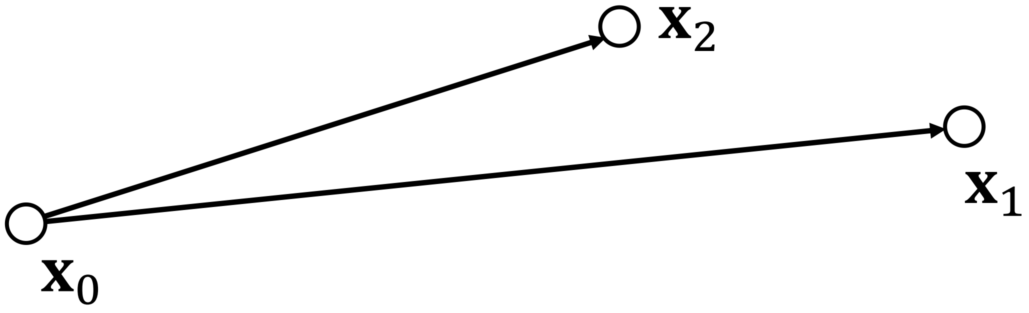
Area:

$$A = \|\mathbf{x}_{10}\| h/2$$

$$= \|\mathbf{x}_{10}\| \|\mathbf{x}_{20}\| \sin\theta / 2$$

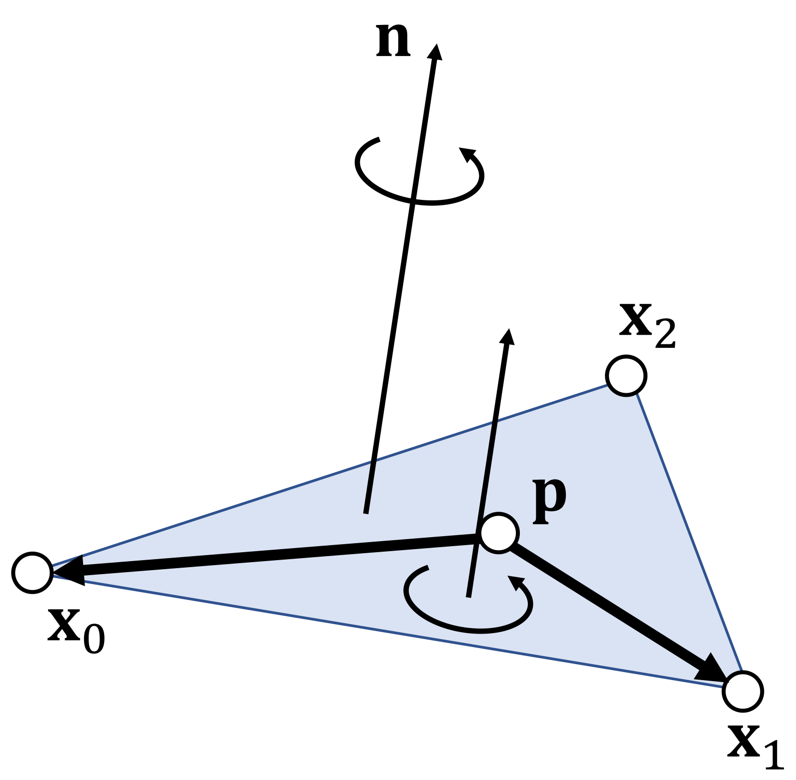
$$= \|\mathbf{x}_{10} \times \mathbf{x}_{20}\| / 2$$

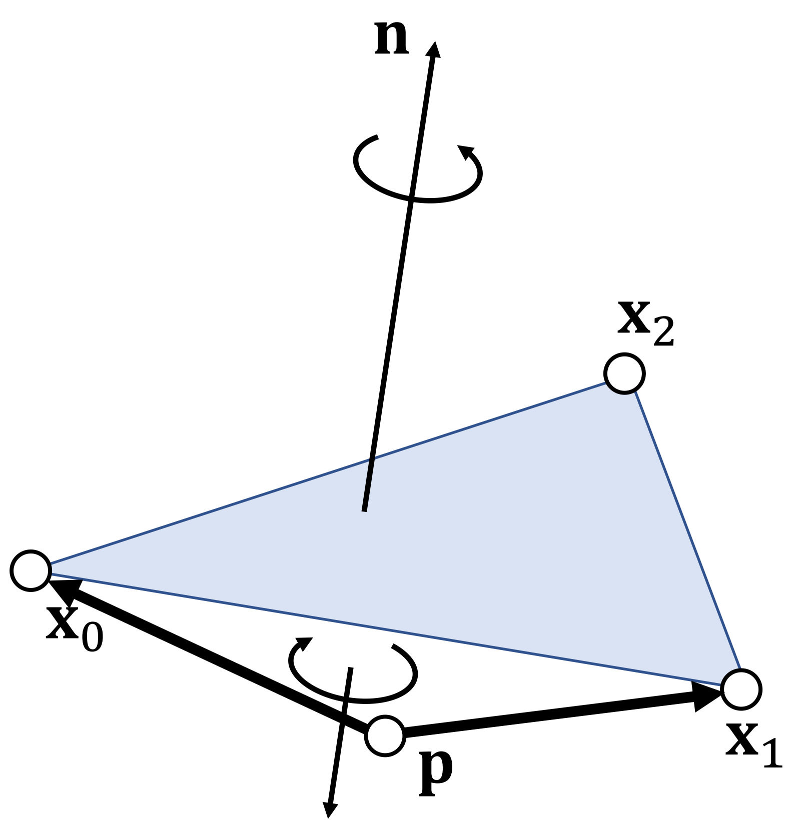
- Cross product gives both the normal and the area.
- The normal depends on the triangle index order, also known as topological order.



Quiz: How to test if three points are on the same line (co-linear)?

Example 6: Triangle Inside/Outside Test





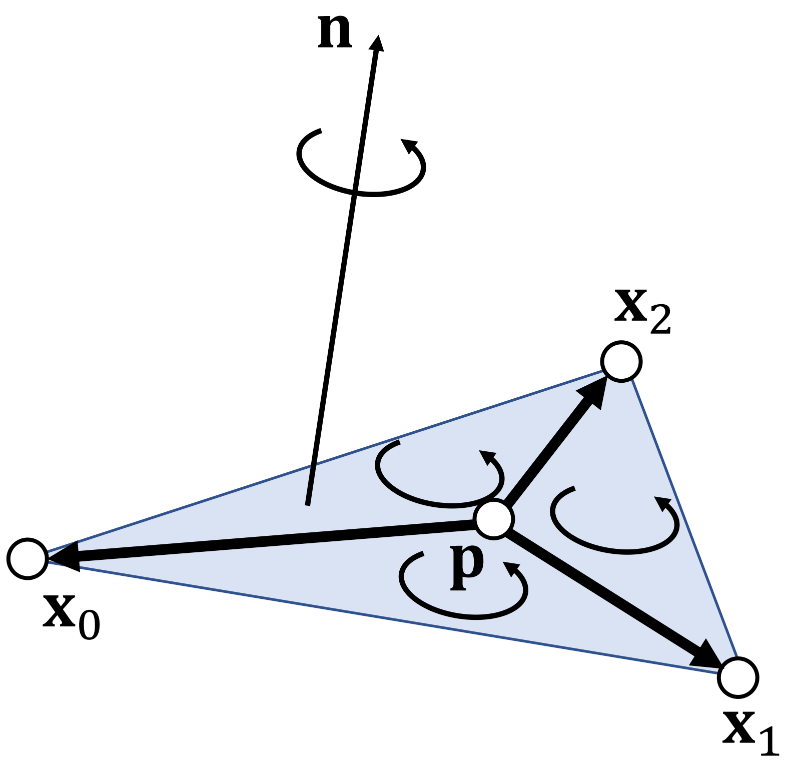
If $\mathbf{p}$ is inside of $\mathbf{x}_0\mathbf{x}_1$, then:

$$(\mathbf{x}_0 - \mathbf{p}) \times (\mathbf{x}_1 - \mathbf{p}) \cdot \mathbf{n} > 0$$

