Vector Calculus

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Reading Material

Lecture notes, Chapter 5

https://mml-book.com

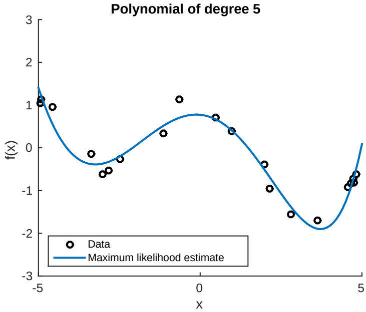
Overview

Optimisation

Differentiation w.r.t. scalars

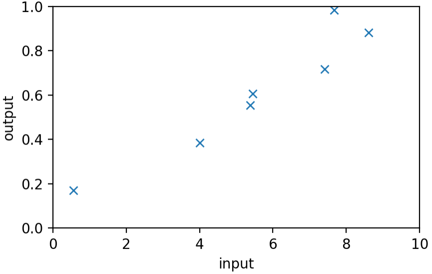
Differentiation w.r.t. vectors

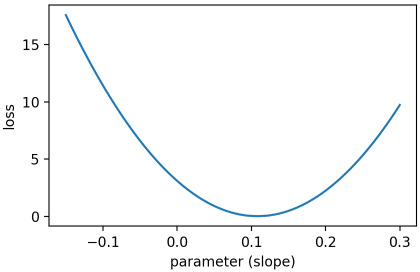
Curve Fitting (Regression) in Machine Learning (2)



- Training the model means finding parameters $\boldsymbol{\theta}^*$, such that $f(\boldsymbol{x}_i, \boldsymbol{\theta}^*) \approx y_i$
- Define a loss function, e.g., $\sum_{i=1}^{N}(y_i - f(\boldsymbol{x}_i, \boldsymbol{\theta}))^2$, which we want to optimize
- Adjust $\boldsymbol{\theta}$ until loss is as small as we can get it: **Minimisation** / **optimisation**.

Example: Minimising the loss





$$f(x) = a \cdot x \qquad L(a) = \sum_{n=1}^{N} (f(x_n, a) - y_n)^2 \tag{1}$$

Let's adjust a.

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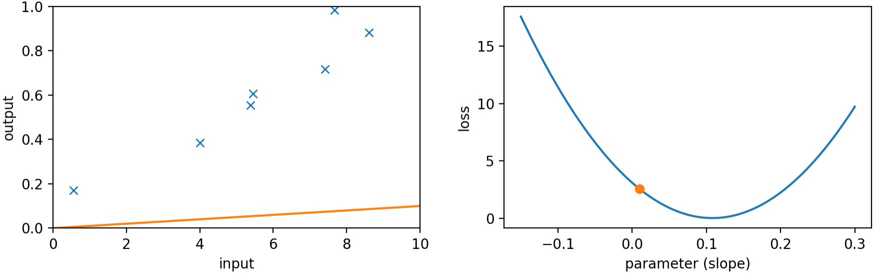

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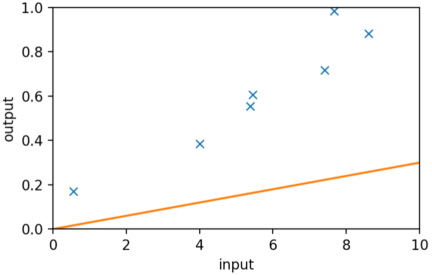

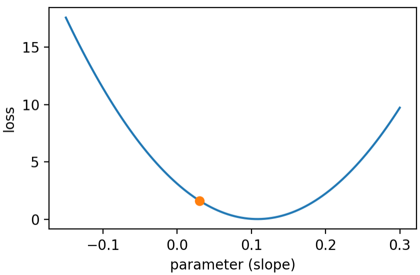

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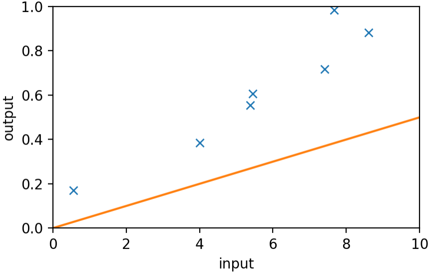

