Lecture 6

Math Foundations Team

BITS Pilani

Pilani | Dubai | Goa | Hyderabad

Introduction

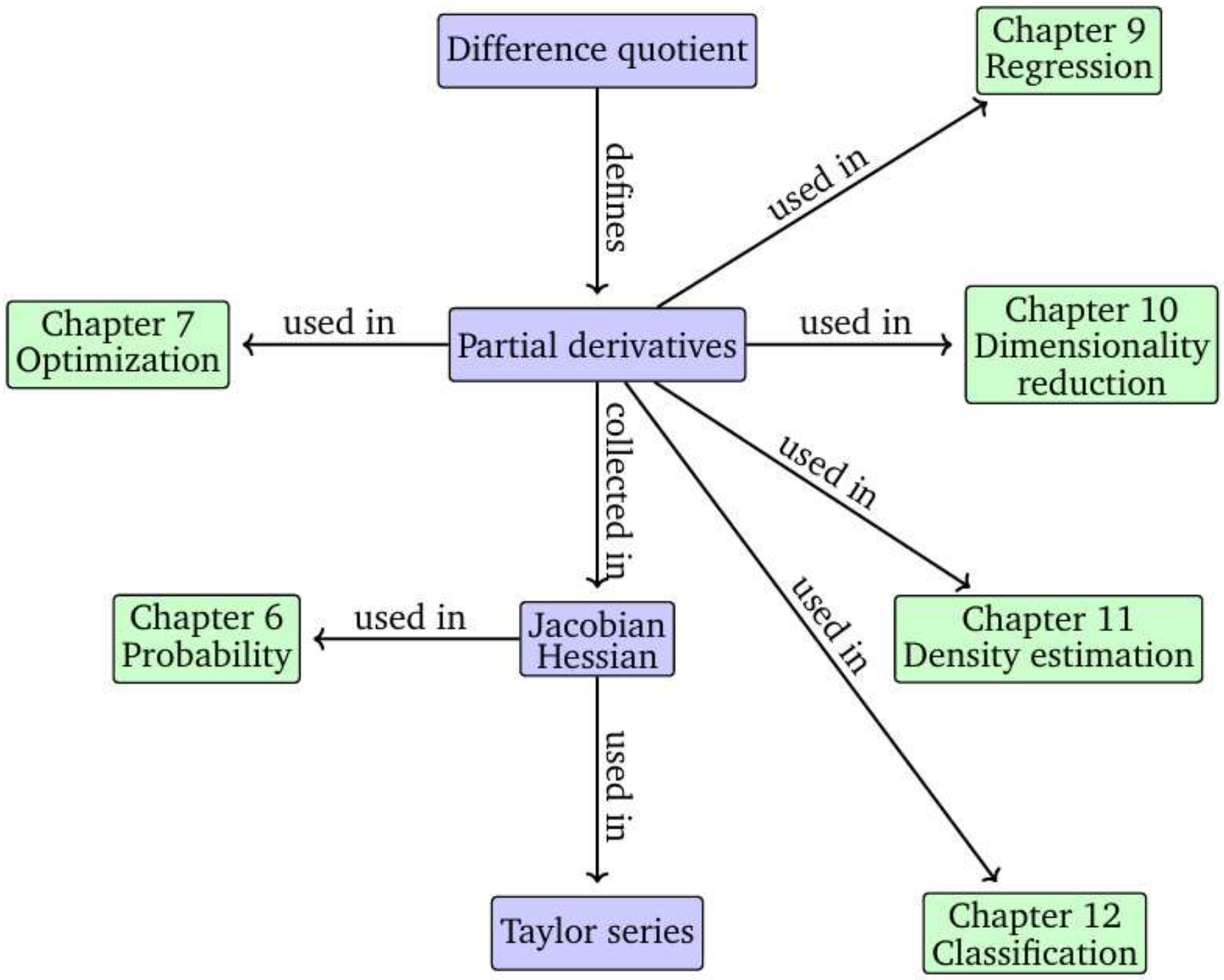
Many algorithms in machine learning optimize an objective function with respect to a set of desired model parameters that control how well a model explains the data: Finding good parameters can be phrased as an optimization problem.

