

Matrix Differentiation

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Derivatives are easy!

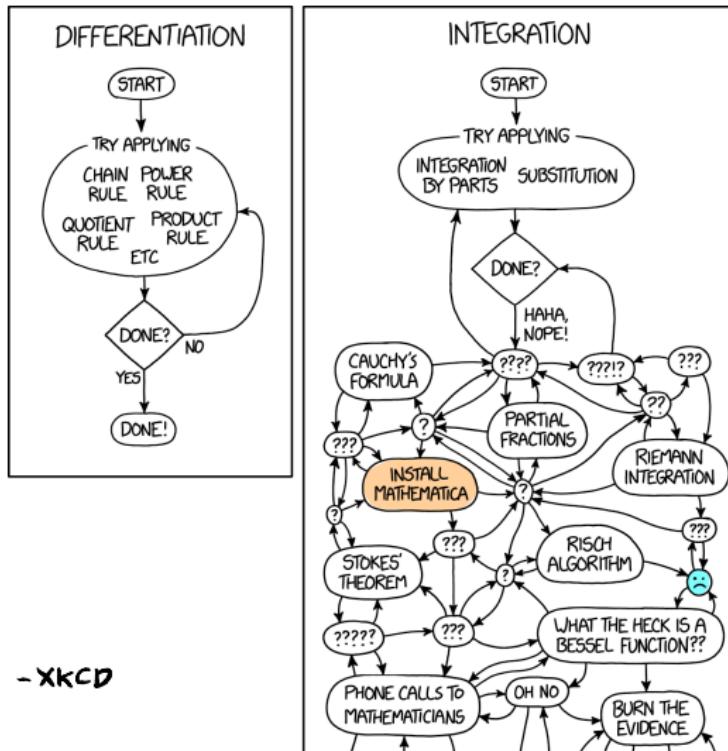


Figure: XKCD: differentiation and integration

What do we want?

In machine learning and many other studies, we often want to optimize functions:

$$\min_x f(x).$$

We know that **extremas** (max,min,saddle points) occur at places with zero derivatives:

$$\frac{df(x)}{dx} \Big|_{x^*} = 0,$$

whether it is a minima or not can be determined by a second order derivative test:

$$\frac{d^2f(x)}{dx^2} \Big|_{x^*} > 0.$$

We denote the point of minima as:

$$x^* = \arg \min_x f(x).$$

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$$\min_{A \in \mathbb{R}^{m \times n}} f(A) \text{ or } \min_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x}),$$

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how do we find the **derivative of a matrix function**? I.e., how do we justify the notation of:

$$\frac{df(A)}{dA} = 0 \text{ or } \frac{df(x)}{dx}?$$

A glimpse of what is to come

So... what kind of functions will we encounter? A prime example is the **squared error**:

$$\mathcal{E} = \|X\mathbf{w} - \mathbf{y}\|^2,$$

where $X \in \mathbb{R}^{m \times n}$, $\mathbf{w} \in \mathbb{R}^n$, $\mathbf{y} \in \mathbb{R}^m$. We would like to find a \mathbf{w} that *best estimates* \mathbf{y} by the approximation:

$$\hat{\mathbf{y}} = X\mathbf{w}.$$

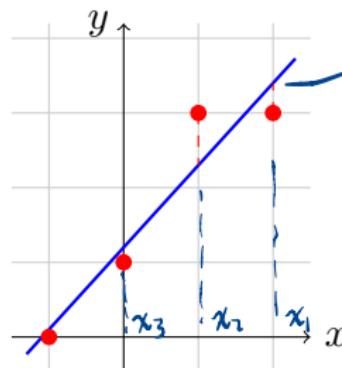
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$$\hat{\mathbf{y}} = a_0 + a_1 x$$

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} a_0 + a_1 x_1 \\ a_0 + a_1 x_2 \\ a_0 + a_1 x_3 \end{bmatrix}$$

$$X = [1, x]$$

$$\mathbf{w} = [a_0, a_1]^\top$$

$$\hat{\mathbf{y}} = a_0 + a_1 x$$

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$$f = \mathbf{x}^T A \mathbf{x}, \det(A), \text{tr}(A), \lambda(A), \dots.$$

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Def. (Transpose)

Flip the matrix along its diagonal:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix}^T = \begin{bmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \\ a_{13} & a_{23} \end{bmatrix}. \quad (1)$$

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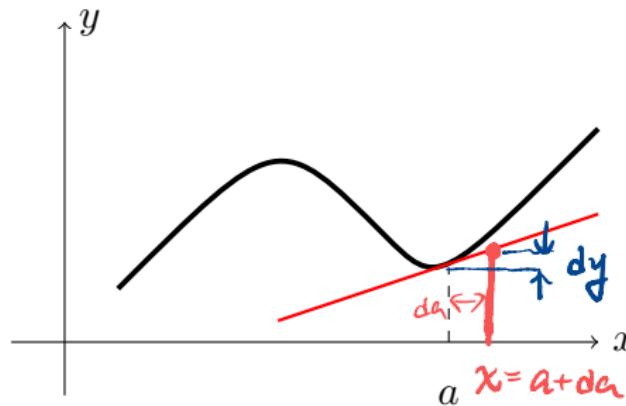
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- 2 Matrix Differentiation
- 3 Examples
- 4 Derivatives of “Matrix Derivatives”

What is a derivative?

Derivatives are linearizations. Consider the easiest case below.



We know that the first order approximation will be

$$y(x) = \frac{dy}{dx} \Big|_a (x - a) + y(a).$$

What is a derivative?

We can rewrite the previous equation into the form below:

$$y(a + dx) = \frac{dy}{dx} \Big|_a dx + y(a)$$

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Thus obtaining:

$$dy = \left(\frac{dy}{dx} \right) dx \quad (2)$$

We don't need to "divide" the dx over to the other side. The equation above works for matrices too.

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Prop. (Derivatives as Linear Approximation)

For $y = f(x)$,

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The above definition holds for x and y being scalars, vectors or matrices so long as the dimensions are compatible.

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e.g.

$$\mathbf{f}(\mathbf{x}) = A\mathbf{x}, \quad A \in \mathbb{R}^{m \times n}, \quad \mathbf{x} \in \mathbb{R}^{n \times 1}$$

矩阵 向量

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$$\frac{d\mathbf{f}}{dx} = A \quad \frac{d(ax)}{dx} = a, \quad \frac{d(ax^2)}{dx} = 2ax$$

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$$\frac{d\mathbf{f}}{dA} \stackrel{?}{=} \mathbf{x}$$

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All works as long as it is linear:

$$\underline{dy} = \mathcal{L}\{\underline{adx_1 + dx_2}\} = \underline{a\mathcal{L}\{dx_1\}} + \underline{\mathcal{L}\{dx_2\}}.$$

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Prop. (Derivatives as Linear Operators (Fréchet derivative))

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Where $\mathcal{L}\{\cdot\}$ is a linear operator, denoting the notion of a derivative.

