Math (P)Review Part II: Vector Calculus

Computer Graphics CMU 15-462/662

Last Time: Linear Algebra

Touched on a variety of topics:

vectors & vector spaces norm L^2 norm/inner product span Gram-Schmidt linear systems quadratic forms

Don't have time to cover everything! But there are some fantastic lectures online:



- vectors as functions inner product
 - linear maps
 - basis
- frequency decomposition
 - bilinear forms
 - matrices

- **3Blue1Brown Essence of Linear Algebra**
- **Robert Ghrist Calculus Blue**

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(Let us know about others online!)





Vector Calculus in Computer Graphics Today's topic: vector calculus.

- Why is vector calculus important for computer graphics?
 - Basic language for talking about spatial relationships, transformations, etc.
 - Much of modern graphics (physically-based animation, geometry processing, etc.) formulated in terms of *partial differential equations* (PDEs) that use div, curl, Laplacian...
 - As we saw last time, vector-valued data is everywhere in graphics!





Euclidean Norm

- Last time, developed idea of norm, which measures total size, length, volume, intensity, etc.
- For geometric calculations, the norm we most often care about is the Euclidean norm
- Euclidean norm is any notion of length preserved by rotations/translations/reflections of space.

In *orthonormal* coordinates:

$$|\mathbf{u}| := \sqrt{u_1^2 + \cdots + u_1^2}$$





WARNING: This quantity does *not* encode geometric length unless vectors are encoded in an orthonormal basis. (Common source of bugs!)



Euclidean Inner Product / Dot Product

- Likewise, lots of possible inner products—intuitively, measure some notion of "alignment."

 $\langle \mathbf{u}, \mathbf{v} \rangle := |\mathbf{u}| |\mathbf{v}| \cos(\theta)$

In orthonormal Cartesian coordinates, can be represented via the dot product

 $\mathbf{u} \cdot \mathbf{v} := u_1 v_1 + \cdots + u_n v_n$

WARNING: As with Euclidean norm, no geometric meaning unless coordinates come from an orthonormal basis.

For geometric calculations, want to use inner product that captures something about geometry!

For n-dimensional vectors, Euclidean inner product defined as

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 θ U U



Cross Product

- Inner product takes two vectors and produces a scalar

Geometrically:

- magnitude equal to parallelogram area
- direction orthogonal to both vectors
- ...but which way?
- Use "right hand rule"

 $\mathbf{u} \times$

(Q: Why only 3D?)

In 3D, cross product is a natural way to take two vectors and get a *vector*, written as "u x v"



Cross Product, Determinant, and Angle More precise definition (that does not require hands):

$$\sqrt{\det(\mathbf{u},\mathbf{v},\mathbf{u}\times\mathbf{v})} =$$

- \bullet is angle between u and v "det" is determinant of three column vectors Uniquely determines coordinate formula:

 $= |\mathbf{u}| |\mathbf{v}| \sin(\theta)$





• Useful abuse of notation in 2D: $\mathbf{u} \times \mathbf{v} := u_1 v_2 - u_2 v_1$



Cross Product as Quarter Rotation



Simple but useful observation for manipulating vectors in 3D: cross product with a unit vector N is equivalent to a quarter-rotation in the plane with normal N:



Matrix Representation of Dot Product Often convenient to express dot product via matrix product:

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^\mathsf{T} \mathbf{v} = \begin{bmatrix} u_1 \end{bmatrix}$$

By the way, what about some other inner product? $\blacksquare E.g., <u,v>:= 2 u1 v1 + u1 v2 + u2 v1 + 3 u2 v2$



Q: Why is matrix representing inner product always symmetric (A^T=A)?



