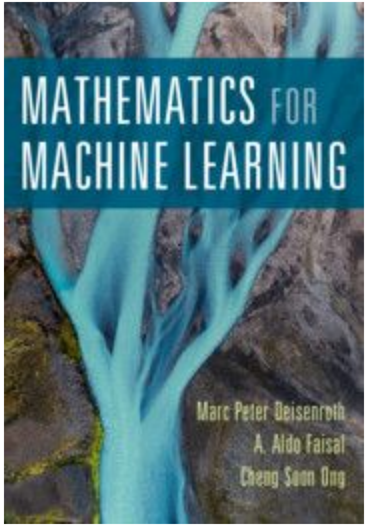

Chapter 5. Vector Calculus

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5.1 Differentiation of Univariate Functions

Definition 5.1 (Difference Quotient). The *difference quotient*

$$\frac{\delta y}{\delta x} := \frac{f(x + \delta x) - f(x)}{\delta x}$$

Derivative:

$$\frac{\mathrm{d}f}{\mathrm{d}x} := \lim_{h \to 0} \frac{f(x + h) - f(x)}{h}$$

Derivative of polynomials

$$\frac{n!}{1!(n-1)!} x^{n-1} = n x^{n-1}$$

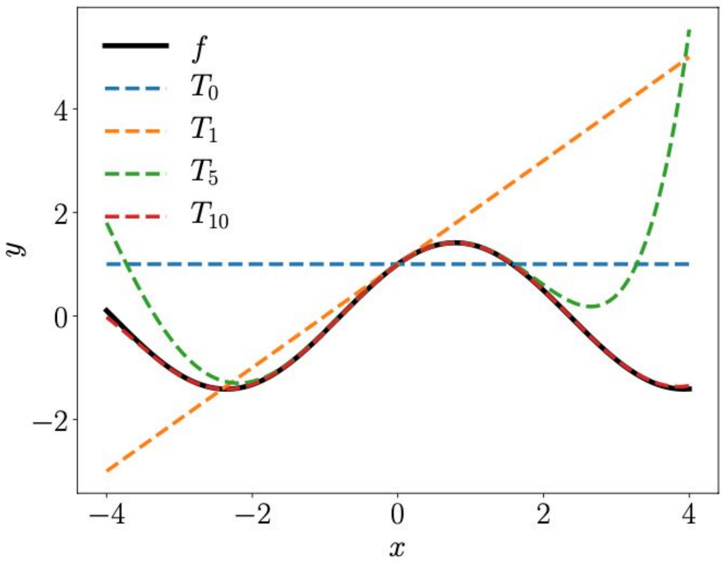
5.1 Differentiation of Univariate Functions

Definition 5.3 (Taylor Polynomial)**.** The *Taylor polynomial* of degree n of $f : \mathbb{R} \to \mathbb{R}$ at x_0 is defined as

$$T_n(x) := \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k \,, \tag{5.7}$$

Maclaurin series is a special case where x = 0

Called “analytic” when it perfectly matches the original function over a given range



5.1 Differentiation of Univariate Functions

Example 5.3 (Taylor Polynomial)
We consider the polynomial

$$f(x) = x^4 \tag{5.9}$$

and seek the Taylor polynomial T_6, evaluated at $x_0 = 1$. We start by computing the coefficients $f^{(k)}(1)$ for $k = 0, \ldots, 6$:

$$f(1) = 1 \tag{5.10}$$
$$f'(1) = 4 \tag{5.11}$$
$$f''(1) = 12 \tag{5.12}$$
$$f^{(3)}(1) = 24 \tag{5.13}$$
$$f^{(4)}(1) = 24 \tag{5.14}$$
$$f^{(5)}(1) = 0 \tag{5.15}$$
$$f^{(6)}(1) = 0 \tag{5.16}$$

Therefore, the desired Taylor polynomial is

$$T_6(x) = \sum_{k=0}^{6} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k \tag{5.17a}$$
$$= 1 + 4(x-1) + 6(x-1)^2 + 4(x-1)^3 + (x-1)^4 + 0\,. \tag{5.17b}$$

Multiplying out and re-arranging yields

$$\begin{aligned} T_6(x) &= (1 - 4 + 6 - 4 + 1) + x(4 - 12 + 12 - 4) \\ &\quad + x^2(6 - 12 + 6) + x^3(4 - 4) + x^4 \end{aligned} \tag{5.18a}$$
$$= x^4 = f(x)\,, \tag{5.18b}$$

i.e., we obtain an exact representation of the original function.

