King Abdullah University of Science and Technology

KAUST

CS 247 – Scientific Visualization
Lecture 11: Scalar Fields, Pt.7 [preview]

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Reading Assignment #6 (until Mar 7)

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):

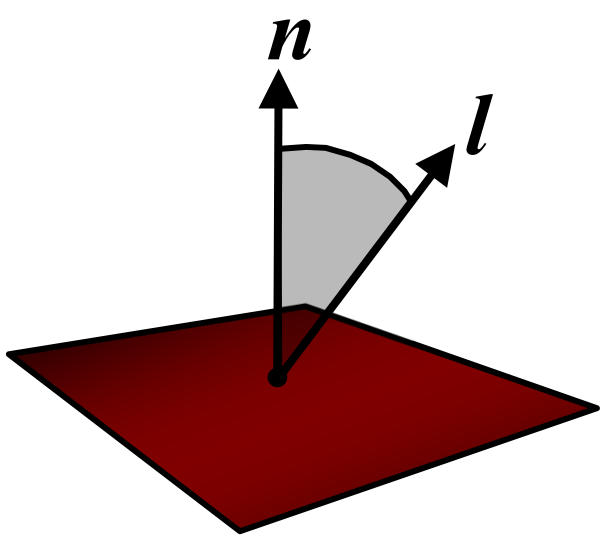
- Riemannian Geometry for Scientific Visualization (notes and videos [part 1])
  `https://vccvisualization.org/RiemannianGeometryTutorial/`

Local Shading Equations

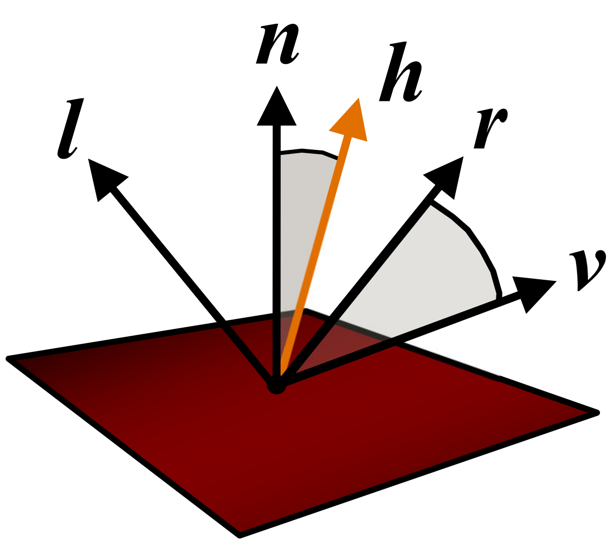
Standard volume shading adapts surface shading

Most commonly Blinn/Phong model

But what about the "surface" normal vector?



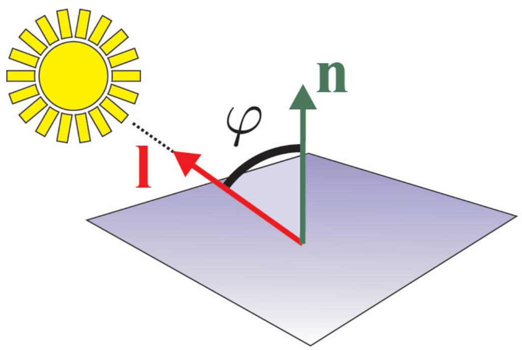
diffuse reflection



specular reflection

Local Illumination Model: Phong Lighting Model

$$\mathbf{I}_{\text{Phong}} = \mathbf{I}_{\text{ambient}} + \mathbf{I}_{\text{diffuse}} + \mathbf{I}_{\text{specular}}$$



$$\begin{aligned} \mathbf{I}_{\text{diffuse}} &= k_d \, \mathbf{M}_d \, \mathbf{I}_d \cos\varphi \qquad \text{if } \varphi \leq \frac{\pi}{2} \\ &= k_d \, \mathbf{M}_d \, \mathbf{I}_d \max((\mathbf{n} \cdot \mathbf{l}), 0) \end{aligned}$$

The Dot Product (Scalar / Inner Product)

