Introduction to AI

Lecture for ASAO Workshop

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AI? What is it?

What for?
What types?

AI: our definition

Despite being present daily in media (even more since ChatGPT), AI often sounds like magic.
Our goal is to introduce some of its technical aspects to get a clearer view of what is AI.

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Our scope of AI

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A computer program able to autonomously react to a context to achieve a goal.

We will focus in particular on data-related AI: **machine learning**.

Controversies

In the media:

- + AI solves all problems: ecology, unemployment, etc.
- - AI is dangerous: "big data is watching you"
- - AI is not fair: biases

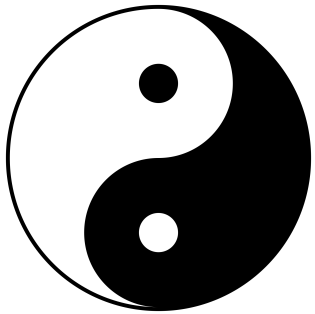
Interesting article about biases in The Consversation.

In the scientific community:

- + AI solves everything: you can predict anything if you have the data
- - AI does not explain anything: it's only black boxes

We will try today to get a fairer judgement on AI.

Impacts of AI in your field



What is the right place of AI?

Manichean views

Think in background of two examples of AI applications (can be softwares, proof of concepts, etc.), one you would characterize as an **opportunity**, the other a **risk** of using AI in your field.
What would be the **impacts** of using AI in your field, and more deeply, the downstream societal impacts.
Let's discuss it in 2h :)

Today's outline

- AI? What for? What types?
- Machine learning
  - Learn from experience (data)
  - Underfitting (beware of biases)
  - Overfitting
- Neural networks
  - Properties
  - Optimizing the loss
  - Architecture matters
- Timeline and future of AI
  - Biases
  - Ethics
  - Open problems

AI what for?

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- Operational (automation of tasks)
  - Robotics (self-driving cars)
  - Indexing images, tagging
- Modelling
  - Extraction of information
  - Prediction (extrapolate data)

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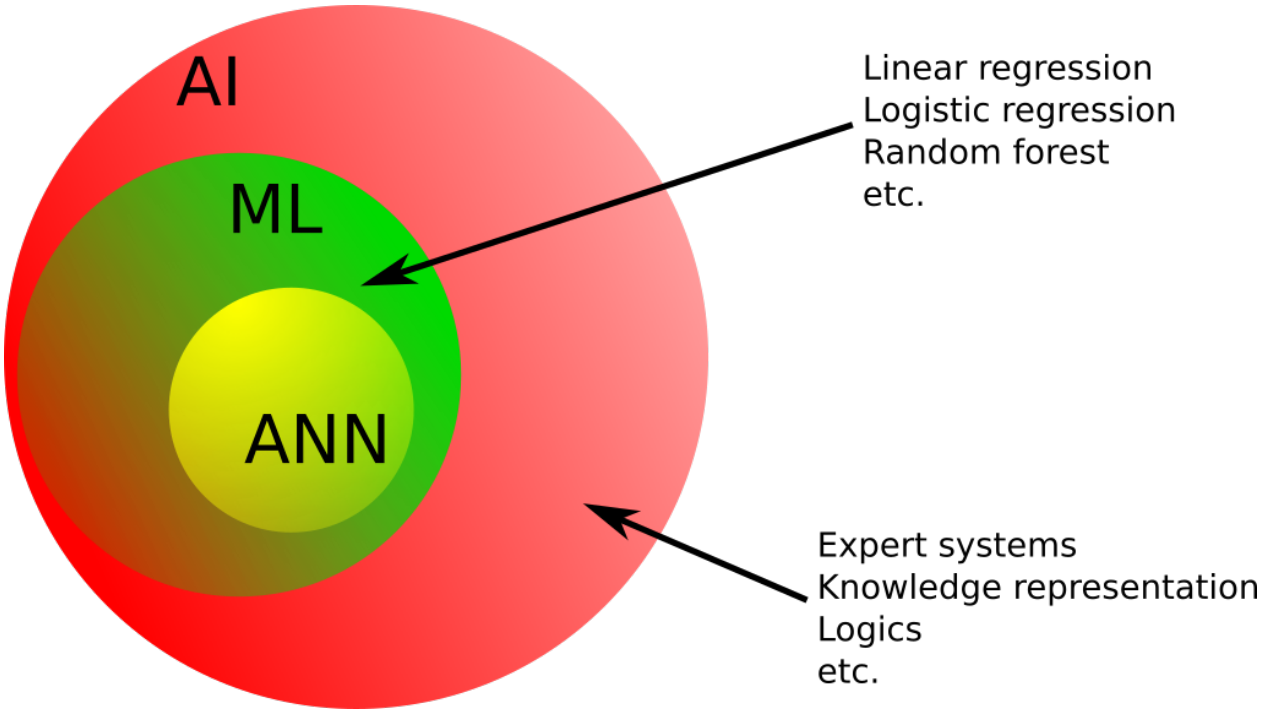
In both cases we are interested by the quality of the prediction, but may be also interested by bound guarantees and avoid "black-boxes".

AI taxonomy



We will focus on the *data science* part of artificial intelligence : **machine learning** and in particular **Artificial Neural Networks (ANN)**.

Lot of machine learning methods

There are many machine learning methods, some you already know. A unified library for implementation of many of these methods is Scikit-Learn.

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For classification tasks:

- Linear Discriminant Analysis (LDA)
- Logistic regression
- Support Vector Machine (SVM)
- Random forests
- Artificial neural networks

For regression tasks:

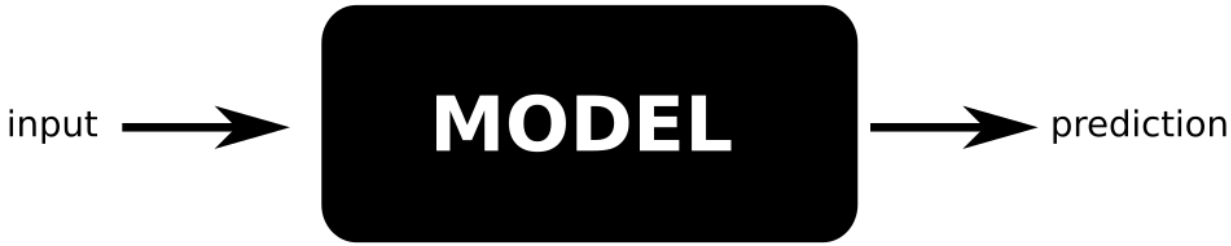
- **Linear regression**
- Regressive artificial neural networks

But also include parts of symbolic AI:

- Grammar inference
- Logic rule inference

Machine learning

Machine learning



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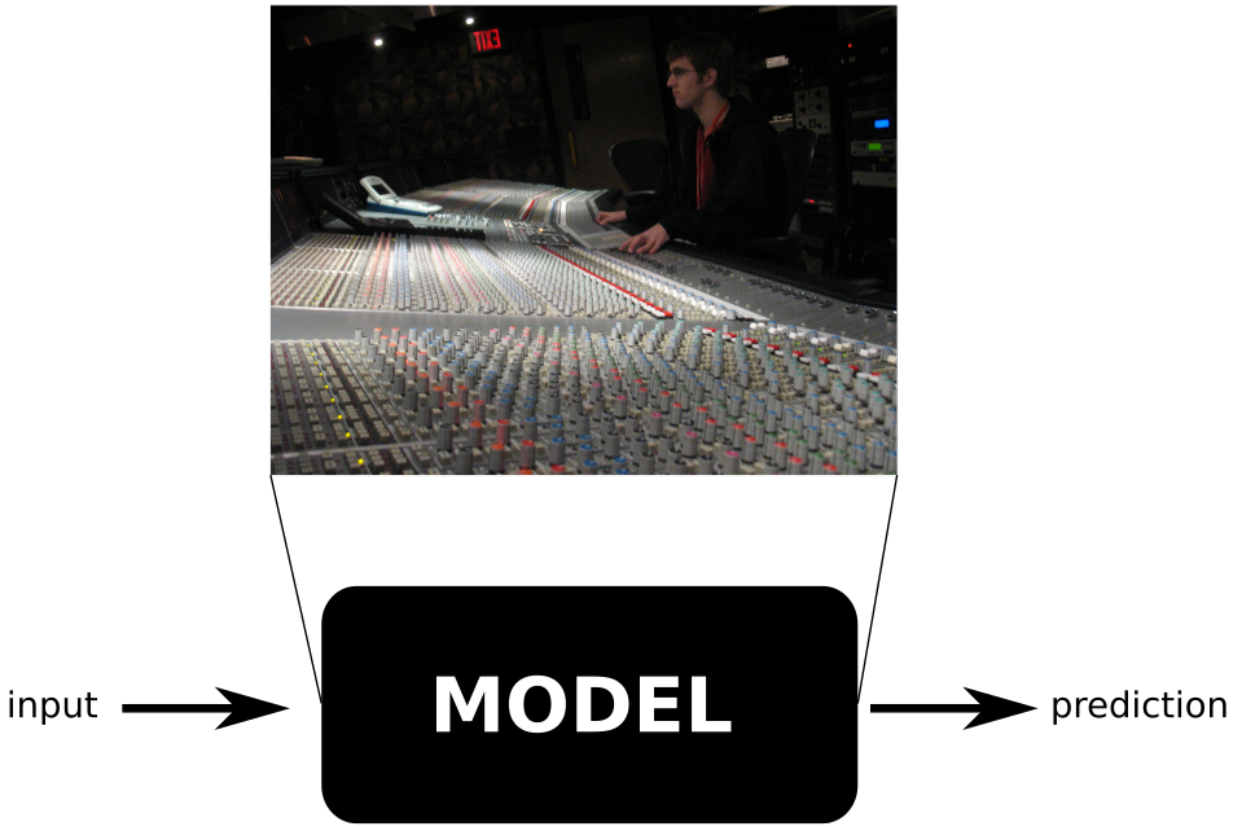

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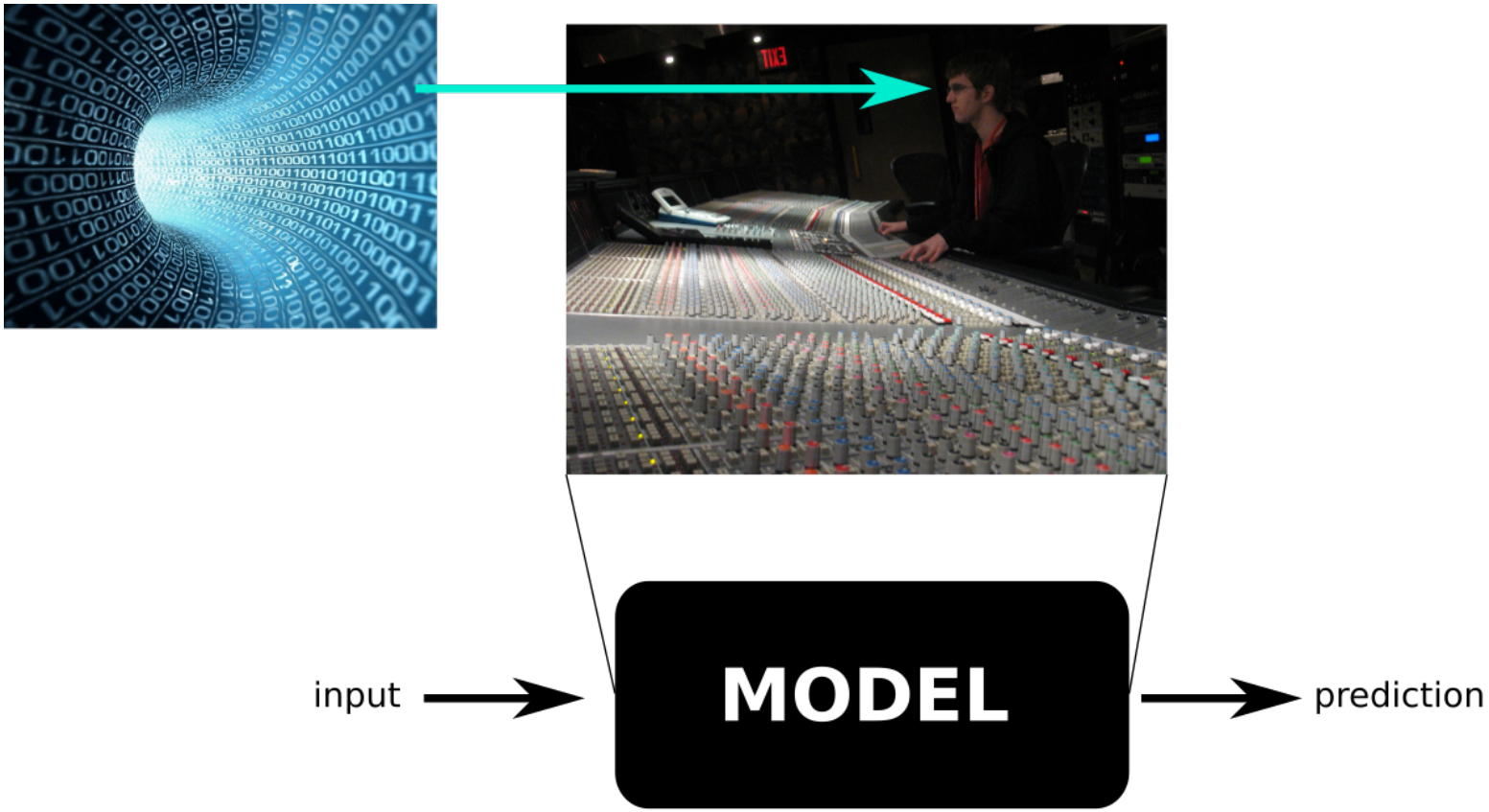

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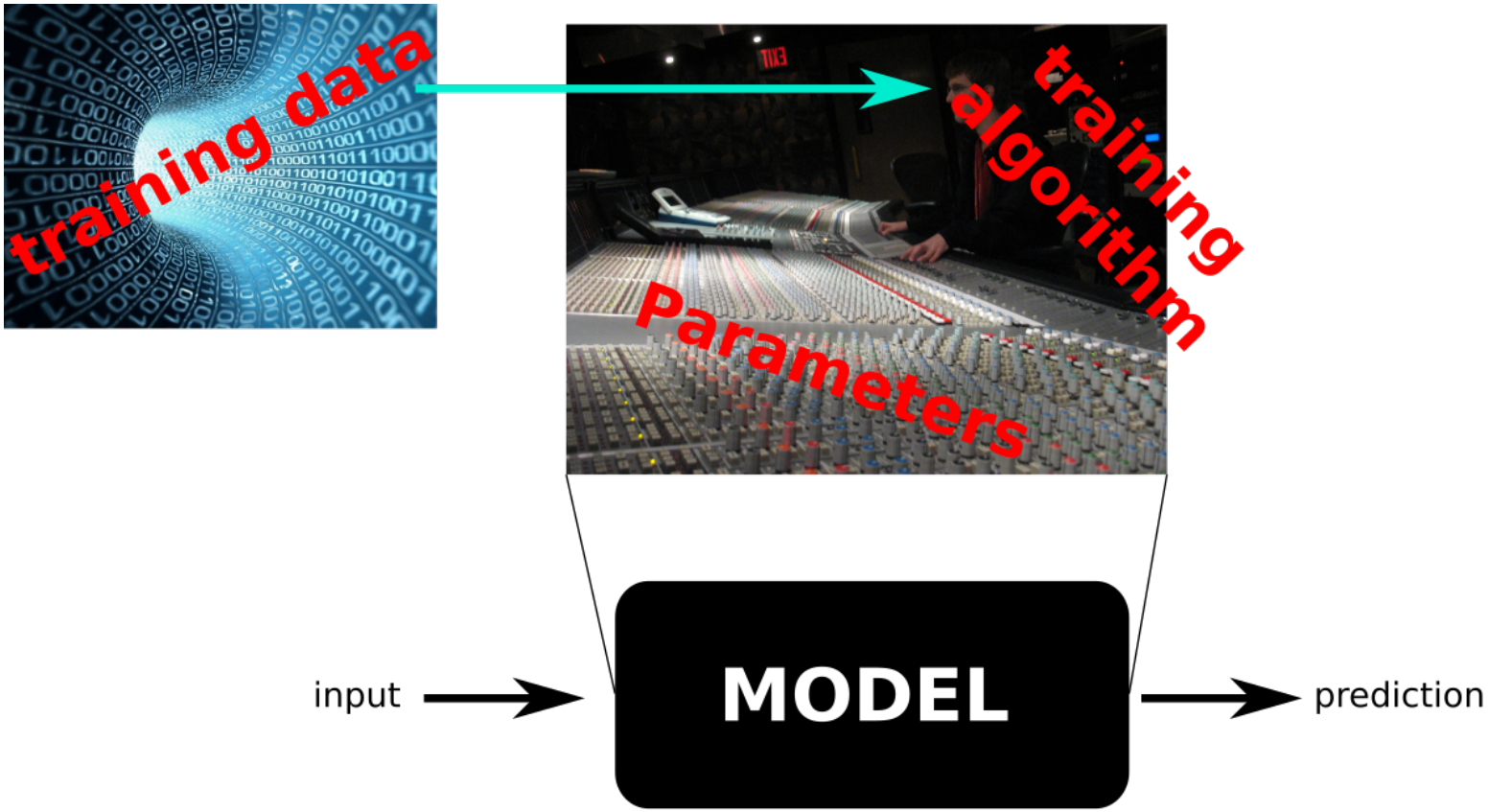

Some order of magnitude: number of parameters

Let's simplify: consider binary parameters (0/1). With N parameters, how many possible combinations?

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How it is possible to train such a model?

[1] [Brown et al. 20]

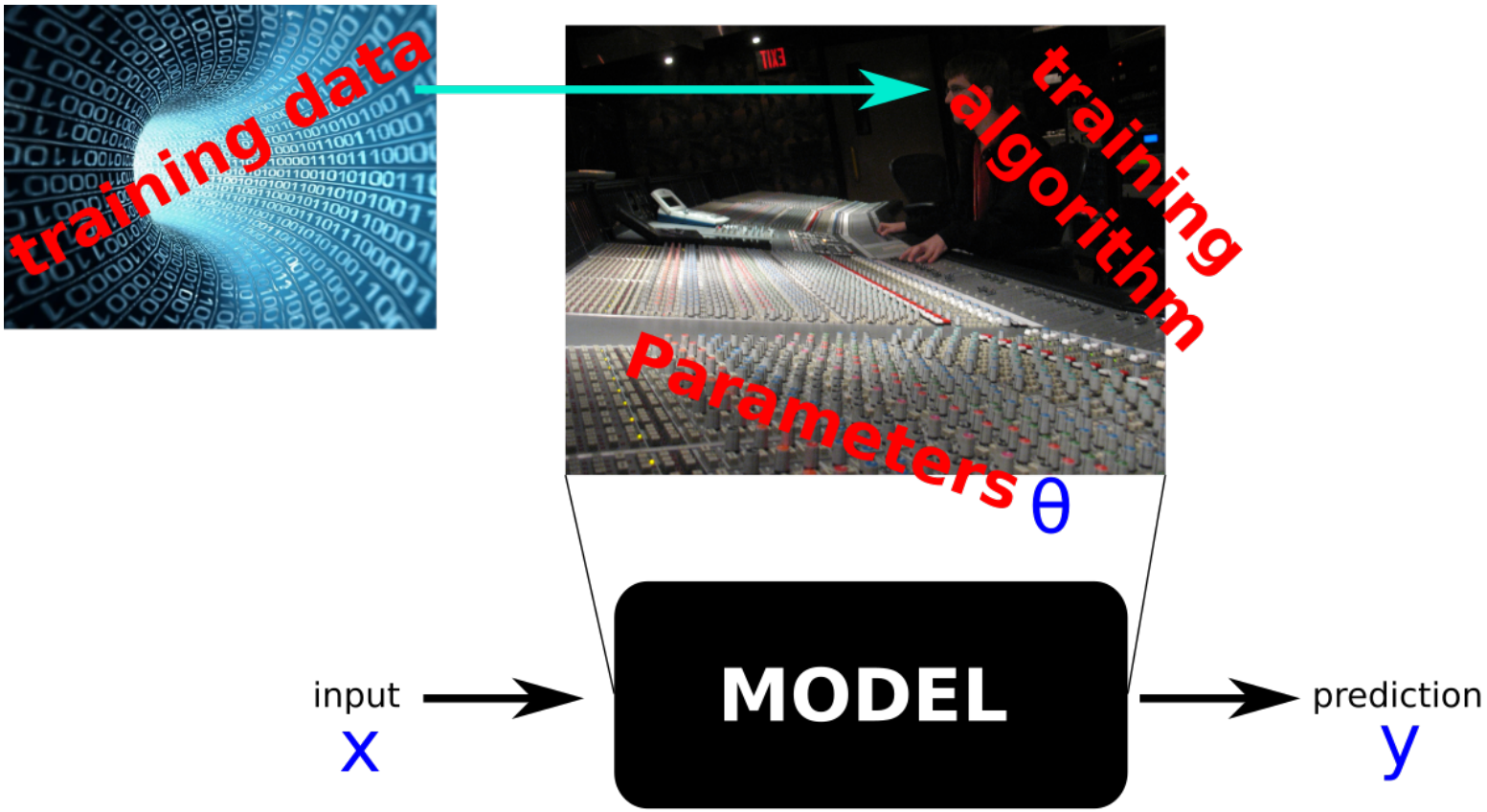
Some order of magnitude: training data

- Recent GPT-3 NLP (Natural Language Processing) model: trained on a corpus of 300B tokens ($\approx 1TB$).

