Vector Calculus

Marc Deisenroth
Centre for Artificial Intelligence
Department of Computer Science
University College London

@mpd37
m.deisenroth@ucl.ac.uk
https://deisenroth.cc

AIMS Rwanda and AIMS Ghana

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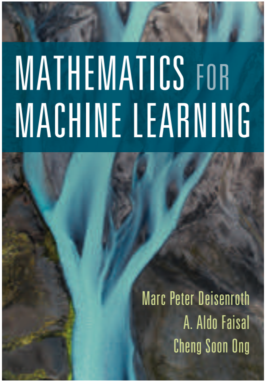
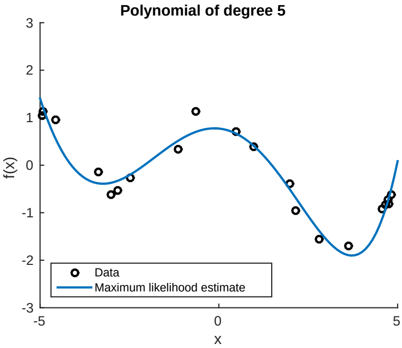


Chapter 5

https://mml-book.com

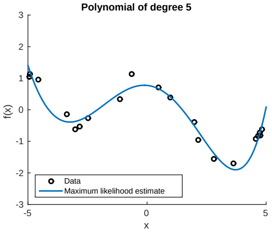
Regression in Machine Learning (1)



- Setting: Inputs $\boldsymbol{x} \in \mathbb{R}^D$, outputs/targets $y \in \mathbb{R}$
- Goal: Find a function that models the relationship between $\boldsymbol{x}$ and y (regression/curve fitting)
- Model f that depends on parameters $\boldsymbol{\theta}$. Examples:
  - Linear model: $f(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \boldsymbol{x}, \quad \boldsymbol{x}, \boldsymbol{\theta} \in \mathbb{R}^D$
  - Neural network: $f(\boldsymbol{x}, \boldsymbol{\theta}) = NN(\boldsymbol{x}, \boldsymbol{\theta})$

Regression in Machine Learning (2)

- Training data, e.g., N pairs $(\boldsymbol{x}_i, y_i)$ of inputs $\boldsymbol{x}_i$ and observations y_i
- Training the model means finding parameters $\boldsymbol{\theta}^*$, such that $f(\boldsymbol{x}_i, \boldsymbol{\theta}^*) \approx y_i$



Regression in Machine Learning (2)

- Training data, e.g., N pairs $(\boldsymbol{x}_i, y_i)$ of inputs $\boldsymbol{x}_i$ and observations y_i
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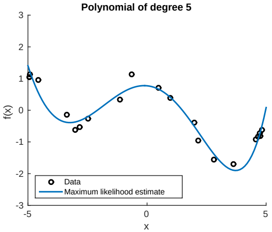


- Define a loss function, e.g., $\sum_{i=1}^{N}(y_i - f(\boldsymbol{x}_i, \boldsymbol{\theta}))^2$, which we want to optimize
- Typically: Optimization based on some form of gradient descent
  - Differentiation required

Types of Differentiation

1. Scalar differentiation: $f : \mathbb{R} \to \mathbb{R}$

   $y \in \mathbb{R}$ w.r.t. $x \in \mathbb{R}$

2. Scalar differentiation of a vector: $f : \mathbb{R} \to \mathbb{R}^N$

   $y \in \mathbb{R}^N$ w.r.t. $x \in \mathbb{R}$

3. Multivariate case: $f : \mathbb{R}^N \to \mathbb{R}$

   $y \in \mathbb{R}$ w.r.t. vector $\boldsymbol{x} \in \mathbb{R}^N$

4. Vector fields: $f : \mathbb{R}^N \to \mathbb{R}^M$

   vector $\boldsymbol{y} \in \mathbb{R}^M$ w.r.t. vector $\boldsymbol{x} \in \mathbb{R}^N$

