



UNIVERSITÉ  
CÔTE D'AZUR

# Lecture 1: Introduction to numerical optimization

Optimization for data sciences

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*inria*



What is optimization?

- Reduce the complexity/overhead of a problem
  - E.g. Network quantization
  - E.g. Computational optimization
- Find the best solution to a problem
  - Numerical optimization
  - Evaluate solutions according to a criterion
  - Look at solutions from some given space of possible solutions to consider

- Reduce the complexity/overhead of a problem
  - E.g. Network quantization
  - E.g. Computational optimization
- **Find the best solution to a problem**
  - **Numerical optimization**
  - **Evaluate solutions according to a criterion**
  - **Look at solutions from some given space of possible solutions to consider**

- You have a balance
  - With 5 weights (1kg, 5kg, 10kg, 50kg, 100kg)
- Object X with unknown mass
- Goal: Find the closest weight



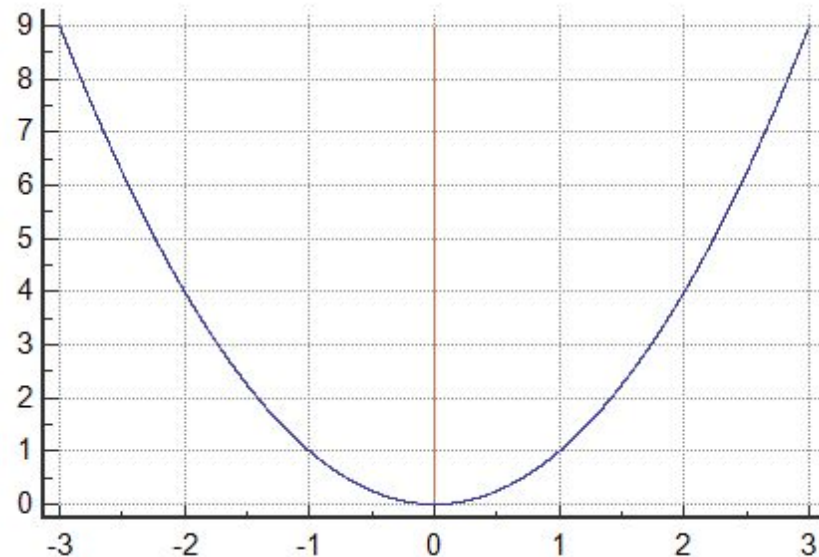
- You have a balance
  - With 5 weights (1kg, 5kg, 10kg, 50kg, 100kg)
- Object X with unknown mass
- Goal: Find the closest weight
  - Criterion: balance reaction



- You have a balance
  - With infinite set of 1kg weight
- Object X with unknown mass
- Goal: Find the closest weight
  - Criterion: balance reaction

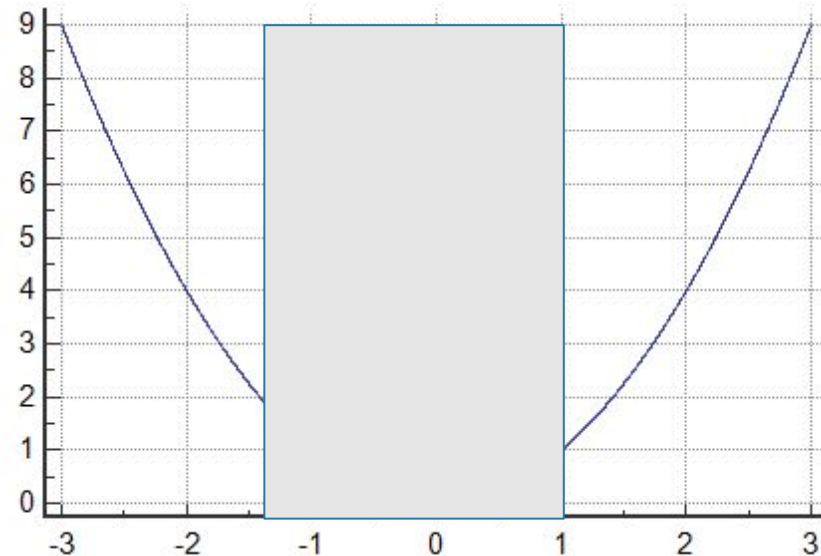


- You have the graph of balance responses
  - “Response for every possible weight values”
- Goal: Find the closest weight
  - Look at the minimum on the graph

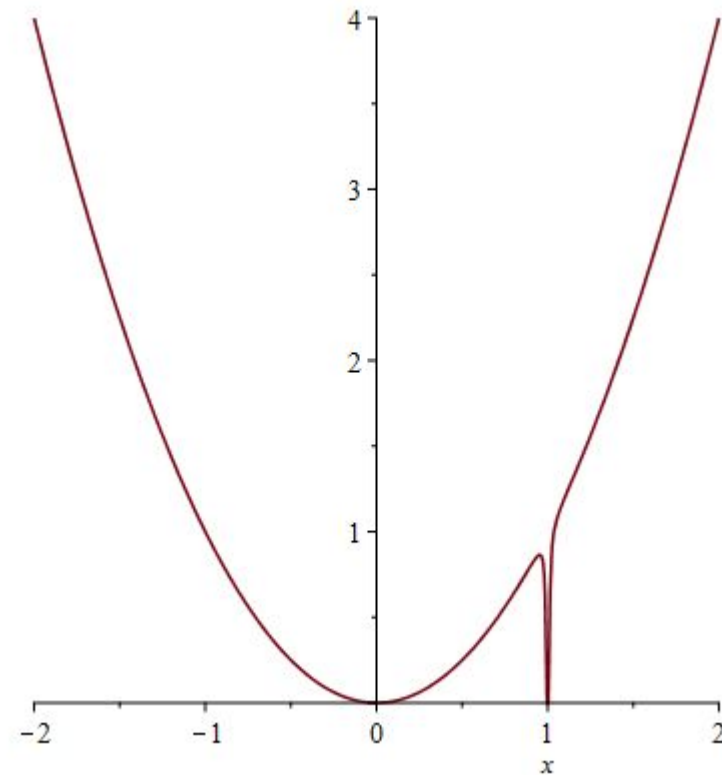




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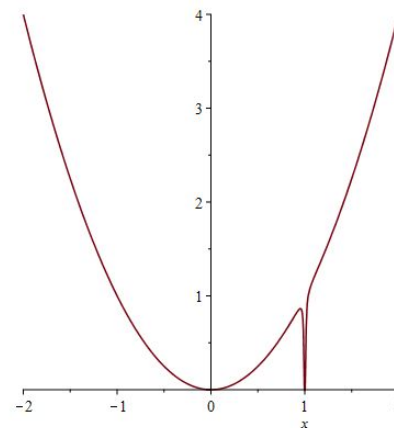
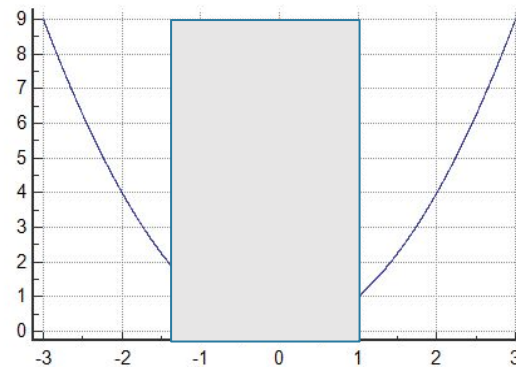
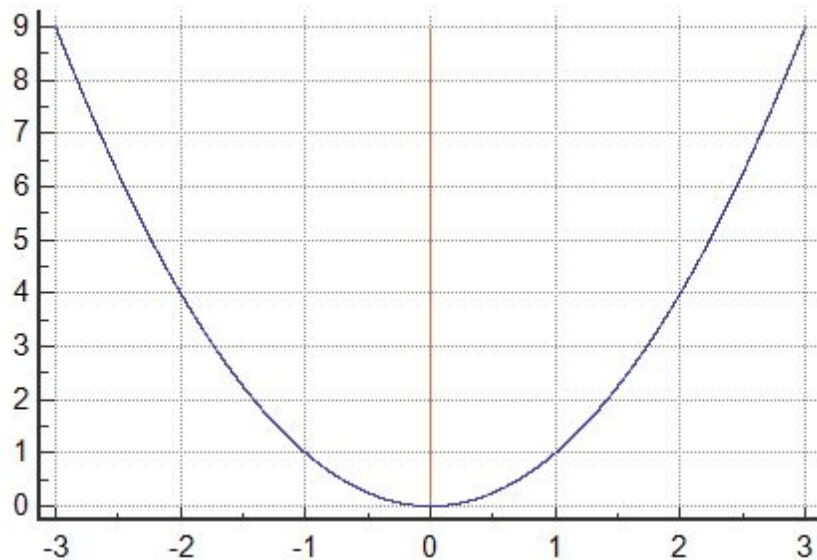


