

Mathematics for Machine Learning

— Vector Calculus: Linearization & Multivariate Taylor Series

Joseph Chuang-Chieh Lin

Department of Computer Science & Engineering,
National Taiwan Ocean University

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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 $f : \mathbb{R}^D \mapsto \mathbb{R}$ 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 k th derivative of f w.r.t. \mathbf{x} evaluated at \mathbf{x}_0 .

Multivariate Taylor Polynomial

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The **Taylor polynomial** of **degree n** of f at \mathbf{x}_0 is

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

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

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

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- $\delta^k \in \mathbb{R}^{\overbrace{D \times D \times \cdots \times D}^{k \text{ times}}}$.
 - $\delta^2 := \delta \otimes \delta = \delta \delta^\top$.
 - $\delta^2[i, j] = \delta[i] \delta[j]$.
 - $\delta^3 := \delta \otimes \delta \otimes \delta$.
 - $\delta^3[i, j, k] = \delta[i] \delta[j] \delta[k]$.

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- Hence,

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

Note & Exercise

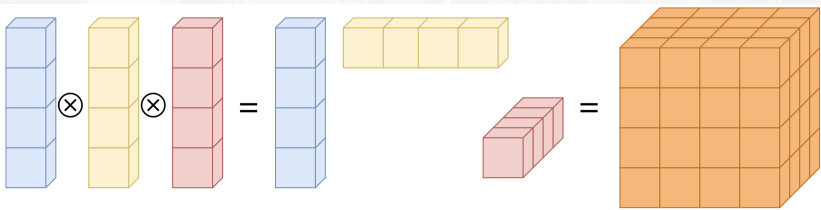
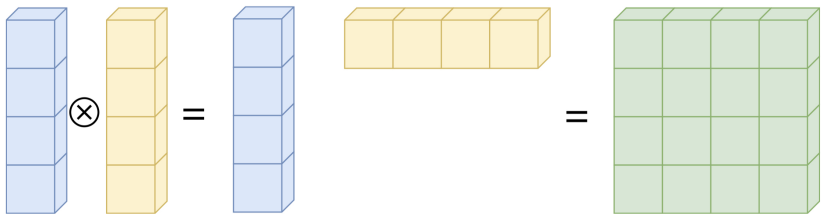
Exercise

Show that

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

where

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

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.

$$f(1, 2) = 13, \quad \delta = [x - 1, y - 2]^T.$$

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

$$\frac{\partial f}{\partial y} = 2x + 3y^2 \implies \frac{\partial f}{\partial y}(1, 2) = 14.$$

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

Example (2/3)

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

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

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$$\begin{aligned} \frac{D_{x,y}^2 f(1, 2)}{2!} \delta^2 &= \frac{1}{2} \delta^\top \mathbf{H}(1, 2) \delta \\ &= \dots = (x-1)^2 + 2(x-1)(y-2) + 6(y-2)^2. \end{aligned}$$

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

Discussions