Vector calculus

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Preliminaries

Function

We say that f is a function if it maps each element of $\mathbb{R}^D$ to a unique element in $\mathbb{R}$. We usually write

$$\begin{aligned} f: \quad & \mathbb{R}^D \mapsto \mathbb{R} \\ & \mathbf{x} \rightarrow f(\mathbf{x}) \end{aligned}$$

Differenciation of univariate function

Let

$$\begin{aligned} f: \quad & \mathbb{R} \mapsto \mathbb{R} \\ & x \to f(x) \end{aligned}$$

be an univariate function. Then the derivative of f at x is given by

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

It refers to the rate of change in the function's f value when moving from x to $x+h$.

Derivation rules

Consider $f, g : \quad \mathbb{R} \mapsto \mathbb{R}$. We have :

1. Product rule : $(f(x)g(x))' = f'(x)g(x) + g'(x)f(x)$
2. Quotient rule : $\left(\frac{f(x)}{g(x)}\right)' = \frac{f'(x)g(x) - g'(x)f(x)}{g(x)^2}$
3. Sum rule : $(f(x) + g(x))' = f'(x) + g'(x)$
4. Chain rule : $(g(f(x)))' = (g \circ f)'(x) = g'(f(x)).f'(x)$.

Example : Chain rule

We want to compute the derivative of the function $h(x) = (2x^2 + 1)^4$.

Partial Derivatives and Gradient Vector

Partial derivatives

Consider the multivariate function

$$\begin{aligned} f: \quad & \mathbb{R}^n \mapsto \mathbb{R} \\ & \mathbf{x} \rightarrow f(\mathbf{x}) \end{aligned}$$

where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^n$.

Partial derivatives

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where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^n$.
A partial derivative of f with respect to $x_i, i = 1..n$ is defined by

$$\frac{\partial f}{\partial x_i} = \lim_{h \to 0} \frac{f(x_1, x_2, \ldots, x_i + h, x_{i+1}, \ldots, x_n) - f((x_1, x_2, \ldots, x_i, x_{i+1}, \ldots, x_n)}{h}$$

Gradient vector

The vector containing first order partial derivatives

$$\nabla f = \frac{df}{d\mathbf{x}} = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}\right] \in \mathbb{R}^{1\times n}$$

is called the Gradient or the Jacobian of f.

We can get the partial derivatives using the chain rule.
Example : $f(x, y) = (x + 2y^3)^2$.

Basic rules of partial differentiation

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1. Product : $\frac{\partial}{\partial \mathbf{x}}(f(\mathbf{x}).g(\mathbf{x})) = \frac{\partial f}{\partial \mathbf{x}}.g(\mathbf{x}) + \frac{\partial g}{\partial \mathbf{x}}.f(\mathbf{x}) \in \mathbb{R}^{1\times n}$.
2. Sum : $\frac{\partial}{\partial \mathbf{x}}(f(\mathbf{x}) + g(\mathbf{x})) = \frac{\partial f}{\partial \mathbf{x}} + \frac{\partial g}{\partial \mathbf{x}} \in \mathbb{R}^{1\times n}$.
3. Chain rule : $\frac{\partial}{\partial \mathbf{x}}(g \circ f)(\mathbf{x}) = \frac{\partial}{\partial \mathbf{x}}(g(f(\mathbf{x}))) = \frac{\partial g}{\partial f} \times \frac{\partial f}{\partial \mathbf{x}} \in \mathbb{R}^{1\times n}$.

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In the case of the chain rule, we have to make sure that dimensions are matching.

Example

Consider the function $g(x, y) = (x^2 + y^2)^3$.

Always with the chain rule

consider the bivariate function $f(x_1, x_2) : \mathbb{R}^2 \mapsto \mathbb{R}$ such that $x_1 = x_1(t)$ and $x_2 = x_2(t)$.