If $\mathbf{p}$ is outside of $\mathbf{x}_0\mathbf{x}_1$, then:

$$(\mathbf{x}_0 - \mathbf{p}) \times (\mathbf{x}_1 - \mathbf{p}) \cdot \mathbf{n} < 0$$

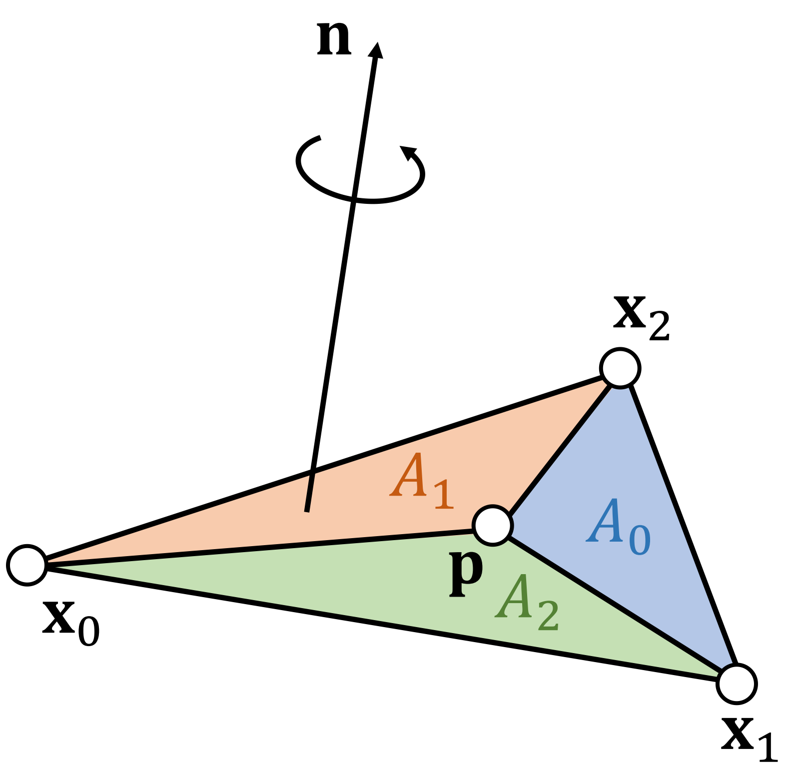
Example 6: Triangle Inside/Outside Test



$$\left.\begin{array}{l}(\mathbf{x}_0 - \mathbf{p}) \times (\mathbf{x}_1 - \mathbf{p}) \cdot \mathbf{n} > 0 \\ (\mathbf{x}_1 - \mathbf{p}) \times (\mathbf{x}_2 - \mathbf{p}) \cdot \mathbf{n} > 0 \\ (\mathbf{x}_2 - \mathbf{p}) \times (\mathbf{x}_0 - \mathbf{p}) \cdot \mathbf{n} > 0\end{array}\right\} \text{Inside of triangle}$$

Otherwise, outside.

Example 7: Barycentric Coordinates



Note that:

$$\frac{1}{2}(\mathbf{x}_0 - \mathbf{p}) \times (\mathbf{x}_1 - \mathbf{p}) \cdot \mathbf{n} = \begin{cases} \frac{1}{2}\|(\mathbf{x}_0 - \mathbf{p}) \times (\mathbf{x}_1 - \mathbf{p})\| & \text{inside} \\ -\frac{1}{2}\|(\mathbf{x}_0 - \mathbf{p}) \times (\mathbf{x}_1 - \mathbf{p})\| & \text{outside} \end{cases}$$

Signed areas:

$$A_2 = \frac{1}{2}(\mathbf{x}_0 - \mathbf{p}) \times (\mathbf{x}_1 - \mathbf{p}) \cdot \mathbf{n}$$

$$A_0 = \frac{1}{2}(\mathbf{x}_1 - \mathbf{p}) \times (\mathbf{x}_2 - \mathbf{p}) \cdot \mathbf{n}$$

$$A_1 = \frac{1}{2}(\mathbf{x}_2 - \mathbf{p}) \times (\mathbf{x}_0 - \mathbf{p}) \cdot \mathbf{n}$$

$$\boxed{A_0 + A_1 + A_2 = A}$$

Barycentric weights of $\mathbf{p}$:

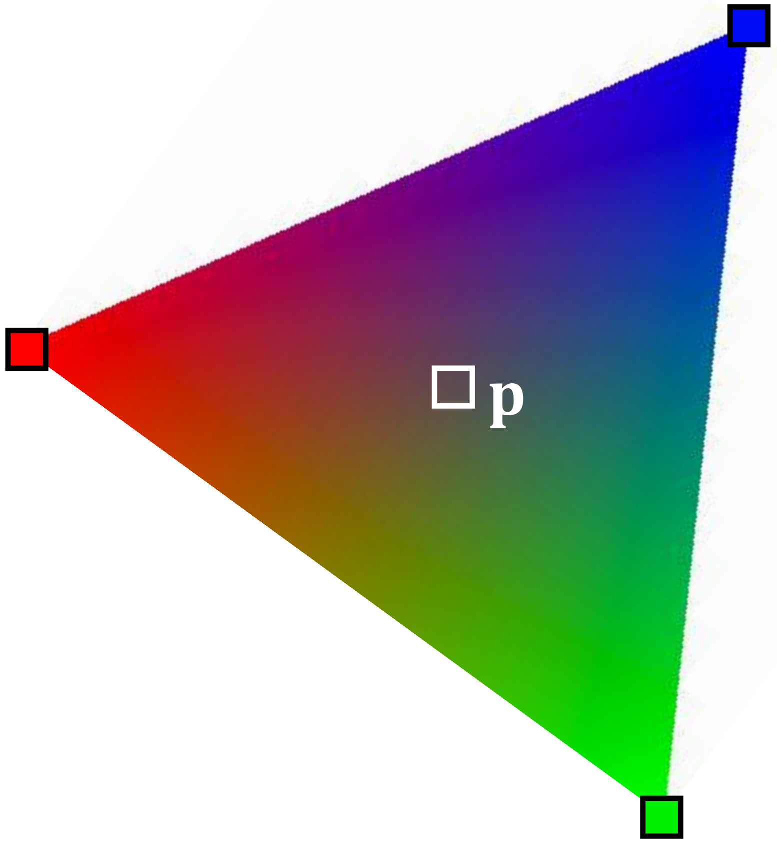
$$b_0 = A_0/A \qquad b_1 = A_1/A \qquad b_2 = A_2/A$$