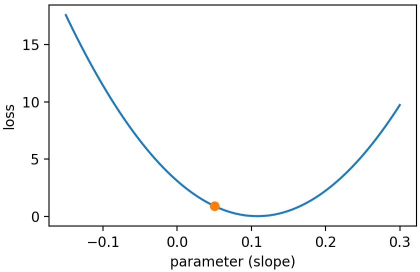

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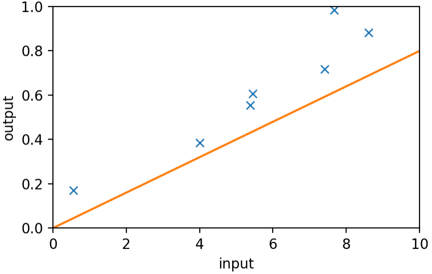

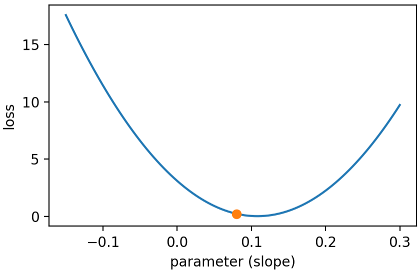

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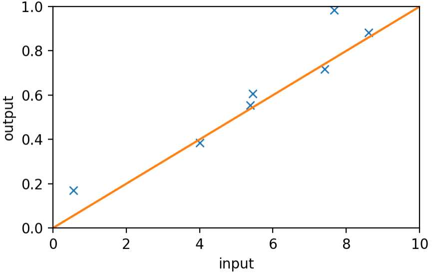

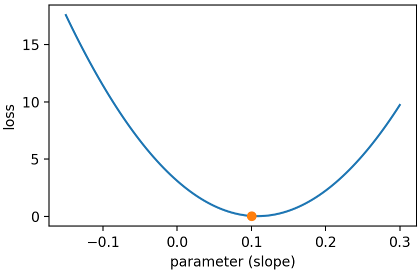

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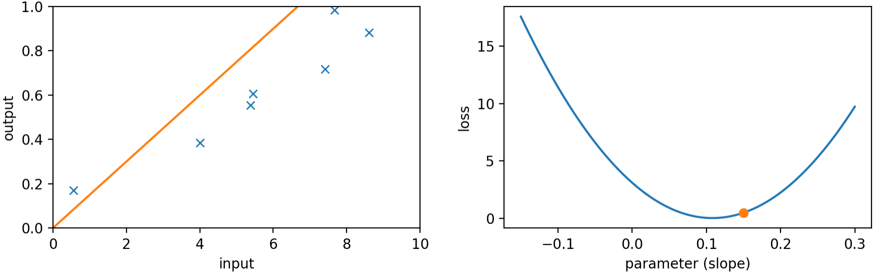

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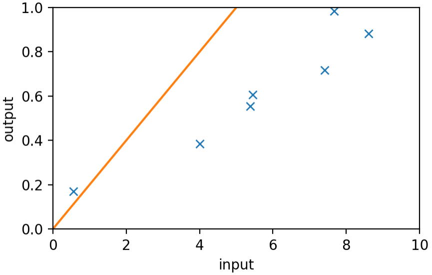

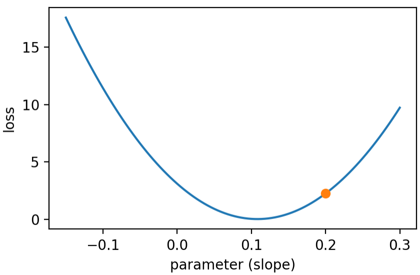

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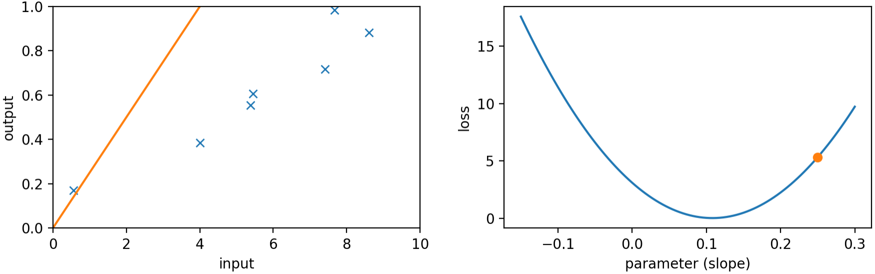

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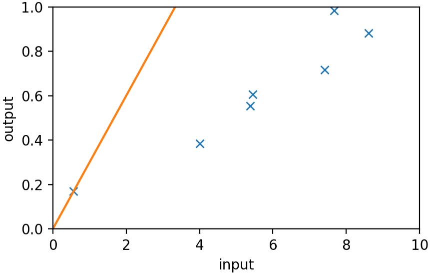