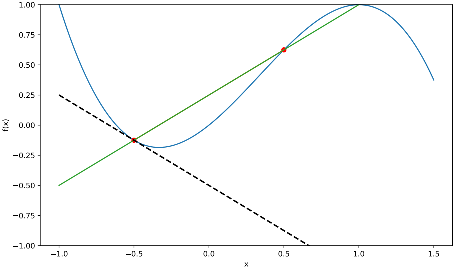
5. General derivatives: $f : \mathbb{R}^{M \times N} \to \mathbb{R}^{P \times Q}$

   matrix $\boldsymbol{y} \in \mathbb{R}^{P \times Q}$ w.r.t. matrix $\boldsymbol{X} \in \mathbb{R}^{M \times N}$

- Derivative defined as the limit of the difference quotient

$$f'(x) = \frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

  - Slope of the secant line through $f(x)$ and $f(x+h)$



Some Examples

$$
\begin{aligned}
f(x) &= x^n & f'(x) &= nx^{n-1} \\
f(x) &= \sin(x) & f'(x) &= \cos(x) \\
f(x) &= \tanh(x) & f'(x) &= 1 - \tanh^2(x) \\
f(x) &= \exp(x) & f'(x) &= \exp(x) \\
f(x) &= \log(x) & f'(x) &= \frac{1}{x}
\end{aligned}
$$

Differentiation Rules

- Sum Rule

$$\big(f(x)+g(x)\big)' = f'(x) + g'(x) = \frac{df(x)}{dx} + \frac{dg(x)}{dx}$$

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- Product Rule

$$\big(f(x)g(x)\big)' = f'(x)g(x) + f(x)g'(x) = \frac{df(x)}{dx}g(x) + f(x)\frac{dg(x)}{dx}$$

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- Chain Rule

$$(g\circ f)'(x) = \big(g(f(x))\big)' = g'(f(x))f'(x) = \frac{dg(f(x))}{df}\frac{df(x)}{dx}$$

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$$(g \circ f)'(x) = \big(g(f(x))\big)' = g'(f(x))f'(x) = \frac{dg(f(x))}{df}\frac{df(x)}{dx}$$

- Quotient Rule

$$\Big(\frac{f(x)}{g(x)}\Big)' = \frac{f(x)'g(x) - f(x)g(x)'}{(g(x))^2} = \frac{\frac{df}{dx}g(x) - f(x)\frac{dg}{dx}}{(g(x))^2}$$

Example: Scalar Chain Rule

$$(g \circ f)'(x) = \big(g(f(x))\big)' = \color{green}{g'(f(x))}\color{blue}{f'(x)} \color{black}{=} \color{green}{\frac{dg}{df}}\color{blue}{\frac{df}{dx}}$$

Beginner

$$\begin{aligned} g(z) &= 6z + 3 \\ z = f(x) &= -2x + 5 \\ (g \circ f)'(x) &= \end{aligned}$$

Advanced

$$\begin{aligned} g(z) &= \tanh(z) \\ z = f(x) &= x^n \\ (g \circ f)'(x) &= \end{aligned}$$

Work it out with your neighbors

Example: Scalar Chain Rule

$$(g \circ f)'(x) = \big(g(f(x))\big)' = g'(f(x))f'(x) = \frac{dg}{df}\frac{df}{dx}$$

Beginner

$$\begin{aligned} g(z) &= 6z + 3 \\ z = f(x) &= -2x + 5 \\ (g \circ f)'(x) &= \underbrace{(6)}_{dg/df}\underbrace{(-2)}_{df/dx} \\ &= -12 \end{aligned}$$

Advanced

$$\begin{aligned} g(z) &= \tanh(z) \\ z = f(x) &= x^n \\ (g \circ f)'(x) &= \underbrace{\left(1 - \tanh^2(x^n)\right)}_{dg/df}\underbrace{nx^{n-1}}_{df/dx} \end{aligned}$$

Scalar Differentiation $f : \mathbb{R} \to \mathbb{R}^N$

$$\boldsymbol{f}(x) = \begin{bmatrix} f_1(x) \\ \vdots \\ f_N(x) \end{bmatrix} \in \mathbb{R}^N, \quad x \in \mathbb{R}$$

- Here, f_n are different functions, e.g.,

$$\boldsymbol{f}(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \end{bmatrix} = \begin{bmatrix} x^2 \\ \sin(x) \end{bmatrix}$$

- Differentiation: Compute derivatives of each f_n:

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}x} = \begin{bmatrix} \frac{\mathrm{d}f_1}{\mathrm{d}x} \\ \vdots \\ \frac{\mathrm{d}f_N}{\mathrm{d}x} \end{bmatrix} \in \mathbb{R}^N$$

- Derivative of a (column) vector w.r.t. a scalar input is a (column) vector

Multivariate Differentiation $f : \mathbb{R}^N \to \mathbb{R}$

$$y = f(\boldsymbol{x}), \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^N$$

- Partial derivative (change one coordinate at a time):

$$\frac{\partial f}{\partial x_i} = \lim_{h \to 0} \frac{f(x_1, \ldots, x_{i-1}, x_i + h, x_{i+1}, \ldots, x_N) - f(\boldsymbol{x})}{h}$$

$$y = f(\boldsymbol{x}) \,, \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^N$$

- Partial derivative (change one coordinate at a time):

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- Jacobian vector (gradient) collects all partial derivatives:

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{1 \times N}$$

Note: This is a **row vector**.

Example: Multivariate Differentiation

Beginner

$$f : \mathbb{R}^2 \to \mathbb{R}$$
$$f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$$

Advanced

$$f : \mathbb{R}^2 \to \mathbb{R}$$
$$f(x_1, x_2) = (x_1 + 2x_2^3)^2 \in \mathbb{R}$$

Partial derivatives? Gradient?

Work it out with your neighbors

Example: Multivariate Differentiation

Beginner

$$f : \mathbb{R}^2 \to \mathbb{R}$$
$$f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$$

Advanced

$$f : \mathbb{R}^2 \to \mathbb{R}$$
$$f(x_1, x_2) = (x_1 + 2x_2^3)^2 \in \mathbb{R}$$

Partial derivatives

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2x_1 x_2 + x_2^3$$
$$\frac{\partial f(x_1, x_2)}{\partial x_2} = x_1^2 + 3x_1 x_2^2$$

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2(x_1 + 2x_2^3) \overbrace{(1)}^{\frac{\partial}{\partial x_1}(x_1 + 2x_2^3)}$$
$$\frac{\partial f(x_1, x_2)}{\partial x_2} = 2(x_1 + 2x_2^3) \underbrace{(6x_2^2)}_{\frac{\partial}{\partial x_2}(x_1 + 2x_2^3)}$$

Example: Multivariate Differentiation

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Partial derivatives

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$$\frac{\partial f(x_1, x_2)}{\partial x_2} = 2(x_1 + 2x_2^3) \underbrace{(6x_2^2)}_{\frac{\partial}{\partial x_2}(x_1 + 2x_2^3)}$$

Gradient $\quad \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f(x_1, x_2)}{\partial x_1} & \frac{\partial f(x_1, x_2)}{\partial x_2} \end{bmatrix} \in \mathbb{R}^{1 \times 2}$

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} 2x_1 x_2 + x_2^3 & x_1^2 + 3x_1 x_2^2 \end{bmatrix}$$
$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} 2(x_1 + 2x_2^3) & 12(x_1 + 2x_2^3) x_2^2 \end{bmatrix}$$

Example: Multivariate Chain Rule

- Consider the function

$$L(\boldsymbol{e}) = \tfrac{1}{2}\|\boldsymbol{e}\|^2 = \tfrac{1}{2}\boldsymbol{e}^\top\boldsymbol{e}$$

$$\boldsymbol{e} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\,, \quad \boldsymbol{x} \in \mathbb{R}^N\,, \boldsymbol{A} \in \mathbb{R}^{M\times N}\,, \boldsymbol{e}, \boldsymbol{y} \in \mathbb{R}^M$$

- Compute the gradient $\frac{\mathrm{d}L}{\mathrm{d}\boldsymbol{x}}$. What is the dimension/size of $\frac{\mathrm{d}L}{\mathrm{d}\boldsymbol{x}}$?