$$\boxed{b_0 + b_1 + b_2 = 1}$$

Barycentric Interpolation

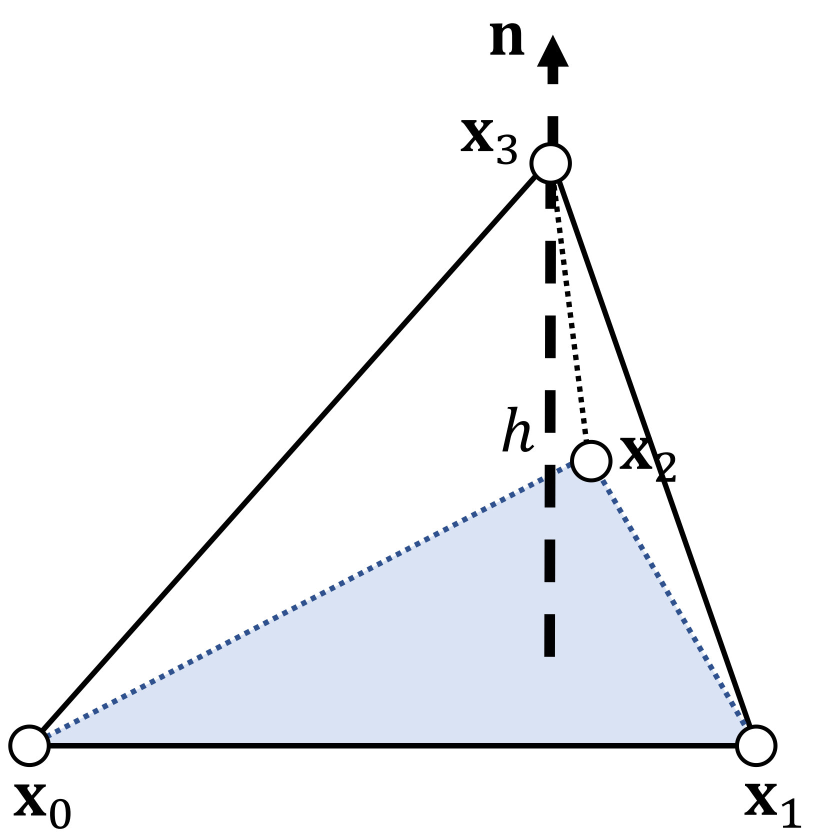
$$\boxed{\mathbf{p} = b_0\mathbf{x}_0 + b_1\mathbf{x}_1 + b_2\mathbf{x}_2}$$

Gouraud Shading



- Barycentric weights allows the interior points of a triangle to be interpolated.
- In a traditional graphics pipeline, pixel colors are calculated at triangle vertices first, and then interpolated within. This is known as *Gouraud shading*.
- It is hardware accelerated.
- It is no longer popular.

Example 9: Tetrahedral Volume



Edge vectors:

$$\mathbf{x}_{10} = \mathbf{x}_1 - \mathbf{x}_0 \quad \mathbf{x}_{20} = \mathbf{x}_2 - \mathbf{x}_0 \quad \mathbf{x}_{30} = \mathbf{x}_3 - \mathbf{x}_0$$

Base triangle area:

$$A = \frac{1}{2}\|\mathbf{x}_{10} \times \mathbf{x}_{20}\|$$

Height:

$$h = \mathbf{x}_{30} \cdot \mathbf{n} = \mathbf{x}_{30} \cdot \frac{\mathbf{x}_{10} \times \mathbf{x}_{20}}{\|\mathbf{x}_{10} \times \mathbf{x}_{20}\|}$$

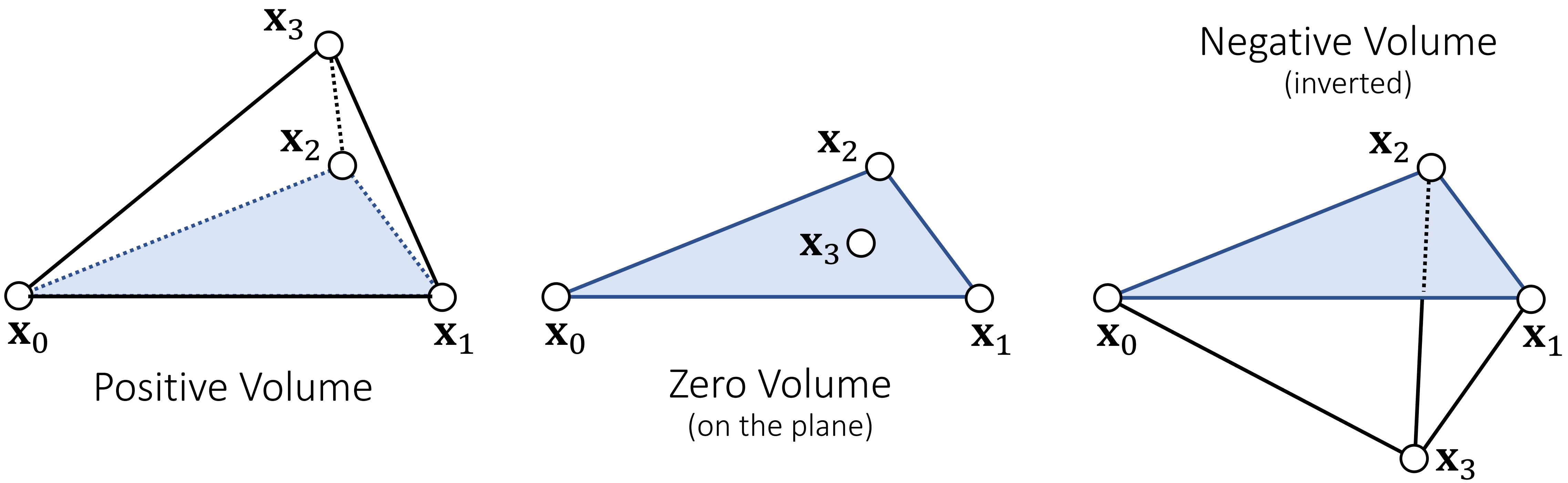
Volume:

$$V = \frac{1}{3}hA = \frac{1}{6}\mathbf{x}_{30} \cdot \mathbf{x}_{10} \times \mathbf{x}_{20}$$

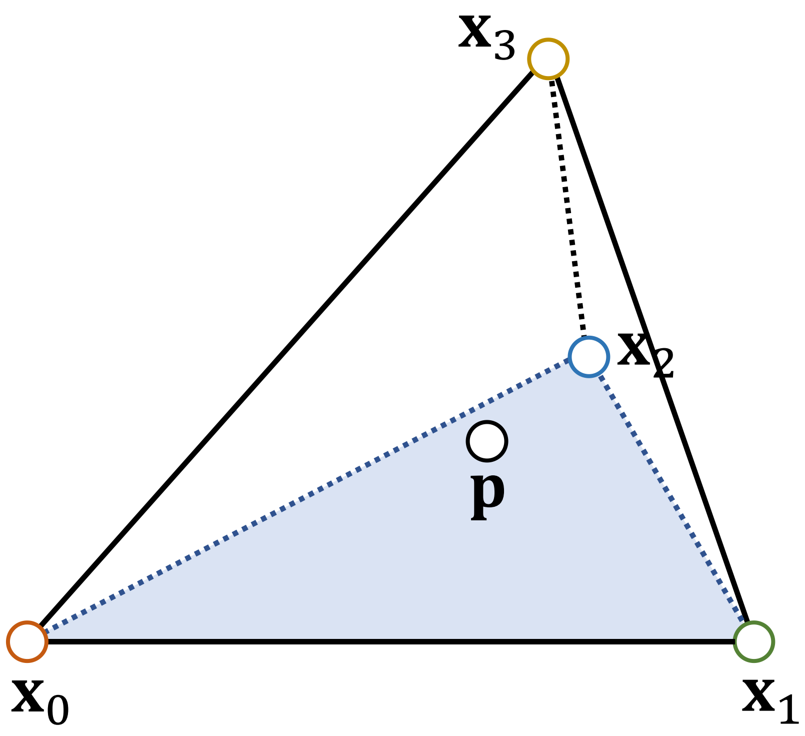
$$= \frac{1}{6}\begin{vmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \mathbf{x}_0 \\ 1 & 1 & 1 & 1 \end{vmatrix}$$

Example 9: Tetrahedral Volume

Note that the volume $V = \frac{1}{3}hA = \frac{1}{6}\mathbf{x}_{30} \cdot \mathbf{x}_{10} \times \mathbf{x}_{20}$ is signed.



Example 10: Barycentric Weights (cont.)