Dataset	Quantity (tokens)	Weight in training mix	Epochs elapsed when training for 300B tokens
Common Crawl (filtered)	410 billion	60%	0.44
WebText2	19 billion	22%	2.9
Books1	12 billion	8%	1.9
Books2	55 billion	8%	0.43
Wikipedia	3 billion	3%	3.4

- Open Image Dataset V6 (18TB):
  - 9M images
  - 2M with labels from 600 classes

Training ML models



What training data?

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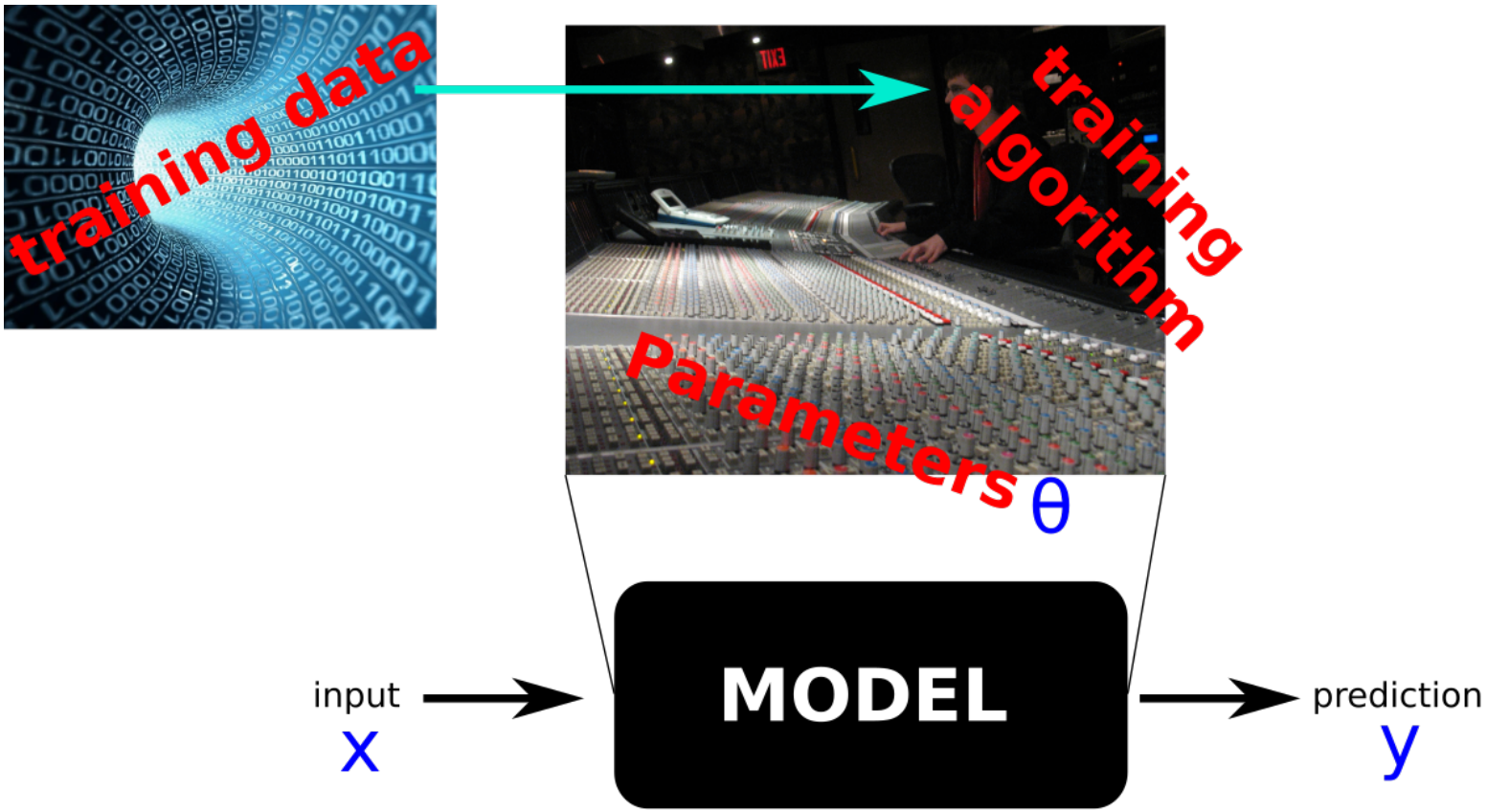

What training data? Observations of (x, y):
$(x_1, y_1), ...(x_T, y_T)$

Worked-out example

You want to know what is the fuel consumption of this car at 180km/h.

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You want to know what is the fuel consumption of this car at 180km/h.

Problem

You **cannot measure it**, because either:

- You don't feel like it  (operational)
- Nobody will do it  (modeling)

What to do?

What to do? Make a model :) !

Worked-out example: choose the model

We want to model the **fuel consumption** y (L/100km) with respect to the **car speed** x (in km/h).

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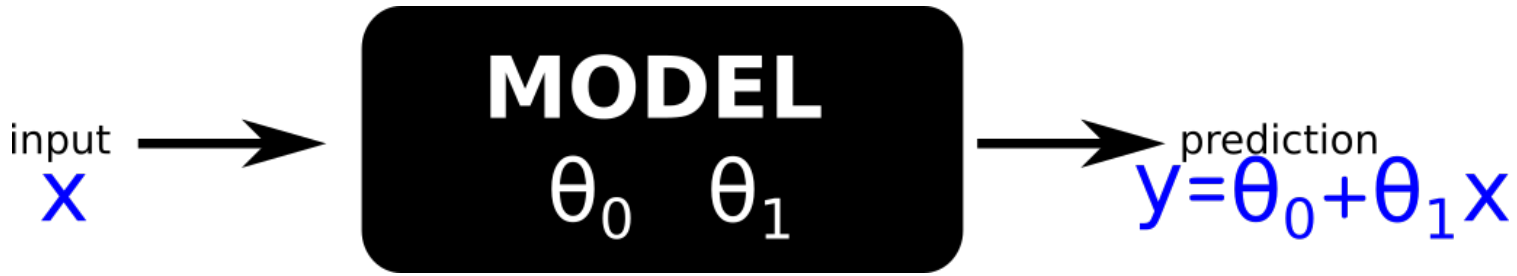

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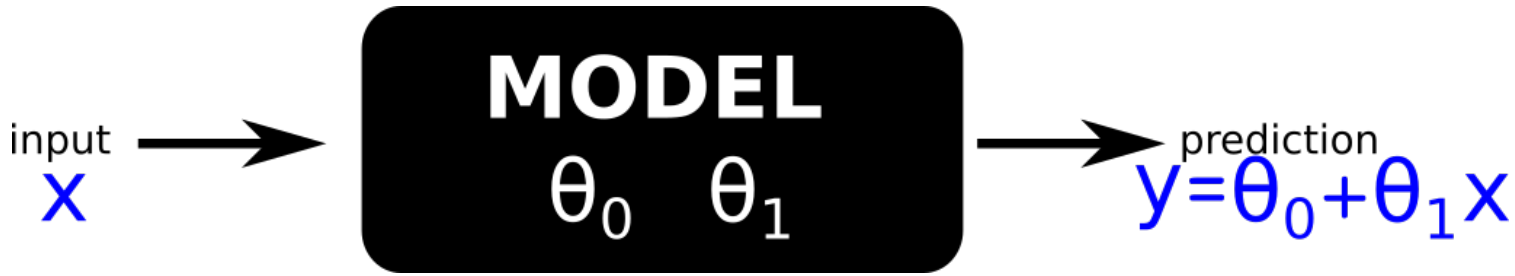
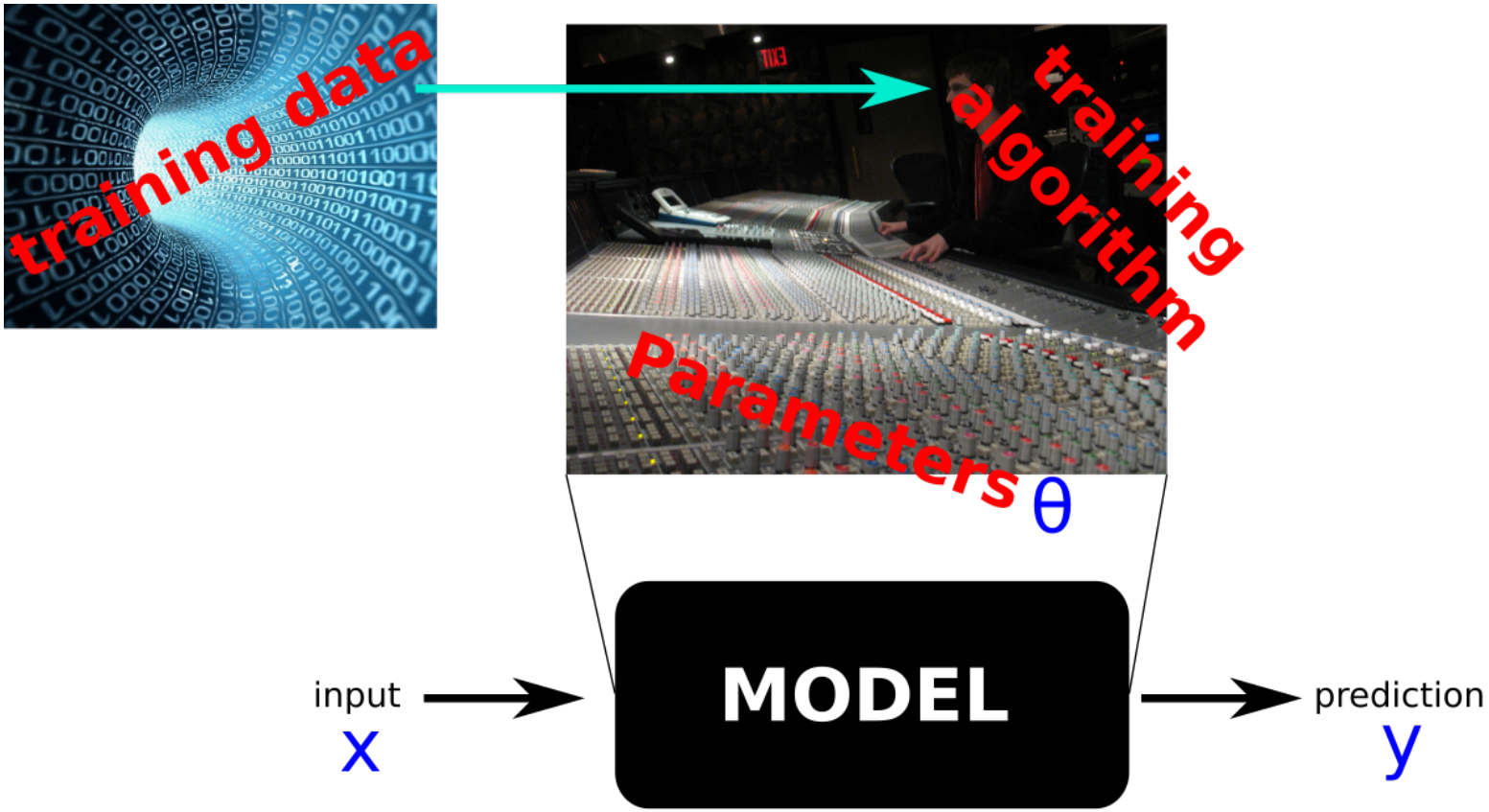


Need to find the right θ_0 and θ_1.
We say we need to **fit** the model.

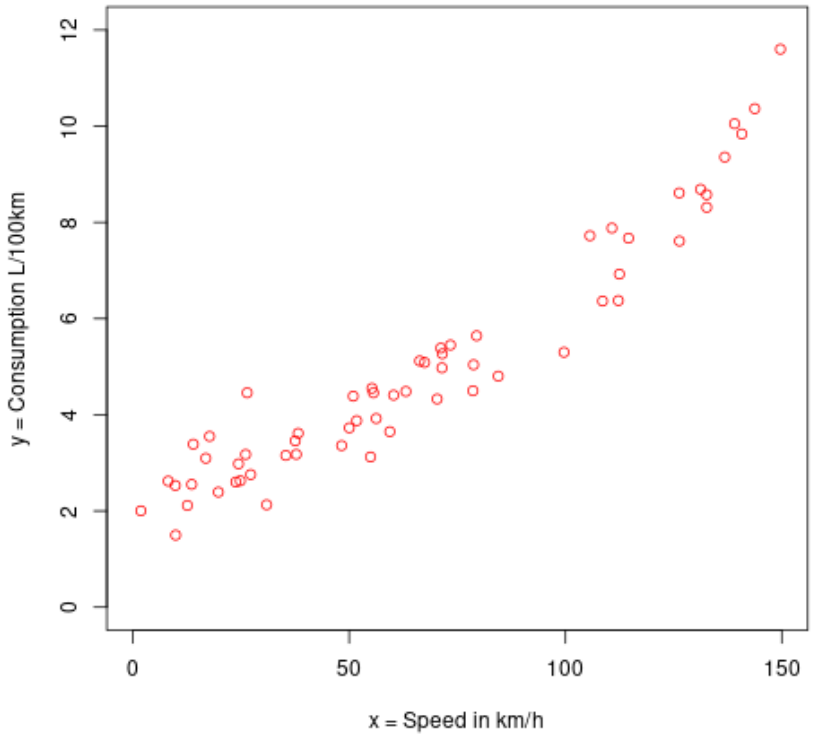
Worked-out example: fitting



Worked-out example: the training data

Your neighbor, gives you her home-made measurements.

It consists in $(x_i, y_i), i = 1, ..60$



Worked-out example: fitting the model

Goal: find optimal θ_0, θ_1 such that:

$$y \approx \theta_0 + \theta_1 . x$$

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Goal: find optimal θ_0, θ_1 such that:
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Goal: find optimal θ_0, θ_1 such that:
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More formally, θ_0, θ_1 such that

$$\mathcal{L}(\theta_0, \theta_1) = \frac{1}{60} \sum_{i=1}^{60} [y_i - (\theta_0 + \theta_1 . x_i)]^2 \quad (1)$$

is **minimal**.

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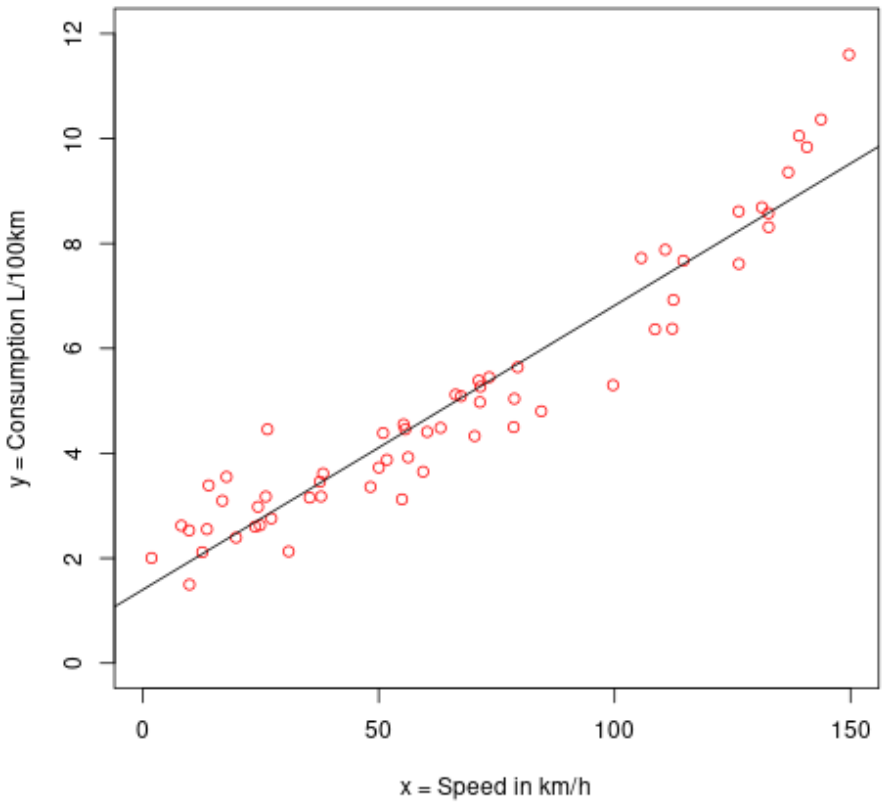
Definition

$\mathcal{L}$ is called a **loss function** for the model[a].

[a] This one in particular is called the *mean squared error*

Worked-out example: the fit



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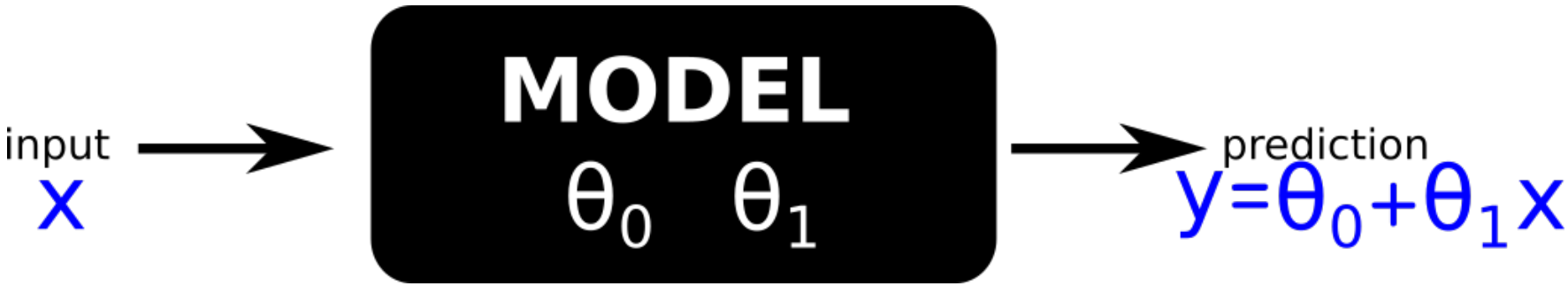

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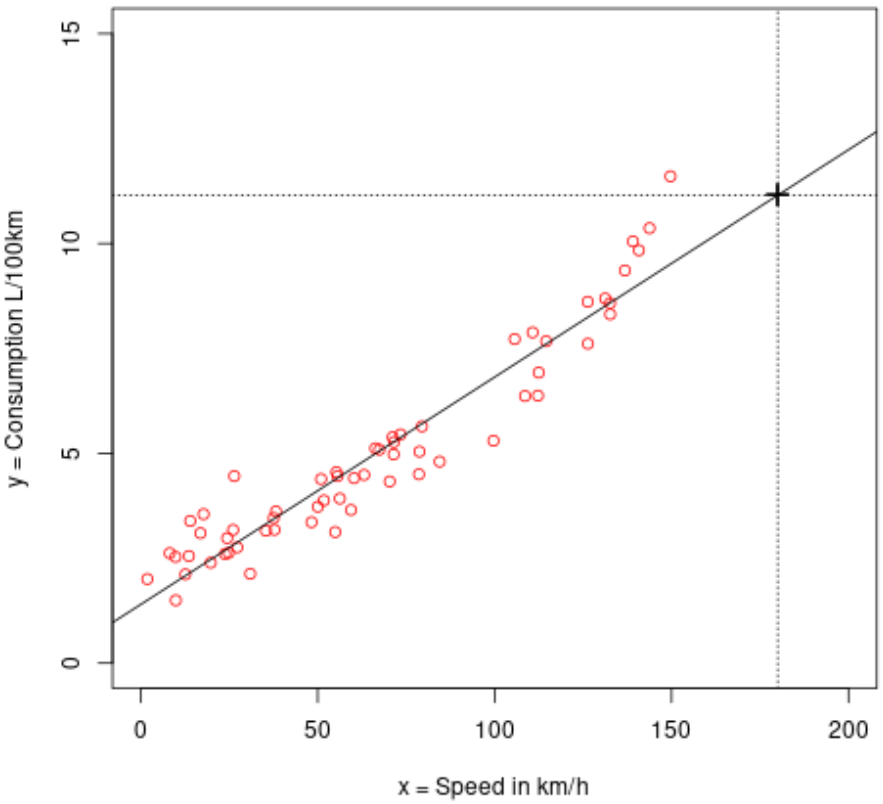
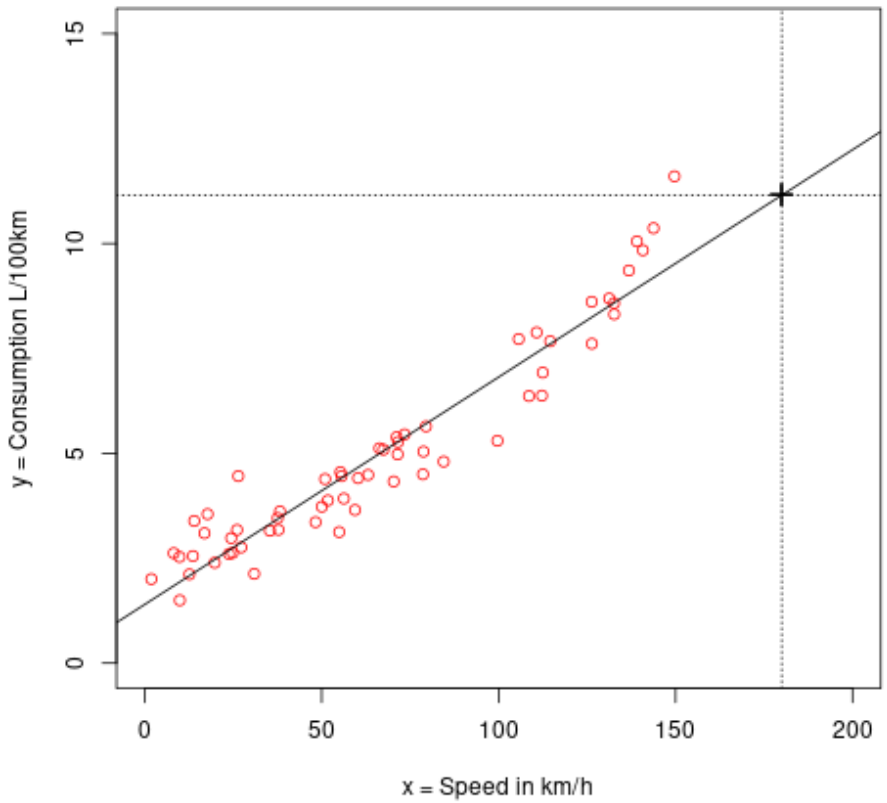