Work it out with your neighbors

Example: Multivariate Chain Rule

- Consider the function

$$L(\boldsymbol{e}) = \tfrac{1}{2}\|\boldsymbol{e}\|^2 = \tfrac{1}{2}\boldsymbol{e}^\top\boldsymbol{e}$$

$$\boldsymbol{e} = \boldsymbol{y} - \boldsymbol{A}\boldsymbol{x}\,, \quad \boldsymbol{x} \in \mathbb{R}^N\,, \boldsymbol{A} \in \mathbb{R}^{M\times N}\,, \boldsymbol{e}, \boldsymbol{y} \in \mathbb{R}^M$$

- Compute the gradient $\frac{\mathrm{d}L}{\mathrm{d}\boldsymbol{x}}$. What is the dimension/size of $\frac{\mathrm{d}L}{\mathrm{d}\boldsymbol{x}}$?

$$\frac{\mathrm{d}L}{\mathrm{d}\boldsymbol{x}} = \frac{\partial L}{\partial \boldsymbol{e}}\frac{\partial \boldsymbol{e}}{\partial \boldsymbol{x}}$$

$$\frac{\partial L}{\partial \boldsymbol{e}} = \boldsymbol{e}^\top \in \mathbb{R}^{1\times M} \tag{1}$$

$$\frac{\partial \boldsymbol{e}}{\partial \boldsymbol{x}} = -\boldsymbol{A} \in \mathbb{R}^{M\times N} \tag{2}$$

$$\Longrightarrow \frac{\mathrm{d}L}{\mathrm{d}\boldsymbol{x}} = \boldsymbol{e}^\top(-\boldsymbol{A}) = -(\boldsymbol{y} - \boldsymbol{A}\boldsymbol{x})^\top\boldsymbol{A} \in \mathbb{R}^{1\times N}$$

Vector Field Differentiation $f : \mathbb{R}^N \to \mathbb{R}^M$

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^M\,, \quad \boldsymbol{x} \in \mathbb{R}^N$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_M(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} f_1(x_1, \ldots, x_N) \\ \vdots \\ f_M(x_1, \ldots, x_N) \end{bmatrix}$$

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- Jacobian matrix (collection of all partial derivatives)

$$\begin{bmatrix} \frac{dy_1}{d\boldsymbol{x}} \\ \vdots \\ \frac{dy_M}{d\boldsymbol{x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{M \times N}$$

Example: Vector Field Differentiation

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

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_M(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + & \cdots & + A_{1N}x_N \\ \vdots \quad\quad \vdots & \vdots & \vdots \\ A_{M1}x_1 + A_{M2}x_2 + & \cdots & + A_{MN}x_N \end{bmatrix}$$

- Compute the gradient $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}}$
  - Dimension of $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}}$:

Example: Vector Field Differentiation

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

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- Compute the gradient $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}}$
  - Dimension of $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}}$: Since $\boldsymbol{f} : \mathbb{R}^N \to \mathbb{R}^M$ it follows that $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{M\times N}$

Example: Vector Field Differentiation

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  - Gradient:

$$f_i(\boldsymbol{x}) = \sum_{j=1}^{N} A_{ij}x_j \qquad \Longrightarrow \quad \frac{\partial f_i}{\partial x_j} = A_{ij}$$

Example: Vector Field Differentiation

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

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  - Gradient:

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

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

Dimensionality of the Gradient

In general: A function $\boldsymbol{f} : \mathbb{R}^{N} \to \mathbb{R}^{M}$ has a gradient that is an $M \times N$-matrix with

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{M \times N}, \qquad \mathrm{d}\boldsymbol{f}[m,n] = \frac{\partial f_m}{\partial x_n}$$

Gradient dimension: # target dimensions $\times$ # input dimensions

Chain Rule

$$\frac{\partial}{\partial \boldsymbol{x}}(g \circ f)(\boldsymbol{x}) = \frac{\partial}{\partial \boldsymbol{x}}\big(g(f(\boldsymbol{x}))\big) = \frac{\partial g(f)}{\partial {\color{red}f}} \frac{\partial {\color{red}f}(\boldsymbol{x})}{\partial \boldsymbol{x}}$$

Example: Chain Rule

- Consider $f : \mathbb{R}^2 \to \mathbb{R}, \quad \boldsymbol{x} : \mathbb{R} \to \mathbb{R}^2$

$$f(\boldsymbol{x}) = f(x_1, x_2) = x_1^2 + 2x_2\,,$$

$$\boldsymbol{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \sin(t) \\ \cos(t) \end{bmatrix}$$

Example: Chain Rule

- Consider $f : \mathbb{R}^2 \to \mathbb{R}, \quad \boldsymbol{x} : \mathbb{R} \to \mathbb{R}^2$

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- What are the dimensions of $\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}}$ and $\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t}$?