Examples include: linear regression, where we look at curve-fitting problems and optimize linear weight parameters to maximize the likelihood; neural-network auto-encoders for dimensionality reduction and data compression.

Topics to be covered

1. Differentiation of Univariate functions
2. Partial Derivatives
3. Gradient of a scalar valued function
4. Gradient of a vector valued function
5. Gradient of a Matrix with respect to a Matrix

Applications of Partial Derivatives in ML

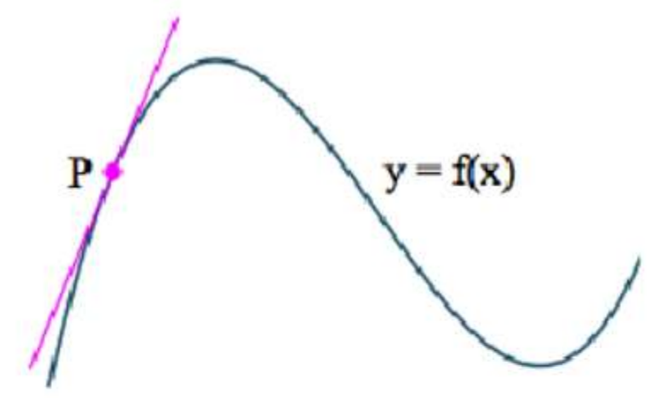


Differentiation of Univariate Functions

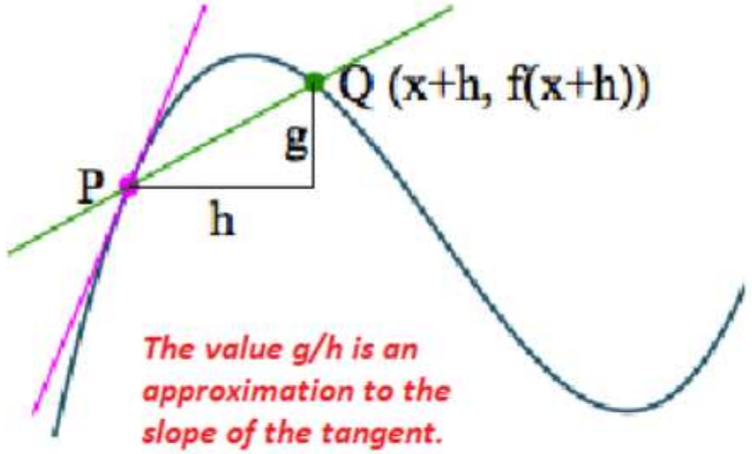
For $h > 0$, the derivative of f at x is defined as the limit

$$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{1}$$

The derivative of f points in the direction of steepest ascent of f.



Slope of the tangent at P.



Slope of the line PQ.

Derivative of a Polynomial

To compute the derivative of $f(x) = x^n \ n \in N$ using the definition

$$\begin{aligned}
\frac{df}{dx} &= \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \\
&= \lim_{h \to 0} \frac{(x+h)^n - x^n}{h} \\
&= \lim_{h \to 0} \frac{\sum_{i=0}^{n} \binom{n}{i} x^{n-i} h^i - x^n}{h} \\
&= \lim_{h \to 0} \frac{\sum_{i=1}^{n} \binom{n}{i} x^{n-i} h^i}{h}
\end{aligned} \tag{2}$$

Derivative of a Polynomial

$$\frac{df}{dx} = \lim_{h\to 0} \sum_{i=1}^{n} \binom{n}{i} x^{n-i} h^{i-1}$$

$$= \lim_{h\to 0} \binom{n}{1} x^{n-1} + \lim_{h\to 0} \sum_{i=2}^{n} \binom{n}{i} x^{n-i} h^{i-1} \quad (3)$$

$$= nx^{n-1}$$

Differentiation Rules

We denote the derivative of f by $f^{'}$

- Product Rule: $(f(x)g(x))^{'} = f^{'}(x)g(x) + f(x)g^{'}(x)$
- Sum Rule: $(f(x) + g(x))^{'} = f^{'}(x) + g^{'}(x)$
- Quotient Rule: $(\frac{f(x)}{g(x)})^{'} = \frac{f^{'}(x)g(x) - f(x)g^{'}(x)}{(g(x))^2}$
- Chain Rule: $(g(f(x))^{'} = (g \circ f)^{'}(x) = g^{'}(f(x))f^{'}(x)$