- Minimize a quantity  $f_0(x)$ 
  - Under inequality and equality constraints
  - Constraints define a domain  $D$
  - Could have no constraint except  $x$  in  $D$

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & g_i(x) = 0, \quad i = 1, \dots, p\end{array}$$



# Can you formalize these problems?



- Invisible engine powering every ML application
  - What actually gives you your good model
  - Better algorithms are constantly found
  - Significant impact on results
- People like to ignore it
  - But it explains a lot about how networks are trained
  - Some problem can be solved easily

- **Introduction to optimization**
  - **A few problems of interest**
  - **Quick mathematical refresher**
- Easy problems
- Duality (for easy problems)
- Descent methods for the general case
- Backpropagation
- Some more properties on stochastic gradient descent

- **Introduction to optimization**
  - **A few problems of interest**
  - **Quick mathematical refresher**
- Convex problems (following Boyd and Vandenberghe)
- Duality (for convex problems)
- Solutions for the convex case
- Descent methods in the general case
- Backpropagation
- Some more properties on stochastic gradient descent

- Reports on lab sessions
  - Labs on jupyter notebooks
    - Not every session
  - Explain the code done in the session
  - Summarize what is done in the practical
- Written Exam
  - Theoretical questions
  - We will do exercises in class



# 0. Some classical optimization problems

$$\begin{array}{ll}\text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & g_i(x) = 0, \quad i = 1, \dots, p\end{array}$$

- ▶  $x \in \mathbf{R}^n$  is (vector) variable to be chosen ( $n$  scalar variables  $x_1, \dots, x_n$ )
- ▶  $f_0$  is the **objective function**, to be minimized
- ▶  $f_1, \dots, f_m$  are the **inequality constraint functions**
- ▶  $g_1, \dots, g_p$  are the **equality constraint functions**
- ▶ variations: maximize objective, multiple objectives, ...

- ▶  $x$  represents some **action**, *e.g.*,
  - trades in a portfolio
  - airplane control surface deflections
  - schedule or assignment
  - resource allocation
- ▶ constraints limit actions or impose conditions on outcome
- ▶ the smaller the objective  $f_0(x)$ , the better
  - total cost (or negative profit)
  - deviation from desired or target outcome
  - risk
  - fuel use

- ▶  $x$  represents the **parameters** in a model
- ▶ constraints impose requirements on model parameters (e.g., nonnegativity)
- ▶ objective  $f_0(x)$  is sum of two terms:
  - a prediction error (or loss) on some observed data
  - a (regularization) term that penalizes model complexity

- ▶ model an entity as taking actions that solve an optimization problem
  - an individual makes choices that maximize expected utility
  - an organism acts to maximize its reproductive success
  - reaction rates in a cell maximize growth
  - currents in a circuit minimize total power
- ▶ (except the last) these are **very crude** models
- ▶ and yet, they often work very well

- ▶ instead of saying how to choose (action, model)  $x$
- ▶ you articulate what you want (by stating the problem)
- ▶ then let an algorithm decide on (action, model)  $x$

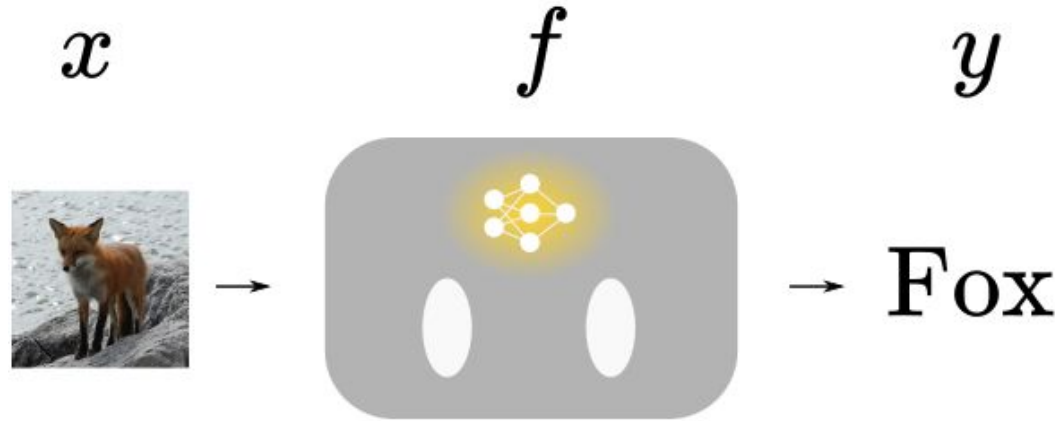
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- ▶ you articulate what you want (by stating the problem)
- ▶ then let an algorithm decide on (action, model)  $x$

## What do we do in Deep Learning?

# 1. The statistical learning problem: Empirical Risk Minimization







- Find (robot)  $f$  that classifies images well
  - Often based on neural networks

$$\forall (x, y) \in \mathcal{D}, f(x) = y$$

- Definitions
  - $X$  set of inputs
  - $Y$  set of labels
  - $\Omega = X \times Y$
  - $\mathcal{D}$  Distribution over  $\Omega$  with probability measure  $p$
- Find function  $f: X \rightarrow Y$  such that

$$\forall (x, y) \in \mathcal{D}, f(x) = y$$

- Finding exact correspondence functions is not always the thing to do
  - No exact matching
  - Other definitions of good solutions
  - Need to use restricted function space
    - Parametric function space

$$\mathcal{F} = \{f_{\theta} | \theta \in \mathbb{R}^d\}$$

- ✓ ● Introduce an assessment of how “good”  $f$  is with a loss  $l$  so that we try to have the lowest quantity  $l(f(x), y)$

- Definitions
  - $X$  set of inputs
  - $Y$  set of labels
  - $\Omega = X \times Y$
  - $\mathcal{D}$  Distribution over  $\Omega$  with probability measure  $p$
  - $l$  loss function assessing fit of  $f(x)$  to  $y$
  - Find  $f$  in function space  $\mathcal{F} = \{f_\theta | \theta \in \mathbb{R}^d\}$

- ✓ ● Minimize the **Risk** over the distribution

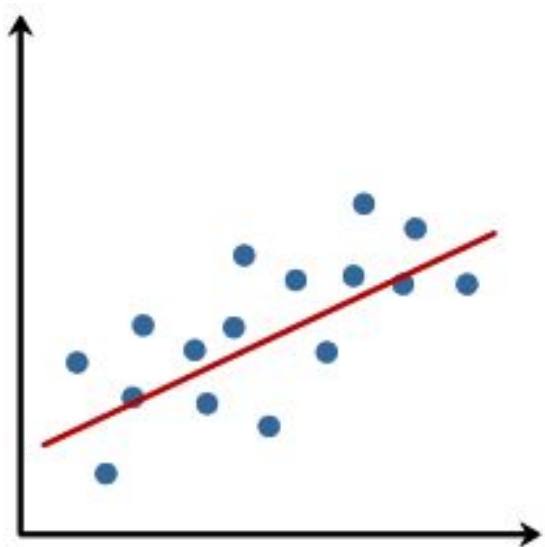
$$\min_{\theta} \mathbb{E}_{x, y \sim \mathcal{D}} [l(f_{\theta}(x), y)]$$

- Problem: we do not know  $\mathcal{D}$  !
  - Solved problem otherwise...
  - Evaluating the risk requires this distribution
- Solution: Use a dataset  $D$  of  $(x,y)$  sampled from  $\mathcal{D}$ 
  - **Empirical Risk Minimization**
  - If the  $(x,y)$  are i.i.d drawn from  $\mathcal{D}$  can be expressed as a mean over the dataset

$$\min_{\theta} \hat{\mathcal{R}}_{\theta} = \frac{1}{N} \sum_{i=0, \dots, N-1} l(f_{\theta}(x_i), y_i)$$

- Core problem: Find function matching inputs to outputs for any  $(x,y)$  of the target distribution
- Optimize over family of parametric functions
  - Assess functions with loss criterion
- Minimize the Risk function
  - Empirical Risk Minimization in practice