Work it out with your neighbors

Example: Chain Rule

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- What are the dimensions of $\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}}$ and $\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t}$?

1×2 and 2×1

- Compute the gradient $\frac{\mathrm{d}f}{\mathrm{d}t}$ using the chain rule:

Example: Chain Rule

- Consider $f : \mathbb{R}^2 \to \mathbb{R}, \quad \boldsymbol{x} : \mathbb{R} \to \mathbb{R}^2$

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1×2 and 2×1

- Compute the gradient $\frac{\mathrm{d}f}{\mathrm{d}t}$ using the chain rule:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}}\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix} = \begin{bmatrix} 2\sin t & 2 \end{bmatrix} \begin{bmatrix} \cos t \\ -\sin t \end{bmatrix}$$
$$= 2\sin t\cos t - 2\sin t = 2\sin t(\cos t - 1)$$

Derivatives with Respect to Matrices

- Recall: A function $\boldsymbol{f} : \mathbb{R}^N \to \mathbb{R}^M$ has a gradient that is an $M \times N$-matrix with

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{M \times N}, \qquad \mathrm{d}\boldsymbol{f}[m,n] = \frac{\partial f_m}{\partial x_n}$$

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  Gradient dimension: # target dimensions $\times$ # input dimensions

- This generalizes to when the inputs (N) or targets (M) are **matrices**

Derivatives with Respect to Matrices

- Recall: A function $\boldsymbol{f} : \mathbb{R}^{N} \to \mathbb{R}^{M}$ has a gradient that is an $M \times N$-matrix with

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{M \times N}, \qquad \mathrm{d}\boldsymbol{f}[m,n] = \frac{\partial f_m}{\partial x_n}$$

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- This generalizes to when the inputs (N) or targets (M) are **matrices**
- Function $\boldsymbol{f} : \mathbb{R}^{M \times N} \to \mathbb{R}^{P \times Q}$, has a gradient that is a $(P \times Q) \times (M \times N)$ object (tensor)

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{X}} \in \mathbb{R}^{(P \times Q) \times (M \times N)}, \qquad \mathrm{d}\boldsymbol{f}[p,q,m,n] = \frac{\partial f_{pq}}{\partial X_{mn}}$$

Example 1: Derivatives with Respect to Matrices

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

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_M(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + & \cdots & + A_{1N}x_N \\ \vdots \quad\quad \vdots & \vdots & \vdots \\ A_{M1}x_1 + A_{M2}x_2 + & \cdots & + A_{MN}x_N \end{bmatrix}$$

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}} \in \mathbb{R}^{?}$$

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$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}} \in \mathbb{R}^{\text{\# target dim} \times \text{\# input dim}} = M \times (M \times N)$$

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}} = \begin{bmatrix} \frac{\partial f_1}{\partial \boldsymbol{A}} \\ \vdots \\ \frac{\partial f_M}{\partial \boldsymbol{A}} \end{bmatrix}, \qquad \frac{\partial f_m}{\partial \boldsymbol{A}} \in \mathbb{R}^{1\times(M\times N)}$$

Example 2: Derivatives w.r.t. Matrices

$$f_m = \sum_{n=1}^{N} A_{mn} x_n, \quad m = 1, \ldots, M$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_i(\boldsymbol{x}) \\ \vdots \\ f_M(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + & \cdots & + A_{1N}x_N \\ \vdots \quad\quad \vdots & \vdots & \vdots \\ A_{i1}x_1 + A_{i2}x_2 + & \cdots & + A_{iN}x_N \\ \vdots \quad\quad \vdots & \vdots & \vdots \\ A_{M1}x_1 + A_{M2}x_2 + & \cdots & + A_{MN}x_N \end{bmatrix}$$

$$\frac{\partial f_m}{\partial A_{mq}} = ? \qquad \frac{\partial f_m}{\partial A_{m,:}} = ? \qquad \frac{\partial f_m}{\partial A_{k \neq m,:}} = ? \qquad \frac{\partial f_m}{\partial \boldsymbol{A}} = ?$$