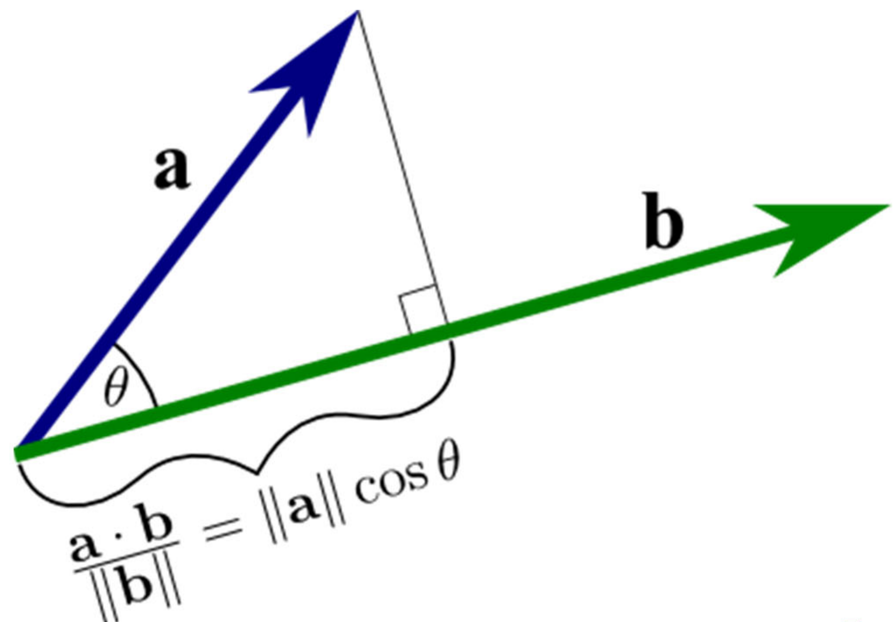
Cosine of angle between two vectors times their lengths

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^{n} a_i b_i \qquad \mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \, \|\mathbf{b}\| \cos\theta$$

(standard inner product in Cartesian coordinates)

Many uses:

- Project vector onto another vector,
  project into basis,
  project into tangent plane,
  ...



The Gradient as Normal Vector

Gradient of the scalar field gives direction+magnitude of fastest change

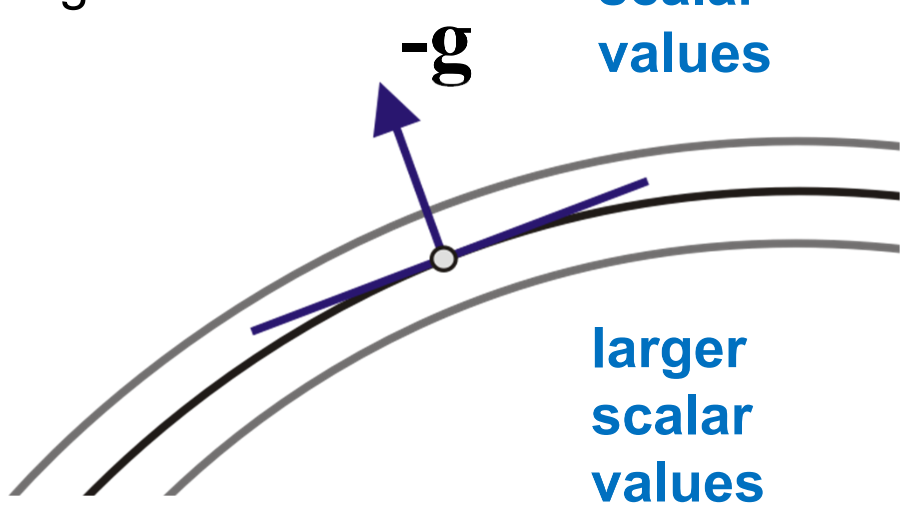
$$\mathbf{g} = \nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right)^{\mathbf{T}}$$

(only correct in Cartesian coordinates [see later lectures])

Local approximation to isosurface at any point:
tangent plane = plane orthogonal to gradient

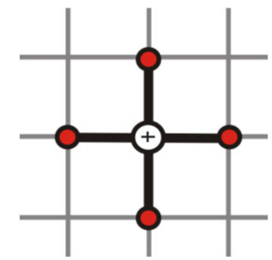
Normal of this isosurface:
normalized gradient vector
(negation is common convention)

$$\mathbf{n} = -\mathbf{g}/|\mathbf{g}|$$



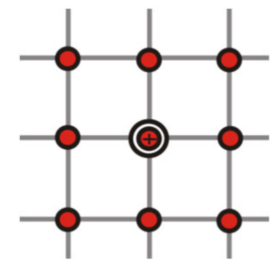
(Numerical) Gradient Reconstruction

We need to reconstruct the derivatives of a continuous function given as discrete samples