## 2. Example: linear regression



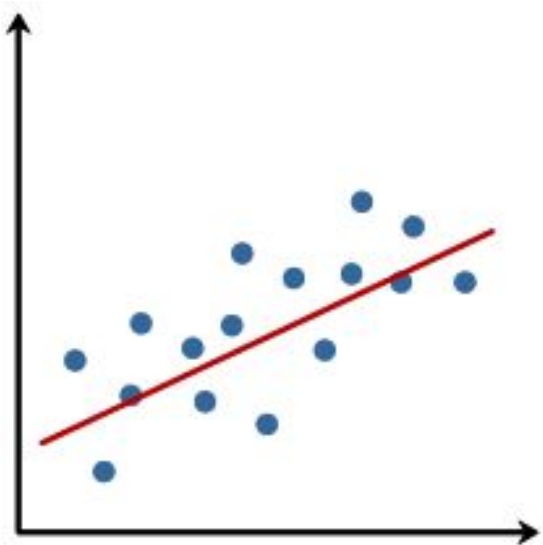
- Linearly correlated data
  - Input  $x$  (e.g. Voltage)
  - Output  $y$  (e.g. Intensity)
- Simple family of linear functions
  - Find linear coefficient

$$f_{\theta}(x) = \theta x$$



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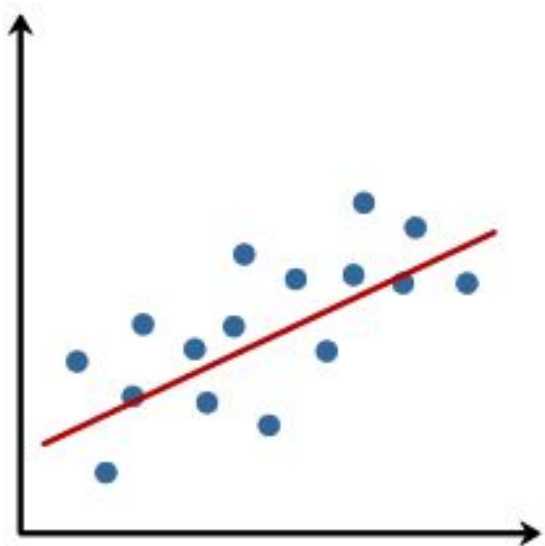
- Minimize the risk

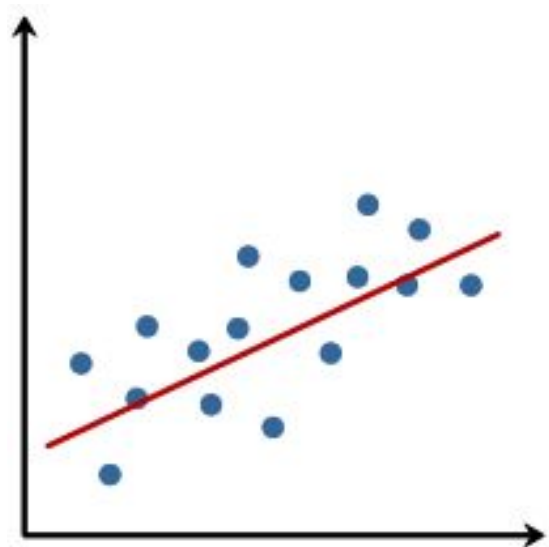


$$f_{\theta}(x) = \theta x$$

- Minimize the risk

$$\min_{\theta} \hat{\mathcal{R}}_{\theta} = \frac{1}{N} \sum_{i=0, \dots, N-1} (y_i - \theta x_i)^2$$



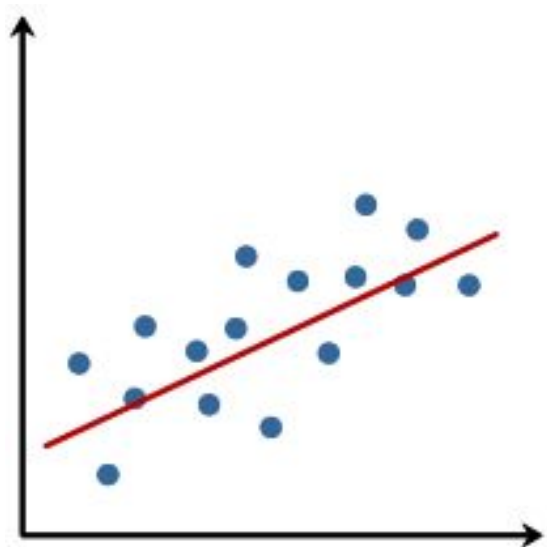


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- How?



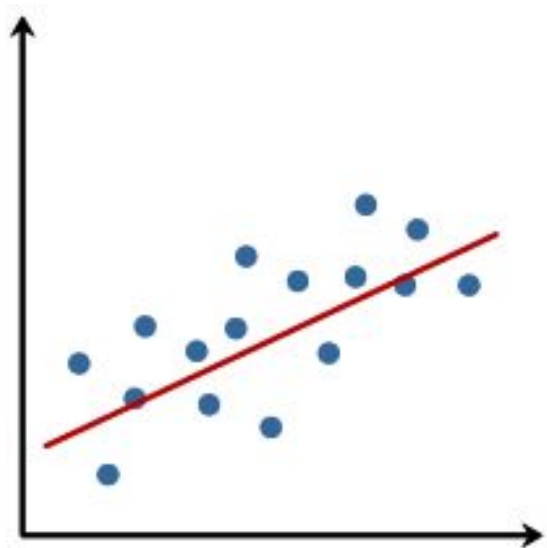
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- How?
  - Convex function!





$$f_{\theta}(x) = \theta x$$

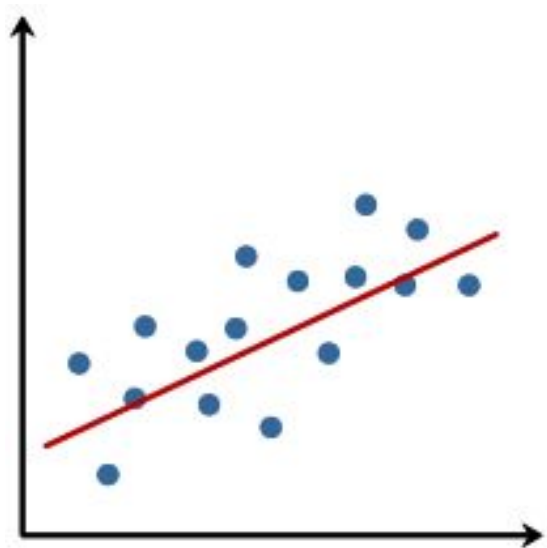
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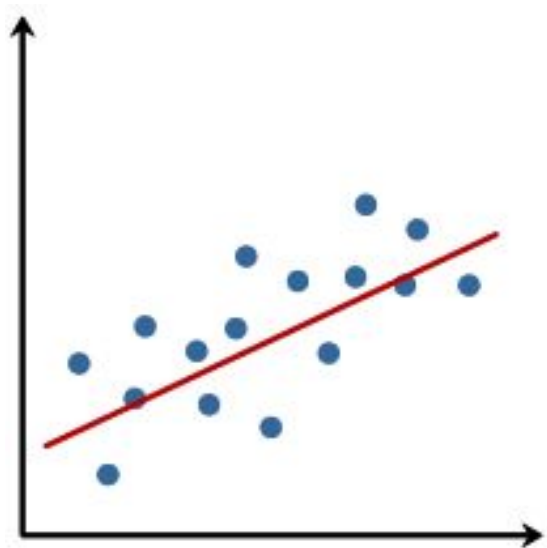
$$\min_{\theta} \hat{\mathcal{R}}_{\theta} = \frac{1}{N} \sum_{i=0, \dots, N-1} (y_i - \theta x_i)^2$$

- How?
  - Convex function!
  - Zero out the gradient!

$$\min_{\theta} \mathcal{R}_{\theta} = \frac{1}{N} \sum_{i=0, \dots, N-1} (y_i - \theta x_i)^2$$

- Deriving gives condition:



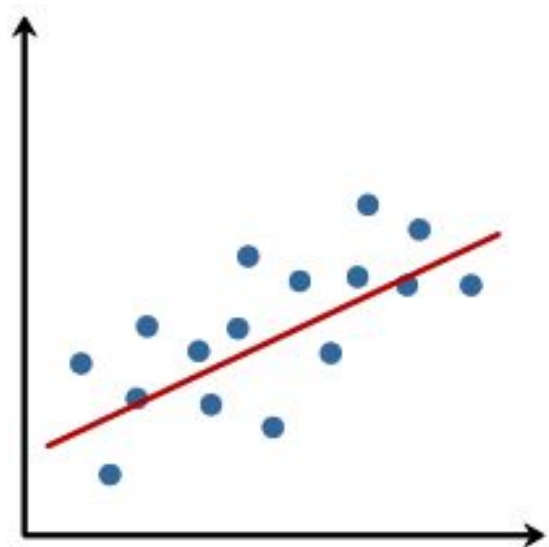


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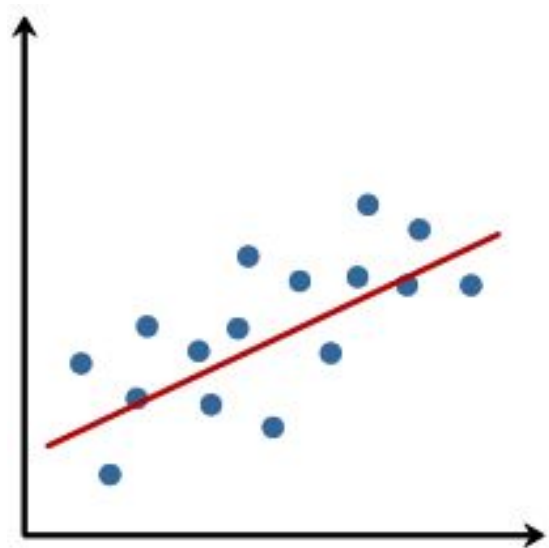
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- Solve for  $\theta$
-