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Let us see some examples of functions where the representation of

$$\mathcal{L}\{\cdot\} = A(\cdot)$$

holds, where A is matrix.

Differentiate by Vectors

(1) Differentiate scalar function f by vector x :

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Given a function $f(x) = f(x_1, \dots, x_n)$ with

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = [x_1 \quad \cdots \quad x_n]^T \in \mathbb{R}^{n \times 1},$$

we know from calculus that its **infinitesimal** change is:

$$df = \frac{df}{dx_i} dx_i \quad df = \frac{\partial f}{\partial x_1} dx_1 + \cdots + \frac{\partial f}{\partial x_n} dx_n. \quad \text{全微分} \quad (4)$$

But this is just the dot product of ∇f and dx !

$$\text{內積 } \vec{a} \cdot \vec{b} = a_1 b_1 + \cdots + a_n b_n$$

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is just the dot product of ∇f and $d\mathbf{x}$:

$$df = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix} \begin{bmatrix} dx_1 \\ \vdots \\ dx_n \end{bmatrix} = (\nabla f)^T d\mathbf{x}.$$

Where the **gradient** $\overset{\text{nabla}}{\nabla f}$ is defined as a column vector.

梯度

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Where the **gradient** ∇f is defined as a column vector. Compare with

$$df = \boxed{\frac{df}{d\mathbf{x}}} d\mathbf{x}. \\ = (\nabla f)^T$$

Differentiate by Vectors

For $f = f(\mathbf{x})$, if we define

$$df = \frac{df}{d\mathbf{x}} d\mathbf{x},$$

then

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \dots & \frac{\partial f}{\partial x_n} \end{bmatrix} = (\nabla f)^\top.$$

Differentiate by Vectors

For $f = f(\mathbf{x})$, if we define

$$df = \frac{df}{d\mathbf{x}} d\mathbf{x}, \quad = [-\nabla f^T] \begin{bmatrix} d\mathbf{x} \\ 1 \end{bmatrix}$$

then

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \dots & \frac{\partial f}{\partial x_n} \end{bmatrix} = (\nabla f)^T.$$

But if we define

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Notice that:

$$\begin{aligned} 1 \times n &\rightarrow \frac{df}{dx} \leftarrow 1 \times 1 \\ &\quad \text{---} \\ n \times 1 &\rightarrow \frac{df}{dx^T} \leftarrow 1 \times n \end{aligned}$$

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Perhaps we could define the derivative as:

$$\underbrace{\frac{df}{dA}}_{m \times n} = \underbrace{\frac{df}{dA}}_{m \times s} \underbrace{\frac{dA}{s \times n}}_{s \times n} \text{ or } \underbrace{\frac{dB}{dB}}_{m \times s} \underbrace{\frac{df}{dB}}_{s \times n}.$$

$$\underbrace{\frac{df}{dA}}_{m \times n} = \underbrace{M_1}_{m \times p} \underbrace{\frac{dA}{P \times Q}}_{P \times Q} \underbrace{M_2}_{Q \times n}$$

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If x is a column vector and f is of the form:

$$f = \begin{bmatrix} f_1(x) \\ \vdots \\ f_m(x) \end{bmatrix},$$

$$\underset{m \times n}{\overbrace{\frac{df}{dx}}} \leftarrow m \times 1 \quad , \quad \underset{m \times 1}{\overbrace{df}} = \underset{m \times n}{\overbrace{\left(\frac{df}{dx} \right)}} \underset{n \times 1}{\overbrace{dx}}$$

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then we have:

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{x}} \\ \vdots \\ \frac{\partial f_m}{\partial \mathbf{x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix},$$

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Remark: the notations $\frac{df}{dx}$ and $\frac{\partial f}{\partial x}$ are used interchangeably.

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- ① Gradient (transpose):

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$\left(\frac{\partial f}{\partial \mathbf{x}} \right)^T$

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e.g. $f(\mathbf{x}) = f(x_1, x_2) = x_1^2 x_2$

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 x_2 \\ x_1^2 \end{bmatrix}$$

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Some terms to introduce: for a scalar function f and position vector $\mathbf{x} = [x_1, \dots, x_n]^\top$,

③ Hessian:

海森矩阵

$$\mathsf{H}(f) := \nabla(\nabla^\top f) = \frac{\partial^2 f}{\partial \mathbf{x}^\top \partial \mathbf{x}} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix} \quad (6)$$

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Some terms to introduce: for a scalar function f and position vector $\mathbf{x} = [x_1, \dots, x_n]^T$,

③ Hessian:

$$\mathsf{H}(f) := \nabla \nabla^T f = \frac{\partial^2 f}{\partial \mathbf{x}^T \partial \mathbf{x}} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix} \quad (6)$$

e.g. $f(\mathbf{x}) = f(x_1, x_2) = x_1^2 x_2$

$$\nabla f = \begin{bmatrix} 2x_1 x_2 \\ x_1^2 \end{bmatrix}, \quad \frac{\partial^2 f}{\partial \mathbf{x}^T \partial \mathbf{x}} = \begin{bmatrix} 2x_2 & 2x_1 \\ 2x_1 & 0 \end{bmatrix}$$

對稱

Differentiate by Vectors

For a vector function $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), \dots, y_n(\mathbf{x})]^T$ and position vector $\mathbf{x} = [x_1, \dots, x_n]^T$,

Differentiate by Vectors

For a vector function $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), \dots, y_m(\mathbf{x})]^T$ and position vector $\mathbf{x} = [x_1, \dots, x_n]^T$,

③ Jacobian:

雅可比

$$J := \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial \mathbf{x}} \\ \vdots \\ \frac{\partial y_m}{\partial \mathbf{x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}, \quad (7)$$

Differentiate by Vectors

For a vector function $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), \dots, y_n(\mathbf{x})]^T$ and position vector $\mathbf{x} = [x_1, \dots, x_n]^T$,

③ Jacobian:

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The Jacobian is useful in coordinate transformations, like the change of variables in integration.

雅可比行列式

$$\int \cdots \int_{\mathbf{y}(\mathcal{X})} f(\mathbf{y}) dy_1 \cdots dy_n = \int \cdots \int_{\mathcal{X}} f(\mathbf{y}(\mathbf{x})) |J| dx_1 \cdots dx_n.$$

$$\int f(y) dy = \int f(y(x)) \left| \frac{dy}{dx} \right| dx$$

Differentiate by Matrices

(3) Differentiate function $f(A)$ by a matrix $A \in \mathbb{R}^{m \times n}$:

$$df = f(A + dA) - f(A)$$

Some examples are as follows:

① $f(A) = Ax$

$$df = (dA)x$$

② $f(A) = \underline{\underline{A}}^T \underline{\underline{A}}$
 $\text{n} \times \text{m}$ $\text{m} \times \text{n}$

$$df = (A + dA)^T (A + dA) - A^T A = (dA)^T A + A^T dA$$

Differentiate by Matrices

For:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \textcolor{red}{a_{31}} & a_{32} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}_{m \times n}, \quad dA = \begin{bmatrix} da_{11} & da_{12} & \cdots \\ da_{21} & da_{22} & \cdots \\ \vdots & \vdots & \ddots \\ da_{m1} & da_{m2} & \cdots \end{bmatrix}_{m \times n}$$

we have that if f is a scalar function:

$$\cancel{df} \neq \frac{\partial f}{\partial A} dA \quad \frac{\partial f}{\partial A} = \begin{bmatrix} \frac{\partial f}{\partial a_{11}} & \frac{\partial f}{\partial a_{21}} & \frac{\partial f}{\partial \textcolor{red}{a_{31}}} & \cdots & \frac{\partial f}{\partial a_{m1}} \\ \frac{\partial f}{\partial a_{12}} & \frac{\partial f}{\partial a_{22}} & \frac{\partial f}{\partial a_{32}} & \cdots & \frac{\partial f}{\partial a_{m2}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial f}{\partial a_{1n}} & \frac{\partial f}{\partial a_{2n}} & \frac{\partial f}{\partial a_{3n}} & \cdots & \frac{\partial f}{\partial a_{mn}} \end{bmatrix}_{n \times m} \quad (8)$$

$$\underline{df} = \frac{\partial f}{\partial a_{11}} da_{11} + \frac{\partial f}{\partial a_{12}} da_{12} + \dots \\ \text{+ } \dots + \frac{\partial f}{\partial a_{mn}} da_{mn} = \mathcal{L} \left\{ \begin{bmatrix} da_{11} & da_{12} & \dots \\ da_{21} & da_{22} & \dots \\ \vdots & \vdots & \ddots \\ da_{m1} & da_{m2} & \dots & da_{mn} \end{bmatrix} \right\} = \mathcal{L} \{ \underline{dA} \}$$

$$df = \text{tr} \left(\frac{\partial f}{\partial A} \cdot dA \right)$$

That's all folks.

$$= \text{tr} \left(\begin{bmatrix} \frac{\partial f}{\partial a_{11}} & \frac{\partial f}{\partial a_{21}} & \frac{\partial f}{\partial a_{31}} & \dots & \frac{\partial f}{\partial a_{m1}} \\ \frac{\partial f}{\partial a_{12}} & \frac{\partial f}{\partial a_{22}} & \frac{\partial f}{\partial a_{32}} & \dots & \frac{\partial f}{\partial a_{m2}} \\ \vdots & \vdots & \ddots & & \vdots \\ \frac{\partial f}{\partial a_{1n}} & \frac{\partial f}{\partial a_{2n}} & \frac{\partial f}{\partial a_{3n}} & \dots & \frac{\partial f}{\partial a_{mn}} \end{bmatrix} \begin{bmatrix} da_{11} & da_{12} & \dots & da_{1n} \\ da_{21} & da_{22} & \dots & da_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ da_{m1} & da_{m2} & \dots & da_{mn} \end{bmatrix} \right)$$

$$= \text{tr} \left[\begin{array}{c|c} \frac{\partial f}{\partial a_{11}} da_{11} + \dots + \frac{\partial f}{\partial a_{m1}} da_{m1} & \frac{\partial f}{\partial a_{12}} da_{12} + \dots + \frac{\partial f}{\partial a_{m2}} da_{m2} \\ \hline \dots & \dots \end{array} \right] \\ = df$$

Time Derivatives

Time derivatives seem like the easiest, just differentiate term by term:

$$\frac{d}{dt} \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} \frac{dv_1}{dt} \\ \vdots \\ \frac{dv_n}{dt} \end{bmatrix}.$$

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By the chain rule, we also have that

$$df = \frac{\partial f}{\partial A} dA \quad \frac{d}{dt} f(A(t)) = \frac{\partial f(A)}{\partial A} \frac{dA}{dt} = \mathcal{L} \left\{ \frac{dA}{dt} \right\}$$

And all the other chain rule, multiplication rule and etc. are satisfied.

Note that, again, the **order of multiplication matters**. And if the matrix derivative is of other form, the time derivative follows suit.

Time Derivatives

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By the chain rule, we also have that

$$\frac{d}{dt} f(A(t)) = \frac{\partial f(A)}{\partial A} \frac{dA}{dt}.$$

E.g. $LHS = \frac{df}{dt} = \frac{d}{dt}(t^4) = 4t^3 = RHS = \frac{\partial f}{\partial \vec{x}} \frac{d\vec{x}}{dt} = [2x_1 x_2 x_1^2] \begin{bmatrix} 1 \\ 2t \end{bmatrix}$

$$\begin{aligned} f(\vec{x}) &= x_1^2 x_2 \\ \vec{x}(t) &= [x_1, x_2]^T = [t, t^2]^T \end{aligned}$$

✓

$$= [2t^3, t^2] \begin{bmatrix} 1 \\ 2t \end{bmatrix} = 4t^3$$

(Recap)

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- ① We should view derivatives of $f(x)$ as a **linear approximation** of $f(x + dx)$.

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(Recap)

- ① We should view derivatives of $f(x)$ as a **linear approximation** of $f(x + dx)$.
- ② Hence, we can represent derivatives as a **linear operator** $\mathcal{L}\{\cdot\}$ satisfying:

$$df(x) = \mathcal{L}\{dx\}.$$

- ③ In working with scalars, vectors or matrices, we can represent derivatives as

$$df(x) = \frac{df}{dx}dx,$$

as long as their dimension matches.

Before we take a break, a short remark is needed.

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Notation

Two conventions exist in when differentiating with matrix/vector:
for y of size $m \times 1$ and x of size $n \times 1$,

- ① Numerator layout:

$\frac{\partial y}{\partial x}$ follows the size of $y \times x^T$, i.e. $m \times n$.

Before we take a break, a short remark is needed.

Notation

Two conventions exist in when differentiating with matrix/vector:
for y of size $m \times 1$ and x of size $n \times 1$,

- ① Numerator layout:

$\frac{\partial y}{\partial x}$ follows the size of $y \times x^T$, i.e. $m \times n$.

