

**ChEESE**

# Artificial Intelligence and Machine Learning for Geosciences

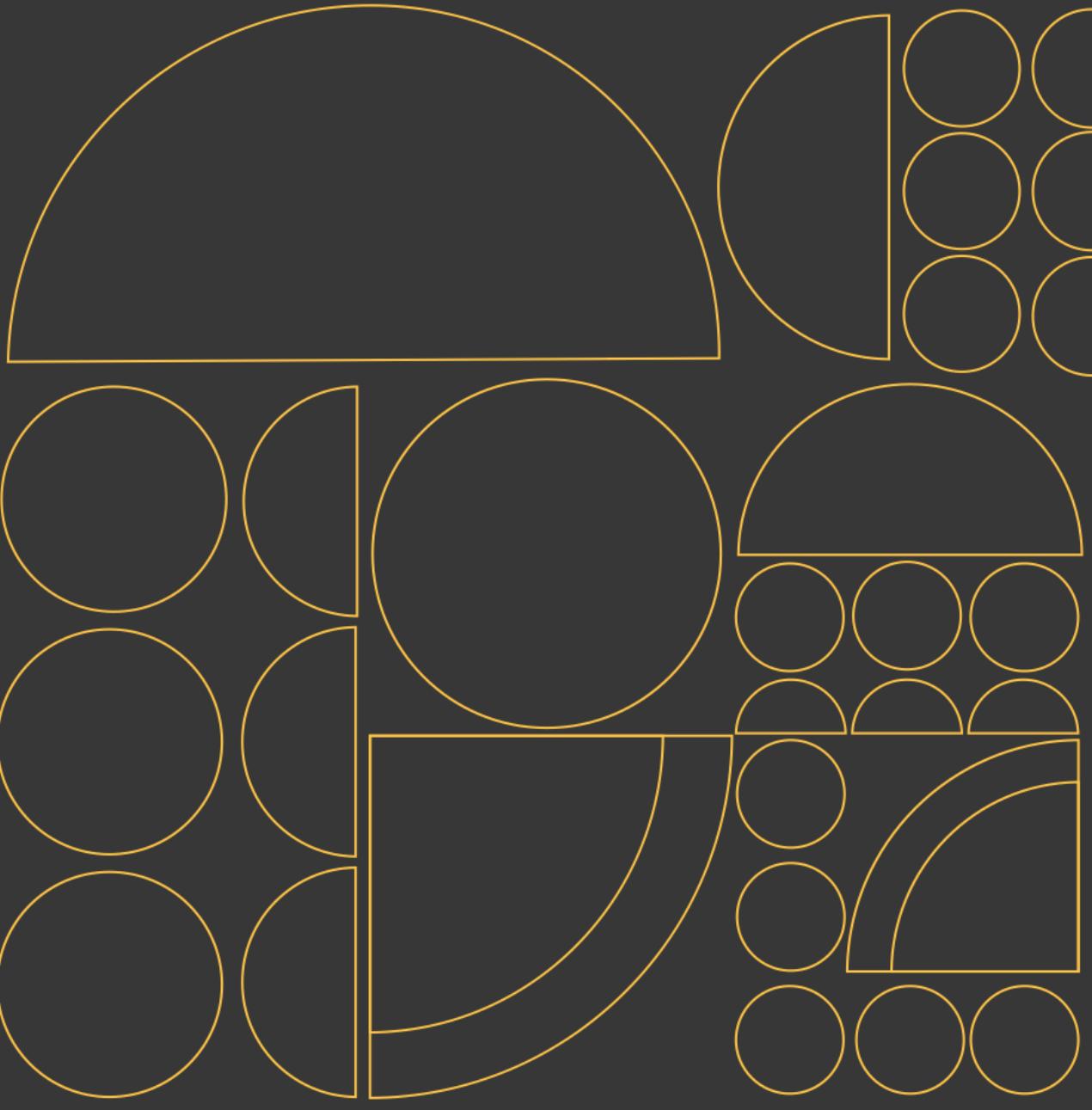
Barcelona November 2024

Léonard Seydoux, Hugo Frezat, Geneviève  
Moguilny & Alexandre Fournier

[leonard-seydoux/cheese-ai-for-geosciences](https://leonard-seydoux/cheese-ai-for-geosciences)



Project funded by EuroHPC under the grant agreement No 101093038.



# Goal: learn about statistical inference and machine learning

1. Identify data-related scientific problems
2. Define the problem and design a solution
3. Learn from examples in the litterature
4. Critisize the litterature
5. Train on real geoscience problems

**RESEARCH**

**REVIEW SUMMARY**

**GEOPHYSICS**

**Machine learning for data-driven discovery in solid Earth geoscience**

Kariann J. Bergen, Paul A. Johnson, Maarten V. de Hoop, Gregory C. Beroza\*

**BACKGROUND:** The solid Earth, oceans, and atmosphere together form a complex interacting geosystem. Processes relevant to understanding Earth's geosystem behavior range in spatial scale from the atomic to the planetary, and in temporal scale from milliseconds to billions of years. Physical, chemical, and biological processes interact and have substantial influence on this complex geosystem, and humans interact with it in ways that are increasingly consequential to the future of both the natural world and civilization as the finitude of Earth becomes increasingly apparent and limits on available energy, mineral resources, and fresh water increasingly affect the human condition. Earth is subject to a variety of geohazards that are poorly understood, yet increasingly impactful as our exposure grows through increasing urbanization, particularly in hazard-prone areas. We have a fundamental need to develop the best possible predictive understanding of how the geosystem works, and that understanding must be informed by both the present and the deep past. This understanding will come through the analysis of increasingly large geo-datasets and from computationally intensive simulations, often connected through inverse problems. Geoscientists are faced with the challenge of extracting as much useful information as possible and gaining new insights from these data, simulations, and the interplay between the two. Techniques from the rapidly evolving field of machine learning (ML) will play a key role in this effort.

**ADVANCES:** The confluence of ultrafast computers with large memory, rapid progress in ML algorithms, and the ready availability of large datasets place geoscience at the threshold of dramatic progress. We anticipate that this progress will come from the application of ML across three categories of research effort: (i) automation to perform a complex prediction task that cannot easily be described by a set of explicit commands; (ii) modeling and inverse problems to create a representation that approximates numerical simulations or captures relationships; and (iii) discovery to reveal new and often unanticipated patterns, structures, or relationships. Examples of automation include geologic mapping using remote-sensing data, characterizing the topology of fracture systems to model subsurface transport, and classifying volcanic ash particles to infer eruptive mechanism. Examples of modeling include approximating the viscoelastic response for complex rheology, determining wave speed models directly from tomographic data, and classifying diverse seismic events. Examples of discovery include predicting laboratory slip events using observations of acoustic emissions, detecting weak earthquake signals using similarity search, and determining the connectivity of subsurface reservoirs using ground-water tracer observations.

**OUTLOOK:** The use of ML in solid Earth geoscience is growing rapidly, but is still in its early stages and making uneven progress. Much remains to be done with existing datasets from long-standing data sources, which in many cases are largely unexplored. Newer, unconventional data sources such as light detection and ranging (LiDAR), fiber-optic sensing, and crowd-sourced measurements may demand new approaches through both the volume and the character of information that they present. Practical steps could accelerate and broaden the use of ML in the geosciences. Wider adoption of open-science principles such as open source code, open data, and open access will better position the solid Earth community to take advantage of rapid developments in ML and artificial intelligence. Benchmark datasets and challenge problems have played an important role in driving progress in artificial intelligence research by enabling rigorous performance comparison and could play a similar role in the geosciences. Testing on high-quality datasets produces better models, and benchmark datasets make these data widely available to the research community. They also help recruit expertise from allied disciplines. Close collaboration between geoscientists and ML researchers will aid in making quick progress in ML geoscience applications. Extracting maximum value from geoscientific data will require new approaches for combining data-driven methods, physical modeling, and algorithms capable of learning with limited, weak, or biased labels. Funding opportunities that target the intersection of these disciplines, as well as a greater component of data science and ML education in the geosciences, could help bring this effort to fruition. ■

**Digital geology.** Digital representation of the geology of the conterminous United States. [Geology of the Conterminous United States at 1:2,500,000 scale; a digital representation of the 1974 P. B. King and H. M. Belknap map by P. G. Schruben, R. E. Arndt, W. J. Bawiec]

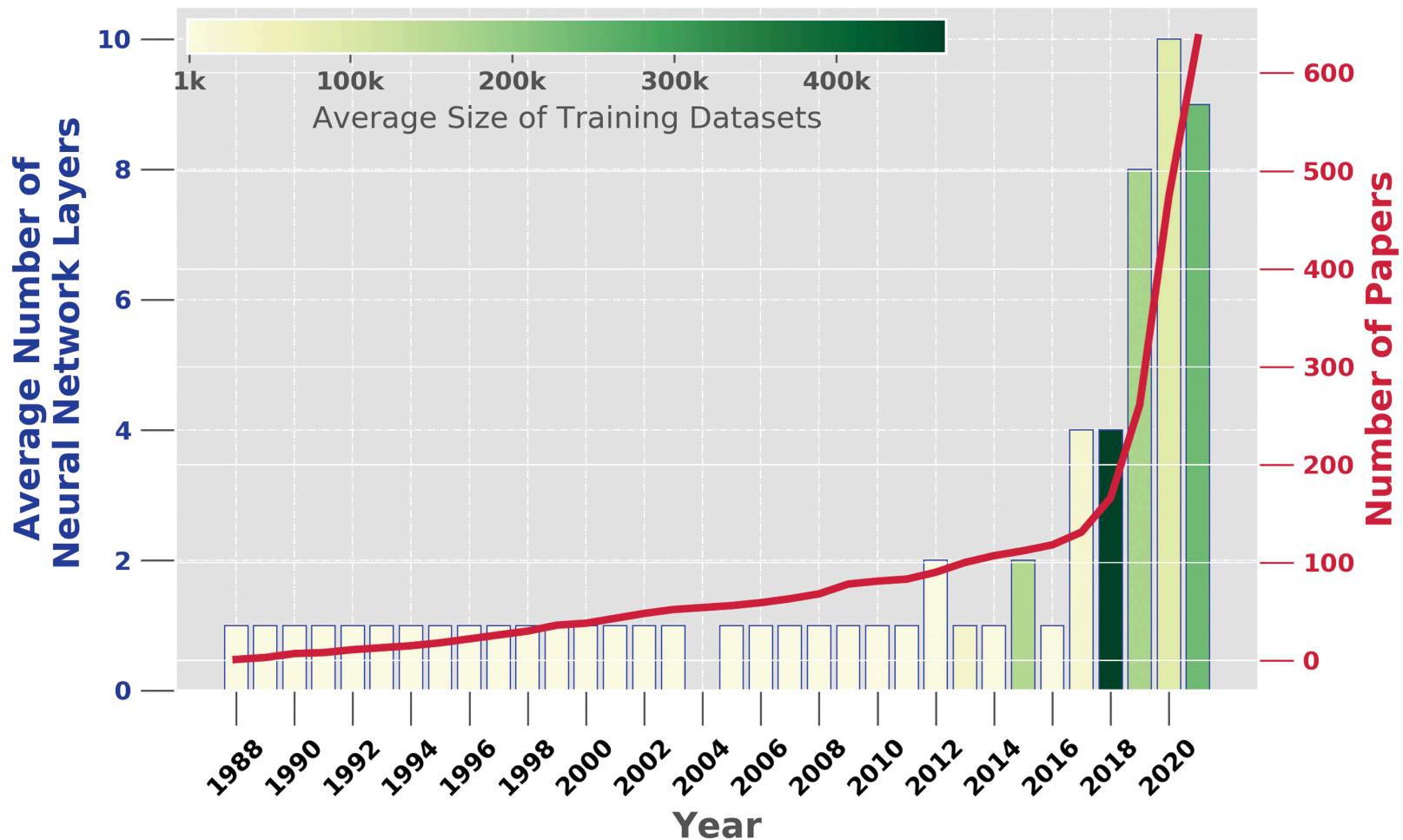
\*Corresponding author. Email: beroza@stanford.edu  
Cite this article as: K. J. Bergen et al., *Science* **363**, eaau0323 (2019). DOI: 10.1126/science.aau0323

Downloaded from https://www.science.org on December 09, 2023

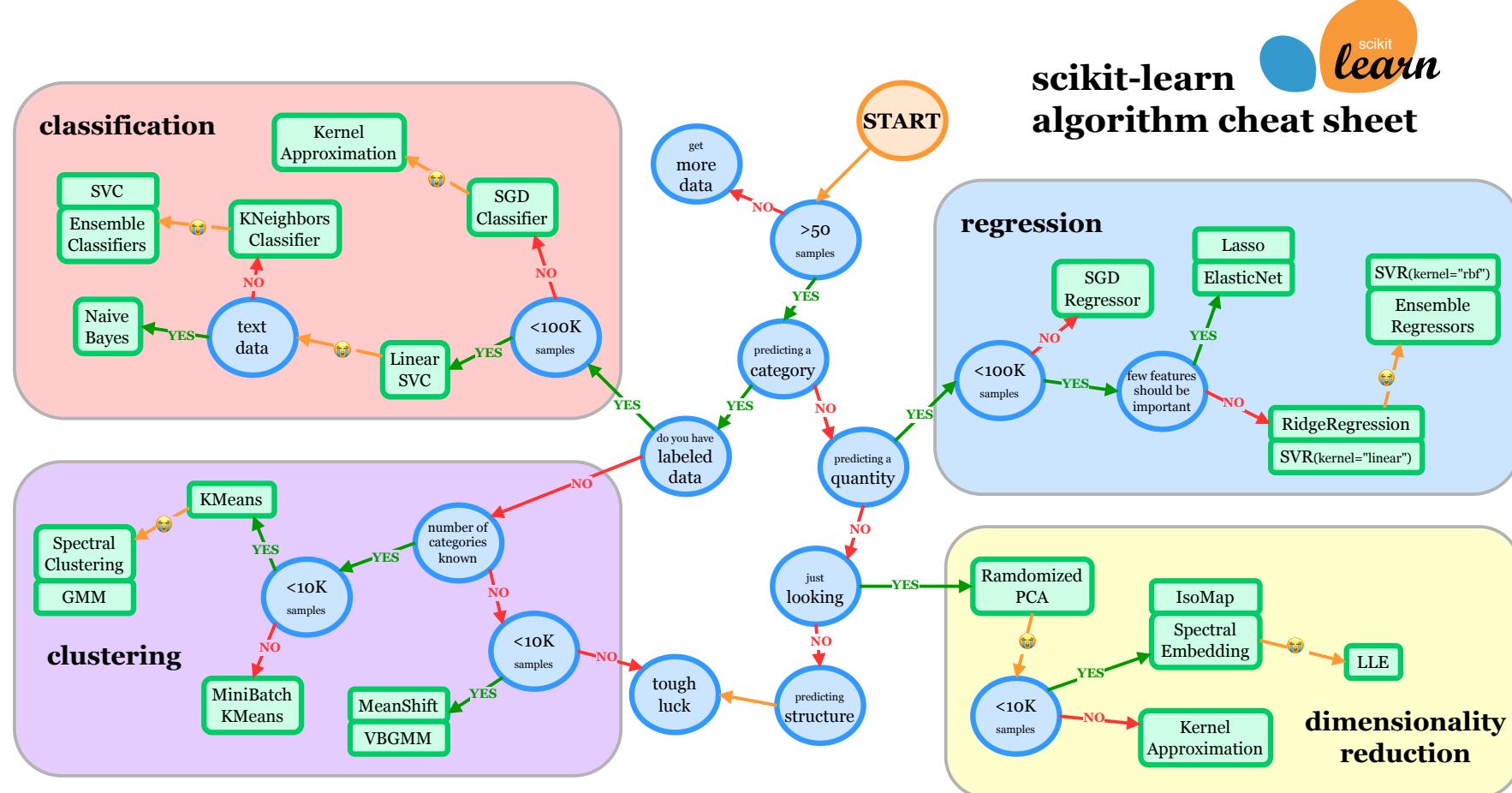
Bergen et al., *Science* **363**, 1299 (2019) 22 March 2019

**1 of 1**

Goal: keep up with the ongoing pace



# Contents of this class make use of the scikit-learn library



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# scikit-learn

*Machine Learning in Python*

Getting Started    Release Highlights for 1.5

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

## Classification

Identifying which category an object belongs to.

**Applications:** Spam detection, image recognition.

**Algorithms:** [Gradient boosting](#), [nearest neighbors](#), [random forest](#), [logistic regression](#), and [more...](#)

## Regression

Predicting a continuous-valued attribute associated with an object.

**Applications:** Drug response, stock prices.

**Algorithms:** [Gradient boosting](#), [nearest neighbors](#), [random forest](#), [ridge](#), and [more...](#)

## Clustering

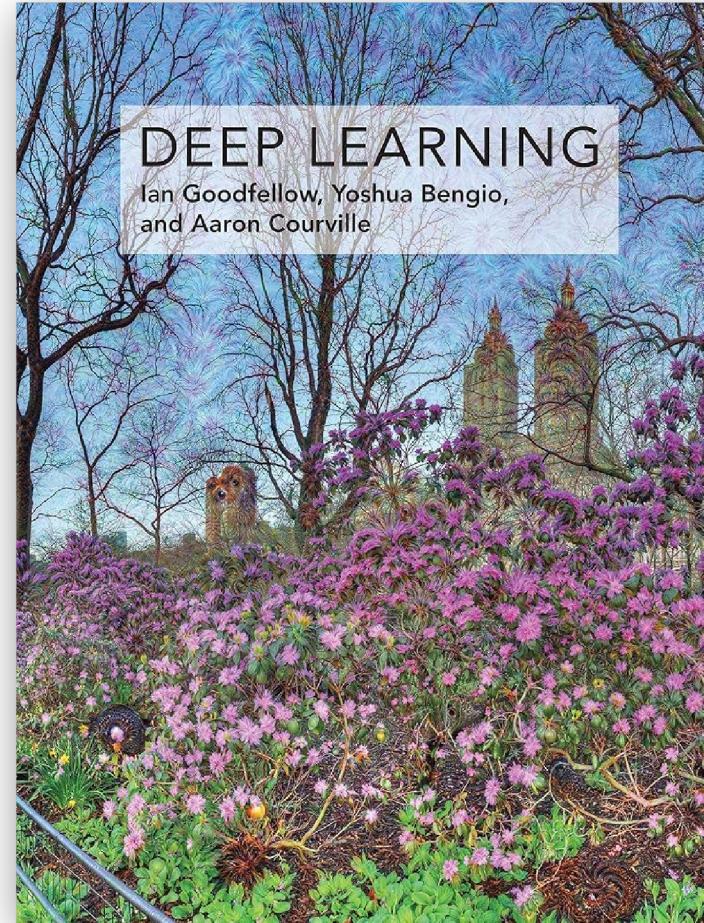
Automatic grouping of similar objects into sets.

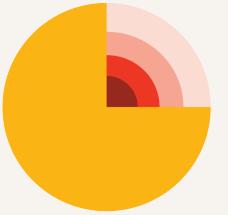
**Applications:** Customer segmentation, grouping experiment outcomes.

**Algorithms:** [k-Means](#), [HDBSCAN](#), [hierarchical clustering](#), and [more...](#)

Lots of resources are also taken from the *Deep learning* book

- Very complete introduction
- Historical aspects
- Starts from scratch (linear algebra)
- Covers machine/deep learning
- Illustrates with examples
- Online free access

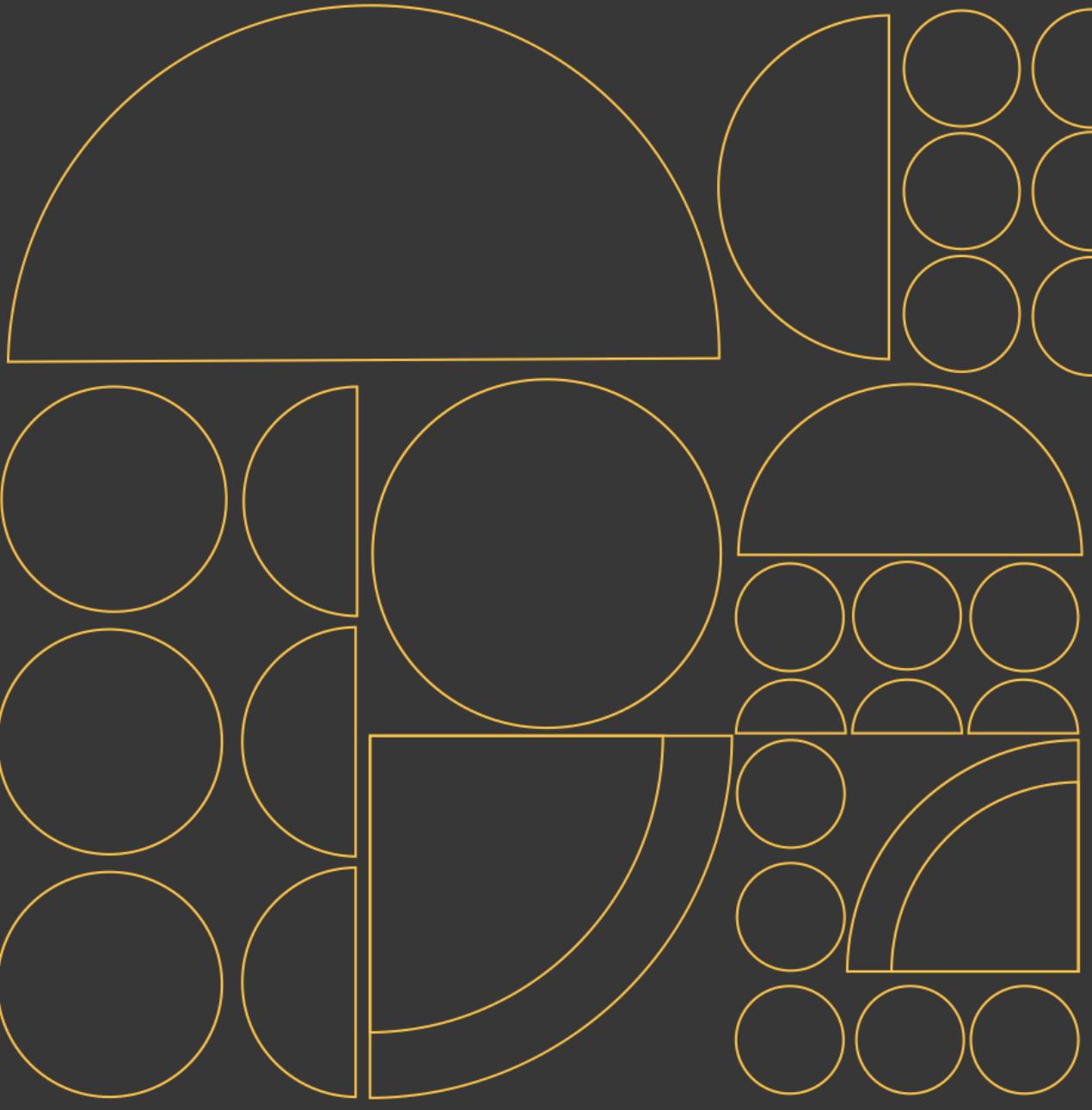




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## 1. Introduction

**Machine learning** for Earth science:  
Why, what, and how? Are any of those  
methods useful for your research? How to  
read papers that use machine learning?



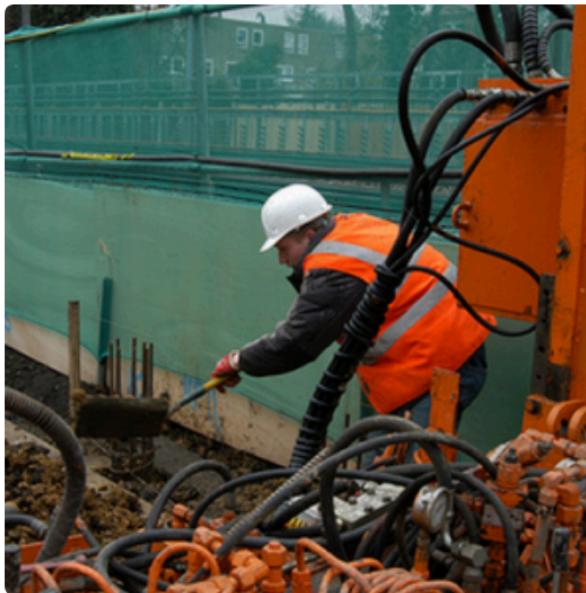
How much time do you need to describe the following images?



# How accurate are those descriptions?



"man in black shirt is playing  
guitar."



"construction worker in orange  
safety vest is working on road."

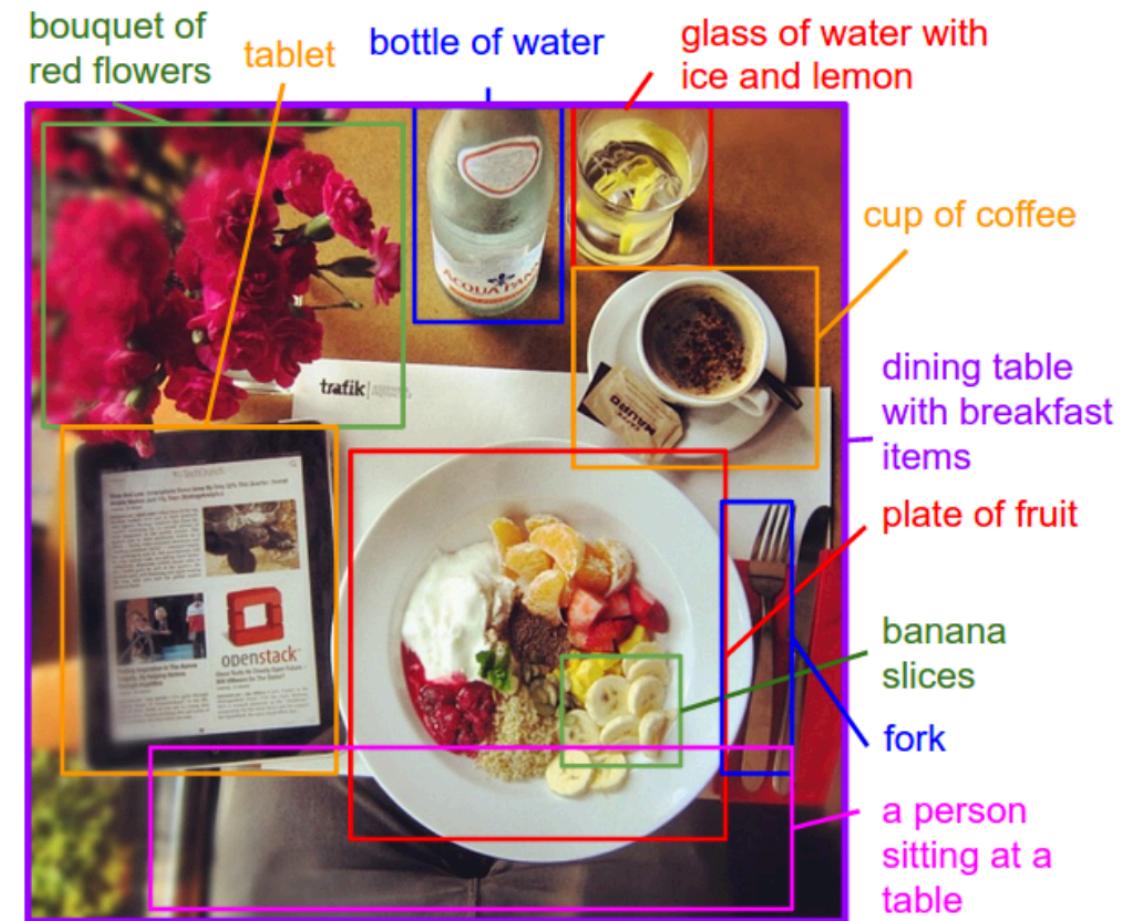


"two young girls are playing with  
lego toy."

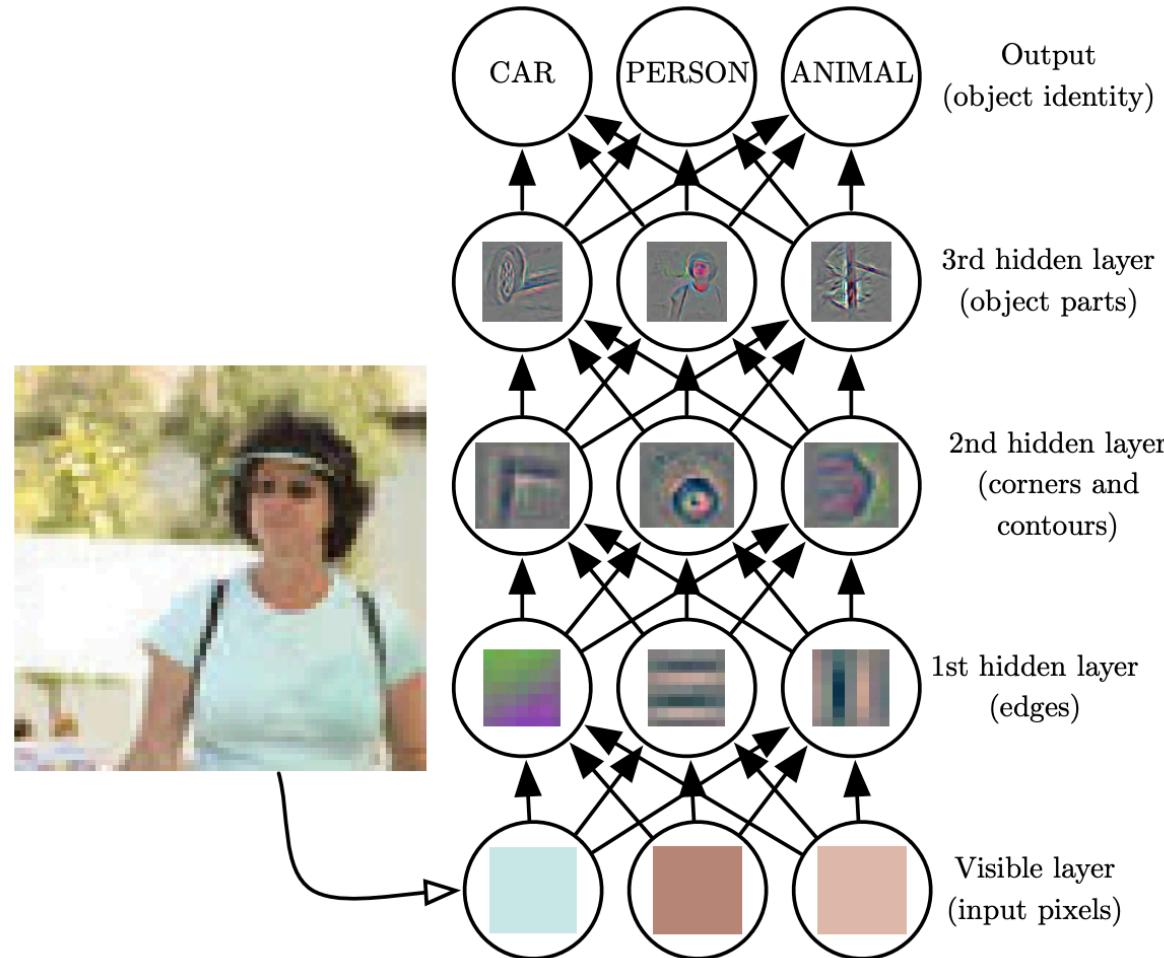
How do we extract such high-level knowledge from data?

## Recipe of image captioning

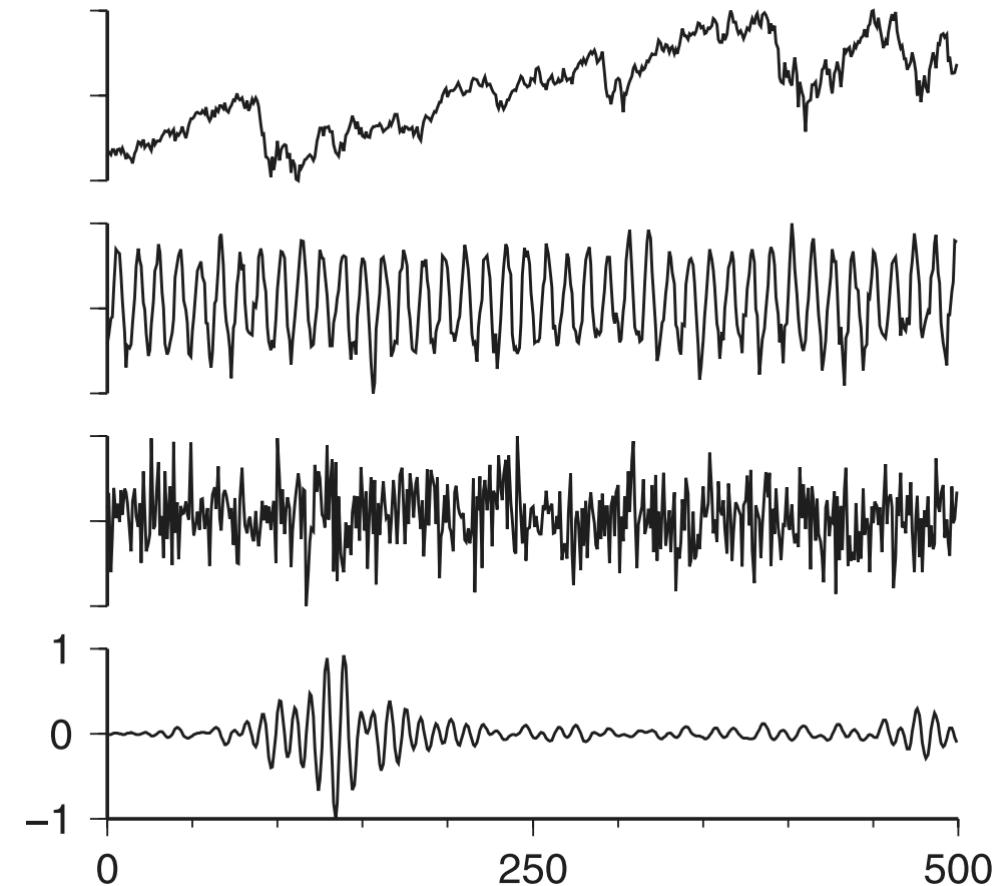
- Identify objects within image
- Recognize objects category
- Understand the link between objects
- Sort links by priority
- Generate text out of it



# Ingredients: hierarchical knowledge extraction



Can you spot the seismogram?

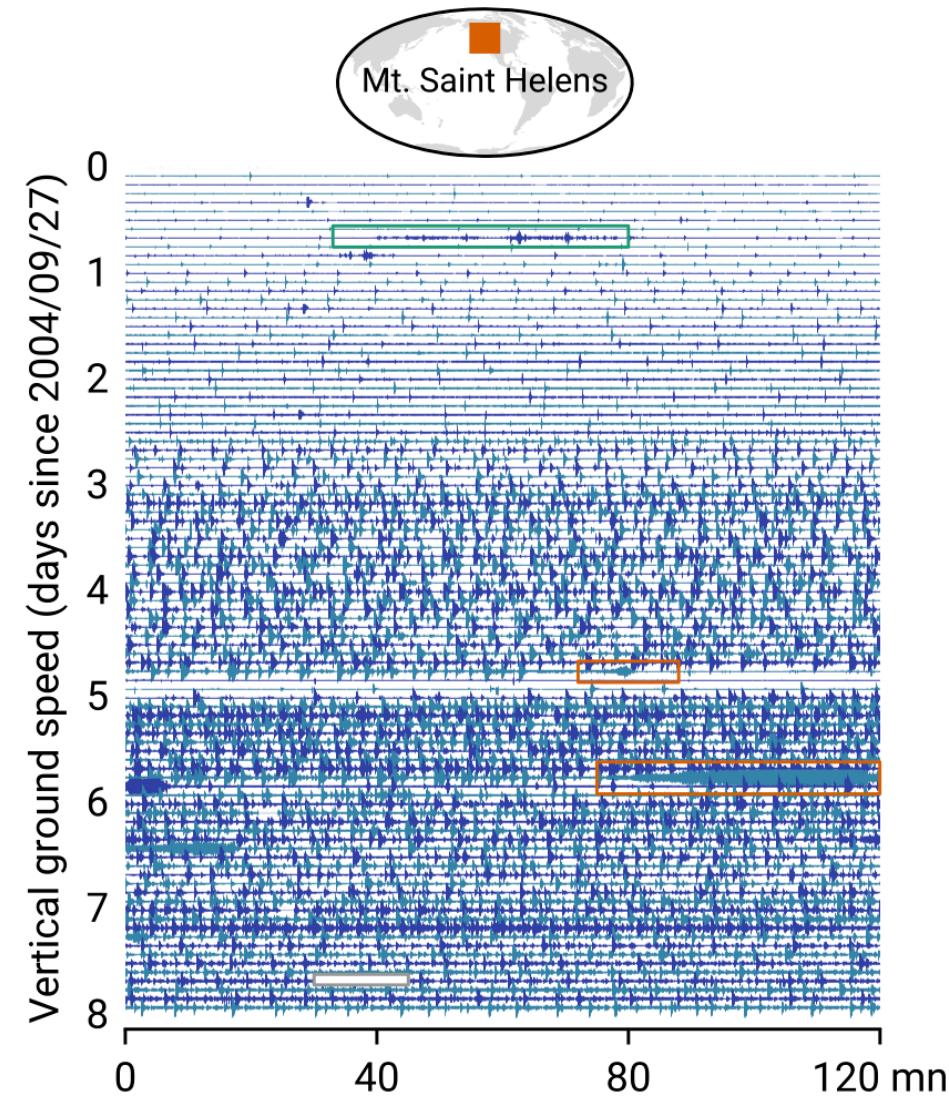


Valentine & Trampert (2012).

Top to bottom: FTSE; Temperature in Central England; Gaussian noise; Long-period seismogram.

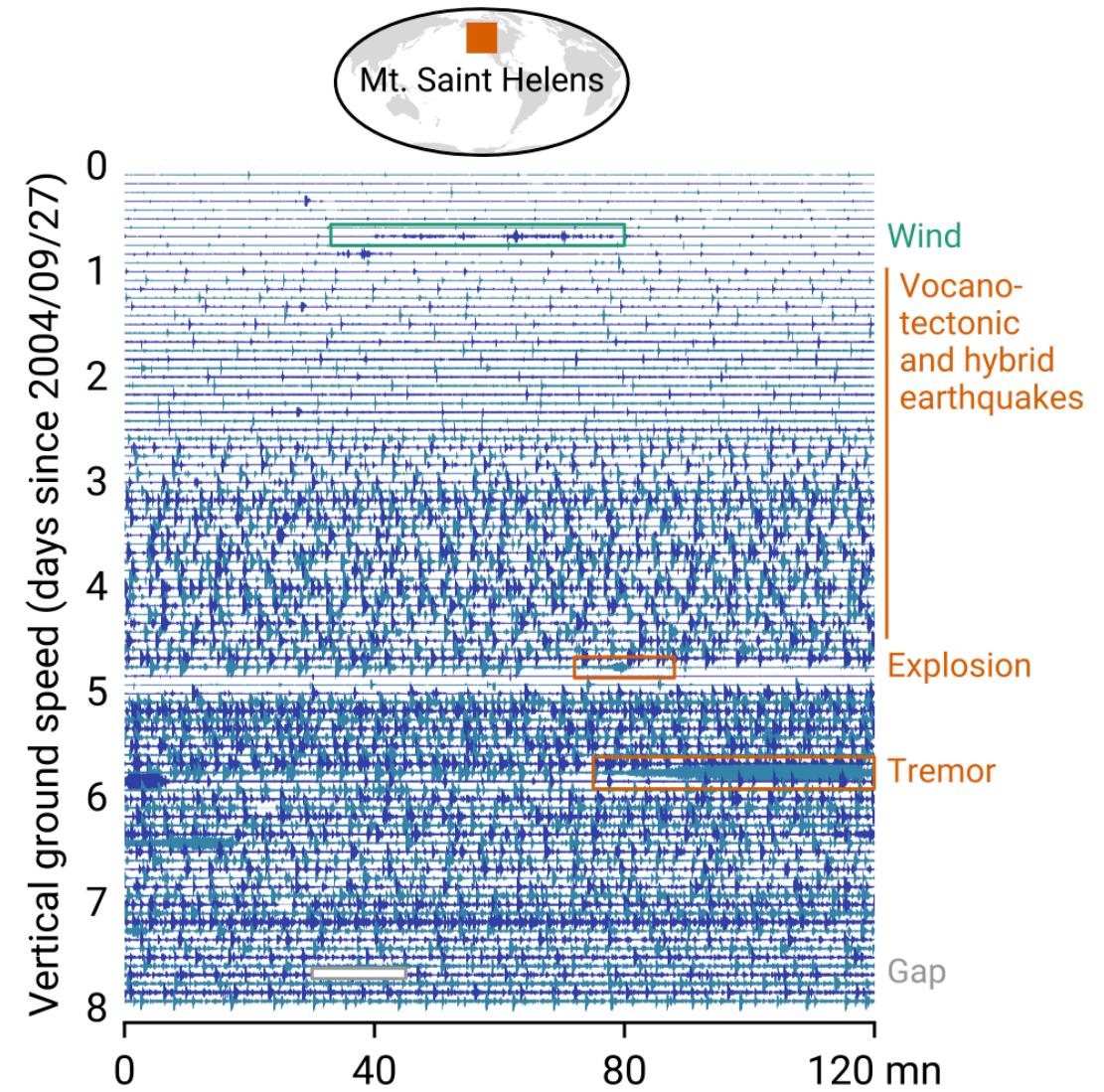
# Detection and classification of events from seismograms

Most humans can pinpoint events.



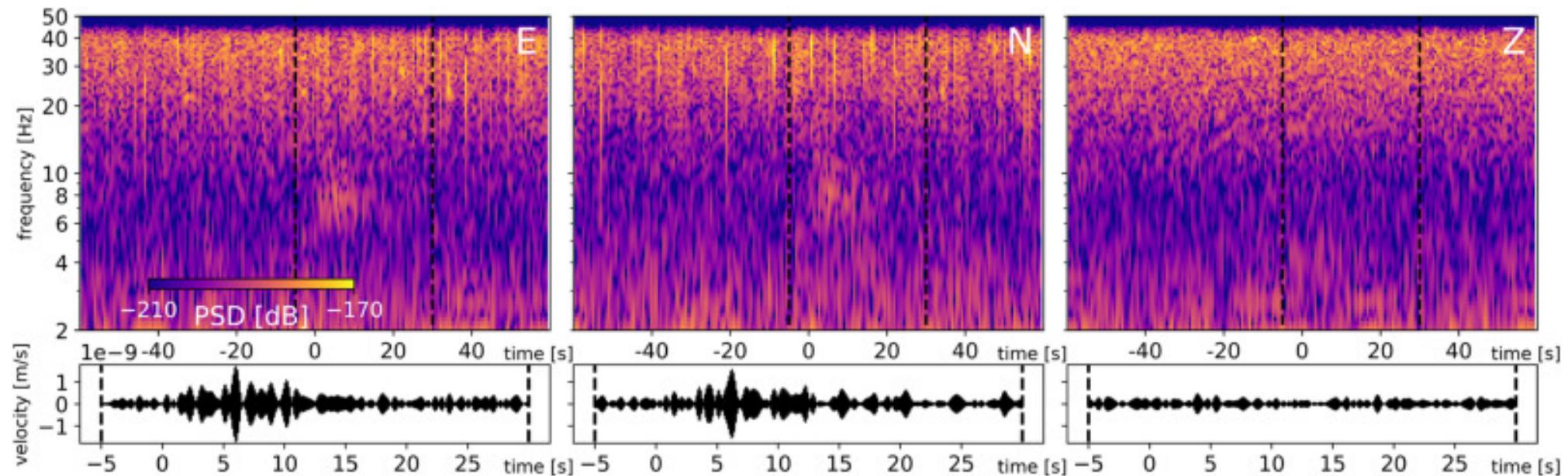
# Detection and classification of events from seismograms

Most humans can pinpoint events.  
Experts can **classify** them.