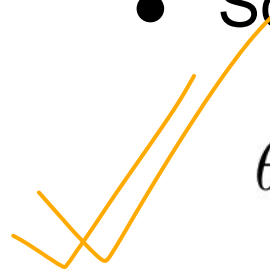


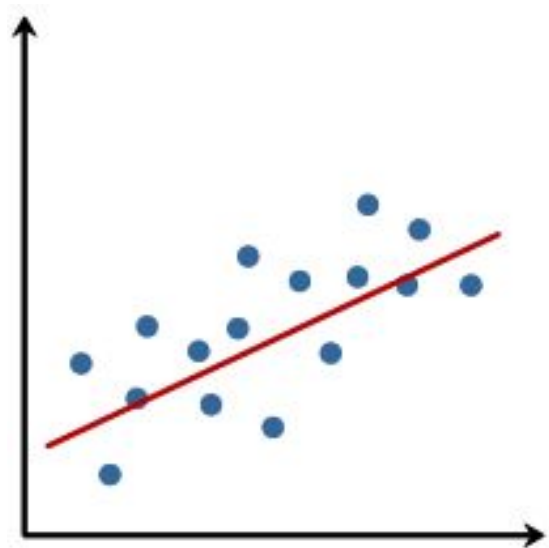
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$$\theta = \frac{\sum_{i=0, \dots, N-1} y_i x_i}{\sum_{i=0, \dots, N-1} x_i^2}$$



$$f_{\theta}(x) = \theta x$$

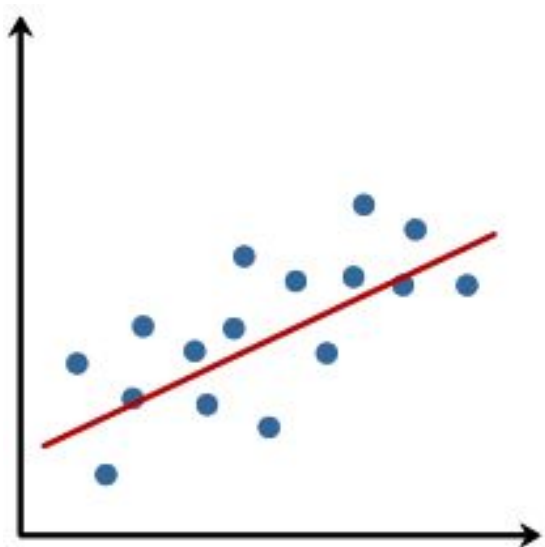
$$\theta = \frac{\sum_{i=0, \dots, N-1} y_i x_i}{\sum_{i=0, \dots, N-1} x_i^2}$$

- If perfectly linear correlation

$$\theta = a \frac{\sum_{i=0, \dots, N-1} x_i^2}{\sum_{i=0, \dots, N-1} x_i^2} = a$$

- Core problem: Find the right function in a family
  - Boils down to finding the right parameters
  - Depends on the data available
- Minimizing the risk is finding the best fit solution
  - Shown on univariate linear regression
  - Generalizes to multiple dimensions
  - ***Pointless if the data does not fit!***