- ② Denominator layout:

$\frac{\partial y}{\partial x}$ follows the size of $x \times y^T$, i.e. $n \times m$.

$$\text{f}(\tilde{x}) = A\tilde{x} \quad , \quad \frac{\partial f}{\partial x} = A^T$$

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- 1 Differentiation Revisited
- 2 Matrix Differentiation
- 3 Examples
- 4 Derivatives of “Matrix Derivatives”

Vector Functions

① $f(\mathbf{x}) = \mathbf{x}$

Vector Functions

$$\textcircled{1} \quad f(\mathbf{x}) = \mathbf{x}$$

$$df = (\mathbf{x} + d\mathbf{x}) - \mathbf{x} = \mathbf{1}d\mathbf{x}$$

$$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} = 1$$

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② $f(\mathbf{x}) = \mathbf{x}^\top$

$$df = (\mathbf{x} + d\mathbf{x})^\top - (\mathbf{x})^\top = (d\mathbf{x})^\top$$

轉置 \rightarrow linear

Vector Functions

Find the derivative with respect to x of the function

$$f(x) = x \cdot x = x^T x.$$

[Sol.]

$$\begin{bmatrix}] \\] \end{bmatrix} \cdot \begin{bmatrix}] \\] \end{bmatrix} = \text{[} \cancel{\text{——}} \text{]} \begin{bmatrix} | \\ | \end{bmatrix}$$

Vector Functions

Find the derivative with respect to \boldsymbol{x} of the function

$$f(\boldsymbol{x}) = \boldsymbol{x} \cdot \boldsymbol{x} = \boldsymbol{x}^\top \boldsymbol{x}.$$

[Sol.]

$$\mathrm{d}f(\boldsymbol{x}) = \mathrm{d}(\boldsymbol{x}^\top \boldsymbol{x}) =$$

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[Sol.]

$$\begin{aligned} df(x) &= d(x^T x) = (x + dx)^T (x + dx) - x^T x \\ &= \cancel{x^T x} + x^T dx + (dx)^T x + (dx)^T dx - \cancel{x^T x} \end{aligned}$$

Vector Functions

Find the derivative with respect to \mathbf{x} of the function

$$f(\mathbf{x}) = \mathbf{x} \cdot \mathbf{x} = \mathbf{x}^\top \mathbf{x}.$$

[Sol.]

$$\begin{aligned} df(\mathbf{x}) &= d(\mathbf{x}^\top \mathbf{x}) = (\mathbf{x} + d\mathbf{x})^\top (\mathbf{x} + d\mathbf{x}) - \mathbf{x}^\top \mathbf{x} \\ &= \mathbf{x}^\top \mathbf{x} + (d\mathbf{x})^\top \mathbf{x} + \mathbf{x}^\top d\mathbf{x} + (d\mathbf{x})^\top d\mathbf{x} - \mathbf{x}^\top \mathbf{x} \end{aligned}$$

Vector Functions

Find the derivative with respect to x of the function

$$f(x) = x \cdot x = x^T x.$$

[Sol.]

$$\begin{aligned} df(x) &= d(x^T x) = (x + dx)^T (x + dx) - x^T x \\ &= x^T x + (dx)^T x + x^T dx + (dx)^T dx - x^T x \\ &= \cancel{(dx)^T x} + x^T \cancel{dx} + \boxed{\cancel{(dx)^T dx}} \rightarrow 0 \end{aligned}$$

$$f(x) = x^2$$

$$f'(x) = \lim_{h \rightarrow 0} \frac{(x+h)^2 - x^2}{h} = \lim_{h \rightarrow 0} \frac{2xh + h^2}{h} = \lim_{h \rightarrow 0} 2x + h = 2x$$

Vector Functions

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$$f(x) = x \cdot x = x^T x.$$

[Sol.]

$$\begin{aligned} df(x) &= d(x^T x) = (x + dx)^T (x + dx) - x^T x \\ &= x^T x + (dx)^T x + x^T dx + (dx)^T dx - x^T x \\ &= (dx)^T x + x^T dx + \cancel{(dx)^T dx} \end{aligned}$$

$dx^T (\dots)$

Ignoring the terms of $O(dx^2)$ and notice that the transpose of a scalar is still itself ($(dx)^T x = x^T dx$), we hence have:

$$df = 2x^T dx = \mathcal{L}\{dx\}. \quad \blacksquare$$

Quadratic Form

Find the derivative with respect to x of the function

$$f(x) = x^T A x. \quad \text{二次型 Quadratic Form}$$

[Sol.]

Quadratic Form

Find the derivative with respect to \mathbf{x} of the function

$$f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}.$$

[Sol.]

$$df = (\mathbf{x} + d\mathbf{x})^T A (\mathbf{x} + d\mathbf{x}) - \mathbf{x}^T \cancel{Ax}$$

Quadratic Form

Find the derivative with respect to \mathbf{x} of the function

$$f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}.$$

[Sol.]

$$\begin{aligned} df &= (\mathbf{x} + d\mathbf{x})^T A (\mathbf{x} + d\mathbf{x}) - \mathbf{x}^T \cancel{\mathbf{x}} \\ &= \mathbf{x}^T A \mathbf{x} + (d\mathbf{x})^T A \mathbf{x} + \mathbf{x}^T A d\mathbf{x} + (d\mathbf{x})^T A d\mathbf{x} - \mathbf{x}^T \cancel{\mathbf{x}} \end{aligned}$$

Quadratic Form

Find the derivative with respect to \mathbf{x} of the function

$$f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}.$$

[Sol.]

$$\begin{aligned}\mathrm{d}f &= (\mathbf{x} + \mathrm{d}\mathbf{x})^T A (\mathbf{x} + \mathrm{d}\mathbf{x}) - \mathbf{x}^T \mathbf{x} \\&= \mathbf{x}^T A \mathbf{x} + (\mathrm{d}\mathbf{x})^T A \mathbf{x} + \mathbf{x}^T A \mathrm{d}\mathbf{x} + (\mathrm{d}\mathbf{x})^T A \mathrm{d}\mathbf{x} - \mathbf{x}^T \mathbf{x} \\&= (\mathrm{d}\mathbf{x})^T A \mathbf{x} + \mathbf{x}^T A \mathrm{d}\mathbf{x} + (\mathrm{d}\mathbf{x})^T A \mathrm{d}\mathbf{x}\end{aligned}$$

Quadratic Form

Find the derivative with respect to \mathbf{x} of the function

$$f(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}.$$

[Sol.]

$$\begin{aligned} df &= (\mathbf{x} + d\mathbf{x})^T A (\mathbf{x} + d\mathbf{x}) - \mathbf{x}^T \mathbf{x} \\ &= \mathbf{x}^T A \mathbf{x} + (d\mathbf{x})^T A \mathbf{x} + \mathbf{x}^T A d\mathbf{x} + (d\mathbf{x})^T A d\mathbf{x} - \mathbf{x}^T \mathbf{x} \\ &= \underline{(d\mathbf{x})^T A \mathbf{x}} + \mathbf{x}^T A d\mathbf{x} + \underline{(d\mathbf{x})^T A d\mathbf{x}} \\ &\quad \text{`}\mathbf{x}^T A^T d\mathbf{x}\text{' } \end{aligned}$$

Ignoring the terms of $O(d\mathbf{x}^2)$, we hence have:

$$df = \mathbf{x}^T (A + A^T) d\mathbf{x} = \mathcal{L}\{d\mathbf{x}\}. \quad \blacksquare$$

Inverse

Given $A = A(t)$, what is

$$\frac{dA^{-1}}{dt}?$$

[Sol.]