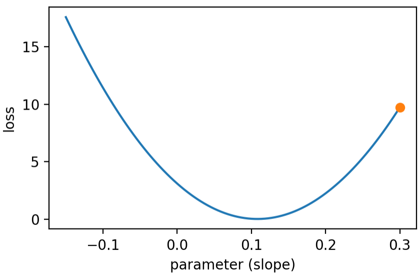

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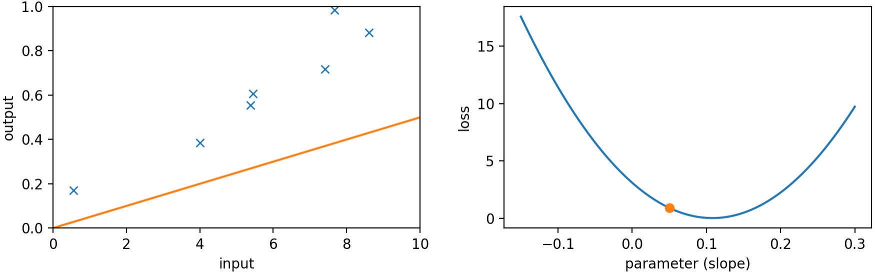

Two questions for now:

- How should we change a to make the loss smaller?
- How do we know when we can't get better?

Overview

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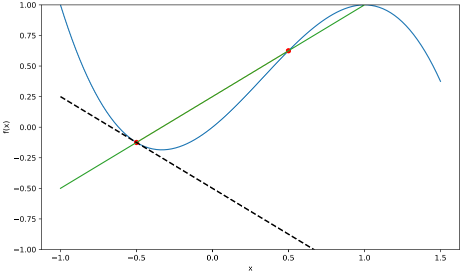
Differentiation w.r.t. vectors

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

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

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- Quotient Rule

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

Example: Scalar Chain Rule

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

Beginner

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

Advanced

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

Work it out with your neighbors

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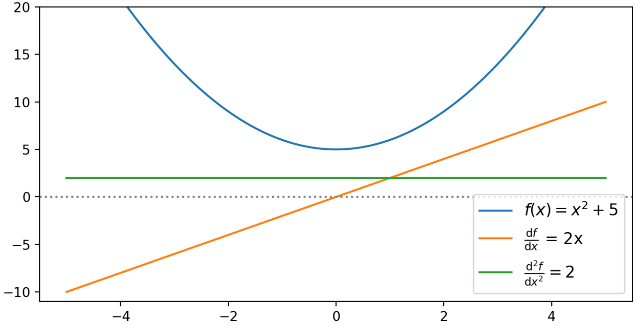
Beginner

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

Advanced

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

Finding minima



Q1: How should we change the input to reduce the output?

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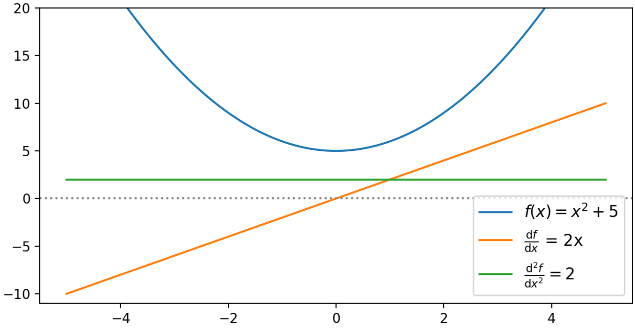

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- Find the derivative function and compute it at a point to find the point's gradient.

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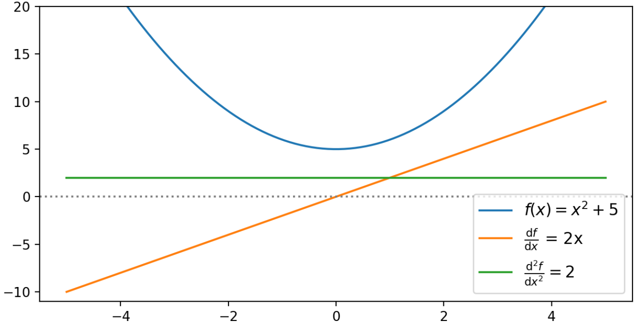

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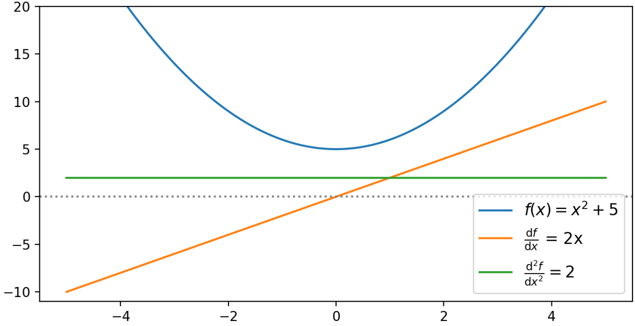
- Increase for negative gradients. Decrease for positive gradients.