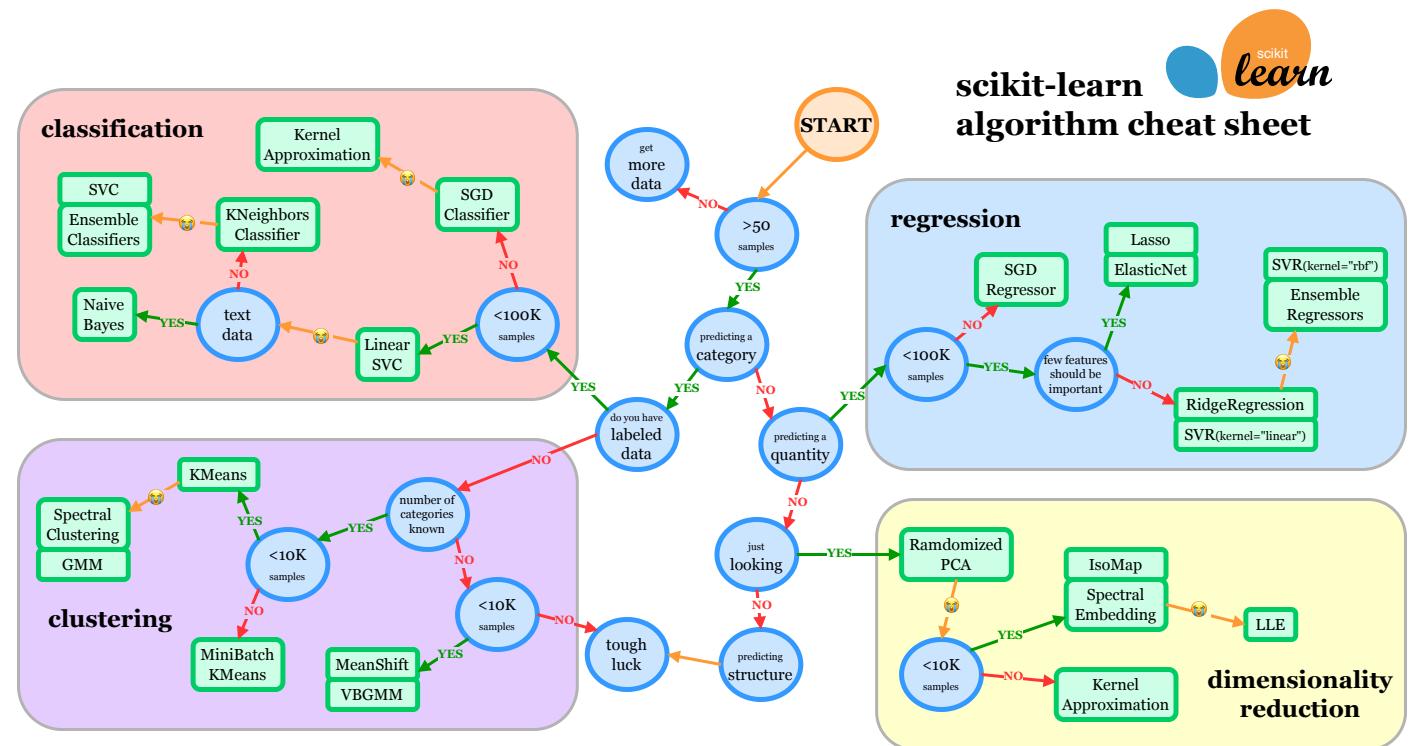
# Diving into previously unseeded data

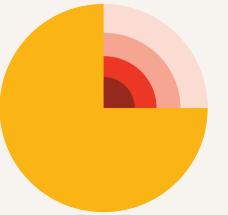
Expert-detected marsquake within continuous insight data



# Target tasks of machine learning

- Time-consuming tasks
- Unprogrammable tasks
- Hard-to-describe tasks
- Exploration of new data

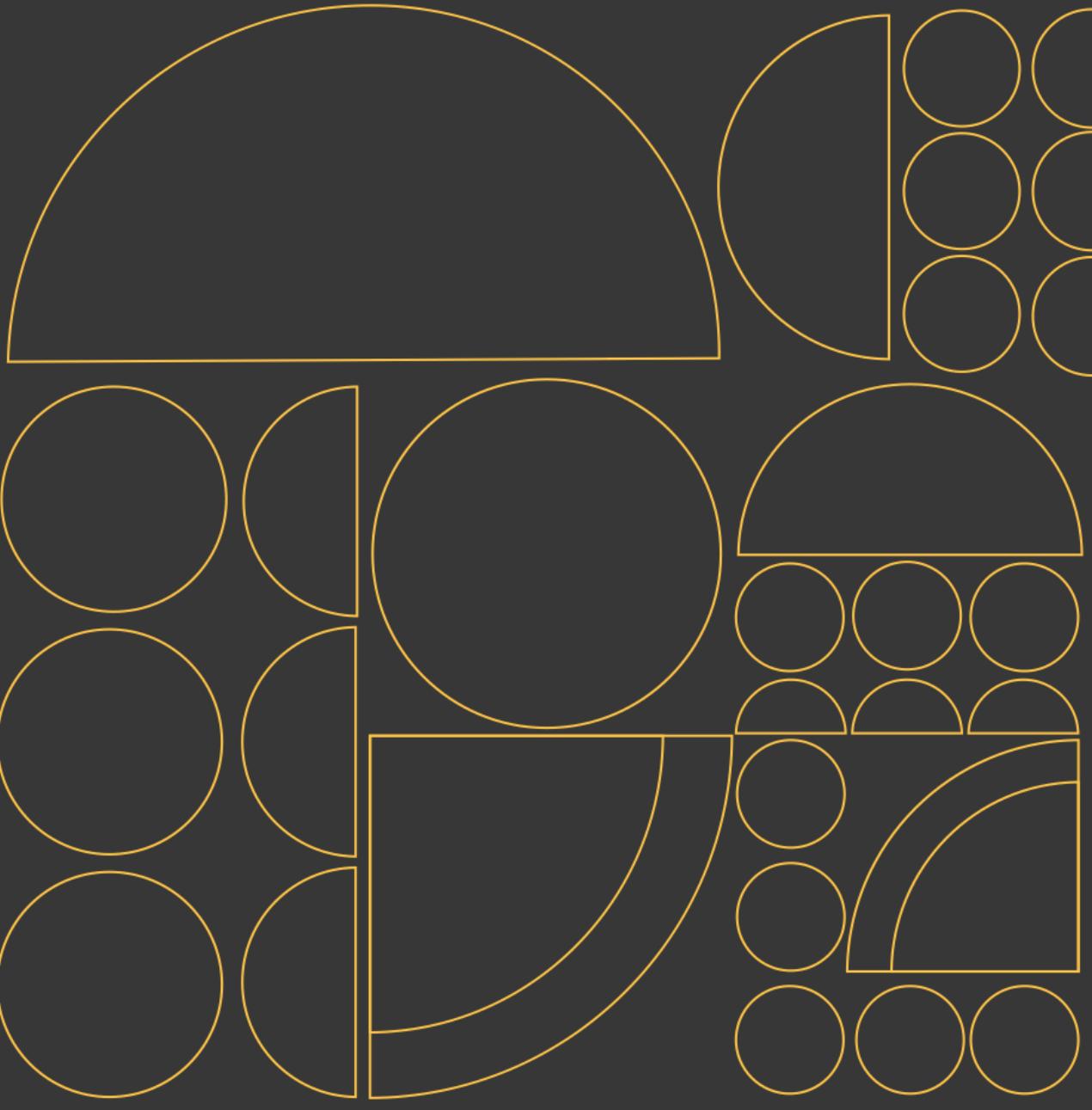




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## 2. Definitions

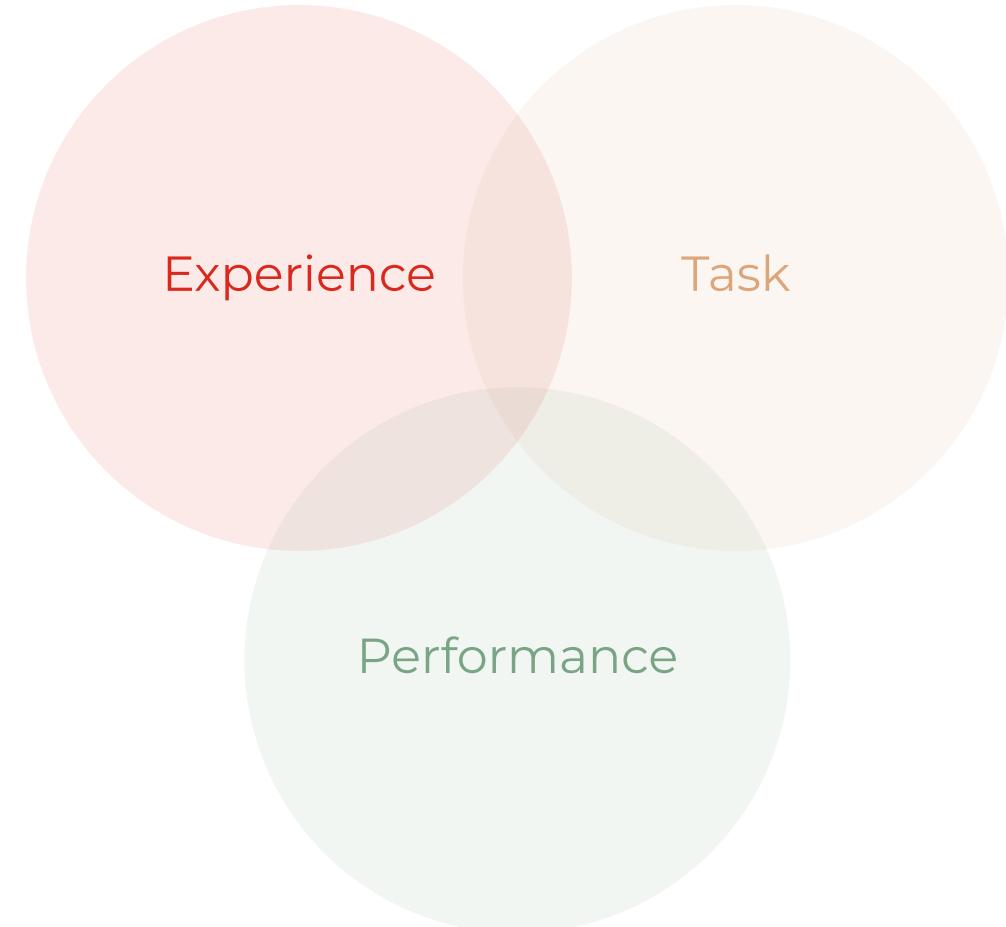
**Machine learning** is a field of study in artificial intelligence concerned with the development and study of statistical algorithms that can effectively generalize and thus perform tasks without explicit instructions.



# General definition of machine learning

An algorithm learns from **experience** with respect to a **task** and **performance**, if its **performance** at solving the **task** improves with **experience**.

**All three elements are required.**



# The data, the model, and the loss



## The data

A set of samples  $\mathbf{x}_i$  and labels  $\mathbf{y}_i$  to learn from:

$$\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$$



## the model

A parametric function  $f_\theta$  that maps data  $\mathbf{x}$  to  $\hat{\mathbf{y}}$

$$f_\theta : \mathbf{x} \mapsto \hat{\mathbf{y}}$$



## the loss

A measurement of the model performance

$$\mathcal{L}(\hat{\mathbf{y}}, \mathbf{y})$$

**Learning** = find the optimal parameters  $\theta^*$  that minimizes the loss  $\mathcal{L}$

$$\theta^* = \arg \min_{\theta} \mathcal{L}(f_\theta(\mathbf{x}), \mathbf{y})$$

# Useful vocabulary and symbols

Symbol	Name
$\{\mathbf{x}_i \in \mathbb{X}\}_{i=1\dots N}$	Collection of <b>data samples</b>
$\{\mathbf{y}_i \in \mathbb{Y}\}_{i=1\dots N}$	Collection of <b>labels</b>
$\mathbf{x} = (x_1, \dots, x_F)$	Set of sample <b>features</b>
$\mathbf{y} = (y_1, \dots, y_T)$	Set of label <b>targets</b>
$N$	Dataset size
$F$	Feature space dimensions
$T$	Target space dimension
$\mathbb{X}$	Data space
$\mathbb{Y}$	Label space

For instance, an image is a sample  $\mathbf{x}$  with

$$\mathbf{x} \in \mathbb{X} = \mathbb{R}^{H \times W \times C}$$

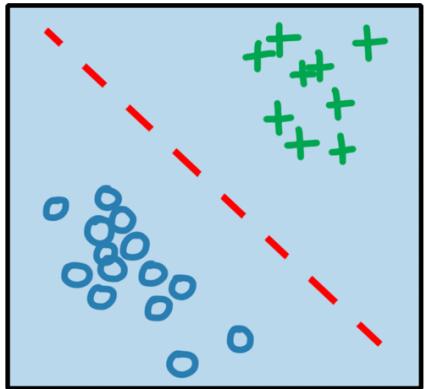
where  $H$  is the height,  $W$  the width, and  $C$  the channels. The label of an image can be represented by a category  $\mathbf{y}$  with

$$\mathbf{y} \in \mathbb{Y} = \{0, 1, \dots, K\}$$

where  $K$  is the number of categories.

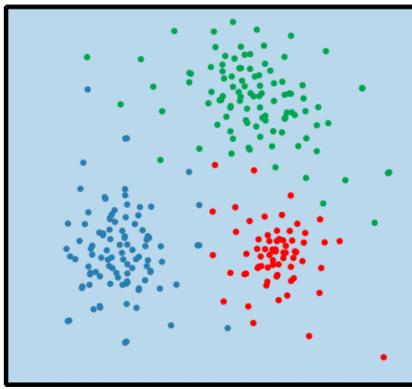
# Main types of machine learning

supervised  
learning



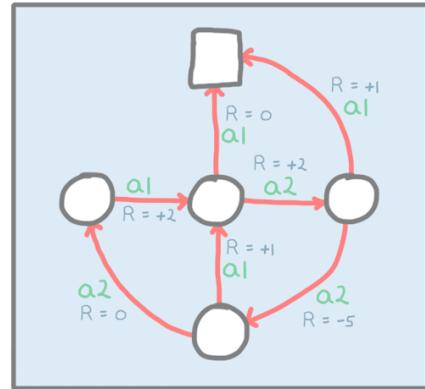
Predict some output  $\mathbf{y}$  from input  $\mathbf{x}$  (regression, classification).

unsupervised  
learning

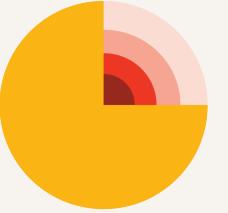


Learn data distribution  $p(\mathbf{x})$  or structure (clustering, reduction).

reinforcement  
learning



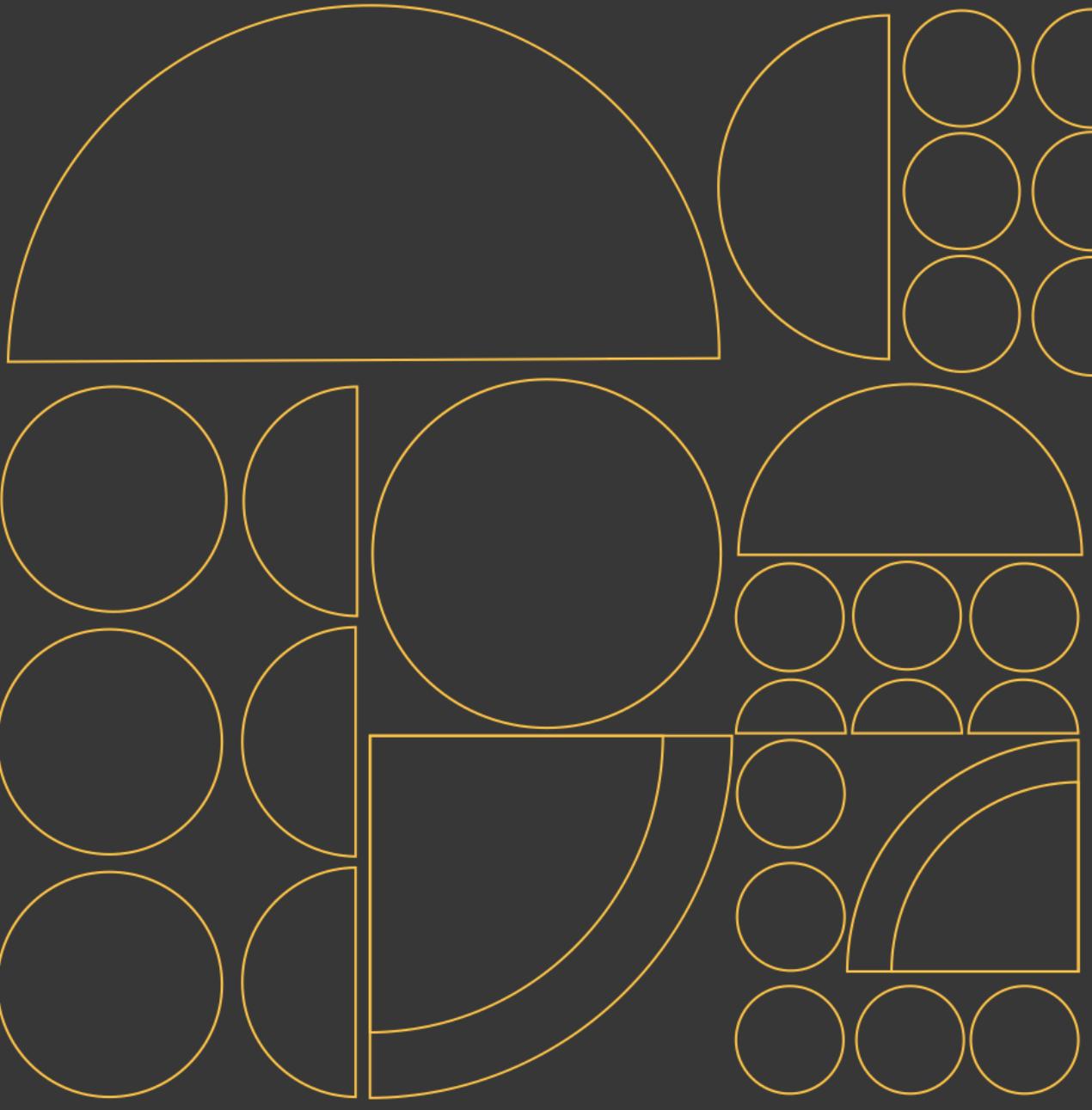
Learns a policy to maximize the reward (game playing, robotics).



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### 3. Supervised machine learning: regression

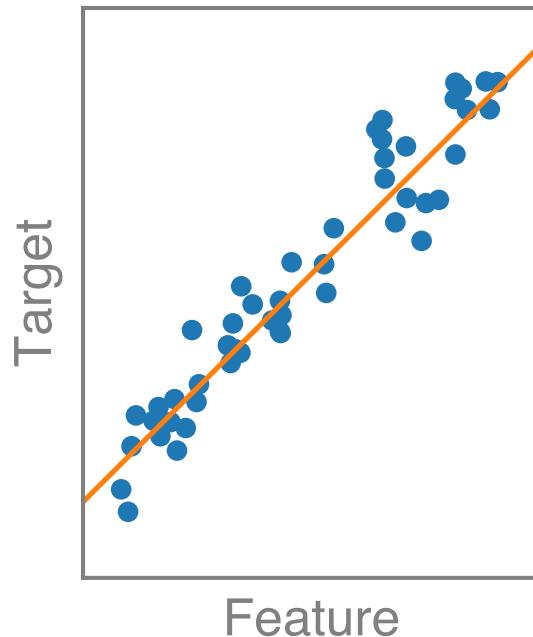
How to solve a regression or classification task with machine learning?



# The two main tasks of supervised machine learning

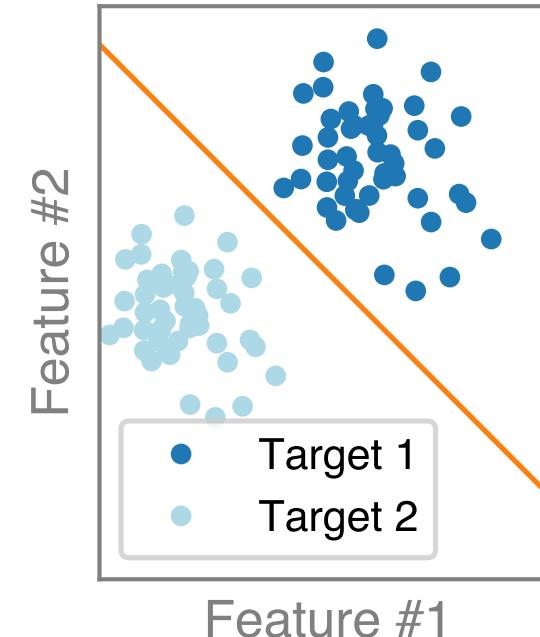
## Regression

$x$  and  $y$  are continuous



## Classification

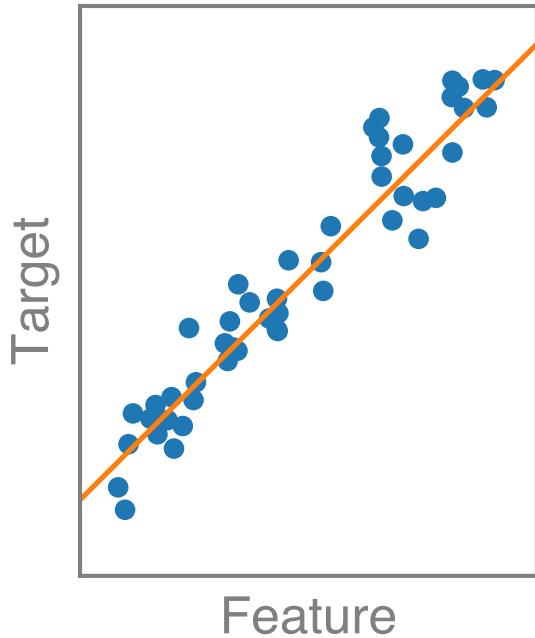
$x$  is continuous and  $y$  is discrete



# The two main tasks of supervised machine learning

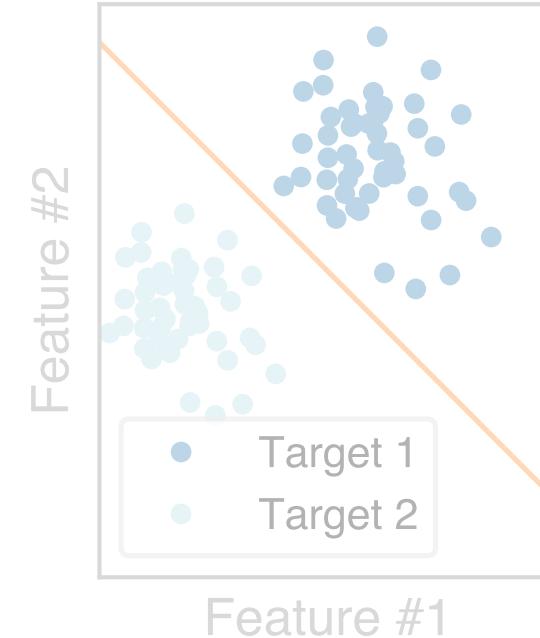
## Regression

$x$  and  $y$  are continuous



## Classification

$x$  is continuous and  $y$  is discrete



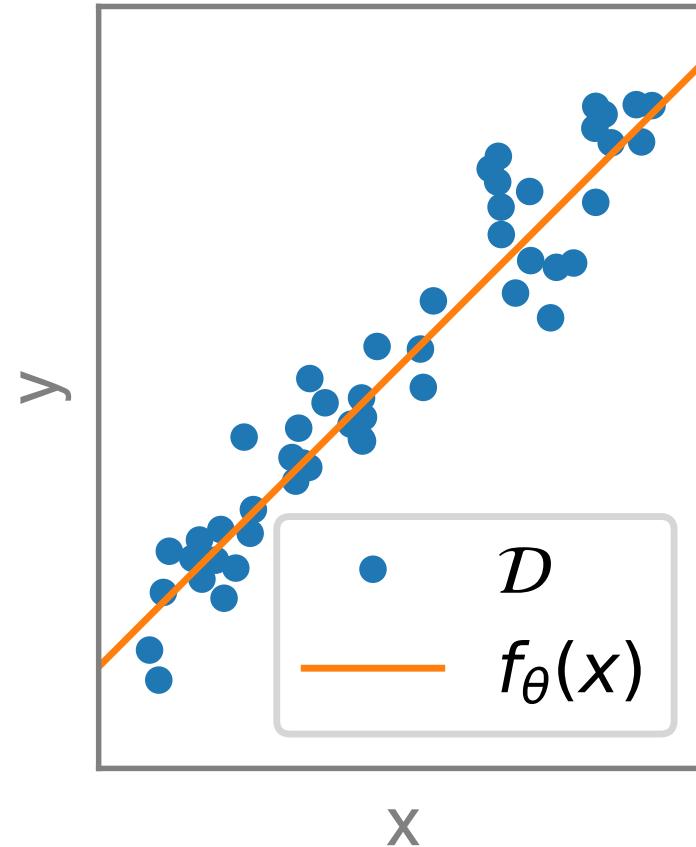
# The regression task

Given a dataset

$$\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N,$$

optimize the parameters  $\theta$  of a function  $f_\theta$  that best predicts the label  $\mathbf{y}$  from the sample  $\mathbf{x}$ , that is find the optimal parameters  $\theta^*$  that minimizes the loss  $\mathcal{L}$ , such as

$$\theta^* = \arg \min_{\theta} \mathcal{L}(f_\theta(\mathbf{x}), \mathbf{y}).$$



# The linear regression

Find the set of coefficients  $\theta = (a, b) \in \mathbb{R}^2$  that best predicts  $y$  from  $x$  so that

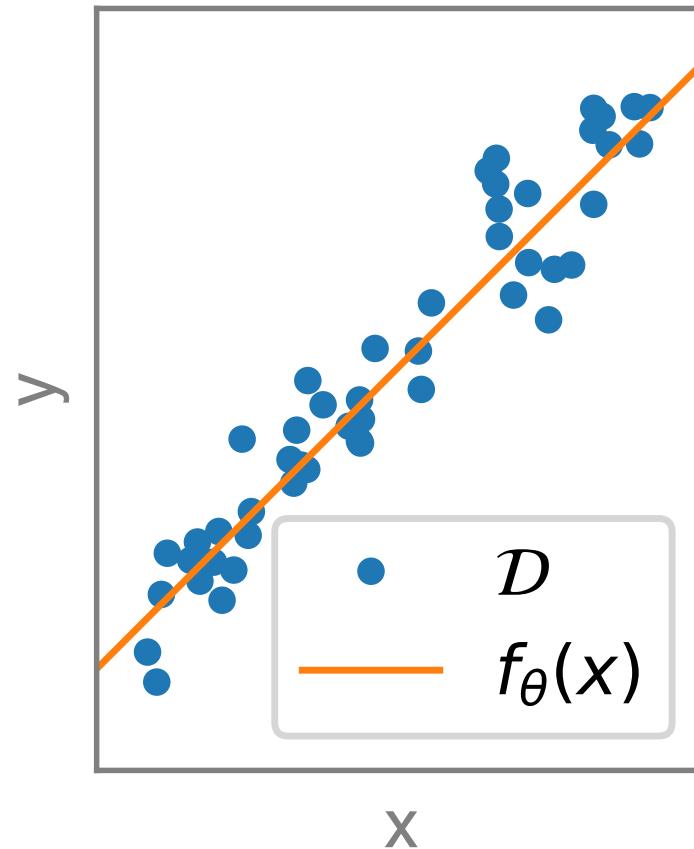
$$f_\theta : x \mapsto ax + b.$$

Here, the best explanation relates to the loss.

For instance, the mean squared error:

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N (f_\theta(x_i) - y_i)^2.$$

**How do we minimize the loss?**

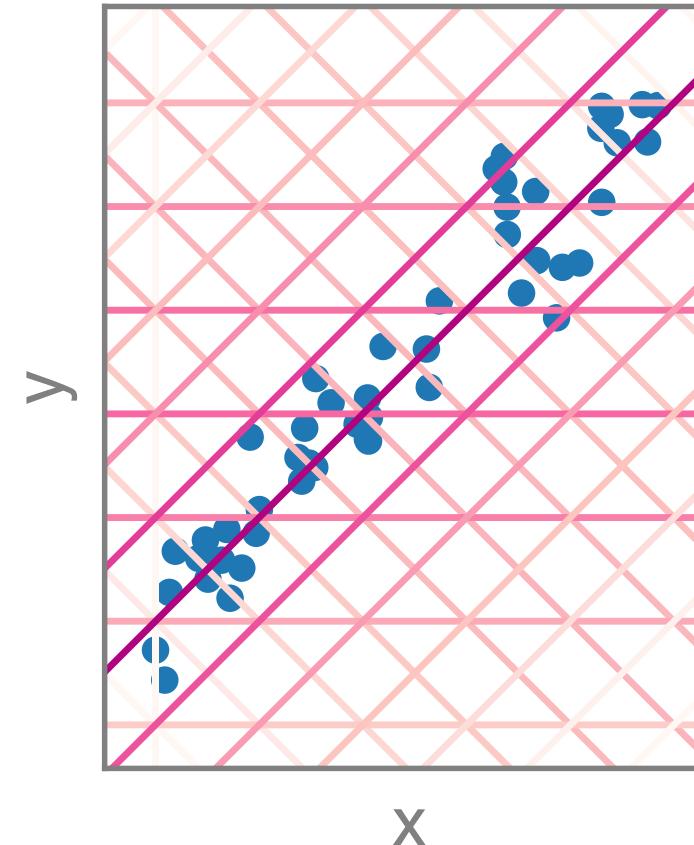


## Naive attempt with a grid search

Find  $\theta^*$  among gridded values of  $\theta$ .

- Pros: easy to implement, exhaustive search, uncertainty estimation.
- Cons: unscalable. If 0.1s / evaluation, then 2 parameters with 100 values each takes 1/2 hour.  
For 5 parameters it takes more than 30 years!

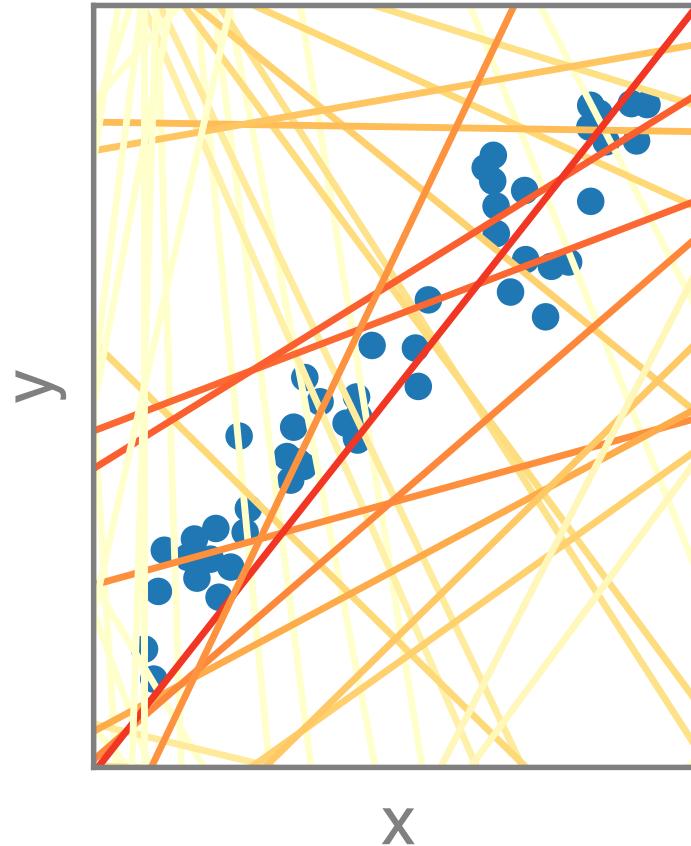
**Any smarter idea?**



## Random search

Random search to find  $\theta^*$ .

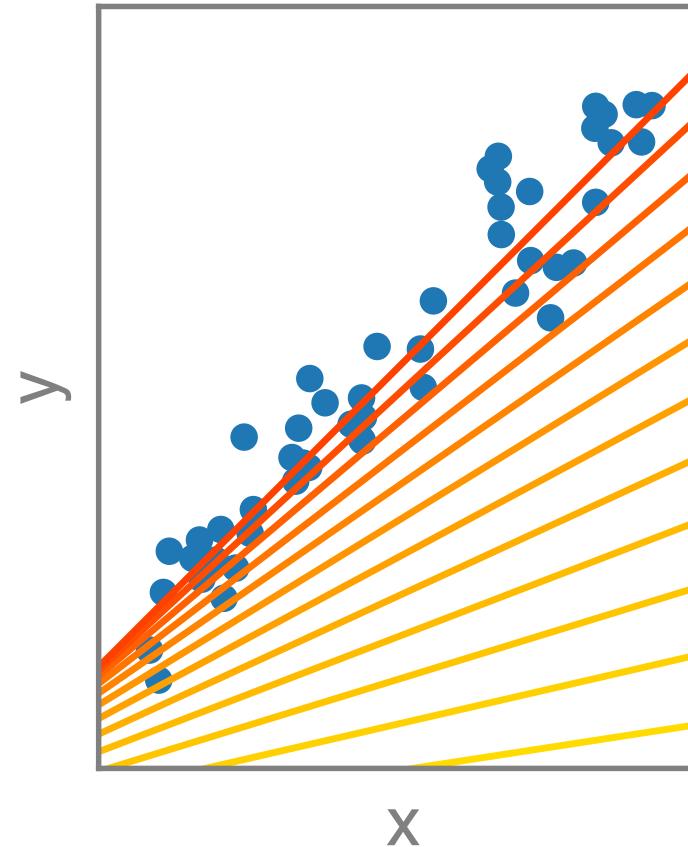
- Pros: easy to implement, scalable, uncertainty estimation, can include prior knowledge.
- Cons: not exhaustive, can be slow to converge.



# Gradient descent

Estimate the gradient of  $\mathcal{L}$  w.r.t. the parameters  $\theta$ , update the parameters towards gradient descent.

- Pros: converges faster than random search.
- Cons: gets stuck in local minima, slow to converge, needs for differentiability.



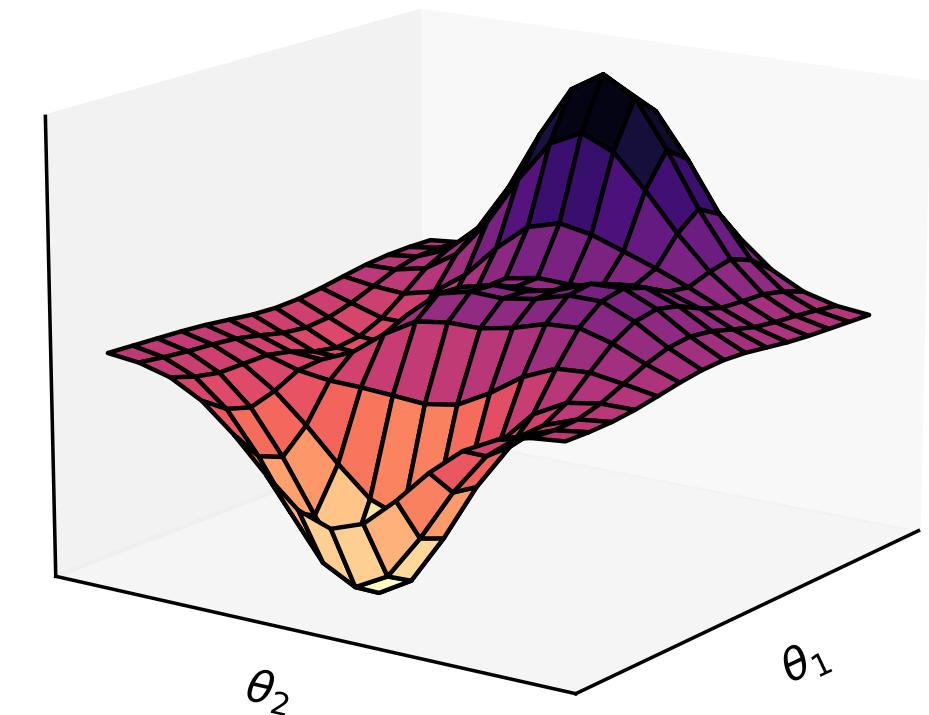
# Gradient descent

## Recipe

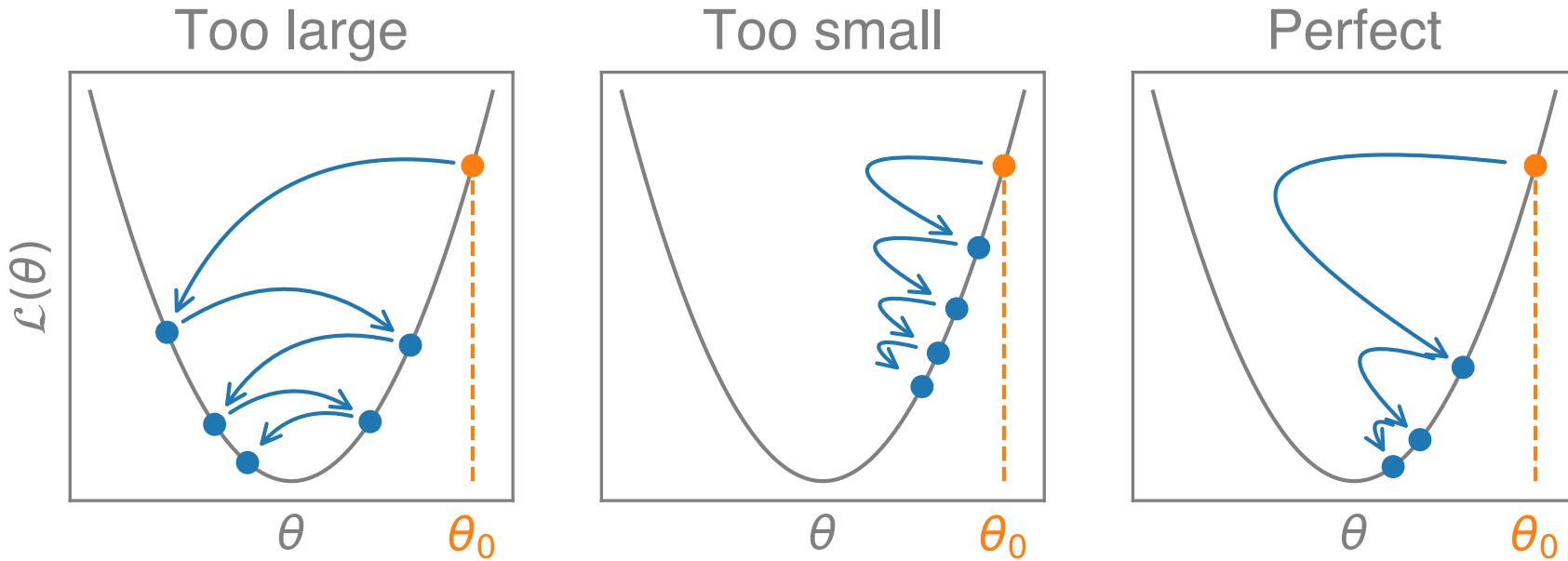
1. Define an initial model  $\theta = (a_0, b_0)$
2. Compute the gradient  $\nabla \mathcal{L}(\theta)$
3. Update the model  $\theta \leftarrow \theta - \eta \nabla \mathcal{L}(\theta)$
4. Repeat until convergence

## Hyperparameters

- The **learning rate**  $\eta$  controls the update.
- An **epoch** is the number of iteration.



# How to deal with learning rate?



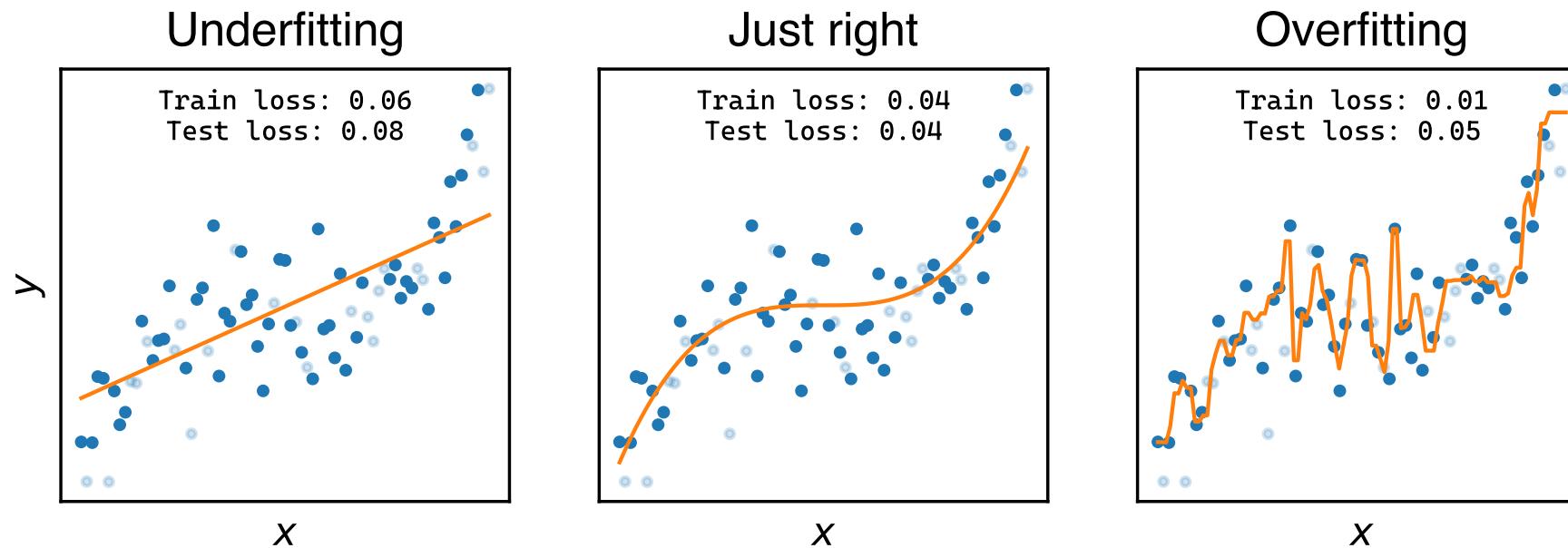
That's part of the **hyperparameters tuning**.  
More about that in the deep learning lectures.

# The problem of overfitting



Having a loss close to 0 does not mean that the model **generalizes** well.

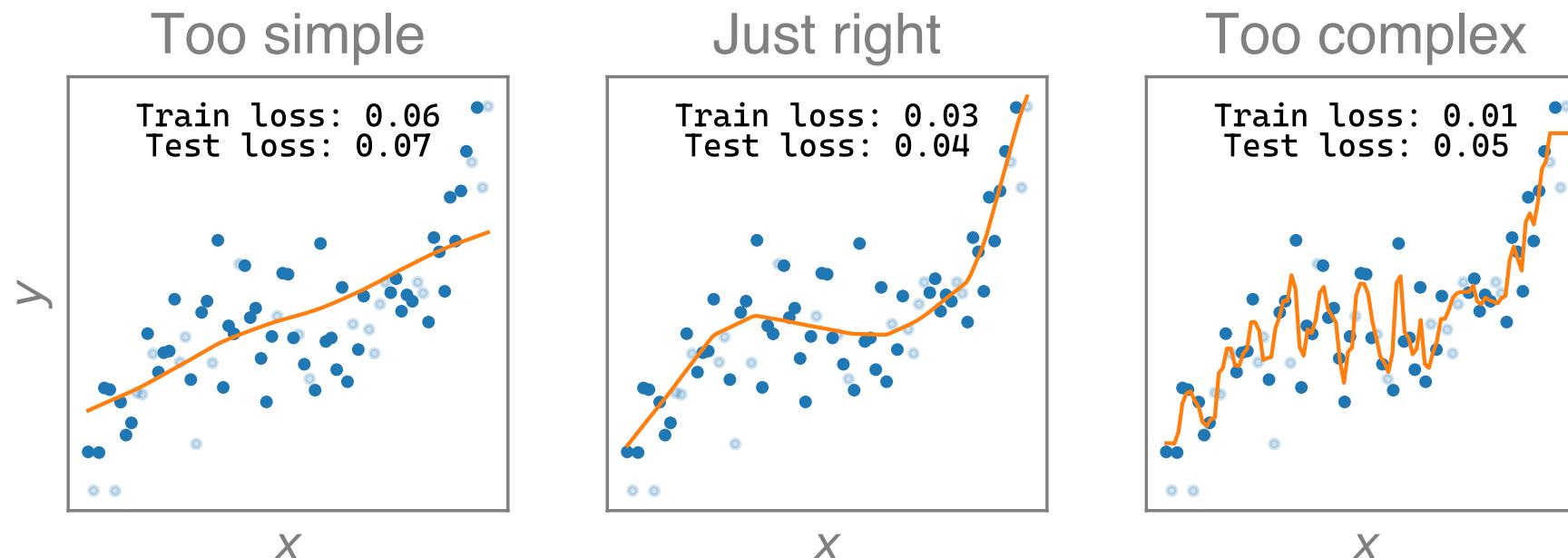
## Key concepts to prevent overfitting: split the dataset



By splitting the dataset into a **training** and a **testing** set,  
we evaluate the performance on unseen (but **similar**) data.