Example: Chain Rule

Compute the derivative of function $h(x) = (2x + 1)^4$

$h(x) = (2x + 1)^4 = g(f(x))$

$f(x) = 2x + 1,$

$g(f) = f^4$

Derivatives of f and g are

$f^{'}(x) = 2$

$g^{'}(f) = 4f^3$

$h^{'}(x) = g^{'}(f)f^{'}(x) = (4f^3).2 = 8(2x + 1)^3$

Partial Differentiation and Gradients

Differentiation applies to functions f of a scalar variable $x \in R$. In the following, we consider the general case where the function f depends on one or more variables $x \in R^n$, e.g.,$f(x) = f(x_1, x_2)$. The generalization of the derivative to functions of several variables is the gradient. We find the gradient of the function f with respect to x by varying one variable at a time and keeping the others constant. The gradient is then the collection of these partial derivatives.

Partial derivatives and Gradients

Definition: For a function $f : \mathbb{R}^n \to \mathbb{R}$, $x \to f(x)$, $x \in R^n$ of n variables $x_1, \ldots, x_n$ we define the *partial derivatives* as

$$\frac{\partial f}{\partial x_1} = \lim_{h \to 0} \frac{f(x_1 + h, x_2, \ldots, x_n) - f(x_1, x_2, \ldots, x_n)}{h}$$

$$\frac{\partial f}{\partial x_2} = \lim_{h \to 0} \frac{f(x_1, x_2 + h, \ldots, x_n) - f(x_1, x_2, \ldots, x_n)}{h}$$

$$\vdots$$

$$\frac{\partial f}{\partial x_n} = \lim_{h \to 0} \frac{f(x_1, x_2, \ldots, x_n + h) - f(x_1, x_2, \ldots, x_n)}{h}$$

We collect them in the row vector called the gradient of f or Jacobian

$$\Delta_x f = gradf = \frac{df}{dx} = \left[\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \ldots, \frac{\partial f(x)}{\partial x_n}\right] \tag{8}$$

Example 1: Find the partial derivatives of $f(x, y) = (x + 2y^3)^2$

$$\frac{\partial f(x,y)}{\partial x} = 2(x + 2y^3)\frac{\partial (x + 2y^3)}{\partial x} = 2(x + 2y^3) \tag{9}$$

$$\frac{\partial f(x,y)}{\partial y} = 2(x + 2y^3)\frac{\partial (x + 2y^3)}{\partial y} = 12y^2(x + 2y^3) \tag{10}$$

here we used the chain rule to compute the partial derivatives.

Example 2

Find the partial derivatives of $f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3$

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2x_1 x_2 + x_2^3 \tag{11}$$

$$\frac{\partial f(x_1, x_2)}{\partial x_2} = x_1^2 + 3x_1 x_2^2 \tag{12}$$

So the gradient is then

$$\frac{df}{dx} = [\frac{\partial f(x_1, x_2)}{\partial x_1}, \frac{\partial f(x_1, x_2)}{\partial x_2}] = [2x_1 x_2 + x_2^3, x_1^2 + 3x_1 x_2^2] \in \mathbb{R}^{1\times 2} \tag{13}$$

Basic rules of partial differentiation

When we compute derivatives with respect to vectors $x \in \mathbb{R}^n$ we need to pay attention: Our gradients now involve vectors and matrices, and matrix multiplication is not commutative i.e., the order matters.

$$\text{Product rule: } \frac{\partial}{\partial x}(f(x)g(x)) = \frac{\partial f}{\partial x}g(x) + f(x)\frac{\partial g}{\partial x} \tag{14}$$

$$\text{Sum rule: } \frac{\partial}{\partial x}(f(x) + g(x)) = \frac{\partial f}{\partial x} + \frac{\partial g}{\partial x} \tag{15}$$

$$\text{chain rule: } \frac{\partial}{\partial x}(g \circ f)(x) = \frac{\partial}{\partial x}(g(f(x)) = \frac{\partial g}{\partial f}\frac{\partial f}{\partial x} \tag{16}$$

Chain Rule

Consider a function $f : \mathbb{R} \to \mathbb{R}$ of two variables x_1, x_2.
Furthermore, $x_1(t)$ and $x_2(t)$ are themselves functions of t.