Worked-out example: toward more complex models



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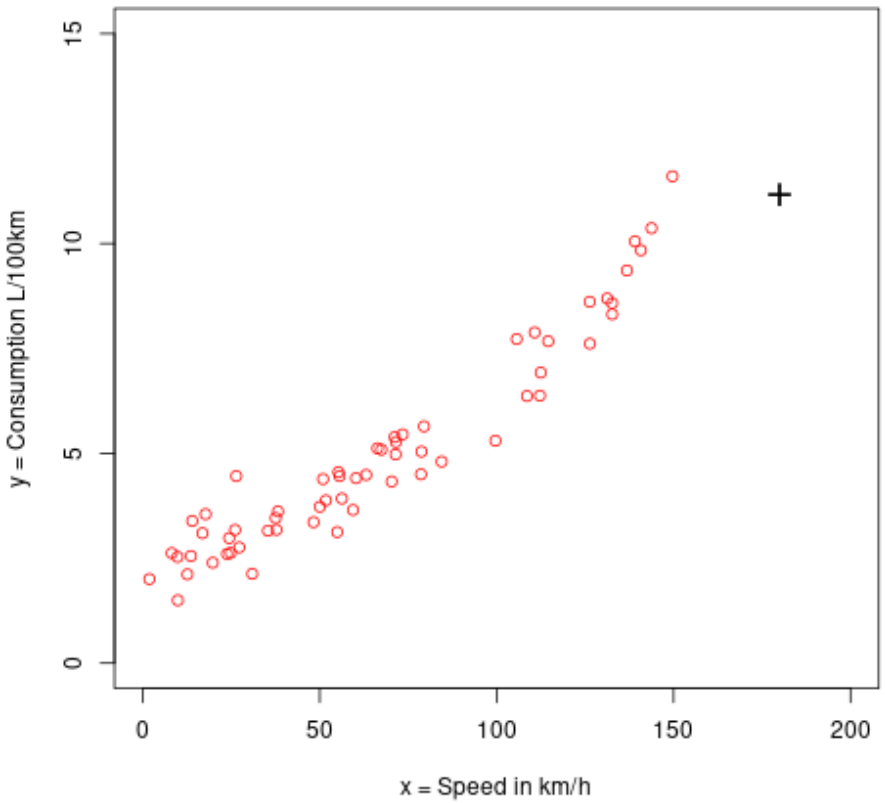

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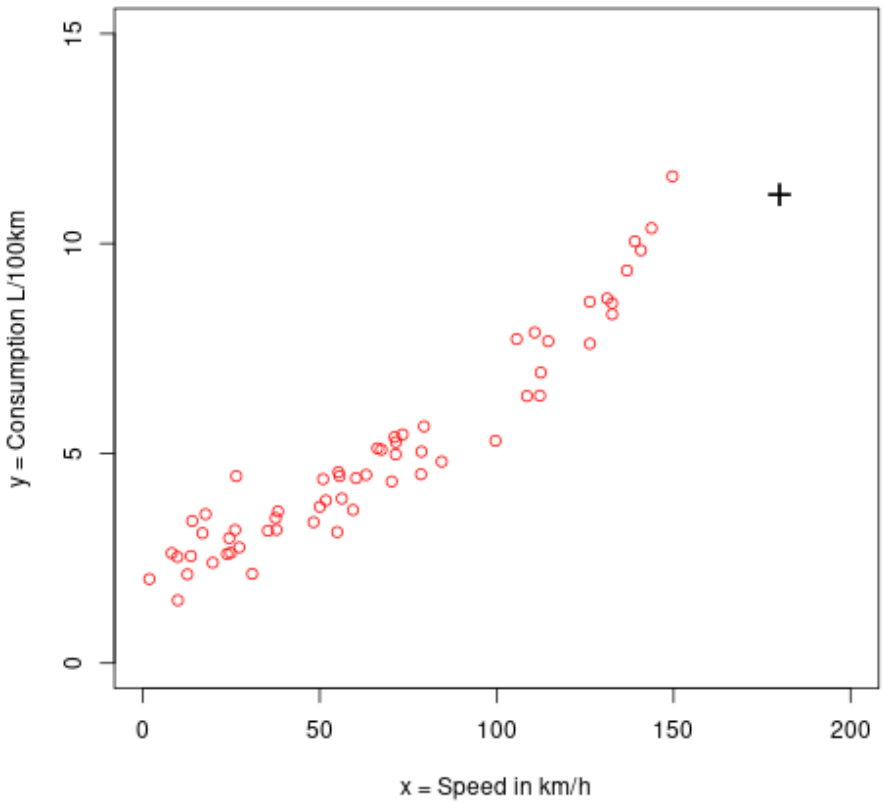

Any comment?

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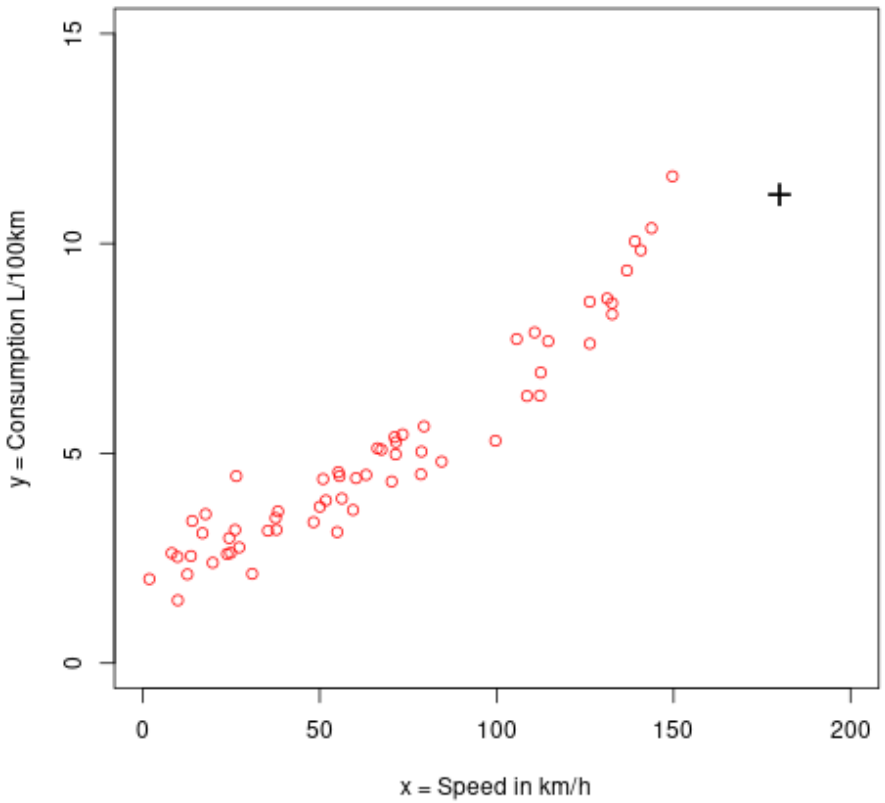

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This phenomenon is known as **underfitting**

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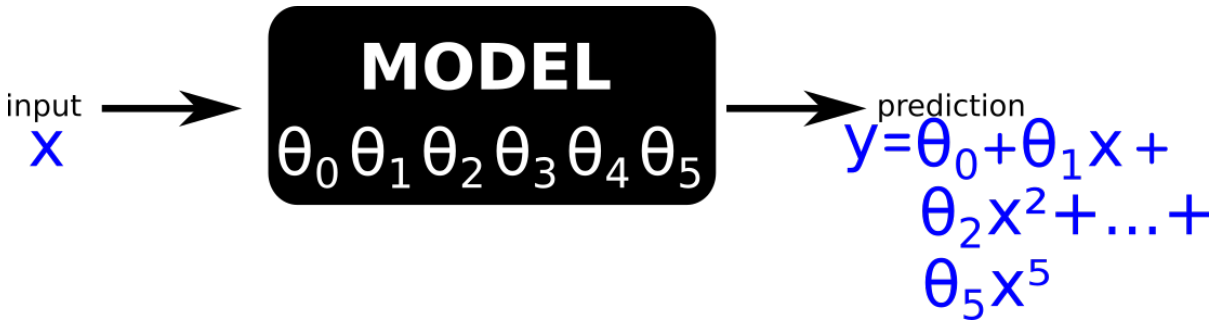

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$\theta_0, \theta_1 ..., \theta_5$ such that

$$\mathcal{L}(\theta_0, ..., \theta_5) = \frac{1}{60} \sum_{i=1}^{60} [y_i - (\sum_{j=0}^{5} \theta_j . x_i^j)]^2 \tag{2}$$

is **minimal**.

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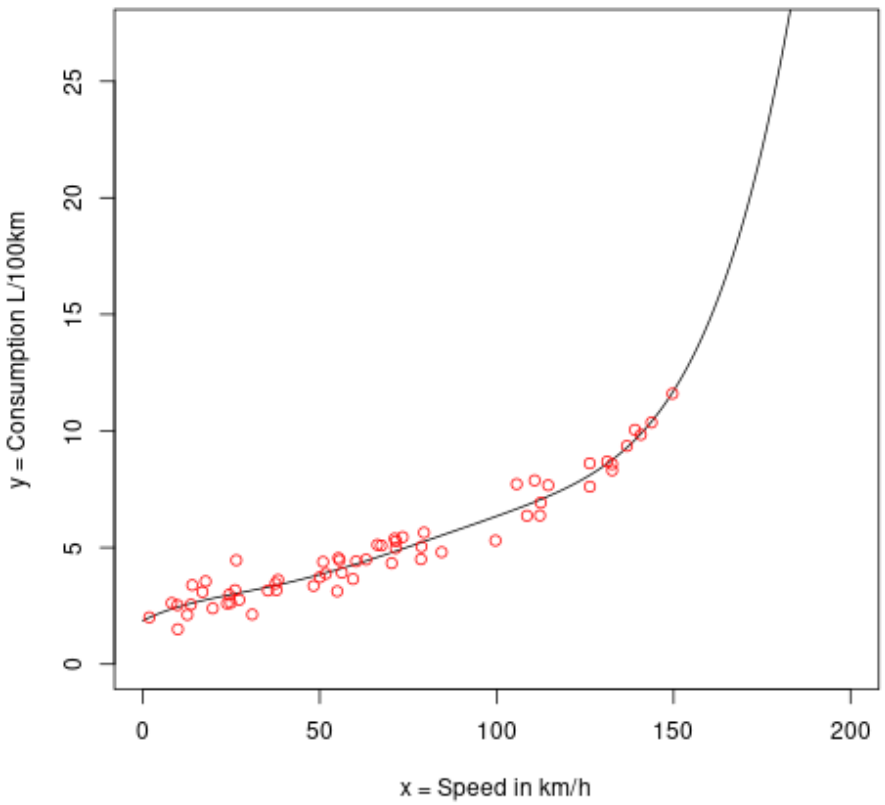

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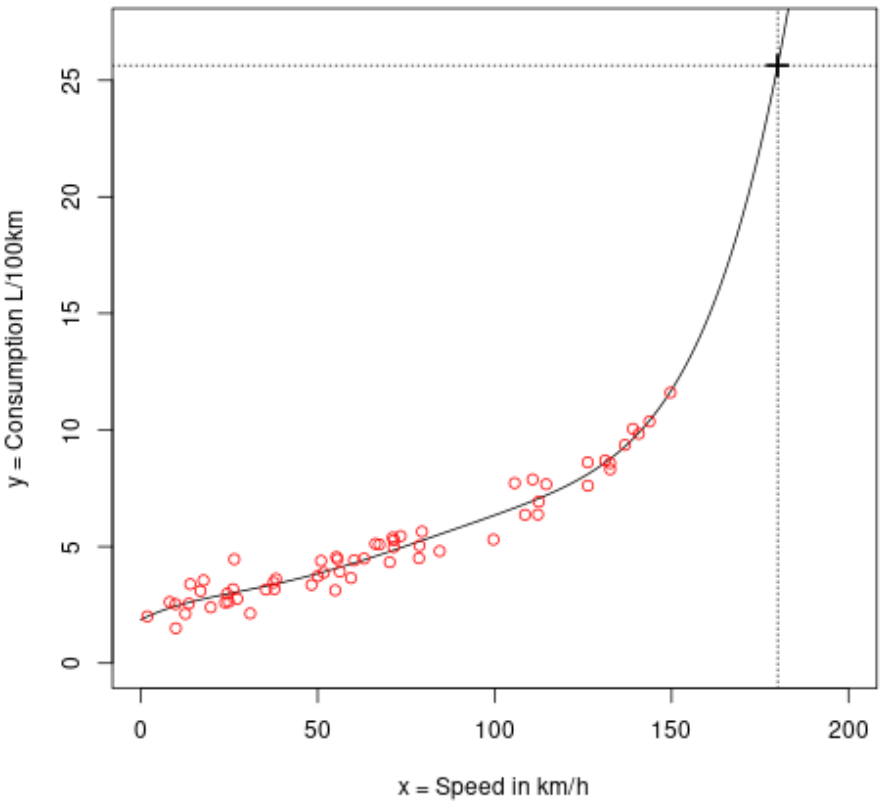

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Informal definition

We will say that the polynomial model of degree 5 is more **expressive** than the linear regression.

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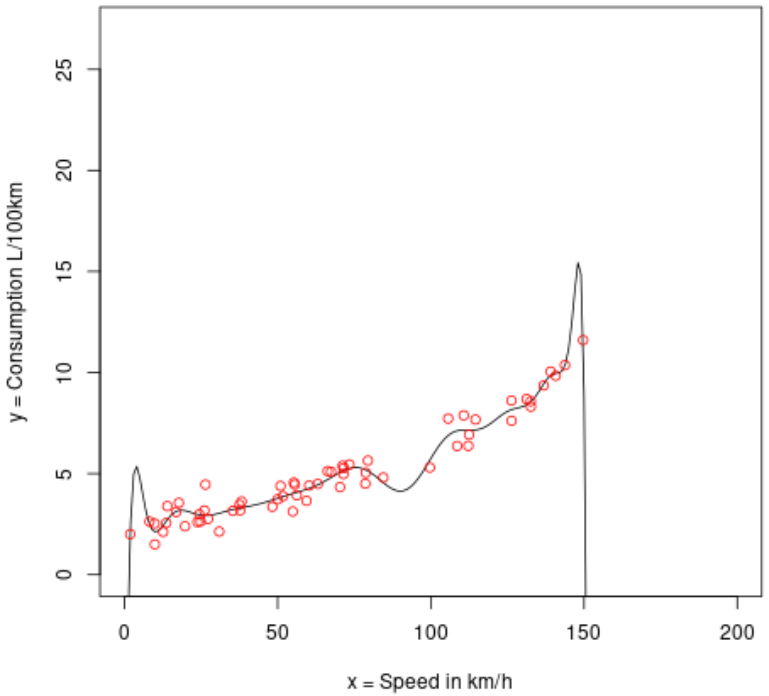
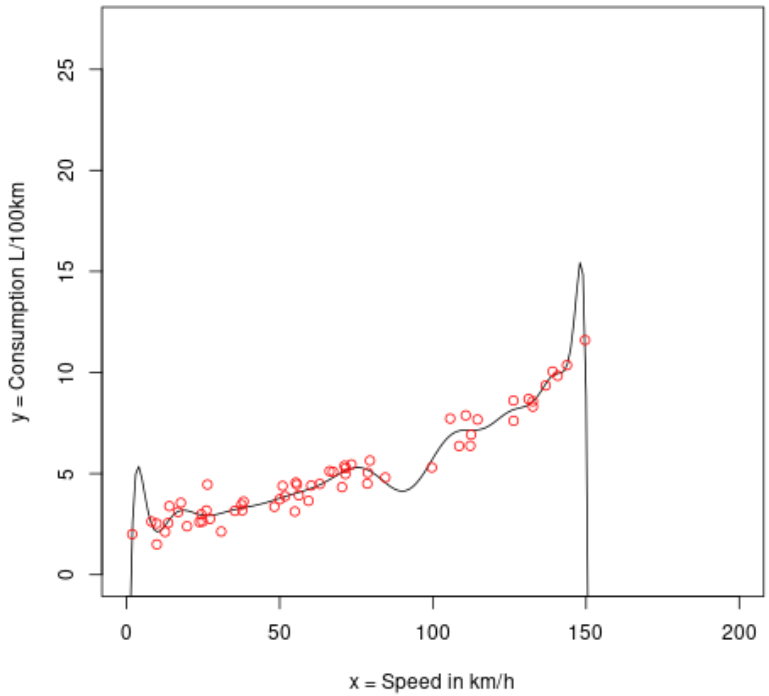


With 30 parameters: $\theta_0, ...\theta_{29}$

Parameters: the more the better?



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Definition

The phenomenon is called **overfitting**.

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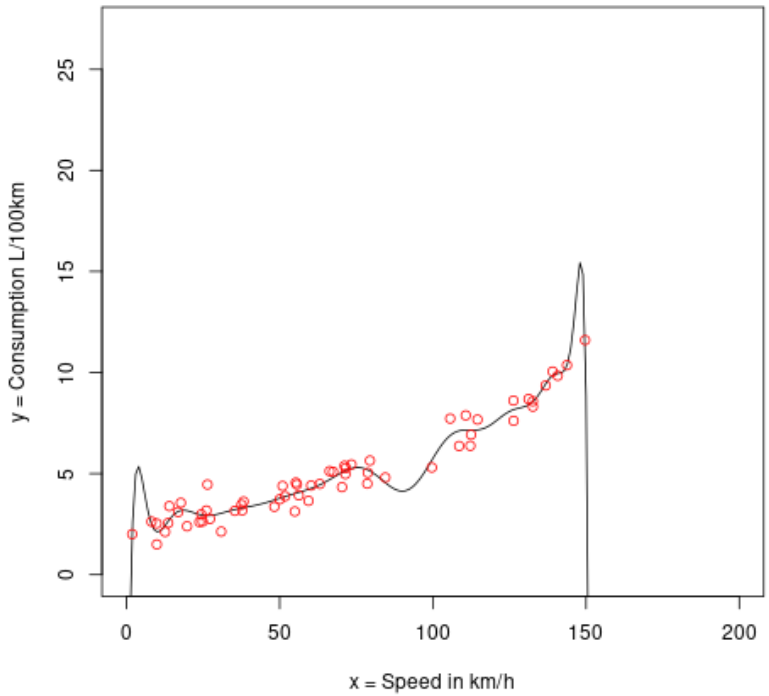

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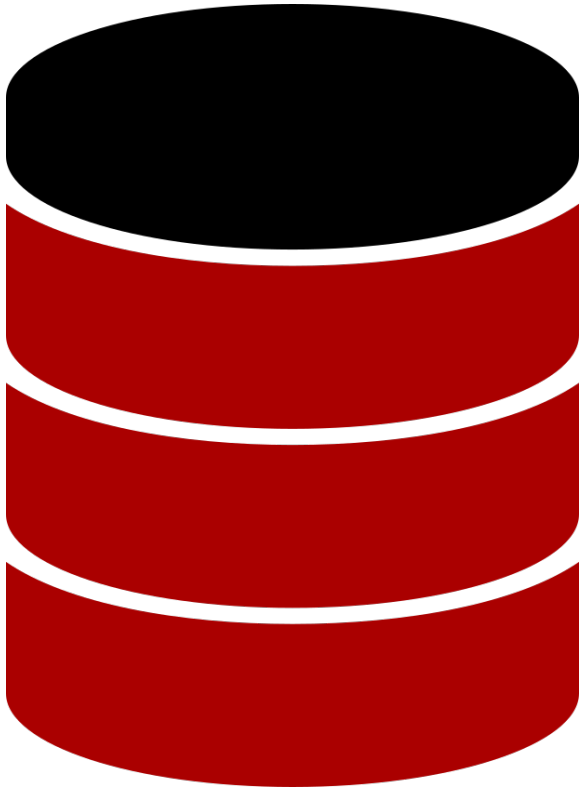
Definition

The phenomenon is called **overfitting**. Mainly happens because of **hyperparametrization**.

How to control overfitting?

