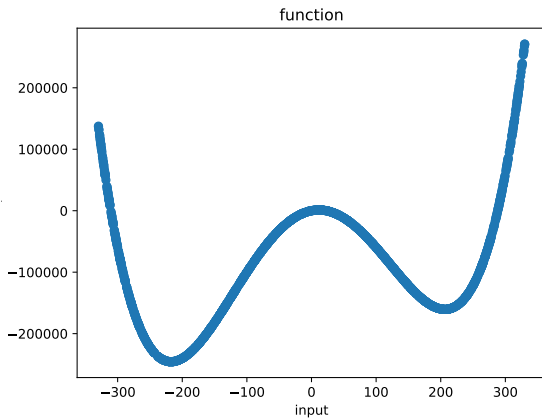


Machine learning I, supervised learning: problem statement



Machine learning (ML)

- ▶ (proposed definition of) **learning** : "Modification of a behavior, based on a life experiment"
- ▶ a **machine learning** system is programmed to learn in a **semi-automatic** way.

Classical programming vs ML

- ▶ Classical program : predict the total amount of money spent, based on the number of fruits bought and the price of each individual fruit (a summation is enough)
- ▶ ML program : predict which fruit(s) a person buys, based on a database of customers and on some information about this person (e.g. buying log, age, profession).

Book

`https://cazencott.info/index.php/pages/
Introduction-au-Machine-Learning`

Use cases of ML

ML is useful for problems :

- ▶ that we cannot solve directly thanks to an explicit representation (such as the amount of money spent in the previous first example).
- ▶ that we can solve in practice, but without a complete understanding of the underlying mechanism (face recognition)
- ▶ that we could solve explicitly, but the computational resources would be too heavy (molecular dynamics), so we **approximate** a solution with ML.

Denomination

- ▶ The name "machine learning" is rather deceitful !
- ▶ It is no more machine driven than any algorithm or coffee machine.
- ▶ The denomination "statistical learning" is sometimes used, and is more explicit.

Mathematical ingredients of machine learning (ML)

ML's main ingredients are (from the mathematics point of view) :

- ▶ statistics and probabilities : most ML objects can (should) be seen as outcomes of **random variables**.
- ▶ optimization : most (but not all) ML problems are formulated as an optimization problem.

Other tools come from :

- ▶ graph theory
- ▶ information theory
- ▶ statistical physics

Deep learning

- ▶ ML is a subset of AI.
- ▶ Deep learning is a subset of ML.

Learning paradigms

- ▶ **supervised learning** : learn to predict an output as a function of an input (predict the energy production of a wind farm based on sensors)
- ▶ **unsupervised learning** : learn information about the structure of data (density estimation, clustering, dimensionality reduction)
- ▶ **reinforcement learning** : learn to perform actions in order to maximize a reward (game player, alphago)

Why is there a hype around machine learning?

Machine learning has received attention and funding because it has reached state-of-the-art efficiency on several problems, such as :

- ▶ computer vision
- ▶ spam classification
- ▶ machine translation
- ▶ speech recognition
- ▶ self-driving cars

Deep learning is involved in several of these setups.

ML revolution

- ▶ Technical progress in the computing and storage capacities
- ▶ Increase in amount of available data. According to IBM, 10^{18} bytes are created each day.
- ▶ Progress in algorithmic methods to analyze the data.

ML revolution II

- ▶ The domain of ML and AI has been evolving at a fast pace since the mid 2000s
- ▶ The speed of evolution has increased again with LLMs (first Chat GPT release : 2022)
- ▶ Spectrum of activities between maths and computer science : the jobs linked to AI and ML evolve. We could argue that the balance is more shifted towards data engineering / devops / computer science in general than 20 years ago.
- ▶ In this course, we will not focus on LLMs, or large models in general, but rather on elementary aspects of ML (also : I am not an LLM expert).

Example 1 : ImageNet

- ▶ A database of images (more than 15M), hand-annotated in order to indicate what objects are present in the image. More than 20000 categories of images.
- ▶ Contest : ImageNet Large Scale Visual Recognition Challenge.
- ▶ The best top 5 score (a measure of the classification error) went from 25% in 2011 to $\simeq 15.3\%$ in 2012.

Example 1 : ImageNet

- ▶ A database of images (more than 15M), hand-annotated in order to indicate what objects are present in the image. More than 20000 categories of images.
- ▶ Contest : ImageNet Large Scale Visual Recognition Challenge.
- ▶ The best top 5 score (a measure of the classification error) went from 25% in 2011 to $\simeq 15.3\%$ in 2012.
- ▶ The technology used was deep learning, exploiting GPUs (AlexNet).