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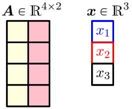
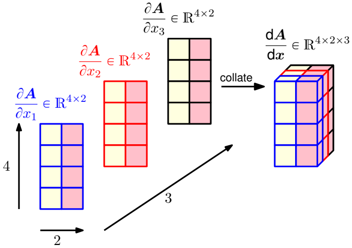
Gradient Computation: Two Alternatives

- Consider $\boldsymbol{f} : \mathbb{R}^3 \to \mathbb{R}^{4\times 2}$, $\quad \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A} \in \mathbb{R}^{4\times 2}$ where the entries A_{ij} depend on a vector $\boldsymbol{x} \in \mathbb{R}^3$
- We can compute $\frac{\mathrm{d}\boldsymbol{A}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{4\times 2\times 3}$ in two equivalent ways:



Partial derivatives:



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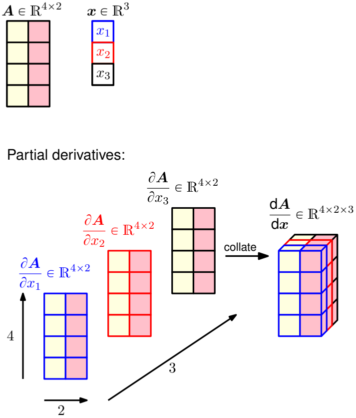
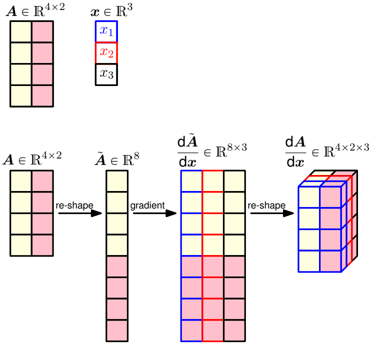
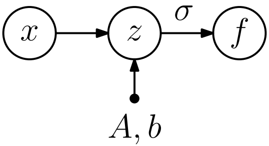




Gradients of a Single-Layer Neural Network



$$\boldsymbol{f} = \tanh(\underbrace{\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}}_{=:\boldsymbol{z}\in\mathbb{R}^M}) \in \mathbb{R}^M, \quad \boldsymbol{x} \in \mathbb{R}^N, \boldsymbol{A} \in \mathbb{R}^{M\times N}, \boldsymbol{b} \in \mathbb{R}^M$$

Gradients of a Single-Layer Neural Network

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$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} = \underbrace{\mathrm{diag}(1 - \tanh^2(\boldsymbol{z}))}_{\in \mathbb{R}^{M\times M}}$$

Gradients of a Single-Layer Neural Network

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$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{b}}[i,j] = \sum_{l=1}^{M} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}}[i,l]\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}[l,j]$$

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Putting Things Together

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- Train single-layer neural network with

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- Find $\boldsymbol{A}, \boldsymbol{b}$, such that the squared loss

$$L(\boldsymbol{\theta}) = \tfrac{1}{2}\|\boldsymbol{e}\|^2 \in \mathbb{R}\,, \quad \boldsymbol{e} = \boldsymbol{y} - \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}) \in \mathbb{R}^M$$

is minimized

Putting Things Together

Partial derivatives:

$$\frac{\partial L}{\partial \boldsymbol{A}} = \frac{\partial L}{\partial \boldsymbol{e}} \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{A}}$$

$$\frac{\partial L}{\partial \boldsymbol{b}} = \frac{\partial L}{\partial \boldsymbol{e}} \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

$$\frac{\partial L}{\partial \boldsymbol{e}} = \underbrace{\boldsymbol{e}^\top}_{\in \mathbb{R}^{1\times M}} \qquad \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{f}} = \underbrace{-\boldsymbol{I}}_{\in \mathbb{R}^{M\times M}} \qquad \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{z}} = \underbrace{\mathrm{diag}(1 - \tanh^2(\boldsymbol{z}))}_{\in \mathbb{R}^{M\times M}}$$