Cross-validation to control overfitting



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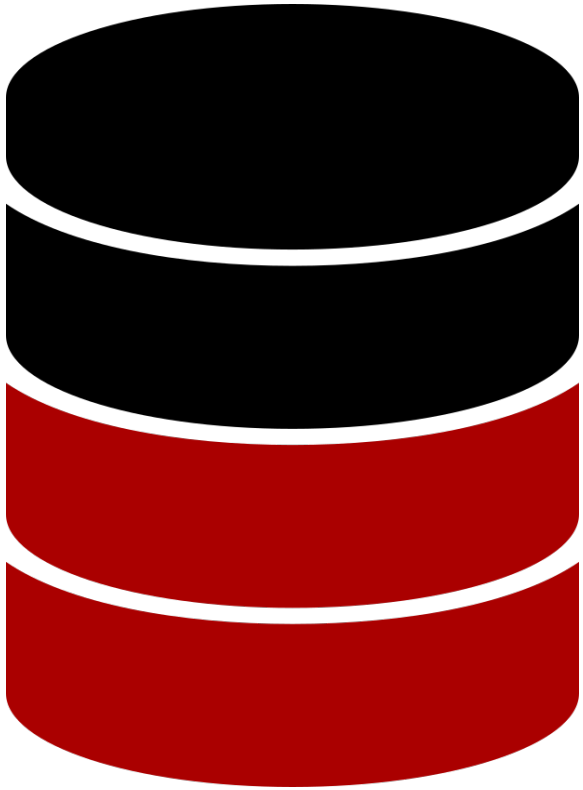

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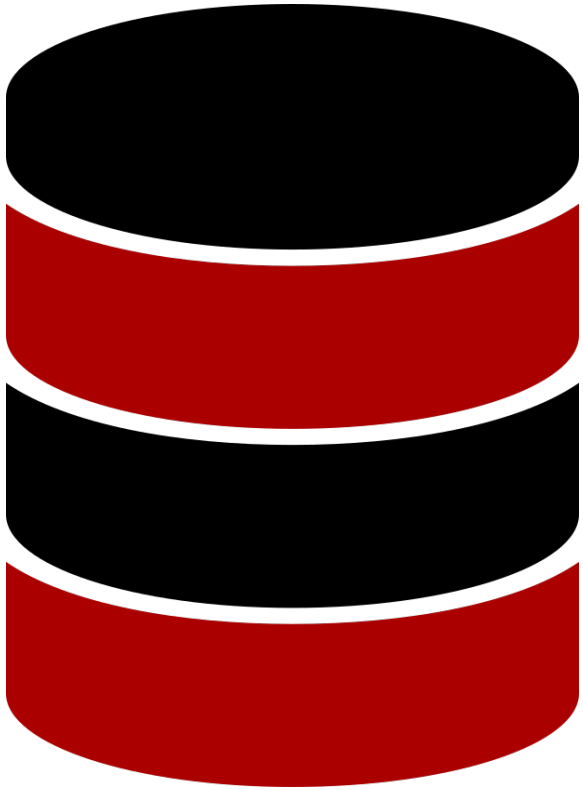

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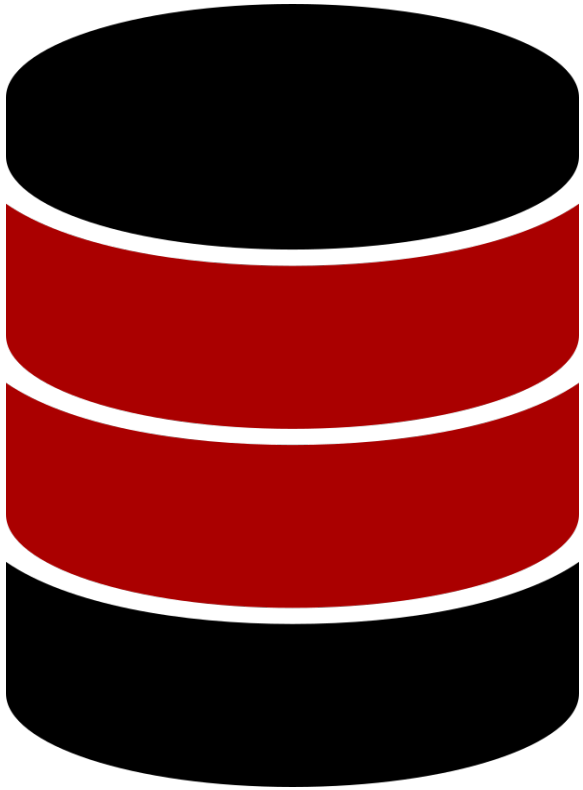
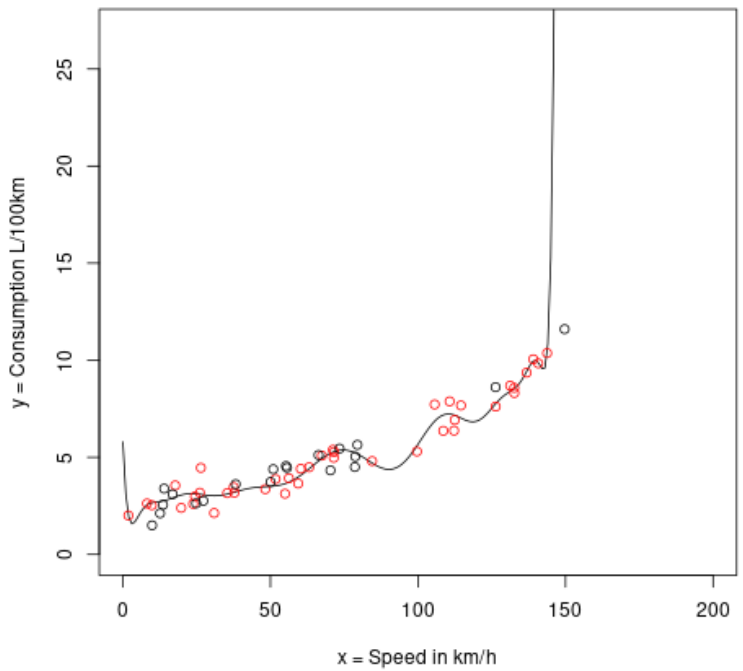


Cross-validation example: 30 parameters

Red: training set Black: validation set



30 parameters, fold 1

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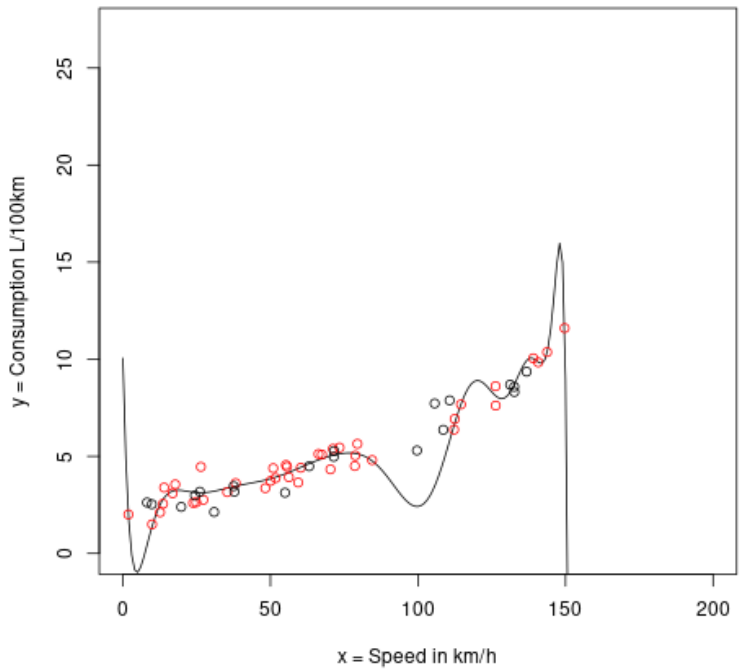

30 parameters, fold 2

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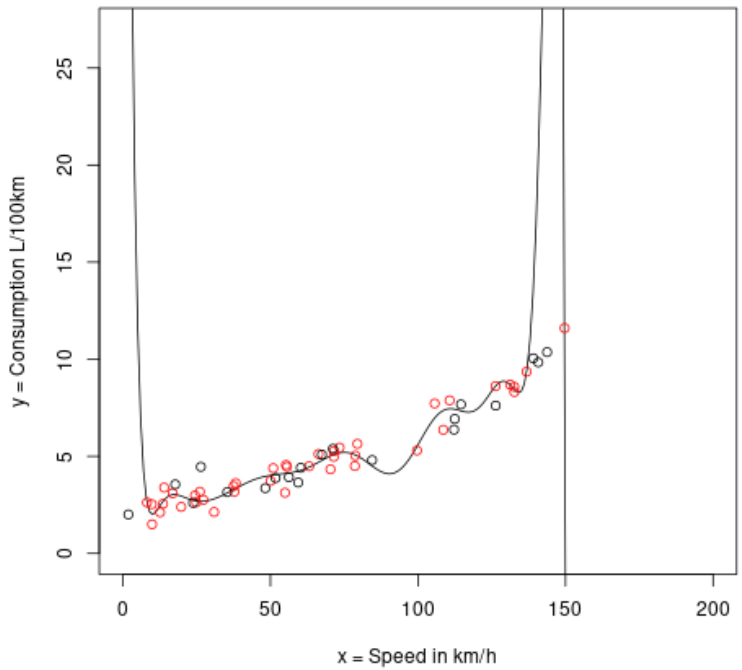

30 parameters, fold 3

Cross-validation example: 6 parameters

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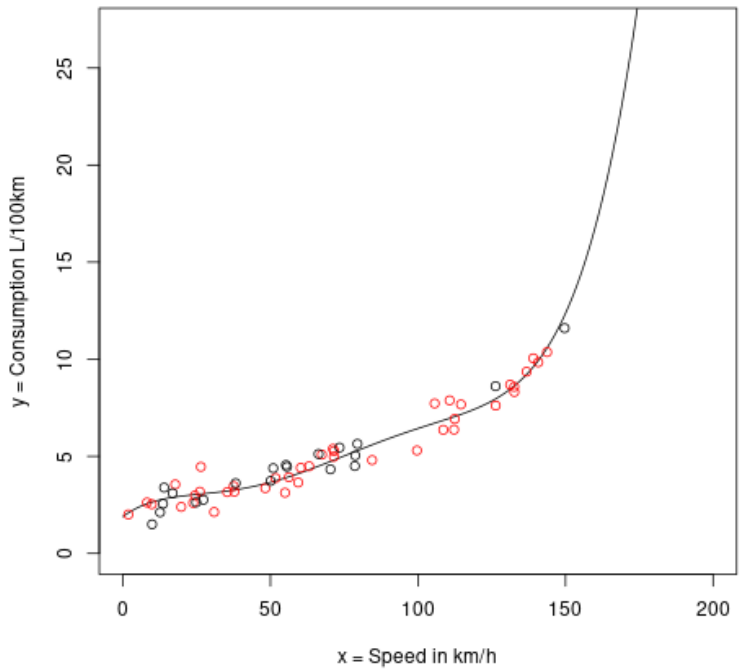

6 parameters, fold 1

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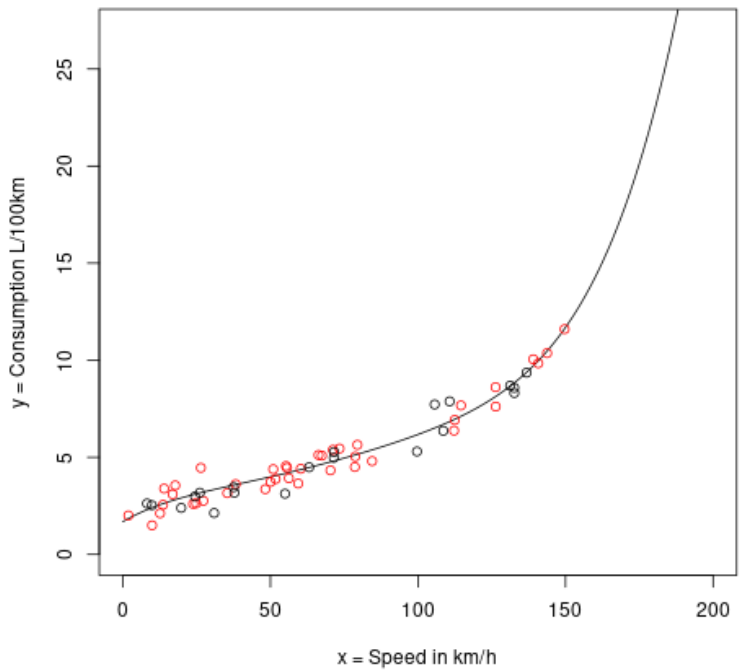

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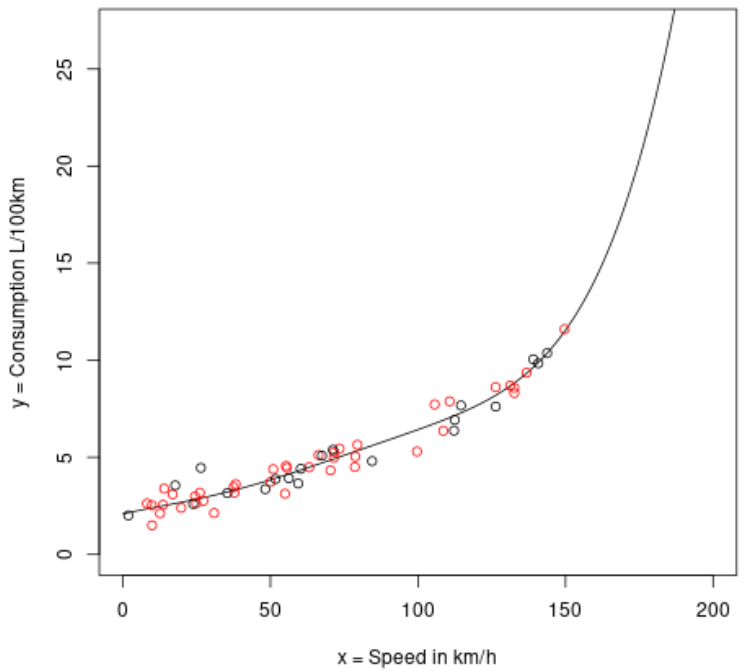

6 parameters, fold 3

What do you observe?

- Lower error on training with ___parameters
- If the error is on the validation is much higher than on training set, it means that the model ___.
- More variance among fits with ___parameters[2]

[2] As we will see, things are different with neural nets

What do you observe?

- Lower error on training with **more** parameters
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More specifically, one can decompose the error of the model as:

$$\begin{aligned}
\mathbb{E}[||y - \hat{y}||^2] &= \mathbb{E}[||y - \mathbb{E}[\hat{y}] + \mathbb{E}[\hat{y}] - \hat{y}||^2] \\
&= \mathbb{E}[||y - \mathbb{E}[\hat{y}]||^2] + 2 \times 0 + \mathbb{E}[||\mathbb{E}[\hat{y}] - \hat{y}||^2] \\
&= ||y - \mathbb{E}[\hat{y}]||^2 + \mathbb{E}[||\mathbb{E}[\hat{y}] - \hat{y}||^2] \\
&= \text{bias}^2 + \text{variance}
\end{aligned} \tag{2}$$

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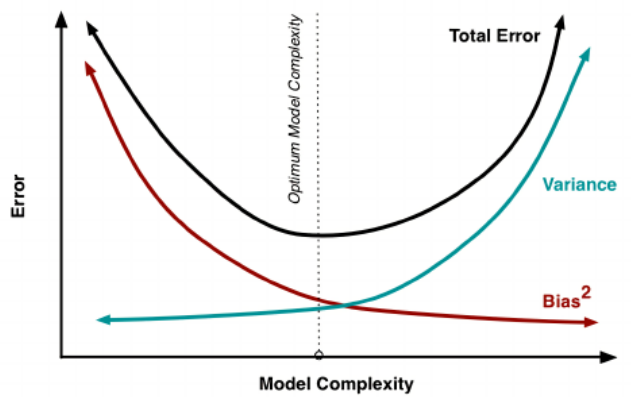
This is known as the **bias-variance trade-off**:



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Quizz - Checkpoint

- We ___ a model by minimizing its ___ function on a ___ set.
- A model can have billion of ___ which make it ___ to try out all combinations.

Quizz - Checkpoint

- We **fit** a model by minimizing its ___ function on a ___ set.
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Quizz - Checkpoint

- We **fit** a model by minimizing its **loss** function on a ___ set.
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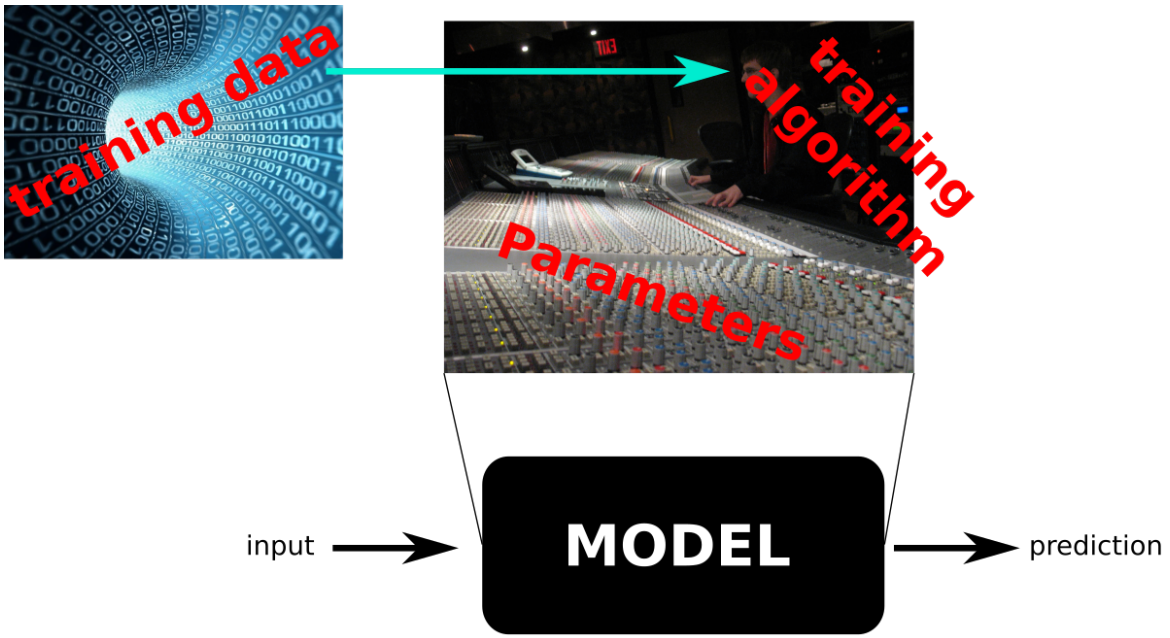

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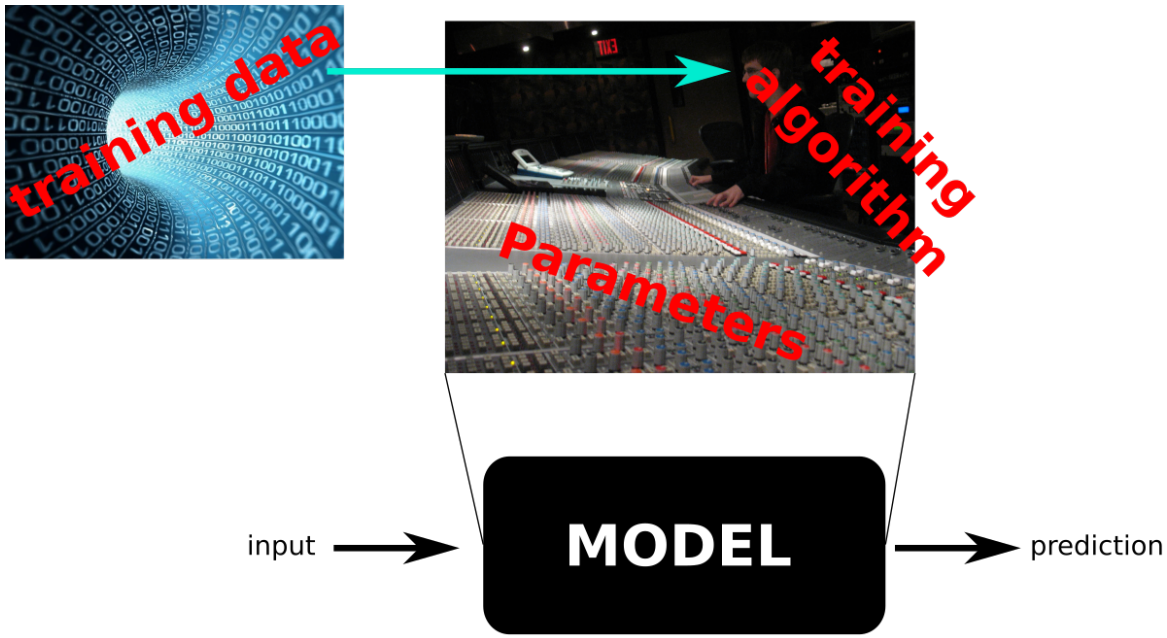

Remaining questions:

- What are the training algorithms?
- How is it possible to train with billions of parameters?

Learning the parameters

Learning algorithms

Of course...

Learning algorithm depends on the model to be fitted.

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Learning algorithm depends on the model to be fitted. But their job is to **minimize** a certain **loss**.

Learning algorithms

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Examples:

- Small discrete models: enumeration and pruning
- Analytic solution for the minimum (*e.g.* linear regression)
- Convex loss function $\rightarrow$ gradient descent methods
- EM algorithms
- etc.

Loss with billions of parameters and datapoints

We would like $\theta_0, \theta_1 ..., \theta_p$ such that

$$\mathcal{L}(\theta_0, ..., \theta_p) = \frac{1}{N} \sum_{i=1}^{N} [y_i - (\sum_{j=0}^{p} \theta_j . x_i^j)]^2 \tag{3}$$

is **minimal**.
One would like to find the minimum of this loss.

Issue: $p, n \sim 10^9$

- Cannot test every parameter combination
- Every computation of the loss is costly.