# Key concepts to prevent overfitting: regularization

Add a penalty term  $\mathcal{R}$  to the loss  $\mathcal{L}_{\mathcal{R}} = \mathcal{L} + \lambda \mathcal{R}$ , where  $\lambda$  is the regularization strength.



The regularization penalizes the model's complexity.

# Why so many regression algorithms?

Because of combination of models, losses, and regularizations. The [scikit-learn.org](https://scikit-learn.org) website provides a unified interface in a **greybox style**.

The model selection is made by experience or **trial and error**.

bagging, voting, stacking

1.12. Multiclass and multioutput algorithms

1.13. Feature selection

1.14. Semi-supervised learning

1.15. Isotonic regression

1.16. Probability calibration

1.17. Neural network models  
(supervised)

2. Unsupervised learning ▾

3. Model selection and evaluation ▾

4. Inspection ▾

5. Visualizations

## 1. Supervised learning

### 1.1. Linear Models

[1.1.1. Ordinary Least Squares](#)

[1.1.2. Ridge regression and classification](#)

[1.1.3. Lasso](#)

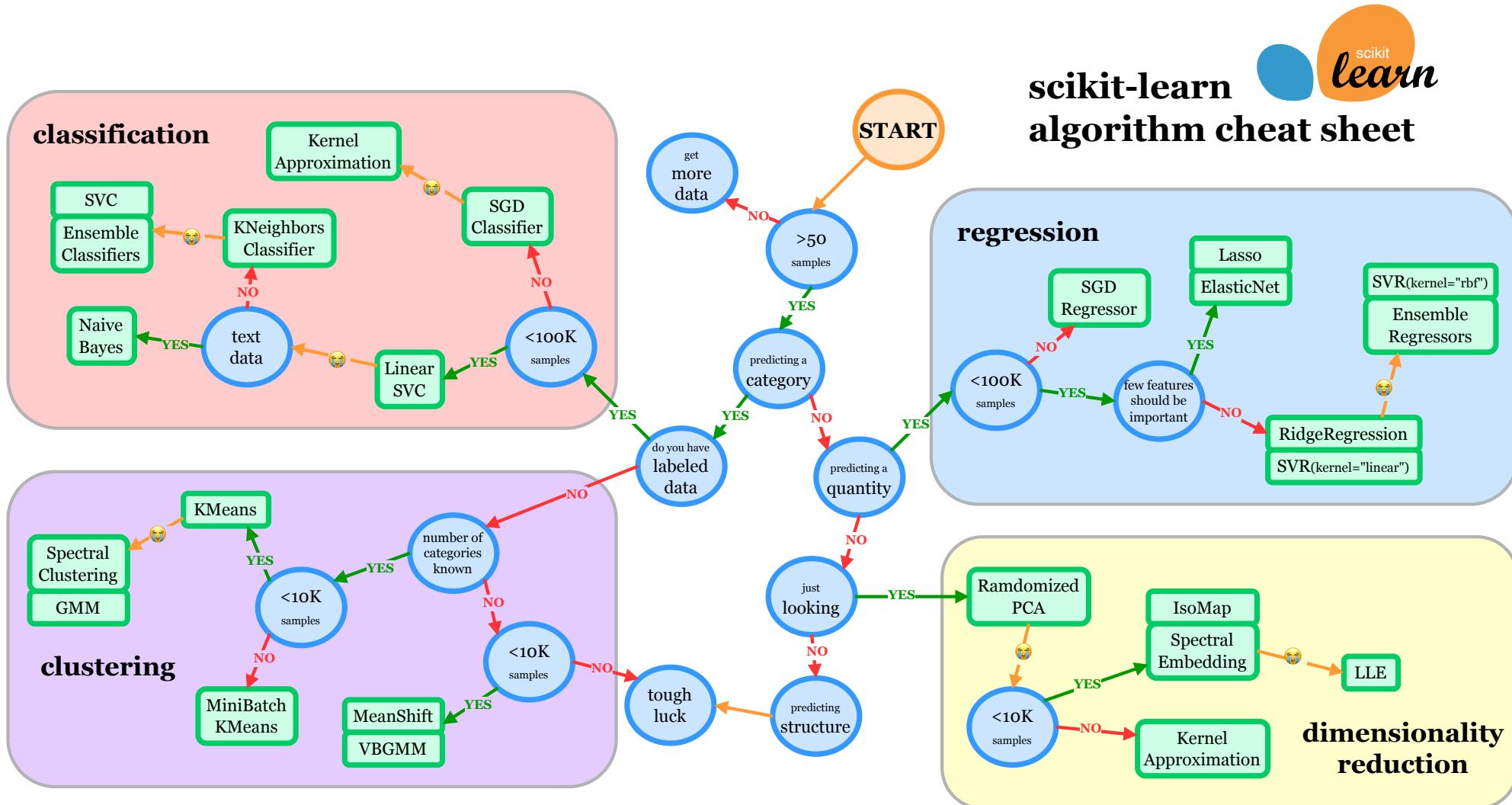
[1.1.4. Multi-task Lasso](#)

[1.1.5. Elastic-Net](#)

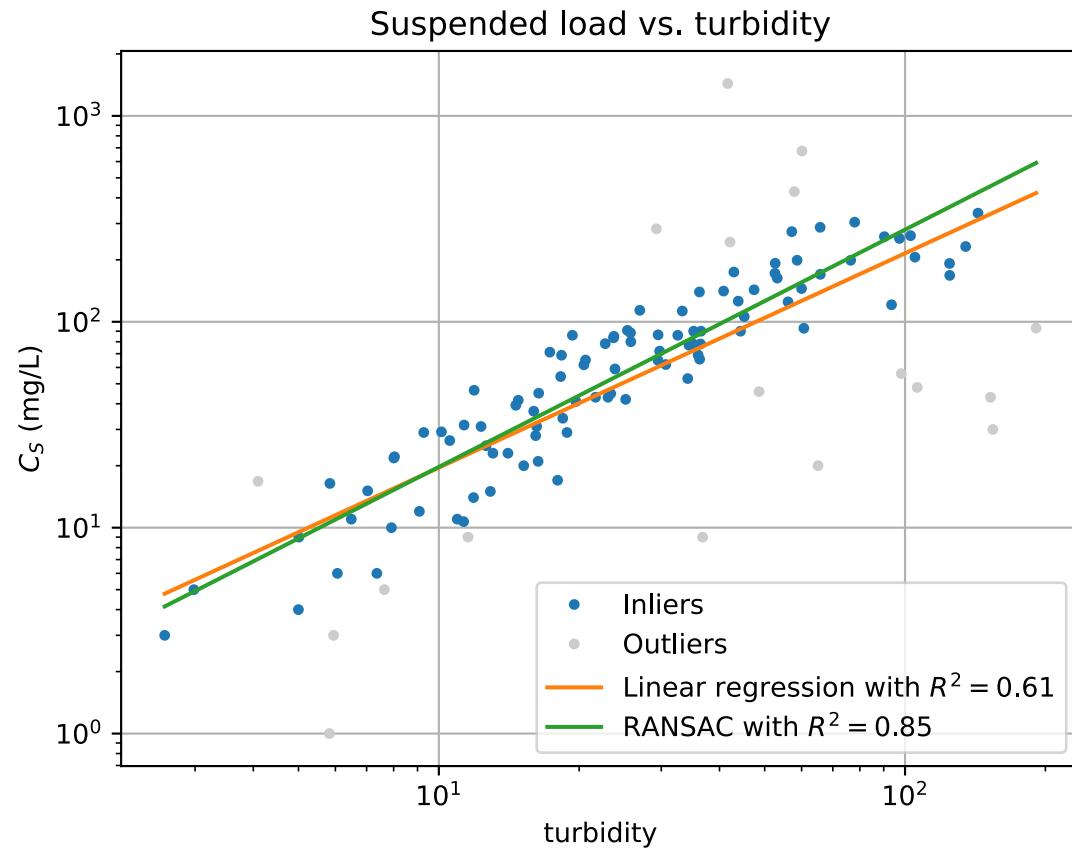
[1.1.6. Multi-task Elastic-Net](#)

[1.1.7. Least Angle Regression](#)

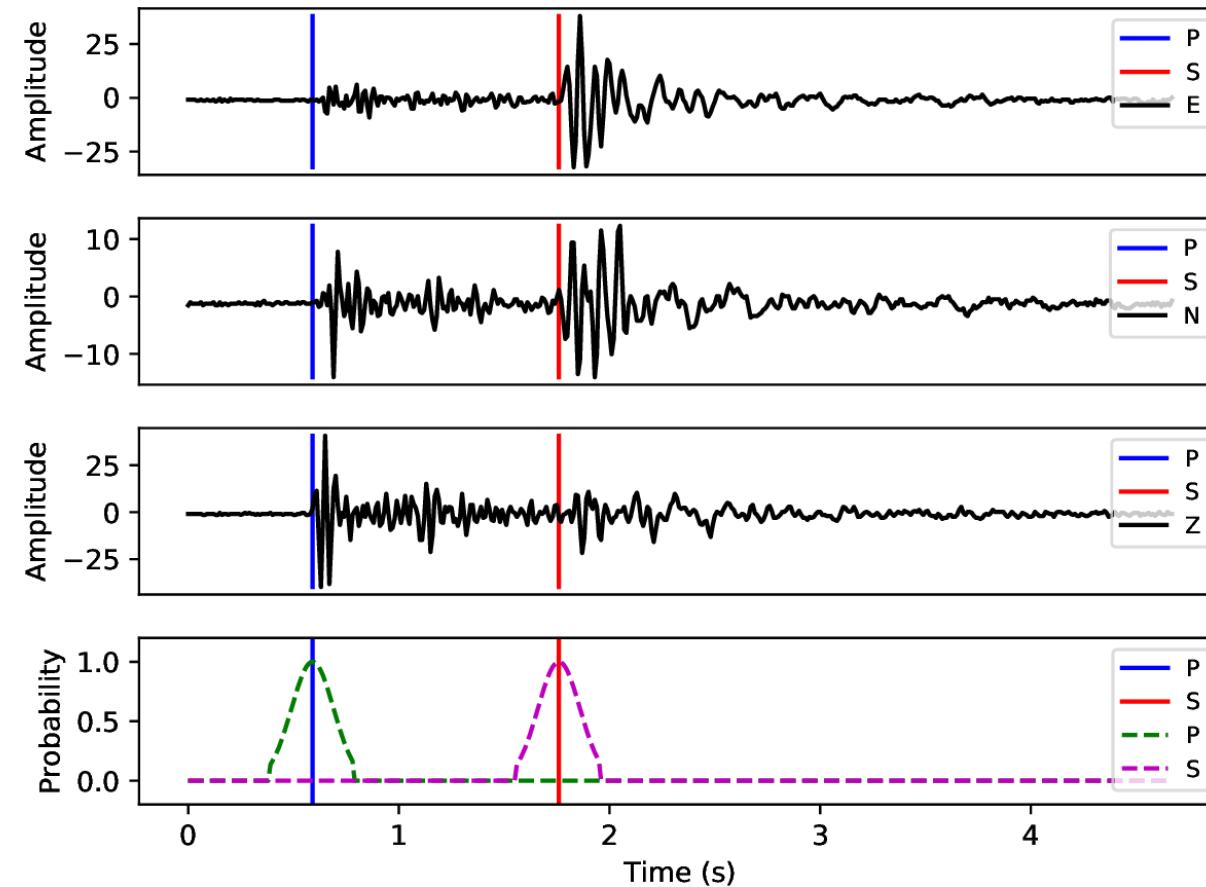
# Guidelines for exploring relevant models



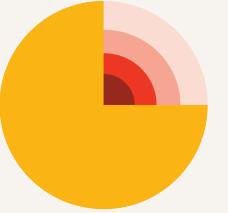
# Calibrate a turbidity sensor to estimate the suspended load in rivers



# Find out $P$ and $S$ waves within continuous seismograms



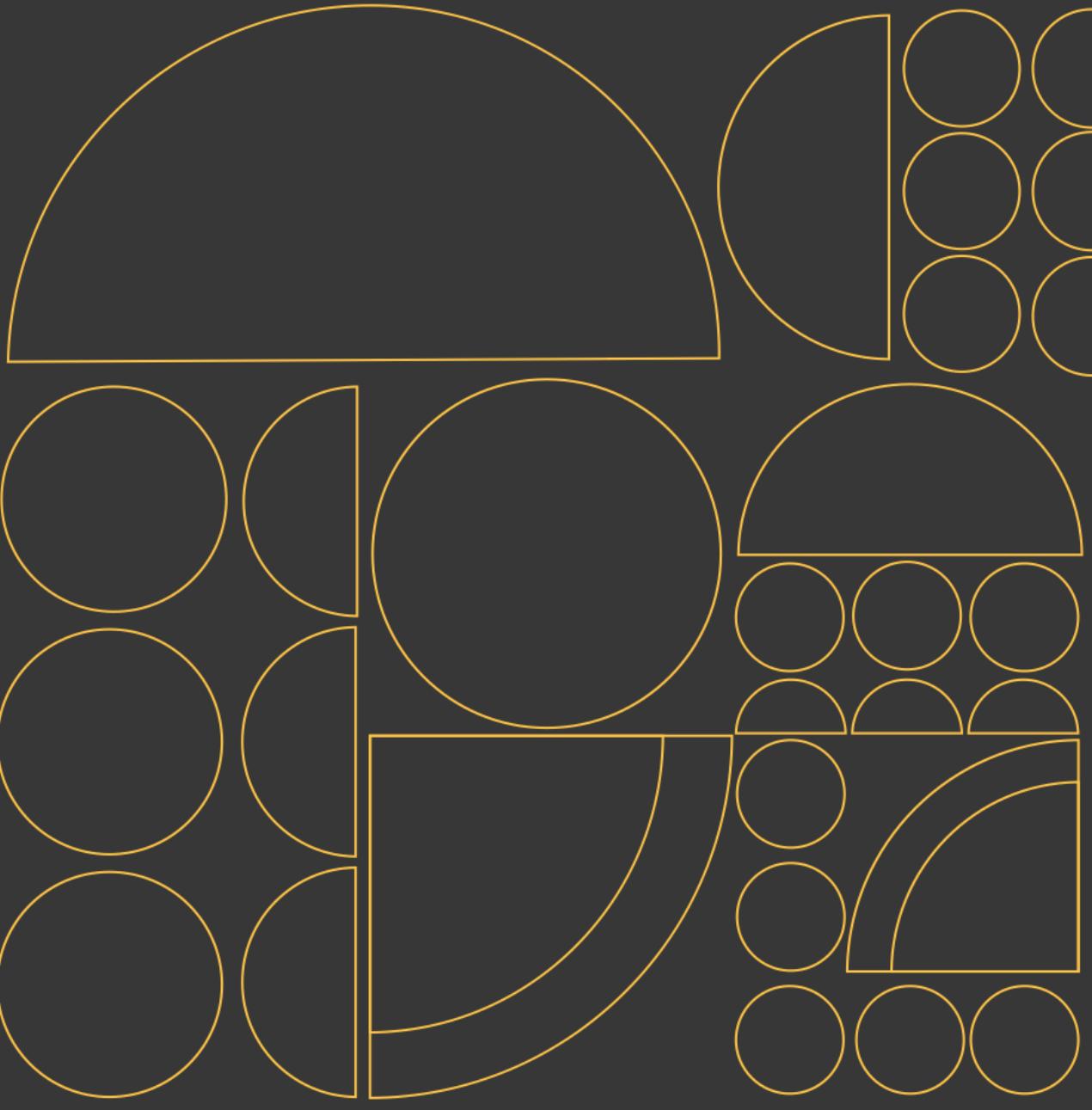
How do you address this regression problem? More after the deep learning lectures.



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## 4. Supervised machine learning: classification

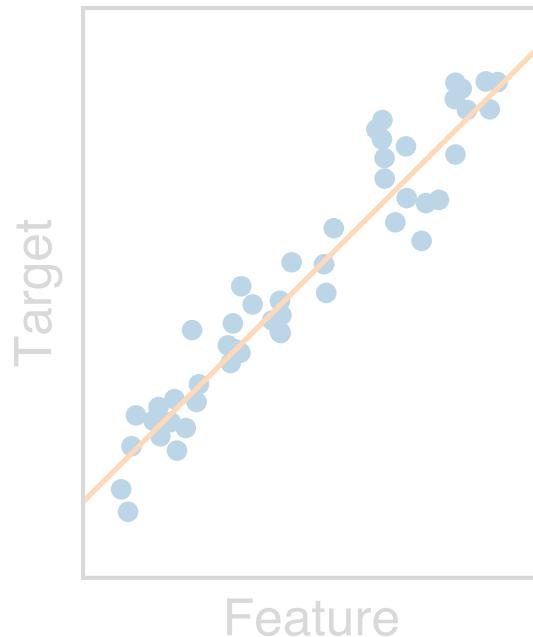
How to solve a regression or classification task with machine learning?



# The two main tasks of supervised machine learning

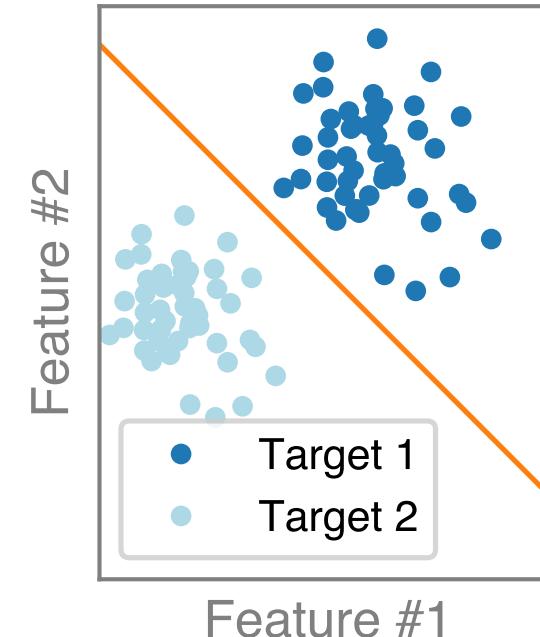
## Regression

$x$  and  $y$  are continuous

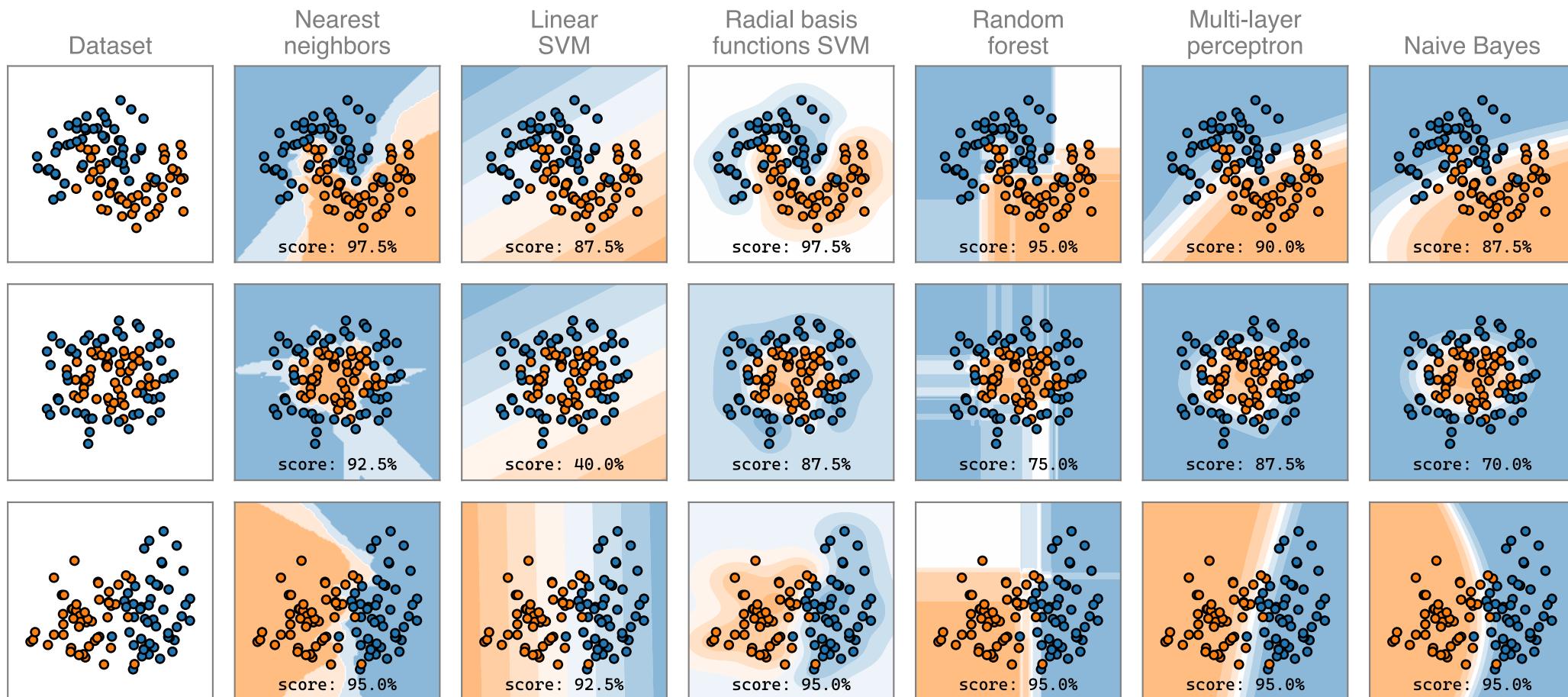


## Classification

$x$  is continuous and  $y$  is discrete



# The classification task



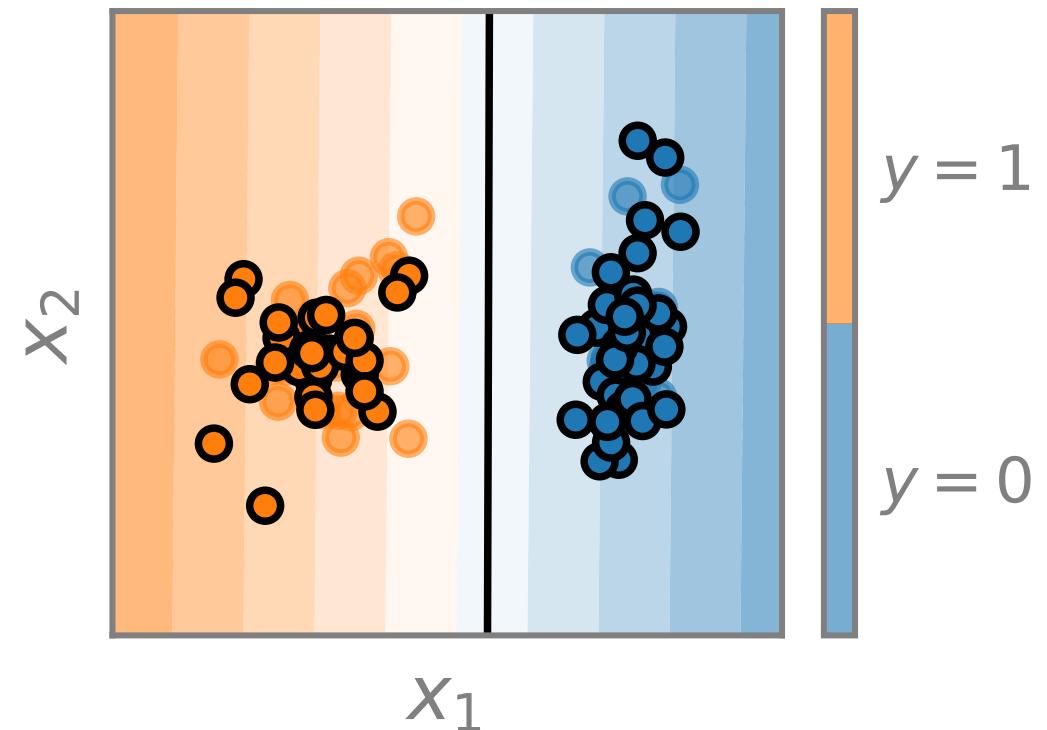
Here again, we have many possibilities.

# The classification task

**Experience:** manual labels  $y \in \{0, 1\}$  obtained from various cases, where two features  $\mathbf{x} \in \mathbb{R}^2$  are measured.

**Task:** predict the category  $\hat{y}$  of the samples  $\mathbf{x}$ .

**Performance:** how should we measure the performance of a classifier?

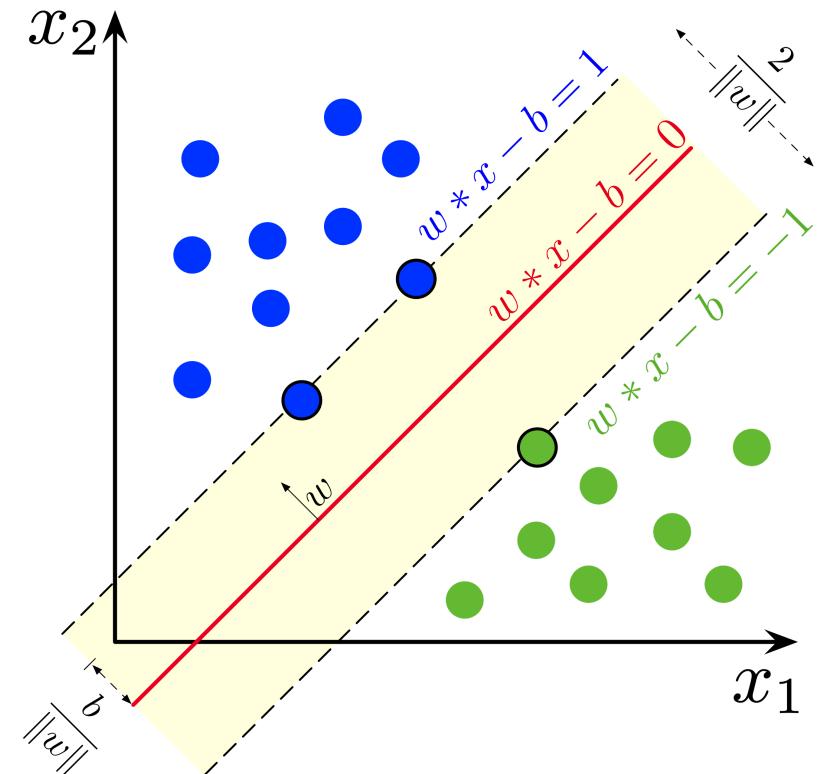


# The classification task with support vector machines (SVM)

Support vector machines search the hyperplane of normal vector  $\mathbf{w}$  and bias  $b$  that split the classes.

Note: in 2D, a hyperplane is a line.

The support vectors are the samples that are closest to the other class.



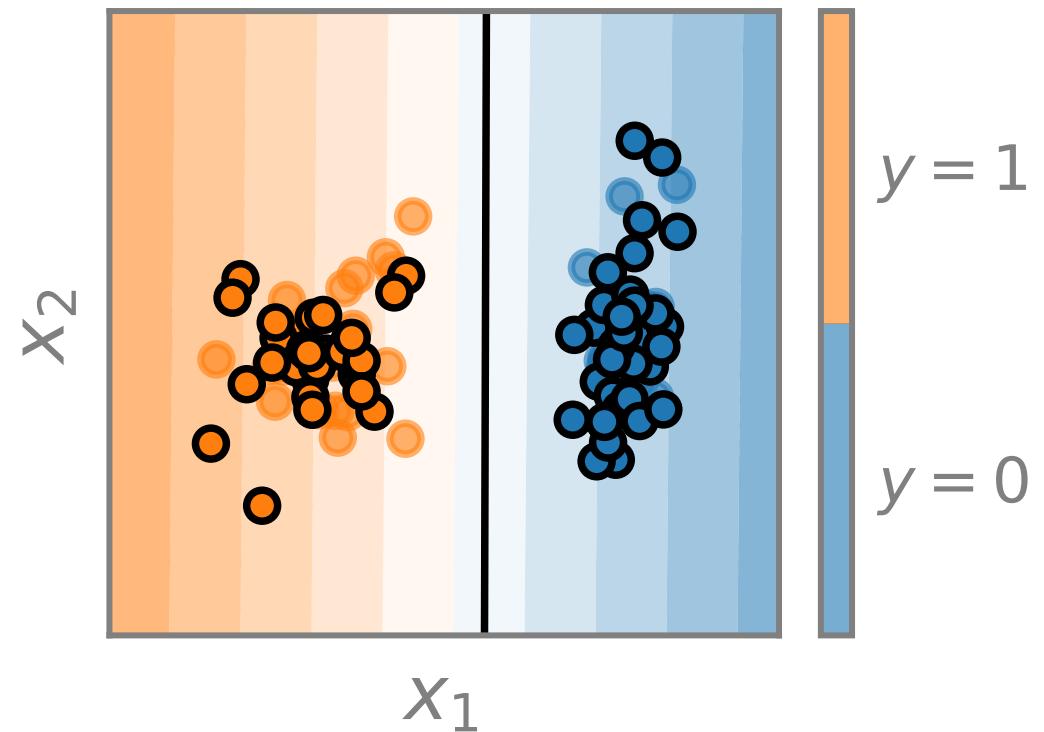
# The classification task with support vector machines (SVM)

The decision function  $f(\mathbf{x})$  depends on the sign of the linear combination of the normal vector and the sample:

$$f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + b$$

The quantity to minimize is the **Hinge loss**:

$$\mathcal{L}(\mathbf{w}, b) = \frac{1}{N} \sum_{i=1}^N \max(0, 1 - y_i (\mathbf{w} \cdot \mathbf{x}_i + b))$$



# The classification task with support vector machines (SVM)

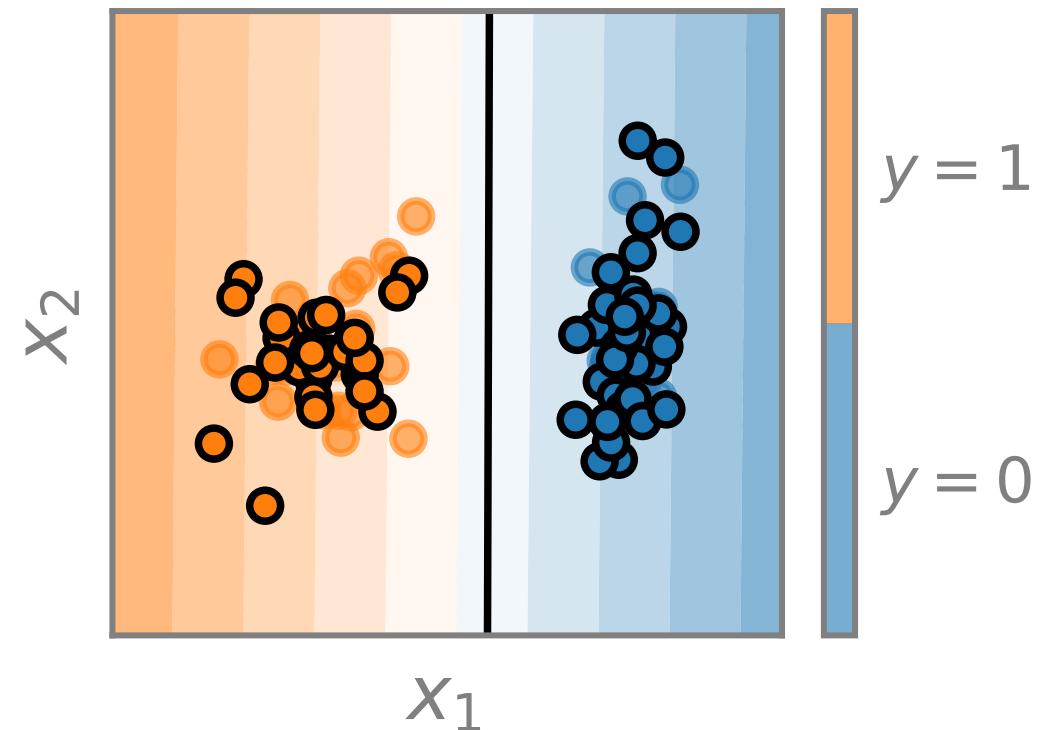
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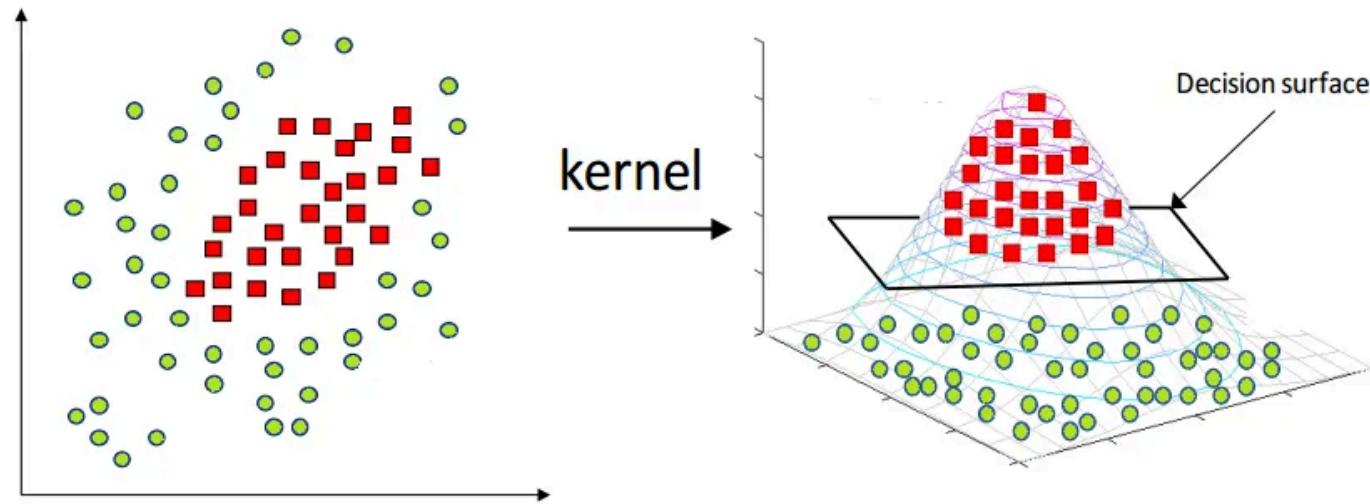
$$\mathcal{L}(\mathbf{w}, b) = \frac{1}{N} \sum_{i=1}^N \max(0, 1 - y_i (\mathbf{w} \cdot \mathbf{x}_i + b))$$

What about non linear problems?



# The kernel trick for non linear classification problems

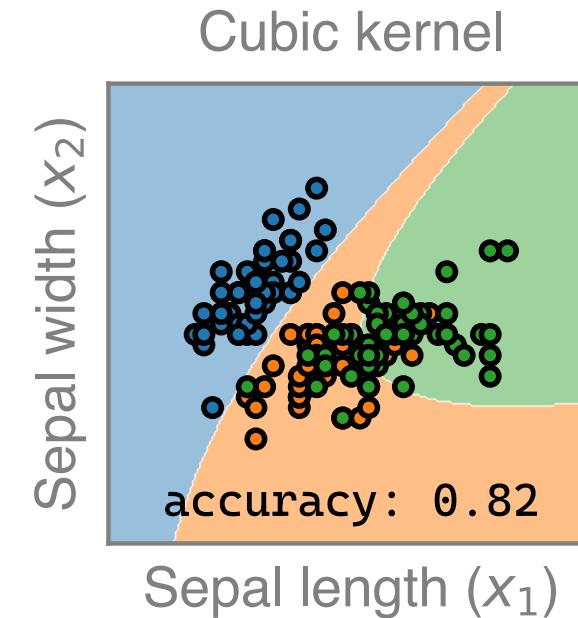
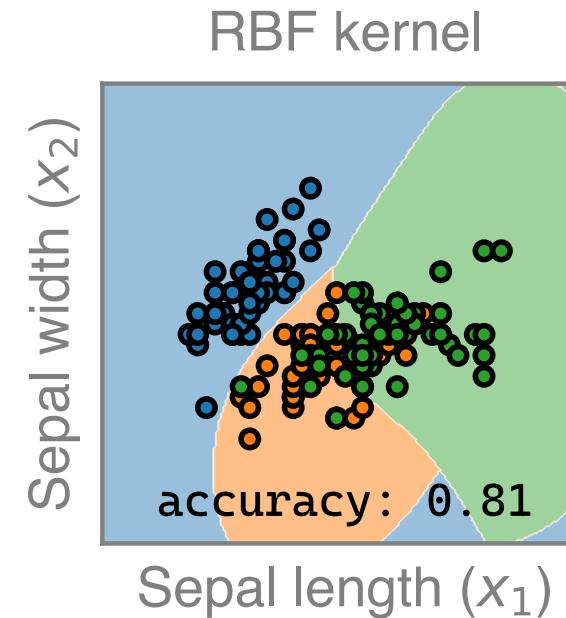
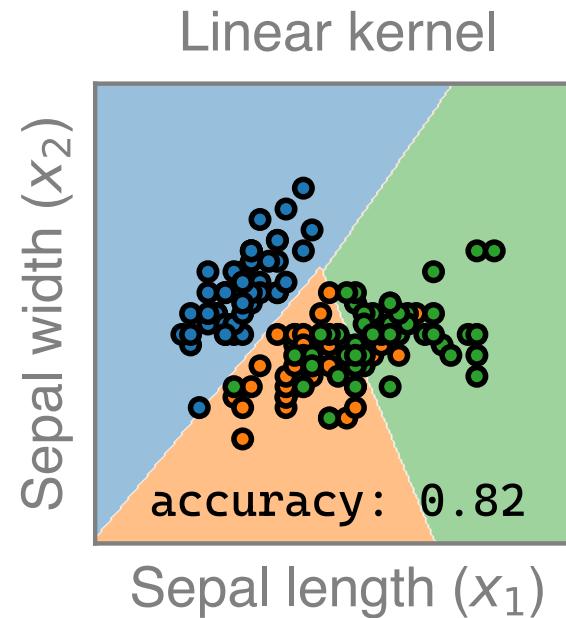
The kernel trick allows to map the data to a **higher dimensional** space made from the input features where the problem is **linearly separable**.



The **Radial Basis Functions** (RBF) is an infinite kernel  $K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2\sigma^2}\right)$

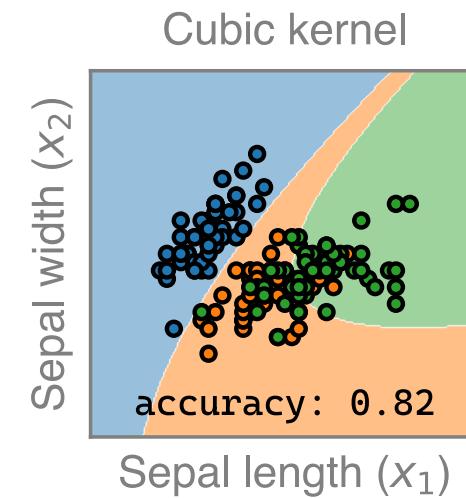
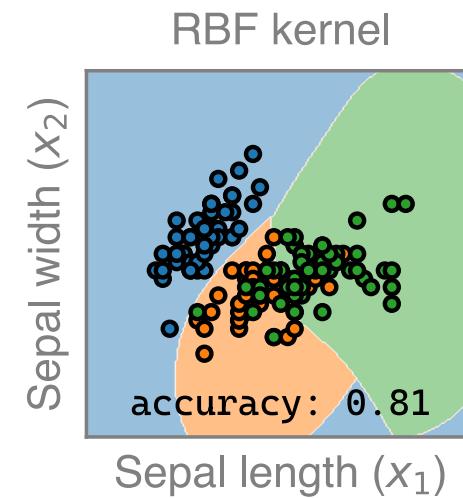
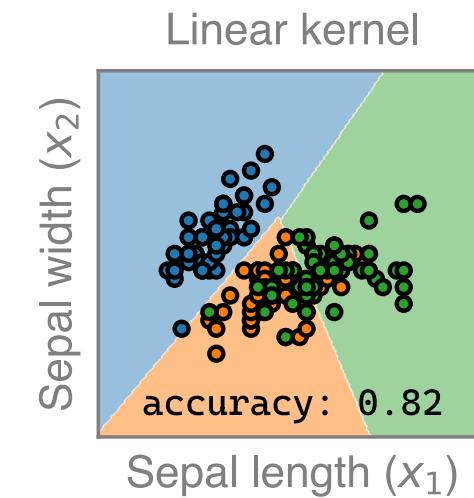
# Generalization of the SVM: the support vector classifier (SVC)

The SVC is a generalization of the SVM that digests more than two classes.



The decision function is linear in the kernel space only.  
We can project it back to the data space to inspect it.

