

**KAUST** 

# CS 247 – Scientific Visualization Lecture 12: Scalar Fields, Pt.8

# Reading Assignment #6 (until Mar 9)



Read (required):

- Real-Time Volume Graphics, Chapter 2 (*GPU Programming*)
- Real-Time Volume Graphics, Chapters 5.5 and 5.6 (you already had to read 5.4) (*Local Volume Illumination*)
- Refresh your memory on eigenvectors and eigenvalues: https://en.wikipedia.org/wiki/Eigenvalues\_and\_eigenvectors

Look at (optional):

• Riemannian Geometry for Scientific Visualization (notes and videos [part 1]) https://vccvisualization.org/RiemannianGeometryTutorial/

### **Gradient and Directional Derivative**



Gradient  $\nabla f(x, y, z)$  of scalar function f(x, y, z):

(in Cartesian coordinates)

$$\nabla f(x, y, z) = \left(\frac{\partial f(x, y, z)}{\partial x}, \frac{\partial f(x, y, z)}{\partial y}, \frac{\partial f(x, y, z)}{\partial z}\right)^T$$

Directional derivative in direction  ${f u}$  :

$$D_{\mathbf{u}}f(x,y,z) = \nabla f(x,y,z) \cdot \mathbf{u}$$

And therefore also:

$$D_{\mathbf{u}}f(x, y, z) = ||\nabla f|| ||\mathbf{u}|| \cos \theta$$

### **Gradient and Directional Derivative**



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(Cartesian vector components; basis vectors not shown)

But: always need **basis vectors**! With Cartesian basis:

$$\nabla f(x, y, z) = \frac{\partial f(x, y, z)}{\partial x} \mathbf{i} + \frac{\partial f(x, y, z)}{\partial y} \mathbf{j} + \frac{\partial f(x, y, z)}{\partial z} \mathbf{k}$$

#### What about the Basis?



On the previous slide, this actually meant

$$\nabla f(x, y, z) = \frac{\partial f(x, y, z)}{\partial x} \mathbf{i}(x, y, z) + \frac{\partial f(x, y, z)}{\partial y} \mathbf{j}(x, y, z) + \frac{\partial f(x, y, z)}{\partial z} \mathbf{k}(x, y, z)$$

It's just that the Cartesian basis vectors are the same everywhere...

But this is not true for many other coordinate systems:



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But this is not true for many other coordinate systems:



# The Gradient as a Differential Form



The gradient as a *differential* (differential 1-form) is the "primary" concept (also "total differential" or "total derivative")

$$df = \frac{\partial f}{\partial x} \, dx + \frac{\partial f}{\partial y} \, dy + \frac{\partial f}{\partial z} \, dz$$

A differential 1-form is a scalar-valued linear function that takes a (direction) vector as input, and gives a scalar as output

Each of the 1-forms df, dx, dy, dz takes direction vector as input, gives scalar output

In the expression of the gradient df above, all 1-forms on the right-hand side get the same vector as input

df is simply a linear combination of the coordinate differentials dx, dy, dz

### The Gradient as a Differential Form



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$$df = \frac{\partial f}{\partial x} \, dx + \frac{\partial f}{\partial y} \, dy + \frac{\partial f}{\partial z} \, dz$$

The directional derivative and the gradient vector

$$D_{\mathbf{u}}f = df(\mathbf{u})$$
$$df(\mathbf{u}) = \nabla f \cdot \mathbf{u}$$

The gradient vector is then *defined*, such that:

$$\nabla f \cdot \mathbf{u} := df(\mathbf{u})$$





the function here is  $f(x,y) = x^2 + y^2$  $\nabla f(x,y) = 2x\mathbf{i} + 2y\mathbf{j}$ 





the function here is  $f(x,y) = x^2 + y^2$   $\nabla f(x,y) = 2x \mathbf{e}_x + 2y \mathbf{e}_y$ df(x,y) = 2x dx + 2y dy

 $df(r, \theta) = 2rdr + 0d\theta = 2rdr$ 





how about in polar coordinates?



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how about in polar coordinates?