Thought experiment: how to minimize the loss

For a set of parameter $\theta_0, ..., \theta_p$, you can ask the value of the loss to a guru:

Exercise

What algorithm can you imagine to minimize the loss?

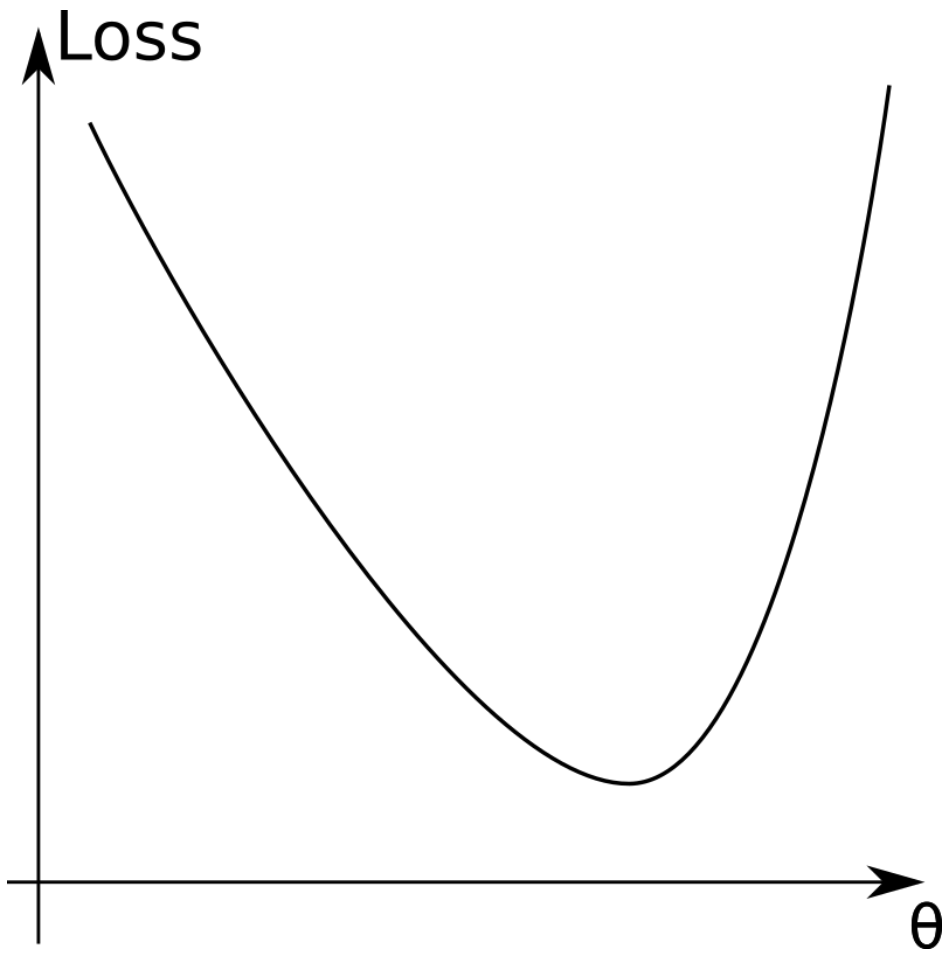
Thought experiment: how to minimize the loss more easily

For a set of parameter $\theta_0, ..., \theta_p$, you can ask the value of the loss **and** which θ_i to reduce or increase, in order to lower the loss. to a guru:

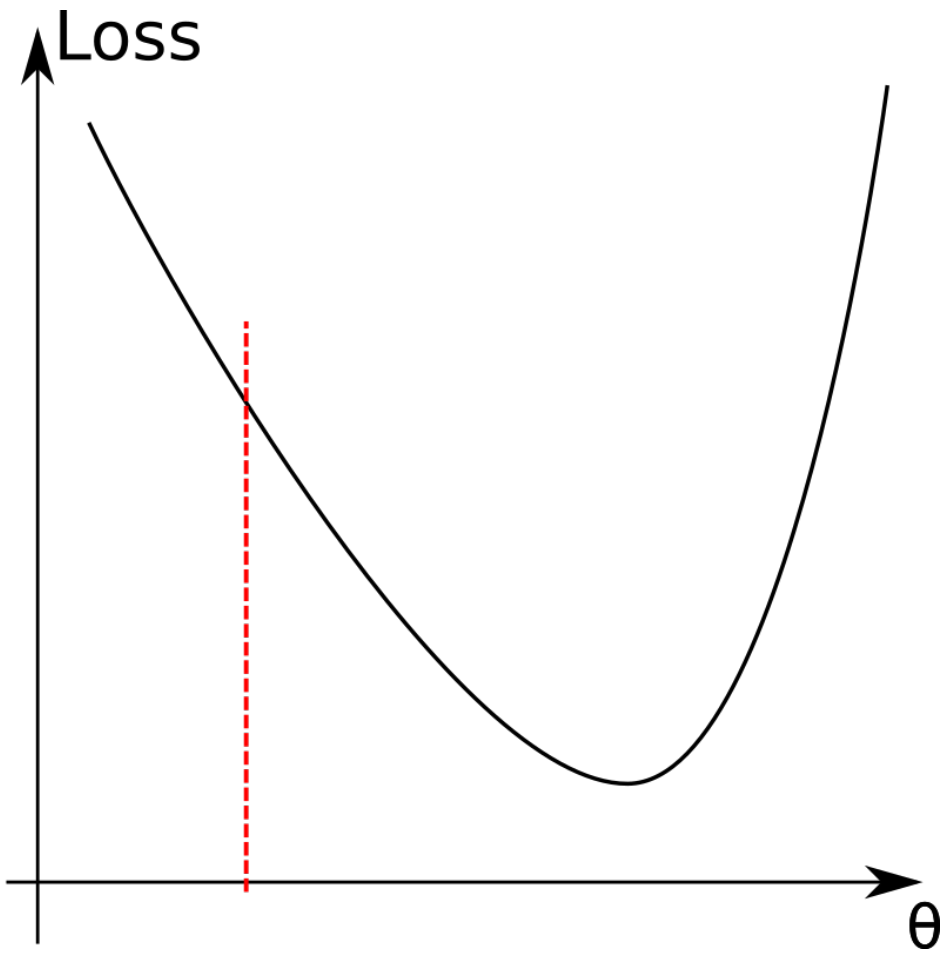
Exercise

What algorithm can you imagine to minimize the loss?

Gradient descent for convex loss



Gradient descent for convex loss



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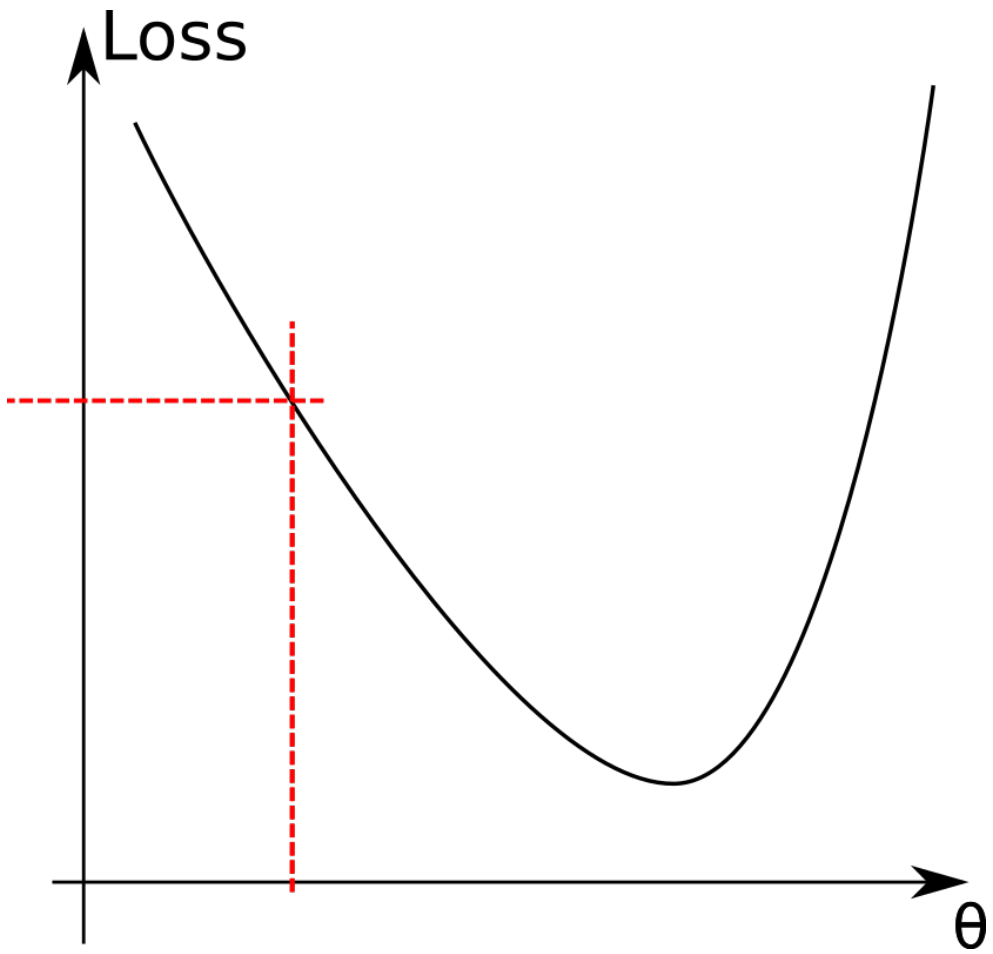

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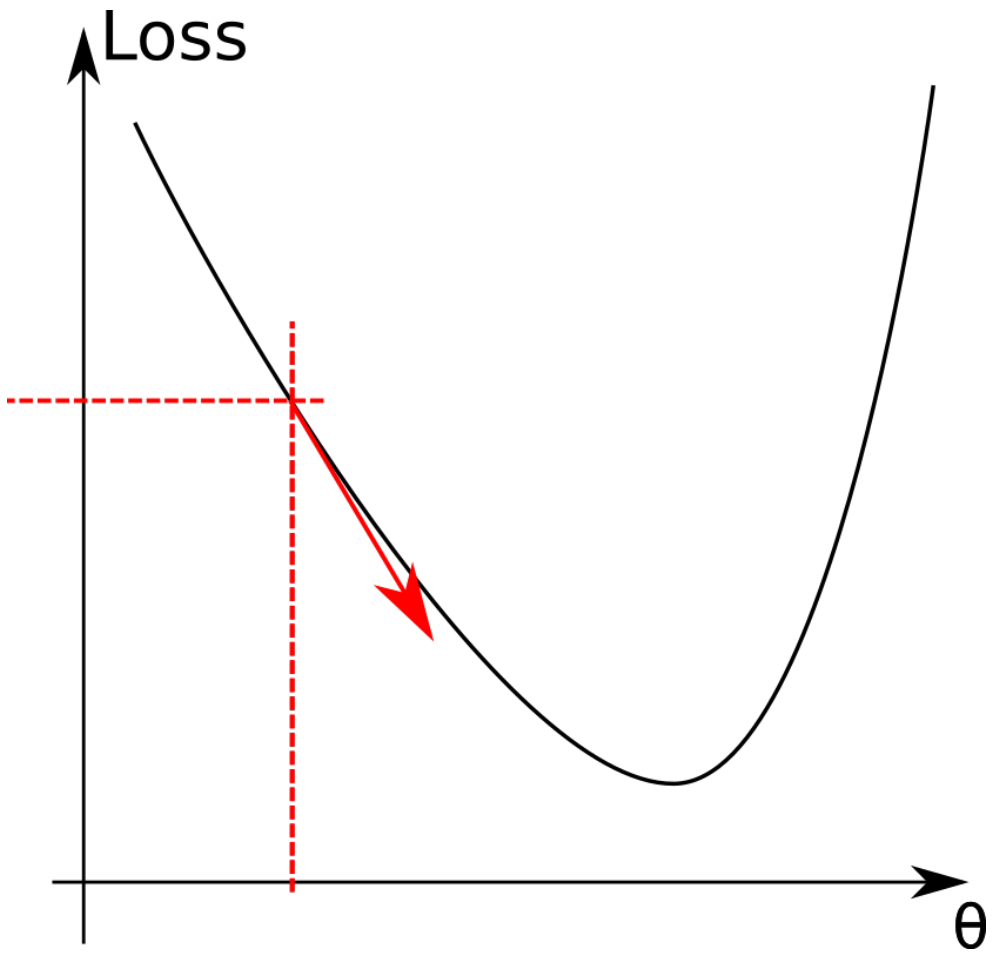

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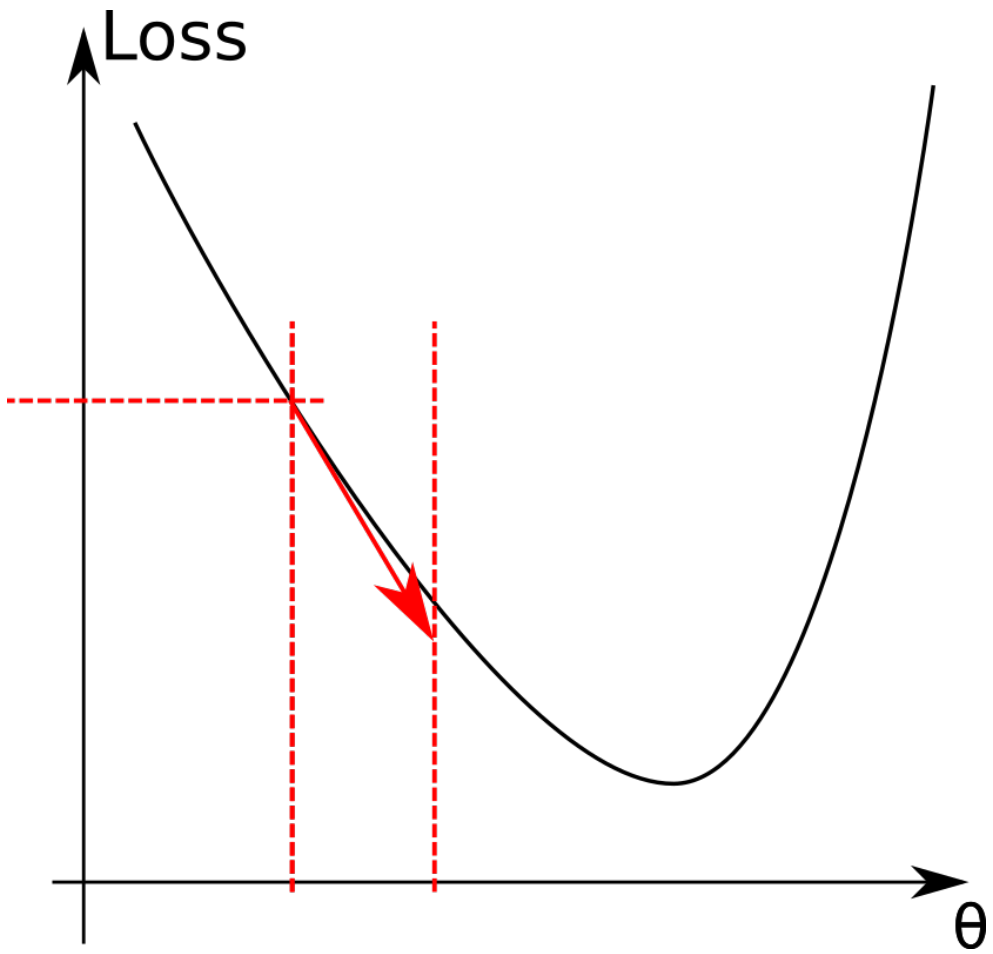

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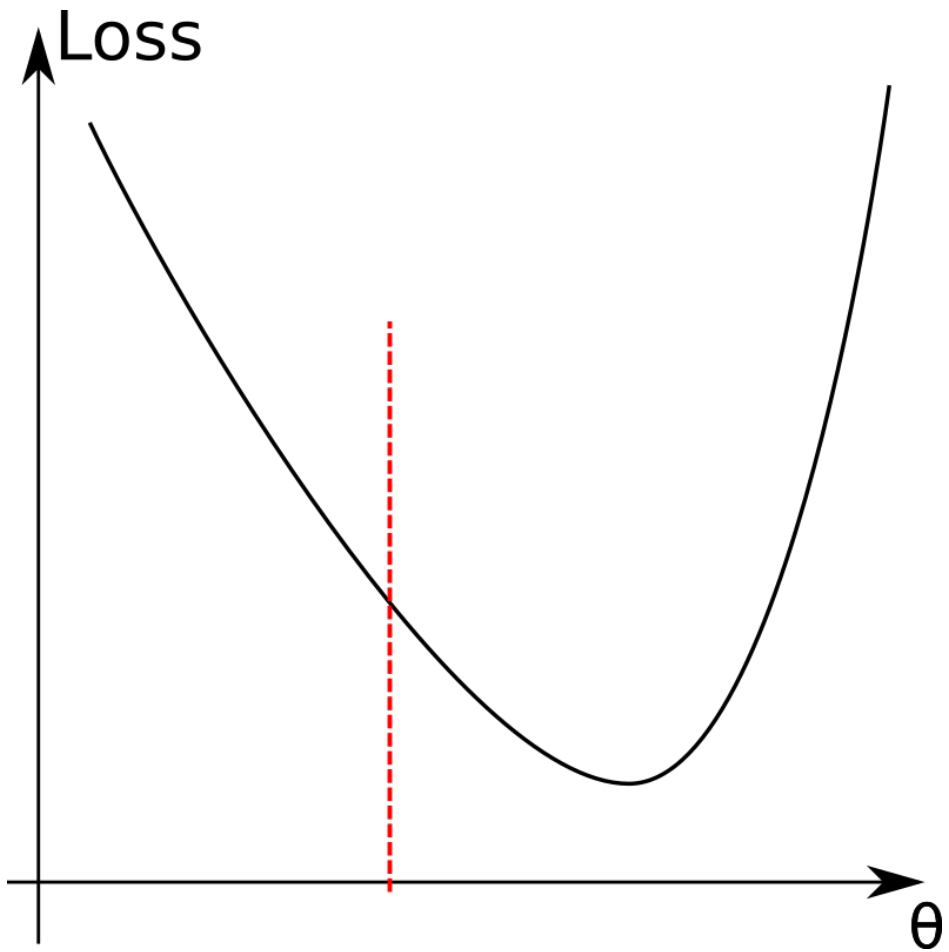

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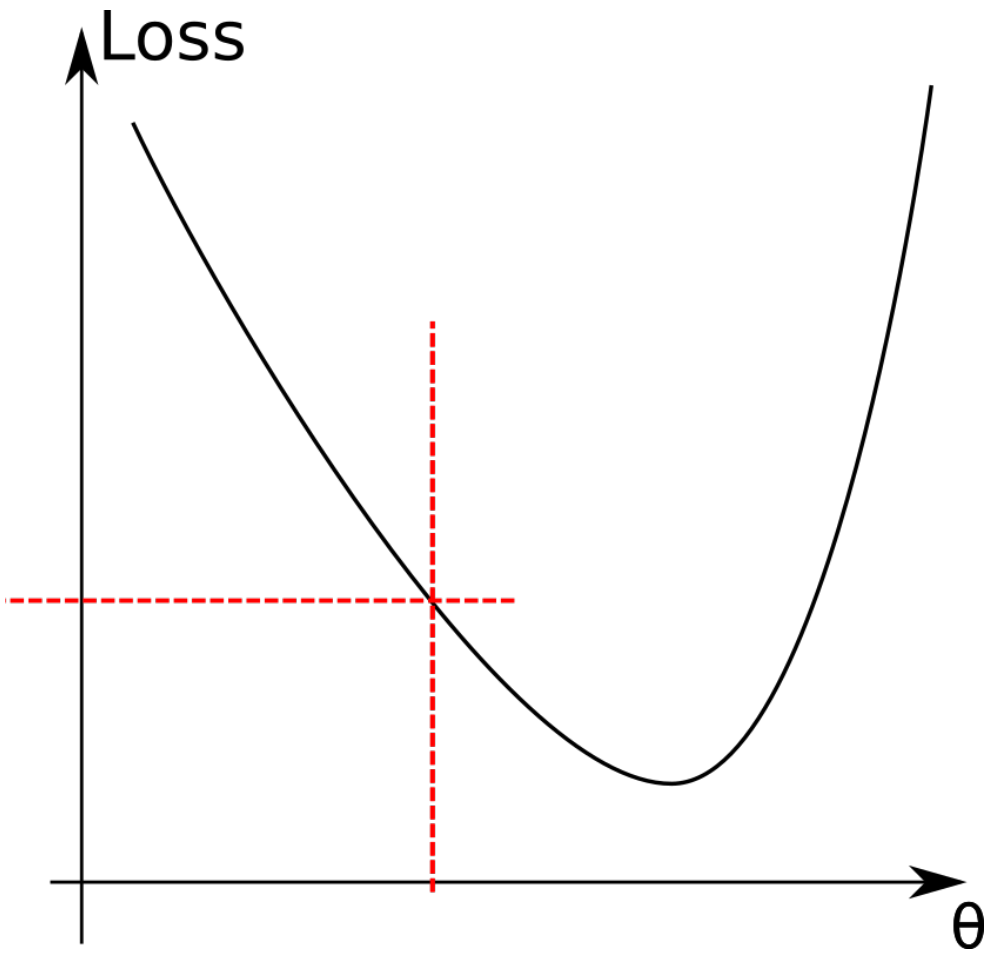