- $\mathbf{p}$ splits the tetrahedron into four sub-tetrahedra:

$$V_0 = \mathrm{Vol}(\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1, \mathbf{p})$$
$$V_1 = \mathrm{Vol}(\mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_0, \mathbf{p})$$
$$V_2 = \mathrm{Vol}(\mathbf{x}_1, \mathbf{x}_0, \mathbf{x}_3, \mathbf{p})$$
$$V_3 = \mathrm{Vol}(\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \mathbf{p})$$

- $\mathbf{p}$ is inside if and only if: $V_0, V_1, V_2, V_3 > 0.$

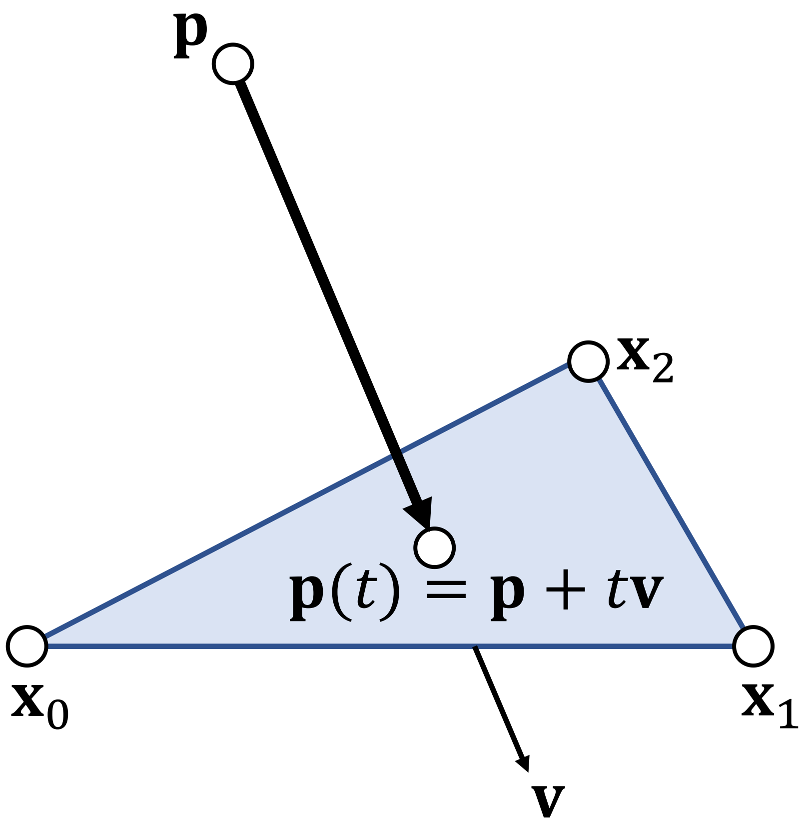
- Barycentric weights:

$$b_0 = V_0/V \quad b_1 = V_1/V \quad b_2 = V_2/V \quad b_3 = V_3/V$$

$$\boxed{b_0 + b_1 + b_2 + b_3 = 1}$$

$$\boxed{\mathbf{p} = b_0\mathbf{x}_0 + b_1\mathbf{x}_1 + b_2\mathbf{x}_2 + b_3\mathbf{x}_3}$$

Example 11: Particle-triangle Intersection



- First, we find t when the particle hits the plane:

$$(\mathbf{p}(t) - \mathbf{x}_0) \cdot \mathbf{x}_{10} \times \mathbf{x}_{20} = 0$$

$$(\mathbf{p} - \mathbf{x}_0 + t\mathbf{v}) \cdot \mathbf{x}_{10} \times \mathbf{x}_{20} = 0$$

$$t = \frac{(\mathbf{p} - \mathbf{x}_0) \cdot \mathbf{x}_{10} \times \mathbf{x}_{20}}{\mathbf{v} \cdot \mathbf{x}_{10} \times \mathbf{x}_{20}}$$

- We then check if $\mathbf{p}(t)$ is inside or not.
  - See Example 6.

Matrices

Matrix: Definition

A *real* matrix is a set of *real* elements arranged in rows and columns.

$$\mathbf{A} = \begin{bmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{bmatrix} = [\mathbf{a}_0 \quad \mathbf{a}_1 \quad \mathbf{a}_2] \in \mathbf{R}^{3\times 3}$$

$$\mathbf{A}^{\mathrm{T}} = \begin{bmatrix} a_{00} & a_{10} & a_{20} \\ a_{01} & a_{11} & a_{21} \\ a_{02} & a_{12} & a_{22} \end{bmatrix}$$

Transpose

$$\begin{bmatrix} a_{00} & & \\ & a_{11} & \\ & & a_{22} \end{bmatrix}$$

Diagonal

$$\mathbf{I} = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$$

Identity

$\mathbf{A}^{\mathrm{T}} = \mathbf{A}$ Symmetric

Matrix: Multiplication

How to do matrix-vector and matrix-matrix multiplication? (Omitted)

- $\mathbf{AB} \neq \mathbf{BA}$ $(\mathbf{AB})\mathbf{x} = \mathbf{A}(\mathbf{Bx})$
- $(\mathbf{AB})^{\mathrm{T}} = \mathbf{B}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}$ $(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{\mathrm{T}} = \boxed{\mathbf{A}^{\mathrm{T}}\mathbf{A}}$ symmetric
- $\mathbf{Ix} = \mathbf{x}$ $\mathbf{AI} = \mathbf{IA} = \mathbf{A}$

- $\mathbf{A}^{-1}$: $\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$ inverse
- $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$
- Not every matrix is invertible, e.g., $\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$.

Matrix: Orthogonality

An orthogonal matrix is a matrix made of orthogonal unit vectors.

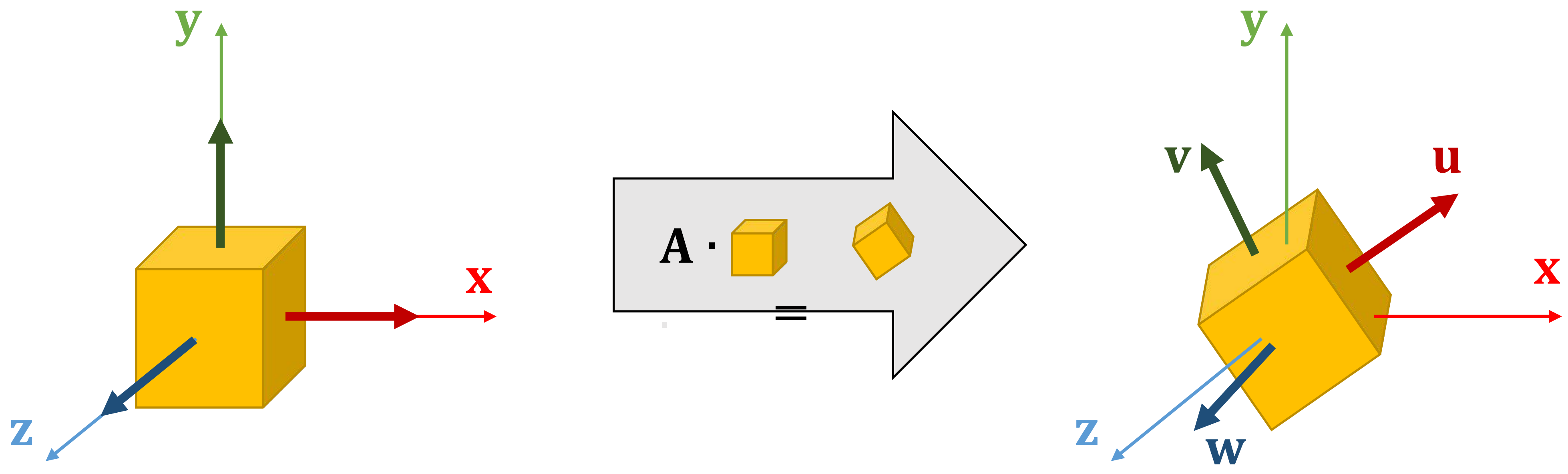
$$\mathbf{A} = [\mathbf{a}_0 \quad \mathbf{a}_1 \quad \mathbf{a}_2] \quad \text{such that} \quad \mathbf{a}_i^{\mathrm{T}}\mathbf{a}_j = \begin{cases} 1, & \text{if } i = j \\ 0. & \text{if } i \neq j \end{cases}$$