[https://paperswithcode.com/sota/
image-classification-on-imagenet](https://paperswithcode.com/sota/image-classification-on-imagenet)

Example 2 : AlphaGo

- ▶ In 2015 : beats a professional player. In 2017 : beats the world champion.
- ▶ Uses several technologies : among them **Deep reinforcement learning**.
- ▶ Improvements : AlphaGo Zero, trained without a database of played games. In 2017, AlphaZero beats AlphaGo Zero after 3 days of learning.

Example 3 : AlphaFold

- ▶ Goal : to predict the spatial configuration of proteins, from their DNA sequence.
- ▶ Achieves a breakthrough performance on the CASP challenge :
 - ▶ 2018 : more than 50% GDT (Global distance test), whereas it was $\leq 40\%$ before then.
 - ▶ 2020 : 92,4% GDT. At a $\geq 90\%$ score, the method is considered competitive with experimental methods..
- ▶ <https://alphafold.ebi.ac.uk/>
- ▶ Also based on Deep learning.

Audio engineering

<https://www.sonible.com/smarteq3/>

<https://www.youtube.com/watch?v=ZGetnk222YU&t=494s>

Supervised learning

Predict an output from an input.

- ▶ discrete output : classification
- ▶ continuous output : regression

We learn from a dataset D_n of n **labeled examples** ;

$$D_n = \{(x_i, y_i), i \in [1, n]\} \quad (1)$$

Supervised Learning : example of regression

- ▶ x : age and height of a person. Here x , is a **vector** containing 2 **features**.
- ▶ y : record on a 100 meters track

Regression : raw inputs

```
16 2.928290359468887800e+01 1.819015686789989559e+02
17 2.894481244139541151e+01 1.808859323280479634e+02
18 1.812029840482161513e+01 1.614667413796399229e+02
19 2.565190120950552100e+01 1.8440068277759839309e+02
20 3.054629307666820637e+01 1.739981941657430866e+02
21 2.600748351639588662e+01 1.811637511224612410e+02
22 1.507418892029618895e+01 1.868432490529089780e+02
23 3.042766519165544281e+01 1.78972790680846270e+02
24 3.658211274235085667e+01 1.785726961288677046e+02
25 2.353156221187539643e+01 1.780926290043428253e+02
26 2.830054102263598281e+01 1.618048901441496241e+02
27 2.327509936340274166e+01 1.908102611218435357e+02
28 3.044525330717638849e+01 1.736836766109009886e+02
29 2.488014451964265206e+01 1.794911044737207232e+02
30 2.226526635755104166e+01 1.788433969242797446e+02
31 1.556357798027287487e+01 1.909257627614161379e+02
32 1.233905436641630615e+01 1.769331920900993964e+02
33 2.430793641280866879e+01 1.712111558087560752e+02
34 3.881928396681708193e+01 1.79459659781927962e+02
35 1.982793868143741671e+01 1.845118060871293721e+02
36 3.118524101800569781e+01 1.636248014144912872e+02
37 2.005698608291917395e+01 1.803034695205161881e+02
38 2.700274799779473511e+01 1.792502475568811064e+02
39 2.506227027010324448e+01 1.762586026486706032e+02
40 1.907377592749981196e+01 1.826560104477087145e+02
41 2.528781623067084183e+01 1.8837580775253261e+02
42 3.232888827510984697e+01 1.767863031548815229e+02
43 2.209651833311454183e+01 1.746617964376699206e+02
44 3.087017061896954573e+01 1.780176276478124180e+02
45 2.20465169371339087e+01 1.927466639363435377e+02
46 2.34704781115108162e+01 1.88940065120515144e+02
47 2.185924634187936633e+01 1.729108385149218358e+02
48 1.808735582805482878e+01 1.719105999524765604e+02
49 1.84475433454114105e+01 1.694675852134845400e+02
50 2.817410966513331855e+01 1.715017351672584027e+02
51 2.532129998240179862e+01 1.79855640705599407e+02
52 1.10989511888699422e+01 1.824644193383422696e+02
53 3.185907680322551404e+01 1.759604448214206229e+02
54 2.969165277770446210e+01 1.875971336737983961e+02
55 2.787730255078729158e+01 1.757878208874049051e+02
56 2.591225877027716606e+01 1.601041967482410087e+02
57 2.498572495922823578e+01 1.721740687961011247e+02
58 2.290736984087771041e+01 1.749157042606373400e+02
59 3.372475127822451876e+01 1.9064072787448299058e+02
60 2.607195861993280062e+01 1.727834180024526347e+02
61 2.600320546710192460e+01 2.021277060723097918e+02
62 2.491918989168637566e+01 1.768863549264245886e+02
63 3.373797890024456163e+01 1.7264789994461313098e+02
64 2.650983933678821103e+01 1.782204896060512169e+02
65 1.908717367205185766e+01 1.817607063871927551e+02
66 2.629780828398855164e+01 1.801754036532959162e+02
NORMAL | master$ git checkout code/examples/X.txt
NERDTreeToggle
```

Input data.