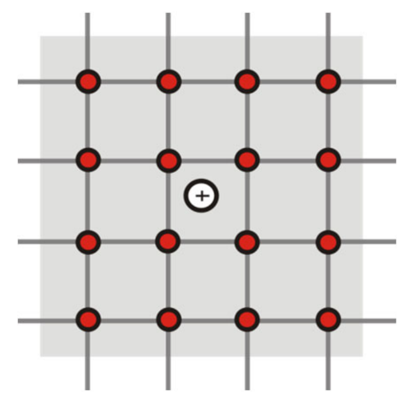
Central differences

- Cheap and quality often sufficient (2*3 neighbors in 3D)



Discrete convolution filters on grid

- Image processing filters; e.g. Sobel (3^3 neighbors in 3D)



Continuous convolution filters

- Derived continuous reconstruction filters
- E.g., the cubic B-spline and its derivatives (4^3 neighbors)

Finite Differences

Obtain first derivative from Taylor expansion

$$
\begin{aligned}
f(x_0+h) &= f(x_0) + \frac{f'(x_0)}{1!}h + \frac{f''(x_0)}{2!}h^2 + \ldots \\
&= \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}h^n .
\end{aligned}
$$

Forward differences / backward differences

$$
f(x_0)' = \frac{f(x_0+h) - f(x_0)}{h} + o(h)
$$

$$
f(x_0)' = \frac{f(x_0) - f(x_0-h)}{h} + o(h)
$$

Finite Differences

Central differences

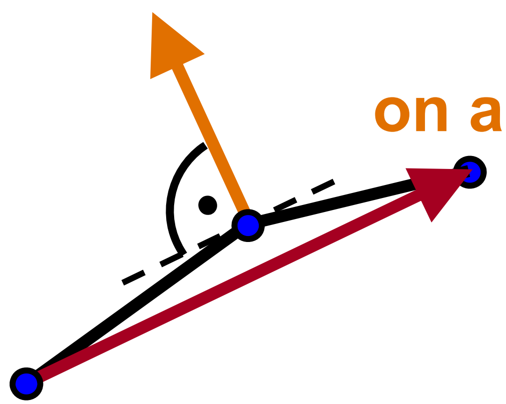
$$
\begin{aligned}
f(x_0 + h) &= f(x_0) + \frac{f'(x_0)}{1!} h + \frac{f''(x_0)}{2!} h^2 + o(h^3) \\
f(x_0 - h) &= f(x_0) - \frac{f'(x_0)}{1!} h + \frac{f''(x_0)}{2!} h^2 + o(h^3)
\end{aligned}
$$