$$\boxed{\mathbf{A}^{\mathrm{T}}\mathbf{A} = \begin{bmatrix} \mathbf{a}_0^{\mathrm{T}} \\ \mathbf{a}_1^{\mathrm{T}} \\ \mathbf{a}_2^{\mathrm{T}} \end{bmatrix} [\mathbf{a}_0 \quad \mathbf{a}_1 \quad \mathbf{a}_2] = \begin{bmatrix} \mathbf{a}_0^{\mathrm{T}}\mathbf{a}_0 & \mathbf{a}_0^{\mathrm{T}}\mathbf{a}_1 & \mathbf{a}_0^{\mathrm{T}}\mathbf{a}_2 \\ \mathbf{a}_1^{\mathrm{T}}\mathbf{a}_0 & \mathbf{a}_1^{\mathrm{T}}\mathbf{a}_1 & \mathbf{a}_1^{\mathrm{T}}\mathbf{a}_2 \\ \mathbf{a}_2^{\mathrm{T}}\mathbf{a}_0 & \mathbf{a}_2^{\mathrm{T}}\mathbf{a}_1 & \mathbf{a}_2^{\mathrm{T}}\mathbf{a}_2 \end{bmatrix} = \mathbf{I}}$$

$$\boxed{\mathbf{A}^{\mathrm{T}} = \mathbf{A}^{-1}}$$

Matrix Transformation

A rotation can be represented by an orthogonal matrix.

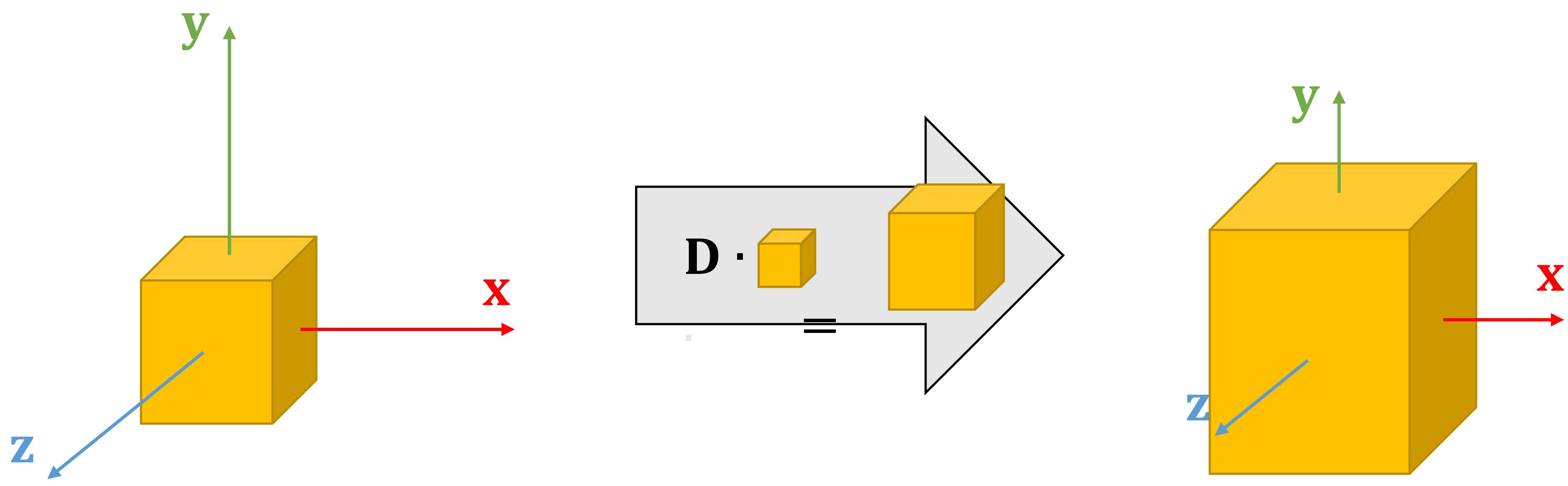


$$\left.\begin{aligned}\mathbf{A}\mathbf{x} &= \mathbf{u}\\ \mathbf{A}\mathbf{y} &= \mathbf{v}\\ \mathbf{A}\mathbf{z} &= \mathbf{w}\end{aligned}\right\} \mathbf{A} = \boxed{[\mathbf{u} \quad \mathbf{v} \quad \mathbf{w}]}$$

Consisting of local coordinate vectors.

Matrix Transformation

A scaling can be represented by a diagonal matrix.



$$\mathbf{D} = \begin{bmatrix} d_x & & \\ & d_y & \\ & & d_z \end{bmatrix}$$

Consisting of scaling factors.

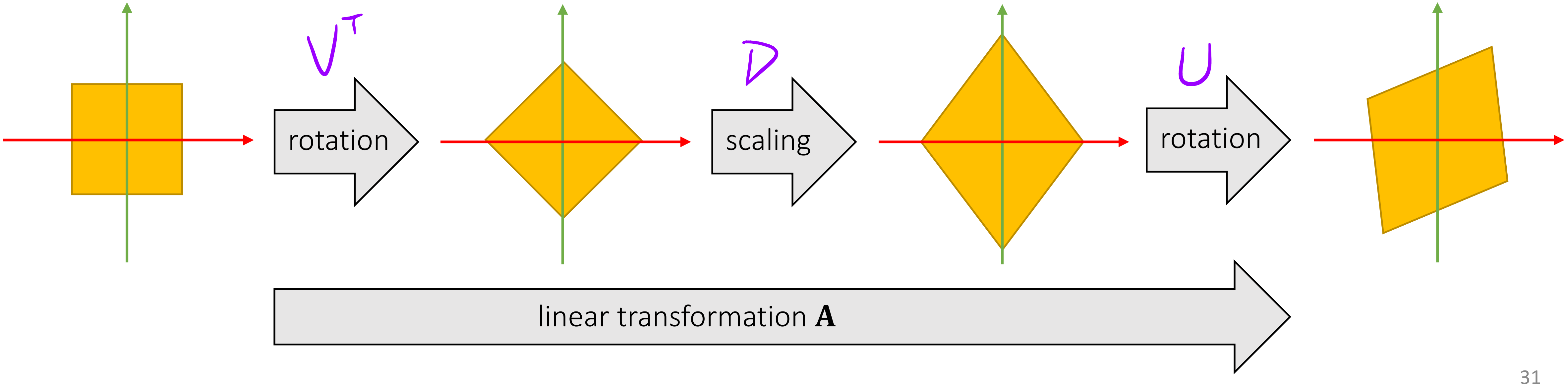
Singular Value Decomposition

A matrix can be decomposed into:

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^{\mathrm{T}}$$ such that $\boxed{\mathbf{D}}$ is diagonal, and $\mathbf{U}$ and $\mathbf{V}$ are orthogonal.

Singular values

Any linear deformation can be decomposed into three steps: rotation, scaling and rotation:



Eigenvalue Decomposition

A symmetric matrix can be decomposed into:

$U^{-1} = U^T$

$\mathbf{A} = \mathbf{U}\boxed{\mathbf{D}}\mathbf{U}^{-1}$ such that $\boxed{\mathbf{D}}$ is diagonal, and $\mathbf{U}$ is orthogonal.

eigenvalues

As in the textbook

Let $\mathbf{U} = [\cdots \quad \mathbf{u}_i \quad \cdots]$, we have:

$$\mathbf{A}\mathbf{u}_i = \mathbf{U}\mathbf{D}\mathbf{U}^{\mathrm{T}}\mathbf{u}_i = \mathbf{U}\mathbf{D}\begin{bmatrix} \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \end{bmatrix} = \mathbf{U}\begin{bmatrix} \vdots \\ 0 \\ d_i \\ 0 \\ \vdots \end{bmatrix} = d_i \, \boxed{\mathbf{u}_i}$$

the eigenvector of d_i

We can apply eigenvalue decomposition to asymmetric matrices too, if we allow eigenvalues and eigenvectors to be complex. **Not considered here**.