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different 1-forms evaluated in some direction





 $df(r,\theta) = 2rdr + 0d\theta = 2rdr$ 

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# Einstein Summation Convention (1)



Implicit summation over paired indices

• Pairs of "upstairs" and "downstairs" indices

$$\mathbf{v} = v^i \, \mathbf{e}_i := \sum_i v^i \, \mathbf{e}_i$$

$$= v^1 \mathbf{e}_1 + v^2 \mathbf{e}_2 + \ldots + v^n \mathbf{e}_n$$

# Einstein Summation Convention (2)



Implicit summation over paired indices

• Pairs of "upstairs" and "downstairs" indices

$$\mathbf{g}(\mathbf{v},\mathbf{w}) = g_{ij} v^i w^j := \sum_{i,j} g_{ij} v^i w^j$$

$$= g_{11} v^1 w^1 + g_{12} v^1 w^2 + \ldots + g_{nn} v^n w^n$$

#### Interlude: Tensor Calculus



In tensor calculus, first-order tensors can be

- Contravariant  $\mathbf{v} = v^i \mathbf{e}_i$
- Covariant

$$\mathbf{v} = v^* \, \mathbf{e}_i$$
$$\boldsymbol{\omega} = v_i \, \boldsymbol{\omega}^i$$

The gradient vector is a contravariant vector  $\mathbf{v} = v^i \partial_i$ The gradient 1-form is a covariant vector (a covector)  $df = \frac{\partial f}{\partial x^i} dx^i$ 

Very powerful; necessary for non-Cartesian coordinate systems On (intrinsically) curved manifolds (sphere, ...): Cartesian coordinates not even possible

#### Interlude: Tensor Calculus



In tensor calculus, first-order tensors can be

- Contravariant  $\mathbf{v} = v^i \mathbf{e}_i$
- Covariant

$$\mathbf{v} = v \mathbf{e}_i$$
$$\boldsymbol{\omega} = v_i \, \boldsymbol{\omega}^i$$

The gradient vector is a contravariant vector  $\mathbf{v} = v^i \partial_i$ The gradient 1-form is a covariant vector (a covector)  $df = \frac{\partial f}{\partial x^i} dx^i$ 

This is also the fundamental reason why in graphics a normal vector transforms differently: as a covector, not as a vector!

(typical graphics rule: **n** transforms with transpose of inverse matrix)



Symmetric, covariant second-order tensor field: *defines* inner product on manifold (in each tangent space)

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



Symmetric, covariant second-order tensor field: *defines* inner product on manifold (in each tangent space)

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$$\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{g}(\mathbf{v}, \mathbf{w})$$

$$= g_{ij} v^{i} w^{j}$$

$$= \mathbf{v}^{T} \mathbf{g} \mathbf{w}$$

$$\| \mathbf{v} \|^{2} = \langle \mathbf{v}, \mathbf{v} \rangle$$

$$= g(\mathbf{v}, \mathbf{v})$$

$$= g_{ij} v^{i} v^{j}$$

$$= \mathbf{v}^{T} \mathbf{g} \mathbf{v}$$



Symmetric, covariant second-order tensor field: *defines* inner product on manifold (in each tangent space)

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

$$g_{ij} = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}$$

$$\left\| \mathbf{v} \|^2 = \langle \mathbf{v}, \mathbf{v} \rangle \\ = \mathbf{g}(\mathbf{v}, \mathbf{w}) \\ = g_{ij} v^i w^j \\ = \mathbf{v}^T \mathbf{g} \mathbf{w} \end{bmatrix} \left\| \mathbf{v} \|^2 = \langle \mathbf{v}, \mathbf{v} \rangle \\ = g_{ij} v^i v^j \\ = \mathbf{v}^T \mathbf{g} \mathbf{v} \end{aligned}$$

$$\left\| \mathbf{v} \|^2 = \begin{bmatrix} v^1 & v^2 \end{bmatrix} \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} v^1 \\ v^2 \end{bmatrix}$$

$$\left\| \mathbf{v} \|^2 = \mathbf{v}^T \mathbf{g} \mathbf{v} \right\|$$

$$\left\| \mathbf{v} \|^2 = \begin{bmatrix} v^1 & v^2 \end{bmatrix} \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} v^1 \\ v^2 \end{bmatrix}$$



Symmetric, covariant second-order tensor field: *defines* inner product on manifold (in each tangent space)