# Various classification metrics from the confusion matrix



True	0	1	2
0	50	0	0
1	0	38	12
2	0	15	35

Predicted

Predicted	0	1	2
0	50	0	0
1	0	31	19
2	0	10	40

Predicted	0	1	2
0	50	0	0
1	0	38	12
2	0	15	35

## Various classification metrics: accuracy, precision, recall

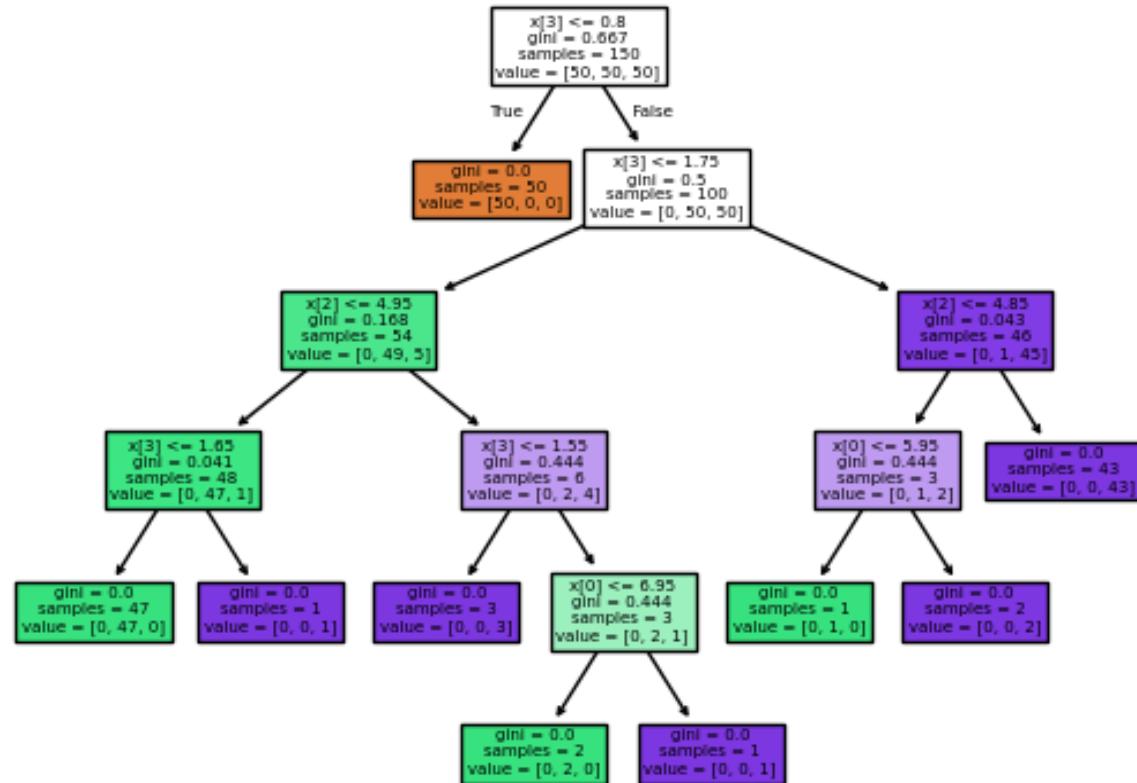
# Decision trees and random forests

**Decision trees** are a set of rules that learns to predict the category.

**Random forests** are an ensemble of decision trees that vote for the category.

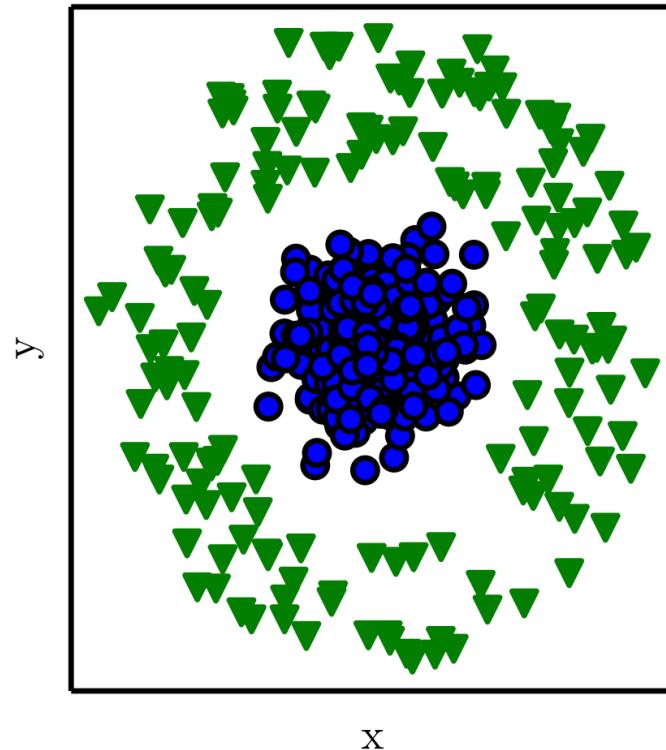
**These algorithms are extremely powerful.**

Decision tree trained on all the iris features

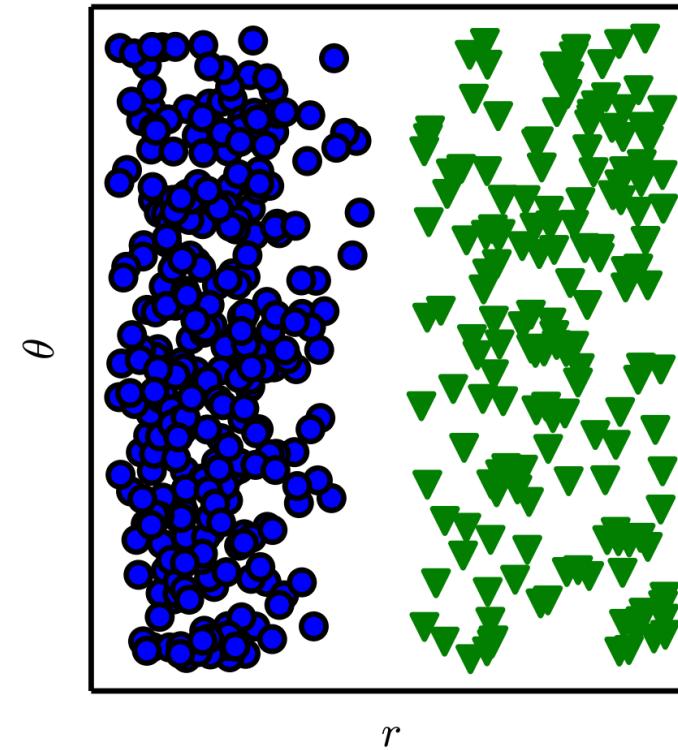


# Representation matters!

Cartesian coordinates



Polar coordinates

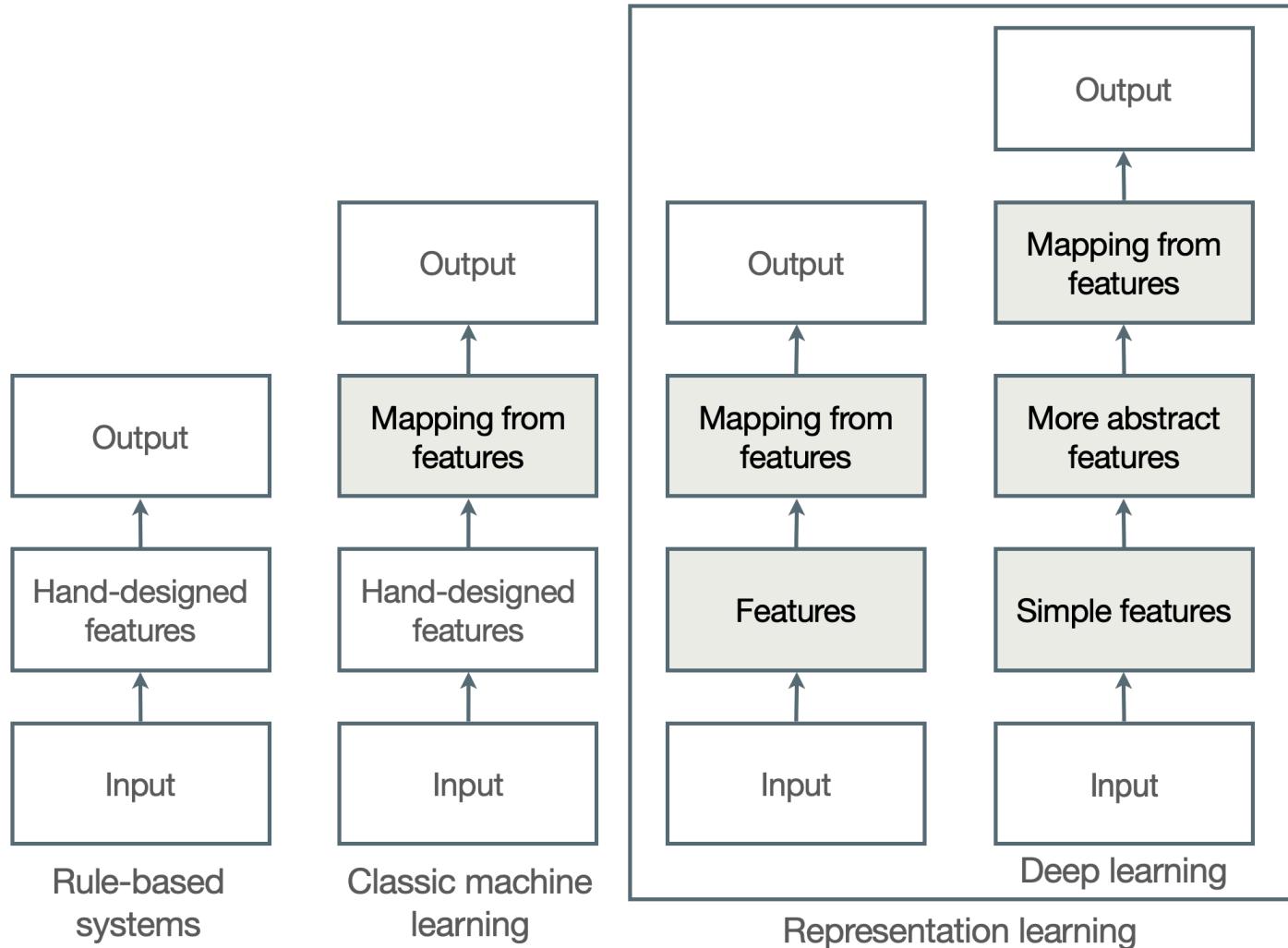


There is no need for a complex model if you have a good **representation** of the data.

# Learning strategies depending on the task complexity

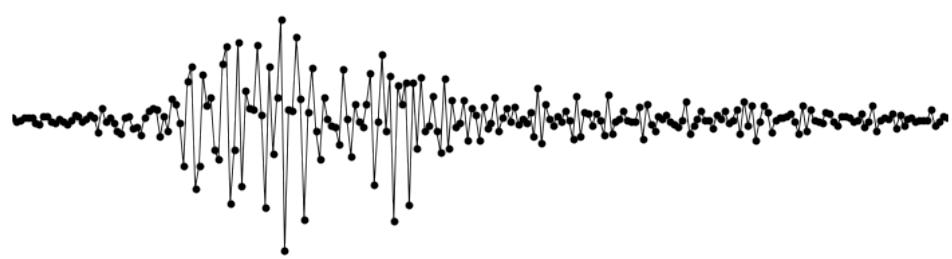
We can engineer features from the raw data to improve the model's performance.

We can also **learn the features** from the data.



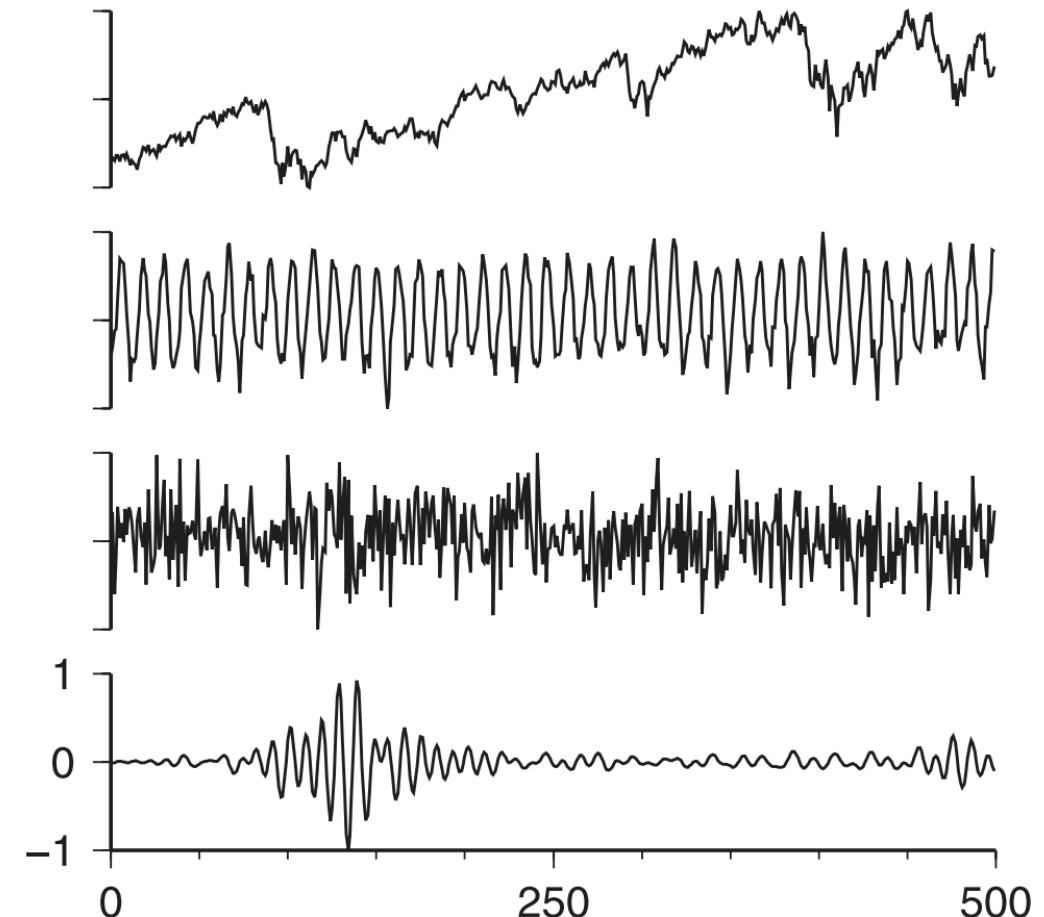
# Why would waveforms not be the best representation of ground motion?

We can see waveforms  $\mathbf{x} \in \mathbb{R}^N$  as points  
of a  $N$ -dimensional space



Yet, seismic waveform do not occupy this  
space fully, likely very sparse.

**Dimension > Information**

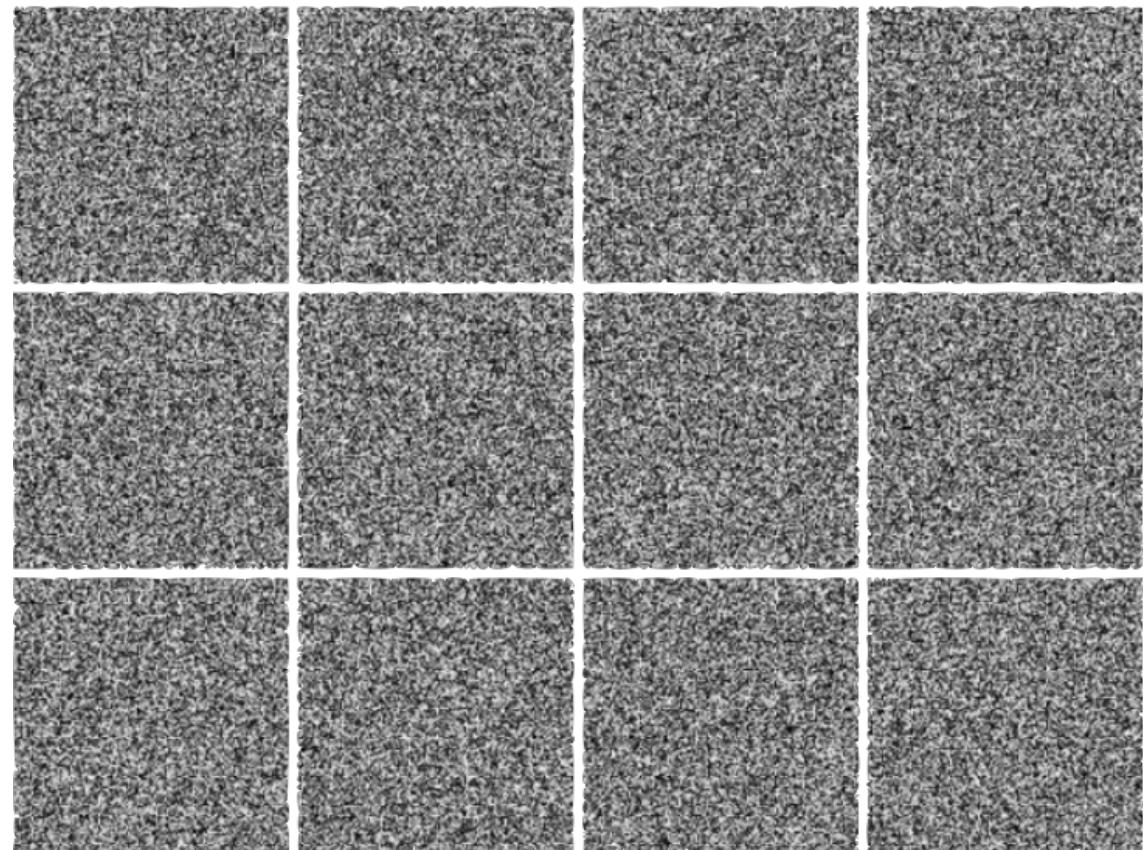


Actually, natural data spaces may be often not fully occupied

Random sampling of the pixels of a face. What is the likelihood that the reshuffled image *is* a face?

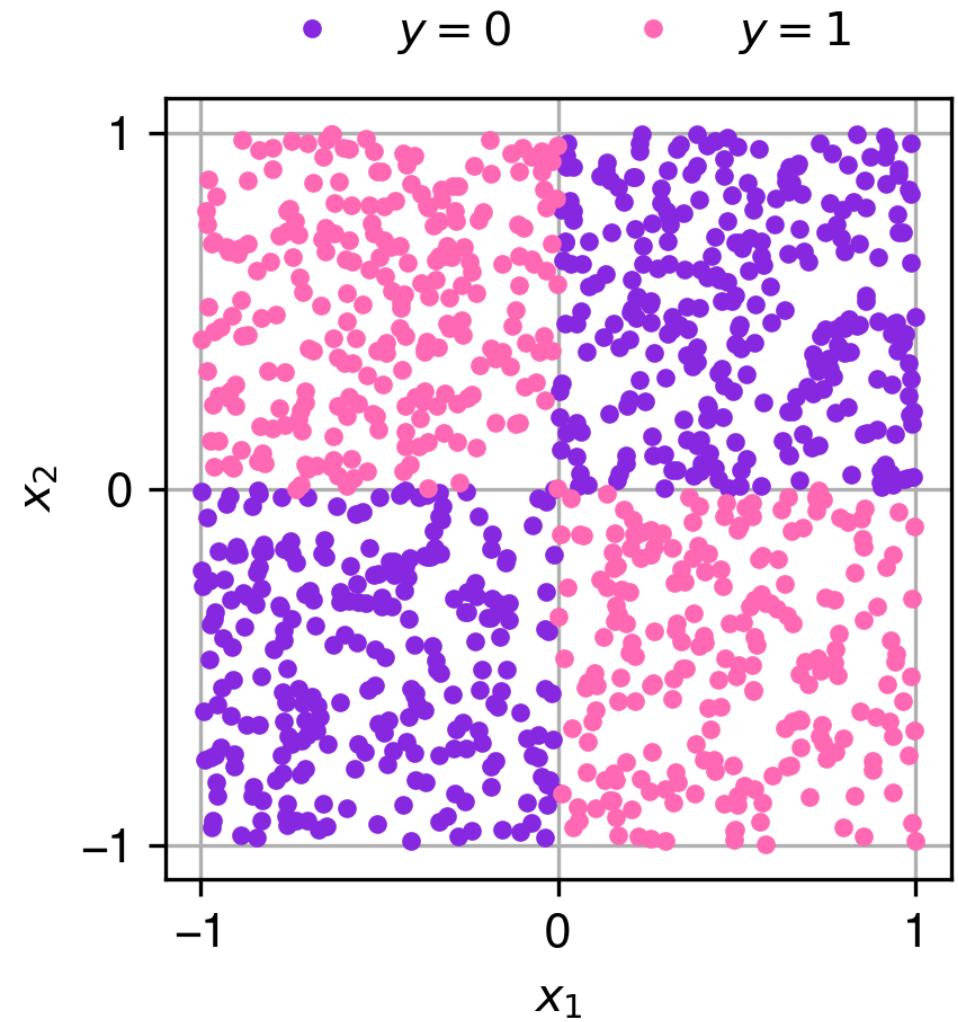


Like waveforms, **images are living on a manifold.**



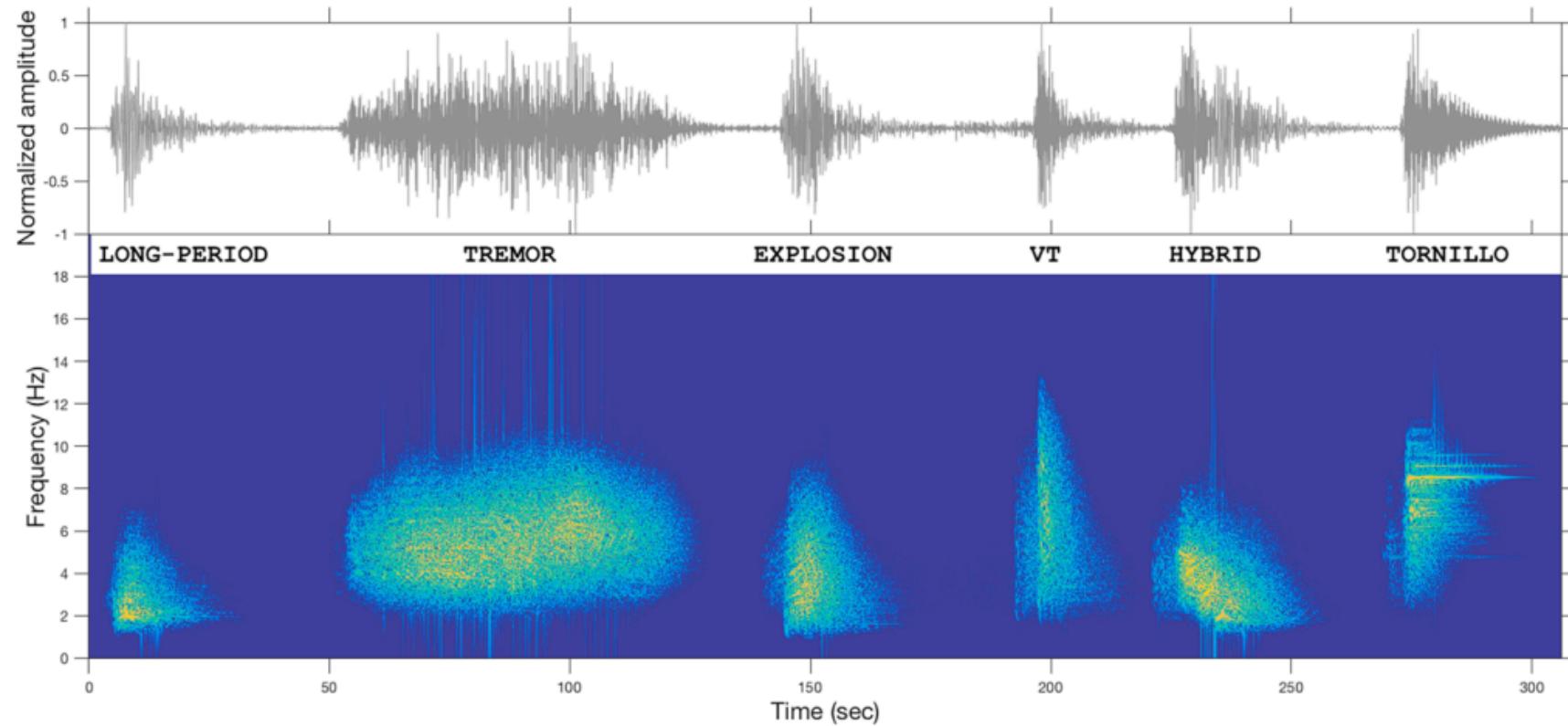
Therefore, we need to find or learn the representation of the data

**The exclusive OR problem** (XOR) is a simple problem not linearly separable, hard to learn using traditional machine learning algorithms. Multi-layer perceptrons can.



# Supervised learning for sismo-volcanic signal classification

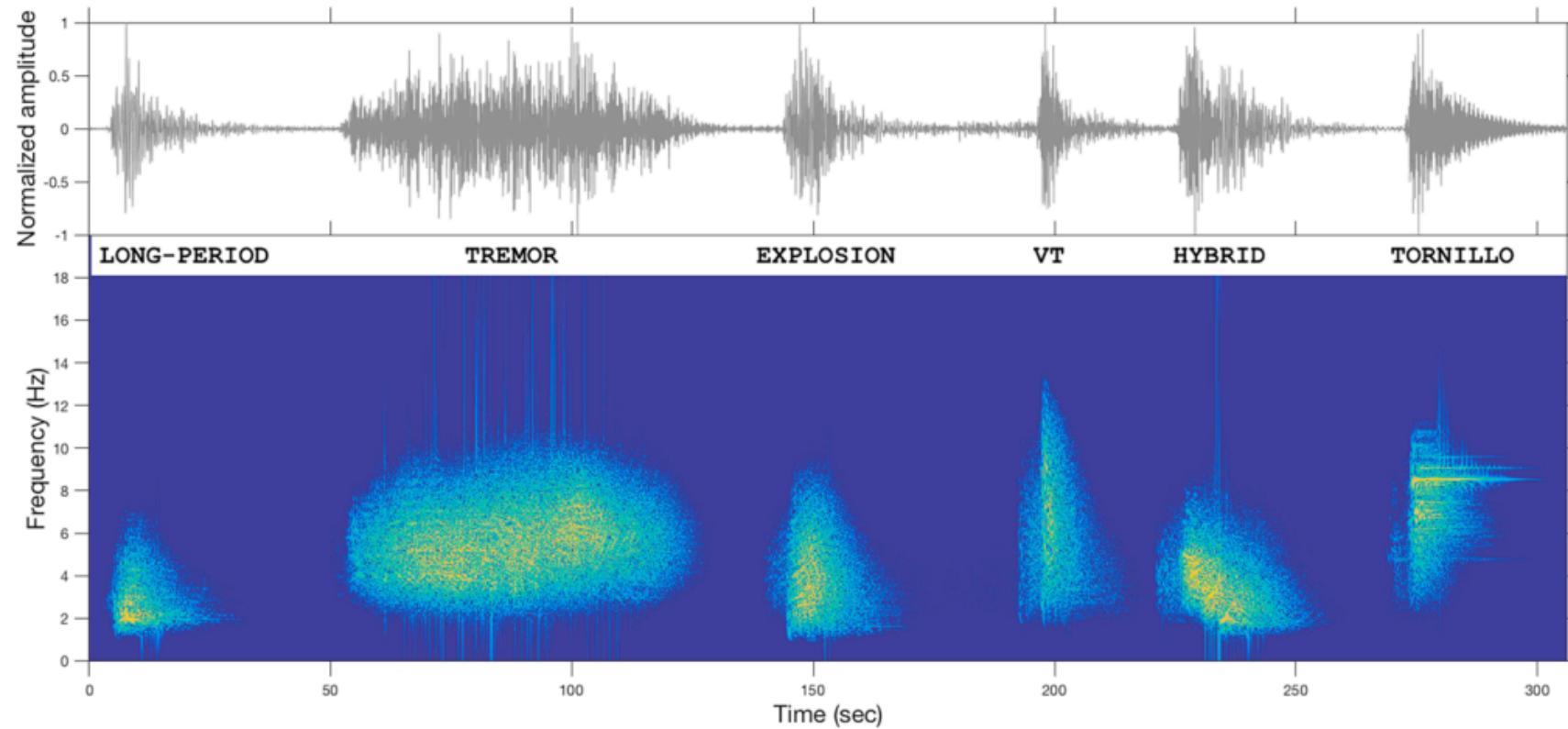
**Supervised learning** experiences a set of examples containing features  $\mathbf{x}_i \in \mathbb{X}$  associated with labels  $\mathbf{y} \in \mathbb{Y}$  to be predicted from the features (here, classification).



# Supervised learning for sismo-volcanic signal classification

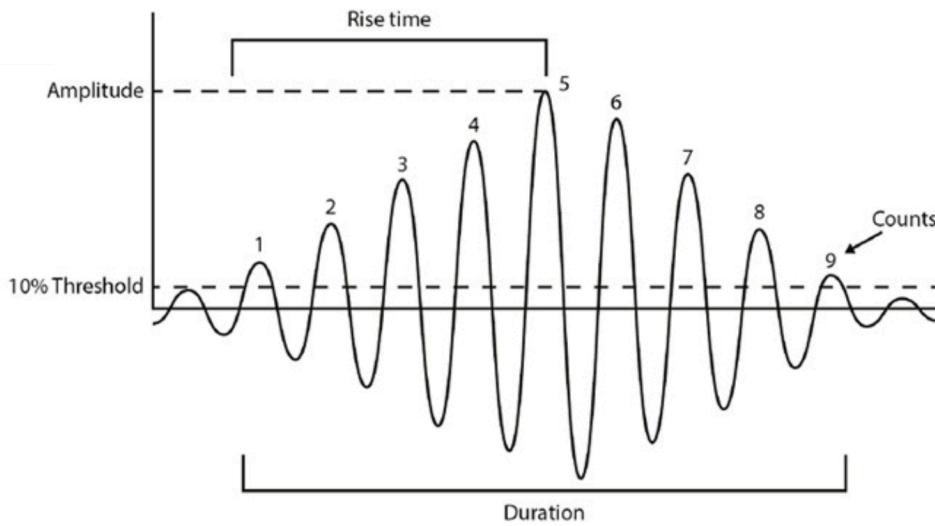
In this case,  $\mathbf{x}$  lies in  $\mathbb{R}^{3 \times N}$ , and  $\mathbf{y}$  in  $[0, \dots, 5]$ .

Which **representation** of  $\mathbf{x}$  works best?



# Handcrafted features for classical machine learning

We need to find relevant descriptors of our data, used as features  $\mathbf{x}$ .



**Table 1**  
*List of Features*

Statistic features		Used in	Ref.
Feature	Definition		
Length	$n = \text{length}(s)$	Tucker and Brown (2005)	1
Mean	$\mu_s = \frac{1}{n} \sum_i s[i]$	Tucker and Brown (2005)	2
Standard deviation	$\sigma_s = \sqrt{\frac{1}{(n-1)} \sum_i (s[i] - \mu_s)^2}$		3
Skewness	$\frac{1}{n} \sum_i \left( \frac{s[i] - \mu_s}{\sigma_s} \right)^3$	Langet (2014) and Hibert et al. (2014)	4
Kurtosis	$\frac{1}{n} \sum_i \left( \frac{s[i] - \mu_s}{\sigma_s} \right)^4$	Langet (2014) and Hibert et al. (2014)	5
$i$ of central energy	$\bar{i} = \frac{1}{E} \cdot \sum_i E_i \cdot i$	(Tucker & Brown, 2005)	6
RMS bandwidth	$B_i = \sqrt{\frac{1}{E} \sum_i i^2 \cdot E_i - \bar{i}^2}$	Tucker and Brown (2005)	7
Mean skewness	$\sqrt{\frac{\sum_i (i-\bar{i})^2 E_i}{E \cdot B_i^3}}$	Tucker and Brown (2005)	8
Mean kurtosis	$\sqrt{\frac{\sum_i (i-\bar{i})^4 E_i}{E \cdot B_i^4}}$	Tucker and Brown (2005)	9
Entropy features (with $p(s_j)$ the probability of amplitude level $s_j$ )		Ref.	
Shannon entropy <sup>a</sup>	$-\sum_j p(s_j) \log_2 (p(s_j))$	Esmaili et al. (2004) and Han et al. (2011)	10 to 12
Rényi entropy <sup>b</sup>	$\frac{1}{1-\alpha} \cdot \log_2 \left( \sum_j p(s_j)^\alpha \right)$	Han et al. (2011)	13 to 18
Shape descriptor features		Ref.	
Rate of attack	$\max_i \left( \frac{s[i] - s[i-1]}{n} \right)$	Tucker and Brown (2005)	19
Rate of decay	$\min_i \left( \frac{s[i] - s[i+1]}{n} \right)$	Tucker and Brown (2005)	20
Ratios	min/mean and max/mean	Langet (2014) and Hibert et al. (2014)	21 to 22
Energy descriptors	Signal energy, maximum, average, standard deviation, skewness, and kurtosis	Tucker and Brown (2005)	23 to 28
Specific values	min, max, $i$ of min, $i$ of max, threshold crossing rate, and silence ratio	Tucker and Brown (2005)	29 to 34

Note. Features computed for a signal  $s[i]_{i=1}^n$  (in which  $i$  might correspond to a temporal, frequency, or cepstral sample).  $E = \sum_{i=1}^n s[i]^2$  and  $E_i = s[i]^2$  describe the signal energy and the energy at sample  $i$ , respectively. Some features have a dimension greater than others; e.g., entropy measurements are made on three different estimations of the amplitude probability (i.e., different histogram bin numbers).

<sup>a</sup>Bin numbers for probability estimation: 5, 30, and 500. <sup>b</sup>Bin numbers for probability estimation: 5, 30, 500,  $\alpha = 2$ , and inf.

# Performance measure, and what can we learn from it?

Accuracy of the predictions measures the model's performance (= confusion matrix)

**Table 3**  
*Confusion Matrix*

		True Class (ground truth)						Precision
		LP	TR	VT	EXP	HYB	TOR	
Predicted Class	LP	<b>58,363</b>	627	8	0	5	1	98.9%
	TR	3,000	<b>4,584</b>	0	1	2	0	60.4%
	VT	478	11	<b>475</b>	5	11	3	48.3%
	EXP	15	16	2	<b>29</b>	0	0	47.8%
	HYB	131	3	28	13	<b>125</b>	0	41.7%
	TOR	43	4	3	0	0	<b>28</b>	35.9%
Accuracy		<b>94.1%</b>	<b>87.4%</b>	<b>92.2%</b>	<b>59.8%</b>	<b>87.1%</b>	<b>84.6%</b>	

What is the guarantee that the features we choose are the best ones?

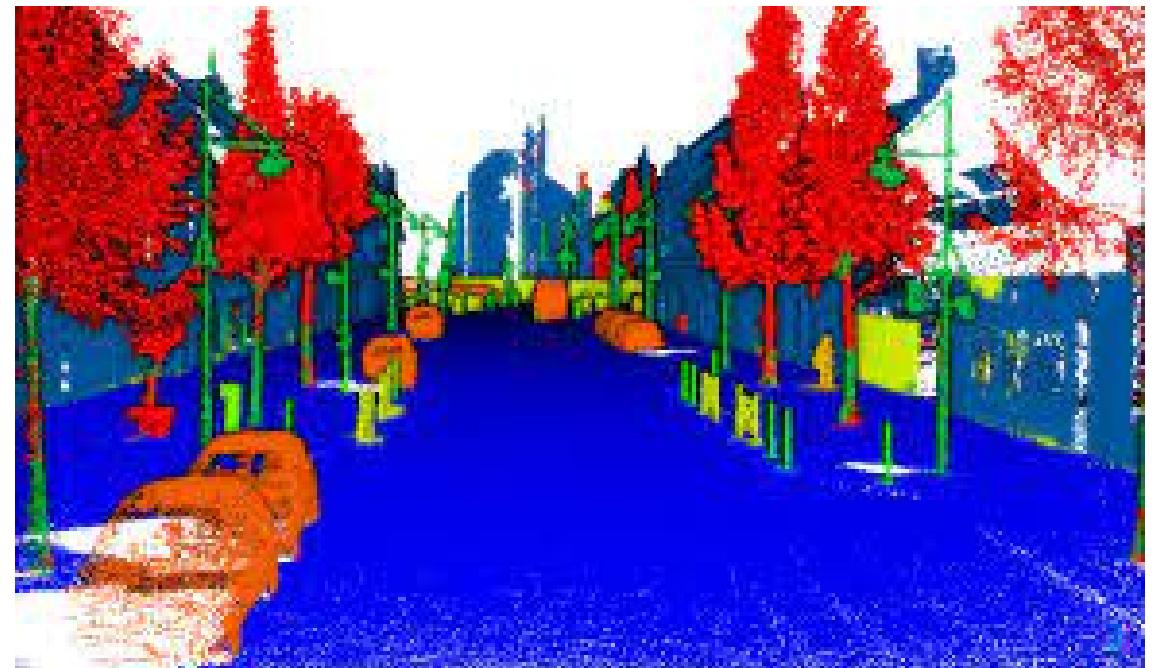
# Notebook: Lidar point cloud classification

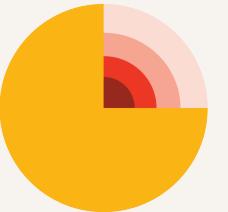
## Problem

Automate the identification of objects in a lidar cloud from labeled subset.

## Objectives

Supervised learning, classification, non-linear models, multi-scale features.

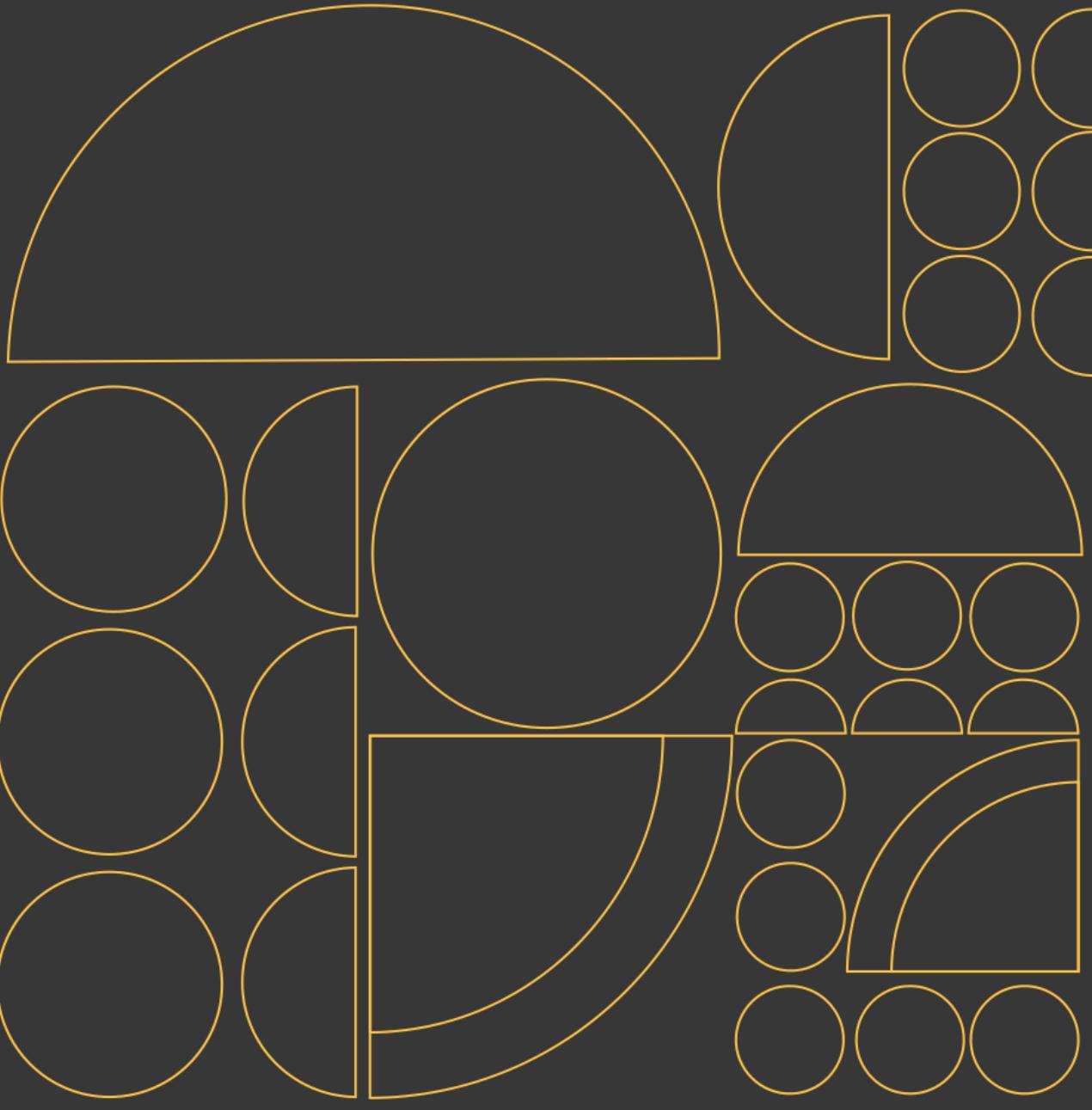




**ChEESE**

## 5. Deep learning: multi-layer perceptrons

How deep learning works? What is a neural network? How to train it, and what for?

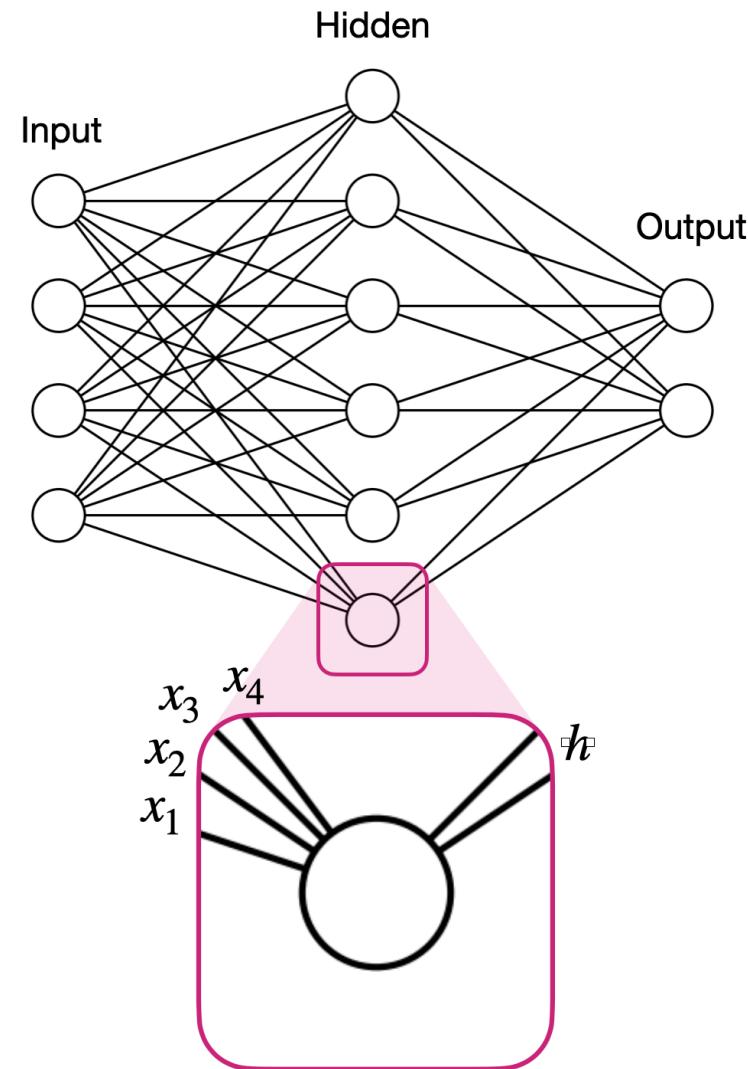


## A general form of an artificial neuron

A **neuron**, or unit, takes a set of inputs  $\mathbf{x}$  and outputs an activation value  $h$ , as

$$h = \varphi \left( \sum_{i=0}^N w_i x_i + b \right)$$

with  $w_i$  the weights,  $b$  the bias,  $\varphi$  is the activation function, and  $N$  is the number of inputs.



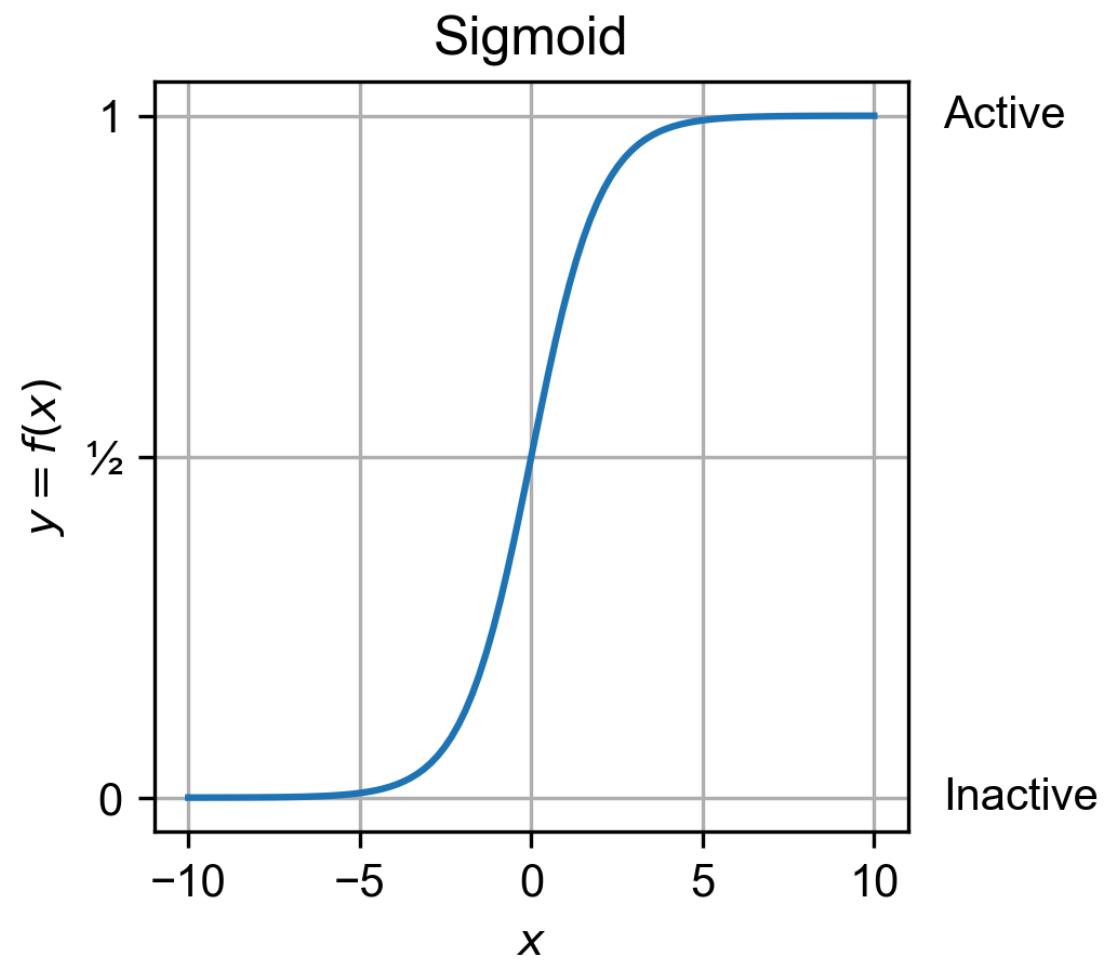
## A famous neuron: the sigmoid unit

A **neuron**, or unit, transforms a set of inputs  $\mathbf{x}$  into an output  $h$ , as

$$h = \varphi \left( \sum_{i=0}^N w_i x_i + b \right)$$

with  $w_i$  the weights,  $b$  the bias,  $\varphi$  is the activation function, and  $N$  is the number of inputs. Common activation functions include the **sigmoid** function, defined as

$$\varphi(z) = \frac{1}{1 + e^{-z}}$$



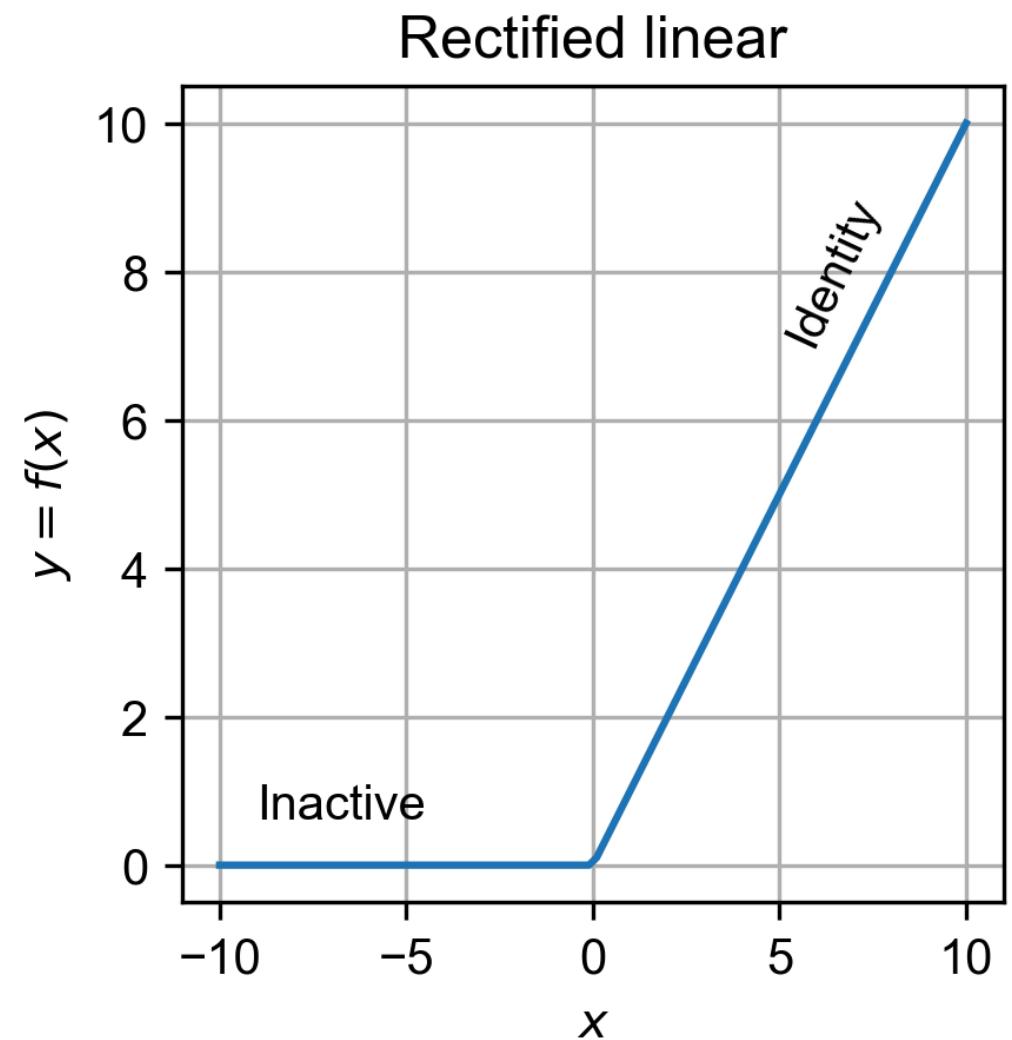
## An even more famous one: the rectified linear unit

A **neuron**, or unit, transforms a set of inputs  $\mathbf{x}$  into an output  $h$ , as

$$h = \varphi \left( \sum_{i=0}^N w_i x_i + b \right)$$

with  $w_i$  the weights,  $b$  the bias,  $\varphi$  is the activation function, and  $N$  is the number of inputs. Common activation functions include the **rectified linear unit** (ReLU), defined as

$$\varphi(z) = \max(0, z)$$



ReLU are empirically preferred to sigmoid units for computational efficiency no saturation when  $x$  is large.