Symmetric Positive Definiteness (s.p.d.)

$\mathbf{A}$ is s.p.d. if only if: $\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} > 0$, for any $\mathbf{v} \neq 0$.

$\mathbf{A}$ is symmetric semi-definite if only if: $\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} \geq 0$, for any $\mathbf{v} \neq 0$.

What does this even mean???

$$d > 0 \quad \Leftrightarrow \quad \mathbf{v}^{\mathrm{T}} d \mathbf{v} > 0, \text{ for any } \mathbf{v} \neq 0$$

$$d_0,\ d_1, \ldots > 0 \quad \Leftrightarrow \quad \mathbf{v}^{\mathrm{T}}\mathbf{D}\mathbf{v} = \mathbf{v}^{\mathrm{T}} \begin{bmatrix} \ddots & & \\ & d_i & \\ & & \ddots \end{bmatrix} \mathbf{v} > 0, \text{ for any } \mathbf{v} \neq 0$$

$d_0,\ d_1, \ldots > 0$

U orthogonal

$$\Leftrightarrow \quad \mathbf{v}^{\mathrm{T}}\boxed{(\mathbf{U}\mathbf{D}\mathbf{U}^{\mathrm{T}})}\mathbf{v} = \mathbf{v}^{\mathrm{T}}\mathbf{U}\mathbf{U}^{\mathrm{T}}(\mathbf{U}\mathbf{D}\mathbf{U}^{\mathrm{T}})\mathbf{U}\mathbf{U}^{\mathrm{T}}\mathbf{v}$$

$$= (\mathbf{U}^{\mathrm{T}}\mathbf{v})^{\mathrm{T}}(\mathbf{D})(\mathbf{U}^{\mathrm{T}}\mathbf{v}) > 0, \text{ for any } \mathbf{v} \neq 0$$

eigenvalue decomposition

Symmetric Positive Definiteness (s.p.d.)

- $\boldsymbol{A}$ is s.p.d. if only if all of its eigenvalues are positive:

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^{\mathrm{T}} \text{ and } d_0,\ d_1, \ldots > 0.$$

- But eigenvalue decomposition is a stupid idea most of the time, since it takes lots of time to compute.
- In practice, people often choose other ways to check if $\boldsymbol{A}$ is s.p.d. For example,

$$a_{ii} > \sum_{i \neq j} \left|a_{ij}\right| \text{ for all } i$$

A diagonally dominant matrix is p.d.

$$\begin{bmatrix} 4 & 3 & 0 \\ -1 & 5 & 3 \\ -8 & 0 & 9 \end{bmatrix}$$

$4 > 3 + 0$
$5 > 1 + 3$
$9 > 8$

- Finally, a s.p.d. matrix must be invertible:

$$\mathbf{A}^{-1} = \left(\mathbf{U}^{\mathrm{T}}\right)^{-1}\mathbf{D}^{-1}\mathbf{U}^{-1} = \mathbf{U}\mathbf{D}^{-1}\mathbf{U}^{\mathrm{T}}.$$

Question

Prove that if $\mathbf{A}$ is s.p.d., then $\mathbf{B} = \begin{bmatrix} \mathbf{A} & -\mathbf{A} \\ -\mathbf{A} & \mathbf{A} \end{bmatrix}$ is symmetric semi-definite.

For any $\mathbf{x}$ and $\mathbf{y}$, we know:

$$[\mathbf{x}^{\mathrm{T}} \quad \mathbf{y}^{\mathrm{T}}]\mathbf{B}\begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = [\mathbf{x}^{\mathrm{T}} \quad \mathbf{y}^{\mathrm{T}}]\begin{bmatrix} \mathbf{A} & -\mathbf{A} \\ -\mathbf{A} & \mathbf{A} \end{bmatrix}\begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix}$$

$$= \mathbf{x}^{\mathrm{T}}\mathbf{A}(\mathbf{x}-\mathbf{y}) - \mathbf{y}^{\mathrm{T}}\mathbf{A}(\mathbf{x}-\mathbf{y}) = (\mathbf{x}-\mathbf{y})^{\mathrm{T}}\mathbf{A}(\mathbf{x}-\mathbf{y})$$

Since $\mathbf{A}$ is s.p.d., we must have:

$$[\mathbf{x}^{\mathrm{T}} \quad \mathbf{y}^{\mathrm{T}}]\mathbf{B}\begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \geq 0$$

Q.E.D. ☐

Linear Solver

Many numerical problems are ended up with solving a linear system:

unknown to be found

$$\mathbf{A}\,\mathbf{x} = \mathbf{b}$$

square matrix   boundary vector

It's expensive to compute $\mathbf{A}^{-1}$, especially if $\mathbf{A}$ is large and sparse. So we cannot simply do: $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$.

There are two popular linear solver approaches: direct and iterative.

Direct Linear Solver

A direct solver is typically based LU factorization, or its variant: Cholesky, LDL^T, etc…

$$\mathbf{A} = \mathbf{LU} = \begin{bmatrix} l_{00} & & \\ l_{10} & l_{11} & \\ \vdots & \cdots & \ddots \end{bmatrix} \begin{bmatrix} \ddots & \cdots & \vdots \\ & u_{n-1,n-1} & u_{n-1,n} \\ & & u_{n,n} \end{bmatrix}$$

lower triangular   upper triangular

First solve: $\mathbf{Ly} = \mathbf{b}$.

$$\begin{bmatrix} l_{00} & & \\ l_{10} & l_{11} & \\ \vdots & \cdots & \ddots \end{bmatrix} \begin{bmatrix} y_0 \\ y_1 \\ \vdots \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \end{bmatrix}$$

Then solve: $\mathbf{Ux} = \mathbf{y}$.

$$\begin{bmatrix} \ddots & \cdots & \vdots \\ & u_{n-1,n-1} & u_{n-1,n} \\ & & u_{n,n} \end{bmatrix} \begin{bmatrix} \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} \vdots \\ y_{n-1} \\ y_n \end{bmatrix}$$

$y_0 = b_0/l_{00}$

$y_1 = (b_1 - l_{10}y_0)/l_{11}$

…

$x_n = y_n/u_{n,n}$

$x_{n-1} = (y_{n-1} - u_{n-1,n}x_n)/u_{n-1,n-1}$

…

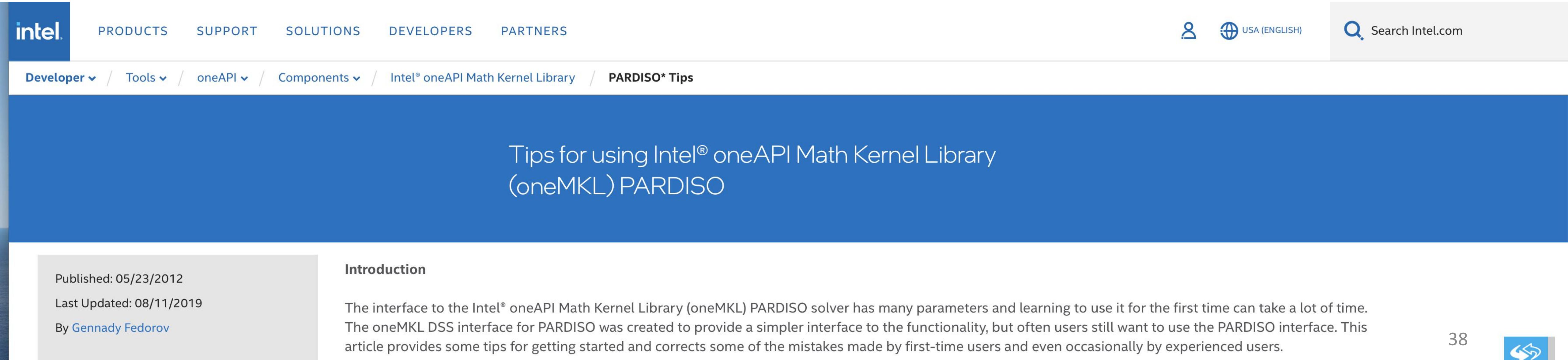
Direct Linear Solver

- When $\mathbf{A}$ is sparse, $\mathbf{L}$ and $\mathbf{U}$ are not so sparse. Their sparsity depends on the permutation. (See matlab)

  → LUP P: 顺序矩阵

- It contains two steps: factorization and solving. If we must solve many linear systems with the same $\mathbf{A}$, we can factorize it only once.