To compute the gradient of f with respect to t, we need to apply the chain rule for multivariate functions as

$$\frac{df}{dt} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1(t)}{\partial t} \\ \frac{\partial x_2(t)}{\partial t} \end{bmatrix} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} \tag{17}$$

where d denotes the gradient and ∂ partial derivatives.

Example

Consider $f(x_1, x_2) = x_1^2 + 2x_2$, where $x_1 = \sin t$ and $x_2 = \cos t$ then

$$\begin{aligned}\frac{df}{dt} &= \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} \\ &= 2\sin t\frac{\partial \sin t}{\partial t} + 2\frac{\partial \cos t}{\partial t} \\ &= 2\sin t\cos t - 2\sin t = 2\sin t(\cos t - 1)\end{aligned}$$

is the corresponding derivative of f with respect to t.

If $f(x_1, x_2)$ is a function of x_1 and x_2, where $x_1(s, t)$ and $x_2(s, t)$ are themselves functions of two variables s and t, the chain rule yields the partial derivatives:

$$\frac{\partial f}{\partial s} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial s} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial s} \tag{18}$$

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} \tag{19}$$

and the gradient is obtained by the matrix multiplication

$$\frac{df}{d(s,t)} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial (s,t)}$$

$$= \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial s} & \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial s} & \frac{\partial x_2}{\partial t} \end{bmatrix}$$

Lecture 6 (ctd)

Math Foundations Team

BITS Pilani

Pilani | Dubai | Goa | Hyderabad

Gradients of Vector-Valued Functions

We have discussed partial derivatives and gradients of functions $f : \mathbb{R}^n \to \mathbb{R}$ mapping to the real numbers. Now we will generalize the concept of the gradient to vector-valued functions $f : \mathbb{R}^n \to \mathbb{R}^m$, where $n \geq 1$ and $m > 1$.
For a function $f : \mathbb{R}^n \to \mathbb{R}^m$ and a vector $x = [x_1, \ldots, x_n]^T$ corresponding vector of function values is given as

$$f(x) = \begin{bmatrix} f_1(x) \\ \vdots \\ f_m(x) \end{bmatrix} \in \mathbb{R}^m \tag{20}$$

where each $f_i : \mathbb{R}^n \to \mathbb{R}$

Gradients of Vector-Valued Functions

Therefore, the partial derivative of a vector-valued function $f : \mathbb{R}^n \to \mathbb{R}^m$ w.r.t. $x_i \in R$, $i = 1, \ldots n$ is given as the vector

$$\frac{\partial f}{\partial x_i} = \begin{bmatrix} \frac{\partial f_1}{\partial x_i} \\ \vdots \\ \frac{\partial f_m}{\partial x_i} \end{bmatrix}$$

$$= \begin{bmatrix} \lim_{h\to 0} \frac{f_1(x_1,\ldots,x_{i-1},x_i+h,x_{i+1},\ldots,x_n)-f_1(x)}{h} \\ \vdots \\ \lim_{h\to 0} \frac{f_m(x_1,\ldots,x_{i-1},x_i+h,x_{i+1},\ldots,x_n)-f_m(x)}{h} \end{bmatrix} \in \mathbb{R}^m$$

Gradients of Vector-Valued Functions

We know that the gradient of f with respect to a vector is the row vector of the partial derivatives. Every partial derivative $\frac{\partial f}{\partial x_i}$ is itself a column vector. Therefore, we obtain the gradient of $f : \mathbb{R}^n \to \mathbb{R}^m$ with respect to $x \in \mathbb{R}^n$ by collecting these partial derivatives:

$$\frac{df(x)}{dx} = \left[\frac{\partial f(x)}{\partial x_1} \cdots \frac{\partial f(x)}{\partial x_n}\right]$$

$$= \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_1} & \cdots & \frac{\partial f_1(x)}{\partial x_n} \\ & \vdots & \\ \frac{\partial f_m(x)}{\partial x_1} & \cdots & \frac{\partial f_m(x)}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{m \times n}$$