Regression : raw ouputs

```
1 1.618446082230515028e+01
2 1.186648764508175882e+01
3 1.464773565654695806e+01
4 1.634498113765004490e+01
5 1.745913980223237516e+01
6 1.166095693440647096e+01
7 1.520870379572047604e+01
8 1.406742858858113319e+01
9 1.280786198800906753e+01
10 1.455705638818248104e+01
11 1.659472777971285644e+01
12 1.545656976520241521e+01
13 1.400667994864794963e+01
14 1.316859968706612349e+01
15 1.850669481499744739e+01
16 1.522353555851539397e+01
17 1.357865817589575563e+01
18 1.575478790439513865e+01
19 1.151989857308148757e+01
20 1.3660895981731065622e+01
21 1.474667733562292504e+01
22 1.420670108820832667e+01
23 1.695499948932924639e+01
24 1.351075264826661382e+01
25 1.421153509268070181e+01
26 1.354265426599408409e+01
27 1.490759453066251261e+01
28 1.60713715989828758e+01
29 1.435965829372504032e+01
30 1.493929537374976135e+01
31 1.286585663123390688e+01
32 1.653170766752944110e+01
33 1.524065698484768028e+01
34 1.421366775637391555e+01
35 1.431635706484540194e+01
36 1.216972043271089277e+01
37 1.3332681272940485513e+01
38 1.628442909496436641e+01
39 1.491744545525017331e+01
40 1.392289095842998847e+01
41 1.237963466793929257e+01
42 1.454636430040251938e+01
43 1.391321928754086912e+01
44 1.517261623645199720e+01
45 1.417429098481692940e+01
46 1.430763524632289752e+01
47 1.426651768644284068e+01
48 1.485261785696788195e+01
49 1.470814688280185104e+01
50 9.800000000000000711e+00
NORMAL | masterE | github/code/examples/t1me.txt
:NERDTreeToggle
```

Output data.

Precision

Exercise 1 :

What order of magnitude of precision do we expect to obtain with this example ?

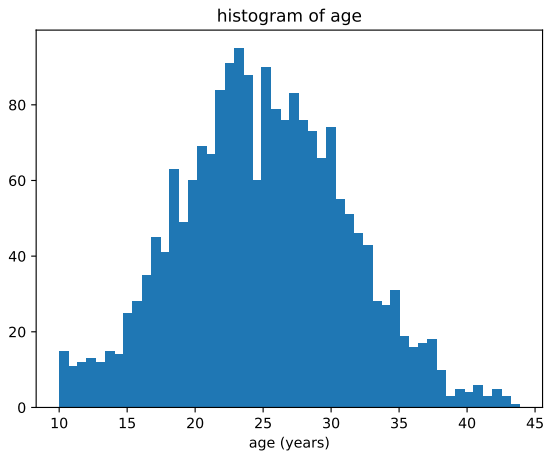
Precision

Exercise 1 :

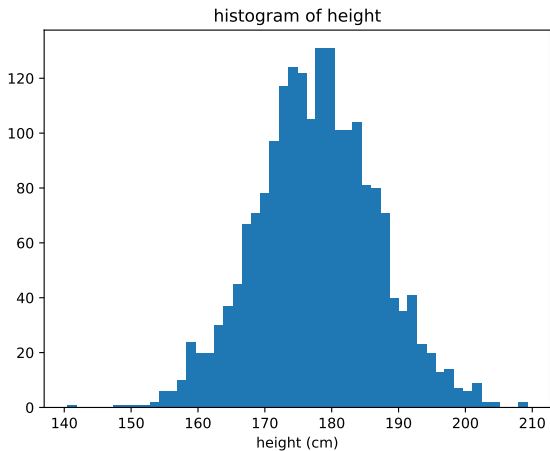
What order of magnitude of precision do we expect to obtain with this example ?

In a machine learning problem, there is (almost) always a statistical error associated to a prediction. Our goal is to minimize it !

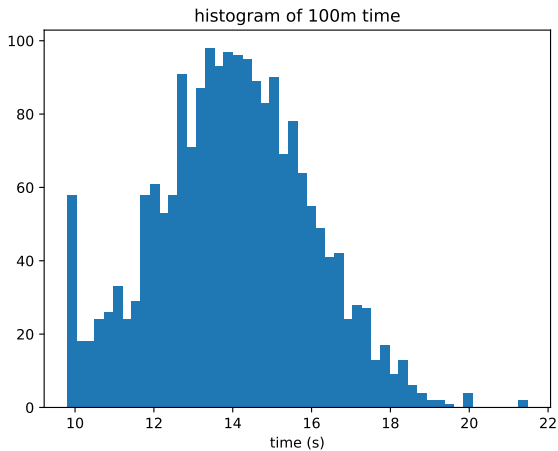
Histograms



Histograms



Histograms



Important question

We assume that there exists a relationship between the inputs x and the output y , given by some **unknown** function f .

$$y = f(x) \quad (2)$$

f is most of the time a function that contains some **randomness**.