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consider the bivariate function $f(x_1, x_2) : \mathbb{R}^2 \mapsto \mathbb{R}$ such that $x_1 = x_1(t)$ and $x_2 = x_2(t)$.
To compute the derivative of f with respect to t, we have to apply the chain rule as follows :

$$\frac{df}{dt} = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}\right] \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix} = \frac{\partial f}{\partial x_1} . \frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2} . \frac{\partial x_2}{\partial t}$$

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where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^n$, with

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Then

$$\frac{df}{dt} = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \frac{\partial x_i}{\partial t}$$

Example

$f(x, y) = x^2 + 2y$, with $x = \sin t$ and $y = \cos t$.

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$$\frac{df}{dt} = \frac{\partial f}{\partial x}.\frac{\partial x}{\partial t} + \frac{\partial f}{\partial y}.\frac{\partial y}{\partial t}$$
$$\frac{df}{ds} = \frac{\partial f}{\partial x}.\frac{\partial x}{\partial s} + \frac{\partial f}{\partial y}.\frac{\partial y}{\partial s}$$

The gradient is obtained by the matrix multiplication :

$$\frac{df}{d(s,t)} = \frac{\partial f}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial (s,t)} = \left[\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right] \begin{bmatrix} \frac{\partial x}{\partial s} & \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial s} & \frac{\partial y}{\partial t} \end{bmatrix}$$

Example

$f(x, y) = xy$
$x = t^2 + 2s$, $y = 3st$.

Gradients of Vector-Valued Functions

Consider the function

$$\begin{aligned} \mathbf{f}: \quad & \mathbb{R}^n \mapsto \mathbb{R}^m \\ & \mathbf{x} \to \mathbf{f}(\mathbf{x}) \end{aligned}$$

where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^n$.

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where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^n$.
The corresponding vector of function values is given by

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ f_m(\mathbf{x}) \end{bmatrix} \tag{1}$$

$\mathbf{f}$ is a vector of functions $[f_1, \ldots, f_m]^\top$ such that $f_i : \mathbb{R}^n \to \mathbb{R}, i = 1..m$.

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$$\frac{\partial \mathbf{f}}{\partial x_i} = \begin{bmatrix} \frac{\partial f_1}{\partial x_i} \\ \vdots \\ \frac{\partial f_m}{\partial x_i} \end{bmatrix} \in \mathbb{R}^m$$

Since every partial derivative $\frac{\partial \mathbf{f}}{\partial x_i}$ is a vector, we obtain the gradient of $\mathbf{f}$ with respect to $\mathbf{x}$ by collecting these vectors and therefore we have :

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

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This matrix is called the Jacobian of $\mathbf{f}$ and is denoted $\mathbf{J}$.

Example 1

Consider the function $\mathbf{f} : \mathbb{R}^3 \to \mathbb{R}^2$, avec $\mathbf{f} = \begin{bmatrix} x^2 - 3y + z \\ x - y^3 + z^2 \end{bmatrix}$

Example 2

Consider the function $\mathbf{f}(\mathbf{x}) = \mathbf{A}\,\mathbf{x} \in \mathbb{R}^n$, with $\mathbf{A} \in \mathbb{R}^{m\times n}, \mathbf{x} \in \mathbb{R}^n$.

Example 2

Consider the function $\mathbf{f}(\mathbf{x}) = \mathbf{A}\,\mathbf{x} \in \mathbb{R}^n$, with $\mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{x} \in \mathbb{R}^n$.

Each function $f_i(\mathbf{x}) = \sum_{i=1}^{n} A_{ij}x_j$. Therefore, $\dfrac{\partial f_i}{\partial x_j} = A_{ij}$.

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \mathbf{A} = \begin{bmatrix} A_{11} & \dots & A_{1n} \\ \vdots & & \vdots \\ A_{m1} & \dots & A_{mn} \end{bmatrix}$$

Gradient of matrices

Gradient of a matrix with respect to a matrix

We may need to compute the gradient of a matrix with respect to a vector or to another matrix.

The gradient of an $m \times n$ matrix of functions $\mathbf{A}$ with respect to an $p \times q$ matrix $\mathbf{B}$ is the Jacobian of size $m \times n \times p \times q$ (tensor), such that $\mathbf{J}_{ijkl} = \dfrac{\partial A_{ij}}{\partial B_{kl}}$.