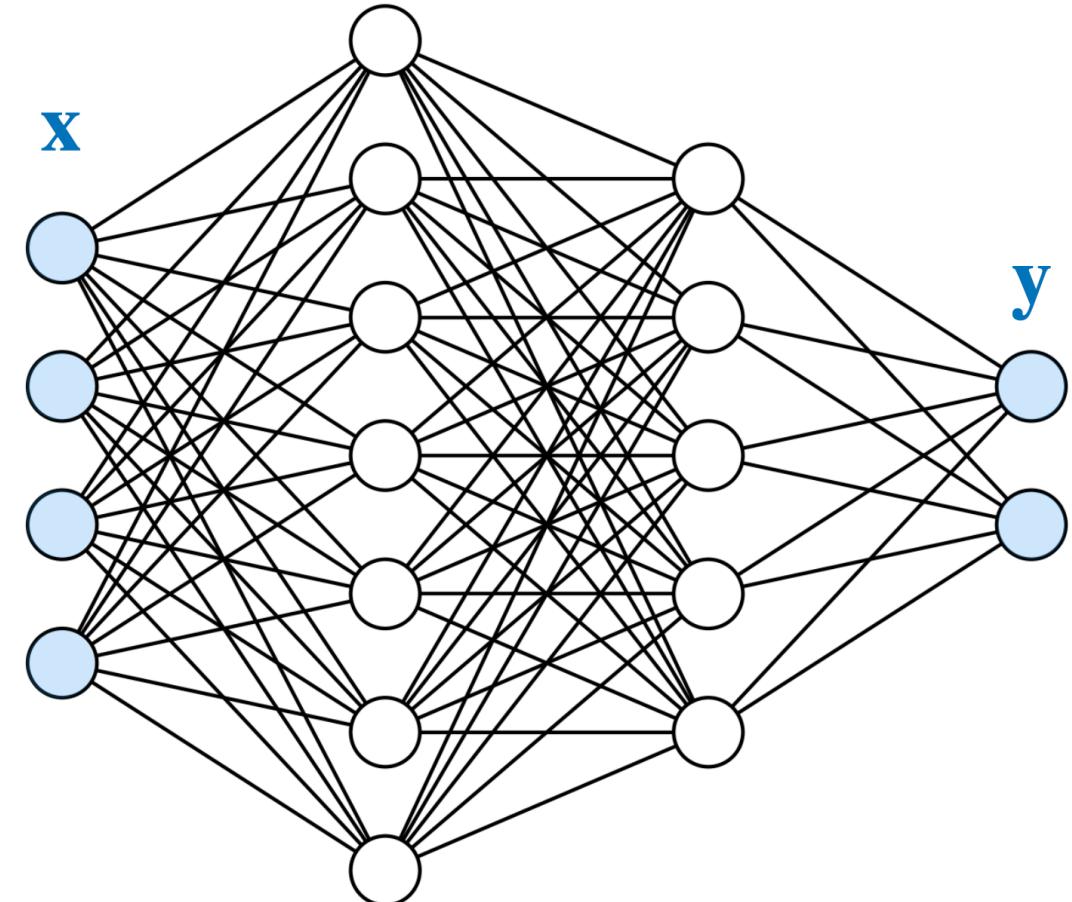
# The multilayer perceptron (MLP)

A **multilayer perceptron** is a neural network with multiple hidden layers:

$$h_i^{(1)} = \varphi^{(1)} \left( \sum_j w_{ij}^{(1)} x_j + b_i^{(1)} \right)$$

$$h_i^{(2)} = \varphi^{(2)} \left( \sum_j w_{ij}^{(2)} h_j^{(1)} + b_i^{(2)} \right)$$

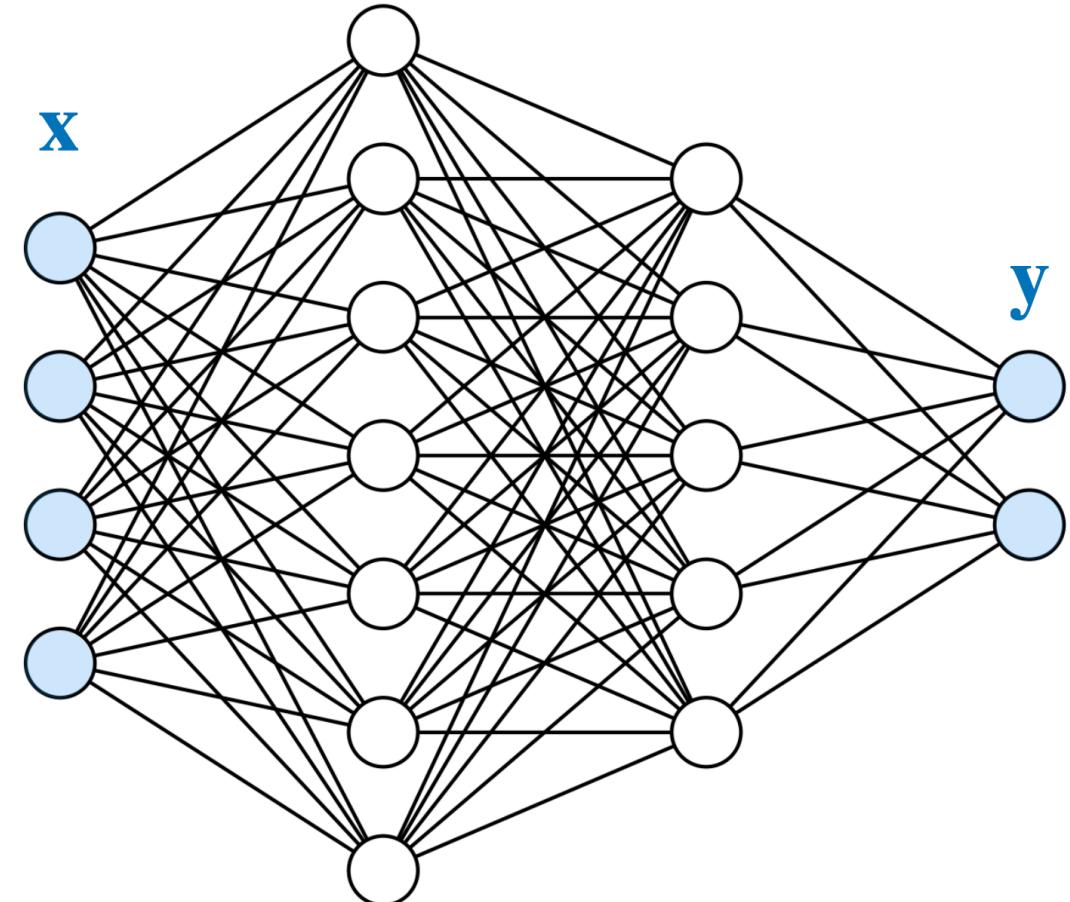
$$y_i = \varphi^{(3)} \left( \sum_j w_{ij}^{(3)} h_j^{(2)} + b_i^{(3)} \right)$$



# The multilayer perceptron (MLP)

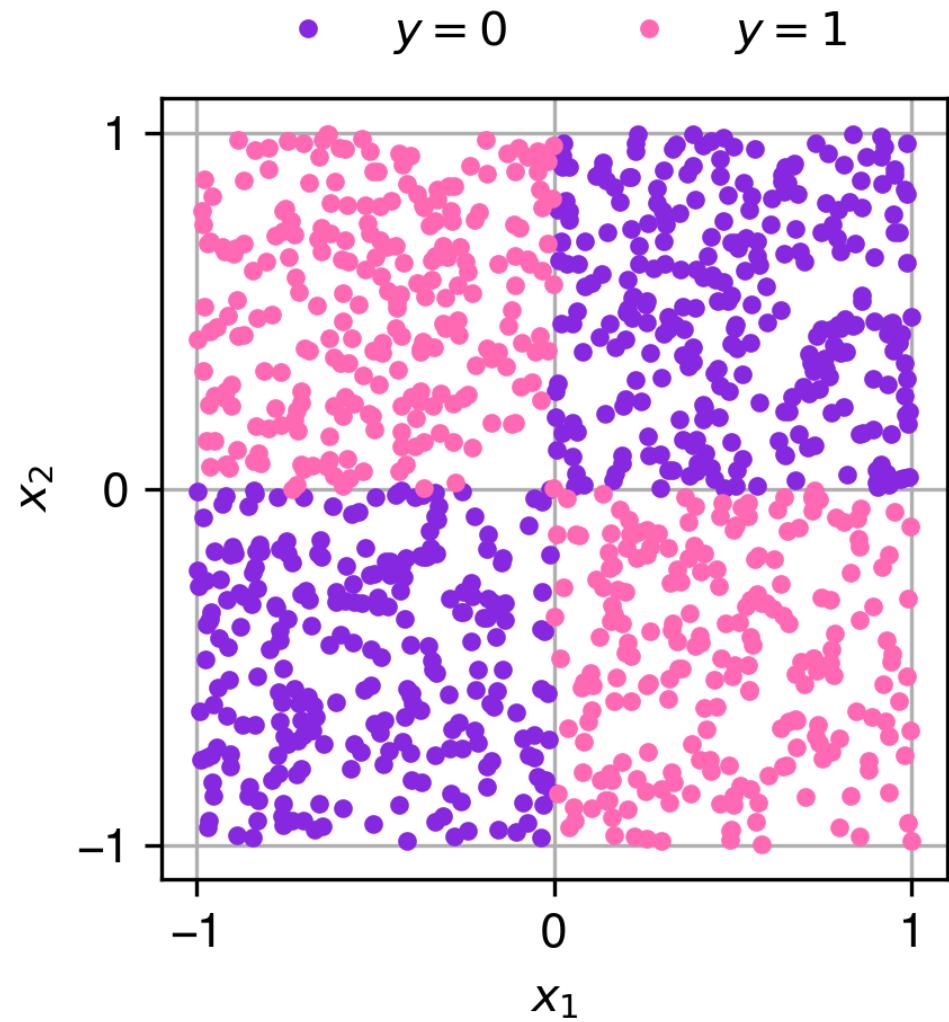
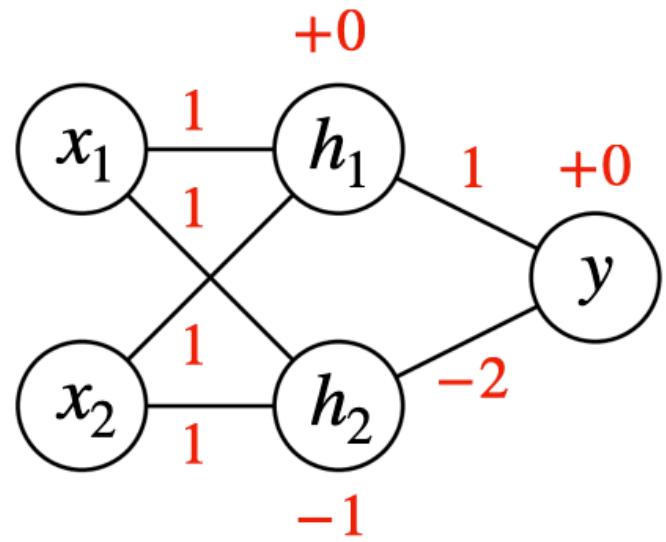
A **multilayer perceptron** is a neural network with multiple hidden layers. Generally speaking (omitting the biases):

$$y = \varphi^{(\ell)} \left( \mathbf{W}^{(\ell)} \varphi^{(\ell-1)} \left( \mathbf{W}^{(\ell-1)} \dots \varphi^{(1)} \left( \mathbf{W}^{(1)} \mathbf{x} \right) \dots \right) \right)$$



## Quick example for solving the XOR problem

Multi-layer perceptrons that solves the XOR problem with binary activations:

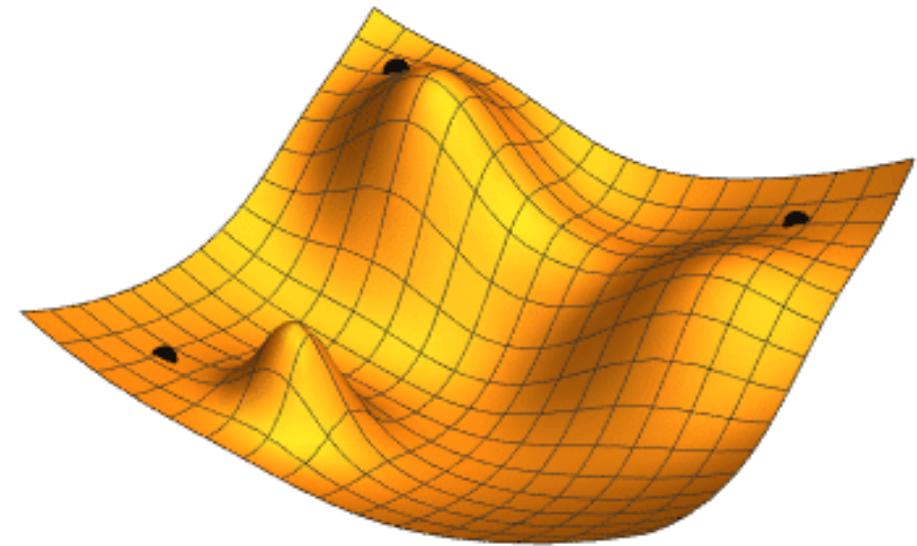


See Section 6.1 of Goodfellow et al. (2016)

# Gradient descent for neural networks

We note  $f_{\theta}(x) : x \mapsto y$  the model, where  $\theta$  are the parameters of the model (including biases and weights).

1. **Learning** is the process of finding the parameters  $\theta^*$  that minimize the loss  $\mathcal{L}$ .
2. The **backpropagation** computes the loss function gradient with respect to  $\theta$ .
3. The **gradient descent** updates  $\theta$  in the direction of the steepest descent.



# Gradient computation with backpropagation

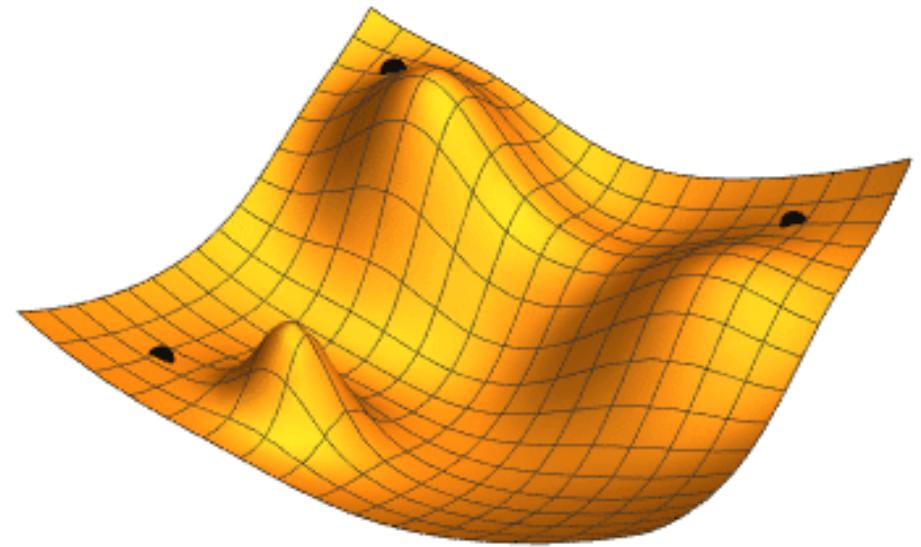
1. **Initialization:** the weights are initialized randomly, the biases to zero
2. **Feed forward:** the input is propagated through the network to compute the output
3. **Loss:** the loss is computed between the output and the target
4. **Back propagation:** computation of the gradient from the loss to the input
5. **Gradient descent:** update the parameters in the direction of the steepest descent

## Gradient-based optimization

Once the gradient is computed, the parameters are updated using the **gradient descent** algorithm:

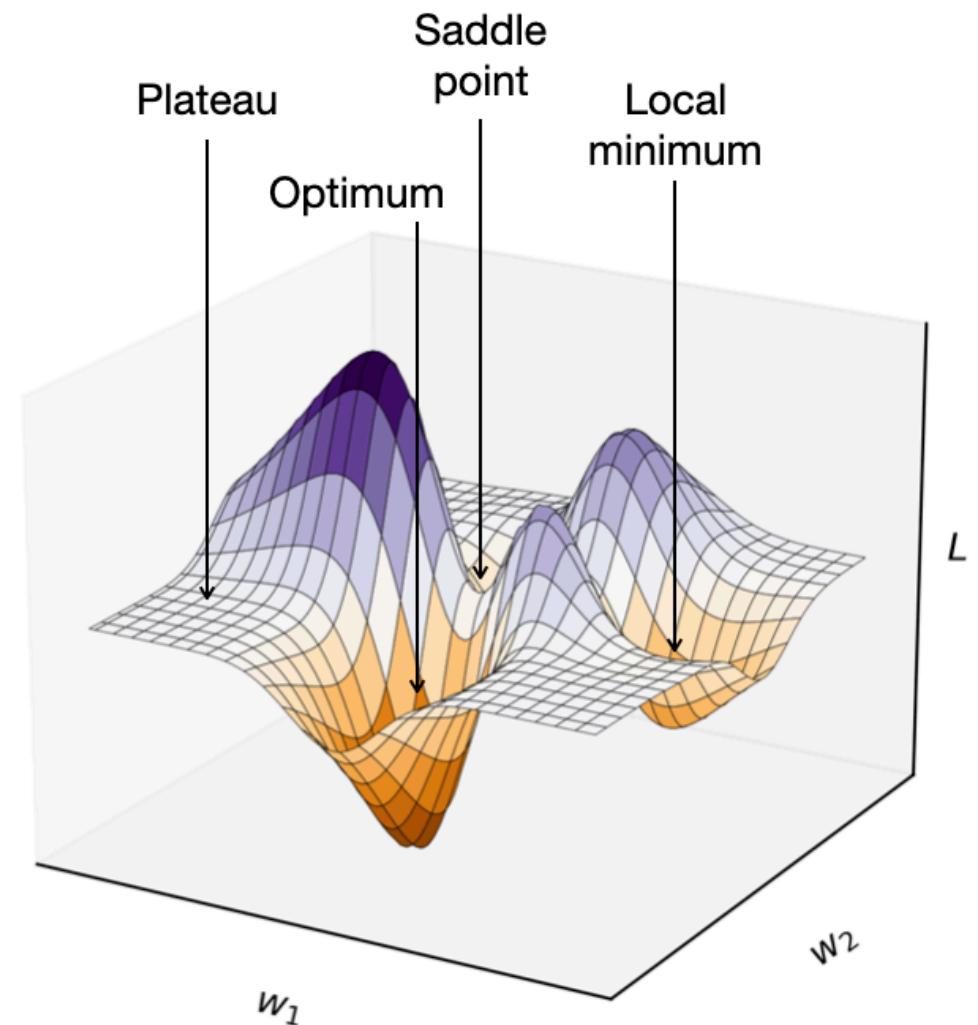
$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$

where  $\eta$  is the **learning rate** that controls the size of the update.

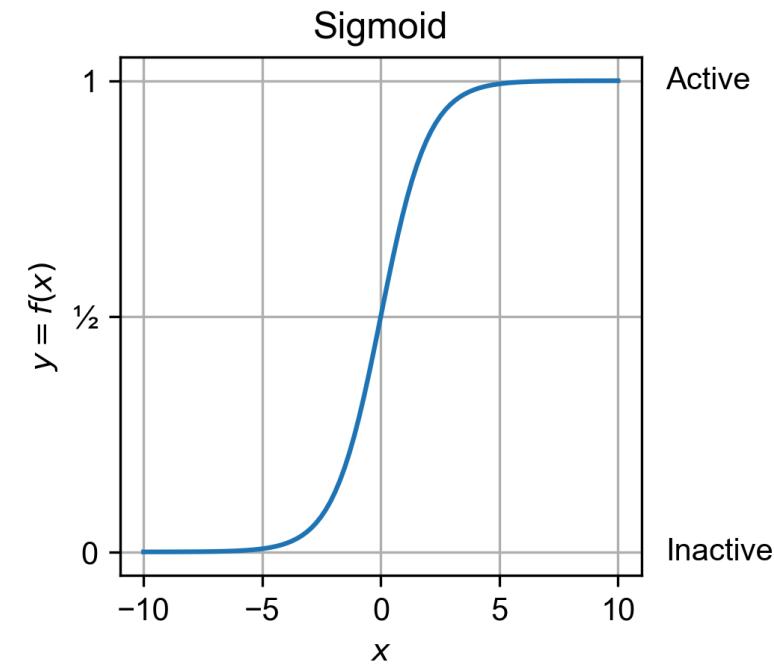
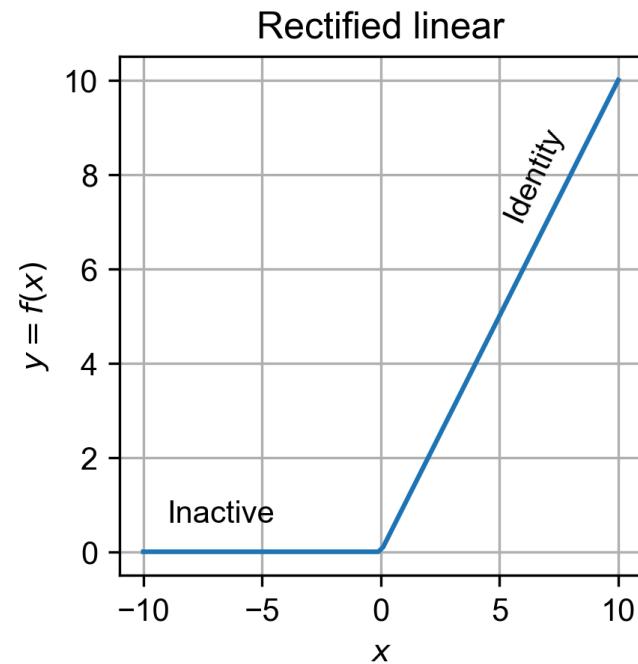


## Gradient descent common issues

- **Local minima:** getting stuck in a local minimum.
- **Sattling points:** behaves as a local minimum but is not.
- **Plateau:** flat loss function, vanishing gradient, slow convergence.



# Gradient descent common issues with plateau



**Plateau** are flat regions of the loss function where the gradient is zero. This can happen with activation functions such as the sigmoid function with saturation. It can also happen with the ReLU function for inputs with negative values.

## Gradient-descent tricks to avoid issue

- **Learning rate**: set up, and maybe adapt it.
- **Momentum**: use the gradient of the previous iteration to update the parameters.
- **Normalization**: normalize the inputs of each layer.
- **Stochastic gradient descent**: use a mini-batch of samples to compute the gradient.
- **Dropout**: randomly drop some neurons during training.

# Gradient descent and learning rate

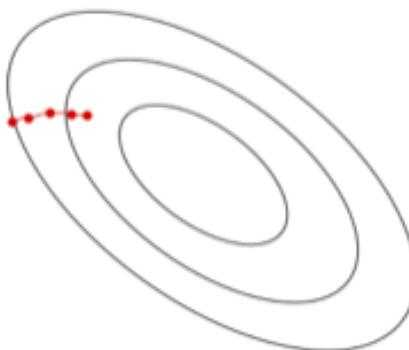
The **learning rate** is a hyperparameter that controls the size of the update of the parameters:

$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$

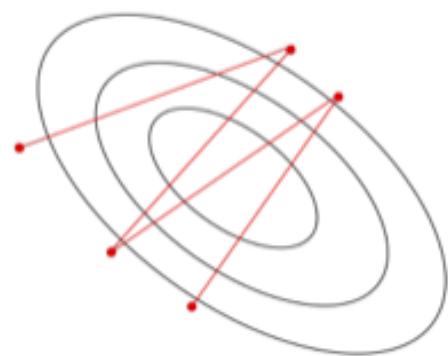
We must look for a learning rate to avoid local minima while still converging fast enough, without diverging.

We can also **adapt** the learning rate.

Too small



Too large

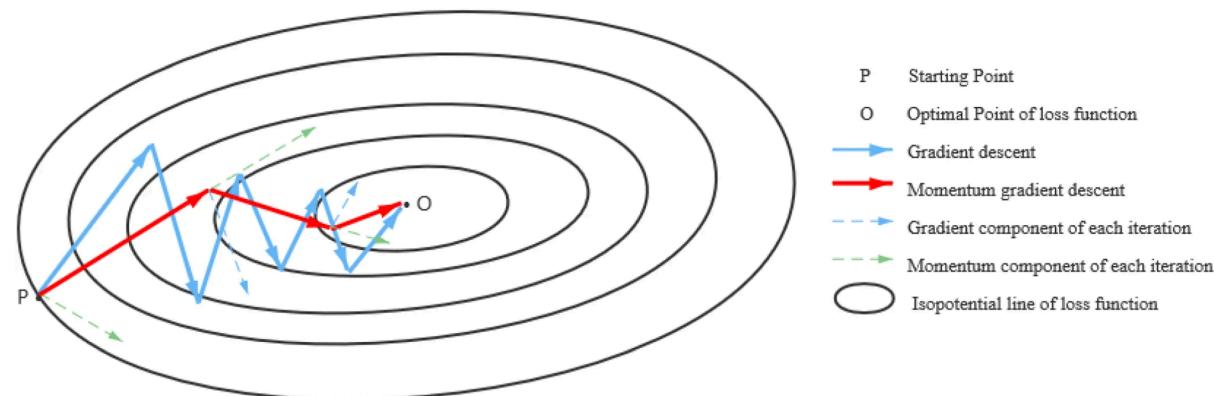


## Gradient descent and momentum

The **momentum** is a technique to accelerate the gradient descent by adding a fraction of the gradient of the previous iteration:

$$p \leftarrow \alpha p - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$
$$\theta \leftarrow \theta + p$$

where  $\alpha$  is the a damping parameter, and  $v_i$  is the **velocity**. Lower values of  $\alpha$  give more weight to the current gradient, higher values give more weight to the previous gradients.



## Data normalization

To avoid getting in the saturation of sigmoidal activation functions, it is important to normalize the data. This can be done by **normalizing the input and the features**:

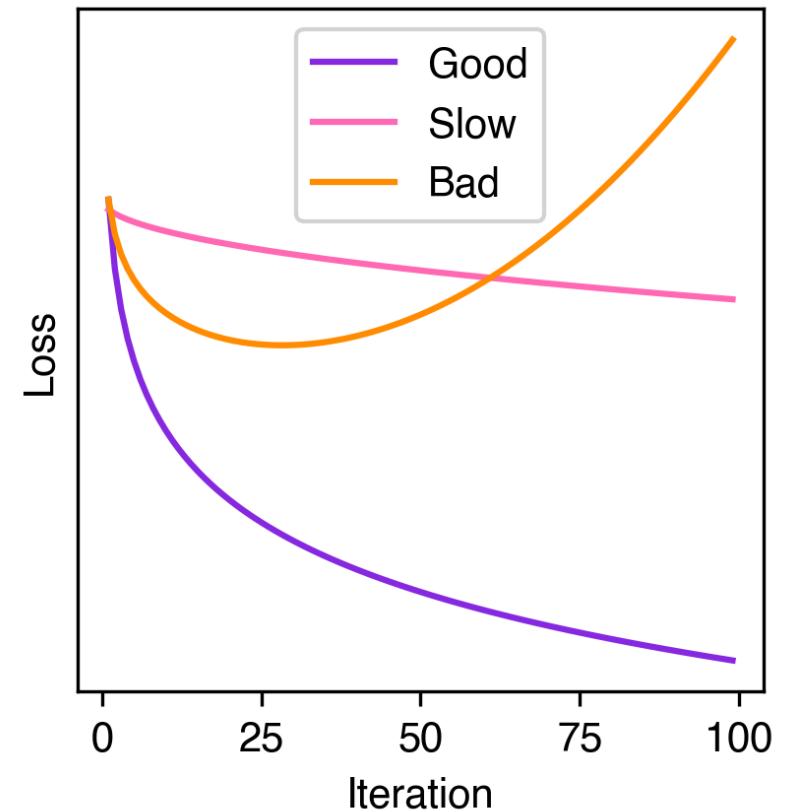
$$\hat{x}_i = \frac{x_i - \mu_i}{\sqrt{\sigma_i^2 + \epsilon}}$$

where  $\mu_i$  is the mean of the input,  $\sigma_i$  is the standard deviation of the input, and  $\epsilon$  is a small constant to avoid division by zero. You can also apply the normalization after the activation function.

## Monitor the training curves

The **training curves** are a good way to monitor the training of a model.

- Slow: increase the learning rate.
- Growing: decrease the learning rate.
- Cross-validation: within 0.0001 to 0.1



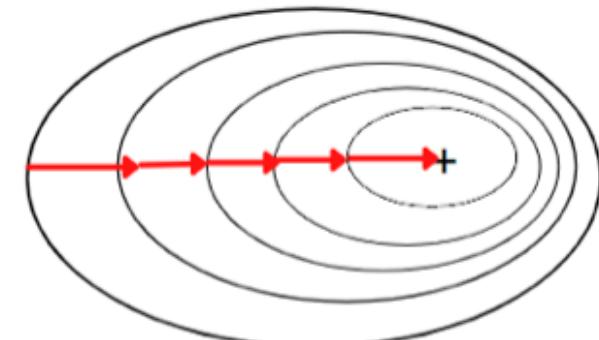
# Stochastic gradient descent

The gradient of the loss function with respect to the parameters  $\theta$  is computed using the **full-batch gradient descent** equal to:

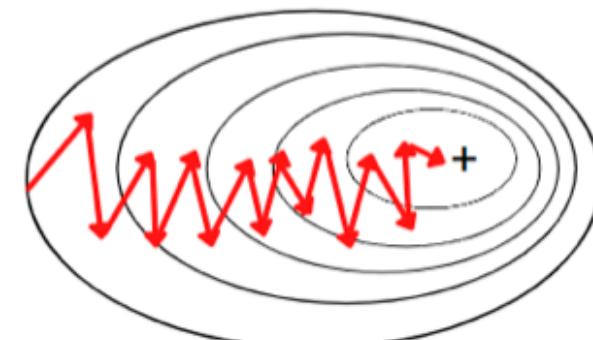
$$\frac{\partial \mathcal{L}}{\partial \theta} = \frac{1}{N} \sum_{i=1}^N \frac{\partial \mathcal{L}^{(i)}}{\partial \theta}$$

The **stochastic gradient descent** is a technique to compute the loss gradient from every sample in the dataset at each iteration.

**Batch Gradient Descent**



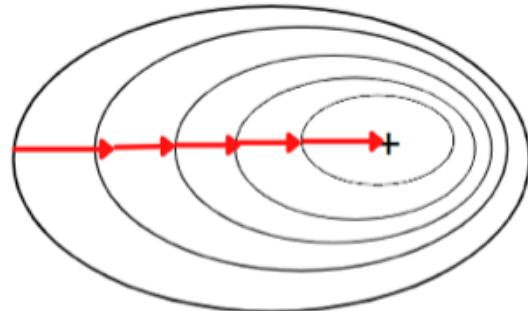
**Stochastic Gradient Descent**



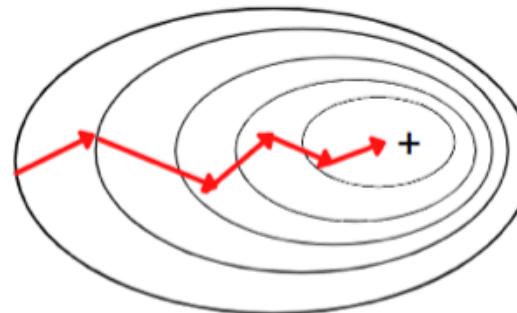
## Mini-batch gradient descent

The **mini-batch gradient descent** is a technique to compute the gradient of the loss function with respect to a subset of the dataset. It is a compromise between the full-batch gradient descent and the stochastic gradient descent.

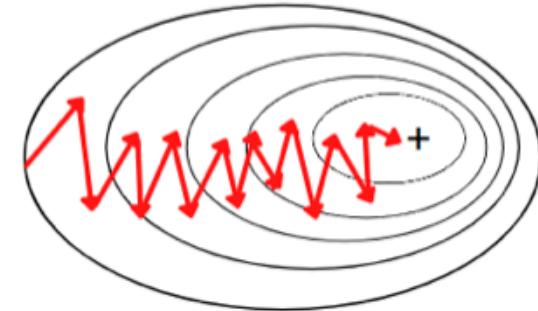
**Batch Gradient Descent**



**Mini-Batch Gradient Descent**



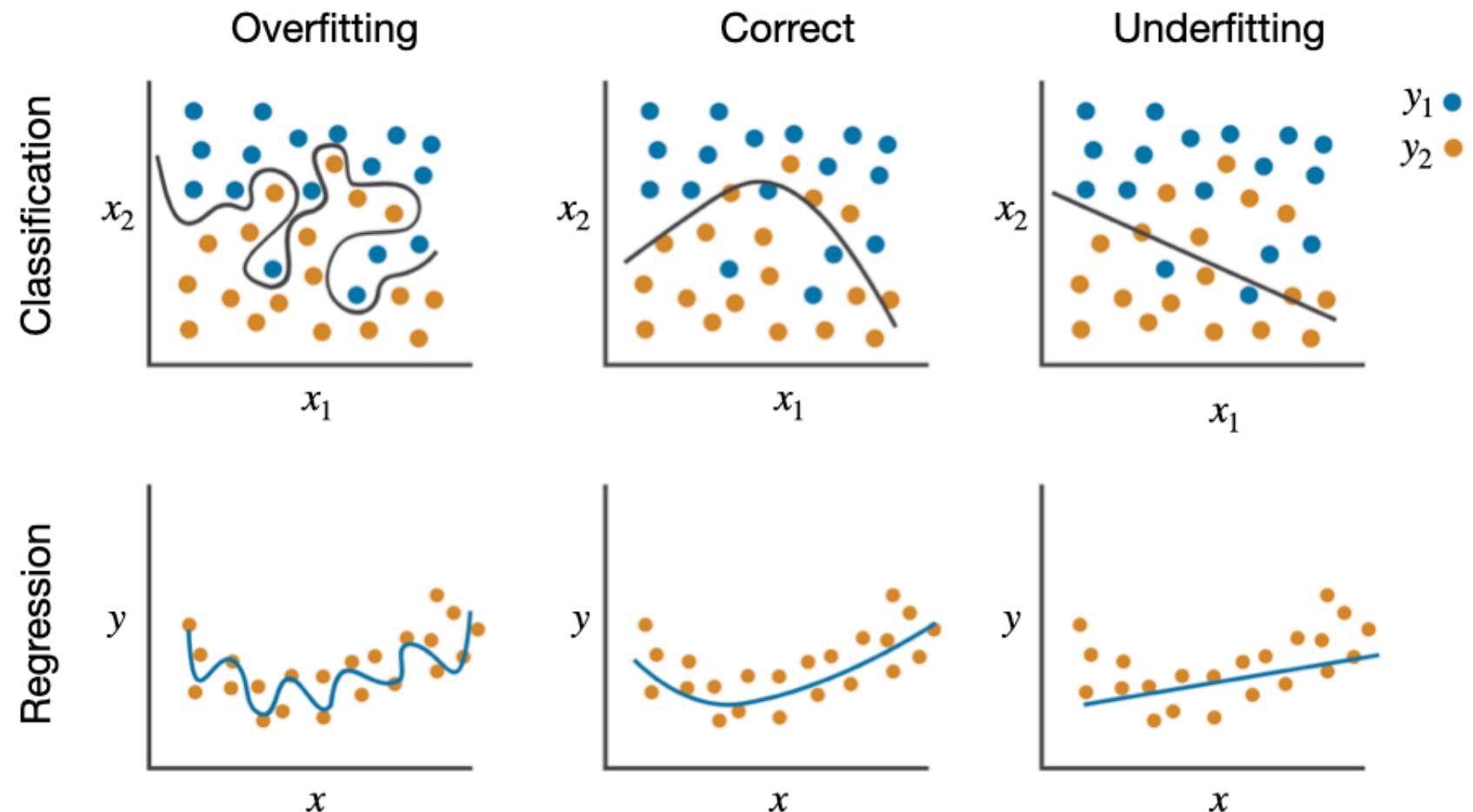
**Stochastic Gradient Descent**



# Overfitting and underfitting

**Overfitting:** too complex model, does not generalize to new data.

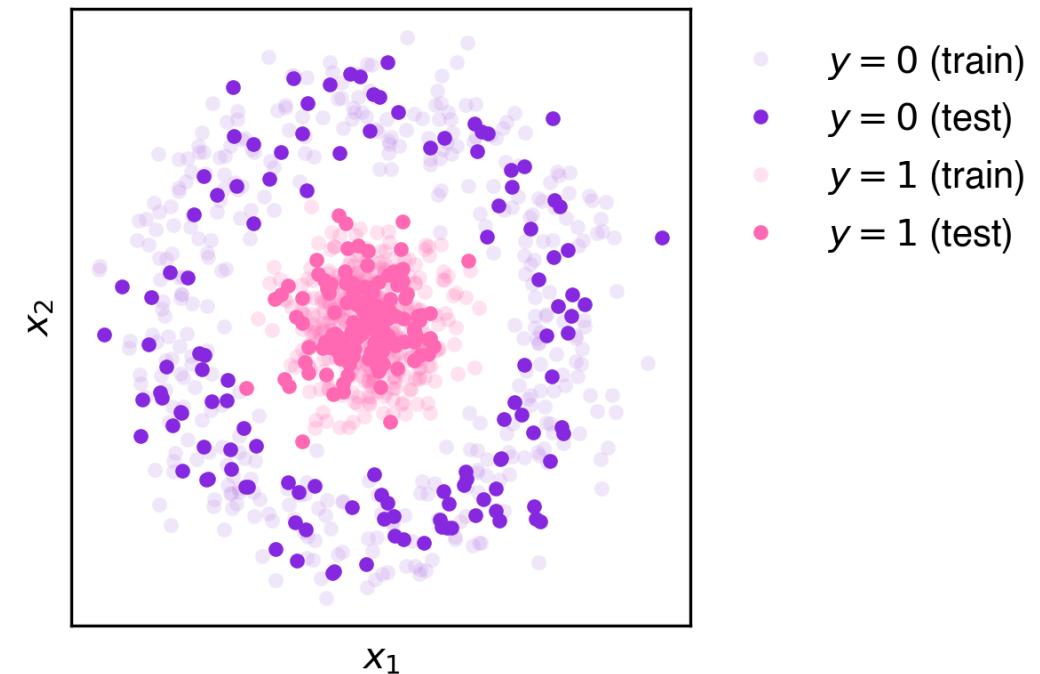
**Underfitting:** too simple model, does not capture the data structure.