Finding minima



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This is the idea behind **gradient descent**.

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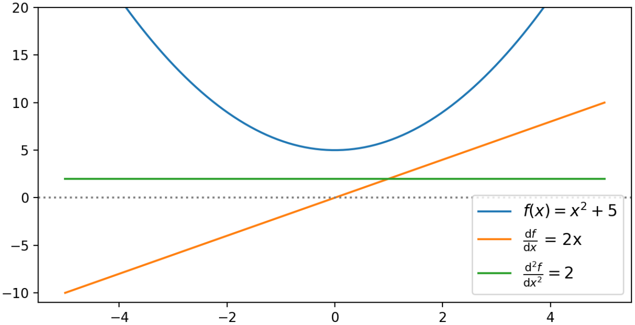

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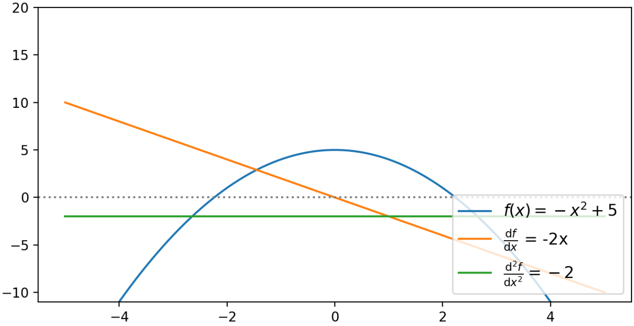

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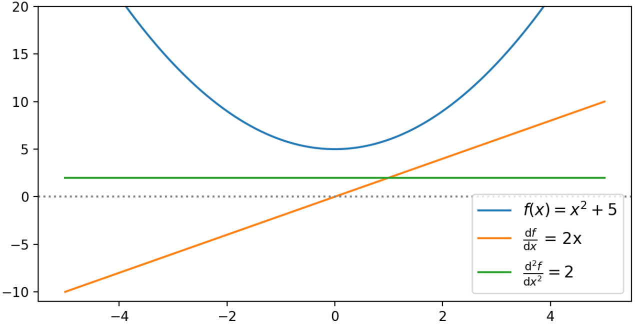

- At a minimum, there is no change we can make that lowers our function value $\implies$ gradient must be zero.
- Zero gradient is not enough!
- For minimum, $f(x)$ must go from decreasing to increasing $\implies$ gradient of gradient positive

Local and global minima

Board.

Example: Linear regression

For the example from earlier, find optimal a:

$$f(x) = a \cdot x \qquad\qquad L(a) = \sum_{n=1}^{N} (f(x_n) - y_n)^2 \tag{2}$$

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$$\frac{\mathrm{d}^2 L}{\mathrm{d}a^2} = \sum_{n=1}^{N} 2x_n^2 \geqslant 0 \tag{6}$$

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Think of a **vector** as parameterising our function:

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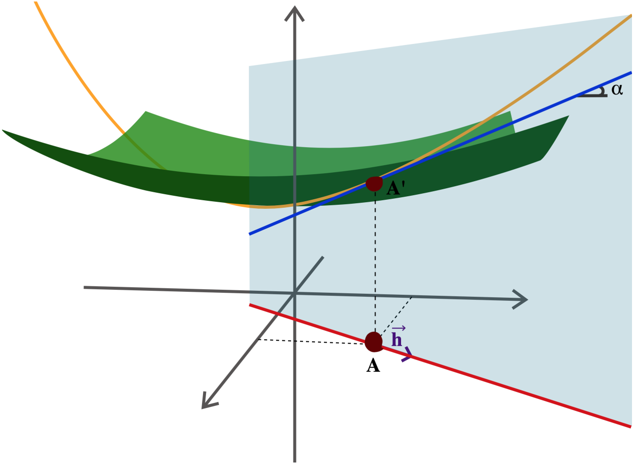
Both can be analysed by
turning the multi-D problem into many 1D problems.