$$] = \begin{bmatrix} u_1 & u_2 \end{bmatrix} \begin{bmatrix} 2v_1 + v_2 \\ v_1 + 3v_2 \end{bmatrix}$$

$$(u_2v_1 + 3u_2v_2).$$
 \checkmark



Matrix Representation of Cross Product

$$\mathbf{u} := (u_1, u_2, u_3)$$

$$\mathbf{u} \times \mathbf{v} = \widehat{\mathbf{u}} \mathbf{v} = \begin{bmatrix} 0 \\ u_3 \\ -u_2 \end{bmatrix}$$

• A: Useful to notice that $v \ge u = -u \ge v \pmod{2}$. Hence,

 $\mathbf{v} \times \mathbf{u} = -$

Can also represent cross product via matrix multiplication:



Q: Without building a new matrix, how can we express v x u?

$$-\widehat{\mathbf{u}}\mathbf{v} = \widehat{\mathbf{u}}^{\mathsf{T}}\mathbf{v}$$



Determinant Q: How do you compute the determinant of a matrix? $\mathbf{A} := \begin{bmatrix} a \\ d \\ g \end{bmatrix}$

A: Apply some algorithm somebody told me once upon a time:



Q: No! What the heck does this number mean?!

$$\begin{array}{c} b & c \\ e & f \\ h & i \end{array} \right]$$

 $det(\mathbf{A}) = a(ei - fh) + b(fg - di) + c(dh - eg)$

Totally obvious... right?



Determinant, Volume and Triple Product



Relationship known as a "triple product formula" Q: What happens if we reverse order of cross product?)

Better answer: det(u,v,w) encodes (signed) volume of parallelepiped with edge vectors u, v, w.

Determinant of a Linear Map Q: If a matrix A encodes a *linear map* f, what does det(A) mean?

(First: need to recall how a matrix encodes a linear map!)

Representing Linear Maps via Matrices Key example: suppose I have a linear map

How do I encode as a matrix? Easy: "a" vectors become matrix columns: $A := \begin{vmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \\ | & | & | & | \end{vmatrix}$ Now, matrix-vector multiply recovers original map: $|u_1| |a_{1,x}u_1 + a_{2,x}|$ $\begin{array}{c|c} u_2 \\ u_3 \end{array} = \begin{bmatrix} a_{1,y}u_1 + a_{2,y}u_1 \\ a_{1,z}u_1 + a_{2,z}u_1 \end{bmatrix}$

	$\begin{bmatrix} a_{1,x} \end{bmatrix}$	$a_{2,x}$	a _{3,x} -
—	<i>a</i> _{1,y}	<i>a</i> _{2,y}	<i>a</i> _{3,y}
	$a_{1,z}$	$a_{2,z}$	<i>a</i> _{3,z}

$$\begin{bmatrix} u_2 + a_{3,x}u_3 \\ u_2 + a_{3,y}u_3 \\ u_2 + a_{3,z}u_3 \end{bmatrix} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$$

Determinant of a Linear Map Q: If a matrix A encodes a *linear map* f, what does det(A) mean?

A: It measures the *change in volume*. Q: What does the *sign* of the determinant tell us, in this case? A: It tells us whether *orientation* was reversed (det(A) < 0)</p>

(Do we really need a *matrix* in order to talk about the determinant of a linear map?)

Other Triple Products Super useful for working w/ vectors in 3D. **E.g., Jacobi identity for the cross product:**

$$\mathbf{u} \times (\mathbf{v} \times \mathbf{w}) + \mathbf{v} \times (\mathbf{w} \times \mathbf{u}) + \mathbf{w} \times (\mathbf{u} \times \mathbf{v}) = 0$$

- Why is it true, geometrically?
 - $\mathbf{u} \times (\mathbf{v} \times \mathbf{w}) = \mathbf{v}(\mathbf{u} \cdot \mathbf{w}) \mathbf{w}(\mathbf{u} \cdot \mathbf{v})$

There *is* a geometric reason, but **not nearly as obvious** as det: has to do w/ fact that triangle's altitudes meet at a point.

Yet another triple product: Lagrange's identity

(Can you come up with a geometric interpretation?)