## Splitting the dataset into train and test sets

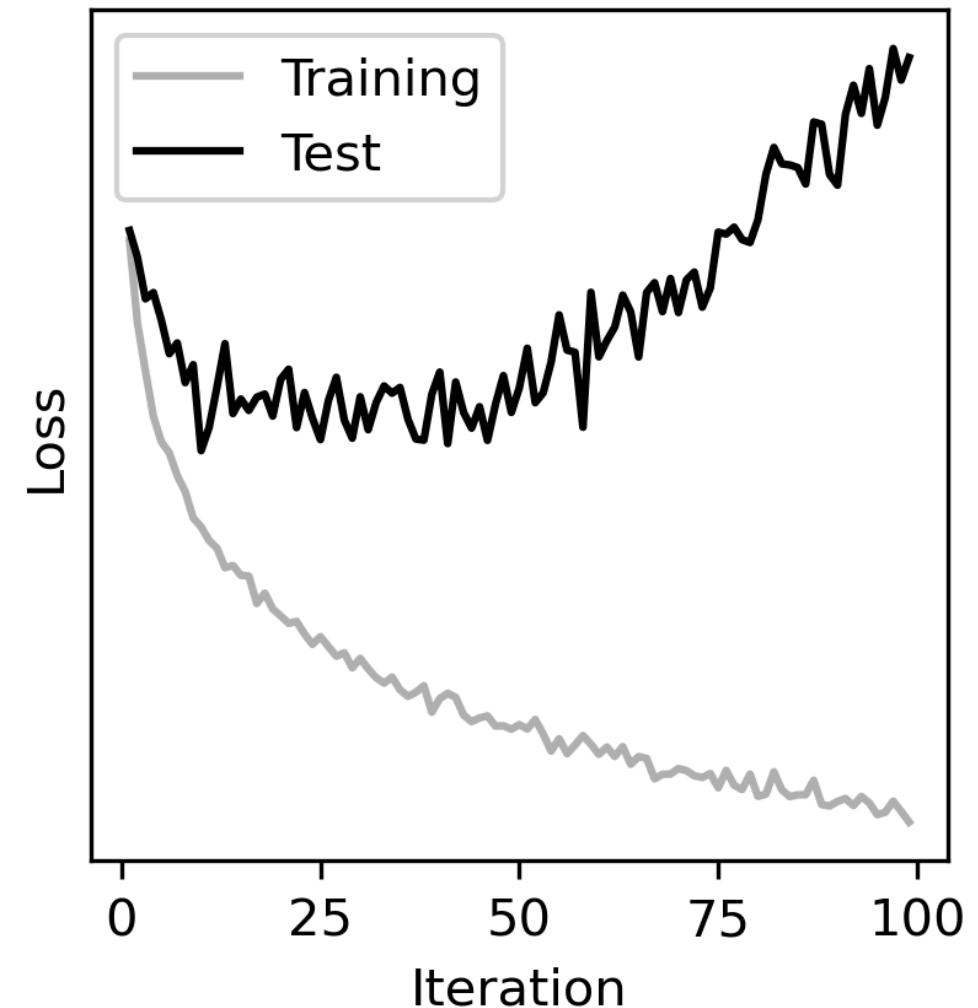
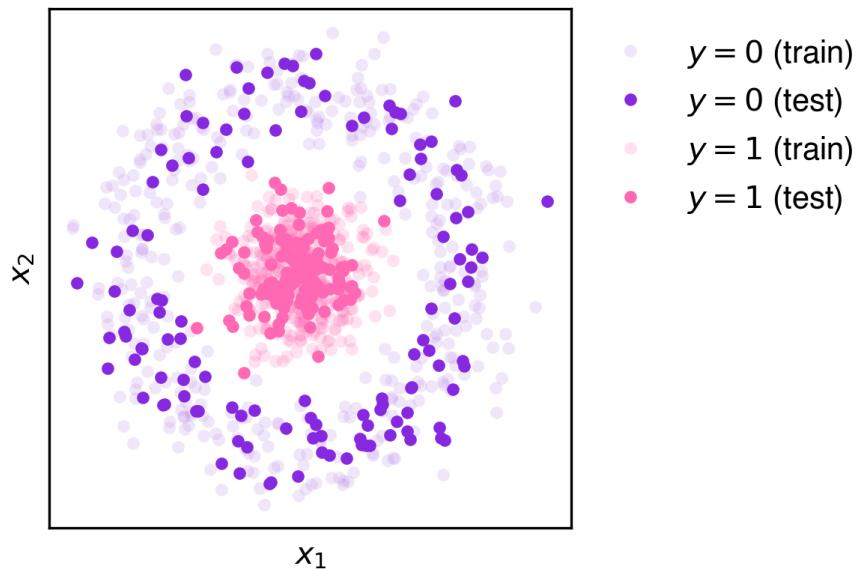
The **training set** is used to train the model. The **test set** is used to evaluate the model generalization error on unseen data.

The typical split is 80% for the training set and 20% for the test set.



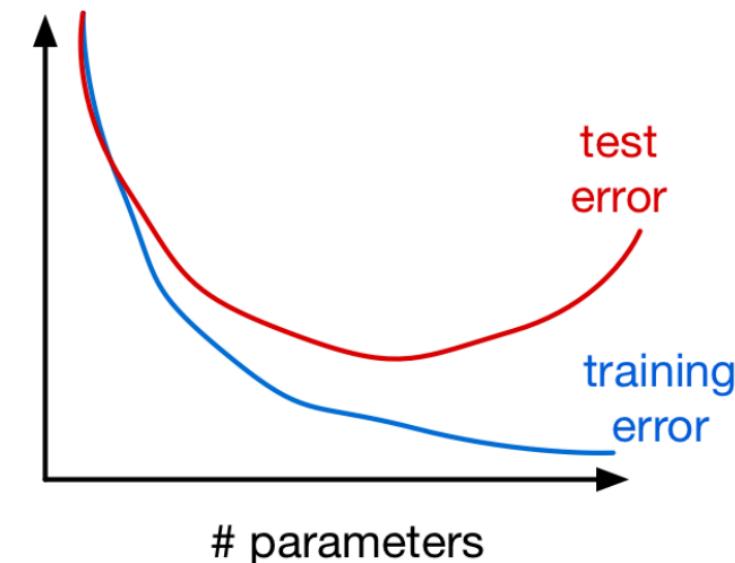
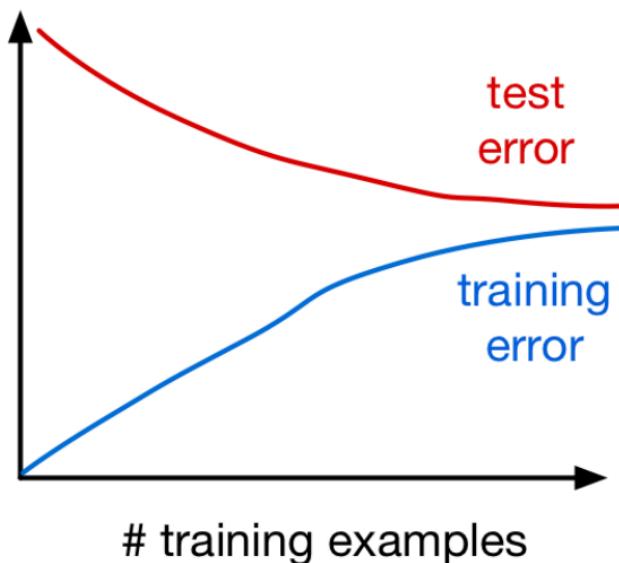
## Training and test learning curves

We must ensure that both the training and test losses decrease. If the training loss is much lower than the test loss, the model **overfits** the training set.



# Targetting the right model complexity

The **model complexity** is roughly the number of parameters of the model. The **model generalization error** is the error on the test set.

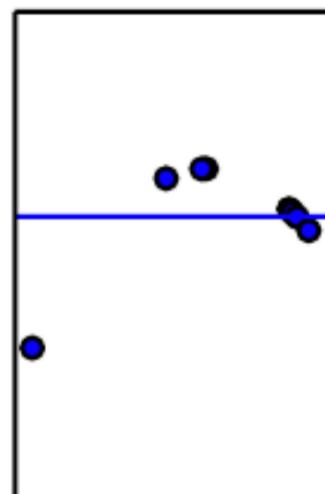


# Regularization

**Regularization** is a technique to control overfitting by adding a penalty term  $\mathcal{R}$  to the loss function. The **regularization parameter**  $\lambda$  controls the strength of the regularization.

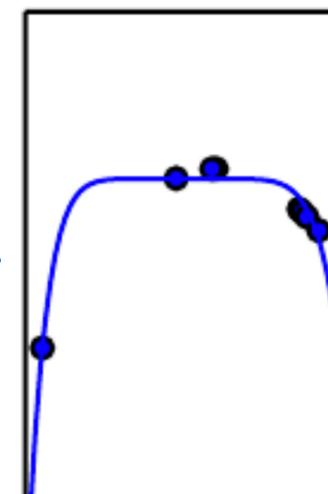
$$\mathcal{L}_{\text{reg}} = \mathcal{L} + \lambda \mathcal{R} = \mathcal{L} + \lambda \|\theta\|_2^2$$

Underfitting  
(Excessive  $\lambda$ )



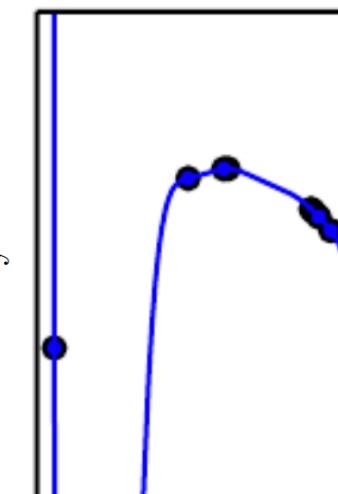
$x_0$

Appropriate weight decay  
(Medium  $\lambda$ )



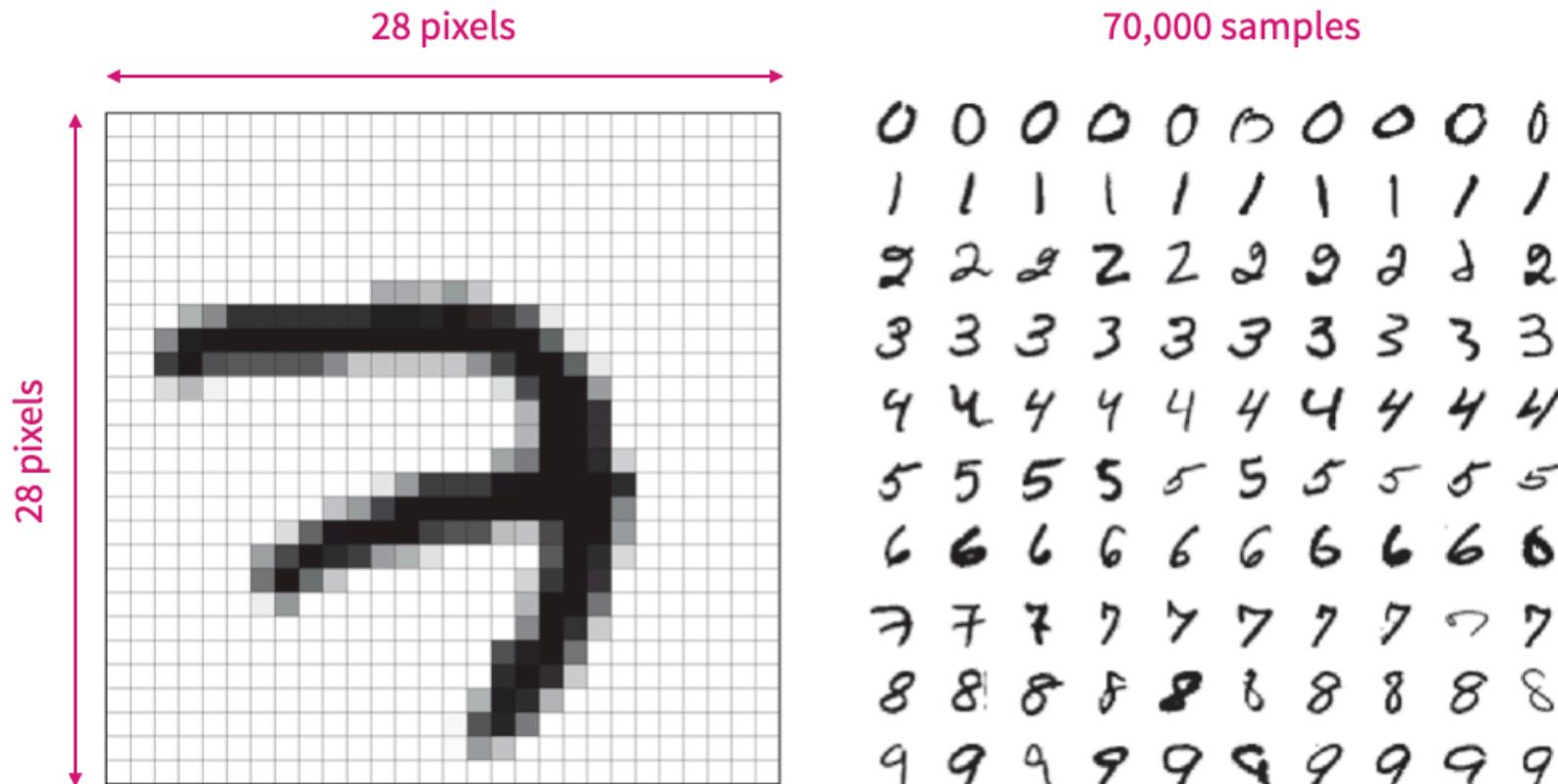
$x_0$

Overfitting  
( $\lambda \rightarrow 0$ )



$x_0$

Handwritten digits set of grayscale images  $x \in \mathbb{R}^{28 \times 28}$  and classes  $y \in \{0, \dots, 9\}$ .

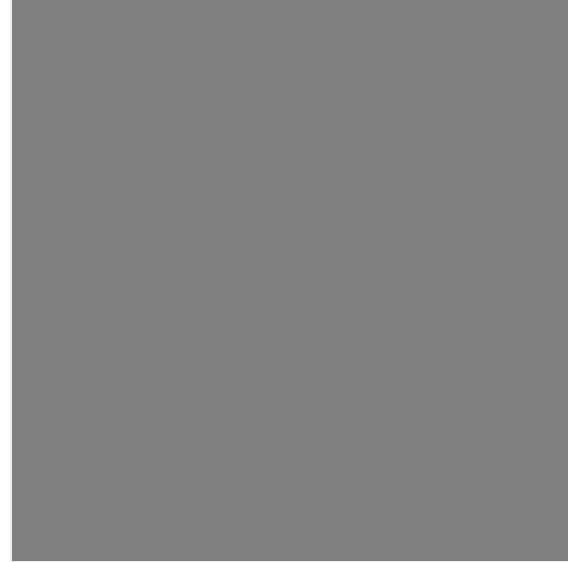


**Goal:** predict the number encoded in the pixels.

# A fully connected network for solving the MNIST classification

FPS

Draw your number here



Downsampled drawing:

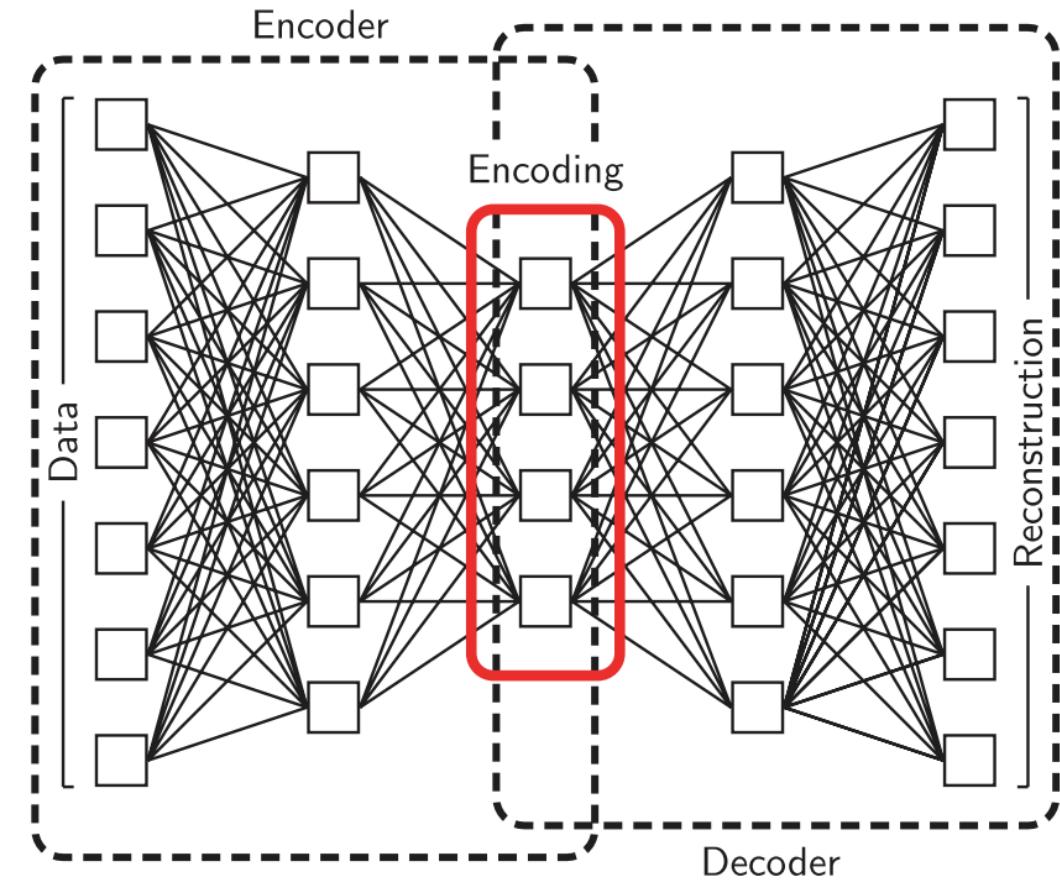
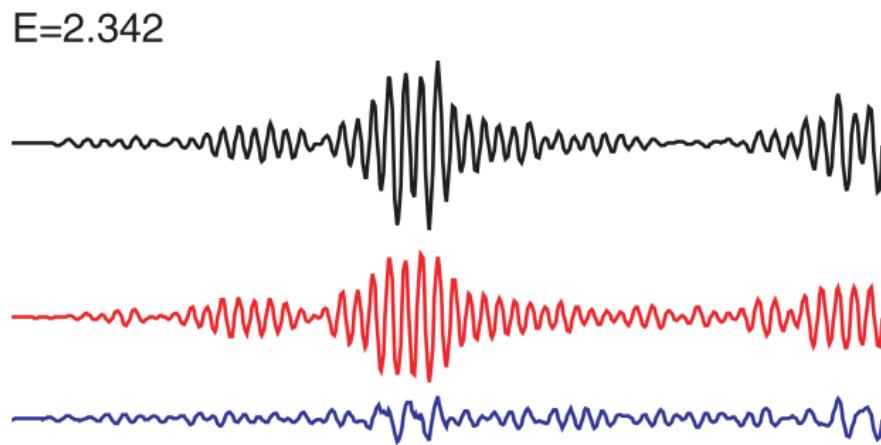
First guess:

Second guess:

# Example in seismology: fully-connected autoencoder

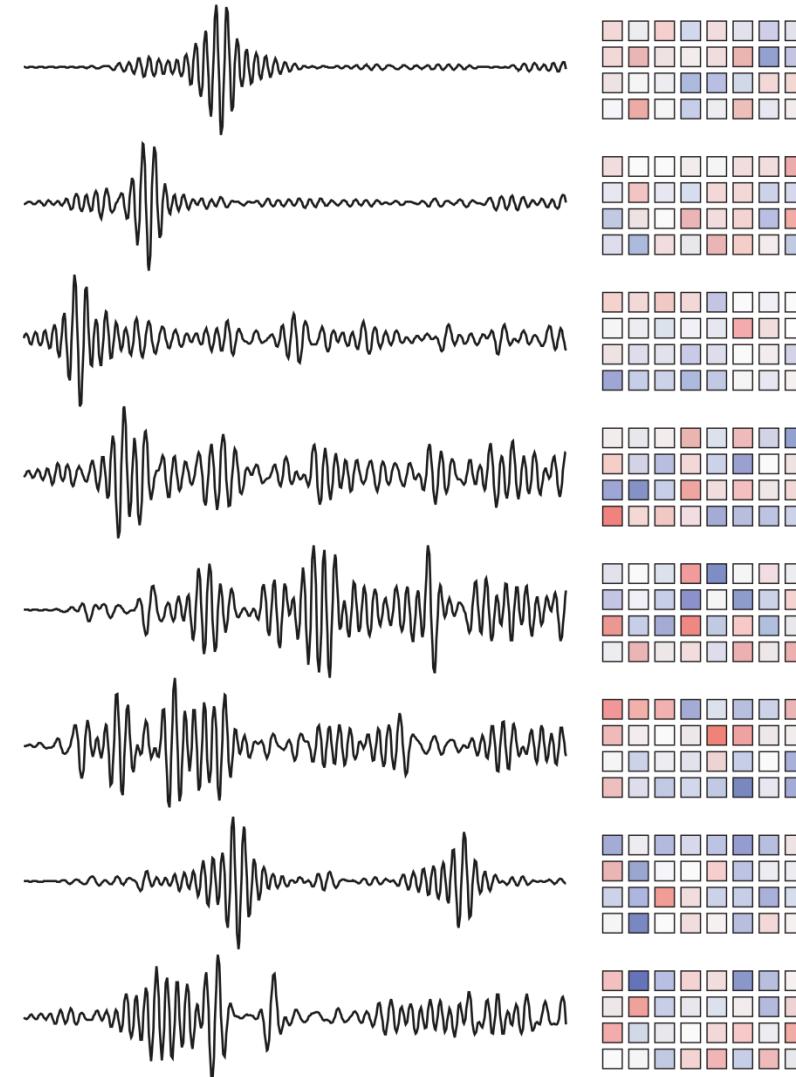
Training of a fully-connected autoencoder on real seismic data.

This is an **unsupervised** learning task: the input and output are the same.



## Example in seismology: fully-connected autoencoder

We learned a low-dimensional representation for the seismic data.

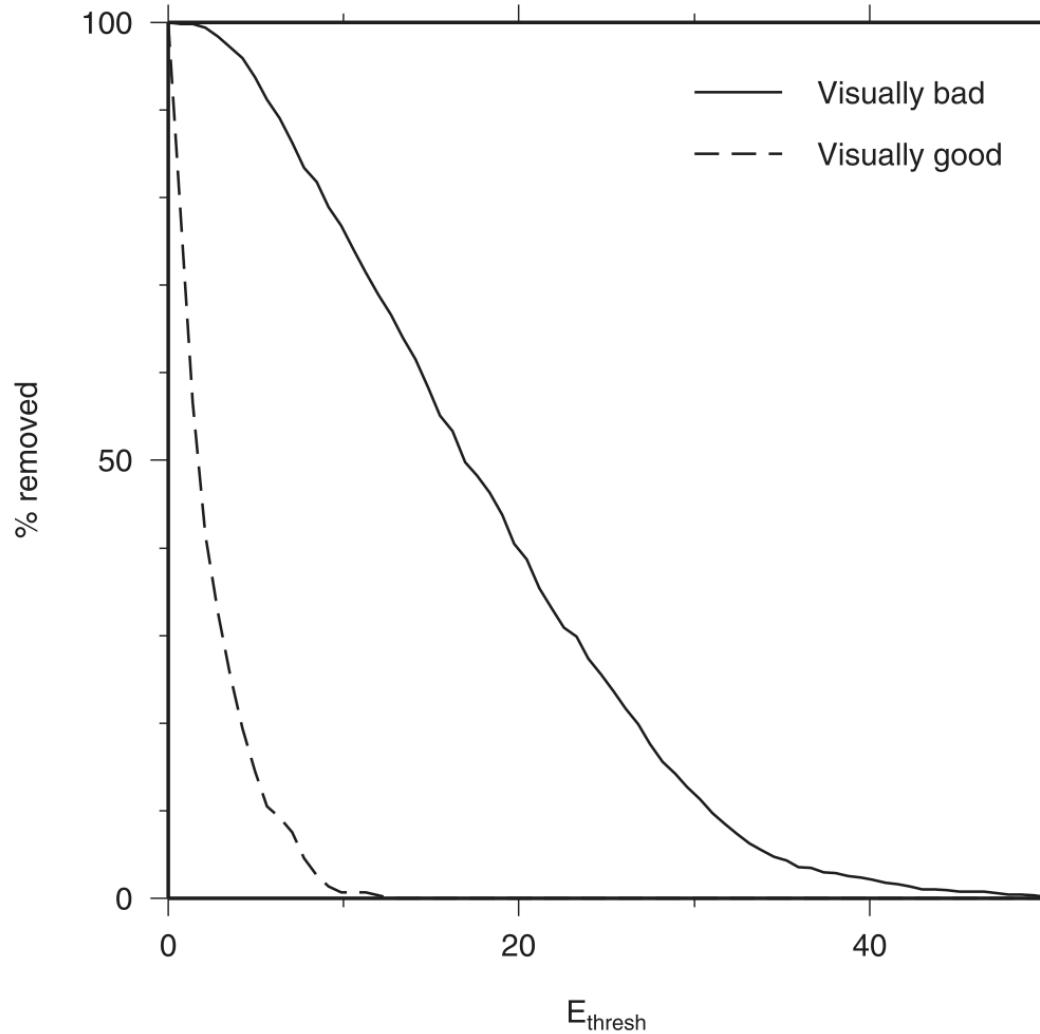


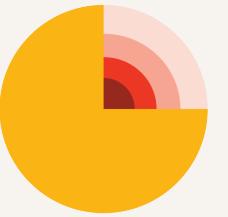
These are the **latent variables** of the autoencoder.

## Example in seismology: fully-connected autoencoder

Example applications:

- quality assessment
- compression

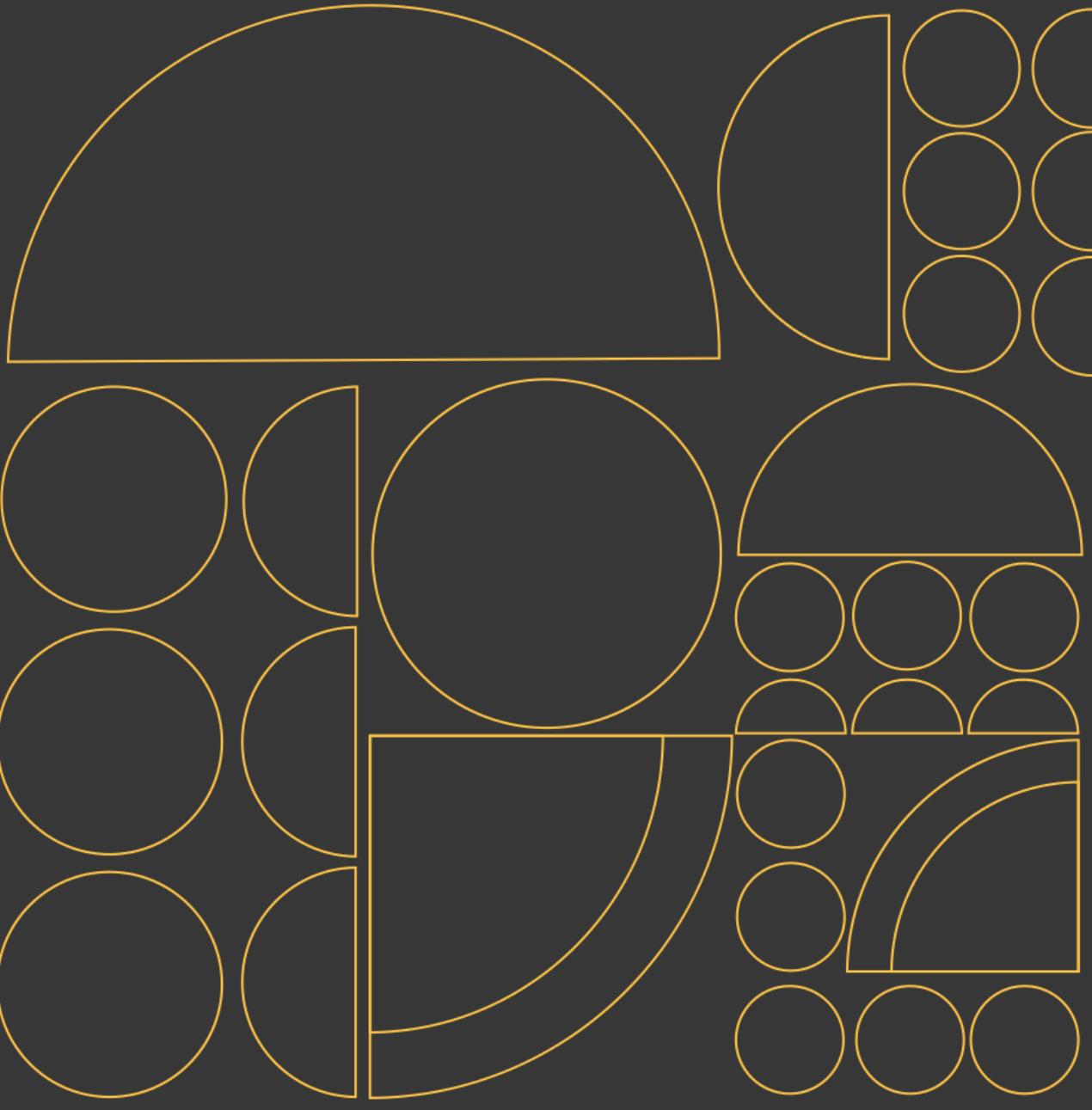




**ChEESE**

## 6. Deep learning: convolutional neural networks

How deep learning works? What is a  
neural network? How to train it, and what  
for?

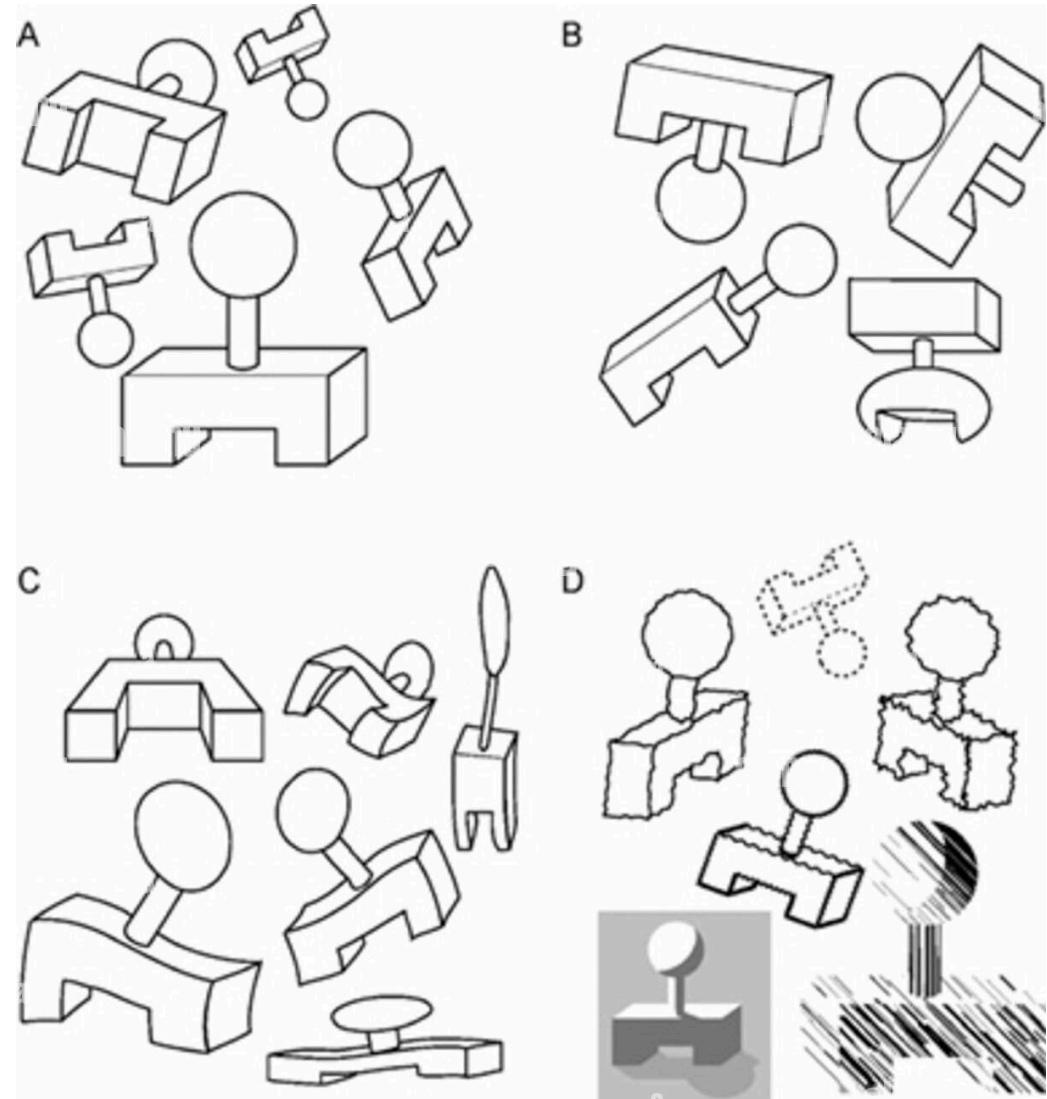


## Limitations of fully connected networks

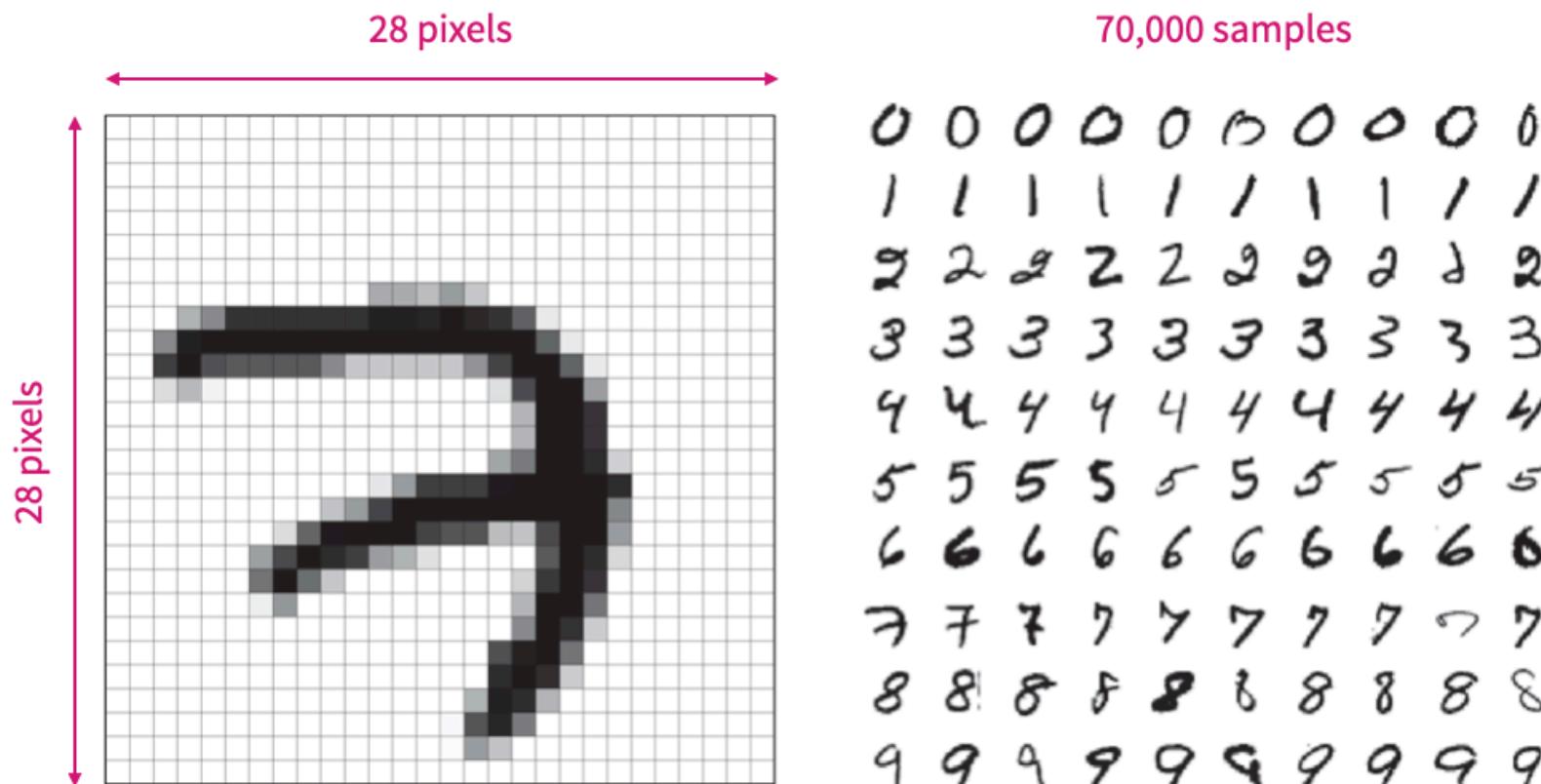
Vision is robust to a lot:

- Translation
- Rotation
- Scaling
- Shearing
- Illumination
- Occlusion

We need invariance to these transformations.



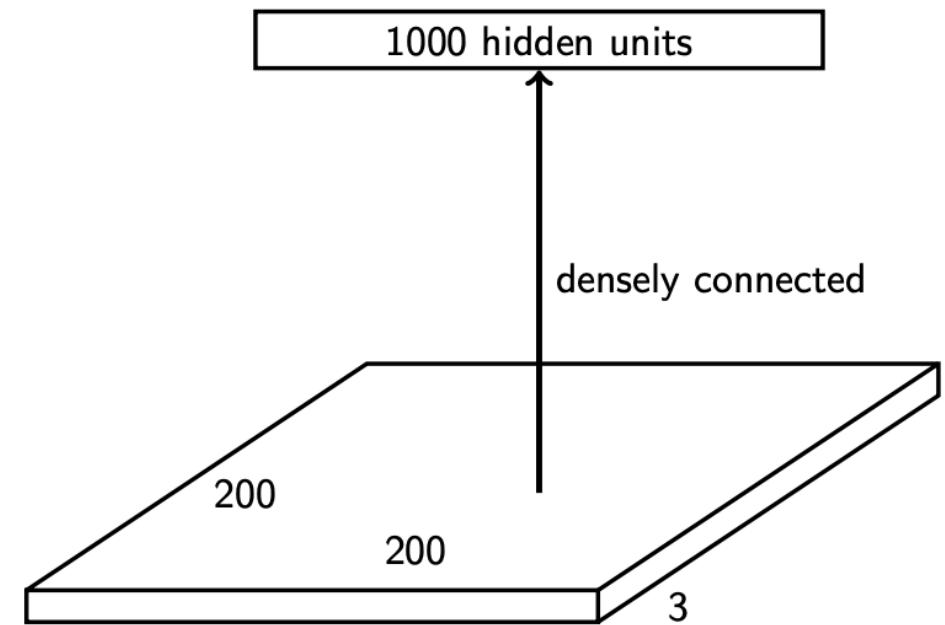
Handwritten digits set of grayscale images  $x \in \mathbb{R}^{28 \times 28}$  and classes  $y \in \{0, \dots, 9\}$ .



## Limitations of fully connected networks

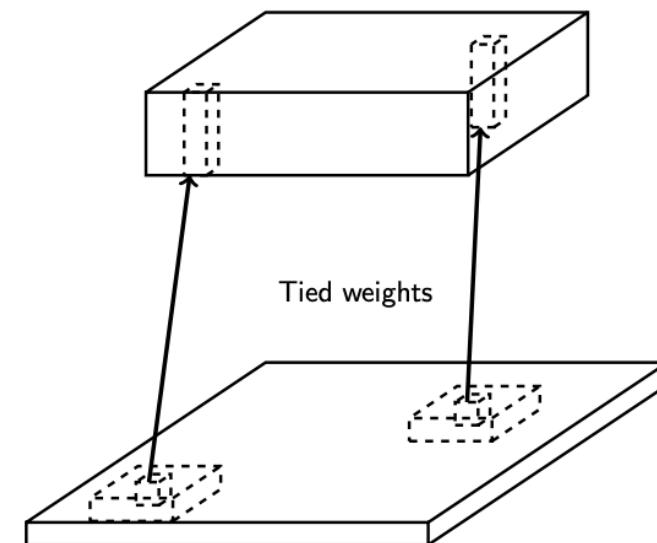
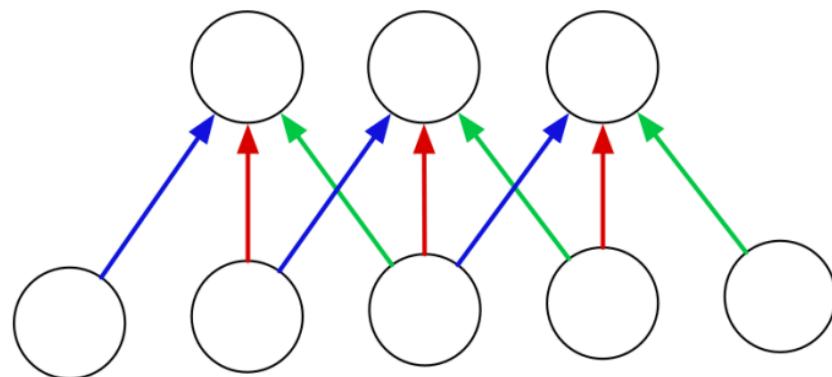
An image may be of  $200 \times 200$  pixels  $\times 3$  color channels. With a **fully connected network** with **1000** hidden units, we would have  $N = 200 \times 200 \times 3 \times 1000 = 120\text{M}$  parameters.

**This clearly does not scale to large images.**



# Convolutional neural networks

**Convolutional layers** are a type of layer that are used in convolutional neural networks. They are composed of a set of learnable filters.



Each hidden unit look a local content from the input image, although the weights are shared across the entire image.

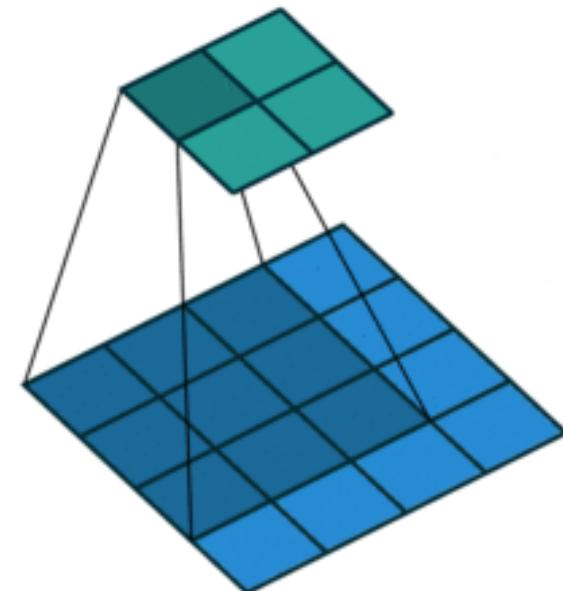
# Convolutional neural networks

Discrete image convolution:

$$(A * B)_{ij} = \sum_n \sum_m A_{nm} B_{i-n, j-m}$$

where  $A$  is a input image, and  $B$  is a convolutional kernel (weights) to learn.

Convolutional layers extract local features from the input image ≠ fully connected layers that extract global features.