5.1 Differentiation of Univariate Functions

Product rule: $(f(x)g(x))' = f'(x)g(x) + f(x)g'(x)$

Quotient rule: $\left(\dfrac{f(x)}{g(x)}\right)' = \dfrac{f'(x)g(x) - f(x)g'(x)}{(g(x))^2}$

Sum rule: $(f(x) + g(x))' = f'(x) + g'(x)$

Chain rule: $\big(g(f(x))\big)' = (g \circ f)'(x) = g'(f(x))f'(x)$

Example 5.5 (Chain Rule)
Let us compute the derivative of the function $h(x) = (2x+1)^4$ using the chain rule. With

$$h(x) = (2x+1)^4 = g(f(x))\,, \tag{5.33}$$
$$f(x) = 2x + 1\,, \tag{5.34}$$
$$g(f) = f^4\,, \tag{5.35}$$

we obtain the derivatives of f and g as

$$f'(x) = 2\,, \tag{5.36}$$
$$g'(f) = 4f^3\,, \tag{5.37}$$

such that the derivative of h is given as

$$h'(x) = g'(f)f'(x) = (4f^3) \cdot 2 \overset{(5.34)}{=} 4(2x+1)^3 \cdot 2 = 8(2x+1)^3\,, \tag{5.38}$$

where we used the chain rule (5.32) and substituted the definition of f in (5.34) in $g'(f)$.

5.2 Partial Differentiation and Gradients

Definition 5.5 (Partial Derivative)**.** For a function $f : \mathbb{R}^n \to \mathbb{R}$, $\boldsymbol{x} \mapsto f(\boldsymbol{x})$, $\boldsymbol{x} \in \mathbb{R}^n$ of n variables $x_1, \dots, x_n$ we define the *partial derivatives* as

$$\begin{aligned} \frac{\partial f}{\partial x_1} &= \lim_{h \to 0} \frac{f(x_1 + h, x_2, \dots, x_n) - f(\boldsymbol{x})}{h} \\ &\vdots \\ \frac{\partial f}{\partial x_n} &= \lim_{h \to 0} \frac{f(x_1, \dots, x_{n-1}, x_n + h) - f(\boldsymbol{x})}{h} \end{aligned} \tag{5.39}$$

Gradient/Jacobian $\left[\frac{\partial f(\boldsymbol{x})}{\partial x_1} \quad \frac{\partial f(\boldsymbol{x})}{\partial x_2} \quad \cdots \quad \frac{\partial f(\boldsymbol{x})}{\partial x_n} \right]$

5.2 Partial Differentiation and Gradients

- In the multivariable case we end up with vectors and matrices
  - Need to be careful because matrix multiplication is not commutative, order matters
- Similar properties with product, sum, chain rule

Example 5.8

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

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} \tag{5.50a}$$

$$= 2\sin t \frac{\partial \sin t}{\partial t} + 2\frac{\partial \cos t}{\partial t} \tag{5.50b}$$

$$= 2\sin t \cos t - 2\sin t = 2\sin t(\cos t - 1) \tag{5.50c}$$

is the corresponding derivative of f with respect to t.

Can verify correctness with finite difference like we used earlier

5.3 Gradients of Vector-Valued Functions

Example 5.9 (Gradient of a Vector-Valued Function)
We are given

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}\,, \qquad \boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^{M}, \quad \boldsymbol{A} \in \mathbb{R}^{M\times N}, \quad \boldsymbol{x} \in \mathbb{R}^{N}\,.$$

To compute the gradient $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{x}$ we first determine the dimension of $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{x}$: Since $\boldsymbol{f} : \mathbb{R}^{N} \to \mathbb{R}^{M}$, it follows that $\mathrm{d}\boldsymbol{f}/\mathrm{d}\boldsymbol{x} \in \mathbb{R}^{M\times N}$. Second, to compute the gradient we determine the partial derivatives of f with respect to every x_j:

$$f_i(\boldsymbol{x}) = \sum_{j=1}^{N} A_{ij}x_j \implies \frac{\partial f_i}{\partial x_j} = A_{ij} \tag{5.67}$$

We collect the partial derivatives in the Jacobian and obtain the gradient

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MN} \end{bmatrix} = \boldsymbol{A} \in \mathbb{R}^{M\times N}\,. \tag{5.68}$$

5.3 Gradients of Vector-Valued Functions

Example 5.11 (Gradient of a Least-Squares Loss in a Linear Model)
Let us consider the linear model

$$\boldsymbol{y} = \boldsymbol{\Phi\theta}\,, \tag{5.75}$$

where $\boldsymbol{\theta} \in \mathbb{R}^D$ is a parameter vector, $\boldsymbol{\Phi} \in \mathbb{R}^{N \times D}$ are input features and $\boldsymbol{y} \in \mathbb{R}^N$ are the corresponding observations. We define the functions

$$L(\boldsymbol{e}) := \|\boldsymbol{e}\|^2\,, \tag{5.76}$$

$$\boldsymbol{e}(\boldsymbol{\theta}) := \boldsymbol{y} - \boldsymbol{\Phi\theta}\,. \tag{5.77}$$

We seek $\frac{\partial L}{\partial \boldsymbol{\theta}}$, and we will use the chain rule for this purpose. L is called a *least-squares loss* function.