Differential Operators - Overview

- Next up: differential operators and vector fields.
- Why is this useful for computer graphics?
 - Many physical/geometric problems expressed in terms of *relative rates of change* (ODEs, PDEs).
 - These tools also provide foundation for numerical optimization—e.g., minimize cost by following the gradient of some objective.

- **Derivative as Slope**
- Consider a function $f(x): R \rightarrow R$
- What does its derivative f' mean?
- **One interpretation "rise over run"**
- **Corresponds to standard definition:**

$$f'(x_0) := \lim_{\varepsilon \to 0} \frac{f(x_0 + \varepsilon) - \varepsilon}{\varepsilon}$$

Careful! What if slope is different when we walk in opposite direction?

$$f^{+}(x_{0}) := \lim_{\varepsilon \to 0} \frac{f(x_{0} + \varepsilon) - \varepsilon}{\varepsilon}$$
$$f^{-}(x_{0}) := \lim_{\varepsilon \to 0} \frac{f(x_{0}) - f(\varepsilon)}{\varepsilon}$$

Differentiable at x0 if $f^+ = f^-$. **Many functions in graphics are NOT differentiable!**

Derivative as Best Linear Approximation Any smooth function f(x) can be expressed as a Taylor series: linear quadratic constant

Replacing complicated functions with a linear (and

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

sometimes quadratic) approximation is a powerful trick in graphics algorithms—we'll see many examples.

Derivative as Best Linear Approximation Intuitively, same idea applies for functions of multiple variables:

How do we think about derivatives for a function that has multiple variables?

Directional Derivative

One way: suppose we have a function f(x1,x2) - Take a "slice" through the function along some line

- Then just apply the usual derivative!
- Called the directional derivative

"nabla" Gradient Given a multivariable function $f(\mathbf{x})$, gradient $\nabla f(\mathbf{x})$ assigns a vector at each point:

* $\int \langle - - \rangle$

Gradient in Coordinates

Most familiar definition: list of partial derivatives I.e., imagine that all but one of the coordinates are just constant values, and take the usual derivative

- Two potential problems:
 - Role of inner product is not clear (more later!)
- Still, extremely common way to calculate the gradient...

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

No way to differentiate *functions of functions* F(f) since we don't have a finite list of coordinates x₁, ..., x_n

Example: Gradient in Coordinates

 $f(\mathbf{x}) := x_1^2 + x_2^2$

 $\frac{\partial f}{\partial x_1} = \frac{\partial}{\partial x_1} x_1^2 + \frac{\partial}{\partial x_1} x_2^2 = 2x_1 + 0$

 $\frac{\partial f}{\partial x_2} = \frac{\partial}{\partial x_2} x_1^2 + \frac{\partial}{\partial x_2} x_2^2 = 0 + 2x_2$

 $\nabla f(\mathbf{x}) = \begin{vmatrix} 2x_1 \\ 2x_2 \end{vmatrix} = 2\mathbf{x}$

Gradient as Best Linear Approximation

Another way to think about it: at each point x0, gradient is the vector $\nabla f(\mathbf{x}_0)$ that leads to the best possible approximation

 $f(\mathbf{x}) \approx f(\mathbf{x}_0) + \langle \nabla f(\mathbf{x}_0), \mathbf{x} - \mathbf{x}_0 \rangle$

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 x_1

Starting at x₀, this term gets:

•smaller if we move in the opposite direction, and

•doesn't change if we move orthogonal to gradient.

The gradient takes you uphill...

 \mathbf{X}_1

 $\nabla f(\mathbf{x}_0)$

 $\nabla f(\mathbf{x}_1)$

- Another way to think about it: direction of "steepest ascent" I.e., what direction should we travel to increase value of function as quickly as possible?
- This viewpoint leads to algorithms for optimization, commonly used in graphics.