Remark

We can rewrite matrices as vectors of dimensions mn and pq. In this case, the Jacobian is of size $mn \times pq$.

Consider the matrix $\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$ With $A_{11} = 2x + 4y$, $A_{12} = xy^2$, $A_{21} = xy$, $A_{22} = x^2 + y$.

Gradient of a vector with respect to a matrix

Consider $\mathbf{f} = \mathbf{A}\,\mathbf{x}$, $\mathbf{f} \in \mathbb{R}^m$, $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{x} \in \mathbb{R}^n$.

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We want to compute the gradient $\dfrac{d\,\mathbf{f}}{d\mathbf{A}} \in \mathbb{R}^{m \times m \times n}$.

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Consider $\mathbf{f} = \mathbf{A}\,\mathbf{x}$, $\mathbf{f} \in \mathbb{R}^m$, $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{x} \in \mathbb{R}^n$.

We want to compute the gradient $\dfrac{d\,\mathbf{f}}{d\mathbf{A}} \in \mathbb{R}^{m \times m \times n}$.

From the definition, we have $\dfrac{d\,\mathbf{f}}{d\mathbf{A}} = \begin{bmatrix} \dfrac{\partial f_1}{\partial \mathbf{A}} \\ \dfrac{\partial f_2}{\partial \mathbf{A}} \\ \vdots \\ \dfrac{\partial f_m}{\partial \mathbf{A}} \end{bmatrix}$, such that

$\dfrac{\partial f_i}{\partial \mathbf{A}} \in \mathbb{R}^{1 \times m \times n}$.

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Thus $\frac{\partial f_i}{\partial A_{iq}} = x_q$. For a row in $\mathbf{A}$, we get

$$\frac{\partial f_i}{\partial A_{i,:}} = \mathbf{x}^\top$$
$$\frac{\partial f_i}{\partial A_{k \neq i,:}} = \mathbf{0}^\top$$

Therefore, we have

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$$\frac{\partial f_i}{\mathbf{A}} = \begin{bmatrix} \mathbf{0}^\top \\ \mathbf{0}^\top \\ \vdots \\ \mathbf{0}^\top \\ \mathbf{x}^\top \\ \vdots \\ \mathbf{0}^\top \end{bmatrix} = \begin{bmatrix} 0 & \dots & 0 \\ \vdots & & \vdots \\ x_1 & \dots & x_n \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{bmatrix}$$

$$\frac{\partial \mathbf{f}}{\partial \mathbf{A}} = \begin{bmatrix} \begin{pmatrix} x_1 & \dots & x_n \\ 0 & \dots & 0 \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & \dots & 0 \\ x_1 & \dots & x_n \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{pmatrix} \\ \vdots \\ \begin{pmatrix} 0 & \dots & 0 \\ \vdots & & \vdots \end{pmatrix} \end{bmatrix}$$

Some useful Formulas

- $\dfrac{\partial}{\partial \mathbf{X}} \mathbf{f}(\mathbf{X})^\top = \left(\dfrac{\partial\, \mathbf{f}(\mathbf{X})}{\partial \mathbf{X}}\right)^\top$
- $\dfrac{\partial\, \mathrm{tr}(\mathbf{f}(\mathbf{X}))}{\partial \mathbf{X}} = \mathrm{tr}\left(\dfrac{\partial\, \mathbf{f}(\mathbf{X})}{\partial \mathbf{X}}\right)$
- $\dfrac{\partial \det(\mathbf{f}(\mathbf{X}))}{\partial \mathbf{X}} = \det(\mathbf{f}(\mathbf{X})).\, \mathrm{tr}\left(\mathbf{f}(\mathbf{X})^{-1} \dfrac{\partial\, \mathbf{f}(\mathbf{X})}{\partial \mathbf{X}}\right)$
- $\dfrac{\partial}{\partial \mathbf{X}} \mathbf{f}(\mathbf{X})^{-1} = -\,\mathbf{f}(\mathbf{X})^{-1} \dfrac{\partial\, \mathbf{f}(\mathbf{X})}{\partial \mathbf{X}}\, \mathbf{f}(\mathbf{X})^{-1}.$
- $\dfrac{\partial a^\top \mathbf{X} b}{\partial \mathbf{X}} = ab^\top.$
- $\dfrac{\partial a^\top \mathbf{X}^{-1} b}{\partial \mathbf{X}} = -\mathbf{X}^{-1} ab^\top (\mathbf{X}^{-1})^\top.$