$$
f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} + o(h^2)
$$

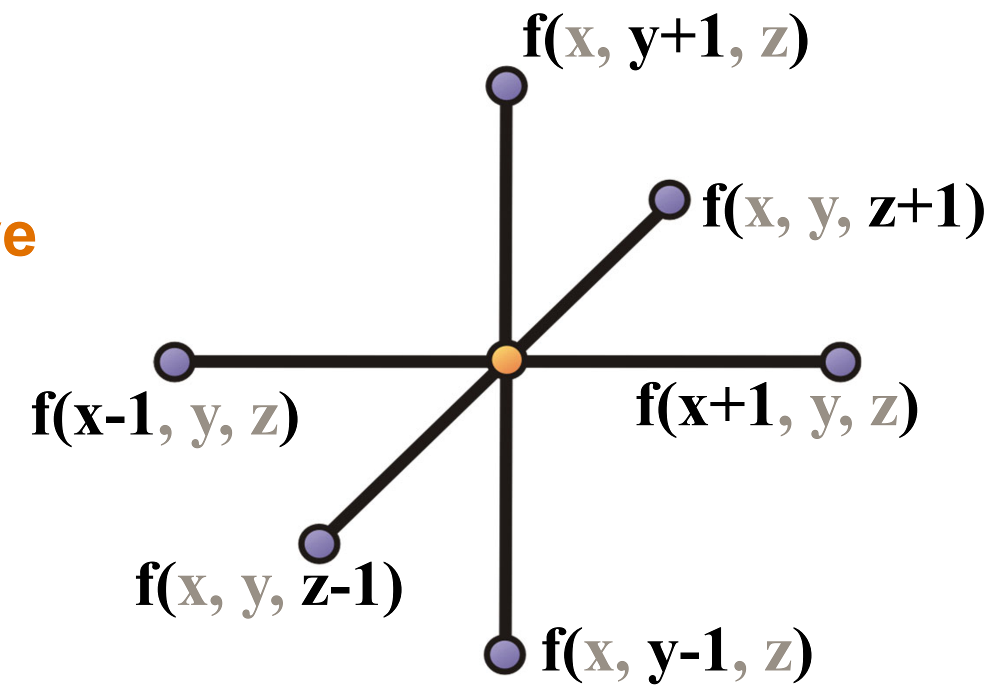
Central Differences

Need only two neighboring voxels per derivative

Most common method



on a curve



$$g_x = 0.5(\ f(x+1,\ y,\ z) - f(x-1,\ y,\ z)\ )$$

$$g_y = 0.5(\ f(x,\ y+1,\ z) - f(x,\ y-1,\ z)\ )$$

$$g_z = 0.5(\ f(x,\ y,\ z+1) - f(x,\ y,\ z-1)\ )$$

in a volume

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 $\mathbf{u}$:

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

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?

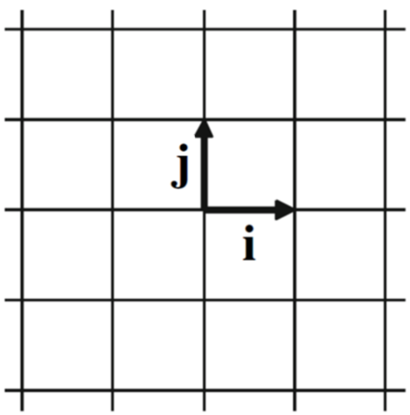
On the previous slide, this actually meant

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

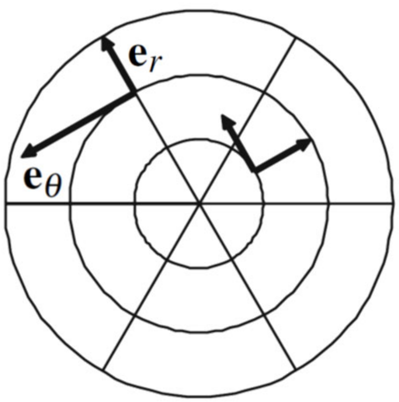
It's just that the Cartesian basis vectors are the same everywhere...

But this is not true for many other coordinate systems:

Cartesian coordinates



polar coordinates



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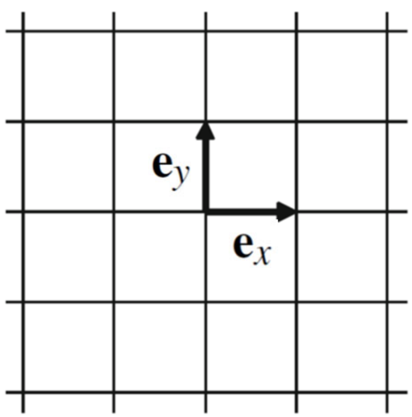

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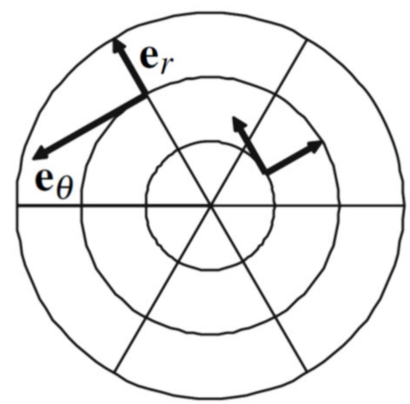