Example 1: Gradients of Vector-Valued Functions

Given $f(x) = Ax, \quad f(x) \in \mathbb{R}^M, \quad A \in \mathbb{R}^{M \times N}, \quad x \in \mathbb{R}^N$
Since $f : \mathbb{R}^N \to \mathbb{R}^M$, it follows that $df/dx \in \mathbb{R}^{M \times N}$. To compute the gradient we determine the partial derivatives of f w.r.t x_j:

$$f_i(x) = \sum_{j=1}^{N} A_{ij} x_j \implies \frac{\partial f_i}{\partial x_j} = A_{ij} \tag{21}$$

We obtain the gradient using Jacobian

$$\frac{df}{dx} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ & \vdots & \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} A_{11} \ldots A_{1N} \\ \vdots \\ A_{M1} \ldots A_{MN} \end{bmatrix} = A \in \mathbb{R}^{M \times N} \tag{22}$$

Example 2: Gradients of Vector-Valued Functions

Consider the function $h : \mathbb{R} \to \mathbb{R}, \quad h(t) = (f \circ g)(t)$ with $f(x) = exp(x_1 x_2^2)$

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = g(t) = \begin{bmatrix} t \cos t \\ t \sin t \end{bmatrix} \tag{23}$$

and compute the gradient of h w.r.t. t. Since $f : \mathbb{R}^2 \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}^2$ we note that

$$\frac{\partial f}{\partial x} \in \mathbb{R}^{1 \times 2} \text{ and } \frac{\partial g}{\partial t} \in \mathbb{R}^{2 \times 1} \tag{24}$$

The desired gradient is computed by applying the chain rule:

$$\frac{dh}{dt} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix}$$

$$= \begin{bmatrix} exp(x_1 x_2^2)x_2^2 & 2exp(x_1 x_2^2)x_1 x_2 \end{bmatrix} \begin{bmatrix} \cos t - t \sin t \\ \sin t + t \cos t \end{bmatrix}$$

$$= exp(x_1 x_2^2)(x_2^2(\cos t - t \sin t) + 2x_1 x_2(\sin t + t \cos t))$$

where $x_1 = t \cos t$ and $x_2 = t \sin t$;

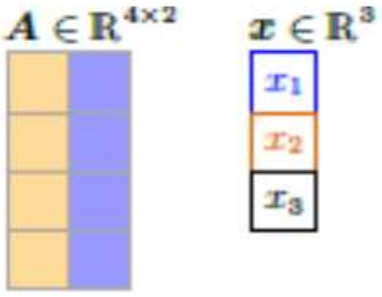
Gradients of Matrices

The gradient of an $m \times n$ matrix A with respect to a $p \times q$ matrix B, the resulting Jacobian would be an $(m \times n) \times (p \times q)$, i.e., a four-dimensional tensor J, whose entries are given as

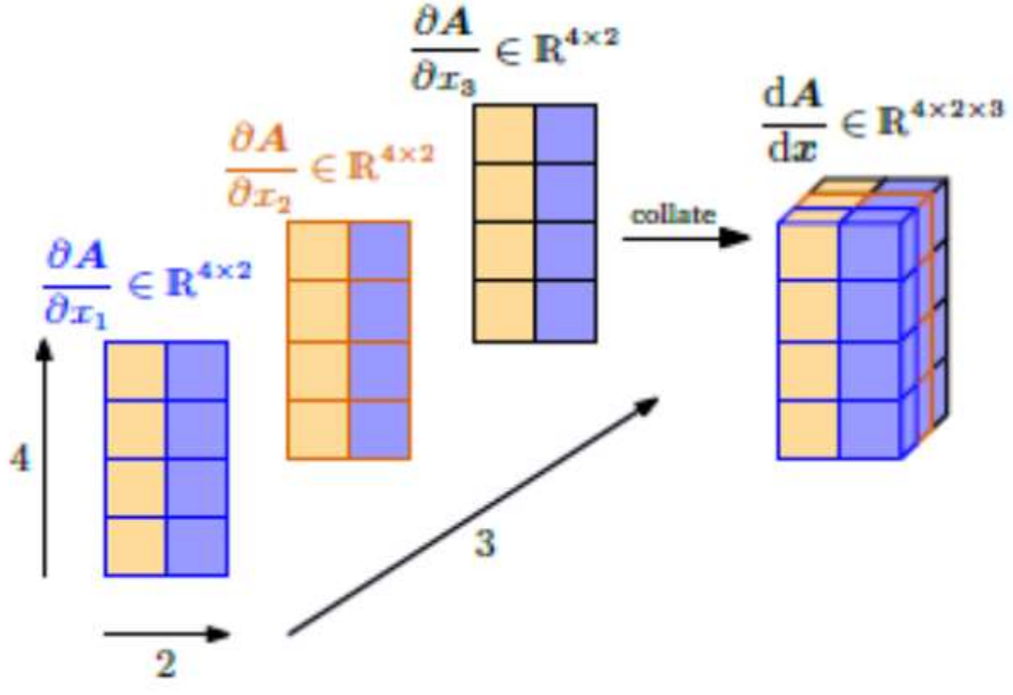
$$J_{ijkl} = \frac{\partial A_{ij}}{\partial B_{kl}}$$