Inverse

Given $A = A(t)$, what is

$$\frac{dA^{-1}}{dt}?$$

[Sol.] Since we have

$$A(t)A^{-1}(t) = 1,$$

(单位矩阵)

Inverse

Given $A = A(t)$, what is

$$\frac{dA^{-1}}{dt}?$$

[Sol.] Since we have

$$A(t)A^{-1}(t) = 1,$$

by chain rule:

$$\frac{d}{dt} \left(AA^{-1} \right) = \frac{dA}{dt} A^{-1} + A \frac{dA^{-1}}{dt} = 0$$

Inverse

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[Sol.] Since we have

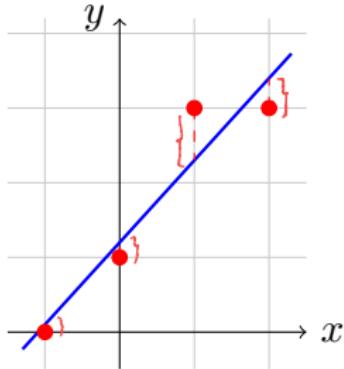
$$A(t)A^{-1}(t) = 1,$$

by chain rule:

$$\begin{aligned}\frac{d}{dt} \left(AA^{-1} \right) &= \frac{dA}{dt} A^{-1} + A \frac{dA^{-1}}{dt} = 0 \\ \frac{dA^{-1}}{dt} &= -A^{-1} \frac{dA}{dt} A^{-1}. \quad \blacksquare\end{aligned}$$

Least Mean Square

Suppose the regression line for the data points is



估測值 $\rightarrow \hat{y} = a_0 + a_1 x$,

we can record the relationship as follows

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \hat{y}_4 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ 1 & x_4 \end{bmatrix}}_X \underbrace{\begin{bmatrix} a_0 \\ a_1 \end{bmatrix}}_w \approx \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}}_y$$

$$\mathcal{E} = \|y - \hat{y}\|^2 = (\hat{y}_1 - y_1)^2 + (\hat{y}_2 - y_2)^2 + \dots$$

Least Mean Square

Def. (LLMSE problem)

The problem of finding the *linear least mean square estimate* is stated as below: given measurements \mathbf{y} over sample points X , find the optimal coefficients (weights) \mathbf{w} that gives the estimate

$$\hat{\mathbf{y}} = X\mathbf{w},$$

such that the mean square error (variance)

$$\mathcal{E} = \|\hat{\mathbf{y}} - \mathbf{y}\|^2$$

is minimized.

It is often used as a cost function in filtering and machine learning. For our talk, we will be focusing on the optimization problem of:

$$\mathbf{w}^* = \arg \min_{\mathbf{w}} \|X\mathbf{w} - \mathbf{y}\|^2.$$

Least Mean Square

By our knowledge of extrema occurs at stationary points, we know that

$$\boldsymbol{w}^* = \arg \min_{\boldsymbol{w}} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2$$

occurs when the derivative is zero at that point, i.e.

$$\left(\frac{\partial}{\partial \boldsymbol{w}} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2 \right) \Bigg|_{\boldsymbol{w}^*} = 0.$$

Least Mean Square

[Sol.]

Least Mean Square

[Sol.]

$$\frac{\partial}{\partial \mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \frac{\partial}{\partial \mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

$$1. \frac{\partial}{\partial \mathbf{x}} \mathbf{x}^\top \mathbf{x} = 2\mathbf{x}^\top = 2(\mathbf{X}\mathbf{w} - \mathbf{y})^\top \mathbf{X}$$

$$2. \frac{\partial}{\partial \mathbf{x}} (\mathbf{A}\mathbf{x} + \mathbf{b}) = \mathbf{A}$$

Least Mean Square

[Sol.]

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 &= \frac{\partial}{\partial \mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \\ &= 2(\mathbf{X}\mathbf{w} - \mathbf{y})^\top \mathbf{X}\end{aligned}$$

$$\begin{aligned}d(\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2) &= (\mathbf{X}\mathbf{w} - \mathbf{y} + \mathbf{X} d\mathbf{w})^\top (\mathbf{X}\mathbf{w} - \mathbf{y} + \mathbf{X} d\mathbf{w}) - (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \\ &= (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X} d\mathbf{w}) + (\mathbf{X} d\mathbf{w})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \\ &= \boxed{2(\mathbf{X}\mathbf{w} - \mathbf{y})^\top \mathbf{X} d\mathbf{w}}\end{aligned}$$

Least Mean Square

[Sol.]

$$\frac{\partial}{\partial \mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \frac{\partial}{\partial \mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

$$= 2(\mathbf{X}\mathbf{w} - \mathbf{y})^\top \mathbf{X}$$

$$(\mathbf{X}\mathbf{w}^* - \mathbf{y})^\top \mathbf{X} = 0$$

Least Mean Square

[Sol.]

$$\frac{\partial}{\partial \mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \frac{\partial}{\partial \mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

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$$(\mathbf{X}\mathbf{w}^* - \mathbf{y})^\top \mathbf{X} = 0$$

$$\mathbf{X}^\top \mathbf{X}\mathbf{w}^* = \mathbf{X}^\top \mathbf{y}$$

Least Mean Square

[Sol.]

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \|X\mathbf{w} - \mathbf{y}\|^2 &= \frac{\partial}{\partial \mathbf{w}} (X\mathbf{w} - \mathbf{y})^\top (X\mathbf{w} - \mathbf{y}) \\ &= 2(X\mathbf{w} - \mathbf{y})^\top X\end{aligned}$$

$$(X\mathbf{w}^* - \mathbf{y})^\top X = 0$$

$$X^\top X \mathbf{w}^* = X^\top \mathbf{y}$$

$$\rightarrow \mathbf{w}^* = (X^\top X)^{-1} X^\top \mathbf{y}. \quad \blacksquare$$

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \end{bmatrix}, \quad X^\top X = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix}$$

$$|X^\top X| = n \sum x_i^2 - (\sum x_i)^2 = n^2 \text{Var}(X) \geq 0, \quad "=\text{" iff } x_i \text{ 同}$$

Least Mean Square

[Sol.]

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 &= \frac{\partial}{\partial \mathbf{w}} (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \\ &= 2(\mathbf{X}\mathbf{w} - \mathbf{y})^\top \mathbf{X}\end{aligned}$$

$$\begin{aligned}(\mathbf{X}\mathbf{w}^* - \mathbf{y})^\top \mathbf{X} &= 0 \\ \mathbf{X}^\top \mathbf{X}\mathbf{w}^* &= \mathbf{X}^\top \mathbf{y} \\ \rightarrow \mathbf{w}^* &= (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}. \quad \blacksquare\end{aligned}$$

The term $(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$ is coined the **matrix pseudo-inverse**.

$$\mathbf{X}\mathbf{w} \approx \mathbf{y} \rightarrow \mathbf{w} = \mathbf{X}^{-1} \mathbf{y}$$

Least Mean Square

We've only checked that $\mathbf{w}^* = (X^T X)^{-1} X^T \mathbf{y}$ is an extrema, but we have yet to check whether its a maxima or a minima. A second derivative test is needed:

Least Mean Square

We've only checked that $\mathbf{w}^* = (X^\top X)^{-1} X^\top \mathbf{y}$ is an extrema, but we have yet to check whether its a maxima or a minima. A second derivative test is needed:

$$\frac{\partial}{\partial \mathbf{w}} ||X\mathbf{w} - \mathbf{y}||^2 = 2(X\mathbf{w} - \mathbf{y})^\top X$$