Some useful Formulas

- $\dfrac{\partial a^\top \mathbf{x}}{\mathbf{x}} = a^\top$.
- $\dfrac{\partial \mathbf{x}^\top a}{\mathbf{x}} = a^\top$.
- $\dfrac{\partial \mathbf{x}^\top \mathbf{B}\mathbf{x}}{\partial \mathbf{x}} = \mathbf{x}^\top (\mathbf{B} + \mathbf{B}^\top)$
- $\dfrac{\partial}{\partial \mathbf{x}} (\mathbf{x} - \mathbf{A}\mathbf{s})\, \mathbf{W}\, (\mathbf{x} - \mathbf{A}\mathbf{s}) = -2\, (\mathbf{x} - \mathbf{A}\mathbf{s})^\top \mathbf{W}\mathbf{A}$, for symmetric $\mathbf{W}$.

Automatic Differentiation and Backpropagation

Automatic Differentiation

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It applies a series of elementary arithmetic operations (addition, multiplication) and elementary functions (sin, cos, exp, log) to compute the gradient of quite complicated functions automatically.

Automatic differentiation

given a function value $\mathbf{y}$ that is computed as a many level function composition :

$$\mathbf{y} = (f_k \circ f_{k-1} \circ \ldots \circ f_1)(\mathbf{x}) = f_k(f_{k-1}(\ldots(f_1(\mathbf{x}))))$$

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$$\mathbf{x} \longrightarrow f_1 \longrightarrow f_2 \dashrightarrow f_{k-1} \longrightarrow f_k$$

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$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial y}{\partial f_k} \cdot \frac{\partial f_k}{\partial f_{k-1}} \cdot \dots \cdot \frac{\partial f_1}{\partial \mathbf{x}}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial y}{\partial f_k} \cdot \frac{\partial f_k}{\partial f_{k-1}} \cdot \dots \cdot \left(\frac{\partial f_2}{\partial f_1} \frac{\partial f_1}{\partial \mathbf{x}} \right) \qquad \text{forward mode}$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \left(\frac{\partial y}{\partial f_k} \cdot \frac{\partial f_k}{\partial f_{k-1}} \right) \cdot \dots \cdot \frac{\partial f_1}{\partial \mathbf{x}} \qquad \text{Reverse mode}$$

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$$
\begin{aligned}
\frac{\partial \mathbf{y}}{\partial \mathbf{x}} &= \frac{\partial y}{\partial f_k} \cdot \frac{\partial f_k}{\partial f_{k-1}} \cdot \dots \cdot \frac{\partial f_1}{\partial \mathbf{x}} \\
\frac{\partial \mathbf{y}}{\partial \mathbf{x}} &= \frac{\partial y}{\partial f_k} \cdot \frac{\partial f_k}{\partial f_{k-1}} \cdot \dots \cdot \left(\frac{\partial f_2}{\partial f_1} \frac{\partial f_1}{\partial \mathbf{x}} \right) \qquad \text{forward mode} \\
\frac{\partial \mathbf{y}}{\partial \mathbf{x}} &= \left(\frac{\partial y}{\partial f_k} \cdot \frac{\partial f_k}{\partial f_{k-1}} \right) \cdot \dots \cdot \frac{\partial f_1}{\partial \mathbf{x}} \qquad \text{Reverse mode}
\end{aligned}
$$

In Deep Learning, it is the reverse mode that is used to compute the partial derivatives. This is called Backpropagation