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

$$g_{ij} = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}$$

$$\left\| \mathbf{v} \right\|^{2} = \langle \mathbf{v}, \mathbf{v} \rangle$$

$$= \mathbf{g}(\mathbf{v}, \mathbf{w})$$

$$= g_{ij} v^{i} w^{j}$$

$$= g_{ij} v^{i} v^{j}$$

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$$\left\| \mathbf{v} \right\|^{2} = \begin{bmatrix} v^{1} & v^{2} \end{bmatrix} \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} v^{1} \\ v^{2} \end{bmatrix}$$

$$Cartesian coordinates: g_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\| \mathbf{v} \|^{2} = \begin{bmatrix} v^{1} & v^{2} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} v^{1} \\ v^{2} \end{bmatrix} = \mathbf{v}^{T} \mathbf{v}$$



Components of metric referred to coordinates

$$g_{ij} := \langle \mathbf{e}_i, \mathbf{e}_j \rangle$$

A second-order tensor field is bi-linear, i.e., linear in each (vector/covector) argument separately

From bi-linearity we immediately get:

$$\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{g} \left( v^i \mathbf{e}_i, w^j \mathbf{e}_j \right)$$
  
=  $v^i w^j \langle \mathbf{e}_i, \mathbf{e}_j \rangle$   
=  $g_{ij} v^i w^j$ 

# Gradient Vector from Differential 1-Form



The metric (and inverse metric) *lower* or *raise* indices (i.e., convert between covariant and contravariant tensors)

$$v^i = g^{ij} v_j$$
$$v_i = g_{ij} v^j$$

$$v^{i}\mathbf{e}_{i} = g^{ij}v_{j}\,\mathbf{e}_{i}$$
$$v_{i}\boldsymbol{\omega}^{i} = g_{ij}v^{j}\boldsymbol{\omega}^{i}$$

Inverse metric (contravariant)

$$[g^{ij}] = [g_{ij}]^{-1}$$

$$g^{ik}g_{kj}=\delta^i_j$$

Kronecker delta behaves like identity matrix

# Gradient Vector from Differential 1-Form



So the gradient vector is

$$\nabla f = \left(g^{ij}\frac{\partial f}{\partial x^j}\right)\mathbf{e}_i$$

$$d\mathbf{r} = dx^i \,\mathbf{e}_i$$
$$d\mathbf{r}(\cdot) = dx^i(\cdot) \,\mathbf{e}_i$$

Directional derivative via inner product:

$$\begin{split} \langle \nabla f, \cdot \rangle &= g_{kj} g^{ik} \frac{\partial f}{\partial x^i} dx^j(\cdot) & \nabla f \cdot d\mathbf{r} = g_{kj} g^{ik} \frac{\partial f}{\partial x^i} dx^j \\ &= \delta^i_j \frac{\partial f}{\partial x^i} dx^j(\cdot) & = \delta^i_j \frac{\partial f}{\partial x^i} dx^j \\ &= \frac{\partial f}{\partial x^i} dx^i(\cdot) & = \frac{\partial f}{\partial x^i} dx^i \end{split}$$

#### **Example: Polar Coordinates**



Metric tensor and inverse metric for polar coordinates

$$g_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & r^2 \end{bmatrix} \qquad \qquad g^{ij} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{r^2} \end{bmatrix}$$



Gradient vector from 1-form: raise index with inverse metric

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial r} & \frac{\partial f}{\partial \theta} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{r^2} \end{bmatrix} \begin{bmatrix} \mathbf{e}_r \\ \mathbf{e}_{\theta} \end{bmatrix} = \frac{\partial f}{\partial r} \mathbf{e}_r + \frac{1}{r^2} \frac{\partial f}{\partial \theta} \mathbf{e}_{\theta}$$

### **Example: Polar Coordinates**



Metric tensor and inverse metric for polar coordinates

$$g_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & r^2 \end{bmatrix} \qquad \qquad g^{ij} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{r^2} \end{bmatrix}$$



Gradient vector from 1-form: raise index with inverse metric

$$\nabla f(r,\theta) = \frac{\partial f(r,\theta)}{\partial r} \mathbf{e}_r(r,\theta) + \frac{1}{r^2} \frac{\partial f(r,\theta)}{\partial \theta} \mathbf{e}_\theta(r,\theta)$$

don't forget that all of this is position-dependent!

#### **Tensor Calculus**

Highly recommended:

Very nice book,

complete lecture on Youtube!

#### **Pavel Grinfeld**

Introduction to Tensor Analysis and the Calculus of Moving Surfaces

D Springer



# Thank you.

#### Thanks for material

- Helwig Hauser
- Eduard Gröller
- Daniel Weiskopf
- Torsten Möller
- Ronny Peikert
- Philipp Muigg
- Christof Rezk-Salama