Gradient and Directional Derivative At each point x, gradient is unique vector $\nabla f(\mathbf{x})$ such that $\langle \nabla f(\mathbf{x}), \mathbf{u} \rangle = D_{\mathbf{u}} f(\mathbf{x})$

Can't happen if function is not differentiable!

(Notice: gradient also depends on choice of *inner product*...)

- for all u. In other words, such that taking the inner product w/ this vector gives you the directional derivative in any direction u.

Example: Gradient of Dot Product Consider the dot product expressed in terms of matrices: $f := \mathbf{u}^{\mathsf{I}} \mathbf{v}$

What is gradient of f with respect to u? One way: write it out in coordinates: $\mathbf{u}^{\mathsf{T}}\mathbf{v} = \sum_{i=1}^{n} u_{i}v_{i} \qquad \text{(equals zero unless i = k)}$ $\frac{\partial}{\partial u_k} \sum_{i=1}^n u_i v_i = \sum_{i=1}^n \frac{\partial}{\partial u_k} (u_i v_i) = v_k$ v_1 $\Rightarrow \nabla_{\mathbf{u}} f = \left| \begin{array}{c} \dots \\ v_n \end{array} \right|$

In other words:

$$abla_{\mathbf{u}}(\mathbf{u}^{\mathsf{T}}\mathbf{v}) = \mathbf{v}$$

Not so different from $\frac{d}{dx}(xy) = y!$

Gradients of Matrix-Valued Expressions

EXTREMELY useful in graphics to be able to differentiate expressions involving matrices

Ultimately, expressions look much like ordinary derivatives

For any two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and **symmetric** matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$:

MATRIX DERIVA

$$\nabla_{\mathbf{x}}(\mathbf{x}^{T}\mathbf{y}) = \mathbf{y}$$
$$\nabla_{\mathbf{x}}(\mathbf{x}^{T}\mathbf{x}) = 2\mathbf{x}$$
$$\nabla_{\mathbf{x}}(\mathbf{x}^{T}A\mathbf{y}) = A\mathbf{y}$$
$$\nabla_{\mathbf{x}}(\mathbf{x}^{T}A\mathbf{y}) = A\mathbf{y}$$

Excellent resource: Petersen & Pedersen, "The Matrix Cookbook"

Then... forget about coordinates altogether!

• • •

| \mathbf{y} \mathbf{x} $\frac{\frac{d}{dx}xy}{\frac{d}{dx}x^2} = 2x$ $\frac{\frac{d}{dx}axy}{\frac{d}{dx}axy} = ay$ $\frac{\frac{d}{dx}ax^2}{\frac{d}{dx}ax^2} = 2ax$ | 7 |
|--|----------|

At least once in your life, work these out meticulously in coordinates (to convince yourself they're true).

Advanced*: L² Gradient

- Consider a function of a function F(f)
- What is the gradient of F with respect to f?
- Can't take partial derivatives anymore!
- Instead, look for function VF such that for all functions u,
 - $\langle \langle \nabla F, u \rangle \rangle = D_u F$
- What is directional derivative of a function of a function?? Don't freak out—just return to good old-fashioned limit:

$$D_{u}F(f) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}$$

*as in, NOT on the test! (But perhaps somewhere in the test of life...)

 $F(f + \varepsilon u) - F(f)$ \mathcal{E}

- This strategy becomes much clearer w/ a concrete example...

Advanced Visual Example: L² Gradient

- Consider function $F(f) := \langle \langle f, g \rangle \rangle$ for f,g: [0,1] \rightarrow R
- I claim the gradient is: $\nabla F = g$
- Does this make sense intuitively? How can we increase inner product with g as quickly as possible?
 - inner product measures how well functions are "aligned"
 - g is definitely function best-aligned with g!
 - so to increase inner product, add a little bit of g to f

Advanced Example: L² Gradient

- At each "point" f0, we want function VF such that for all functions u

$$\langle\!\langle \nabla F(f_0), u \rangle\!\rangle = \lim_{\varepsilon \to 0} \frac{F(f_0 + \varepsilon u) - F(f_0)}{\varepsilon}$$