Example

Consider the function

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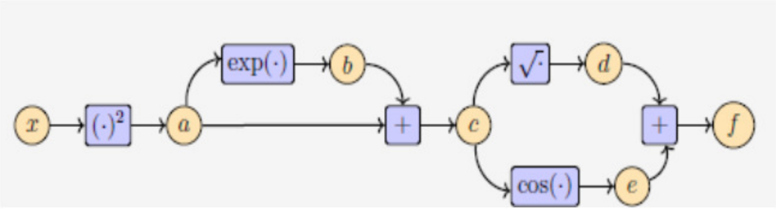
We define the variables :

$$
\begin{aligned}
a &= x^2, \\
b &= \exp(a), \\
c &= a + b, \\
d &= \sqrt{c}, \\
e &= \cos(c), \\
f &= d + e,
\end{aligned}
$$

Example of a computation graph



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$$\frac{\partial a}{\partial x} = 2x,$$
$$\frac{\partial b}{\partial a} = \exp(a),$$
$$\frac{\partial c}{\partial a} = \frac{\partial c}{\partial b} = 1,$$
$$\frac{\partial d}{\partial c} = \frac{1}{2\sqrt{c}},$$
$$\frac{\partial e}{\partial c} = \sin(c),$$
$$\frac{\partial f}{\partial d} = \frac{\partial f}{\partial e} = 1.$$

Going back to the computation graph, we can deduce that

$$
\begin{aligned}
\frac{\partial f}{\partial c} &= \frac{\partial f}{\partial d} \cdot \frac{\partial d}{\partial c} + \frac{\partial f}{\partial e} \cdot \frac{\partial e}{\partial c} \\
\frac{\partial f}{\partial b} &= \frac{\partial f}{\partial c} \cdot \frac{\partial c}{\partial b} = \frac{\partial f}{\partial c} \\
\frac{\partial f}{\partial a} &= \frac{\partial f}{\partial c} \cdot \frac{\partial c}{\partial a} = \frac{\partial f}{\partial c} \\
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial a} \cdot \frac{\partial a}{\partial x}.
\end{aligned}
$$

Example 2

Consider the bivariate function

$$y = f(x_1, x_2) = \frac{x_1^2 - 2x_2}{\sqrt{x_1 x_2 - \sin(x_2)}}$$

Automatic differentiation

Let $x_1, \dots, x_d$ be the input variables to the function and $x_{d+1}, \dots, x_{D-1}$ be the intermediate variables and x_D the output variable. Then the computation graph can be expressed as follows :

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where g_i is an elementary function and $x_{P(x_i)}$ are the parent nodes (predecessors) of the variable x_i in the graph.

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where g_i is an elementary function and $x_{P(x_i)}$ are the parent nodes (predecessors) of the variable x_i in the graph. Therefore, we have

$$\frac{\partial f}{\partial x_D} = 1$$
$$\frac{\partial f}{\partial x_i} = \sum_{x_j : x_i \in P(x_j)} \frac{\partial f}{\partial x_j} \cdot \frac{\partial x_j}{\partial x_i}$$

Backpropagation in a Neural Network

Consider a function value $\mathbf{y}$ that is computed as a many level function composition :

$$\mathbf{y} = (f_k \circ f_{k-1} \circ \ldots \circ f_1)(\mathbf{x}) = f_k(f_{k-1}(\ldots(f_1(\mathbf{x}))))$$

where $\mathbf{x}$ are the input, $\mathbf{y}$ represents the observations, and every function $f_i, i = 1..k$ has its own parameters.

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$\mathbf{A}_{i-1}$ is the matrix of weights between layers $i-1$ and i,

Backpropagation in a Neural Network

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x_{i-1} denotes the output of the layer $i-1$ ($x_0 = \mathbf{x}$) ,

$\mathbf{A}_{i-1}$ is the matrix of weights between layers $i-1$ and i,

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Our goal is then to compute the gradient of the function

$$\mathcal{L}(\Theta) = \|\, \mathbf{y} - f_k(\Theta, \mathbf{x})\|^2$$

with $\Theta = \{\mathbf{A}_0, \mathbf{b}_0, \ldots, \mathbf{A}_{k-1}, \mathbf{b}_{k-1}\}$.