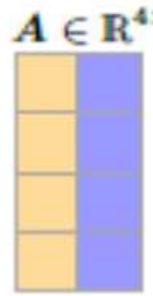
Since, we can consider $\mathbb{R}^{m \times n}$ as $\mathbb{R}^{mn}$, we can shape our matrix into vectors of length mn and pq respectively. The gradient using mn vectors results in a Jacobian of size $mn \times pq$

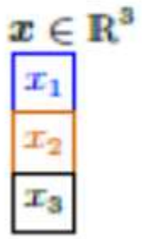
Gradients of Matrices

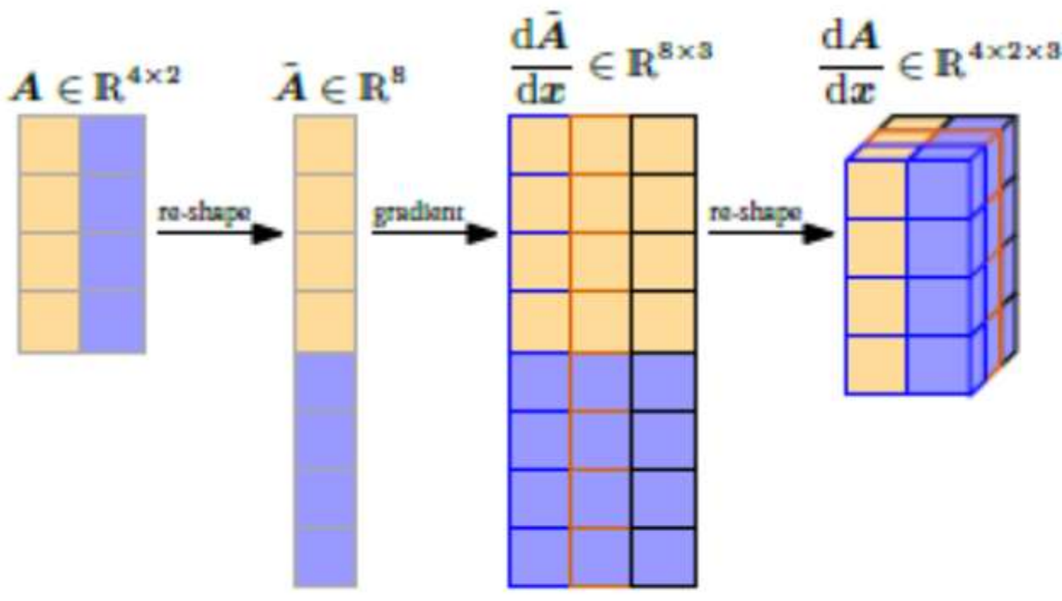


Partial derivatives:









Gradients of Matrices

Gradient of Vector values functions with respect to Matrices - Example

Let $f = Ax$ where $A \in \mathbb{R}^{m \times n}$, and $x \in \mathbb{R}^n$, then

$$\frac{\partial f}{\partial A} \in \mathbb{R}^{m \times (m \times n)}$$

By definition

$$\frac{\partial f}{\partial A} = \begin{bmatrix} \frac{\partial f_1}{\partial A} \\ \vdots \\ \frac{\partial f_m}{\partial A} \end{bmatrix}, \frac{\partial f_i}{\partial A} \in \mathbb{R}^{1 \times (m \times n)}$$

Gradients of Matrices

Now, we have

$$f_i = \sum_{j=1}^{n} A_{ij} x_j, i = 1, \cdots, m.$$

Therefore, by taking partial derivatives with respect to A_{iq}

$$\frac{\partial f_i}{\partial A_{iq}} = x_q.$$

Hence, i^{th} row becomes

$$\frac{\partial f_i}{\partial A_{i,:}} = x^T \in \mathbb{R}^{1 \times 1 \times n}$$

$$\frac{\partial f_i}{\partial A_{k,:}} = 0^T \in \mathbb{R}^{1\times 1\times n}, \text{for} k \neq i$$

Hence, by stacking the partial derivatives, we get

$$\frac{\partial f_i}{\partial A_{k,:}} = \begin{bmatrix} 0^T \\ \vdots \\ x^T \\ \vdots \\ 0^T \end{bmatrix} \in \mathbb{R}^{1\times m\times n}$$

Gradients of Matrices with respect to Matrices

Let $B \in \mathbb{R}^{m \times n}$ and $f : \mathbb{R}^{m \times n} \to \mathbb{R}^{n \times n}$ with

$$f(B) = B^T B =: K \in \mathbb{R}^{n \times n}$$

Then, we have

$$\frac{\partial K}{\partial B} \in \mathbb{R}^{(n \times n) \times (m \times n)}.$$

Moreover

$$\frac{\partial K_{pq}}{\partial B} \in \mathbb{R}^{1 \times (m \times n)}, \text{for} p, q = 1, \cdots n$$

where K_{pq} is the $(p, q)^{th}$ entry of $K = f(B)$

Gradients of Matrices with respect to Matrices

Let i^{th} column of B be b_i, then

$$K_{pq} = r_p^T r_q = \sum_{l=1}^{m} B_{lp} B_{lq}$$

Computing the partial derivative, we get

$$\frac{\partial K_{pq}}{\partial B_{ij}} = \sum_{l=1}^{m} \frac{\partial}{\partial B_{ij}} B_{lp} B_{lq} = \partial_{pqij}$$

Gradients of Matrices with respect to Matrices

Clearly, we have

$$\begin{aligned}
\partial_{pqij} &= B_{iq} \quad \text{if } j = p, p \neq q \\
\partial_{pqij} &= B_{ip} \quad \text{if } j = q, p \neq q \\
\partial_{pqij} &= 2B_{iq} \quad \text{if } j = p, p = q \\
\partial_{pqij} &= 0 \qquad \text{otherwise}
\end{aligned}$$

where $p, q, j = 1, \cdots, n$ $i = 1, \cdots, m$

Useful Identities for Computing Gradients

- $\frac{\partial}{\partial X} f(X)^T = (\frac{\partial f(X)}{\partial X})^T$
- $\frac{\partial}{\partial X} tr(f(X)) = tr(\frac{\partial f(X)}{\partial X})$
- $\frac{\partial}{\partial X} det(f(X)) = det(f(X)) tr(f(X)^{-1} \frac{\partial f(X)}{\partial X})$
- $\frac{\partial}{\partial X} f(X)^{-1} = -f(X)^{-1} \frac{\partial f(X)}{\partial X} f(X)^{-1}$

Useful Identities for Computing Gradients

- $\frac{\partial a^T X^{-1} b}{\partial X} = -(X^{-1})^T a b^T (X^{-1})^T$
- $\frac{\partial x^T a}{\partial x} = a^T$
- $\frac{\partial a^T x}{\partial x} = a^T$
- $\frac{\partial a^T X b}{\partial X} = a b^T$
- $\frac{\partial x^T B}{\partial x} = x^T (B + B^T)$
- $\frac{\partial}{\partial s}(x - As)^T W (x - As) = -2(x - As)^T WA$

for symmetric W.