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$$\frac{\partial}{\partial \mathbf{w}} \|X\mathbf{w} - \mathbf{y}\|^2 = 2(X\mathbf{w} - \mathbf{y})^\top X$$

$$\frac{\partial^2}{\partial \mathbf{w}^\top \partial \mathbf{w}} \|X\mathbf{w} - \mathbf{y}\|^2 = \frac{\partial}{\partial \mathbf{w}^\top} 2(X\mathbf{w} - \mathbf{y})^\top X = 2X^\top X$$

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Hence we know that the second derivative is **positive definite**, i.e. for all $d\mathbf{w} \neq 0$,

$$\begin{aligned} \|X(\mathbf{w}^* + d\mathbf{w}) - \mathbf{y}\|^2 - \|X\mathbf{w}^* - \mathbf{y}\|^2 &= (d\mathbf{w})^\top (2X^\top X)d\mathbf{w} > 0, \\ &= 2(Xd\mathbf{w})^\top (Xd\mathbf{w}) \end{aligned}$$

it is therefore a minima.

Definiteness

Def. (Definiteness)

A matrix A is called **positive definite** if for any non-zero vector x it satisfies: $A^T = A$ 正定

$$x^T Ax > 0 \iff A \succ 0.$$

Moreover, we have:

(positive semi-definite) $x^T Ax \geq 0 \iff A \succeq 0$

(negative definite) $x^T Ax < 0 \iff A \prec 0$

(negative semi-definite) $x^T Ax \leq 0 \iff A \preceq 0$

If none of the above are satisfied, then the matrix is termed **indefinite**.

Taylor Expansion

From the derivation of LLMSE solution above, we can find a second order approximation of a scalar-valued function $f(\mathbf{x})$ of vector \mathbf{x} by:

$$f(\mathbf{x}) = f(\mathbf{a}) + \underbrace{\frac{\partial f(\mathbf{a})}{\partial \mathbf{x}} (\mathbf{x} - \mathbf{a})}_{\text{linear approx. term}} + \underbrace{\frac{1}{2!} (\mathbf{x} - \mathbf{a})^T \frac{\partial^2 f(\mathbf{a})}{\partial \mathbf{x} \partial \mathbf{x}^T} (\mathbf{x} - \mathbf{a})}_{\text{quadratic approx. term}} + \dots, \quad (9)$$

or as

$$f(\mathbf{x}) = f(\mathbf{a}) + f'(\mathbf{a})(\mathbf{x} - \mathbf{a}) + \frac{1}{2} f''(\mathbf{a})(\mathbf{x} - \mathbf{a})^2 + \dots$$

$$f(\mathbf{a} + d\mathbf{x}) = f(\mathbf{a}) + \underbrace{\nabla^T f(\mathbf{a}) d\mathbf{x}}_{\text{gradient}} + \frac{1}{2} (d\mathbf{x})^T \underbrace{\mathbf{H}(f(\mathbf{a}))}_{\text{Hessian}} d\mathbf{x}. \quad (10)$$



Regression

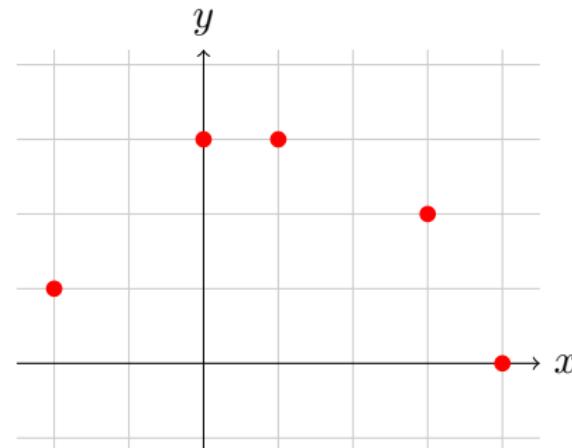
Given a set of data points (x, y) , find a function that interpolates them with the least mean square error.

x	y
-2	1
0	3
1	3
3	2
4	0

Find a quadratic:

$$\hat{y} = a_0 + a_1x + a_2x^2$$

such that the mean square error is minimized.



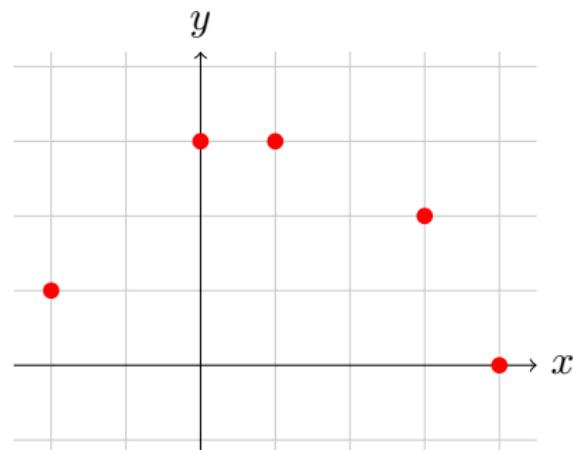
Regression

Given a set of data points (x, y) , find a function that interpolates them with the least mean square error.

We can rewrite the estimation equation as:

$$\hat{y} = \begin{bmatrix} 1 & x & x^2 \\ 1 & -2 & 4 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = Xw$$

$$y = [1, 3, 3, 2, 0]^T$$



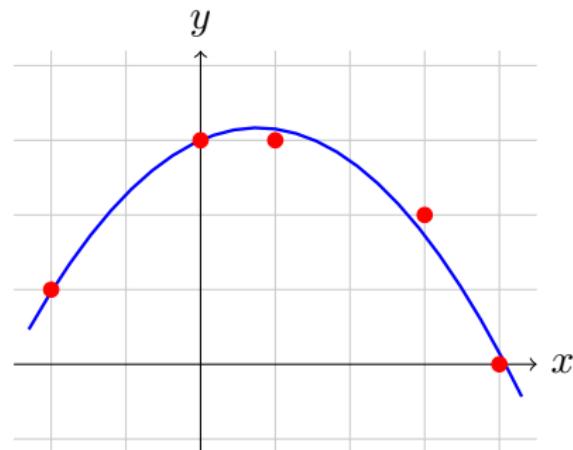
Regression

Given a set of data points (x, y) , find a function that interpolates them with the least mean square error.

$$(X^T X)^{-1} X^T = \begin{bmatrix} 0.14 & 0.43 & 0.43 & 0.14 & -0.14 \\ -0.28 & 0.047 & 0.12 & 0.10 & 0.00 \\ 0.06 & -0.05 & -0.06 & -0.01 & 0.06 \end{bmatrix}$$

$$\mathbf{w}^* = \begin{bmatrix} 3.0000 \\ 0.4394 \\ -0.2879 \end{bmatrix}$$

$$\hat{y} = 3 + 0.44x - 0.29x^2$$



HTML

HTML, HW3

Q6. Let the cross-entropy error function for $E_{\text{in}}(\mathbf{w})$ be:

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \ln \left(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n) \right).$$

Find the Hessian of the function. Express it in diagonalized form of
 $\nabla^\top \nabla E_{\text{in}} = XDX^\top$.