Chain rule allows us to compute the partial derivatives of $\mathcal{L}$ with respect to parameters $\theta_i = \{\mathbf{A}_i, \mathbf{b}_i\}$:

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$$\vdots$$

$$\frac{\partial \mathcal{L}}{\partial \theta_{i}} = \frac{\partial \mathcal{L}}{\partial f_k} \cdot \frac{\partial f_k}{\partial f_{k-1}} \cdot \frac{\partial f_{k-1}}{\partial f_{k-2}} \cdots \boxed{\frac{\partial f_{i+2}}{\partial f_{i+1}} \cdot \frac{\partial f_{i+1}}{\partial \theta_{i}}}$$

Second Order Derivatives

$$
\begin{aligned}
f: \quad & \mathbb{R}^n \mapsto \mathbb{R} \\
& \mathbf{x} \to f(x)
\end{aligned}
$$

where $\mathbf{x} = [x_1, x_2, \ldots, x_n]^\top \in \mathbb{R}^n$.

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$$\mathbf{x} \rightarrow f(\ x)$$

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The second order partial derivatives are obtained by deriving the first order partial derivatives function with respect to all variables.

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The second order partial derivatives are obtained by deriving the first order partial derivatives function with respect to all variables.
Thus we have, for $i, j = 1..n$:

$$\frac{\partial(\frac{\partial f}{\partial x_i})}{\partial x_j} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

The Hessian Matrix

The *Hessian* matrix of f is a matrix of second-order partial derivatives :

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$$\text{i.e. } [(\mathbf{H})_{ij}] = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

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The Hessian is used in some optimization algorithms such as Newton's method.

It is expensive to calculate but can drastically reduce the number of iterations needed to converge to a local minimum by providing information about the curvature of f.

Example

Consider the function $f = xy^2 - 3z^2$.

Remark

If $\mathbf{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$, then the Hessian is a $m \times n \times n$ tensor.

For instance, $\mathbf{f} = \begin{pmatrix} x^2y + \exp(z) \\ xy^2z - \ln(x) \end{pmatrix}$

Taylor's Theorem

Taylor's theorem has natural generalizations to multivariate and vector functions :

Theorem ((Taylor's theorem))

Suppose $f : \mathbb{R}^d \to \mathbb{R}$ *is continuously differentiable, and let* $\mathbf{h} \in \mathbb{R}^d$*. Then there exists* $t \in [0, 1]$ *such that*

$$f(\mathbf{x} + \mathbf{h}) = f(\mathbf{x}) + \nabla f(\mathbf{x} + t\mathbf{h})\mathbf{h}$$

Furthermore, if f *is twice continuously differentiable, then there exists* $t \in [0, 1]$ *such that*

$$f(\mathbf{x} + \mathbf{h}) = f(\mathbf{x}) + \nabla f(\mathbf{x})\mathbf{h} + \frac{1}{2}\boldsymbol{h}^T\mathbf{H}(\mathbf{x} + t\mathbf{h})\mathbf{h}$$

Example

Consider the function $f(x, y) = x^2 + y^2$. We want to compute $f(\mathbf{x})$ with $\mathbf{x} = (1, 1; 1, 1)^\top$.

Taylor's theorem is used to give approximation of any differentiable function by a polynomial function and particularly linear and quadratic approximation in the neighborhood of a point $\mathbf{x} = \mathbf{x}_0 + \mathbf{h}$. We can thus write

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x_0}) + o(\|\mathbf{x} - \mathbf{x_0}\|)$$

And

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)(\mathbf{x} - \mathbf{x_0}) + \frac{1}{2}(\mathbf{x} - \mathbf{x_0})^\top \mathbf{H}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x_0}) + o(\|\mathbf{x} - \mathbf{x_0}\|^2)$$

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It is also used in proofs about conditions for local minima of unconstrained optimization problems.