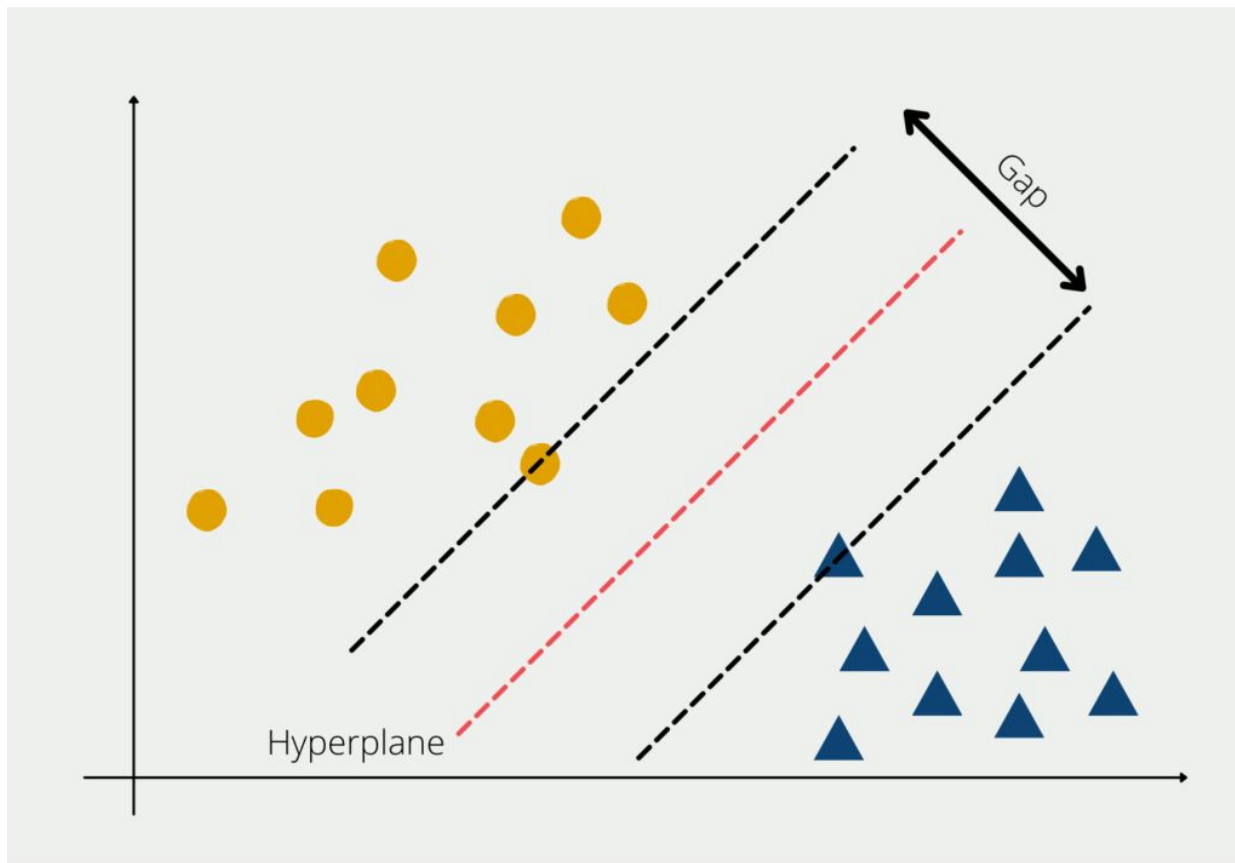
### 3. A few classical functions



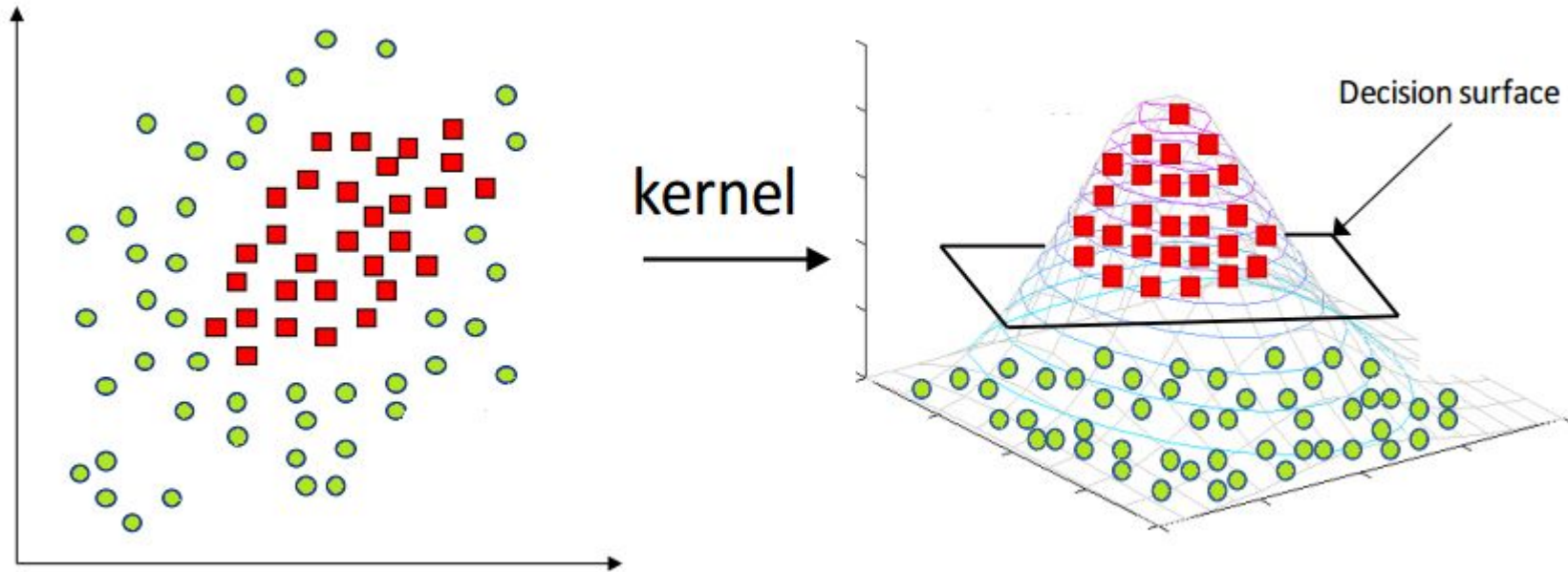
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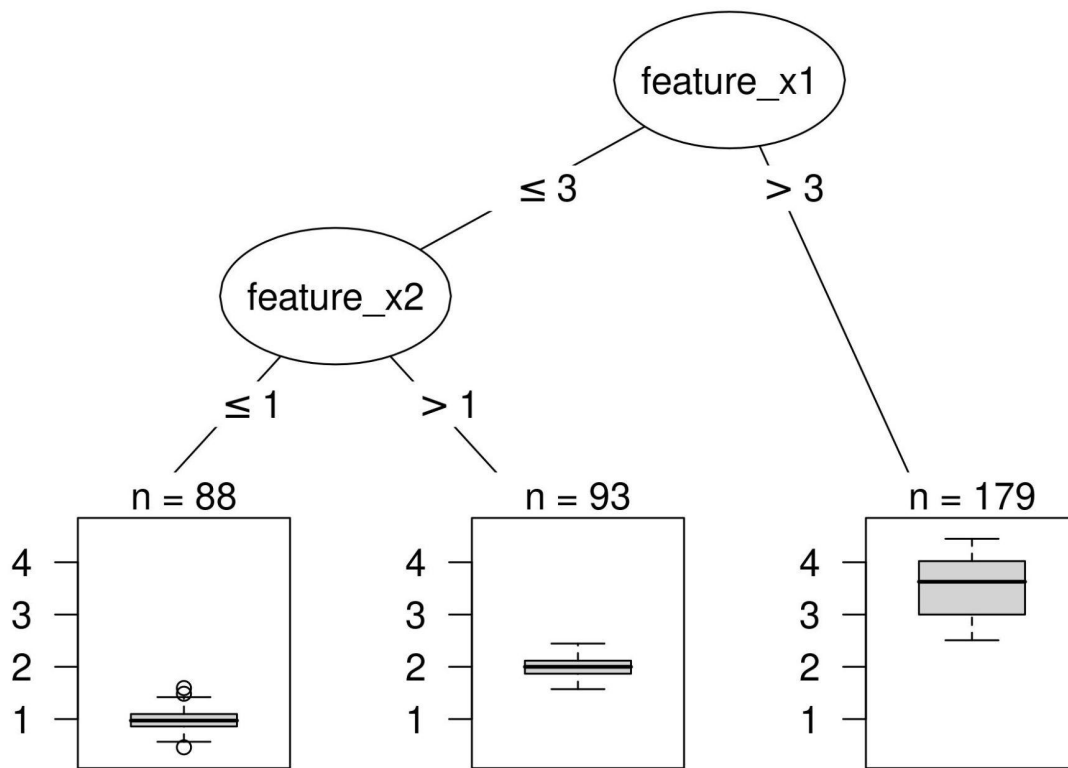
$$f_{\theta}(x) = \theta x$$

# Separating hyperplane (SVM)

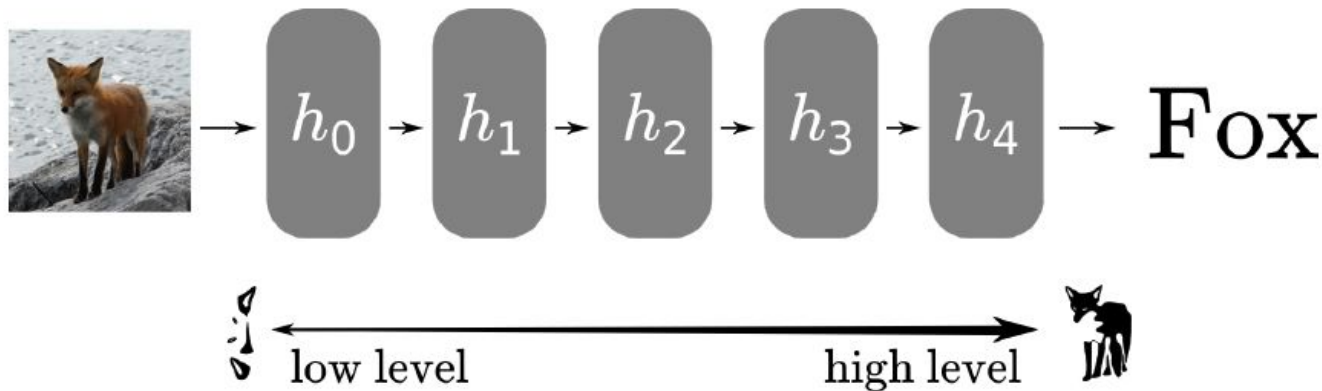


# Separating hyperplane (SVM with kernel)



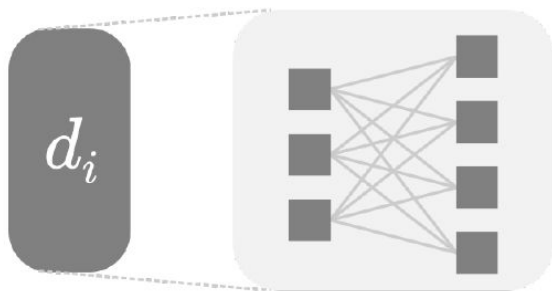
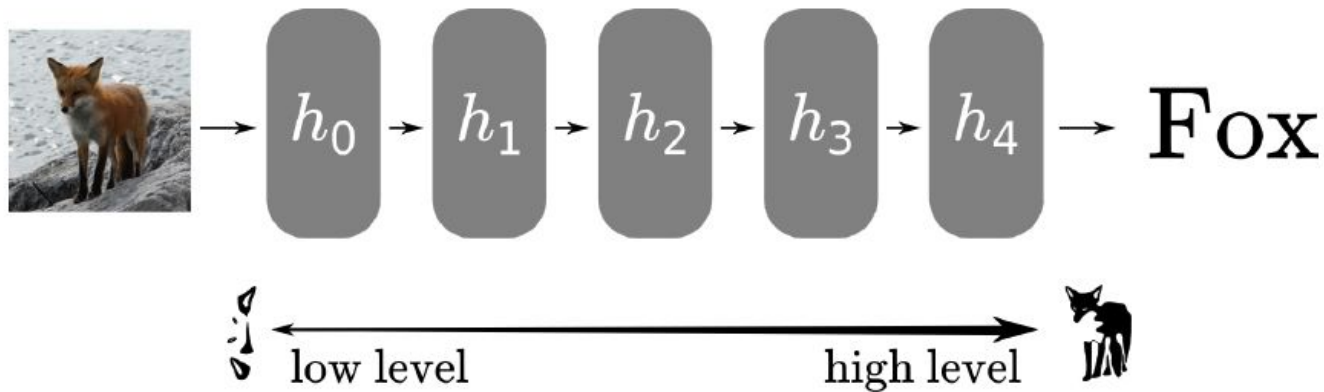