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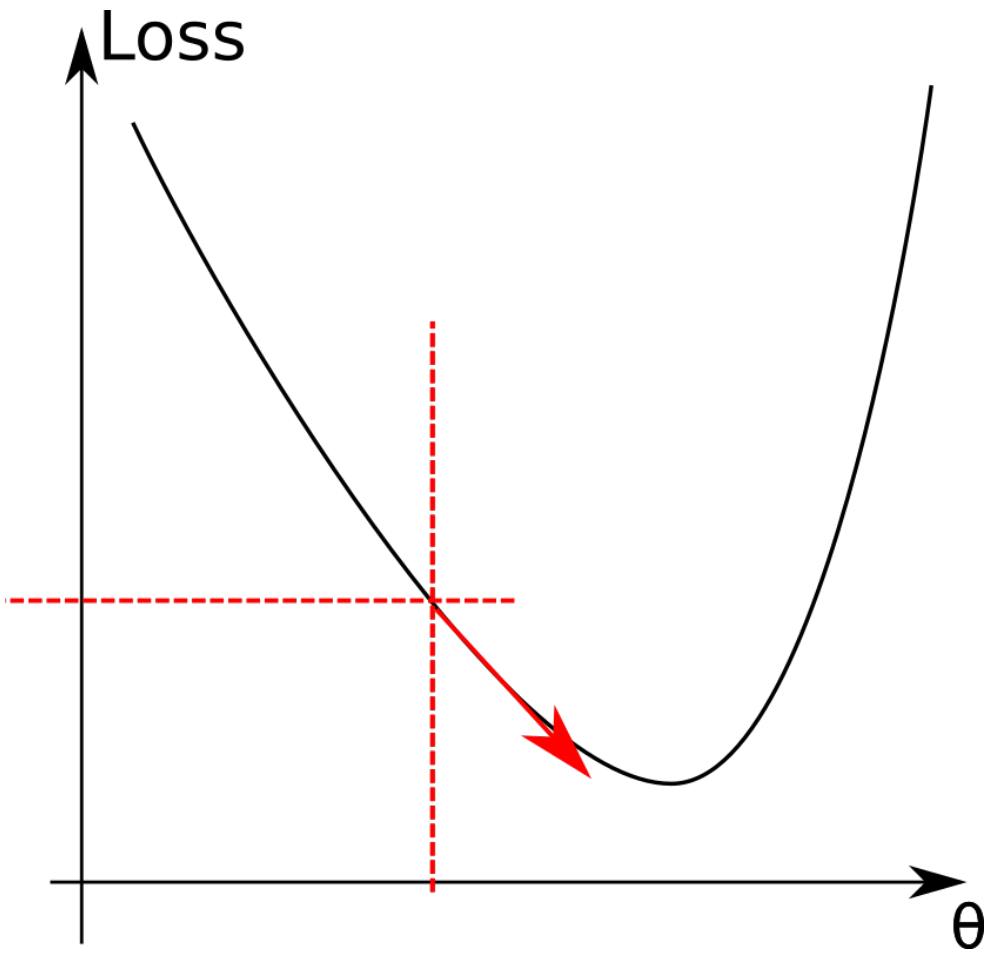

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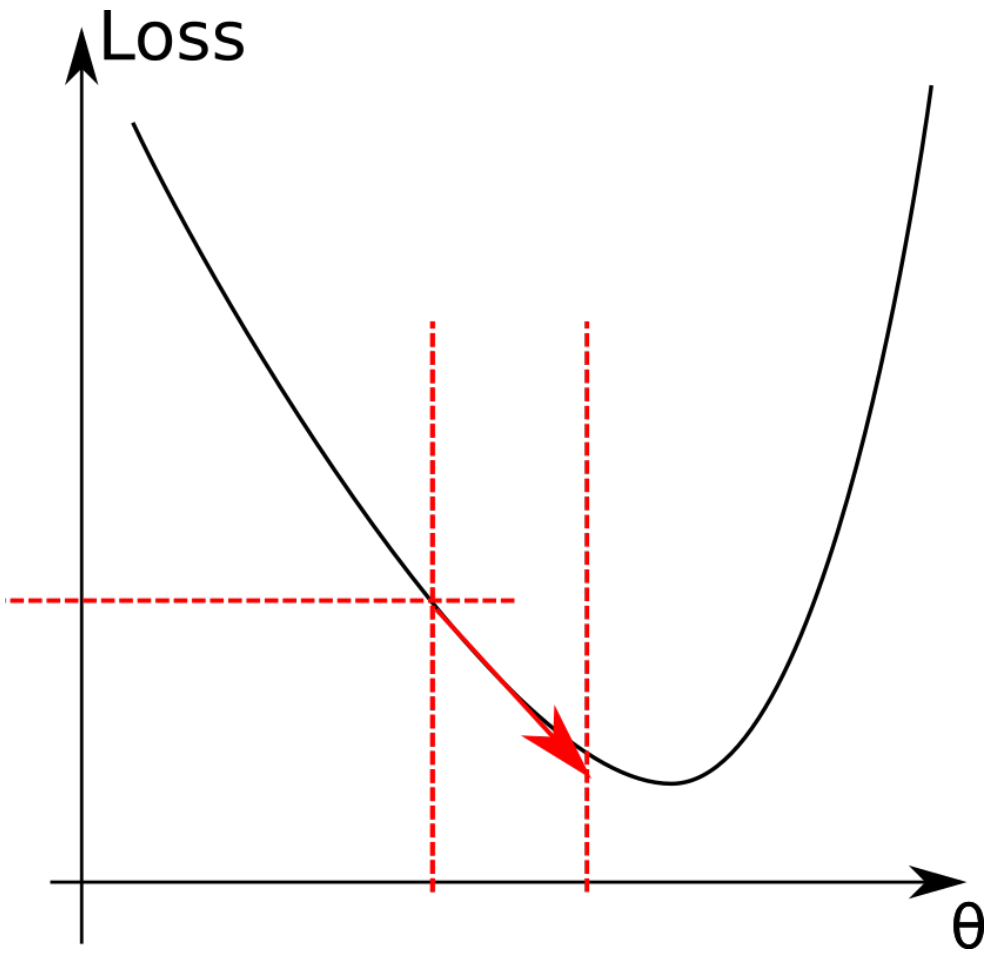

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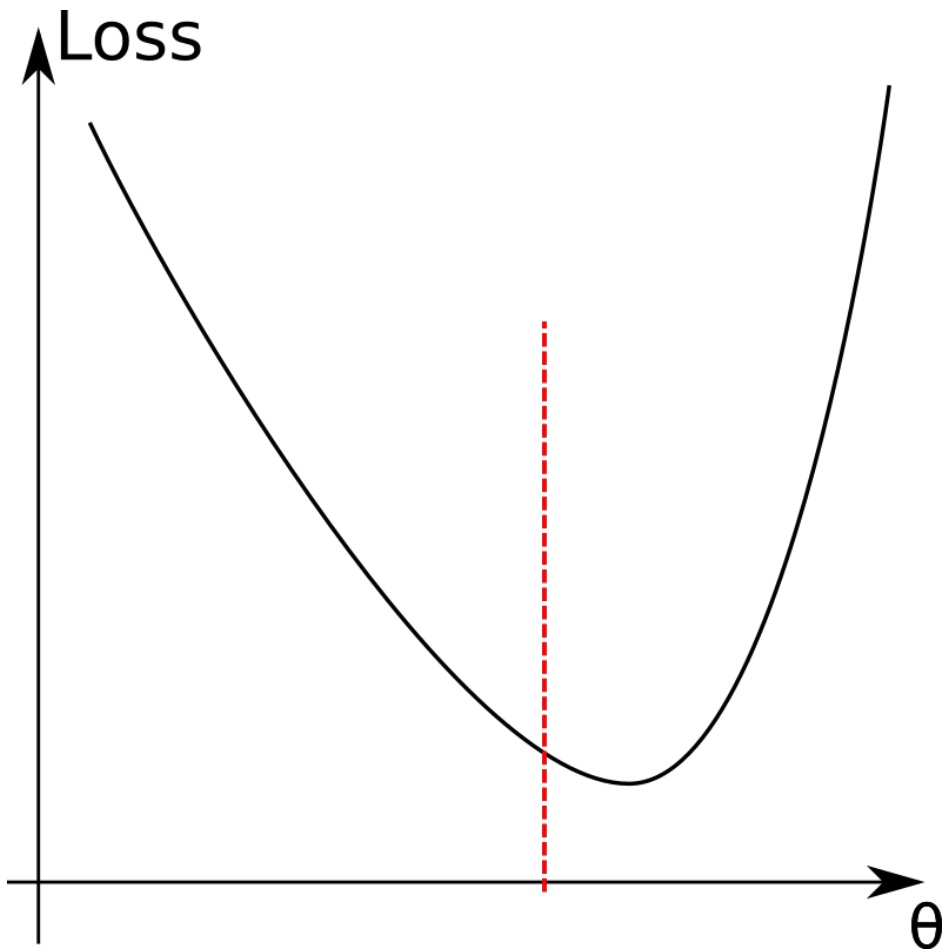

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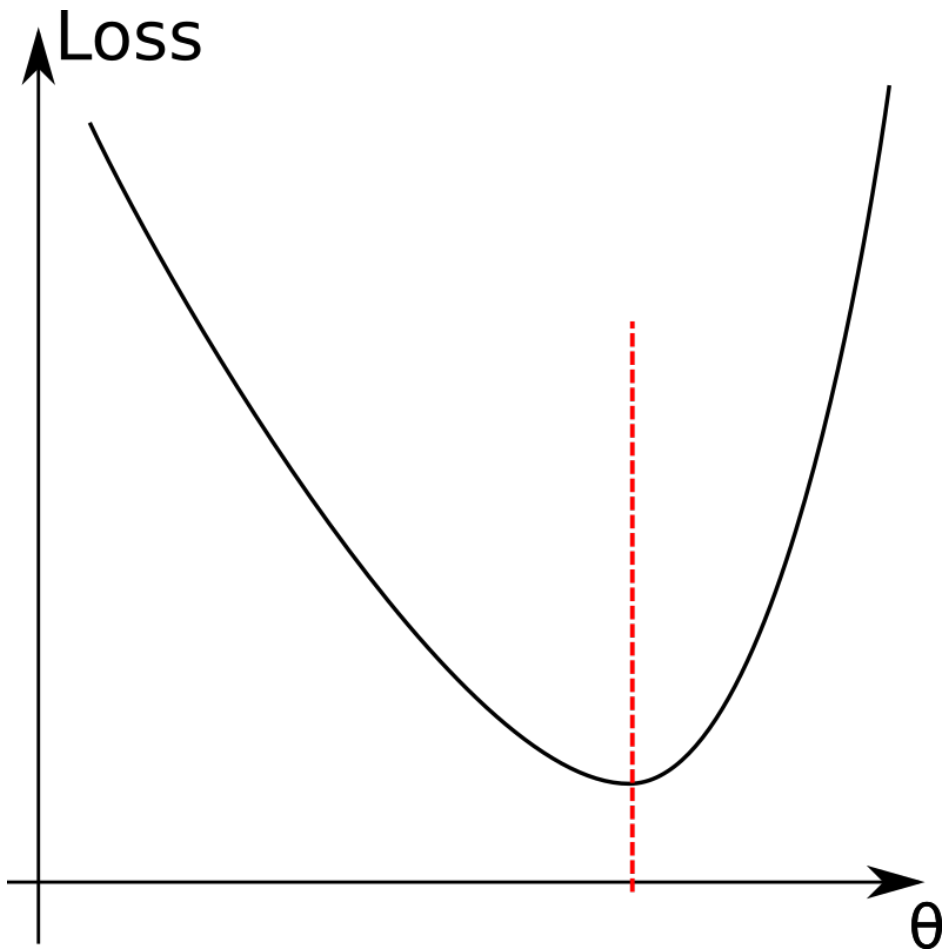
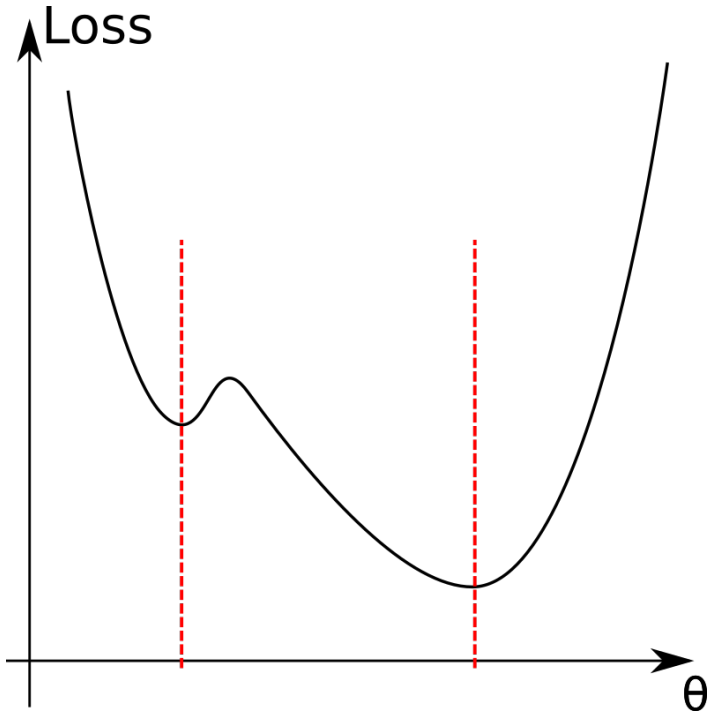
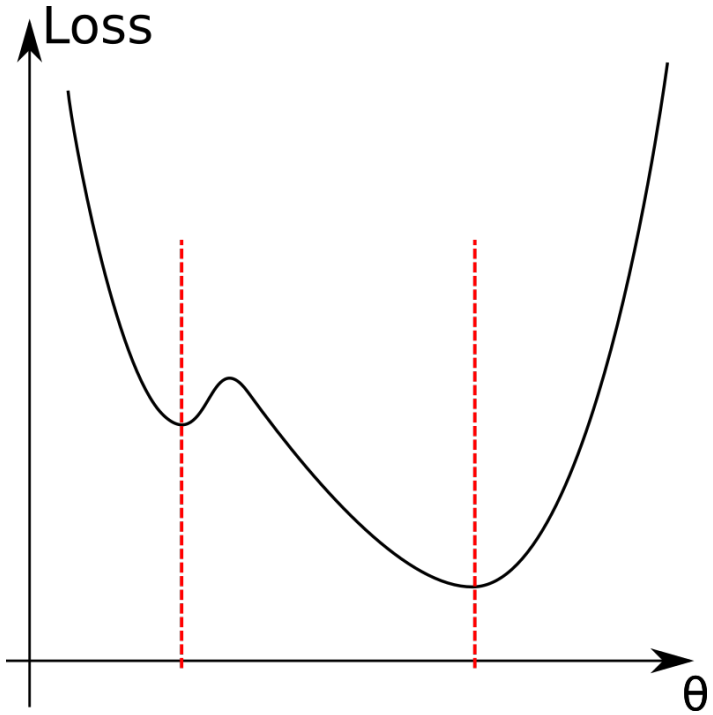


Gradient descent for **non**-convex loss



The gradient descent stops when it reaches a **critical point**: $\nabla \mathcal{L}(\theta_n) = \vec{0}$

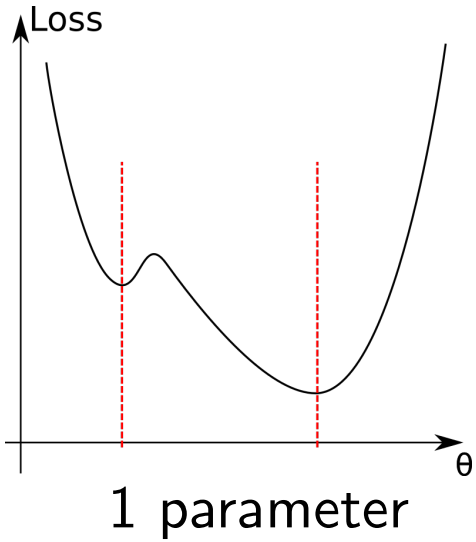
Gradient descent for **non**-convex loss



The gradient descent stops when it reaches a **critical point**: $\nabla \mathcal{L}(\theta_n) = \vec{0}$

What are the possible *types* of critical points?

Critical points in higher dimension



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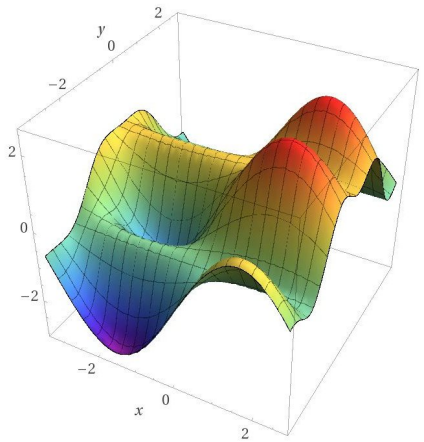
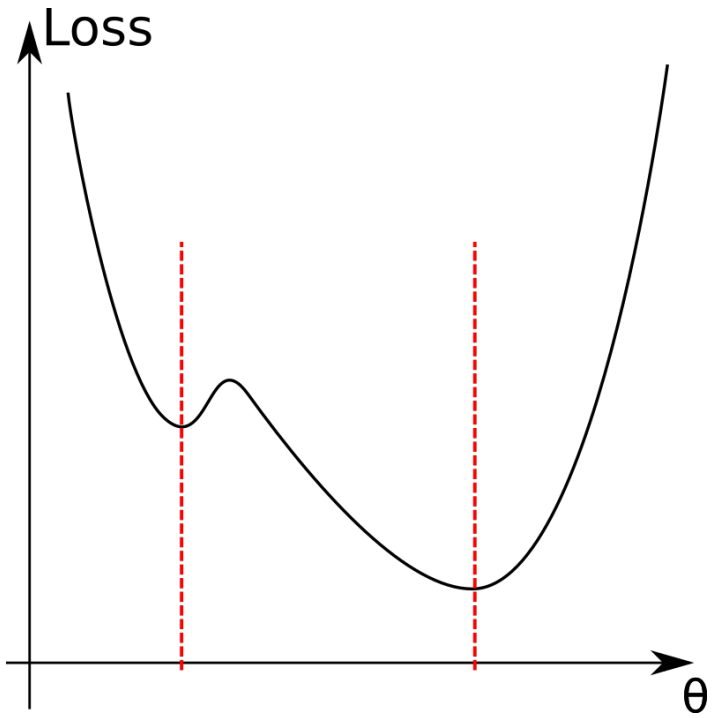


≥ 2 parameters

Escaping *easy* local minima



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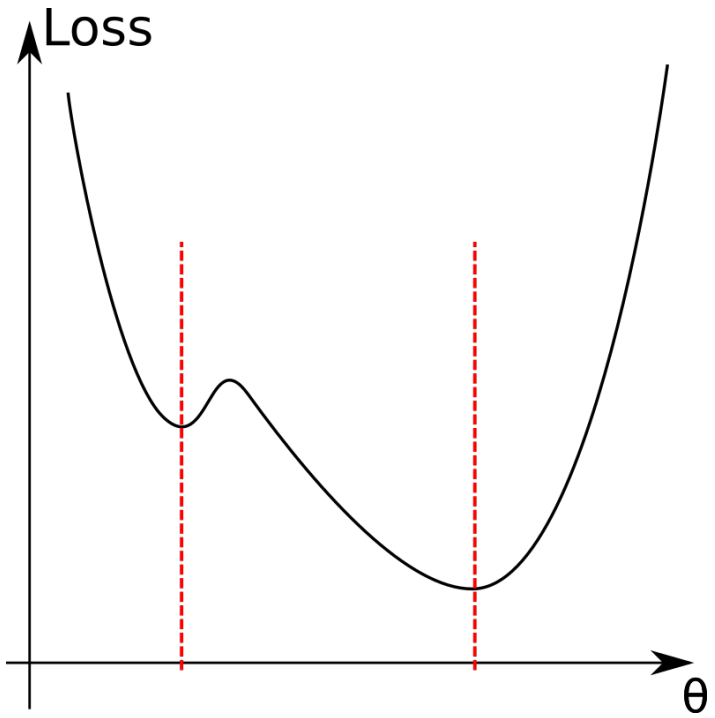

Gradient descent works well in practice for "small" non convexities by adding an inertia term:

$$\begin{aligned} \text{grad}_{n+1} &= \nabla \mathcal{L}(\theta_n) \\ \theta_{n+1} &= \theta_n - \eta_{n+1} \text{grad}_{n+1} \end{aligned} \tag{4}$$

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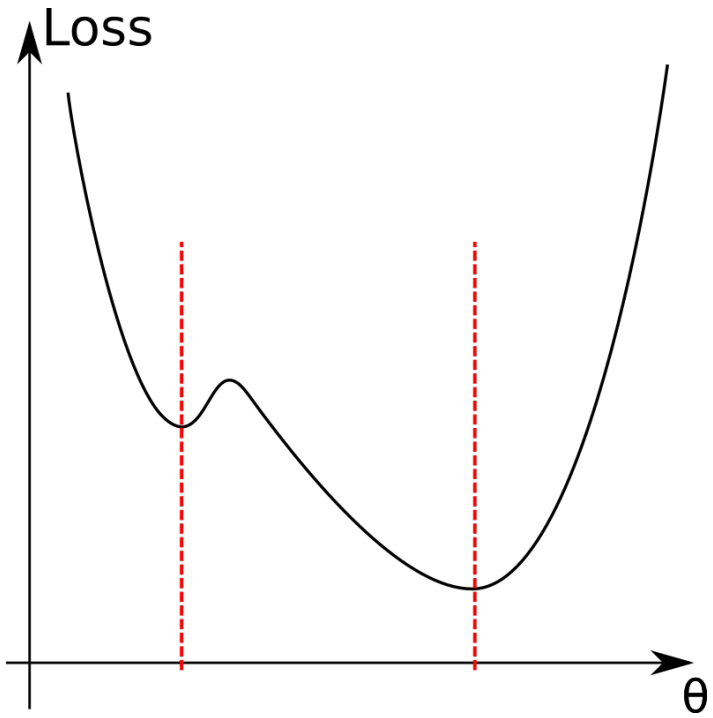

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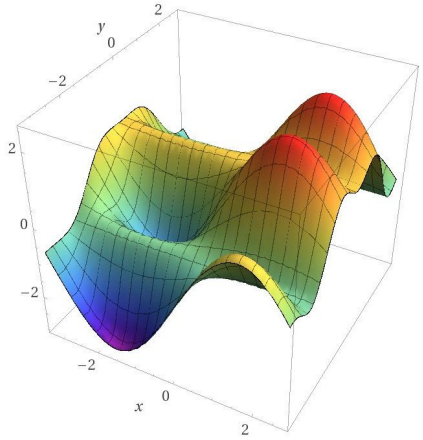
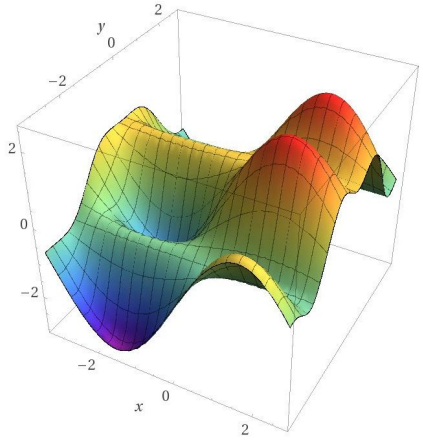
Escaping local non-minimal critical points



How is it possible to escape a critical point that is **not** a minimum?

