Mathematics for Machine Learning
— Vector Calculus
Linearization & Multivariate Taylor Series

Joseph Chuang-Chieh Lin

Department of Computer Science & Engineering,
National Taiwan Ocean University

Fall 2025

Credits for the resource

- The slides are based on the textbooks:
  - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
  Francesco Orabona: A Modern Introduction to Online Learning. https://arxiv.org/abs/1912.13213

Linear Approximation of a Function

The gradient ∇f of a function f can be used for locally linear approximation of f around $\mathbf{x}_0$:

$$f(\mathbf{x}) \approx f(\mathbf{x_0}) + (\nabla_{\mathbf{x}} f)(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0)$$

- $(\nabla_{\mathbf{x}} f)(\mathbf{x}_0)$: the gradient of f w.r.t. $\mathbf{x}$ evaluated at $\mathbf{x}_0$.

Multivariate Taylor Series

Multivariate Taylor Series

Consider a function $f : \mathbb{R}^D \to \mathbb{R}$ which is smooth (i.e., infinitely differentiable) at $\mathbf{x}_0$.

Define the difference vector $\boldsymbol{\delta} := \mathbf{x} - \mathbf{x}_0$.

The multivariate Taylor series of f at $\mathbf{x_0}$ is

$$f(\mathbf{x}) = \sum_{k=0}^{\infty} \frac{D_{\mathbf{x}}^k f(\mathbf{x}_0)}{k!} \boldsymbol{\delta}^k,$$

where $D_{\mathbf{x}}^k f(\mathbf{x}_0)$ is the kth derivative of f w.r.t. $\mathbf{x}$ evaluated at $\mathbf{x}_0$.

Multivariate Taylor Polynomial

Multivariate Taylor Polynomial

The Taylor polynomial of degree n of f at $\mathbf{x_0}$ is

$$T_n(\mathbf{x}) = \sum_{k=0}^{n} \frac{D_{\mathbf{x}}^k f(\mathbf{x}_0)}{k!} \boldsymbol{\delta}^k,$$

where $D_{\mathbf{x}}^k f(\mathbf{x}_0)$ is the kth derivative of f w.r.t. $\mathbf{x}$ evaluated at $\mathbf{x}_0$.

- It contains the first $n+1$ components of the Taylor series.

Notice

- $\boldsymbol{\delta}^k$ is undefined for $\mathbf{x} \in \mathbb{R}^D$, $D > 1$ and $k > 1$.

Notice

- $\boldsymbol{\delta}^k$ is undefined for $\mathbf{x} \in \mathbb{R}^D$, $D > 1$ and $k > 1$.
- $D_{\mathbf{x}}^k$ and $\boldsymbol{\delta}^k$ are kth order tensors (i.e., k-dimensional arrays).

Notice

- $\boldsymbol{\delta}^k$ is undefined for $\mathbf{x} \in \mathbb{R}^D$, $D > 1$ and $k > 1$.
- $D_{\mathbf{x}}^k$ and $\boldsymbol{\delta}^k$ are kth order tensors (i.e., k-dimensional arrays).
- $\boldsymbol{\delta}^k \in \mathbb{R}^{\overbrace{D \times D \times \cdots \times D}^{k \text{ times}}}$.

Notice

- $\boldsymbol{\delta}^k$ is undefined for $\mathbf{x} \in \mathbb{R}^D$, $D > 1$ and $k > 1$.
- $D_{\mathbf{x}}^k$ and $\boldsymbol{\delta}^k$ are kth order tensors (i.e., k-dimensional arrays).
- $\boldsymbol{\delta}^k \in \mathbb{R}^{\overbrace{D \times D \times \cdots \times D}^{k \text{ times}}}$.
  - $\boldsymbol{\delta}^2 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\top$.
    - $\boldsymbol{\delta}^2[i,j] = \delta[i]\delta[j]$.
  - $\boldsymbol{\delta}^3 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta}$.
    - $\boldsymbol{\delta}^3[i,j,k] = \delta[i]\delta[j]\delta[k]$.