- Expanding 1st term in numerator, we get $||f_0 + \varepsilon u||^2 = ||f_0||^2$
- Hence, limit becomes $\lim_{\varepsilon \to 0} (\varepsilon ||u||^2 + 2\langle \langle f_0 \rangle$
- The only solution to $\langle \langle \nabla F($

• Consider function $F(f) := ||f||^2$ for arguments f: [0,1] \rightarrow R

$$|^{2} + \varepsilon^{2}||u||^{2} + 2\varepsilon\langle\langle f_{0}, u\rangle\rangle$$

$$(f_0, u) \rangle = 2\langle\langle f_0, u \rangle\rangle$$

 $(f_0), u \rangle = 2\langle\langle f_0, u \rangle\rangle$ for all u is

 $\nabla F(f_0) = 2f_0$ | \leftarrow not much different from $\frac{d}{dx}x^2 = 2x!$

Key idea: **Once you get the hang of taking the gradient** of ordinary functions, it's (superficially) not much harder for more exotic objects like matrices, functions of functions, ...

Vector Fields

- Gradient was our first example of a vector field **E.g.**, can think of a 2-vector field in the plane as a map $X: \mathbb{R}^2 \to \mathbb{R}^2$
- For example, we saw a gradient field
 - $\nabla f(x, y) = (2x)$
 - (for the function $f(x,y) = x^2$

In general, a vector field assigns a vector to each point in space

Q: How do we measure the *change* in a vector field?

Divergence and Curl

Two basic derivatives for vector fields:

"How much is field shrinking/expanding?" "How much is field spinning?"

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curl Y

Divergence • Also commonly written as $\nabla \cdot X$ Suggests a coordinate definition for divergence ■ Think of ∇ as a "vector of derivatives" $\nabla = \left(\frac{\partial}{\partial u_1}, \cdots, \frac{\partial}{\partial u_n}\right)$

Think of X as a "vector of functions" $X(\mathbf{u}) = (X_1(\mathbf{u}), \ldots,$

Then divergence is

$$\nabla \cdot X := \sum_{i=1}^{n} \frac{\partial X_i}{\partial u_i}$$

$$X_n(\mathbf{u}))$$

 $\nabla \cdot X$

Divergence - Example

• Consider the vector field $X(u, v) := (\cos(u), \sin(v))$ Divergence is then

$\nabla \cdot X = \frac{\partial}{\partial u} \cos(u) + \frac{\partial}{\partial v} \sin(v) = -\sin(u) + \cos(v).$

Curl Also commonly written as $\nabla \times X$ Suggests a coordinate definition for curl ■ This time, think of **V** as a vector of just *three* derivatives: $\nabla = \left(\frac{\partial}{\partial u_1}, \frac{\partial}{\partial u_2}, \frac{\partial}{\partial u_3}\right)$ Think of X as vector of three functions: $X(\mathbf{u}) = (X_1(\mathbf{u}), X_2(\mathbf{u}), X_3(\mathbf{u}))$ Then curl is $\nabla \times X := \begin{bmatrix} \frac{\partial X_3}{\partial u_2} - \frac{\partial X_2}{\partial u_2} \\ \frac{\partial X_1}{\partial u_3} - \frac{\partial X_3}{\partial u_1} \end{bmatrix}$ $\partial X_2 / \partial u_1 - \partial X_1 / \partial u_2$ (2D"curl": $\nabla \times X := \partial X_2 / \partial u_1 - \partial X_1 / \partial u_2$)

Curl - Example

• Consider the vector field $X(u, v) := (-\sin(v), \cos(u))$ ■ (2D) Curl is then

$\nabla \times X = \frac{\partial}{\partial u} \cos(u) - \frac{\partial}{\partial v} (-\sin(v)) = -\sin(u) + \cos(v).$

Notice anything about the relationship between curl and divergence?

