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

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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 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

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

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

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- $\boldsymbol{\delta}^k \in \mathbb{R}^{\overbrace{D \times D \times \cdots \times D}^{k \text{ times}}}$.

  - $\boldsymbol{\delta}^2 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\top$.
    - $\boldsymbol{\delta}^2[i, j] = \delta[i]\delta[j]$.

  - $\boldsymbol{\delta}^3 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta}$.
    - $\boldsymbol{\delta}^3[i, j, k] = \delta[i]\delta[j]\delta[k]$.

Notice

- δ^k is not defined for $\mathbf{x} \in \mathbb{R}^D$, $D > 1$ and $k > 1$.

- $D_{\mathbf{x}}^k$ and δ^k are kth order tensors (i.e., k-dimensional arrays).

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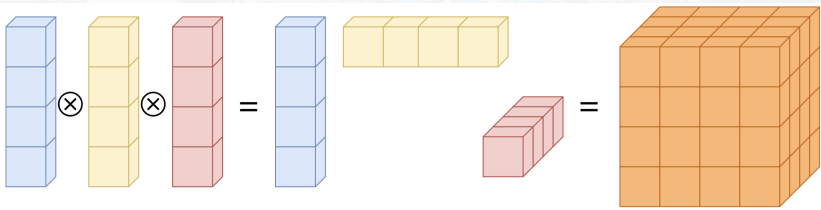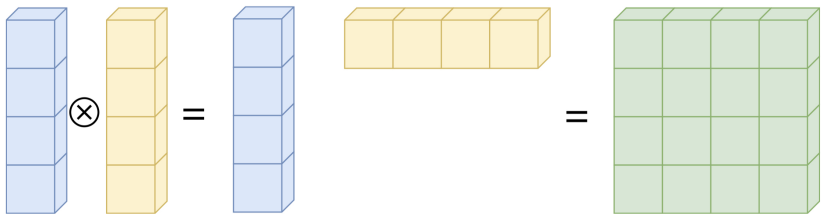
Note & Exercise

Exercise

Show that

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

where

$$\boldsymbol{H} = \left[\begin{array}{cc} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \, \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \, \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{array} \right].$$

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.

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

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

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

Example (2/3)

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

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

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

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

Example (3/3)

Now, compute

$$D_{x,y}^3 f =$$

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

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

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

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

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

Discussions