5.4 Gradients of Matrices

- Possible to scale to matrices
  - Gets messy
  - Easiest to define the known shape and then fill everything in

5.5 Useful Identities for Computing Gradients

$$\frac{\partial}{\partial \boldsymbol{X}} \boldsymbol{f}(\boldsymbol{X})^\top = \left(\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right)^\top \tag{5.99}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \mathrm{tr}(\boldsymbol{f}(\boldsymbol{X})) = \mathrm{tr}\left(\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right) \tag{5.100}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \det(\boldsymbol{f}(\boldsymbol{X})) = \det(\boldsymbol{f}(\boldsymbol{X}))\mathrm{tr}\left(\boldsymbol{f}(\boldsymbol{X})^{-1}\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right) \tag{5.101}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \boldsymbol{f}(\boldsymbol{X})^{-1} = -\boldsymbol{f}(\boldsymbol{X})^{-1}\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\boldsymbol{f}(\boldsymbol{X})^{-1} \tag{5.102}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{X}^{-1}\boldsymbol{b}}{\partial \boldsymbol{X}} = -(\boldsymbol{X}^{-1})^\top \boldsymbol{a}\boldsymbol{b}^\top (\boldsymbol{X}^{-1})^\top \tag{5.103}$$

$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{a}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \tag{5.104}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \tag{5.105}$$

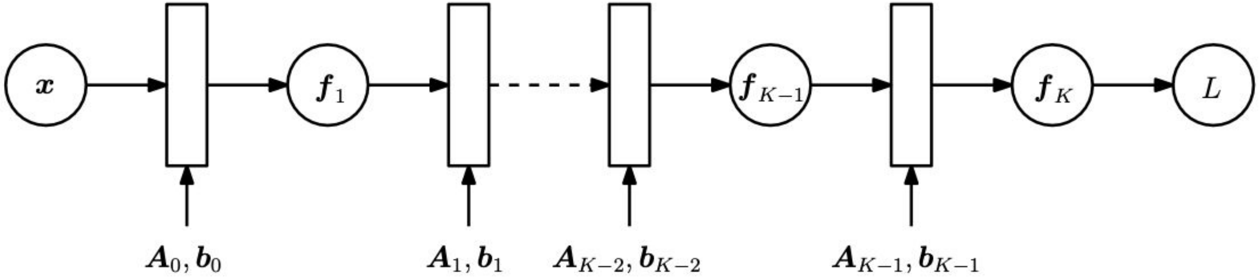
$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{X}\boldsymbol{b}}{\partial \boldsymbol{X}} = \boldsymbol{a}\boldsymbol{b}^\top \tag{5.106}$$

$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{B}\boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{x}^\top(\boldsymbol{B} + \boldsymbol{B}^\top) \tag{5.107}$$

$$\frac{\partial}{\partial \boldsymbol{s}}(\boldsymbol{x} - \boldsymbol{A}\boldsymbol{s})^\top \boldsymbol{W}(\boldsymbol{x} - \boldsymbol{A}\boldsymbol{s}) = -2(\boldsymbol{x} - \boldsymbol{A}\boldsymbol{s})^\top \boldsymbol{W}\boldsymbol{A} \quad \text{for symmetric } \boldsymbol{W} \tag{5.108}$$

5.6 Backpropagation and Automatic Differentiation

- Writing out the full gradient formula is often impractical
  - Can become much more expensive than just running the function
- Backpropagation
  - Chain rule, each layer is a function
- Special case of automatic differentiation
- Can go in both directions, forward and backward



5.7 Higher-Order Derivatives

- We can go beyond first order derivatives, but becomes expensive quickly
- Hessian - collection of all second-order partial derivatives

5.8 Linearization and Multivariate Taylor Series

- It is possible to use multivariate taylor series that is locally accurate
- Computing n-th order partial derivative gets messy quickly

Example 5.15 (Taylor Series Expansion of a Function with Two Variables)
Consider the function

$$f(x, y) = x^2 + 2xy + y^3 \,. \tag{5.161}$$