Divergence vs. Curl (2D) Divergence of X is the same as curl of 90-degree rotation of X:

Playing these kinds of games w/ vector fields plays an important role in algorithms (e.g., fluid simulation)

Question (Q: Can you come up with an analogous relationship in 3D?)

$\nabla \cdot X = \nabla \times X^{\perp}$

Example: Fluids w/ Stream Function

$\min_{\Psi} ||u^* - \nabla \times \Psi||^2$ $u = \nabla \times \Psi$

Ando et al, "A Stream Function Solver for Liquid Simulations" (SIGGRAPH 2015)

$$\Delta p = \nabla \cdot u^*$$

$$u = u^* - \nabla p$$

Laplacian

- One more operator we haven't seen yet: the Laplacian
- Unbelievably important object in graphics, showing up across geometry, rendering, simulation, imaging
 - basis for Fourier transform / frequency decomposition
 - used to define model PDEs (Laplace, heat, wave equations)
 - encodes rich information about geometry

Laplacian—Visual Intuition

Likewise, Laplacian measures "curvature" of a function.

For further interpretations of the Laplacian, see https://youtu.be/oEq9R0I9Umk

Laplacian—Many Definitions

- Usually* denoted by Δ -----"Delta"
- Many starting points for Laplacian:

 - by analogy: graph Laplacian
 - variation of surface area
 - trace of Hessian ...

*Or by ∇^2 , but we'll reserve this symbol for the *Hessian*

Maps a scalar function to another scalar function (*linearly!*)

Laplacian—Example • Let's use coordinate definition: $\Delta f := \sum_i \frac{\partial^2 f}{\partial x_i^2}$ We have

$$\frac{\partial^2}{\partial x_1^2} f = \frac{\partial^2}{\partial x_1^2} \cos(3x_1) + \frac{\partial^2}{\partial x_1} \sin(3x_1) = \frac{\partial^2}{\partial x_1}$$
and

$$\frac{\partial^2}{\partial x_2^2}f = -9\sin(3x_2).$$

Hence,

 $\Delta f = -9(\cos(3x_1) + \sin(3x_2))$

• Consider the function $f(x_1, x_2) := \cos(3x_1) + \sin(3x_2)$

 $= -9\cos(3x_1).$

Hessian

- Recall our Taylor series

How do we do this for multivariable functions?

Already talked about best linear approximation, using gradient:

Our final differential operator—Hessian will help us locally approximate complicated functions by a few simple terms

 $f(\mathbf{x}) \approx f(\mathbf{x}_0) + \langle \nabla f(\mathbf{x}_0), \mathbf{x} - \mathbf{x}_0 \rangle$

Hessian gives us next, "quadratic" term.

Hessian in Coordinates

- **Typically denote Hessian by symbol** $abla^2$
- Just as gradient was "vector that gives us partial derivatives of the *function*," Hessian is "operator that gives us partial derivatives of the *gradient*":
- For a function $f(x): \mathbb{R}^n \to \mathbb{R}$, can be more explicit:

 $(\nabla^2 f)\mathbf{u} := D_{\mathbf{u}}(\nabla f)$

Taylor Series for Multivariable Functions Using Hessian, can now write 2nd-order approximation of any smooth, multivariable function f(x) around some point x₀:

Can write this in matrix form as

Will see later on how this approximation is *very* useful for optimization!

 $f(\mathbf{u}) \approx \frac{1}{2}\mathbf{u}^{\mathsf{T}}\mathbf{A}\mathbf{u} + \mathbf{b}^{\mathsf{T}}\mathbf{u} + c, \quad \mathbf{u} := \mathbf{x} - \mathbf{x}_0$

Next time: Rasterization

Next time, we'll talk about how to draw triangles

A lot more interesting (and difficult!) than it might seem...

Leads to a deep understanding of modern graphics hardware