- ▶ **Objective** : find a good **estimation** \tilde{f} , of f .
- ▶ \tilde{f} maps an input to an output, deterministically. For the input x_i , we predict $\tilde{f}(x_i)$.
- ▶ In order to measure the quality of \tilde{f} , we use **loss functions**.

Example loss function for a regression problem

- ▶ The loss function should be a measure of the discrepancy between our prediction and the correct label.
- ▶ For an individual sample, a discrepancy is the least-square loss

$$(\tilde{f}(x_i) - y_i)^2 \quad (3)$$

Loss function

- ▶ Taking into account the whole dataset, the **loss function** writes :

$$\sum_{i=1}^n (\tilde{f}(x_i) - y_i)^2 \quad (4)$$

- ▶ Several other loss functions are possible :

$$\sum_{i=1}^n |\tilde{f}(x_i) - y_i| \quad (5)$$

Loss function

- ▶ The loss function is a **real number** measuring the relevance of a **collection** of parameters (\tilde{f} is defined by these parameters.)
- ▶ The number of parameters depends on the situation, and varies between 1 (e.g. for a simple linear model) and millions (e.g. for some deep neural networks).

Important question II

- ▶ To what subset of functions does \tilde{f} belong?

More supervised learning examples : I

Predict the winning team of an NBA game at half-time.

- ▶ Dataset : 15 years of games (comments, text) : approximately 17000 games.
- ▶ The dataset is preprocessed to have as an input a time-series : each time contains the score **and** 10 technical features (rebounds, etc.). So for each time the dimension is 11. Each game is a matrix of size 1440×11 , reorganized as a line vector.
- ▶ Output : Receiving team wins or loses (classification)
- ▶ Evaluation metric : classification error ("0-1" loss).

Example II

Predict the quantity of oil in a rock.

- ▶ Input : tomographic image of a rock.
- ▶ Output : material of the rock, average presence of residual oil in the rock (regression).

Example III

Detect issues in wind farms.

- ▶ Input : sensors on the wind turbine (wind direction, air temperature, electric tension, rotation speed, component temperature, etc.) as a time series. Each step represents 10 minutes (several years).
- ▶ Output : Power generated by the turbine (regression)
- ▶ Evaluation metric : MAE (mean absolute error).

Difficulties of machine learning

- ▶ hard optimization problem
- ▶ overfitting / statistical guarantees
- ▶ curse of dimensionality

Optimization problem

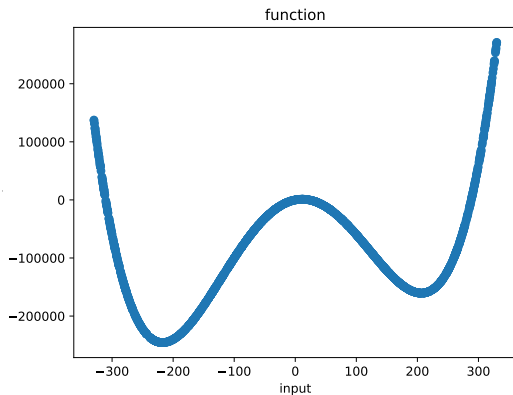
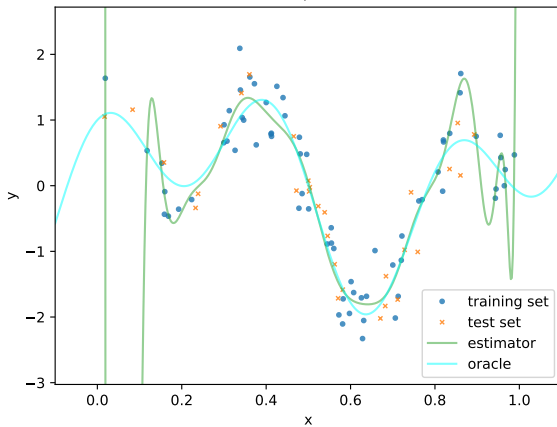


Figure – Loss function

Overfitting

Polynomial fit on training set, degree=22
train error $1.11\text{E-}01$, test error $7.83\text{E+}01$



Curse of dimensionality

Two numbers are important in machine learning :

- ▶ n : number of samples
- ▶ d : dimension (number of features) of a unique sample

Both can be large and prohibitive for some algorithms.

Curse of dimensionality

- ▶ n is large when the dataset has many samples.
- ▶ d is large if each sample has many features :
 - ▶ image
 - ▶ DNA sequence
 - ▶ text
 - ▶ audio/video file