Directional derivative



How does the function change if we move in a particular *direction*?

Directional derivative

Define **directional derivative** $\nabla_{\mathbf{v}} L(\boldsymbol{\theta})$ as how much the function changes if we move in direction $\mathbf{v}$:

$$\nabla_{\mathbf{v}} L(\boldsymbol{\theta}) = \lim_{h \to 0} \frac{L(\boldsymbol{\theta} + h\mathbf{v}) - L(\boldsymbol{\theta})}{h}$$

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$$= \lim_{h \to 0} \frac{L(\theta_1 + h', \theta_2 + h'\frac{v_2}{v_1}) - L(\theta_1, \theta_2 + h'\frac{v_2}{v_1})}{h'/v_1} + \frac{L(\theta_1, \theta_2 + h'') - L(\theta_1, \theta_2)}{h''/v_2}$$

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$$= \frac{\partial L}{\partial \theta_1} v_1 + \frac{\partial L}{\partial \theta_2} v_2$$

Directional derivative

Define **directional derivative** $\nabla_{\mathbf{v}} L(\boldsymbol{\theta})$ as how much the function changes if we move in direction $\mathbf{v}$:

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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):

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

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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**.

Steepest descent direction

Directional derivative:

$$\nabla_{\boldsymbol{v}} f(\boldsymbol{\theta}) = \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\theta}}\boldsymbol{v} \tag{9}$$

(inner product, row vector times column vector)

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$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\theta}}\boldsymbol{v} = |\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{\theta}}||\boldsymbol{v}|\cos\beta \tag{10}$$

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- Choose unit vector $\boldsymbol{v}$

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- Angle between vectors β should be zero $\implies \cos\beta = 1$.

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Steepest descent points in direction of Jacobian/gradient 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

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Partial derivatives

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

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

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

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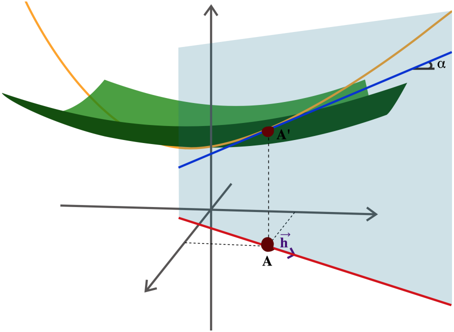
Gradient $\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \left[\frac{\partial f(x_1,x_2)}{\partial x_1} \quad \frac{\partial f(x_1,x_2)}{\partial x_2}\right] \in \mathbb{R}^{1\times 2}$

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \left[2x_1 x_2 + x_2^3 \quad x_1^2 + 3x_1 x_2^2\right]$$

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \left[2(x_1 + 2x_2^3) \quad 12(x_1 + 2x_2^3)x_2^2\right]$$

Optima, minima, maxima

What is an optimum for a function of a vector?



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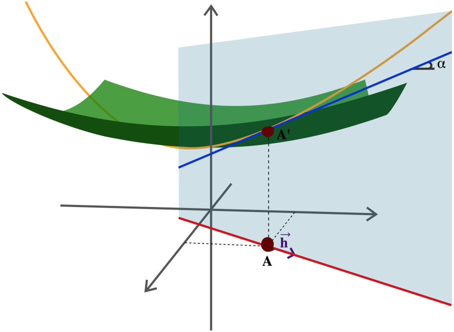

- Directional derivative should be zero *in all directions* $\implies \frac{\mathrm{d}f}{\mathrm{d}x} = \mathbf{0}$.

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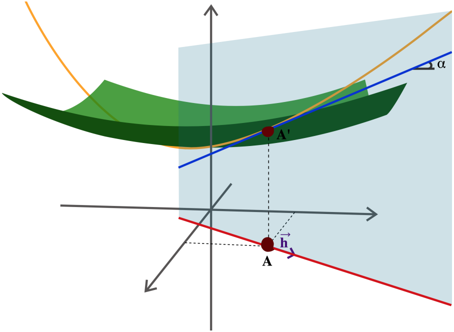

- Directional derivative should be zero *in all directions* $\implies \frac{\mathrm{d}f}{\mathrm{d}x} = \mathbf{0}$.
- For minimum: second directional derivative should be positive *in all directions*.

Summary

Motivation: Want to optimise functions of several variables

- Directional derivative
- Partial derivatives $\Longrightarrow$ gradient vector
- Steepest descent direction
- At an optimum $\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \boldsymbol{0}$