The Gradient as a Differential Form

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

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

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

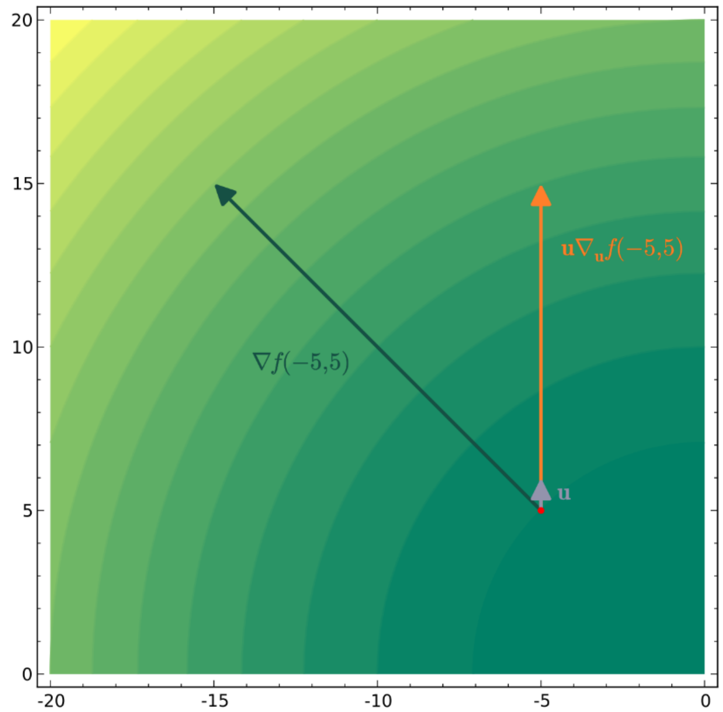
The directional derivative and the gradient vector

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

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

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

Gradient Vectors and Differential 1-Forms

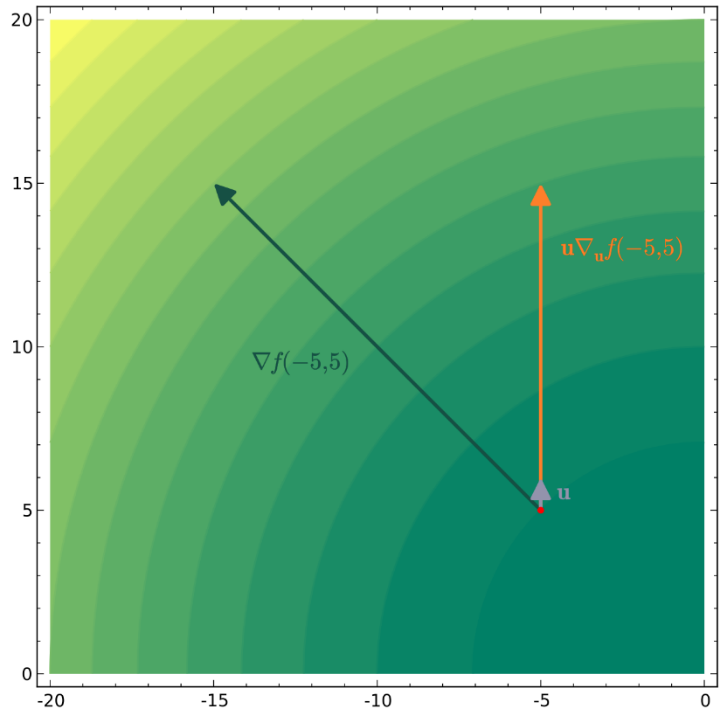


from Wikipedia (for **u** a unit vector),

the function here is $f(x,y) = x^2 + y^2$

$$\nabla f(x,y) = 2x\,\mathbf{i} + 2y\,\mathbf{j}$$

Gradient Vectors and Differential 1-Forms



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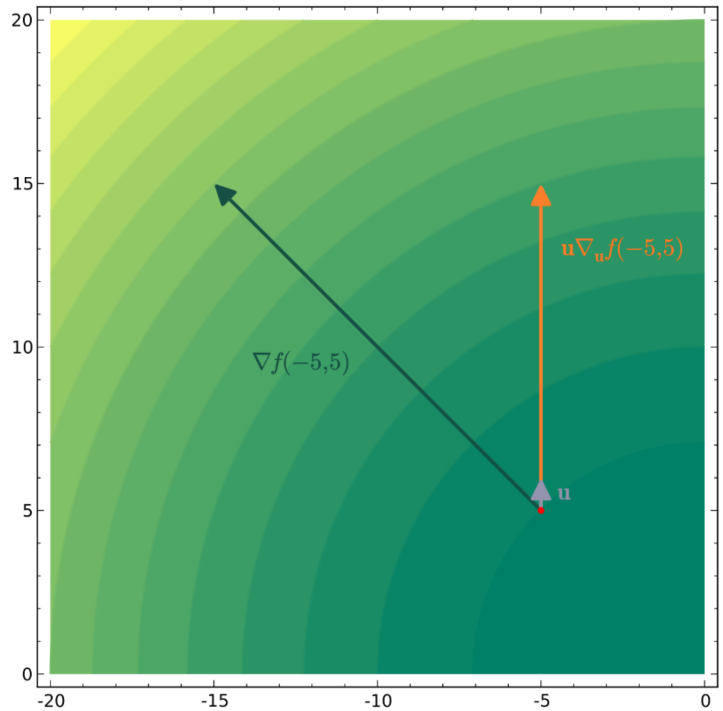
$$\nabla f(x,y) = 2x\,\mathbf{e}_x + 2y\,\mathbf{e}_y$$