- Cannot be easily parallelized: Intel MKL PARDISO



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Developer / Tools / oneAPI / Components / Intel® oneAPI Math Kernel Library / PARDISO* Tips

Tips for using Intel® oneAPI Math Kernel Library (oneMKL) PARDISO

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By Gennady Fedorov

Introduction

The interface to the Intel® oneAPI Math Kernel Library (oneMKL) PARDISO solver has many parameters and learning to use it for the first time can take a lot of time. The oneMKL DSS interface for PARDISO was created to provide a simpler interface to the functionality, but often users still want to use the PARDISO interface. This article provides some tips for getting started and corrects some of the mistakes made by first-time users and even occasionally by experienced users.

Iterative Linear Solver

An iterative solver has the form:

$$\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \overbrace{\alpha}^{\text{relaxation}} \underbrace{\mathbf{M}}_{\text{iterative matrix}}{}^{-1} (\underbrace{\mathbf{b} - \mathbf{A}\mathbf{x}^{[k]}}_{\text{residual error}})$$

Why does it work?

$$\begin{aligned} \mathbf{b} - \mathbf{A}\mathbf{x}^{[k+1]} &= \mathbf{b} - \mathbf{A}\mathbf{x}^{[k]} - \alpha\mathbf{A}\mathbf{M}^{-1}(\mathbf{b} - \mathbf{A}\mathbf{x}^{[k]}) \\ &= (\mathbf{I} - \alpha\mathbf{A}\mathbf{M}^{-1})(\mathbf{b} - \mathbf{A}\mathbf{x}^{[k]}) = (\mathbf{I} - \alpha\mathbf{A}\mathbf{M}^{-1})^{k+1}(\mathbf{b} - \mathbf{A}\mathbf{x}^{[0]}) \end{aligned}$$

So,

$$\mathbf{b} - \mathbf{A}\mathbf{x}^{[k+1]} \rightarrow 0, \text{ if } \boxed{\rho(\mathbf{I} - \alpha\mathbf{A}\mathbf{M}^{-1})} < 1.$$

spectral radius (the largest absolute value of the eigenvalues)

Iterative Linear Solver

An iterative solver has the form:

$$\mathbf{x}^{[k+1]} = \mathbf{x}^{[k]} + \overbrace{\alpha}^{\text{relaxation}} \underbrace{\mathbf{M}^{-1}}_{\text{iterative matrix}} (\underbrace{\mathbf{b} - \mathbf{A}\mathbf{x}^{[k]}}_{\text{residual error}})$$

$\mathbf{M}$ must be easier to solve:

$\mathbf{M} = \mathrm{diag}(\mathbf{A})$ Jacobi Method	$\mathbf{M} = \mathrm{lower}(\mathbf{A})$ Gauss-Seidel Method

The convergence can be accelerated: Chebyshev, Conjugate Gradient, … (Omitted here.)

simple | fast for inexact solution | parallelable

convergence condition | slow for exact solution

Tensor Calculus

Basic Concepts: 1st-Order Derivatives

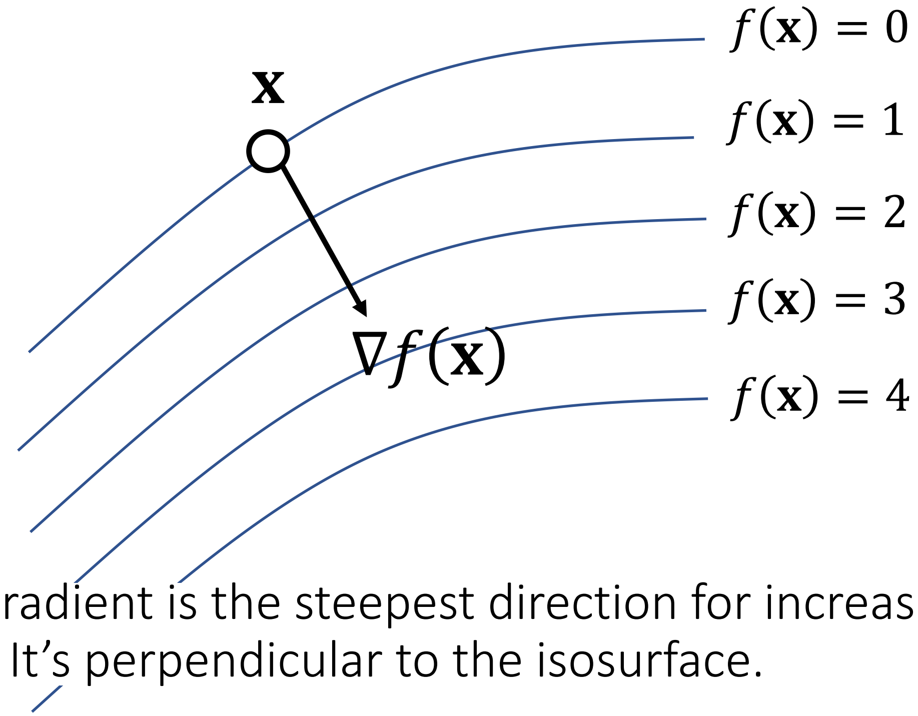
If $f(\mathbf{x}) \in \mathbf{R}$, then $df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz = \begin{bmatrix}\frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z}\end{bmatrix}\begin{bmatrix}dx \\ dy \\ dz\end{bmatrix}$.

$$\frac{\partial f}{\partial \mathbf{x}} = \begin{bmatrix}\frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z}\end{bmatrix}$$

or

$$\nabla f(\mathbf{x}) = \begin{bmatrix}\frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial z}\end{bmatrix}$$

gradient



Gradient is the steepest direction for increasing f. It’s perpendicular to the isosurface.

Basic Concepts: 1st-Order Derivatives

If $\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f(\mathbf{x}) \\ g(\mathbf{x}) \\ h(\mathbf{x}) \end{bmatrix} \in \mathbf{R}^3$, then:

$$\mathbf{J}(\mathbf{x}) = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} & \frac{\partial f}{\partial z} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} & \frac{\partial g}{\partial z} \\ \frac{\partial h}{\partial x} & \frac{\partial h}{\partial y} & \frac{\partial h}{\partial z} \end{bmatrix}$$

Jacobian

$$\nabla \cdot \mathbf{f} = \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial h}{\partial z}$$

Divergence

$$\nabla \times \mathbf{f} = \begin{bmatrix} \frac{\partial h}{\partial y} - \frac{\partial g}{\partial z} \\ \frac{\partial f}{\partial z} - \frac{\partial h}{\partial x} \\ \frac{\partial g}{\partial x} - \frac{\partial f}{\partial y} \end{bmatrix}$$

Curl

Basic Concepts: 2nd-Order Derivatives

If $f(\mathbf{x}) \in \mathbf{R}$, then:

$$\mathbf{H} = \mathbf{J}(\nabla f(\mathbf{x})) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial x \partial z} & \frac{\partial^2 f}{\partial y \partial z} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix}$$