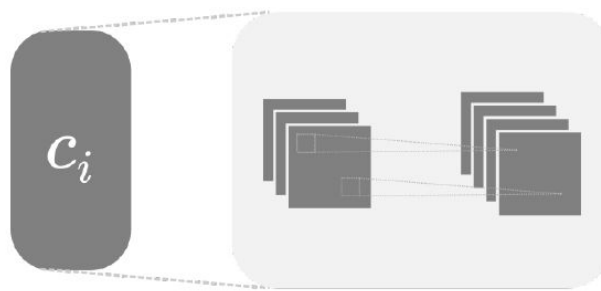


- Neural networks are sequences of simple functions

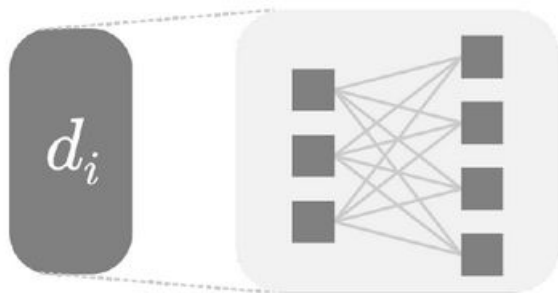
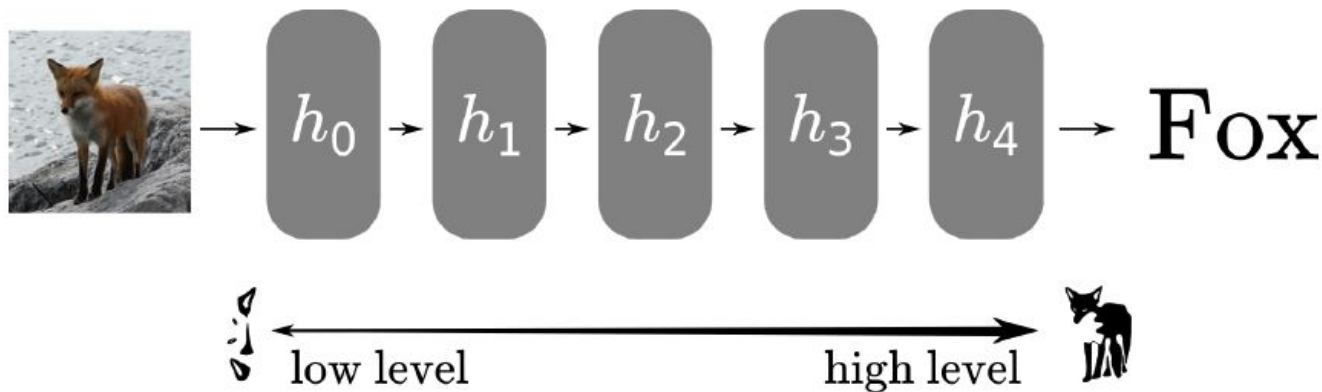
$$f_{\theta} = h_{\theta}^0 \circ h_{\theta}^1 \circ \dots \circ h_{\theta}^{L-1}$$



(a) Dense layer



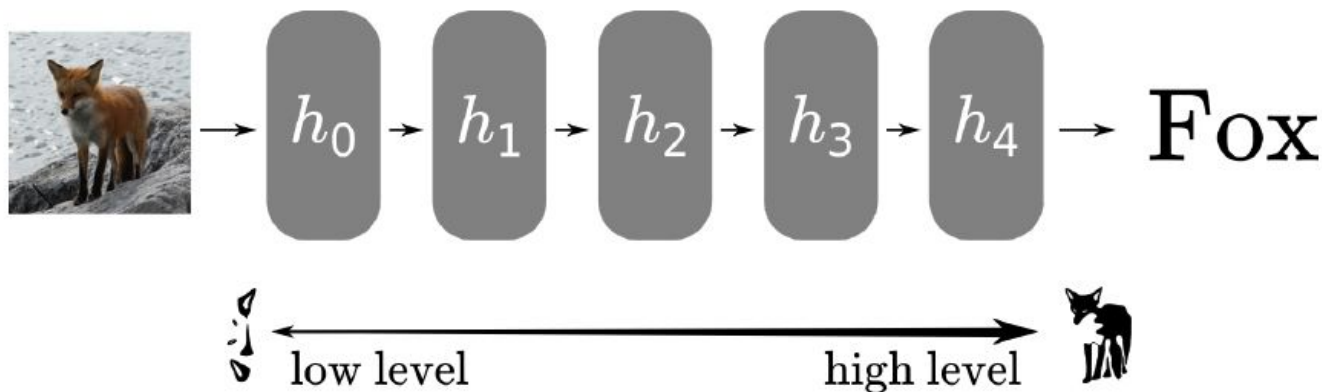
(b) Convolutional layer



(a) Dense layer

$$d_{\theta}(x) = \sigma(W_{\theta}x^T + b_{\theta})$$

$$\sigma(x) = \text{ReLU}(x) = \max(0, x)$$

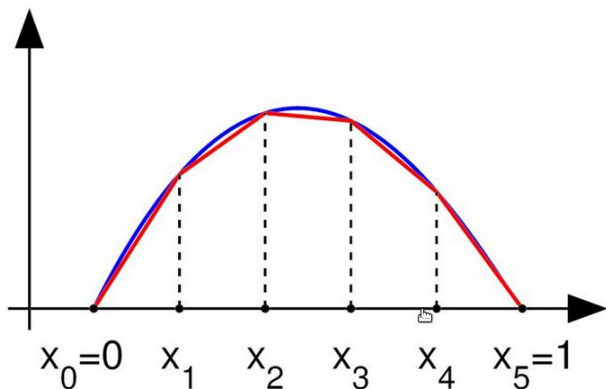
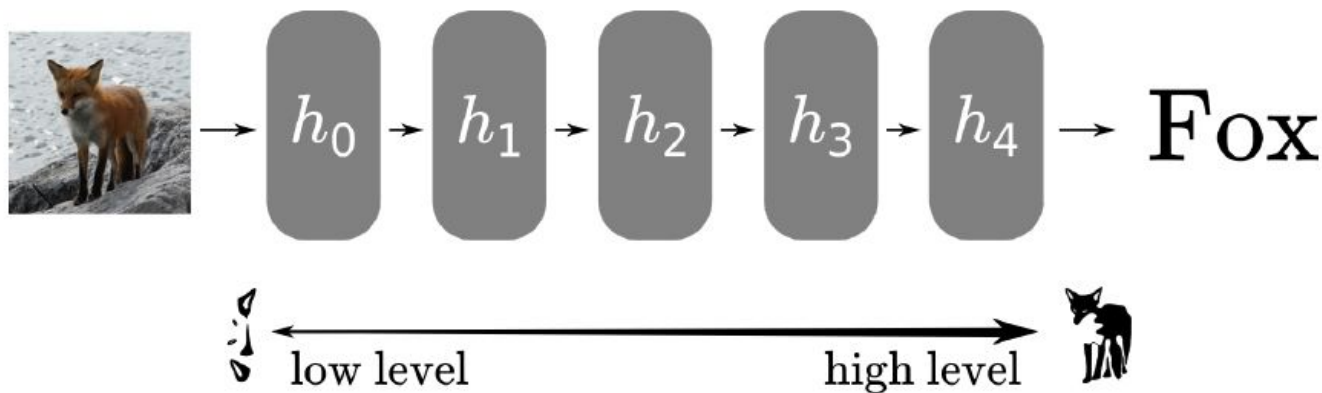


$$d_{\theta}(x) = \sigma(W_{\theta}x^T + b_{\theta})$$

$$\sigma(x) = \text{ReLU}(x) = \max(0, x)$$

**Piecewise linear!**

*Individual layers are piecewise linear, composition preserves piecewise linearity*



- Highly expressive
  - Can fit many types of distributions

- Upper bound on number of linear pieces wrt number of layers and units per layer
  - Exercise: Proof by recurrence
- Similar properties with other deep networks
  - Piecewise polynomial with other  $\sigma$
  - Similar reasoning on convolutional layers
- Universal approximation theorem [Cybenko '89]
  - Proof by contradiction

- Neural networks composed of simple functions
  - Typical linear layer operations
  - Non-linear activation functions
- High expressive power
  - Universal approximation with enough neurons
  - ReLU Feedforward networks are piecewise linear

# Mathematical foundations



- Set of vectors  $V$ 
  - Preserved by addition and scalar product
  - We work in finite dimensions
- Addition operation between vectors
- Scalar product between real numbers and vectors

# 1. Inner product, norms and basic topology



$$\langle x, y \rangle = x^T y = \sum_{i=1}^n x_i y_i,$$

- Traditional product between vectors
- Elementwise product into sum

$$\|x\|_2 = (x^T x)^{1/2} = (x_1^2 + \dots + x_n^2)^{1/2}.$$

- Inner product of  $x$  with itself
- Classical euclidean norm from traditional geometry

$$\langle X, Y \rangle = \text{tr}(X^T Y) = \sum_{i=1}^m \sum_{j=1}^n X_{ij} Y_{ij},$$



- Let  $X$  and  $Y$  be matrices  $m \times n$
- Sum of elementwise products
  - Matricial inner product

$$\|X\|_F = (\text{tr}(X^T X))^{1/2} = \left( \sum_{i=1}^m \sum_{j=1}^n X_{ij}^2 \right)^{1/2} .$$

- Let  $X$  be a matrix  $m \times n$
- Product of  $X$  to itself again
  - Euclidean norm on matrix space

A function  $f : \mathbf{R}^n \rightarrow \mathbf{R}$  with  $\text{dom } f = \mathbf{R}^n$  is called a *norm* if