$$df(x,y) = 2x\,dx + 2y\,dy$$

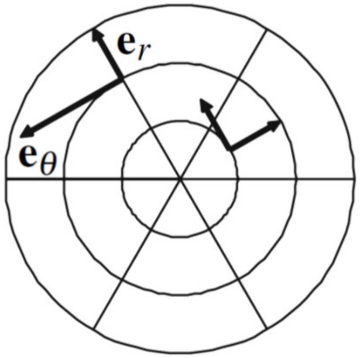
Gradient Vectors and Differential 1-Forms



from Wikipedia (for **u** a unit vector),

the function here is $f(r,\theta) = r^2$

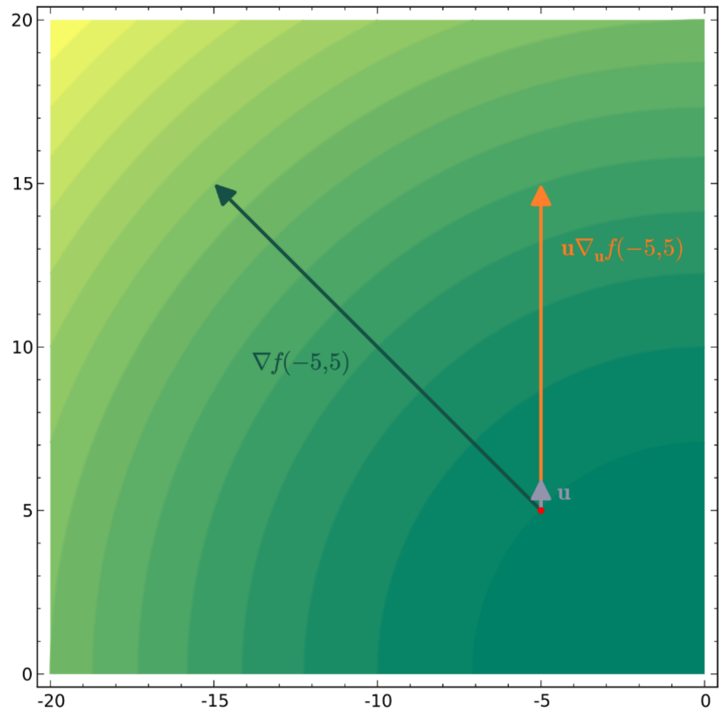
how about in polar coordinates?



$$\nabla f(r,\theta) = 2r\,\mathbf{e}_r + 0\frac{1}{r^2}\,\mathbf{e}_\theta = 2r\,\mathbf{e}_r$$

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

Gradient Vectors and Differential 1-Forms



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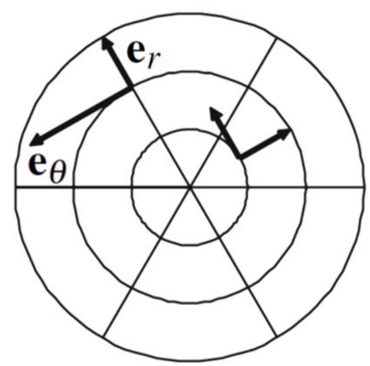