HTML

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \ln \left(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n) \right)$$

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{\partial E_{\text{in}}}{\partial \mathbf{w}^\top} = \frac{\partial}{\partial \mathbf{w}^\top} \left(\frac{1}{N} \sum_{n=1}^N \ln \left(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n) \right) \right)$$

HTML

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \ln \left(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n) \right)$$

$$\begin{aligned}\nabla E_{\text{in}}(\mathbf{w}) &= \frac{\partial E_{\text{in}}}{\partial \mathbf{w}^\top} = \frac{\partial}{\partial \mathbf{w}^\top} \left(\frac{1}{N} \sum_{n=1}^N \ln \left(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n) \right) \right) \\ &= \frac{1}{N} \sum_{n=1}^N \frac{1}{1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)} \frac{\partial}{\partial \mathbf{w}^\top} \left(\exp(-y_n \mathbf{w}^\top \mathbf{x}_n) \right)\end{aligned}$$

HTML

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N \ln \left(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n) \right)$$

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HTML

$$\frac{\partial^2 E_{\text{in}}}{\partial \mathbf{w} \partial \mathbf{w}^\top} = \frac{\partial}{\partial \mathbf{w}} \left(\frac{1}{N} \sum_{n=1}^N \frac{-y_n \mathbf{x}_n \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)}{1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)} \right)$$

HTML

$$\begin{aligned}\frac{\partial^2 E_{\text{in}}}{\partial \mathbf{w} \partial \mathbf{w}^T} &= \frac{\partial}{\partial \mathbf{w}} \left(\frac{1}{N} \sum_{n=1}^N \frac{-y_n \mathbf{x}_n \exp(-y_n \mathbf{w}^T \mathbf{x}_n)}{1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)} \right) \\ &= \sum_{n=1}^N \frac{-y_n \mathbf{x}_n - y_n \mathbf{x}_n^T \exp(-y_n \mathbf{w}^T \mathbf{x}_n) (1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)) + y_n \mathbf{x}_n^T (\exp(-y_n \mathbf{w}^T \mathbf{x}_n))^2}{N (1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n))^2}\end{aligned}$$

HTML

$$\begin{aligned}\frac{\partial^2 E_{\text{in}}}{\partial \mathbf{w} \partial \mathbf{w}^\top} &= \frac{\partial}{\partial \mathbf{w}} \left(\frac{1}{N} \sum_{n=1}^N \frac{-y_n \mathbf{x}_n \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)}{1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)} \right) \\ &= \sum_{n=1}^N \frac{-y_n \mathbf{x}_n - y_n \mathbf{x}_n^\top \exp(-y_n \mathbf{w}^\top \mathbf{x}_n) (1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)) + y_n \mathbf{x}_n^\top (\exp(-y_n \mathbf{w}^\top \mathbf{x}_n))^2}{N (1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n))^2} \\ &= \sum_{i=1}^N \left(\frac{y_n^2 \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)}{N (1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n))^2} \right) \mathbf{x}_n \mathbf{x}_n^\top.\end{aligned}$$

HTML

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Diagonalized (spectral decomposition):

$$E_{\text{in}} = XDX^\top = \sum_{n=1}^N \lambda_n \mathbf{x}_n \mathbf{x}_n^\top. \quad (11)$$

$$\begin{matrix} \mathbf{x}_1 \dots \mathbf{x}_N \\ \parallel \\ \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{bmatrix} \begin{bmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_N^\top \end{bmatrix} \end{matrix}$$

HTML

$$\frac{\partial^2 E_{\text{in}}}{\partial \mathbf{w} \partial \mathbf{w}^\top} = \sum_{i=1}^N \left(\frac{y_n^2 \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)}{N(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n))^2} \right) \mathbf{x}_n \mathbf{x}_n^\top$$

Diagonalized (spectral decomposition):

$$E_{\text{in}} = XDX^\top = \sum_{n=1}^N \lambda_n \mathbf{x}_n \mathbf{x}_n^\top. \quad (11)$$

This is the Hessian in its diagonalized form, with \mathbf{x}_n being the eigenvectors associated with the eigenvalues of

$$\frac{y_n^2 \exp(-y_n \mathbf{w}^\top \mathbf{x}_n)}{N(1 + \exp(-y_n \mathbf{w}^\top \mathbf{x}_n))^2}.$$

Table of Contents

- 1 Differentiation Revisited
- 2 Matrix Differentiation
- 3 Examples
- 4 Derivatives of "Matrix Derivatives"

Matrix Derivatives

We'll go over the derivative of objects including the trace, the determinant, eigenvalues, and singular values.

Trace

Def. (Trace)

The trace of a square matrix is the sum of its diagonals.

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$$\text{tr} \left(\begin{bmatrix} a_{11} & * & \cdots & * \\ * & a_{22} & \cdots & * \\ \vdots & \vdots & \ddots & \vdots \\ * & * & \cdots & a_{nn} \end{bmatrix} \right) = \sum_{i=1}^n a_{ii}. \quad (12)$$

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It can easily be checked that the derivative operator and trace operator are commutative:

$$\frac{d}{dt} \text{tr}(A(t)) = \text{tr} \left(\frac{d}{dt} A(t) \right).$$

Determinant

Lemma

The following identity holds for all square matrices A :

$$\det(e^A) = e^{\text{tr}(A)}. \quad (13)$$

It can be immediately proven by Jordan canonical form of matrices.

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It can be immediately proven by Jordan canonical form of matrices.

e.g. $A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$, $e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!} = \sum_{n=0}^{\infty} \frac{A^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \frac{A^{2n+1}}{(2n+1)!}$

$$\begin{aligned} A^2 &= -\mathbb{1} & = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \mathbb{1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} A \\ &= (\cos 1) \mathbb{1} + (\sin 1) A = \begin{bmatrix} \cos 1 & \sin 1 \\ -\sin 1 & \cos 1 \end{bmatrix} \end{aligned}$$

Determinant

Lemma

The following identity holds for all square matrices A :

$$\det(e^A) = e^{\text{tr}(A)}. \quad (13)$$

It can be immediately proven by Jordan canonical form of matrices.

e.g. $A = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$ $e^A = \begin{bmatrix} \cos 1 & \sin 1 \\ -\sin 1 & \cos 1 \end{bmatrix}$, $\det(e^A) = 1$

$\text{tr}(A) = 0$, $e^{\text{tr}(A)} = 1$

Determinant

Hence if the matrix $A(t)$ is expressible as an exponential:

$$A(t) = e^{B(t)},$$

then a (pseudo-)proof is as follows:

$$\frac{d}{dt} \det(A(t)) =$$

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$$\therefore \frac{d}{dt} A(t) = e^{B(t)} \frac{d}{dt} B(t)$$

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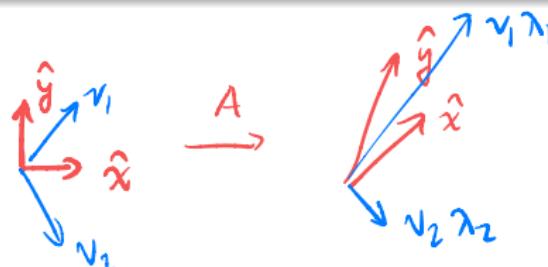
Eigenvalues

Def. (Eigenvalues and Eigenvectors)

For a given square matrix A , it has **eigenvalues** $\{\lambda_i\}$ such that they satisfy:

$$A\mathbf{v}_i = \lambda_i \mathbf{v}_i,$$

where \mathbf{v}_i is the associated (right) **eigenvector**.