- $f$  is nonnegative:  $f(x) \geq 0$  for all  $x \in \mathbf{R}^n$
- $f$  is definite:  $f(x) = 0$  only if  $x = 0$
- $f$  is homogeneous:  $f(tx) = |t|f(x)$ , for all  $x \in \mathbf{R}^n$  and  $t \in \mathbf{R}$
- $f$  satisfies the triangle inequality:  $f(x + y) \leq f(x) + f(y)$ , for all  $x, y \in \mathbf{R}^n$


$$\text{dist}(x, y) = \|x - y\|.$$


- Norm of the difference vector
- Easily shown to be equivalent to standard distance definition for euclidean norm



$$\mathcal{B} = \{x \in \mathbf{R}^n \mid \|x\| \leq 1\},$$

- All elements with norm less or equal to 1
- Often used for a number of things
- Immediately defined by simple constraint

Suppose that  $\|\cdot\|_a$  and  $\|\cdot\|_b$  are norms on  $\mathbf{R}^n$ . A basic result of analysis is that there exist positive constants  $\alpha$  and  $\beta$  such that, for all  $x \in \mathbf{R}^n$ ,

$$\alpha\|x\|_a \leq \|x\|_b \leq \beta\|x\|_a.$$

- Norm on real vector space tend to have similar properties (convergence, ...)
  - Given by the inequalities

An element  $x \in C \subseteq \mathbf{R}^n$  is called an interior point of  $C$  if there exists an  $\epsilon > 0$  for which

$$\{y \mid \|y - x\|_2 \leq \epsilon\} \subseteq C,$$

- Interior are points  $x$  such that there is a ball/neighborhood centered on  $x$  is entirely in  $C$ 
  - Not all sets have an non-empty interior!



- $\text{Int}(C) = C$

- All the points of  $C$  are in its interior
- You can find a neighborhood of any point  $x$  in  $C$  that remains in  $C$

$$\text{cl } C = \mathbf{R}^n \setminus \text{int}(\mathbf{R}^n \setminus C),$$

- Closure is the complement of the interior of the complement
- Any sequence of the  $\text{cl } C$  that converges converges in the closure

- Complement is an open set
  - Similar to the closure definition
- $C \mid C = C$ 
  - Same thing as interior and open sets

$$\mathbf{bd} C = \mathbf{cl} C \setminus \mathbf{int} C.$$

- Points “on the edge” of the set
  - Outer envelope

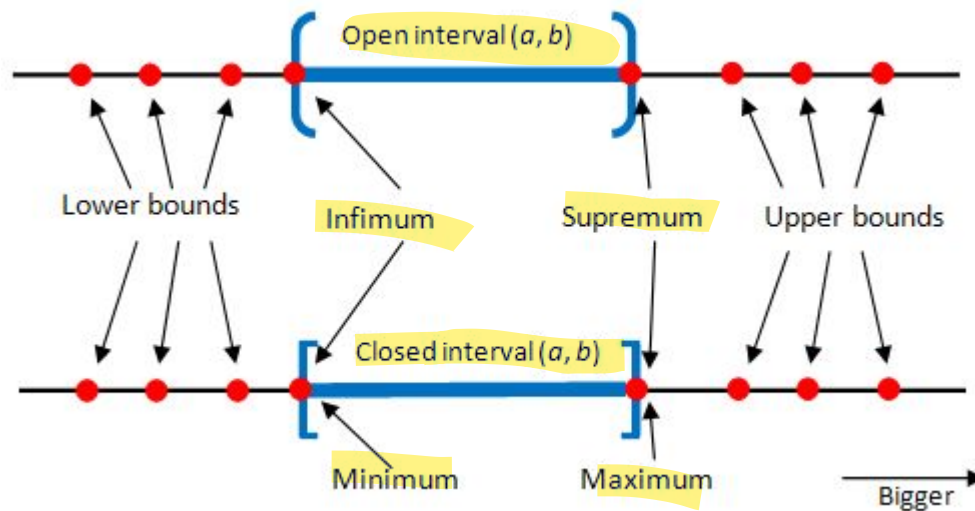
A *boundary point*  $x$  (i.e., a point  $x \in \mathbf{bd} C$ ) satisfies the following property: For all  $\epsilon > 0$ , there exists  $y \in C$  and  $z \notin C$  with

$$\|y - x\|_2 \leq \epsilon, \quad \|z - x\|_2 \leq \epsilon,$$

- Closed and bounded set for our purposes
  - Heine Borel
- Every sequence has a convergent subsequence
  - Useful property!



- Supremum
  - Smallest upper bound
- Infimum
  - Largest lower bound



## 2. Function

$$f : A \rightarrow B$$

- Function maps set A to set B
  - f is the function
  - A is the input set
  - B is the output set
- Dom f is the set of inputs f is defined over
  - Usually A unless specified otherwise

A function  $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$  is *continuous* at  $x \in \mathbf{dom} f$  if for all  $\epsilon > 0$  there exists a  $\delta$  such that

$$y \in \mathbf{dom} f, \quad \|y - x\|_2 \leq \delta \implies \|f(y) - f(x)\|_2 \leq \epsilon.$$

- Can be described in terms of limits

$$\lim_{i \rightarrow \infty} f(x_i) = f\left(\lim_{i \rightarrow \infty} x_i\right).$$

- $F$  is continuous if it is continuous for every  $x$

$$\min_{x \in \Omega} f(x) \quad (1)$$

We say that  $x^* \in \Omega$  is

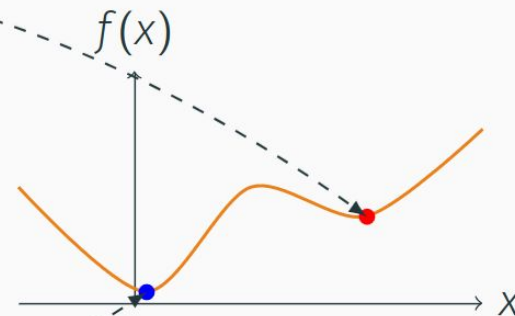
- a **local** minimizer of (Opt), if there exists a neighborhood  $\mathcal{O}$  of  $x^*$  such that

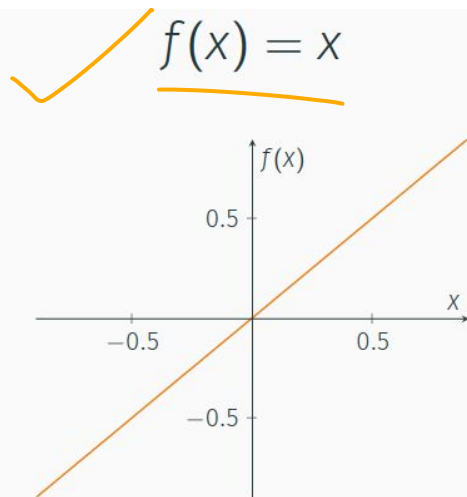
$$\forall x \in \Omega \cap \mathcal{O}, \quad f(x) \geq f(x^*)$$