Notice

- $\boldsymbol{\delta}^k$ is undefined for $\mathbf{x} \in \mathbb{R}^D$, $D > 1$ and $k > 1$.
- $D_{\mathbf{x}}^k$ and $\boldsymbol{\delta}^k$ are kth order tensors (i.e., k-dimensional arrays).
- $\boldsymbol{\delta}^k \in \mathbb{R}^{\overbrace{D \times D \times \cdots \times D}^{k \text{ times}}}$.
    - $\boldsymbol{\delta}^2 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\top$.
        - $\boldsymbol{\delta}^2[i, j] = \delta[i]\delta[j]$.
    - $\boldsymbol{\delta}^3 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta}$.
        - $\boldsymbol{\delta}^3[i, j, k] = \delta[i]\delta[j]\delta[k]$.
- Hence,

$$D_{\mathbf{x}}^k f(\mathbf{x}_0)\boldsymbol{\delta}^k = \sum_{i_1=1}^{D} \cdots \sum_{i_k=1}^{D} D_{\mathbf{x}}^k f(\mathbf{x}_0)[i_1, \ldots, i_k]\delta[i_1] \cdots \delta[i_k].$$

Note & Exercise

Exercise

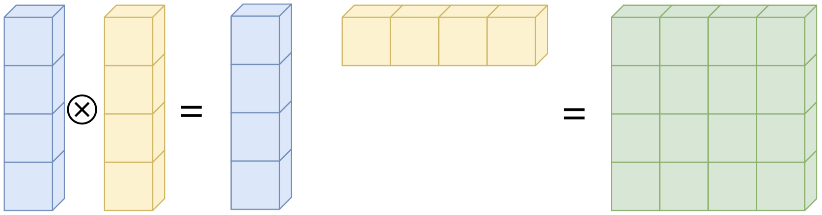
Suppose $\mathbf{x} = (x_1, x_2)$. Show that

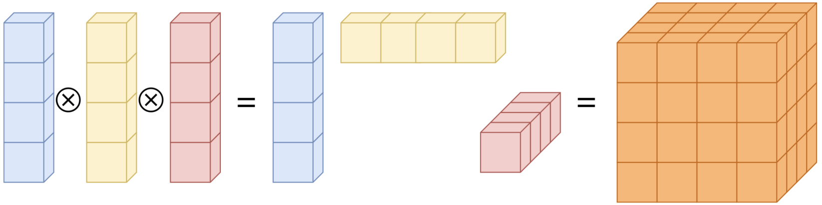
$$D_{\mathbf{x}}^2 f(\mathbf{x}_0)\boldsymbol{\delta}^2 = \boldsymbol{\delta}^\top \boldsymbol{H}(\mathbf{x}_0)\boldsymbol{\delta},$$

where

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \, \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \, \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}.$$

δ^2 & δ^3





Example (1/3)

Example

Consider the function $f(x, y) = x^2 + 2xy + y^3$ and $(x_0, y_0) = (1, 2)$.

- Note: f is a polynomial of degree 3.

$$f(1, 2) = 13, \quad \boldsymbol{\delta} = [x - 1,\ y - 2]^\top.$$
$$\frac{\partial f}{\partial x} = 2x + 2y \Longrightarrow \frac{\partial f}{\partial x}(1, 2) = 6.$$
$$\frac{\partial f}{\partial y} = 2x + 3y^2 \Longrightarrow \frac{\partial f}{\partial y}(1, 2) = 14.$$

Example (1/3)

Example

Consider the function $f(x, y) = x^2 + 2xy + y^3$ and $(x_0, y_0) = (1, 2)$.

- Note: f is a polynomial of degree 3.

$$f(1,2) = 13, \quad \boldsymbol{\delta} = [x - 1,\ y - 2]^\top.$$
$$\frac{\partial f}{\partial x} = 2x + 2y \Longrightarrow \frac{\partial f}{\partial x}(1,2) = 6.$$
$$\frac{\partial f}{\partial y} = 2x + 3y^2 \Longrightarrow \frac{\partial f}{\partial y}(1,2) = 14.$$

$$\therefore D^1_{x,y} f(1,2) = \nabla_{x,y} f(1,2) = \begin{bmatrix} \frac{\partial f}{\partial x}(1,2) & \frac{\partial f}{\partial y}(1,2) \end{bmatrix} = [6 \quad 14] \in \mathbb{R}^{1\times 2}.$$

Example (1/3)

Example

Consider the function $f(x, y) = x^2 + 2xy + y^3$ and $(x_0, y_0) = (1, 2)$.

- Note: f is a polynomial of degree 3.

$$
\begin{aligned}
f(1,2) = 13, \quad \boldsymbol{\delta} = [x-1,\ y-2]^\top. \\
\frac{\partial f}{\partial x} = 2x + 2y \Longrightarrow \frac{\partial f}{\partial x}(1,2) = 6. \\
\frac{\partial f}{\partial y} = 2x + 3y^2 \Longrightarrow \frac{\partial f}{\partial y}(1,2) = 14.
\end{aligned}
$$

$$
\therefore D^1_{x,y} f(1,2) = \nabla_{x,y} f(1,2) = \left[\frac{\partial f}{\partial x}(1,2) \quad \frac{\partial f}{\partial y}(1,2) \right] = [6 \quad 14] \in \mathbb{R}^{1\times 2}.
$$

$$
\Longrightarrow \frac{D^1_{x,y} f(1,2)}{1!} \boldsymbol{\delta} = [6 \quad 14] \begin{bmatrix} x-1 \\ y-2 \end{bmatrix} = 6(x-1) + 14(y-2).
$$