Hessian

$$\nabla \cdot \nabla f(\mathbf{x}) = \nabla^2 f(\mathbf{x}) = \Delta f(\mathbf{x}) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

Laplacian

Taylor Expansion

If $f(x) \in R$, then: $f(x) = f(x_0) + \frac{\partial f(x_0)}{\partial x}(x - x_0) + \frac{1}{2}\frac{\partial f^2(x_0)}{\partial x^2}(x - x_0)^2 + \cdots$

If $f(\underline{x}) \in R$, then: $f(\underline{x}) = f(\underline{x}_0) + \frac{\partial f(\underline{x}_0)}{\partial \underline{x}}(\underline{x} - \underline{x}_0) + \frac{1}{2}(\underline{x} - \underline{x}_0)^T \frac{\partial f^2(\underline{x}_0)}{\partial \underline{x}^2}(\underline{x} - \underline{x}_0)^2 + \cdots$

$= f(\underline{x}_0) + \nabla f(\underline{x}_0) \cdot (\underline{x} - \underline{x}_0) + \frac{1}{2}(\underline{x} - \underline{x}_0)^T H (\underline{x} - \underline{x}_0) + \cdots$

Quiz:

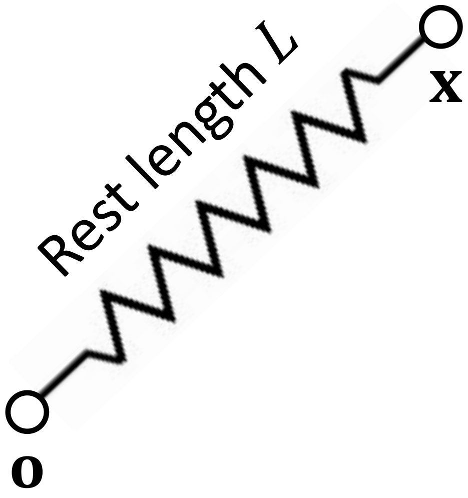
$$\frac{\partial\|\mathbf{x}\|}{\partial\mathbf{x}} = ?$$

$$\frac{\partial\|\mathbf{x}\|}{\partial\mathbf{x}} = \frac{\partial\left(\mathbf{x}^{\mathrm{T}}\mathbf{x}\right)^{1/2}}{\partial\mathbf{x}} = \frac{1}{2}\left(\mathbf{x}^{\mathrm{T}}\mathbf{x}\right)^{-1/2}\frac{\partial\left(\mathbf{x}^{\mathrm{T}}\mathbf{x}\right)}{\partial\mathbf{x}} = \frac{1}{2\|\mathbf{x}\|}2\mathbf{x}^{\mathrm{T}} = \frac{\mathbf{x}^{\mathrm{T}}}{\|\mathbf{x}\|}$$

$$\frac{\partial\left(\mathbf{x}^{\mathrm{T}}\mathbf{x}\right)}{\partial\mathbf{x}} = \frac{\partial(x^2+y^2+z^2)}{\partial\mathbf{x}} = [2x \quad 2y \quad 2z] = 2\mathbf{x}^{\mathrm{T}}$$

Example: A Spring

$$\frac{\partial\|\mathbf{x}\|}{\partial\mathbf{x}} = \frac{\mathbf{x}^{\mathrm{T}}}{\|\mathbf{x}\|}$$



Energy:

$$E(\mathbf{x}) = \frac{k}{2}(\|\mathbf{x}\| - L)^2$$

Force:

$$\mathbf{f}(\mathbf{x}) = -\nabla E(\mathbf{x}) = -k(\|\mathbf{x}\| - L)\left(\frac{\partial\|\mathbf{x}\|}{\partial\mathbf{x}}\right)^{\mathrm{T}}$$

$$= -k(\|\mathbf{x}\| - L)\frac{\mathbf{x}}{\|\mathbf{x}\|}$$

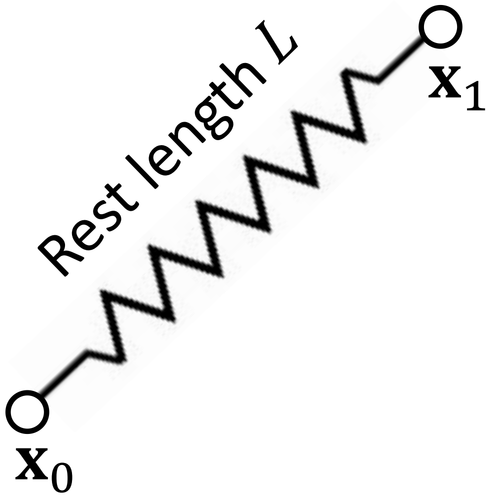
Tangent stiffness:

$$\mathbf{H}(\mathbf{x}) = -\frac{\partial\mathbf{f}(\mathbf{x})}{\partial\mathbf{x}} = k\frac{\mathbf{x}\mathbf{x}^{\mathrm{T}}}{\|\mathbf{x}\|^2} + k(\|\mathbf{x}\| - L)\frac{\mathbf{I}}{\|\mathbf{x}\|} - k(\|\mathbf{x}\| - L)\frac{\mathbf{x}}{\|\mathbf{x}\|^2}\frac{\mathbf{x}^{\mathrm{T}}}{\|\mathbf{x}\|}$$

$$= k\frac{\mathbf{x}\mathbf{x}^{\mathrm{T}}}{\|\mathbf{x}\|^2} + k\left(1 - \frac{L}{\|\mathbf{x}\|}\right)\left(\mathbf{I} - \frac{\mathbf{x}\mathbf{x}^{\mathrm{T}}}{\|\mathbf{x}\|^2}\right)$$

Choi and Ko. 2002. Stable But Responive Cloth. TOG (SIGGRAPH)

Example: A Spring with Two Ends



$$\mathbf{x}_{01} = \mathbf{x}_0 - \mathbf{x}_1$$

$$\boxed{\frac{\partial \|\mathbf{x}\|}{\partial \mathbf{x}} = \frac{\mathbf{x}^{\mathrm{T}}}{\|\mathbf{x}\|}}$$

Energy:

$$E(\mathbf{x}) = \frac{k}{2}(\|\mathbf{x}_{01}\| - L)^2$$

Force:

$$\mathbf{f}(\mathbf{x}) = -\nabla E(\mathbf{x}) = \begin{bmatrix} -\nabla_0 E(\mathbf{x}) \\ -\nabla_1 E(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} \mathbf{f}_e \\ -\mathbf{f}_e \end{bmatrix} \quad R^6$$

$$\mathbf{f}_e = -k(\|\mathbf{x}_{01}\| - L)\frac{\mathbf{x}_{01}}{\|\mathbf{x}_{01}\|}$$

Tangent stiffness:

$$\mathbf{H}(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 E}{\partial \mathbf{x}_0^2} & \frac{\partial^2 E}{\partial \mathbf{x}_0 \partial \mathbf{x}_1} \\ \frac{\partial^2 E}{\partial \mathbf{x}_0 \partial \mathbf{x}_1} & \frac{\partial^2 E}{\partial \mathbf{x}_1^2} \end{bmatrix} = \begin{bmatrix} \mathbf{H}_e & -\mathbf{H}_e \\ -\mathbf{H}_e & \mathbf{H}_e \end{bmatrix}$$

$$\mathbf{H}_e = k\frac{\mathbf{x}_{01}\mathbf{x}_{01}^{\mathrm{T}}}{\|\mathbf{x}_{01}\|^2} + k\left(1 - \frac{L}{\|\mathbf{x}_{01}\|}\right)\left(\mathbf{I} - \frac{\mathbf{x}_{01}\mathbf{x}_{01}^{\mathrm{T}}}{\|\mathbf{x}_{01}\|^2}\right)$$