- a **(global)** minimizer if

$$\forall x \in \Omega, \quad f(x) \geq f(x^*)$$

The set of global minimizers of  $f$  is denoted  $\operatorname{argmin} f$

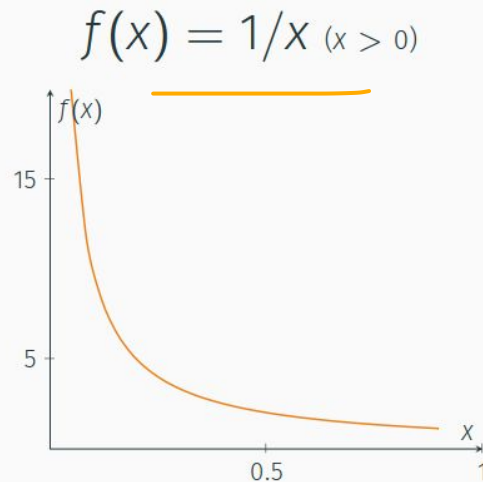




Unbounded from below

$$\inf f = -\infty$$

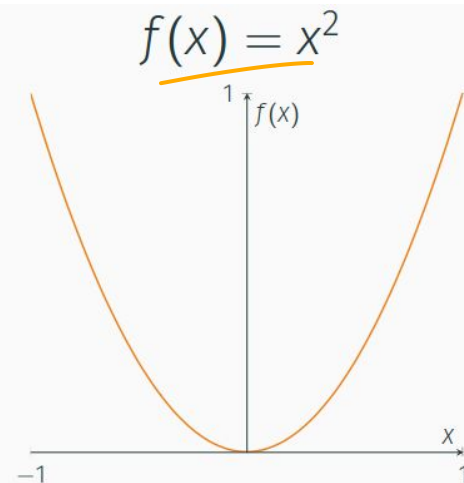
$$\operatorname{argmin} f = \emptyset$$



Bounded but not achieved

$$\inf f = 0$$

$$\operatorname{argmin} f = \emptyset$$



Bounded and achieved

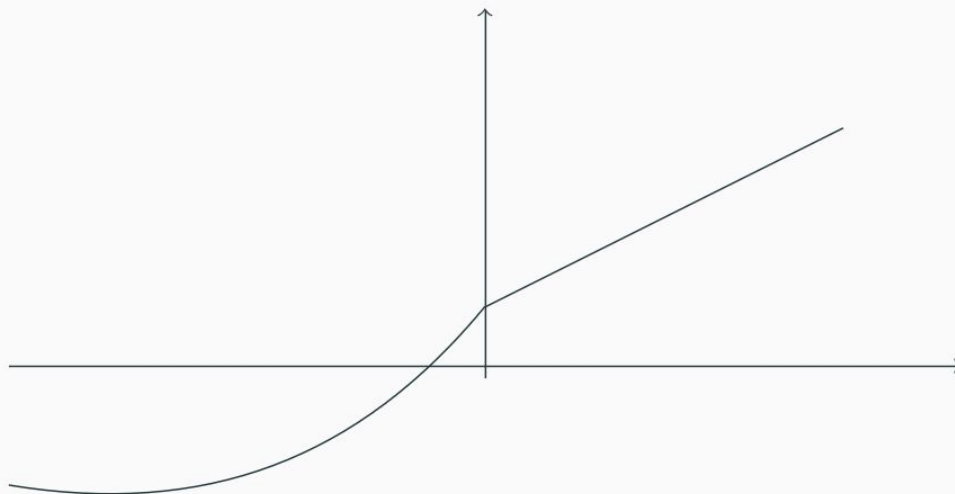
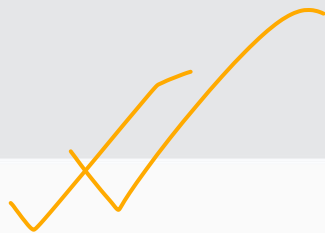
$$\inf f = 0$$

$$\operatorname{argmin} f = \{0\}$$

## Definition

$\phi : \Omega \subseteq E \rightarrow F$  is  $L$ -Lipschitz continuous if

$$\forall x, y \in \Omega, \quad \|\phi(x) - \phi(y)\|_E \leq L \|x - y\|_F.$$



(live)



Suppose  $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$  and  $x \in \text{int dom } f$ . The function  $f$  is differentiable at  $x$  if there exists a matrix  $Df(x) \in \mathbf{R}^{m \times n}$  that satisfies

$$\lim_{z \in \text{dom } f, z \neq x, z \rightarrow x} \frac{\|f(z) - f(x) - Df(x)(z - x)\|_2}{\|z - x\|_2} = 0,$$

- $Df$  (or Jacobian) is the derivative at  $x$
- $f$  is differentiable if  $\text{dom } f$  open and  $f$  has a derivative at every  $x$



- F can be approximated locally
  - Start at value at point
  - Move a little along line given by derivatives

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left. \frac{d^n f(x)}{dx^n} \right|_{x=x_0} (x-x_0)^n$$

$$f(x) = f(x_0) + \left. \frac{df(x)}{dx} \right|_{x=x_0} (x-x_0) + \frac{d^2 f(x)}{2! dx^2} \Big|_{x=x_0} (x-x_0)^2 + \dots$$

$y = f(x)$	$\frac{dy}{dx} = f'(x)$
$k$ , any constant	0
$x$	1
$x^2$	$2x$
$x^3$	$3x^2$
$x^n$ , any constant $n$	$nx^{n-1}$
$e^x$	$e^x$
$e^{kx}$	$ke^{kx}$
$\ln x = \log_e x$	$\frac{1}{x}$
$\sin x$	$\cos x$
$\sin kx$	$k \cos kx$
$\cos x$	$-\sin x$
$\cos kx$	$-k \sin kx$
$\tan x = \frac{\sin x}{\cos x}$	$\sec^2 x$

$\sin^{-1} x$	$\frac{1}{\sqrt{1-x^2}}$
$\cos^{-1} x$	$\frac{-1}{\sqrt{1-x^2}}$
$\tan^{-1} x$	$\frac{1}{1+x^2}$
$\cosh x$	$\sinh x$
$\sinh x$	$\cosh x$
$\tanh x$	$\operatorname{sech}^2 x$
$\operatorname{sech} x$	$-\operatorname{sech} x \tanh x$
$\operatorname{cosech} x$	$-\operatorname{cosech} x \coth x$
$\coth x$	$-\operatorname{cosech}^2 x$
$\cosh^{-1} x$	$\frac{1}{\sqrt{x^2-1}}$
$\sinh^{-1} x$	$\frac{1}{\sqrt{x^2+1}}$
$\tanh^{-1} x$	$\frac{1}{1-x^2}$

Rules	Function	Derivative
Multiplication by constant	$cf$	$cf'$
Power Rule	$x^n$	$nx^{n-1}$
Sum Rule	$f + g$	$f' + g'$
Difference Rule	$f - g$	$f' - g'$
Product Rule	$fg$	$fg' + f'g$
Quotient Rule	$f/g$	$\frac{f'g - g'f}{g^2}$
Reciprocal Rule	$1/f$	$-f'/f^2$

When  $f$  is real-valued (*i.e.*,  $f : \mathbf{R}^n \rightarrow \mathbf{R}$ ) the derivative  $Df(x)$  is a  $1 \times n$  matrix, *i.e.*, it is a *row* vector. Its transpose is called the *gradient* of the function:

$$\nabla f(x) = Df(x)^T,$$

which is a (column) vector, *i.e.*, in  $\mathbf{R}^n$ . Its components are the partial derivatives of  $f$ :

$$\nabla f(x)_i = \frac{\partial f(x)}{\partial x_i}, \quad i = 1, \dots, n.$$

The first-order approximation of  $f$  at a point  $x \in \mathbf{int\,dom\,}f$  can be expressed as (the affine function of  $z$ )

$$f(x) + \nabla f(x)^T(z - x).$$

Suppose  $f : \mathbf{R}^n \rightarrow \mathbf{R}^m$  is differentiable at  $x \in \mathbf{int\,dom\,} f$  and  $g : \mathbf{R}^m \rightarrow \mathbf{R}^p$  is differentiable at  $f(x) \in \mathbf{int\,dom\,} g$ . Define the composition  $h : \mathbf{R}^n \rightarrow \mathbf{R}^p$  by  $h(z) = g(f(z))$ . Then  $h$  is differentiable at  $x$ , with derivative

$$Dh(x) = Dg(f(x))Df(x).$$


$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx},$$

$$\nabla^2 f(x)_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}, \quad i = 1, \dots, n, \quad j = 1, \dots, n,$$

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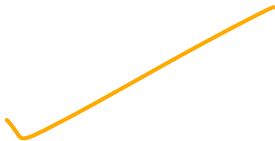
- Differentiate twice
  - Differentiate the derivate
  - If possible

### 3. Linear algebra

$$\mathcal{R}(A) = \{Ax \mid x \in \mathbf{R}^n\}.$$


- Space induced by transforming the input space by the linear function  $A$ 
  - Subspace
  - Dimension is the rank of  $A$



$$\mathcal{N}(A) = \{x \mid Ax = 0\}.$$


- 
- Space of elements  $x$  such that  $Ax$  is null
    - Also a subspace
- 

If  $\mathcal{V}$  is a subspace of  $\mathbf{R}^n$ , its *orthogonal complement*, denoted  $\mathcal{V}^\perp$ , is defined as

$$\mathcal{V}^\perp = \{x \mid z^T x = 0 \text{ for all } z \in \mathcal{V}\}.$$

(As one would expect of a complement, we have  $\mathcal{V}^{\perp\perp} = \mathcal{V}$ .)


A basic result of linear algebra is that, for any  $A \in \mathbf{R}^{m \times n}$ , we have

$$\mathcal{N}(A) = \mathcal{R}(A^T)^\perp.$$

$$Ax = \lambda x$$


- $\lambda$  Is an eigenvalue of the matrix/function  $A$ 
  - $x$  is an associated eigenvector
  - Multiple eigenvalues that can be ranked

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$$


$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{-1}$$

The matrix  $\mathbf{A}$  is represented by a 3x3 grid.

The matrix  $\mathbf{Q}$  is formed by the eigen vectors  $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$  of  $\mathbf{A}$ .

The matrix  $\mathbf{\Lambda}$  is a diagonal matrix containing the eigen values  $\lambda_1, \lambda_2, \lambda_3$  of  $\mathbf{A}$ .

The matrix  $\mathbf{Q}^{-1}$  is the inverse of  $\mathbf{Q}$ , also formed by the eigen vectors  $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$  of  $\mathbf{A}$ .