Example (2/3)

Example

$$\frac{\partial^2 f}{\partial x^2} = 2 \implies \frac{\partial^2 f}{\partial x^2}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial y^2} = 6y \implies \frac{\partial^2 f}{\partial y^2}(1,2) = 12$$

$$\frac{\partial^2 f}{\partial y\,\partial x} = 2 \implies \frac{\partial^2 f}{\partial y\,\partial x}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial x\,\partial y} = 2 \implies \frac{\partial^2 f}{\partial x\,\partial y}(1,2) = 2$$

Example (2/3)

Example

$$\frac{\partial^2 f}{\partial x^2} = 2 \implies \frac{\partial^2 f}{\partial x^2}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial y^2} = 6y \implies \frac{\partial^2 f}{\partial y^2}(1,2) = 12$$

$$\frac{\partial^2 f}{\partial y\, \partial x} = 2 \implies \frac{\partial^2 f}{\partial y\, \partial x}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial x\, \partial y} = 2 \implies \frac{\partial^2 f}{\partial x\, \partial y}(1,2) = 2$$

Hessian:

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x\, \partial y} \\ \frac{\partial^2 f}{\partial y\, \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 6y \end{bmatrix}$$

Example (2/3)

Example

$$\frac{\partial^2 f}{\partial x^2} = 2 \implies \frac{\partial^2 f}{\partial x^2}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial y^2} = 6y \implies \frac{\partial^2 f}{\partial y^2}(1,2) = 12$$

$$\frac{\partial^2 f}{\partial y\,\partial x} = 2 \implies \frac{\partial^2 f}{\partial y\,\partial x}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial x\,\partial y} = 2 \implies \frac{\partial^2 f}{\partial x\,\partial y}(1,2) = 2$$

Hessian:

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x\,\partial y} \\ \frac{\partial^2 f}{\partial y\,\partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 6y \end{bmatrix}$$

$$\Rightarrow \boldsymbol{H}(1,2) = \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \in \mathbb{R}^{2\times 2}.$$

Example (2/3)

Example

$$\frac{\partial^2 f}{\partial x^2} = 2 \implies \frac{\partial^2 f}{\partial x^2}(1,2) = 2$$
$$\frac{\partial^2 f}{\partial y^2} = 6y \implies \frac{\partial^2 f}{\partial y^2}(1,2) = 12$$
$$\frac{\partial^2 f}{\partial y\,\partial x} = 2 \implies \frac{\partial^2 f}{\partial y\,\partial x}(1,2) = 2$$
$$\frac{\partial^2 f}{\partial x\,\partial y} = 2 \implies \frac{\partial^2 f}{\partial x\,\partial y}(1,2) = 2$$

Hessian:

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x\,\partial y} \\ \frac{\partial^2 f}{\partial y\,\partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 6y \end{bmatrix}$$

$$\Rightarrow \boldsymbol{H}(1,2) = \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \in \mathbb{R}^{2\times 2}.$$

$$\begin{aligned} \frac{D^2_{x,y} f(1,2)}{2!}\boldsymbol{\delta}^2 &= \frac{1}{2}\boldsymbol{\delta}^\top \boldsymbol{H}(1,2)\boldsymbol{\delta} \\ &= \cdots \end{aligned}$$

Example (2/3)

Example

$$\frac{\partial^2 f}{\partial x^2} = 2 \implies \frac{\partial^2 f}{\partial x^2}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial y^2} = 6y \implies \frac{\partial^2 f}{\partial y^2}(1,2) = 12$$

$$\frac{\partial^2 f}{\partial y\,\partial x} = 2 \implies \frac{\partial^2 f}{\partial y\,\partial x}(1,2) = 2$$

$$\frac{\partial^2 f}{\partial x\,\partial y} = 2 \implies \frac{\partial^2 f}{\partial x\,\partial y}(1,2) = 2$$

Hessian:

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x\,\partial y} \\ \frac{\partial^2 f}{\partial y\,\partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 6y \end{bmatrix}$$

$$\Rightarrow \boldsymbol{H}(1,2) = \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \in \mathbb{R}^{2\times 2}.$$

$$\begin{aligned} \frac{D^2_{x,y} f(1,2)}{2!}\boldsymbol{\delta}^2 &= \frac{1}{2}\boldsymbol{\delta}^\top \boldsymbol{H}(1,2)\boldsymbol{\delta} \\ &= \cdots = (x-1)^2 + 2(x-1)(y-2) + 6(y-2)^2. \end{aligned}$$