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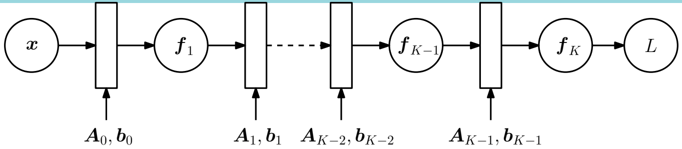
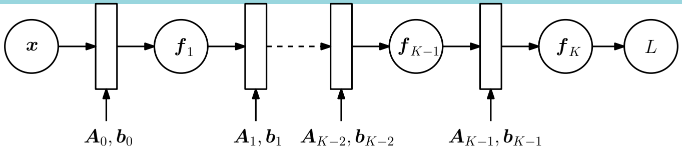
Gradients of a Multi-Layer Neural Network



- Inputs $\boldsymbol{x}$, observed outputs $\boldsymbol{y}$
- Train multi-layer neural network with

$$\boldsymbol{f}_0 = \boldsymbol{x}$$
$$\boldsymbol{f}_i = \sigma_i(\boldsymbol{A}_{i-1}\boldsymbol{f}_{i-1} + \boldsymbol{b}_{i-1}), \quad i = 1, \ldots, K$$

Gradients of a Multi-Layer Neural Network



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- Train multi-layer neural network with

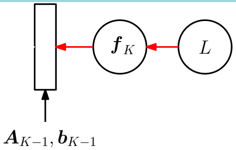
$$\boldsymbol{f}_0 = \boldsymbol{x}$$
$$\boldsymbol{f}_i = \sigma_i(\boldsymbol{A}_{i-1}\boldsymbol{f}_{i-1} + \boldsymbol{b}_{i-1})\,, \quad i = 1, \ldots, K$$

- Find $\boldsymbol{A}_j, \boldsymbol{b}_j$ for $j = 0, \ldots, K-1$, such that the squared loss

$$L(\boldsymbol{\theta}) = \|\boldsymbol{y} - \boldsymbol{f}_{K,\boldsymbol{\theta}}(\boldsymbol{x})\|^2$$

is minimized, where $\boldsymbol{\theta} = \{\boldsymbol{A}_j, \boldsymbol{b}_j\}\,, \quad j = 0, \ldots, K-1$

Gradients of a Multi-Layer Neural Network



$$\frac{\partial L}{\partial \boldsymbol{\theta}_{K-1}} = \frac{\partial L}{\partial \boldsymbol{f}_K} \frac{\partial \boldsymbol{f}_K}{\partial \boldsymbol{\theta}_{K-1}}$$

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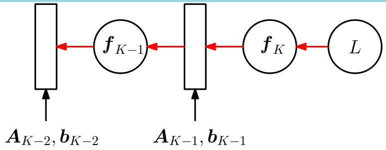

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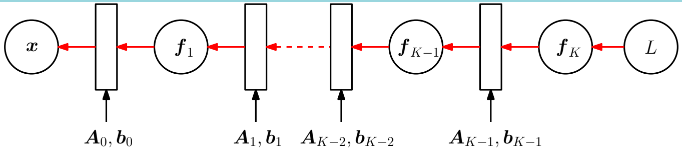

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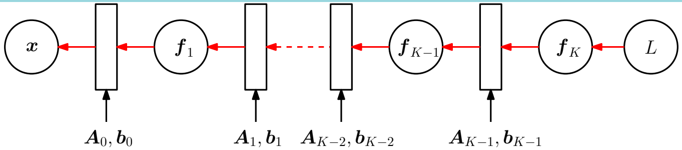

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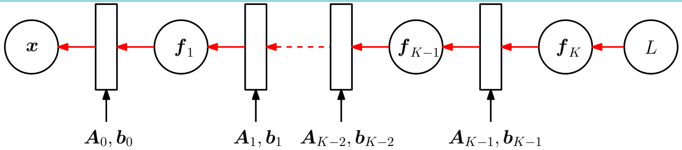

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- Intermediate derivatives are stored during the forward pass

- Linear regression with a neural network parametrized by $\boldsymbol{\theta}$:

$$y = f_{\boldsymbol{\theta}}(\boldsymbol{x}) + \epsilon\,, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_\epsilon^2\big)$$

Example: Regression with Neural Networks

- Linear regression with a neural network parametrized by $\boldsymbol{\theta}$:

$$y = f_{\boldsymbol{\theta}}(\boldsymbol{x}) + \epsilon\,, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_\epsilon^2\big)$$