[3]Would need to invert a 175.10^9 dimensional matrix for GPT3... $\approx 5.3.10^{33}$ operations :-/

Escaping local non-minimal critical points



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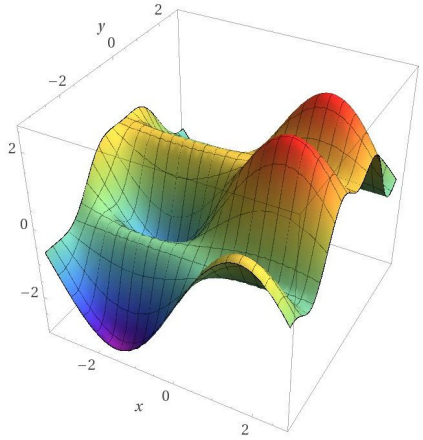
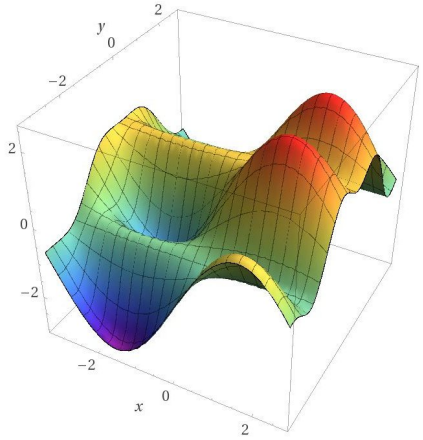


How is it possible to escape a critical point that is **not** a minimum?

- By computing the curvature (too big if a lot of parameters[3])

[3] Would need to invert a 175.10^9 dimensional matrix for GPT3... $\approx 5.3.10^{33}$ operations :-/

Escaping local non-minimal critical points



How is it possible to escape a critical point that is **not** a minimum?

- By computing the curvature (too big if a lot of parameters[3])
- **Add "noise" to the gradient !**

How to add some noise?

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Stochastic gradient descent (SGD)

$$\mathcal{L}(\theta) = \sum_{i=1}^{N} l(\theta, x_i, y_i)$$

where $\{(x_i, y_i)\}$ is the training set.

[4] By linearity of expectation: $\mathbb{E}_{\mathcal{B}}[\mathcal{L}_{\mathcal{B}}(\theta, X, Y)] = \mathcal{L}(\theta, X, Y)$

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If one computes instead the gradient on a **random subset** $\mathcal{B}$ (coined a **batch**) of the training set, one has an unbiased[4] **noisy** estimate of the gradient:

$$\mathcal{L}_{\mathcal{B}}(\theta, X, Y) = \sum_{i \in \mathcal{B}} l(\theta, x_i, y_i) \tag{5}$$

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SGD properties

- SGD is guaranteed to converge to the minimum for a convex loss.
- SGD can escape *easy* saddle points
- the computational cost is **much reduced**! See: $N_{\text{updates}} \times |\mathcal{B}|$
- with small batches can take advantage of modern hardware (GPUs)
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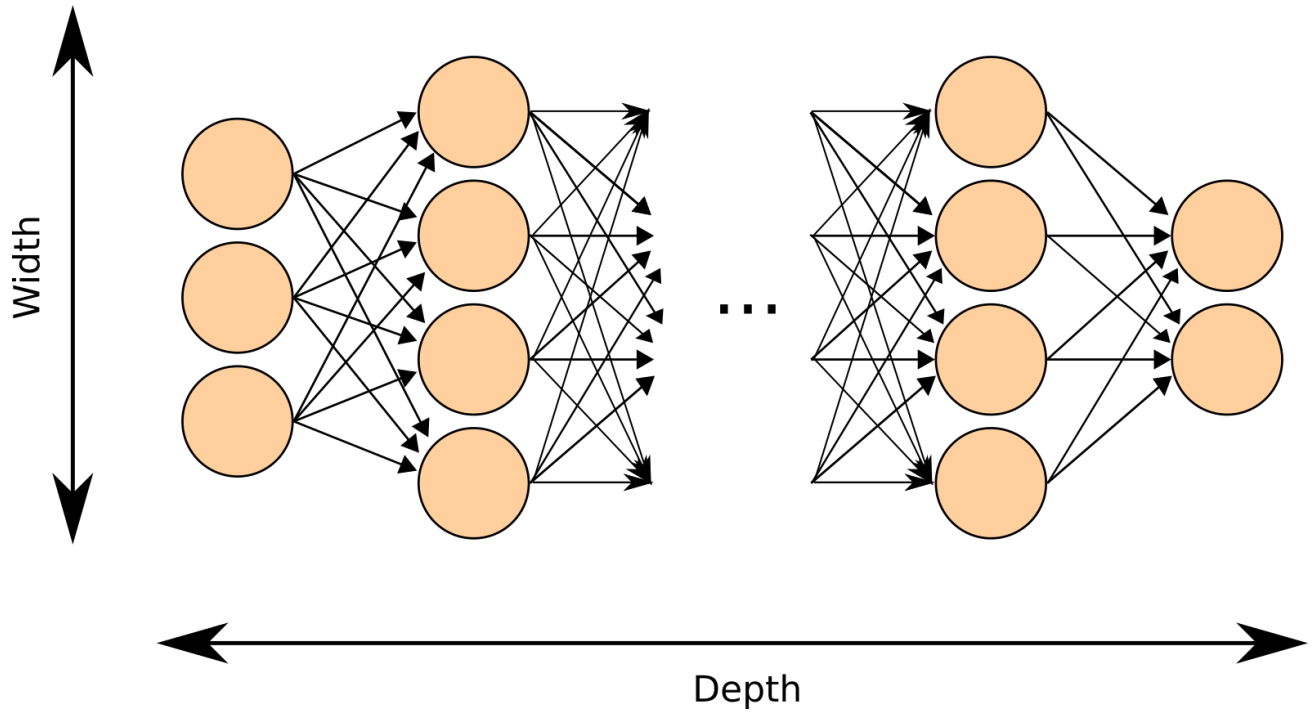
It seems that we have a candidate to train a model with billions of parameters...

Neural Networks

Neural networks

Neural networks are just a specific type of model that propagates input values through a network of connected neurons.
The way the neurons are connected and the reaction of each neurons to its neighbours' activation is decided by the modeller and it is coined the architecture of the neural network.
We will go through some examples of architectures.

Dense feed-forward neural network



Activation of neuron i in layer l: $z_{i,l} = \sigma_l(\sum_{k \in \mathcal{I}_{i,l}} w_{l,i,k} z_{k,l-1})$

Parameters[5]: $w_{j,k}$'s.

σ_l: activation functions.

[5] GPT-3 has 96 layers and 175B parameters

Input and outputs

Inputs are vectors in $\mathbb{R}^m$, and output vectors in $\mathbb{R}^n$.

It can be:

-  in $\rightarrow$  out

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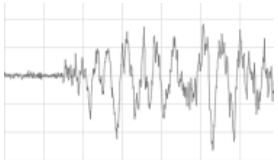
-  in $\rightarrow$ *"plant"* out

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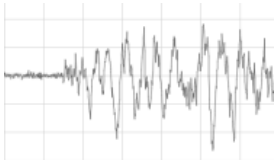
-  in $\rightarrow$ *"plant"* out
- ...

Images can be encoded as 1 px = 1 dimension of the vector, a signal as 1 time point = 1 dimension, etc.

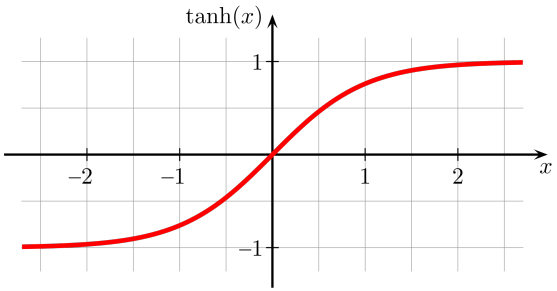
Time to play

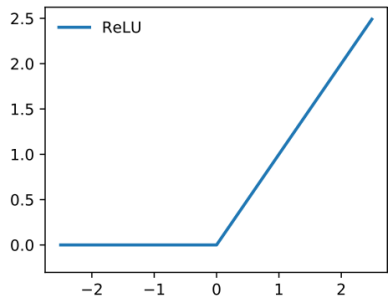
Let's see how an ANN looks like in practice:
https://playground.tensorflow.org

Activation function

What activation function?

- Its gradient has to be simple to compute
- It should "make sense"





Note that the linear regression can be recovered with 1 single output neuron and $f(x) = x$ as activation function.

Neural networks as a *"universal"* model

Theorem [Lu et al. NIPS'18]

For any $\epsilon > 0$, and any Lebesgue-integrable function $f : \mathbb{R}^m \to \mathbb{R}$, there exists a ReLU neural network η such that:

$$\int |f(x) - \eta(x)| dx < \epsilon \tag{6}$$

Moreover, one can also restict the maximal width to $m + 4$.

There are theoretical results ensuring that neural nets can approximate arbitrarily well any well-behaved function.

Time to play

Let's see how ReLU and depth allow to model complex data:
https://playground.tensorflow.org

Training: SGD to the rescue!

Which training algorithm?

- + Automatic computation of the gradient of the loss using *automatic differentiation*.
- - The loss is non-convex even with linear activation functions [Kawaguchi NIPS'16] .

Nevertheless...

Gradient descent works very well in practice.

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Gradient descent works very well in practice.

We now have some theoretical results explaining (a bit) why it SGD works well for deep neural networks [Hardt et al. 16] (SGD and generalization error), [Chaudhari and Soatto ICLR'18] (SGD naturally regularizes).

Training a neural network: the big picture

A (dense) NN is therefore simply a function
$f_w(x) = \sigma_d(\sum_{k_d} w_{d,1,k_d} \sigma_{d-1}(\sum ... \sigma_1(\sum_{k_1} w_{1,i,k_1} x_{k_1})))$.
How to fit the parameters $w_{j\,k\,l}$?

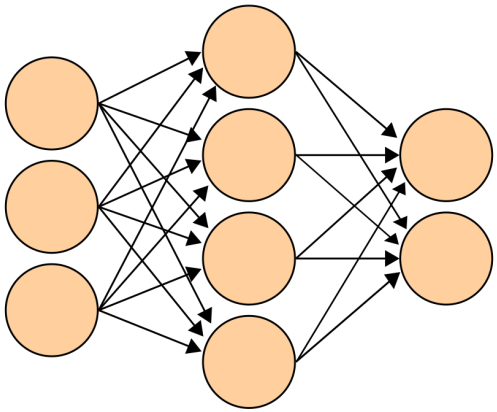
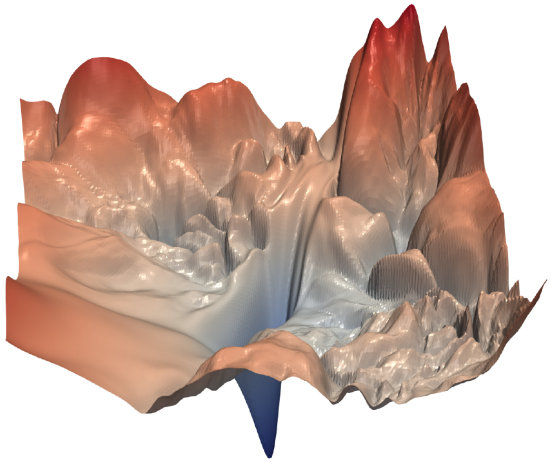
- Get a traning set (x_s, y_s), can range from kB to TB of data[6].
- Define a loss function, for instance $\mathcal{L}(w) = \sum_s [y_s - f_w(x_s)]^2$.
- Then compute[7] the derivatives $\frac{\partial \mathcal{L}}{\partial w_{i,j}}$
- Use your favorite variant of SGD, and find a good minimum of the loss.

[6] the more the better

[7] An analytical formula can be obtain by a computer for well-chosen activation functions

Architecture matters for training: resNet example

The loss function can change dramatically depending on the NN architecture.

	Architecture	Loss landscape
Dense		

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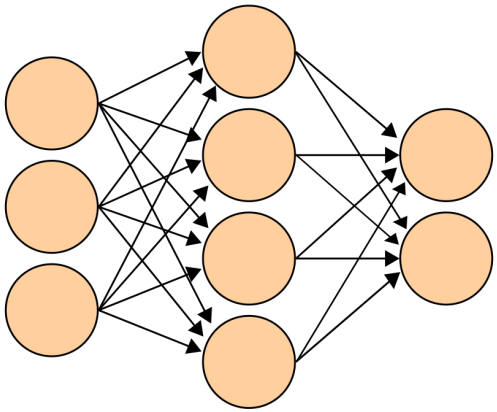
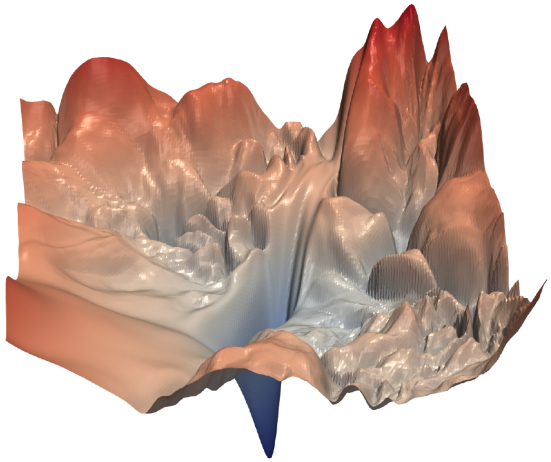
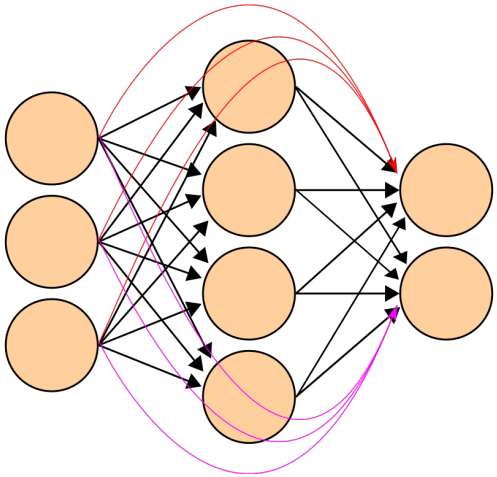
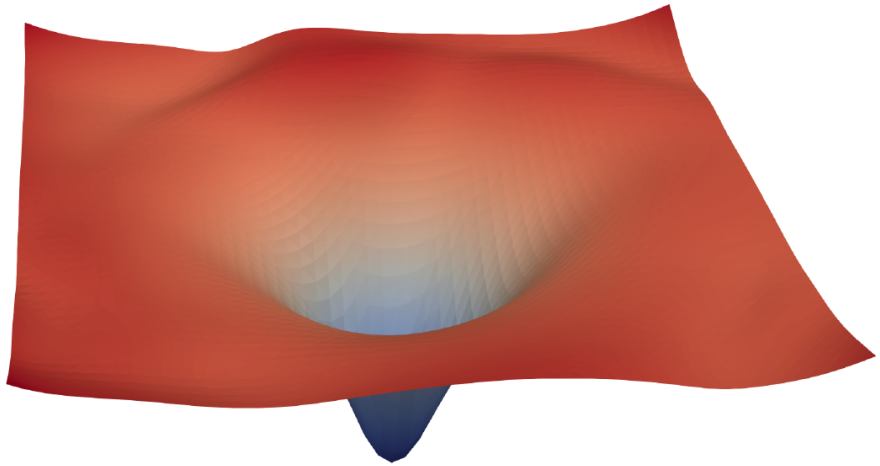
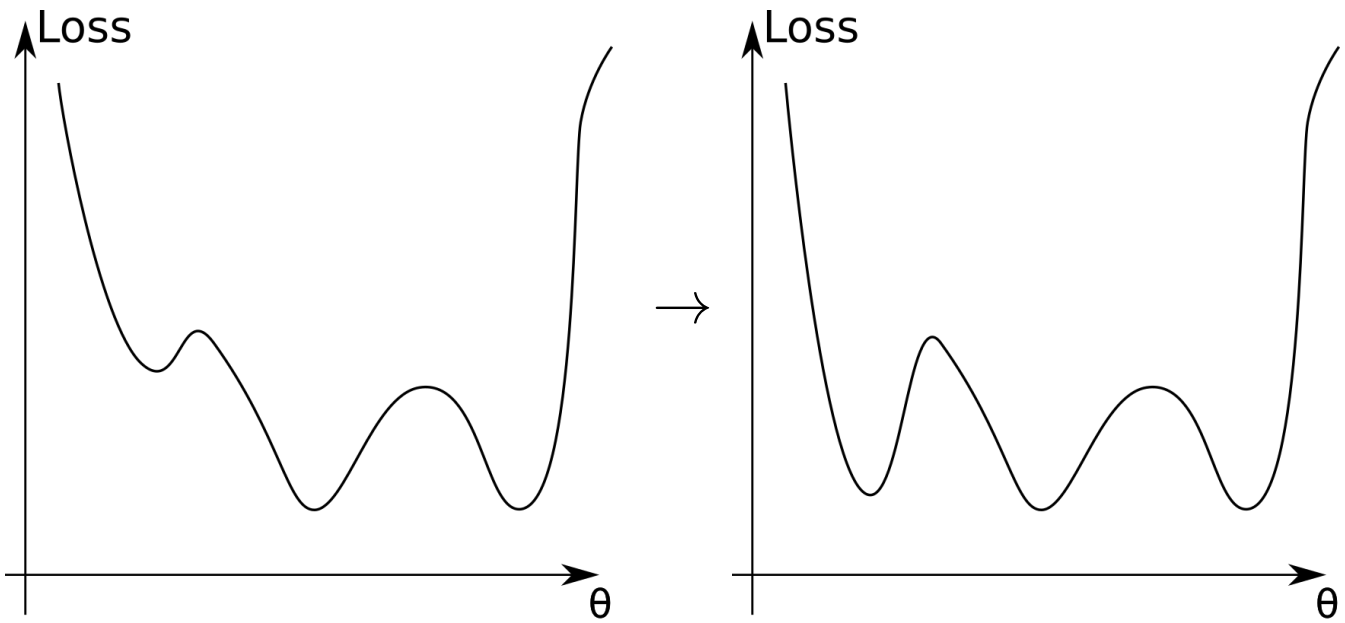
Dense		
resNet		

Architecture matters for training: depth

[Choromanska et al. 15] (spin-glass model)

The bigger the network, the fewer bad local minima.



ANN and optimization

The loss of neural networks is ___.
The loss landscape depends on the ___. It therefore makes sense to use an architecture for which local minima are of ___ quality (like deep or specific like ResNet).
So... ___ neural networks are universal models that can be trained efficiently using ___. But the deeper the ANN, the ___ parameters are involved... so even with a huge load of data, it should ___, right?!