## Convolution operation

$$(A * B)_{ij} = \sum_n \sum_m A_{nm} B_{i-n,j-m}$$

Input image

200 pixels



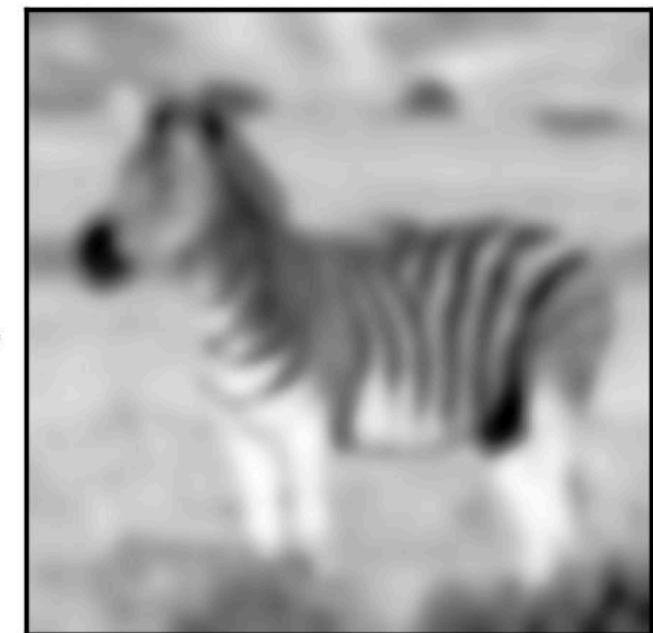
200 pixels

\*      Kernel  
5 pixels      5 pixels

=

200 pixels

Filtered image



200 pixels

## Convolution operation

$$(A * B)_{ij} = \sum_n \sum_m A_{nm} B_{i-n,j-m}$$

Input image

200 pixels



200 pixels

$$\begin{matrix} & \text{Kernel} \\ * & \begin{matrix} 3 \text{ pixels} \\ \text{---} \\ 3 \text{ pixels} \end{matrix} \\ & \text{---} \\ & \text{---} \end{matrix} =$$

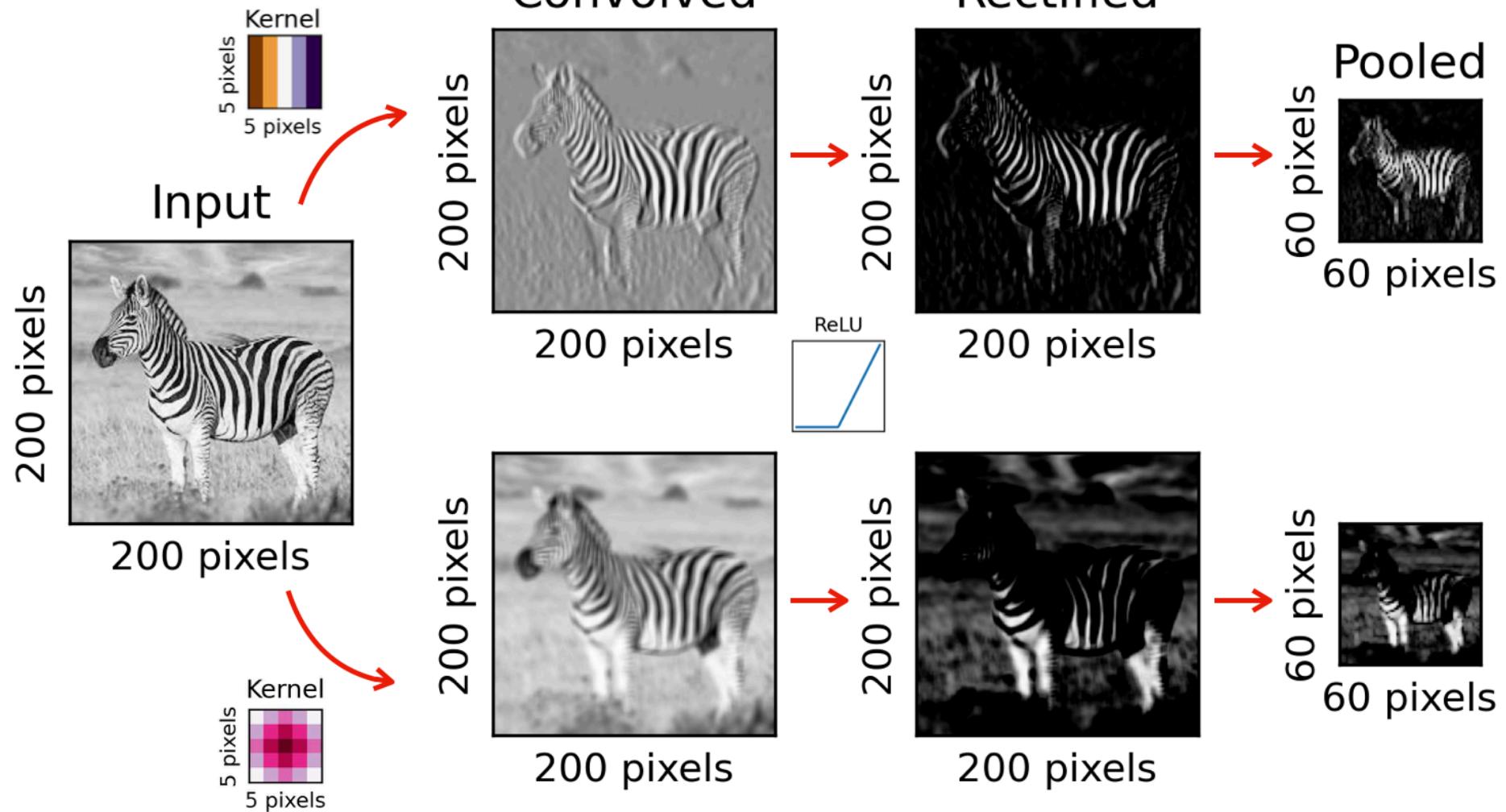
Filtered image

200 pixels



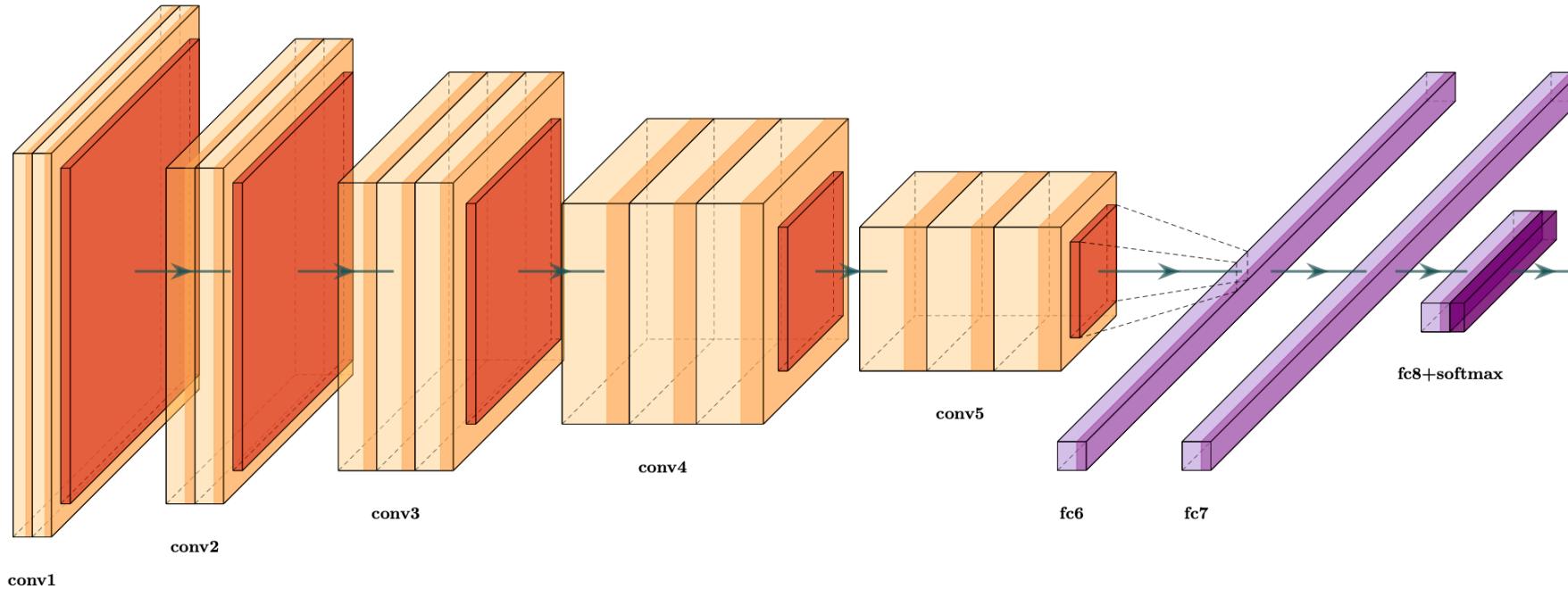
200 pixels

## Convolution unit



# Convolutional neural network: example with VGG16

Now, we can understand this winning architecture for image classification.

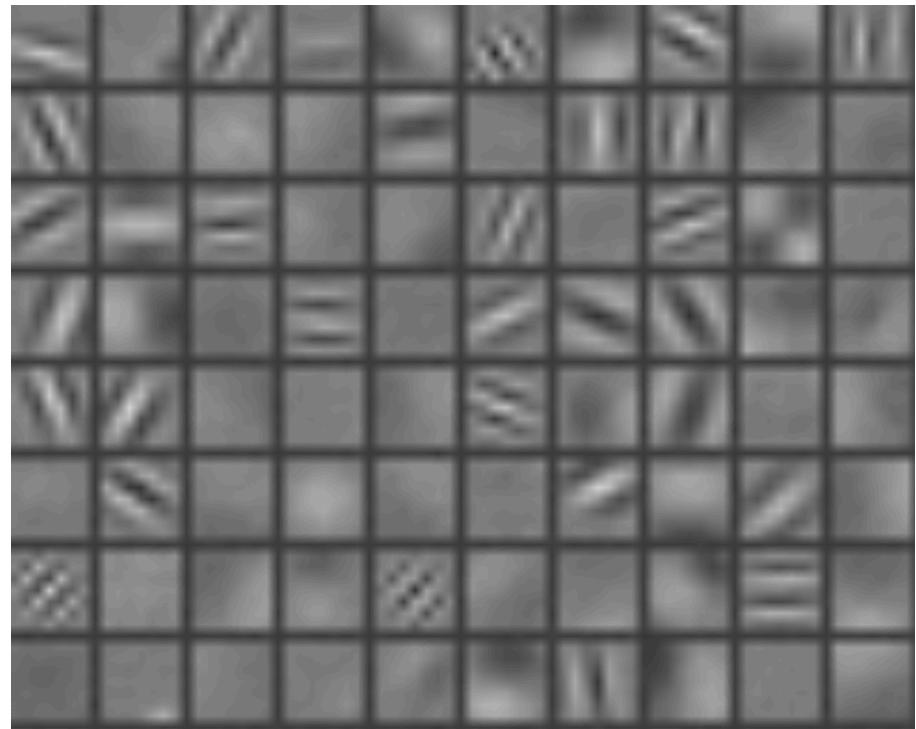
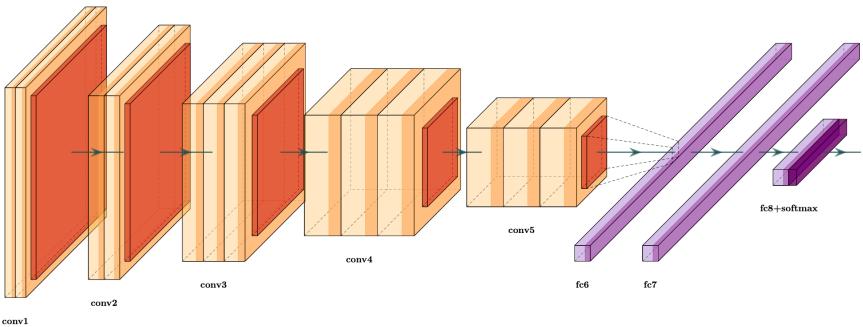


Note the last three layers are **fully connected**.

When extracting low-dimensional data from images, this is often needed.

# Convolutional neural network: example with VGG16

Here are the **filters from the first layer** of VGG16 after training on 100k+ images. These filters collect various shapes, scales, colors, etc.



# A convolutional network for solving the MNIST classification

FPS

Draw your number here



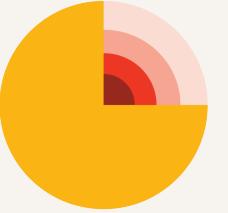
Downsampled drawing:

First guess:

Second guess:

Layer visibility

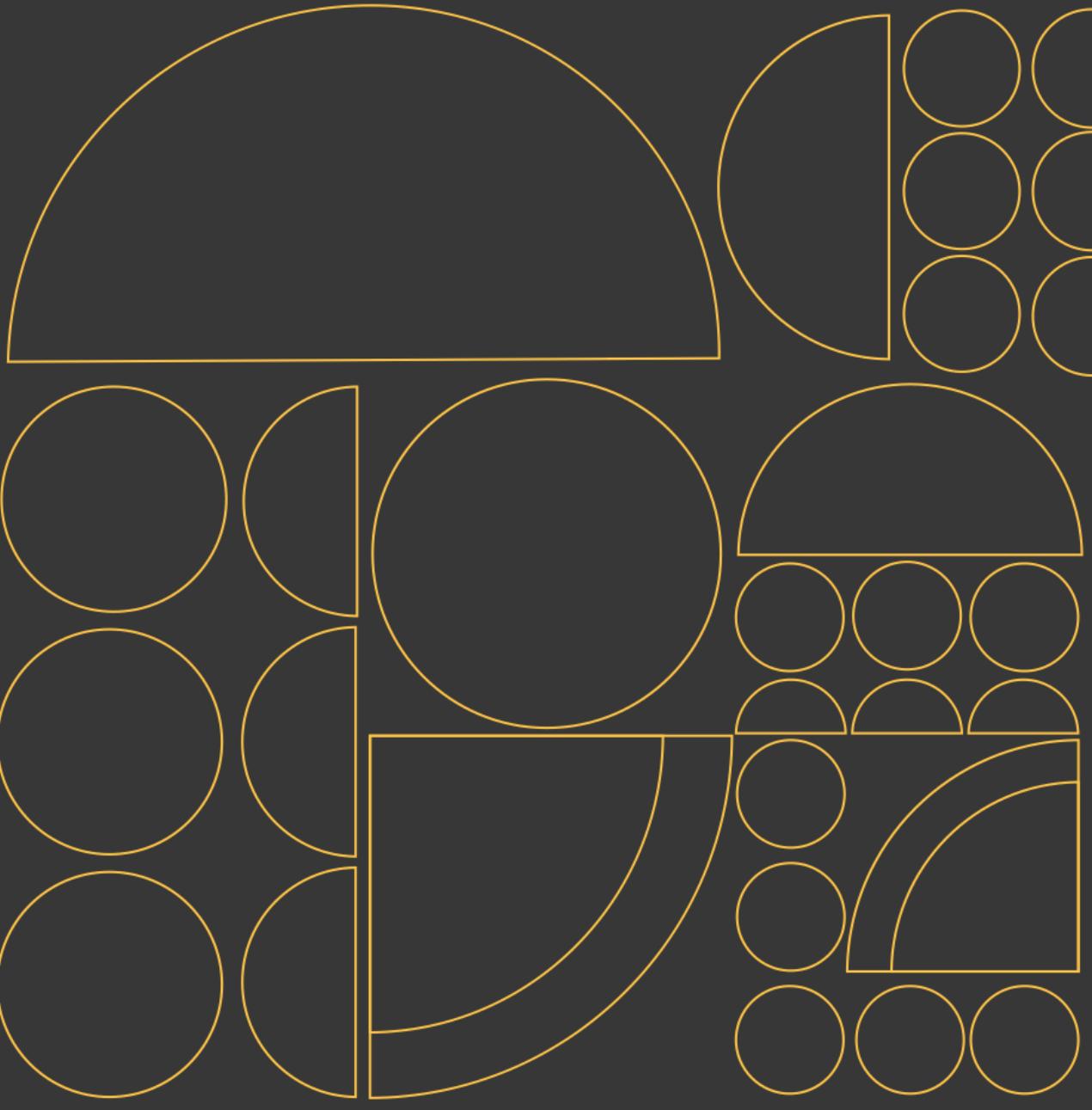
Input layer	wordS
Convolution layer 1	wordS
Downsampling layer 1	wordS
Convolution layer 2	wordS
Downsampling layer 2	wordS
Fully-connected layer 1	wordS
Fully-connected layer 2	wordS
Output layer	wordS



**ChEESE**

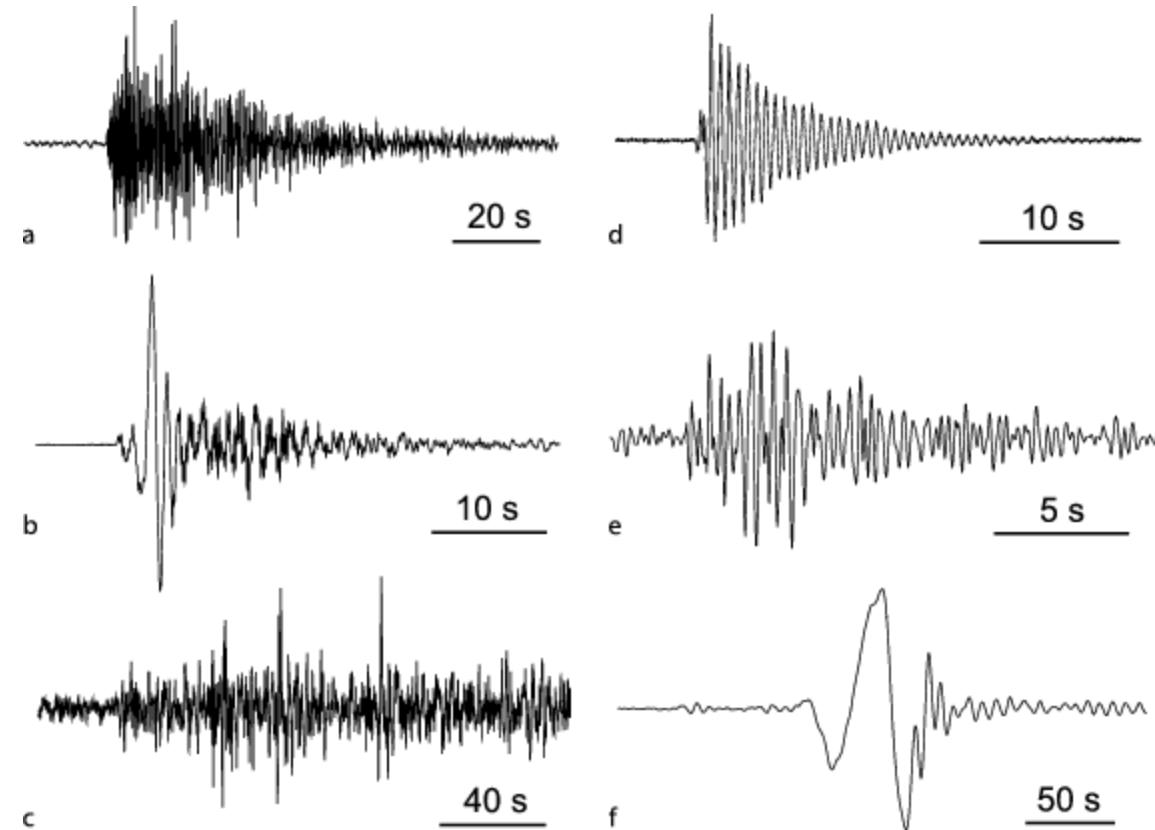
## 7. Applications

The illustration of the previous concepts with examples from seismology. And then you will be ready to apply these concepts to your own problems!



# Deep-learning applications in seismology

- Signal detection, pattern recognition
- Classification
- Source localization from sparse or evolving datasets
- Denoising and compression



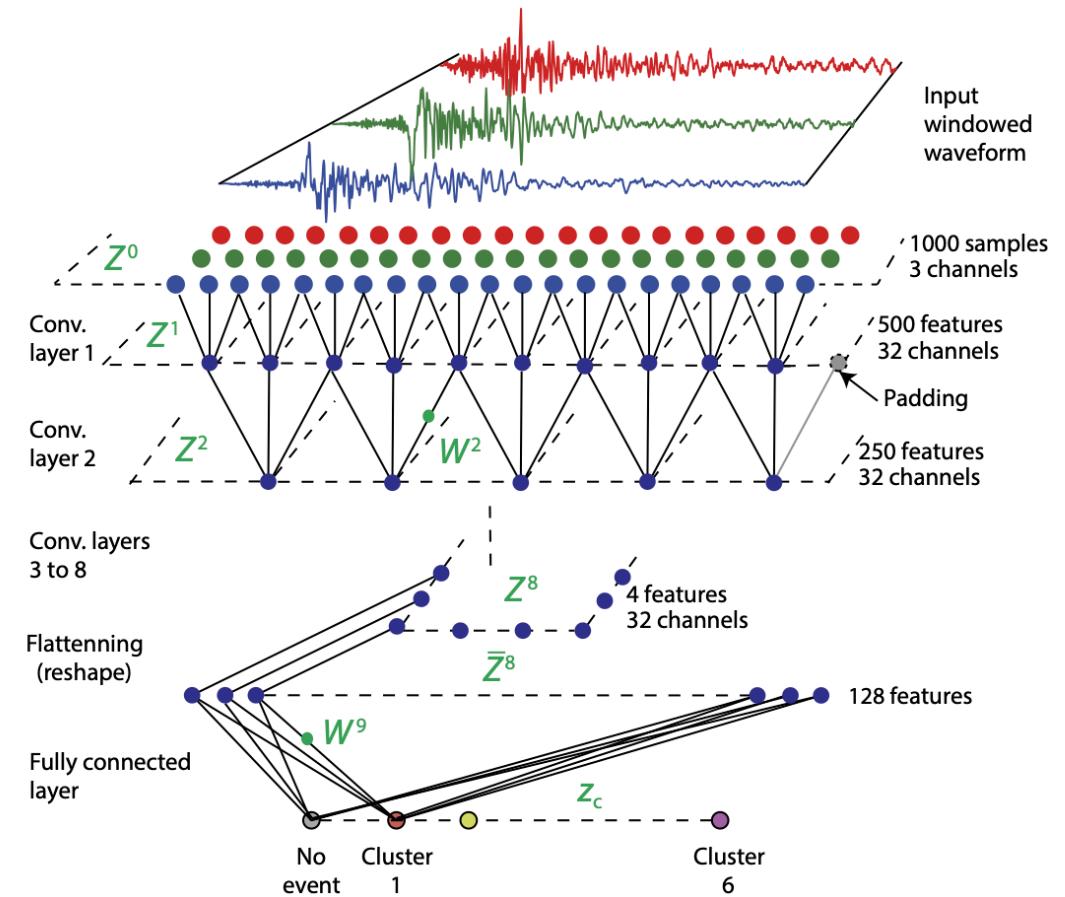
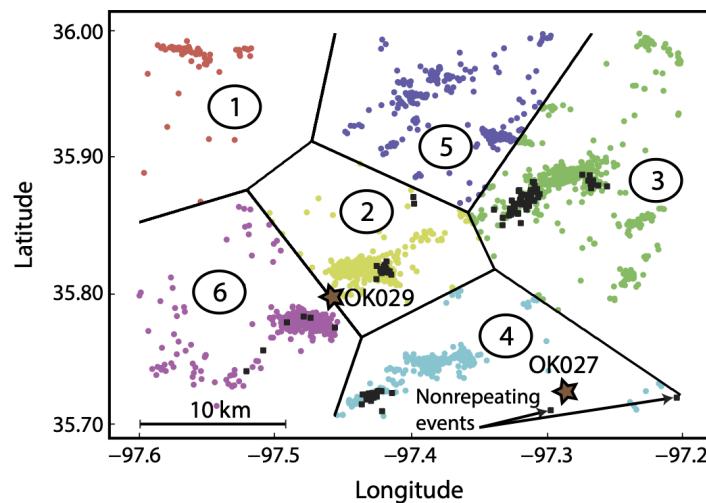
# Earthquake detection and location with ConvNetQuake

**Features:** 3-comp. waveform  $\mathbf{x} \in \mathbb{R}^{N \times 3}$

**Target:** prob. of event in cell **1** to **6**

**Loss:** cross-entropy with regularization  $\mathcal{L} =$

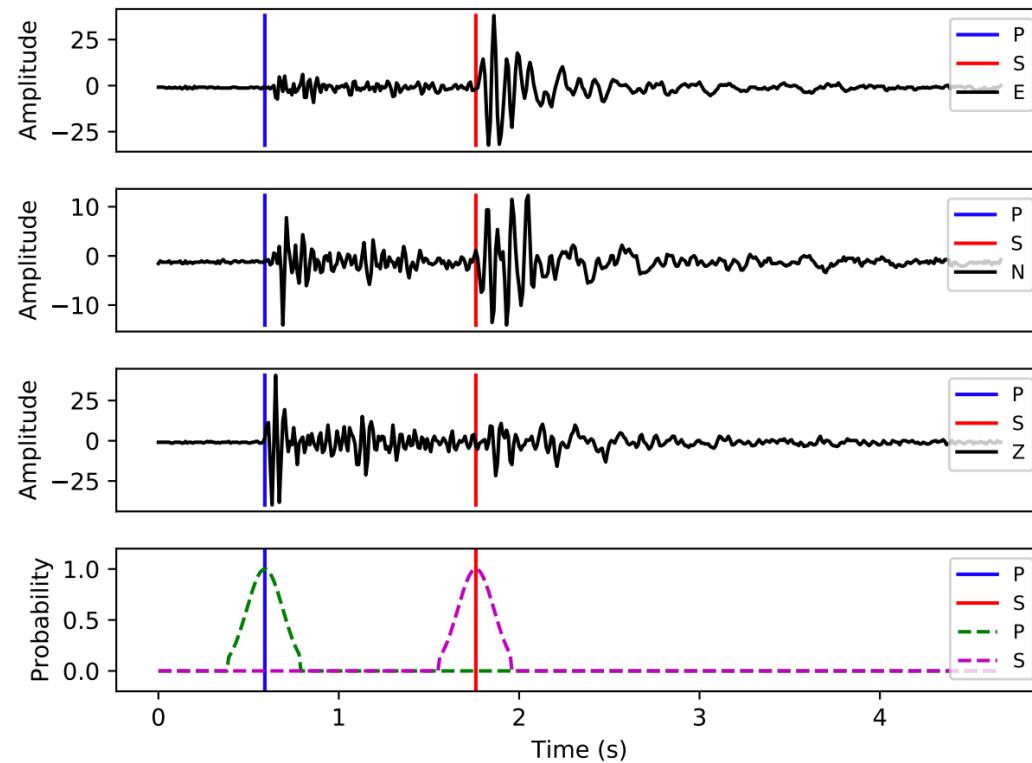
$$-\sum_c q_c \log p_c + \lambda \|\mathbf{w}\|_2^2$$



# Seismic phase picking with PhaseNet

**Features:** 3-component seismic signal  $\mathbf{x} \in \mathbb{R}^{3000 \times 3}$

**Targets:** probabilities  $p_i(\mathbf{x})$  of  $P$ ,  $S$ , and  $N$ oise over time =  $\mathbf{y} \in \mathbb{R}^{3000 \times 3}$

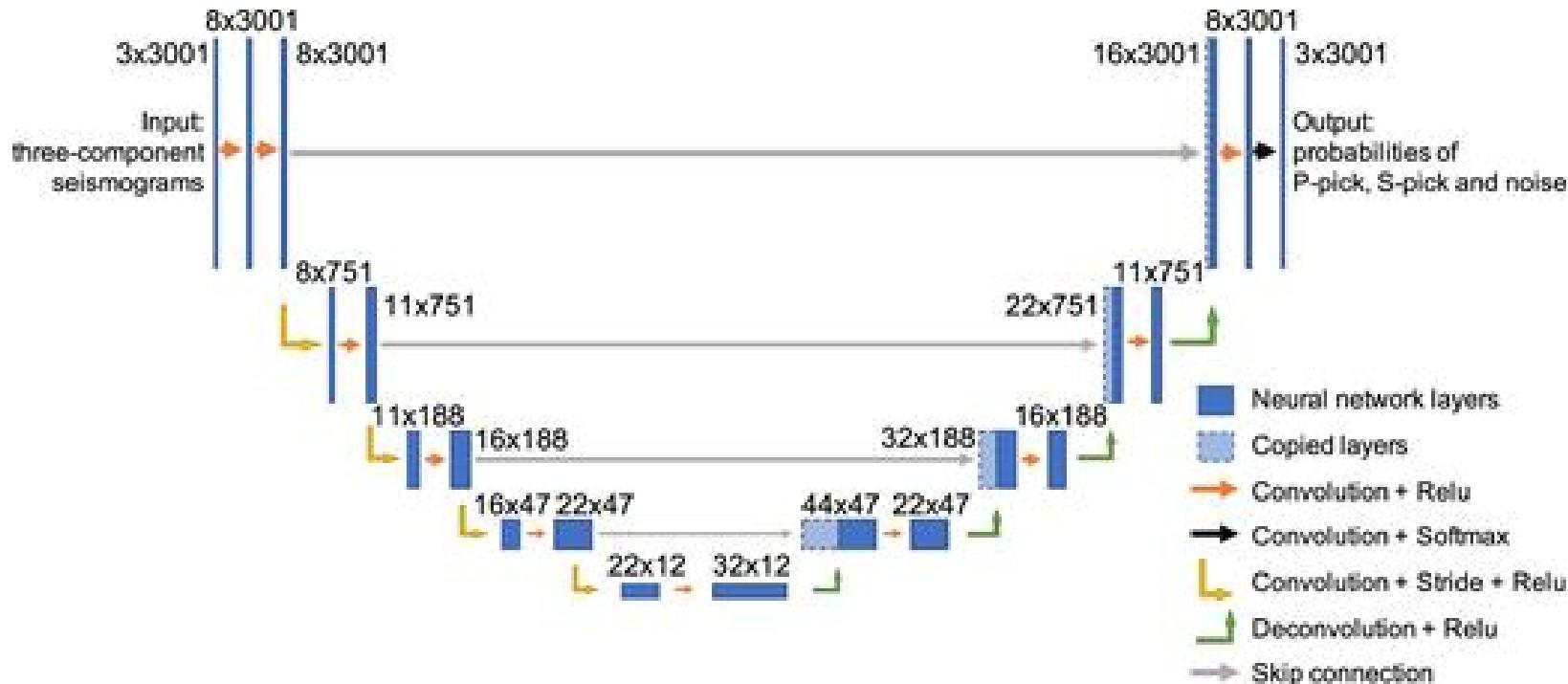


# Seismic phase picking with PhaseNet

**Features:** 3-component seismic signal  $x \in \mathbb{R}^{3000 \times 3}$

**Targets:** probabilities  $p_i(x)$  of  $P$ ,  $S$ , and Noise over time =  $y \in \mathbb{R}^{3000 \times 3}$

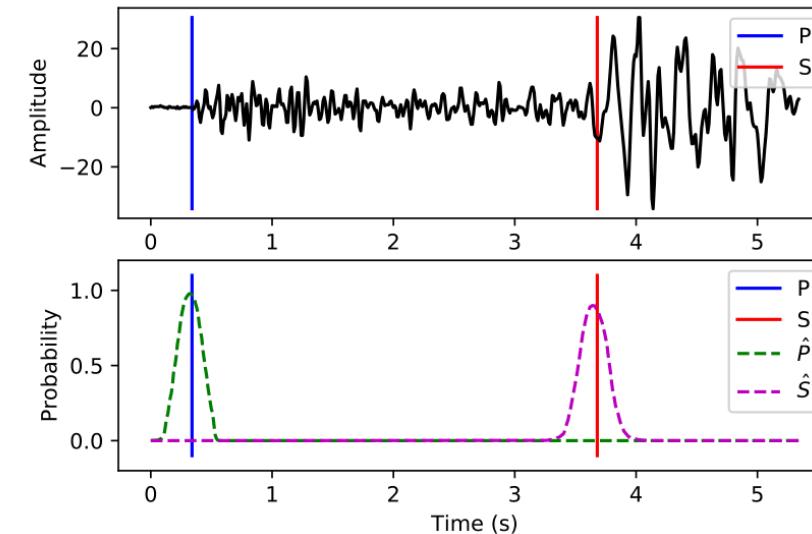
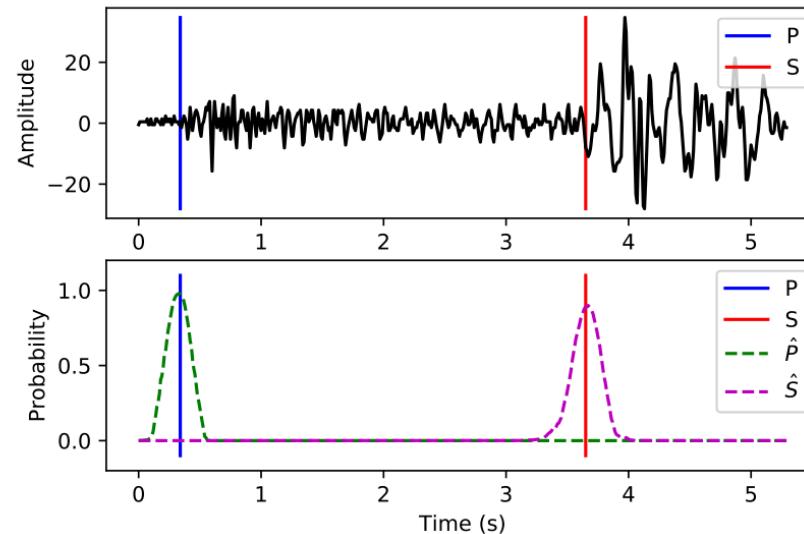
**Loss:** cross-entropy  $\mathcal{L} = -\sum_i \sum_x p(x) \log(q(x))$



# Seismic phase picking with PhaseNet

**Features:** 3-component seismic signal  $\mathbf{x} \in \mathbb{R}^{3000 \times 3}$

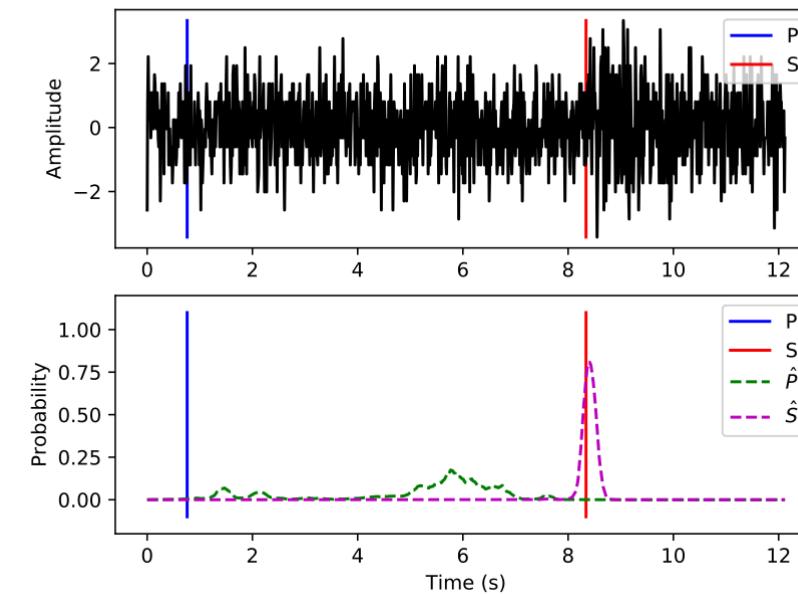
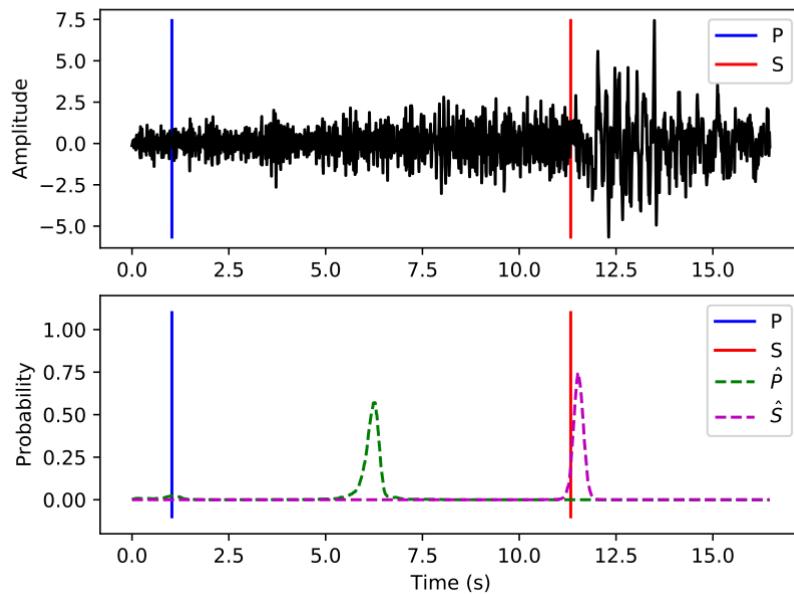
**Predictions:** likelihood  $q_i(\mathbf{x})$  of  $P$ ,  $S$ , and  $N$ oise over time



# Seismic phase picking with PhaseNet

**Features:** 3-component seismic signal  $\mathbf{x} \in \mathbb{R}^{3000 \times 3}$

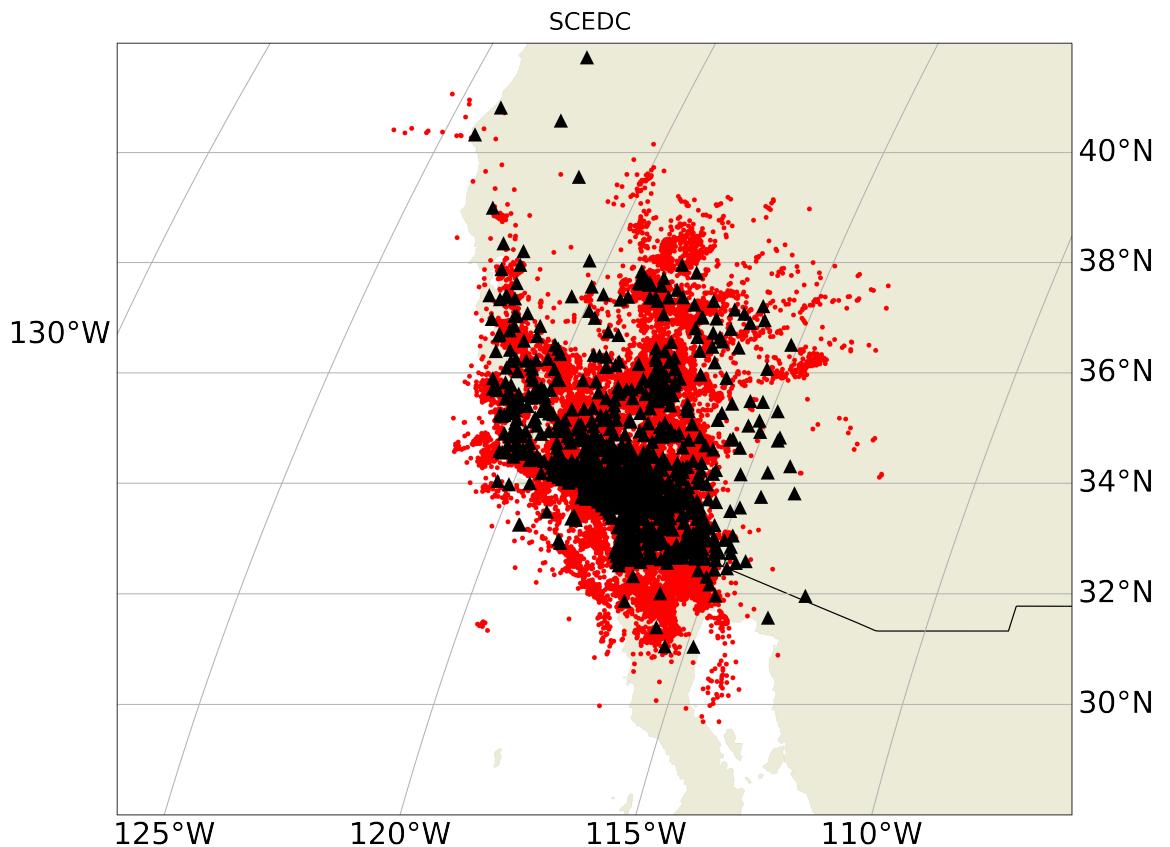
**Predictions:** likelihood  $q_i(\mathbf{x})$  of  $P$ ,  $S$ , and  $N$ oise over time



# Transfer learning and fine-tuning

**Transfer learning** is the use of a pre-trained model  $f_\alpha = f_{\theta^*}$  on a new task as a initial point for training a new model  $f_\alpha \rightarrow f_{\alpha^*}$ .

**Fine-tuning** is the partial re-training of a pre-trained model on a new task, while keeping the weights of the pre-trained layers fixed.



# Deep-learning libraries in Julia and Python

## Warning

Libraries are constantly evolving,  
and the documentation is often  
incomplete.



## Scikit-Learn toolbox documentation

- Machine learning in Python
- Online examples
- Explanation of algorithms
- Grey-box models

The screenshot shows the official scikit-learn documentation website. At the top, the title "scikit-learn" is displayed in large, bold, blue letters, followed by "Machine Learning in Python" in a smaller, italicized blue font. Below the title, there are two main navigation links: "Getting Started" and "Release Highlights for 1.5". To the right of these links is a vertical column of bullet points summarizing the toolbox's features. At the bottom of the page, there are three large callout boxes: "Classification" (describing identifying object categories), "Regression" (describing predicting continuous values), and "Clustering" (describing grouping similar objects). Each callout box also includes a "Applications" section with an example.

- Simple and efficient tools for predictive data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

**Classification**  
Identifying which category an object belongs to.  
**Applications:** Spam

**Regression**  
Predicting a continuous-valued attribute associated with an object.

**Clustering**  
Automatic grouping of similar objects into sets.  
**Applications:** Customer segmentation, grouping

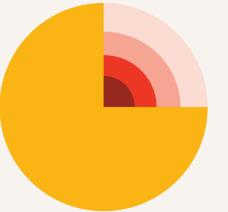
# Learning visually with the TensorFlow playground

### What do 50 million drawings look like?

Over 15 million players have contributed millions of drawings playing [Quick, Draw!](#). These doodles are a unique data set that can help developers train new neural networks, help researchers see patterns in how people around the world draw, and help artists create things we haven't begun to think of. That's why [we're open-sourcing them](#), for anyone to play with.