- Given inputs $\boldsymbol{x}_n$ and corresponding (noisy) observations y_n, $n = 1, \dots, N$, find parameters $\boldsymbol{\theta}^*$ that minimize the squared loss

$$L(\boldsymbol{\theta}) = \sum_{n=1}^{N} (y_n - f_{\boldsymbol{\theta}}(\boldsymbol{x}_n))^2 = \|\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{X})\|^2$$

Training NNs as Maximum Likelihood Estimation

- Training a neural network in the above way corresponds to maximum likelihood estimation:
  - If $\boldsymbol{y} = NN(\boldsymbol{x}, \boldsymbol{\theta}) + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}\big(\boldsymbol{0},\, \boldsymbol{I}\big)$ then the log-likelihood is

$$\log p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) = -\tfrac{1}{2}\|\boldsymbol{y} - NN(\boldsymbol{x}, \boldsymbol{\theta})\|^2$$

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  - Find $\boldsymbol{\theta}^*$ by minimizing the negative log-likelihood:

$$\begin{aligned}\boldsymbol{\theta}^* &= \arg\min_{\boldsymbol{\theta}} -\log p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}) \\ &= \arg\min_{\boldsymbol{\theta}} \tfrac{1}{2}\|\boldsymbol{y} - NN(\boldsymbol{x}, \boldsymbol{\theta})\|^2 \\ &= \arg\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta})\end{aligned}$$

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- Maximum likelihood estimation can lead to overfitting (interpret noise as signal)

Example: Linear Regression (1)

- Linear regression with a polynomial of order M:

$$y = f(x, \boldsymbol{\theta}) + \epsilon\,, \quad \epsilon \sim \mathcal{N}\big(0,\, \sigma_\epsilon^2\big)$$

$$f(x, \boldsymbol{\theta}) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_M x^M = \sum_{i=0}^{M} \theta_i x^i$$

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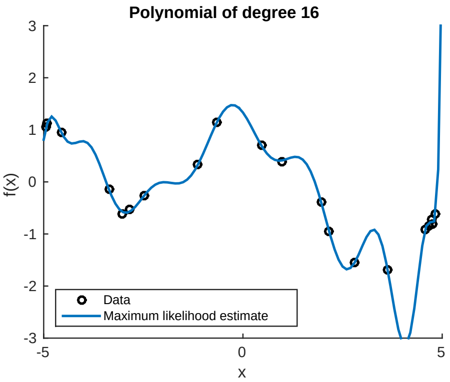
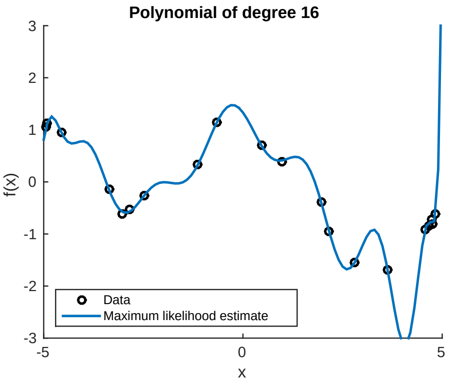
- Given inputs x_i and corresponding (noisy) observations y_i, $i = 1, \ldots, N$, find parameters $\boldsymbol{\theta} = [\theta_0, \ldots, \theta_M]^\top$, that minimize the squared loss (equivalently: maximize the likelihood)

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{N} (y_i - f(x_i, \boldsymbol{\theta}))^2$$

Example: Linear Regression (2)

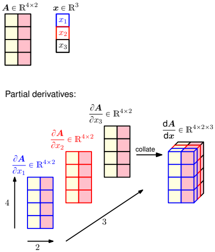


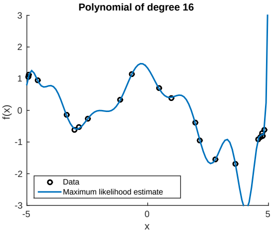
Example: Linear Regression (2)

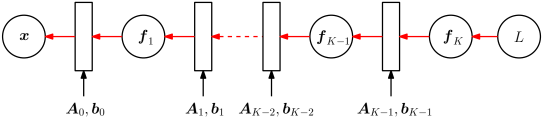


- Regularization, model selection etc. can address overfitting
- Alternative approach based on integration

Summary







- Vector-valued differentiation
- Chain rule
- Check the dimension of the gradients