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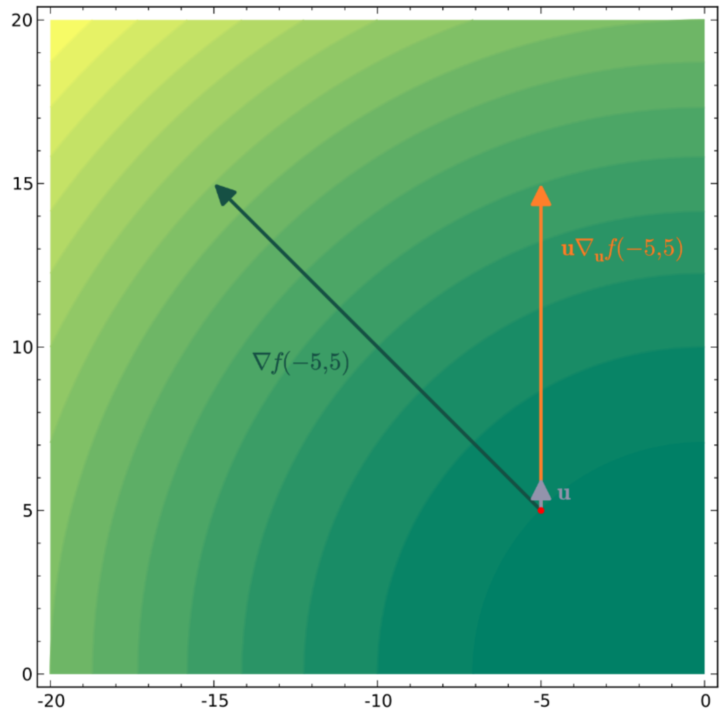
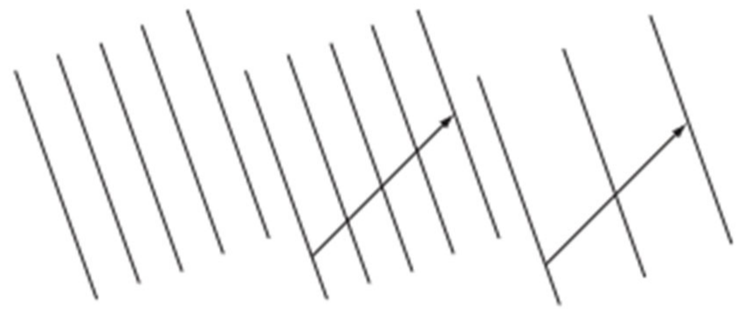
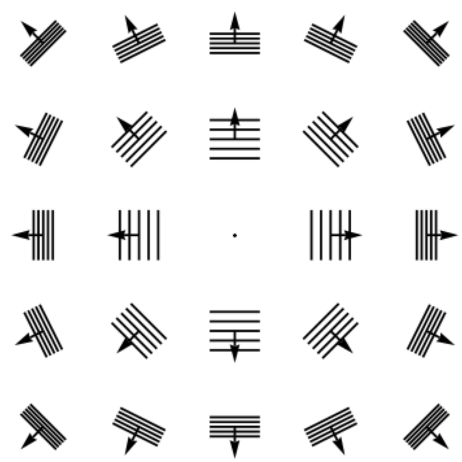
Gradient Vectors and Differential 1-Forms



different 1-forms
evaluated in some direction



1-form (field) df



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

Interlude: Tensor Calculus

In tensor calculus, first-order tensors can be

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

The gradient vector is a contravariant vector $\mathbf{v} = v^i \, \boldsymbol{\partial}_i$

The gradient 1-form is a covariant vector (a covector) $df = \dfrac{\partial f}{\partial x^i} \, dx^i$

Very powerful; necessary for non-Cartesian coordinate systems

On (intrinsically) curved manifolds (sphere, ...):
Cartesian coordinates not even possible

Interlude: Tensor Calculus

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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)

Einstein Summation Convention (1)

Implicit summation over paired indices

- Pairs of “upstairs” and “downstairs” indices

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

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

Einstein Summation Convention (2)

Implicit summation over paired indices

- Pairs of “upstairs” and “downstairs” indices

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

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

Inner Products and Metric Tensor (Field)

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

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

Inner Products and Metric Tensor (Field)

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

Inner Products and Metric Tensor (Field)

Symmetric, covariant second-order tensor field:
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$$\boxed{\langle \mathbf{v}, \mathbf{w} \rangle := \mathbf{g}(\mathbf{v}, \mathbf{w}) = \|\mathbf{v}\| \, \|\mathbf{w}\| \cos\theta}$$

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

(2D)

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

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

Inner Products and Metric Tensor (Field)

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

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

$$g_{ij} = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}$$ (2D)

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

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

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

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

Inner Products and Metric Tensor (Field)

Components of metric referred to coordinates

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

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

From bi-linearity we immediately get:

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

Gradient Vector from Differential 1-Form

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

$$\boxed{\begin{aligned} v^i &= g^{ij} v_j \\ v_i &= g_{ij} v^j \end{aligned}}$$

$$v^i \mathbf{e}_i = g^{ij} v_j \mathbf{e}_i$$
$$v_i \boldsymbol{\omega}^i = g_{ij} v^j \boldsymbol{\omega}^i$$

Inverse metric (contravariant)

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

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

Kronecker delta behaves
like identity matrix

Gradient Vector from Differential 1-Form

So the gradient vector is

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

Vector-valued 1-form

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

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

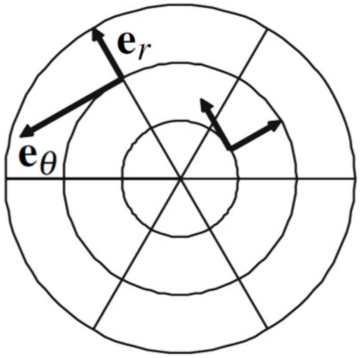
Directional derivative via inner product:

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

$$\begin{aligned} \nabla f \cdot d\mathbf{r} &= g_{kj} g^{ik} \frac{\partial f}{\partial x^i} dx^j \\ &= \delta^i{}_j \frac{\partial f}{\partial x^i} dx^j \\ &= \frac{\partial f}{\partial x^i} dx^i \end{aligned}$$

Example: Polar Coordinates

Metric tensor and inverse metric for polar coordinates



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

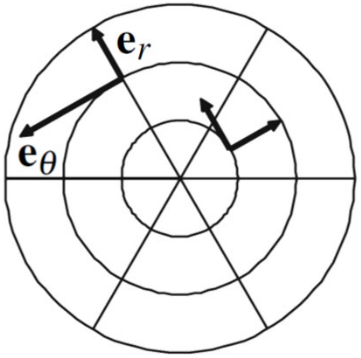
Gradient vector from 1-form: raise index with inverse metric

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

Example: Polar Coordinates

Metric tensor and inverse metric for polar coordinates

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



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

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

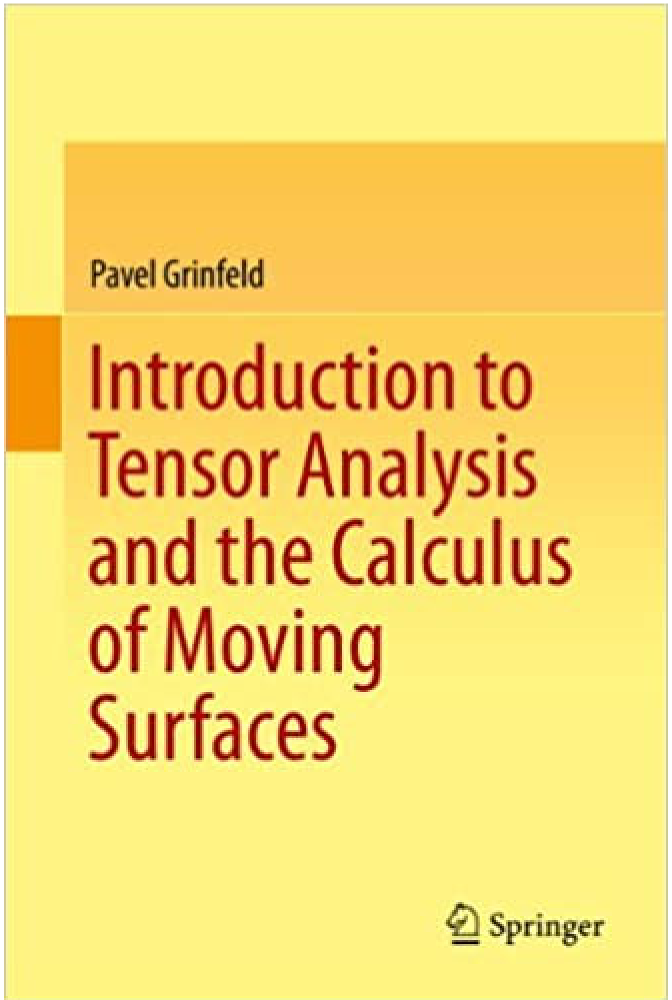
don't forget that all of this is position-dependent!

Tensor Calculus

Highly recommended:

Very nice book,

complete lecture on Youtube!



Thank you.

Thanks for material

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