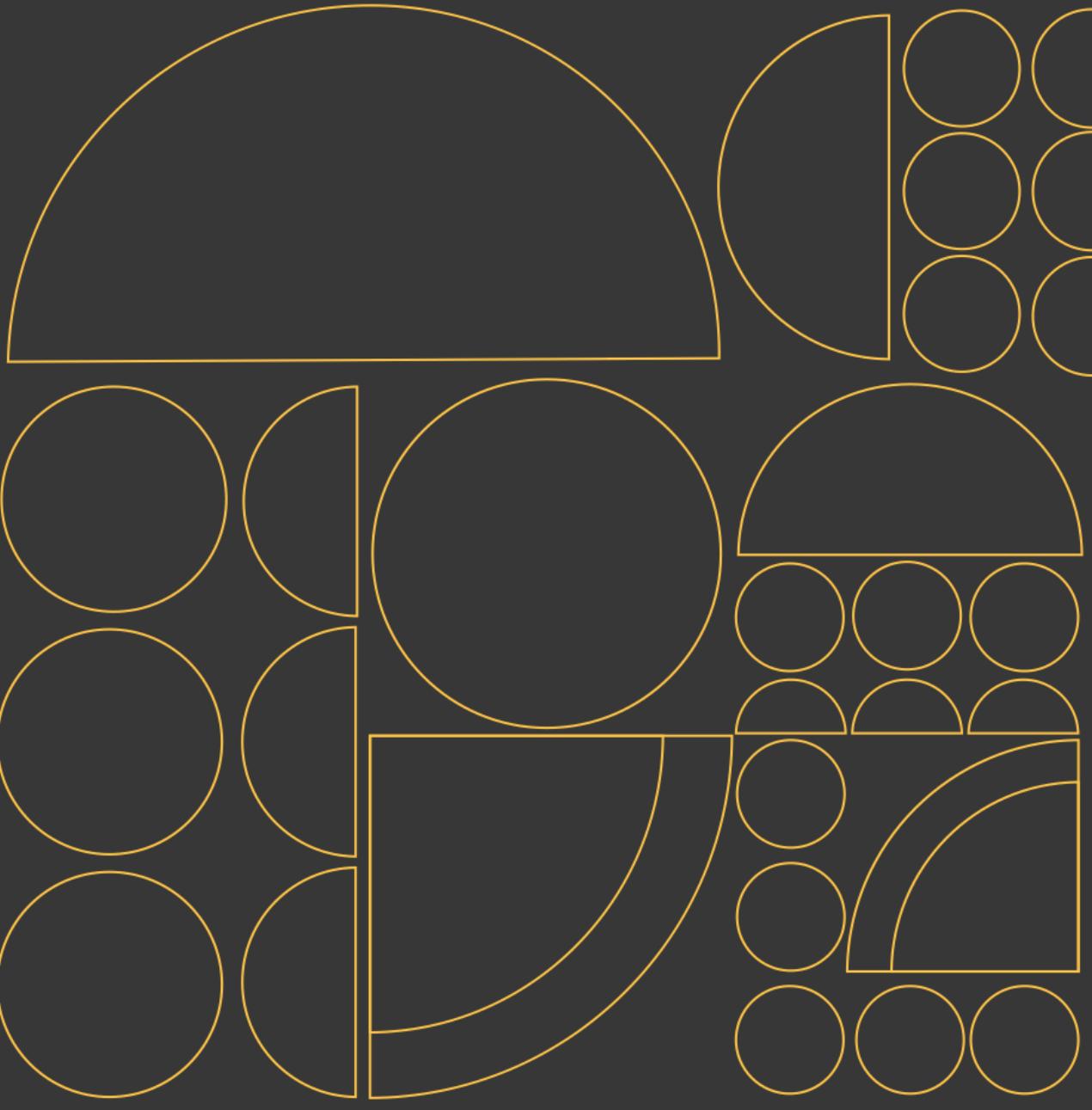
Select a drawing





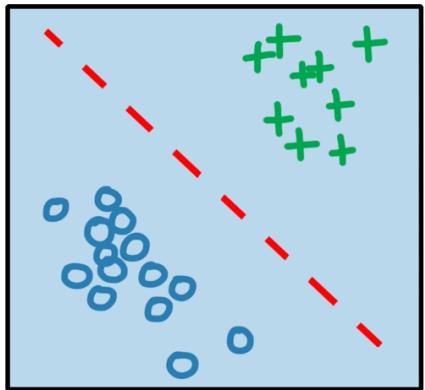
**ChEESE**

## 8. Unsupervised learning



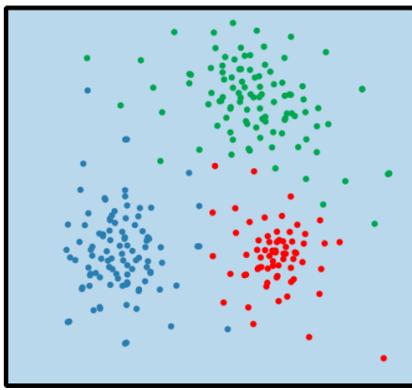
# Main types of machine learning

supervised  
learning



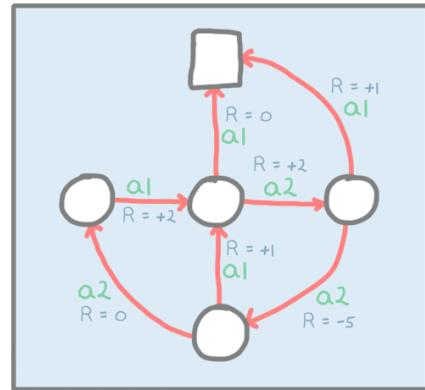
Predict some output  $\mathbf{y}$  from input  $\mathbf{x}$  (regression, classification).

unsupervised  
learning



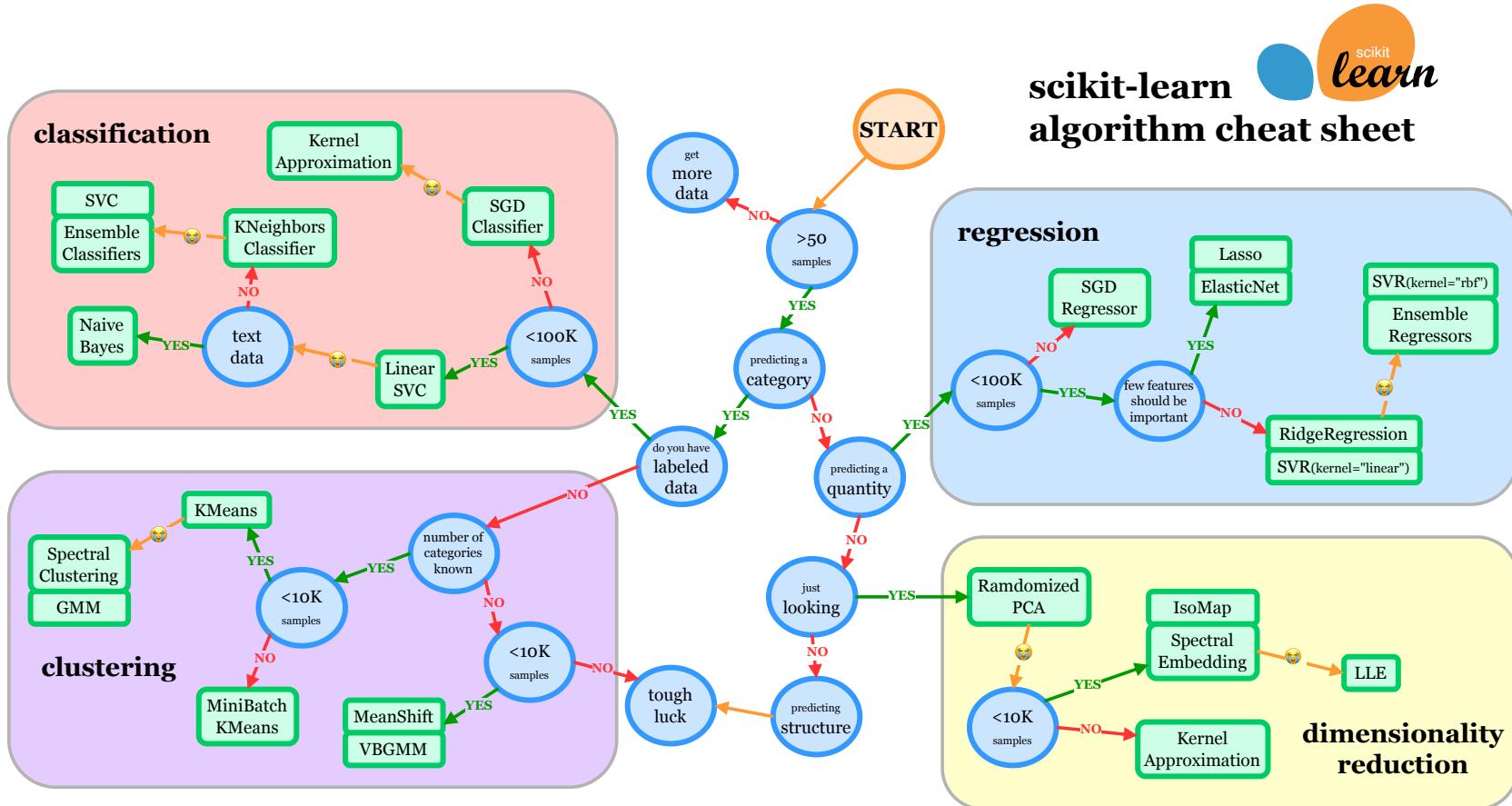
Learn data distribution  $p(\mathbf{x})$  or structure (clustering, reduction).

reinforcement  
learning



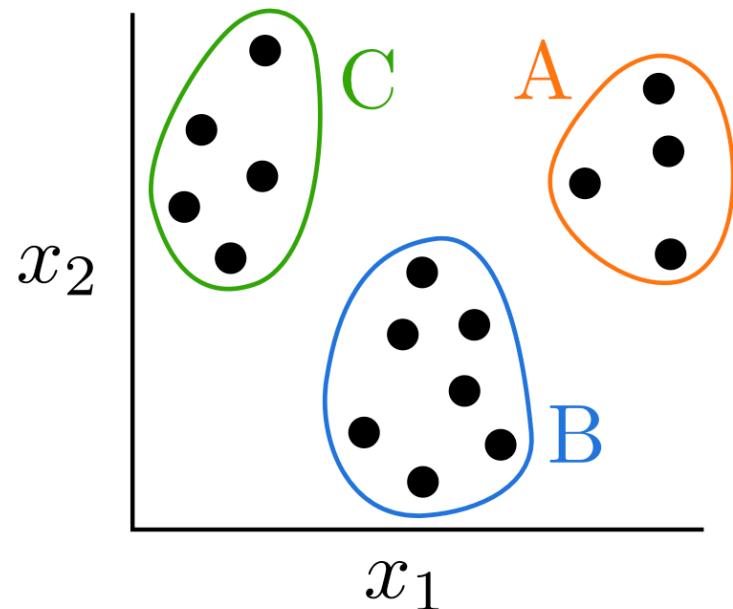
Learns a policy to maximize the reward (game playing, robotics).

# Contents of this class make use of the scikit-learn library



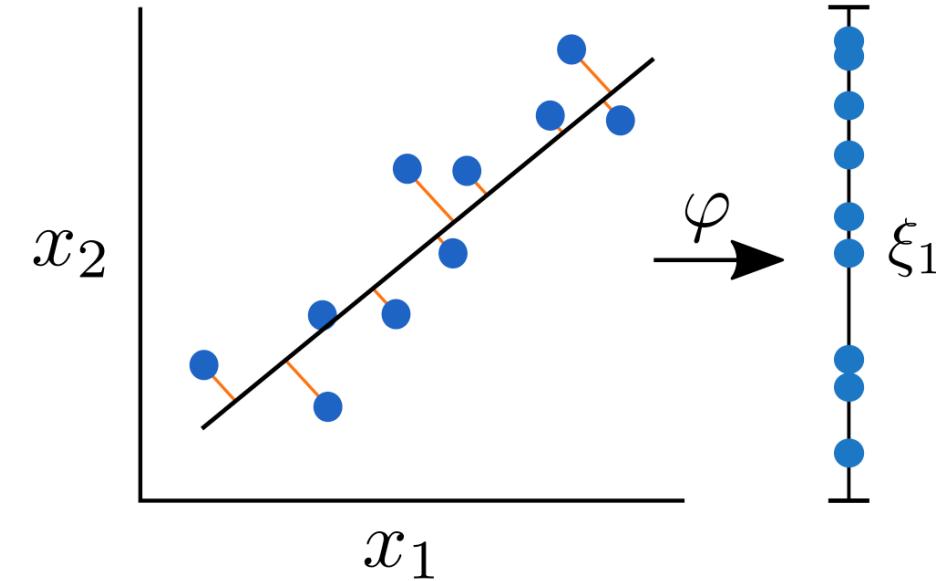
# Unsupervised learning: learning the structure of the data without labels

**Clustering**



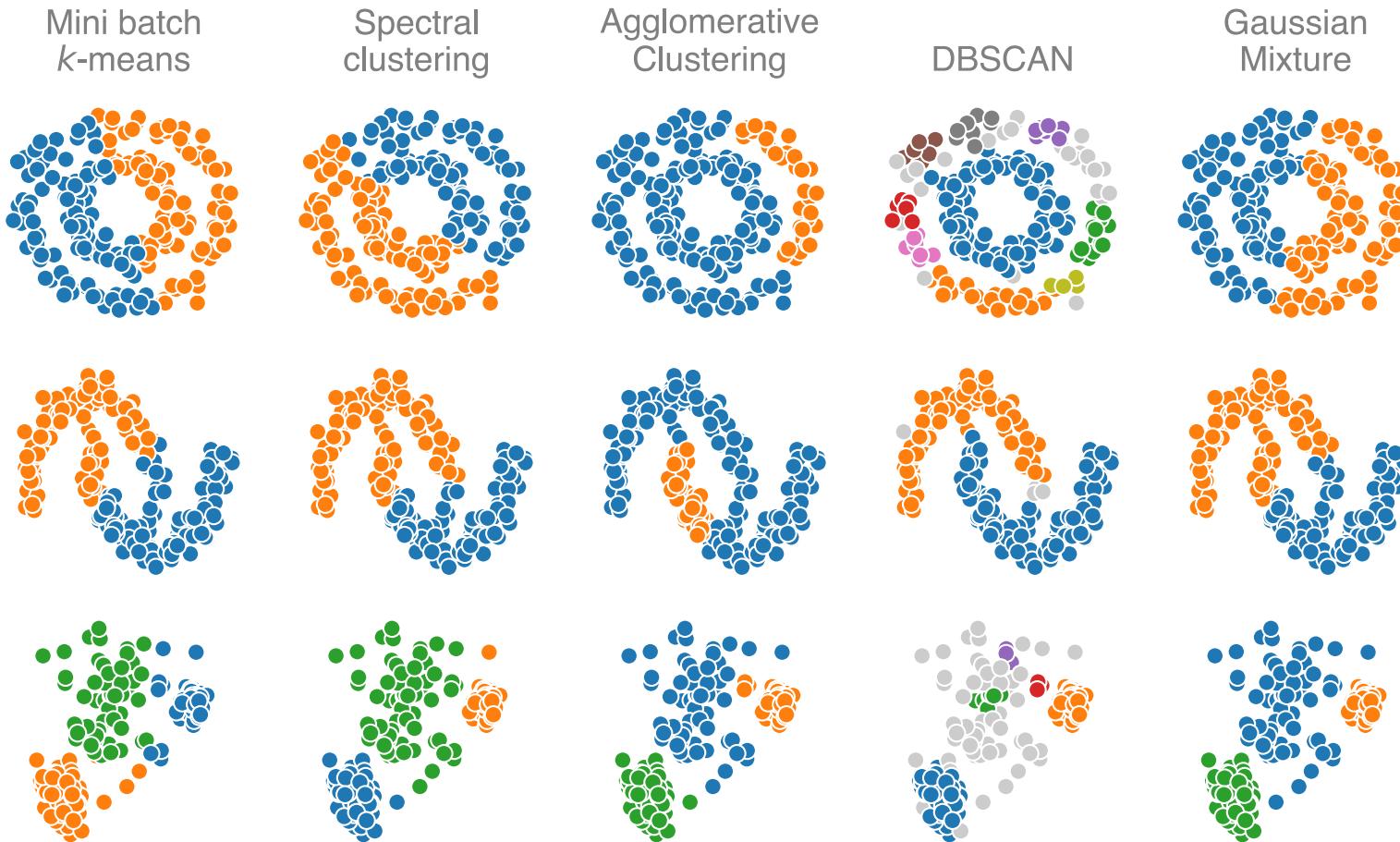
Group similar data points together based on some similarity measure.

**Dimensionality reduction**

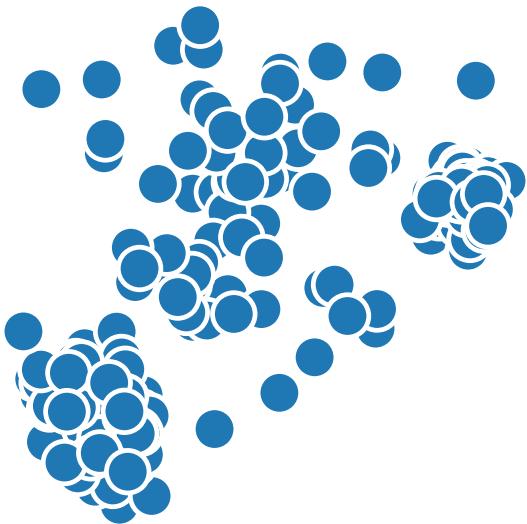


Find a low-dimensional representation of the data.

# Clustering – class-membership identification without labels



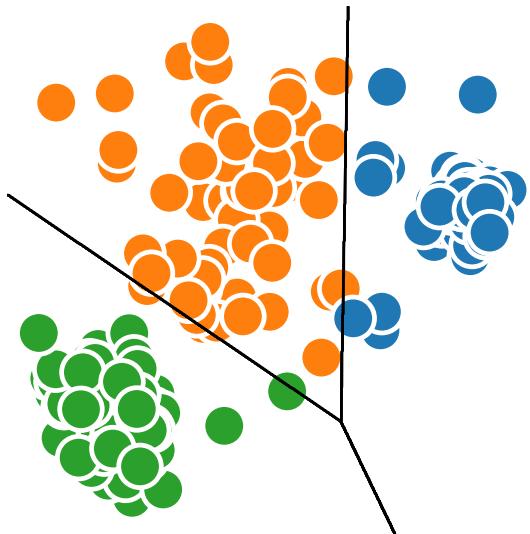
# Definitions of clustering



Two main definitions of clustering:

- Top-bottom: partition the heterogeneous data into **homogeneous** subsets.
  - Bottom-up: group the data samples based on some criterion of **similarity**.
- We need to provide a definition of **similarity** or **homogeneity**.

## Example of clustering with $k$ -means



$k$ -means is a clustering algorithm that partitions the data into  $k$  clusters by minimizing the **inertia**:

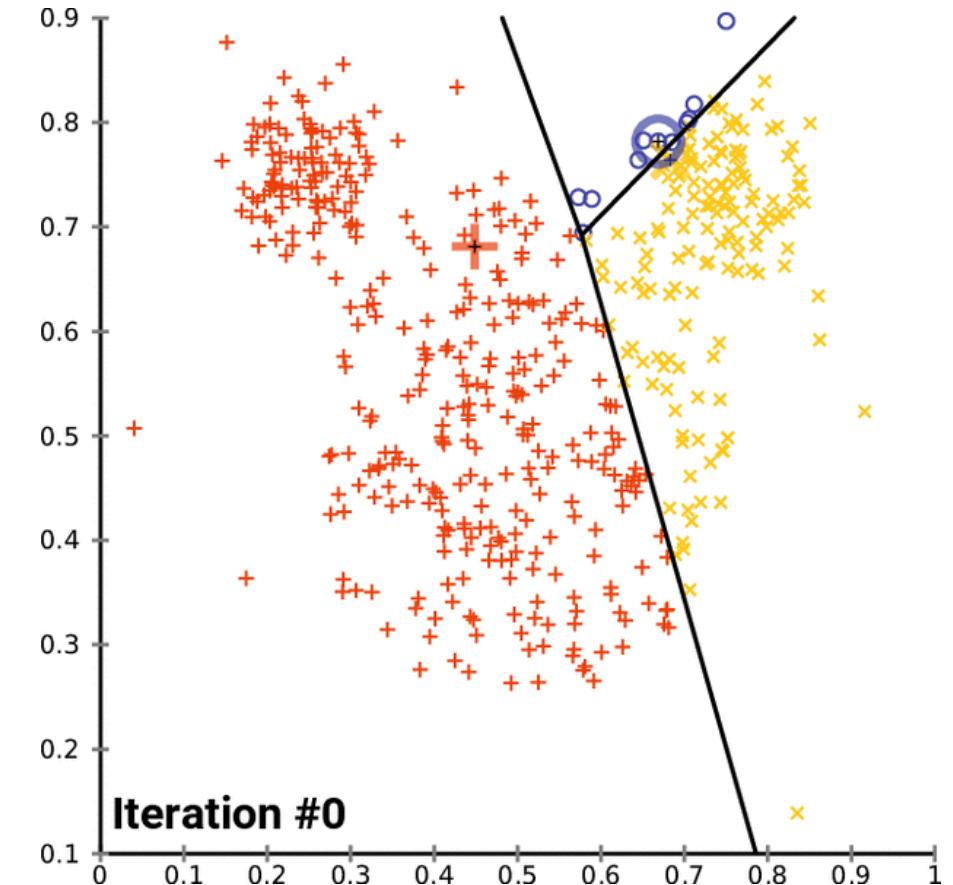
$$\arg \min_{\mathbf{C}} \sum_{i=1}^k \sum_{\mathbf{x}_j \in C_i} \|\mathbf{x}_j - \mu_i\|^2$$

where  $\mu_i$  is the centroid of cluster  $C_i$ .

# Example of clustering with $k$ -means

In practice, we need to provide the number of clusters  $k$ , and the algorithm will find the best partition:

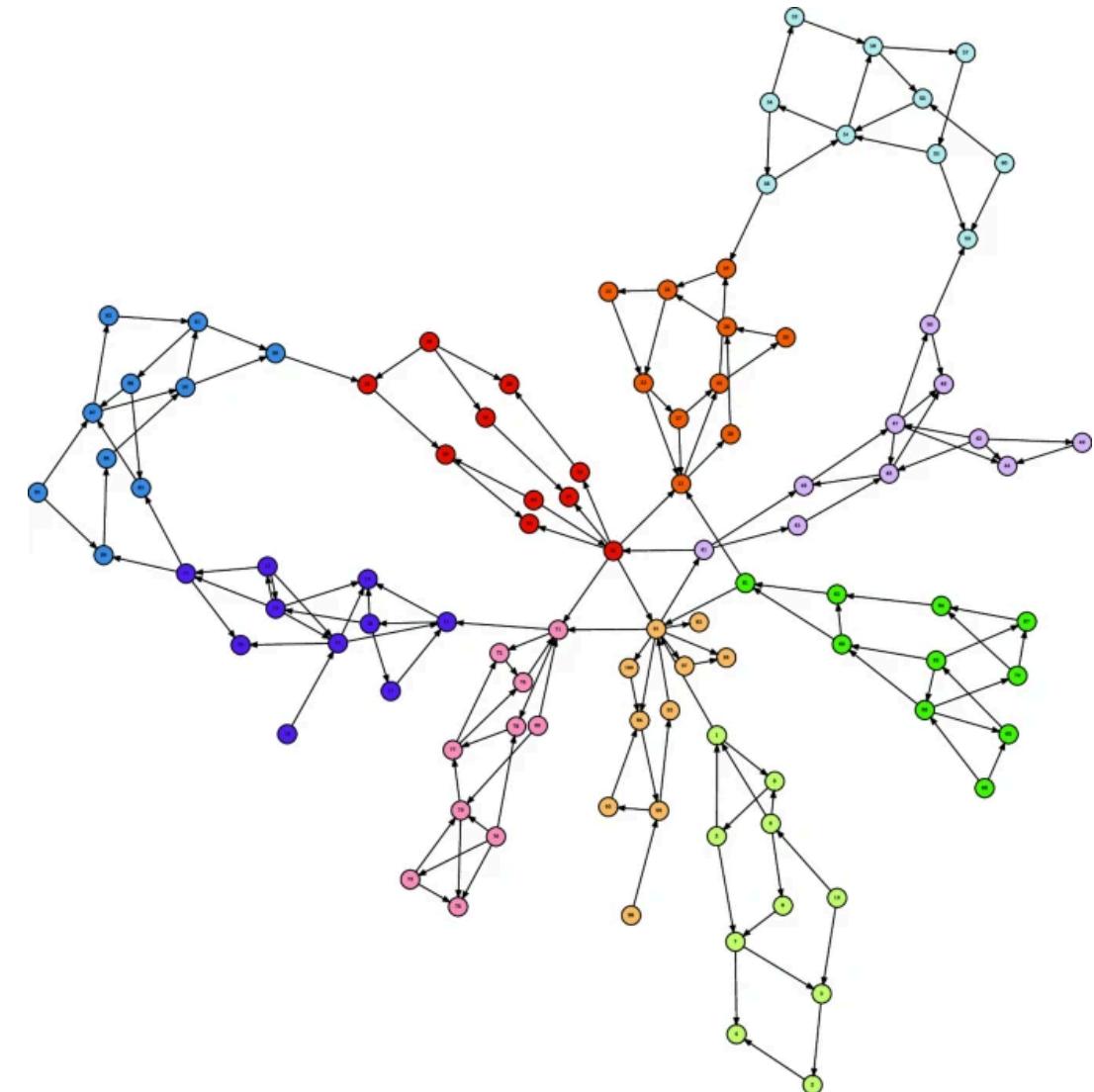
1. Initialize the centroids  $\mu_i$  randomly.
2. Assign each sample to the closest centroid.
3. Update the centroids with the new samples.
4. Repeat until convergence.



# Example of clustering with spectral clustering

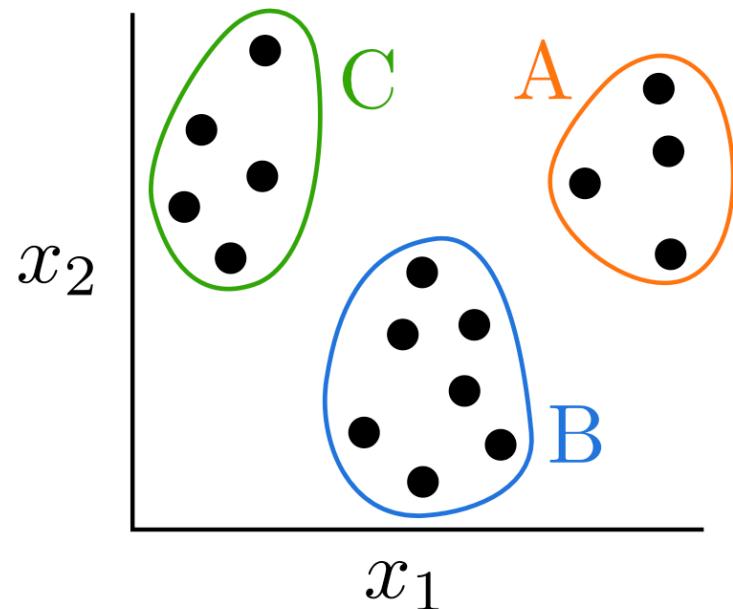
Spectral clustering uses the eigenvectors of the similarity matrix to find the clusters.

1. Compute the adjacency matrix.
2. Compute the Laplacian matrix.
3. Get the first  $m$  eigenvectors.
4. Cluster the data using  $k$ -means.



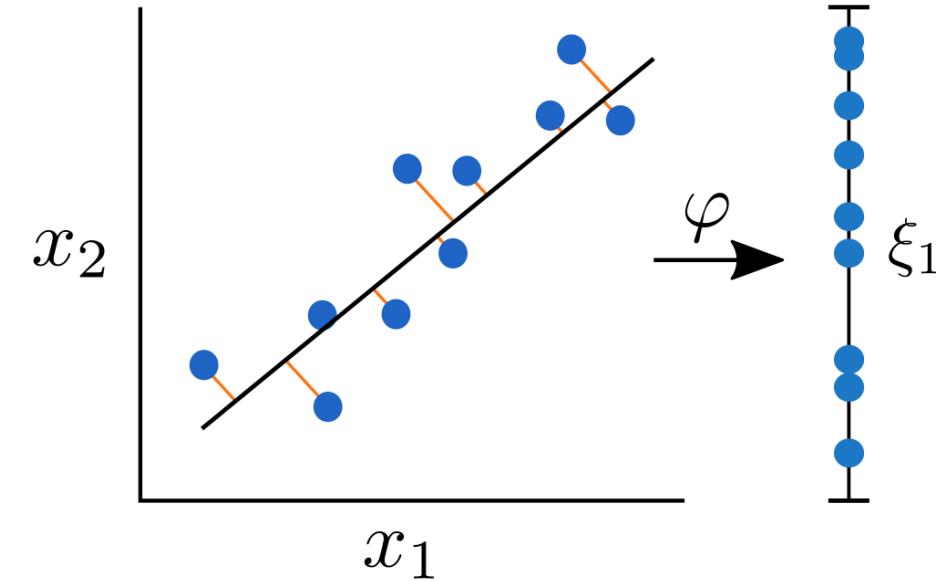
# Unsupervised learning: learning the structure of the data without labels

**Clustering**



Group similar data points together based on some similarity measure.

**Dimensionality reduction**



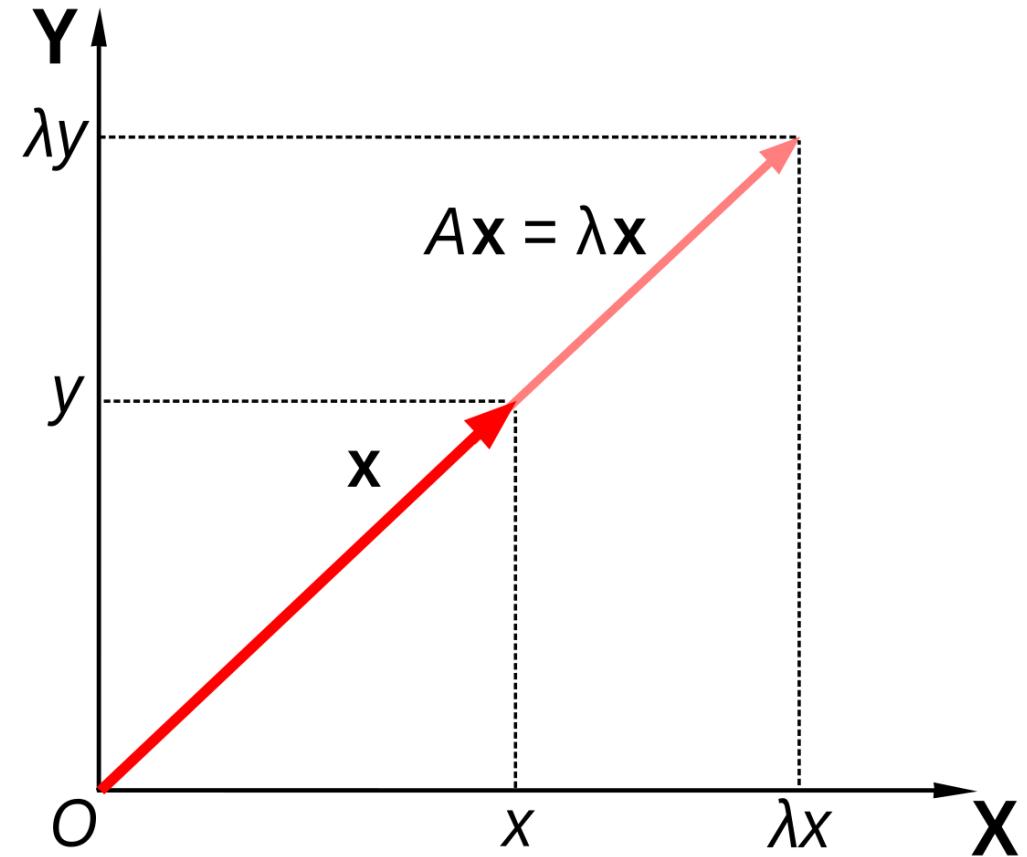
Find a low-dimensional representation of the data.

## Eigenvectors of a matrix

The eigenvectors of a matrix are obtained by solving the eigenvalue problem:

$$\mathbf{Ax} = \lambda \mathbf{x}$$

where  $\mathbf{A}$  is a square matrix,  $\mathbf{x}$  is the eigenvector, and  $\lambda$  is the eigenvalue.



# Singular value decomposition

The singular value decomposition (SVD) of a matrix  $\mathbf{A}$  is defined as:

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$$

where  $\mathbf{U}$  and  $\mathbf{V}$  are orthogonal matrices, and  $\Sigma$  is a diagonal matrix.

$$\begin{matrix} \text{A} \\ m \times n \end{matrix} = \begin{matrix} \text{U} \\ m \times m \end{matrix} \begin{matrix} \Sigma \\ m \times n \end{matrix} \begin{matrix} \text{V}^* \\ n \times n \end{matrix}$$

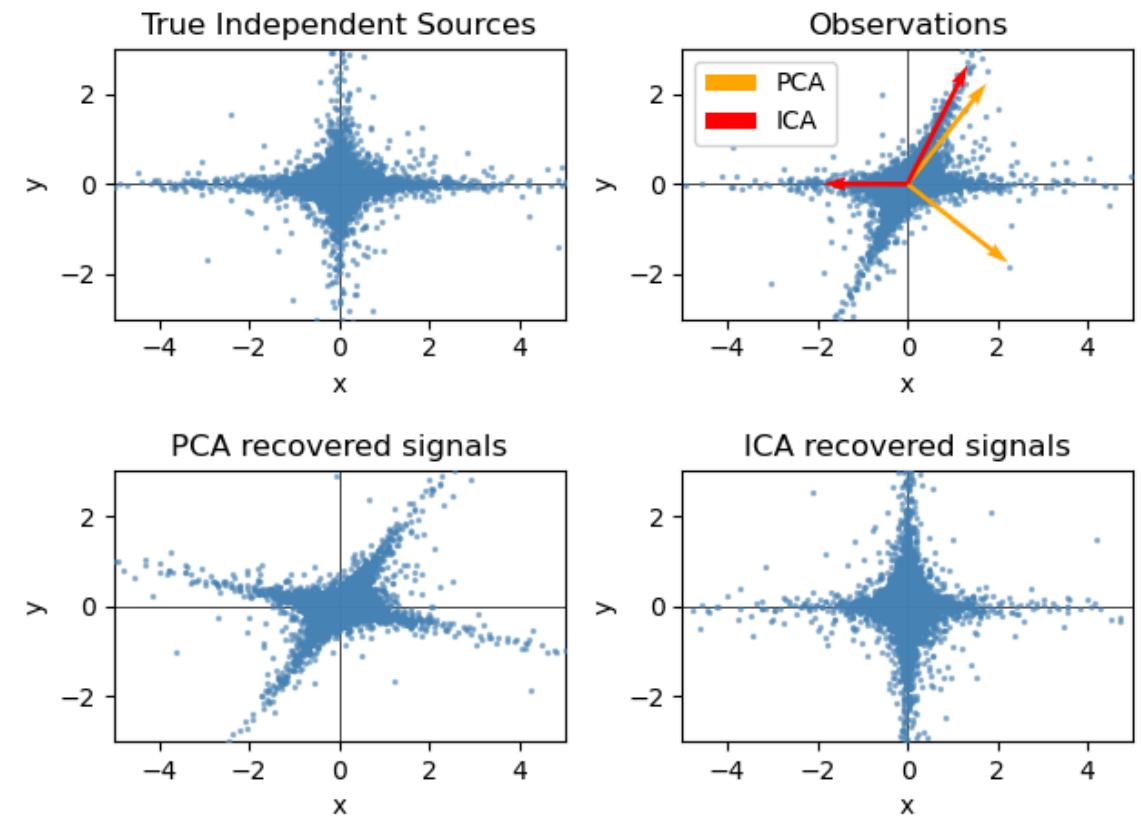
## Example of dimensionality reduction with principal component analysis

Principal component analysis (PCA) is a dimensionality reduction technique that uses eigendecomposition:

1. Compute the data covariance matrix.
2. Compute the eigenvectors.
3. Project the data onto the eigenvectors.

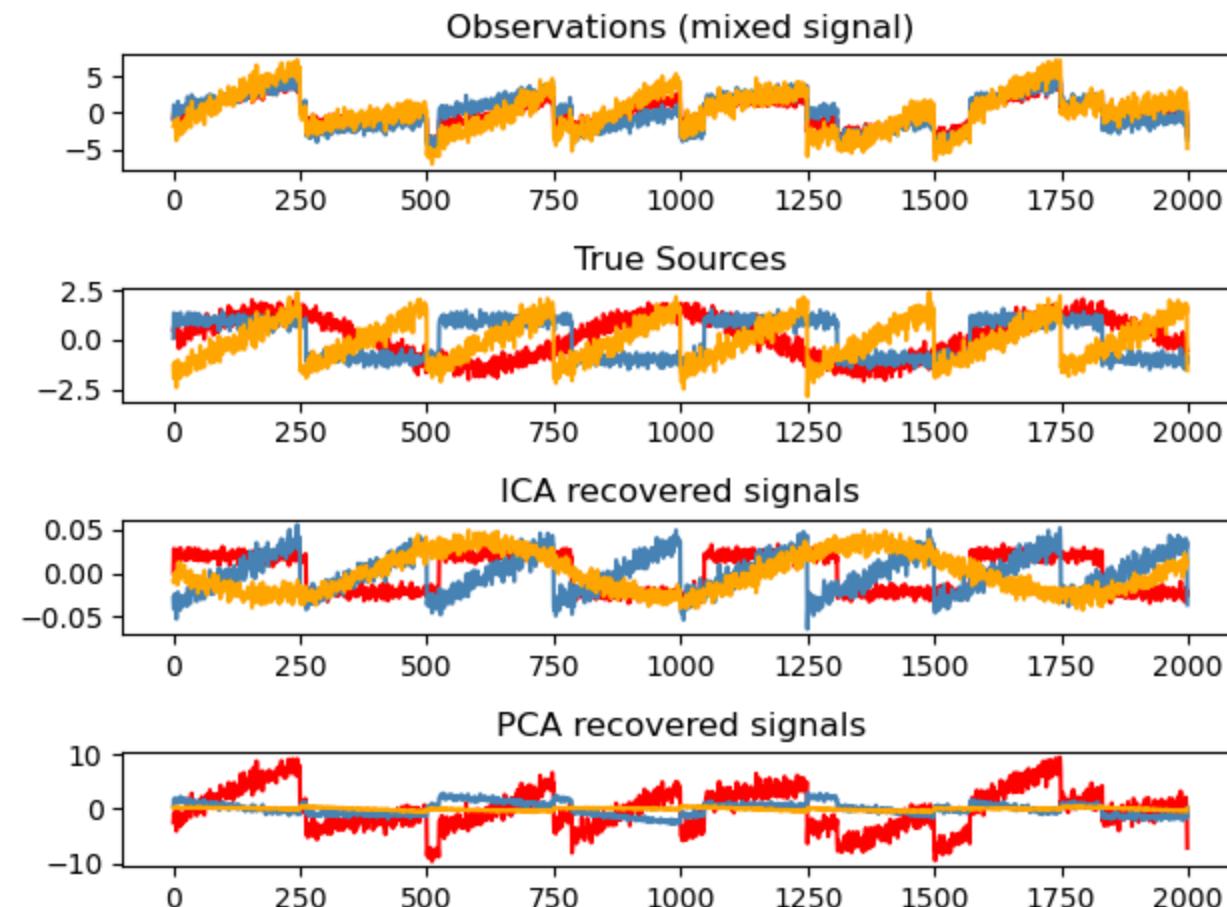
# Example of dimensionality reduction with independent component analysis

Independent component analysis (ICA) is a dimensionality reduction technique that maximizes the independence of the components.



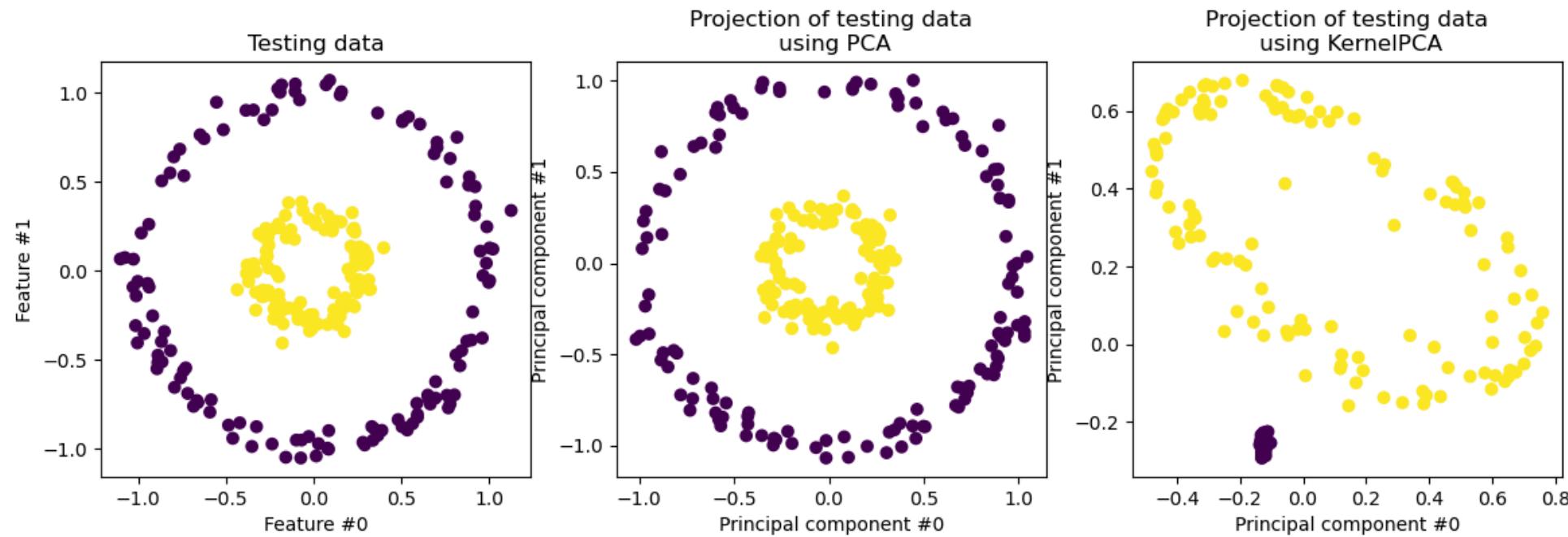
# Principal vs. independent component analysis

For blind source separation, ICA is preferred over PCA.



## Kernel PCA, of course

Kernel PCA is a non-linear dimensionality reduction technique that uses the kernel trick to project the data onto a higher-dimensional space.



# Deep unsupervised learning

Deep neural networks can be used for unsupervised learning:

**Autoencoders**: learn a low-dimensional representation of the data.

**Generative adversarial networks**: learn a generative model of the data.

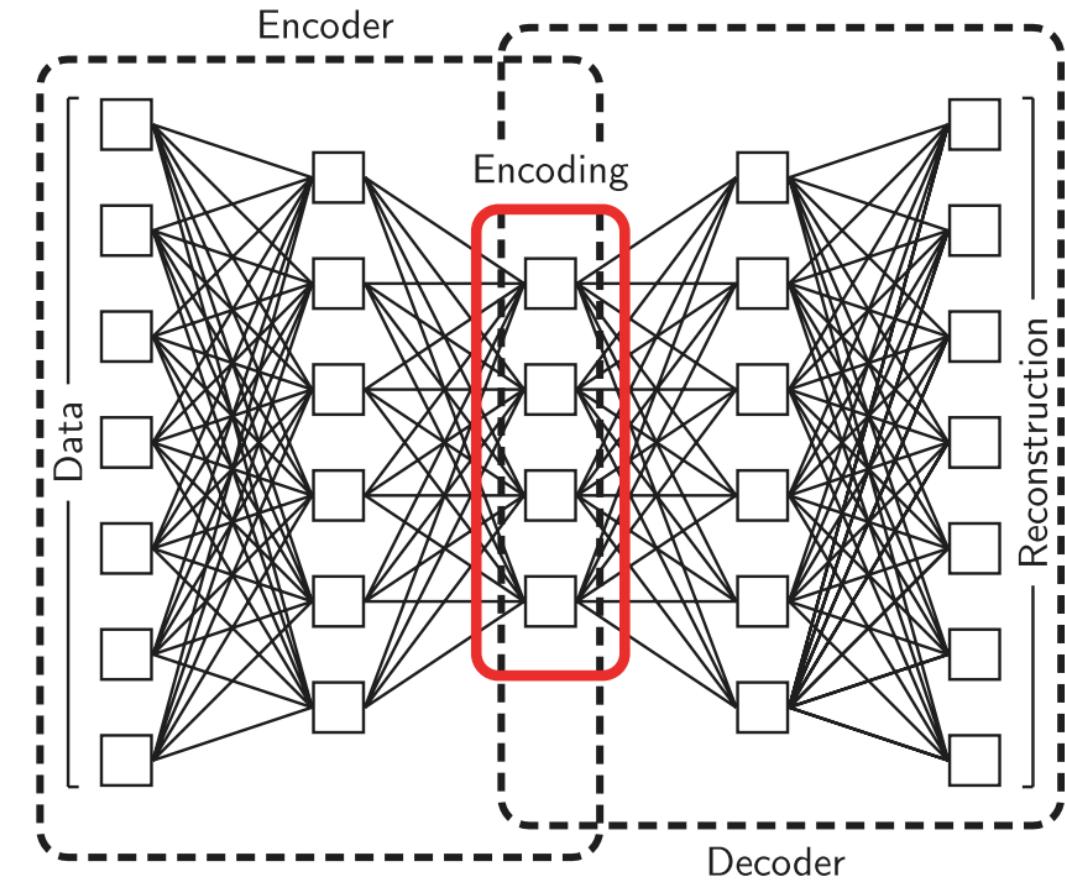
# Autoencoders

Autoencoders are neural networks that learn a low-dimensional representation of the data. They are composed of an **encoder** and a **decoder**.

The input  $\mathbf{x}$  is encoded into a latent representation  $\mathbf{z}$ , and decoded into  $\mathbf{x}'$ .

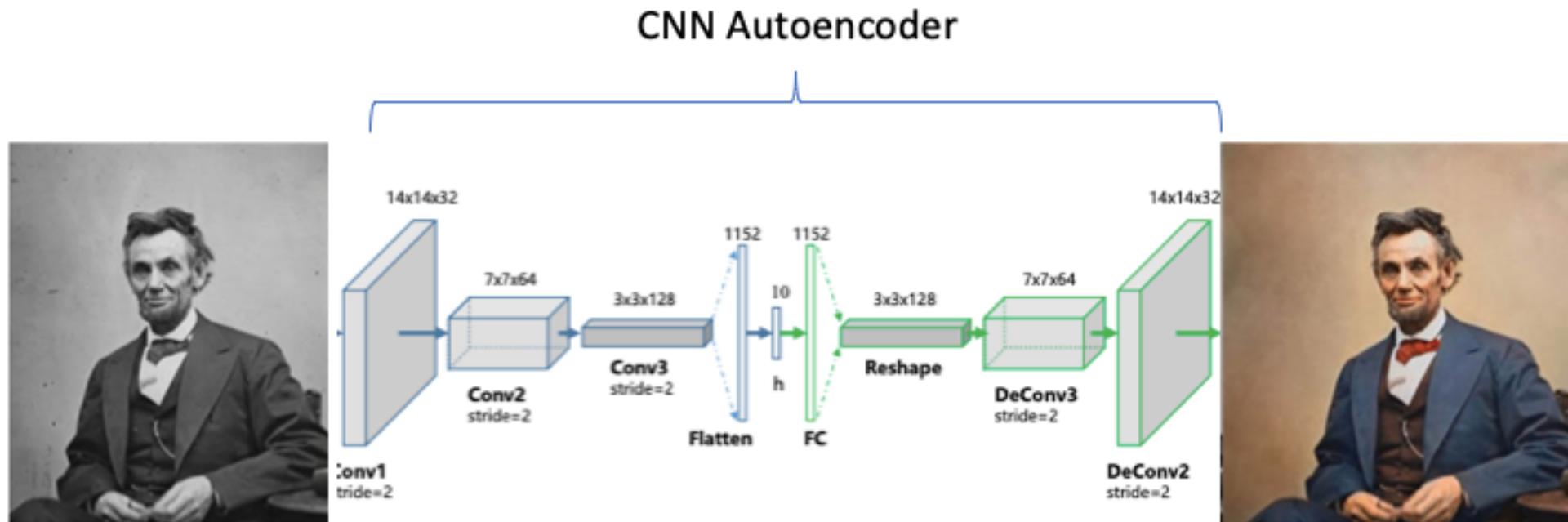
The loss function is the difference between the input and the reconstruction:

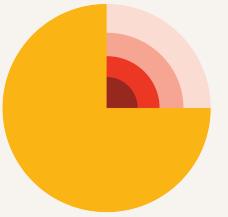
$$\mathcal{L} = \|\mathbf{x} - \mathbf{x}'\|^2$$



# Convolutional autoencoders

Convolutional autoencoders use convolutional layers instead of fully connected layers. They are used for image denoising, compression, and quality assessment.





**ChEESE**

*The end!*