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then \mathbf{u}_i is the associated left eigenvector.

Written in the language of matrices:

$$AV = A \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_n \end{bmatrix} = \begin{bmatrix} \mathbf{v}_1 & \cdots & \mathbf{v}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} = V\Lambda$$

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Written in the language of matrices:

$$U^T A = [\mathbf{u}_1 \ \dots \ \mathbf{u}_n]^T A = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} [\mathbf{u}_1 \ \dots \ \mathbf{u}_n]^T = \Lambda U^T$$

Eigenvalues

Some theorems of linear algebra:

Eigenvalues

Some theorems of linear algebra: since we have $AV = V\Lambda$,

Thm. (Diagonalization)

If V is full rank, i.e., V^{-1} exists, then the matrix A can be diagonalized via:

$$\Lambda = V^{-1}AV.$$

$$\begin{cases} AV = V\Lambda \\ V^T A = \Lambda V^T \end{cases} \rightarrow \begin{matrix} \Lambda = V^{-1}AV \\ [\lambda_1 \dots \lambda_n] \quad [**] \end{matrix} \rightarrow \begin{cases} A = V\Lambda V^{-1} \\ A = U^T \Lambda U^T \end{cases}$$

$$\Lambda = U^T A U^{-T} \quad \Lambda^n = \begin{bmatrix} \lambda_1^n & 0 \\ 0 & \lambda_2^n \end{bmatrix} \quad A = V\Lambda U^T$$

$$A^n = V\Lambda^n V^{-1} \quad = [v_1 \dots v_n] \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \begin{bmatrix} u_1^T \\ \vdots \\ u_n^T \end{bmatrix}$$

$$= \sum_{i=1}^n \lambda_i v_i u_i^T$$

Eigenvalues

Some theorems of linear algebra: since we have $AV = V\Lambda$,

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If V is full rank, i.e., V^{-1} exists, then the matrix A can be diagonalized via:

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By expanding out $A = V\Lambda V^{-1}$ and setting $V = [\mathbf{v}_1, \dots, \mathbf{v}_n]$,
 $(V^{-1})^\top = [\mathbf{u}_1, \dots, \mathbf{u}_n]$,

Thm. (Spectral Decomposition)

The $n \times n$ matrix A can be decomposed by

$$A = \sum_{i=1}^n \lambda_i \mathbf{v}_i \mathbf{u}_i^\top.$$

Eigenvalues

For a time varying $A(t)$, what is $\frac{d\lambda_i(t)}{dt}$?

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[Sol.]

Let us consider $\lambda_i(t)$ with its associated right and left eigenvectors: $v_i(t)$ and $u_i(t)$ that has length satisfying:

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$$u_i^T (t) A(t) \underline{\lambda_i v_i} = \lambda_i(t)$$

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Then,

$$\mathbf{u}_i^T(t) A(t) \mathbf{v}_i(t) = \lambda_i(t)$$

$$\frac{d\lambda_i}{dt} = \frac{d\mathbf{u}_i^T}{dt} A \mathbf{v}_i + \mathbf{u}_i^T \frac{dA}{dt} \mathbf{v}_i + \mathbf{u}_i^T A \frac{d\mathbf{v}_i}{dt}$$

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$$\frac{d\lambda_i}{dt} = \frac{d\mathbf{u}_i^\top}{dt} A \mathbf{v}_i + \mathbf{u}_i^\top \frac{dA}{dt} \mathbf{v}_i + \mathbf{u}_i^\top A \frac{d\mathbf{v}_i}{dt}$$

But we also have

$$\begin{aligned}\frac{d\mathbf{u}_i^\top}{dt} A \mathbf{v}_i + \mathbf{u}_i^\top A \frac{d\mathbf{v}_i}{dt} &= \lambda_i \left(\frac{d\mathbf{u}_i^\top}{dt} \mathbf{v}_i + \mathbf{u}_i^\top A \cancel{\frac{d\mathbf{v}_i}{dt}} \right) \\ &= \lambda_i \frac{d}{dt} (\mathbf{u}_i^\top \mathbf{v}_i) = 0\end{aligned}$$

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$$\rightarrow \frac{d\lambda_i}{dt} = \mathbf{u}_i^\top \frac{dA}{dt} \mathbf{v}_i$$

Singular Values

Def. (Singular Value Decomposition, SVD)

For a real (complex) matrix A of size $m \times n$ (WLOG let $m > n$), then it can be decomposed into a sandwich product of diagonal matrix Σ by two orthogonal (unitary) matrices U and V :

$$A = \underbrace{U}_{m \times m} \underbrace{\Sigma}_{m \times n} \underbrace{V^T}_{n \times n} = \begin{bmatrix} | & & | \\ u_1 & \cdots & u_m \\ | & & | \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ \hline & 0 & & 0 \end{bmatrix} \begin{bmatrix} v_1^T \\ \vdots \\ v_n^T \end{bmatrix} \quad (14)$$

where $U^T U = 1$, $V^T V = 1$, and $\sigma_1 \geq \cdots \geq \sigma_r \geq 0$.

Note that for the case of complex A , the transposition are replaced by conjugate-transpose.

Singular Values

Thm. (Spectral Decomposition)

The result of singular value decomposition can also be written as:

$$A = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^\top.$$

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The result of singular value decomposition can also be written as:

$$A = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^\top.$$

The same derivation can be applied for finding the time derivative of singular values. By utilizing:

$$AV = U\Sigma V^\top V = U\Sigma, \quad U^\top A = U^\top U\Sigma V^\top = \Sigma V^\top$$

Singular Values

Thm. (Spectral Decomposition)

The result of singular value decomposition can also be written as:

$$A = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^\top.$$

The same derivation can be applied for finding the time derivative of singular values. By utilizing:

$$AV = U\Sigma V^\top V = U\Sigma, \quad U^\top A = U^\top U\Sigma V^\top = \Sigma V^\top$$

the solution is given by

$$\frac{d\sigma_i}{dt} = \mathbf{u}_i^\top \frac{dA}{dt} \mathbf{v}_i, \quad (15)$$

where $\mathbf{u}_i(t)$ and $\mathbf{v}_i(t)$ are the left and right singular vector associated with the singular value $\sigma_i(t)$.

That's all folks.