Example (3/3)

Now, compute

$$D^3_{x,y} f =$$

Example (3/3)

Now, compute

$$D^3_{x,y} f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times 2\times 2}$$

Example (3/3)

Now, compute

$$D^3_{x,y} f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times2\times2}$$

$$\frac{\partial \boldsymbol{H}}{\partial x} = \begin{bmatrix} \frac{\partial^3 f}{\partial x^3} & \frac{\partial^3 f}{\partial x^2 \partial y} \\ \frac{\partial^3 f}{\partial x \partial y \partial x} & \frac{\partial^3 f}{\partial x \partial y^2} \end{bmatrix}, \quad \frac{\partial \boldsymbol{H}}{\partial y} = \begin{bmatrix} \frac{\partial^3 f}{\partial y \partial x^2} & \frac{\partial^3 f}{\partial y \partial x \partial y} \\ \frac{\partial^3 f}{\partial y^2 \partial x} & \frac{\partial^3 f}{\partial y^3} \end{bmatrix}$$

Example (3/3)

Now, compute

$$D^3_{x,y} f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times 2\times 2}$$

$$\frac{\partial \boldsymbol{H}}{\partial x} = \begin{bmatrix} \frac{\partial^3 f}{\partial x^3} & \frac{\partial^3 f}{\partial x^2 \, \partial y} \\ \frac{\partial^3 f}{\partial x \, \partial y \, \partial x} & \frac{\partial^3 f}{\partial x \, \partial y^2} \end{bmatrix}, \quad \frac{\partial \boldsymbol{H}}{\partial y} = \begin{bmatrix} \frac{\partial^3 f}{\partial y \, \partial x^2} & \frac{\partial^3 f}{\partial y \, \partial x \, \partial y} \\ \frac{\partial^3 f}{\partial y^2 \, \partial x} & \frac{\partial^3 f}{\partial y^3} \end{bmatrix}$$

We only need to compute $\frac{\partial^3 f}{\partial y^3} = 6 \implies \frac{\partial^3 f}{\partial y^3}(1, 2) = 6.$

Example (3/3)

Now, compute

$$D^3_{x,y} f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times 2\times 2}$$

$$\frac{\partial \boldsymbol{H}}{\partial x} = \begin{bmatrix} \frac{\partial^3 f}{\partial x^3} & \frac{\partial^3 f}{\partial x^2 \partial y} \\ \frac{\partial^3 f}{\partial x \partial y \partial x} & \frac{\partial^3 f}{\partial x \partial y^2} \end{bmatrix}, \quad \frac{\partial \boldsymbol{H}}{\partial y} = \begin{bmatrix} \frac{\partial^3 f}{\partial y \partial x^2} & \frac{\partial^3 f}{\partial y \partial x \partial y} \\ \frac{\partial^3 f}{\partial y^2 \partial x} & \frac{\partial^3 f}{\partial y^3} \end{bmatrix}$$

We only need to compute $\frac{\partial^3 f}{\partial y^3} = 6 \implies \frac{\partial^3 f}{\partial y^3}(1,2) = 6.$

$$\frac{D^3_{x,y} f(1,2)}{3!} \boldsymbol{\delta}^3 = (y-2)^3.$$

Example (3/3)

Now, compute

$$D^3_{x,y} f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times 2\times 2}$$

$$\frac{\partial \boldsymbol{H}}{\partial x} = \begin{bmatrix} \frac{\partial^3 f}{\partial x^3} & \frac{\partial^3 f}{\partial x^2\,\partial y} \\ \frac{\partial^3 f}{\partial x\,\partial y\,\partial x} & \frac{\partial^3 f}{\partial x\,\partial y^2} \end{bmatrix}, \quad \frac{\partial \boldsymbol{H}}{\partial y} = \begin{bmatrix} \frac{\partial^3 f}{\partial y\,\partial x^2} & \frac{\partial^3 f}{\partial y\,\partial x\,\partial y} \\ \frac{\partial^3 f}{\partial y^2\,\partial x} & \frac{\partial^3 f}{\partial y^3} \end{bmatrix}$$

We only need to compute $\frac{\partial^3 f}{\partial y^3} = 6 \implies \frac{\partial^3 f}{\partial y^3}(1,2) = 6.$

$$\frac{D^3_{x,y} f(1,2)}{3!}\boldsymbol{\delta}^3 = (y-2)^3.$$

Check if $f(x) = f(1,2) + D^1_{x,y} f(1,2)\boldsymbol{\delta} + \frac{D^2_{x,y} f(1,2)}{2!}\boldsymbol{\delta}^2 + \frac{D^3_{x,y} f(1,2)}{3!}\boldsymbol{\delta}^3.$

Discussions