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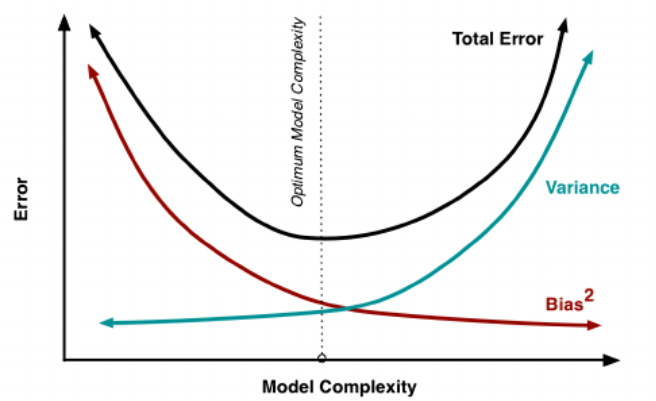

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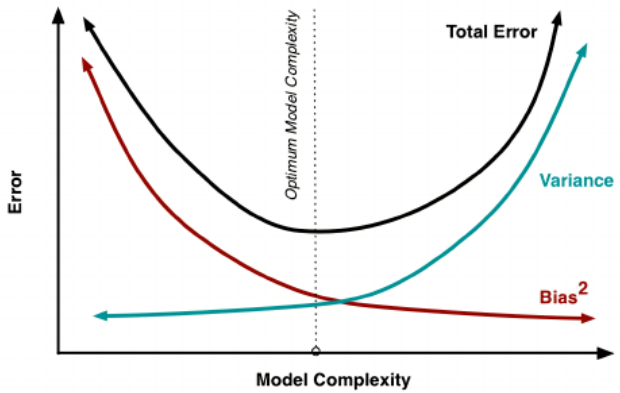

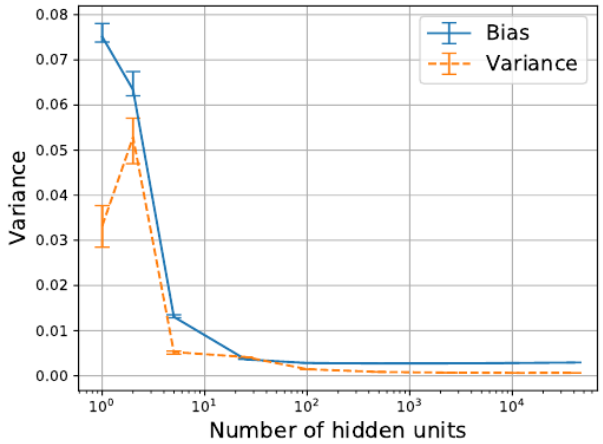

[Neal et al. 19]

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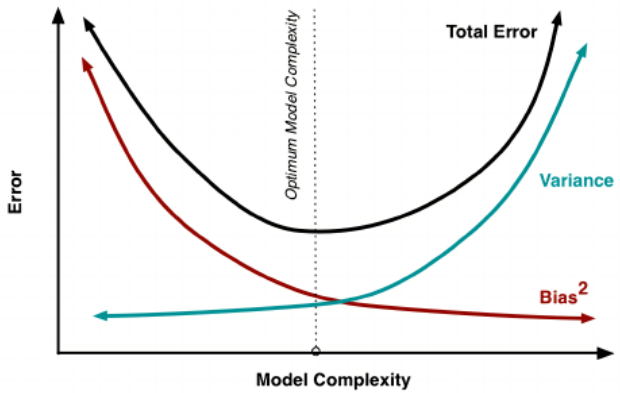

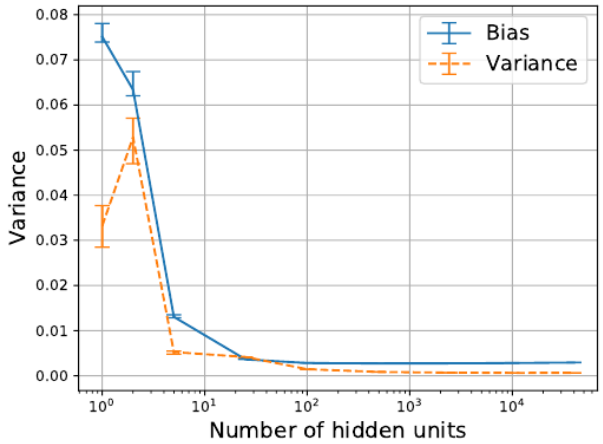

[Neal et al. 19]

A big insight [Achille and Soatto JMLR'18]

One should rather measure the amount of information from the training data that is transferred to the weights during the fit: less and less amount is transfered the deeper you go.

Time to play

Let's see what neurons learn with respect to depth:
https://playground.tensorflow.org

Summary: neural nets, why does it work that well?

No real "breakthrough" but rather a concordance of events:

[8] Actually it may be also why biological neural nets have been selected by evolution

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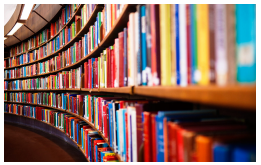

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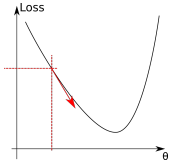

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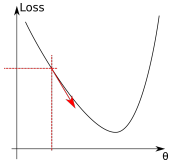

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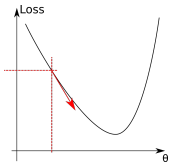
- Better optimization algorithms (SGD and its variants) 

- Better hardware (GPUs for parallel computations) 

- Some luck[8]: ANN tend *not* to overfit (but it has been noticed afterwards) 

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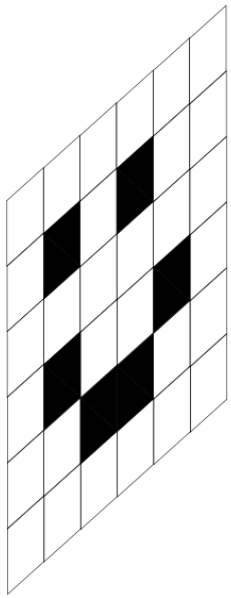
Some architecture you need to know

What architecture are allowed?

What architecture are allowed?

Virtually any, as soon as you can compute the gradient of the loss :)

Image processing: dense NN?



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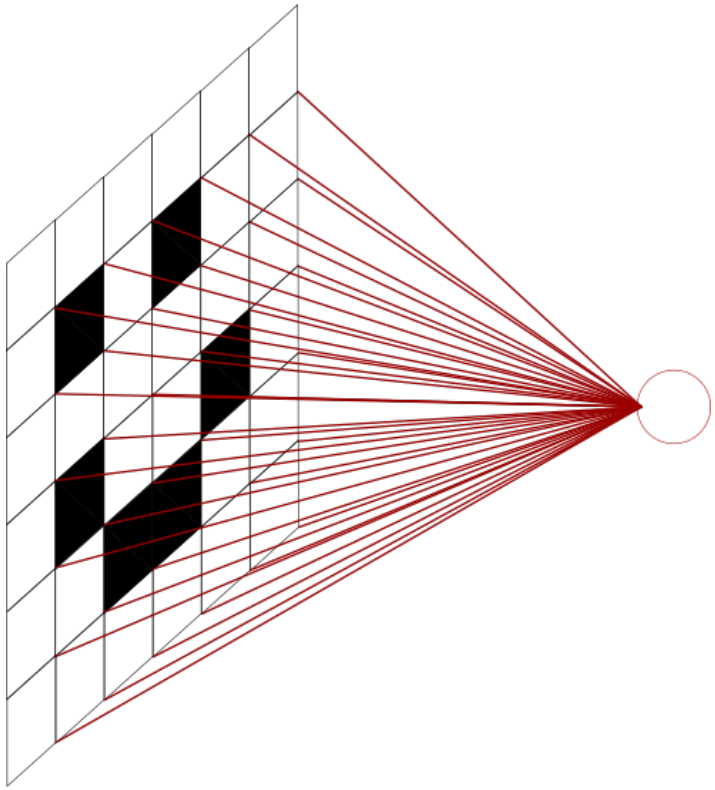

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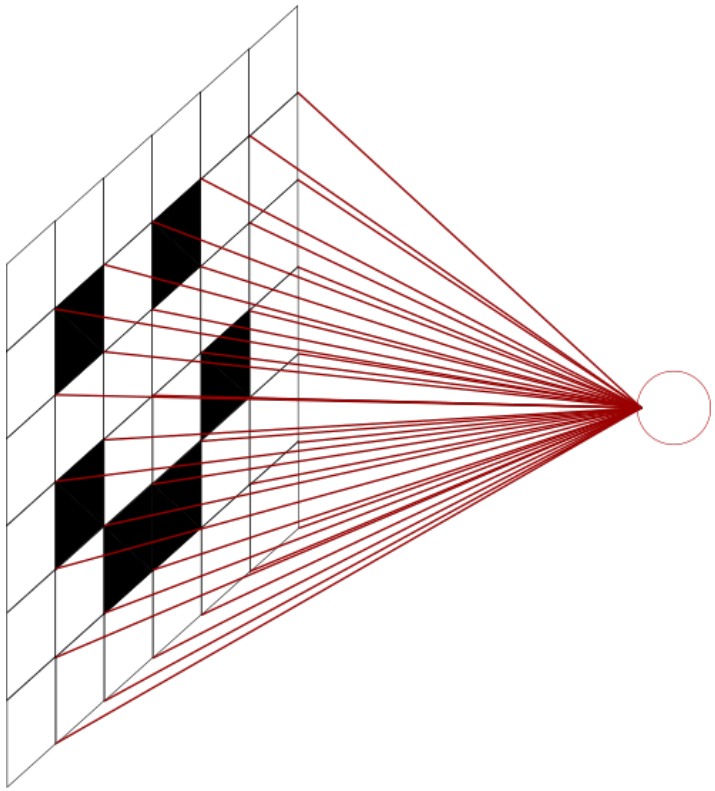
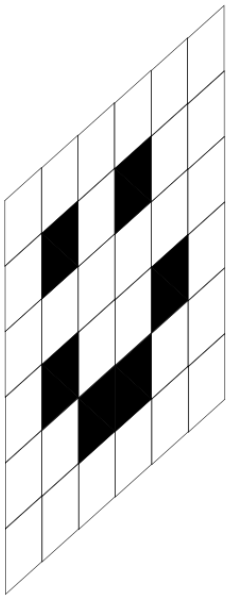


- How many parameters do we need?
- What happens if we shift the whole dataset by 1px?

Image processing: convolutional neural nets (CNN)



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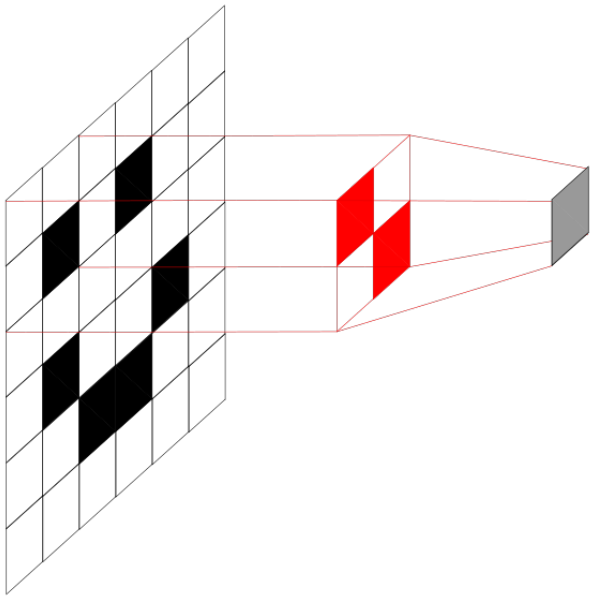

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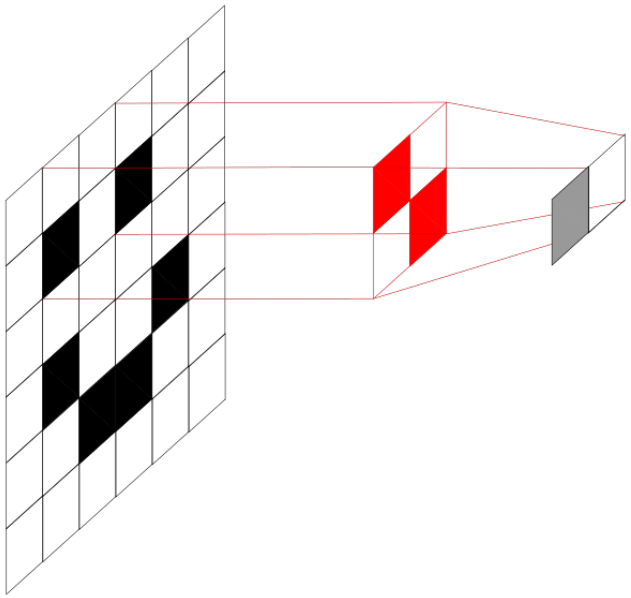

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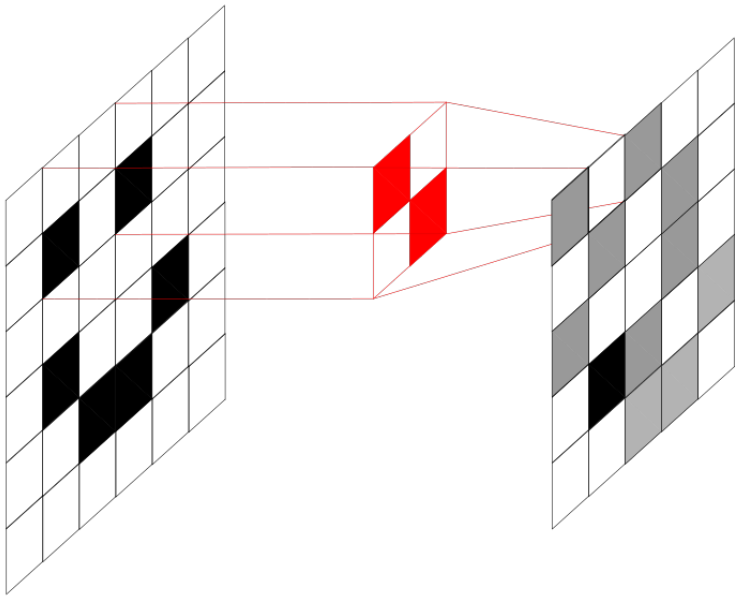

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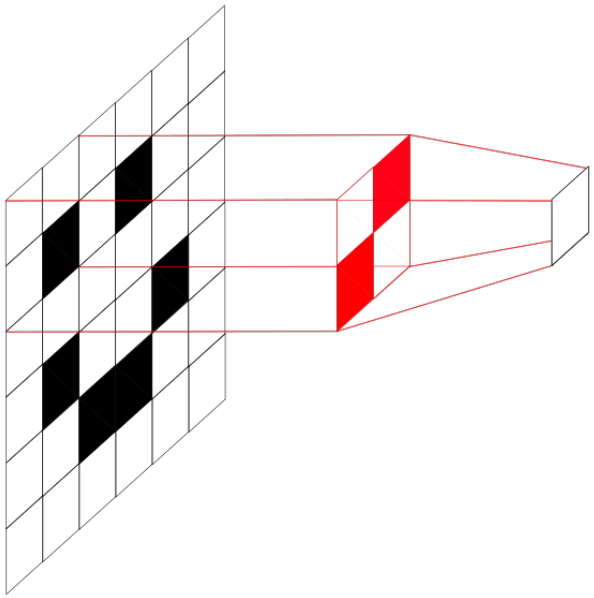
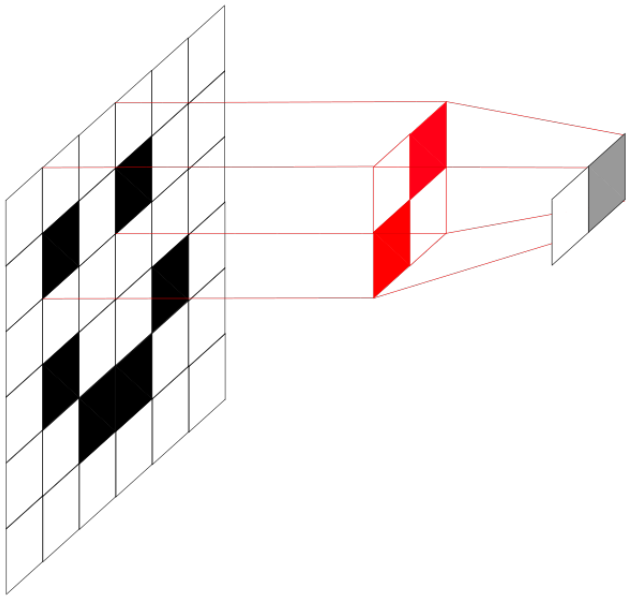


Image processing: convolutional neural nets (CNN)



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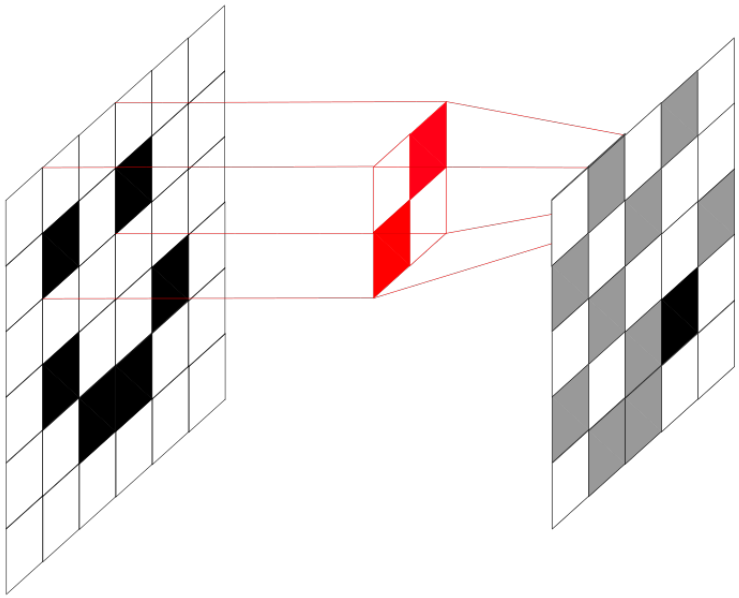

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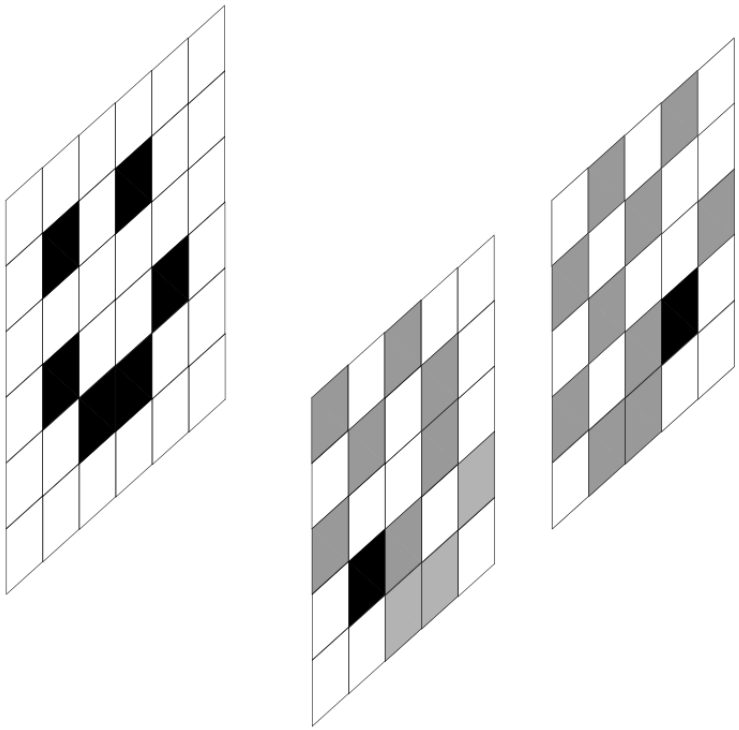

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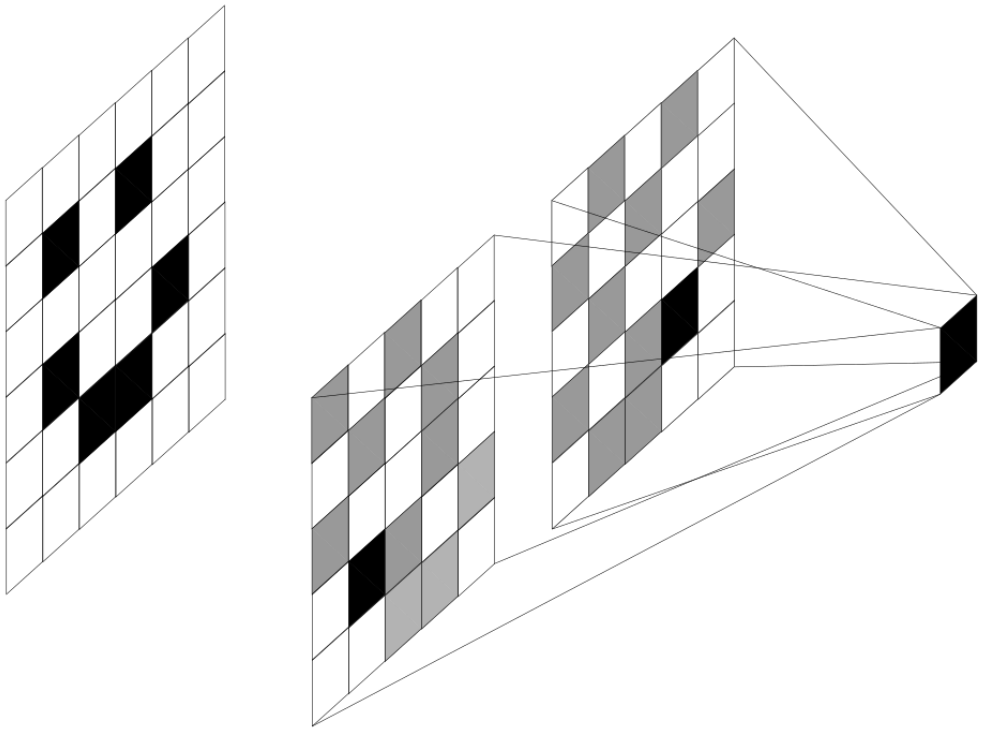
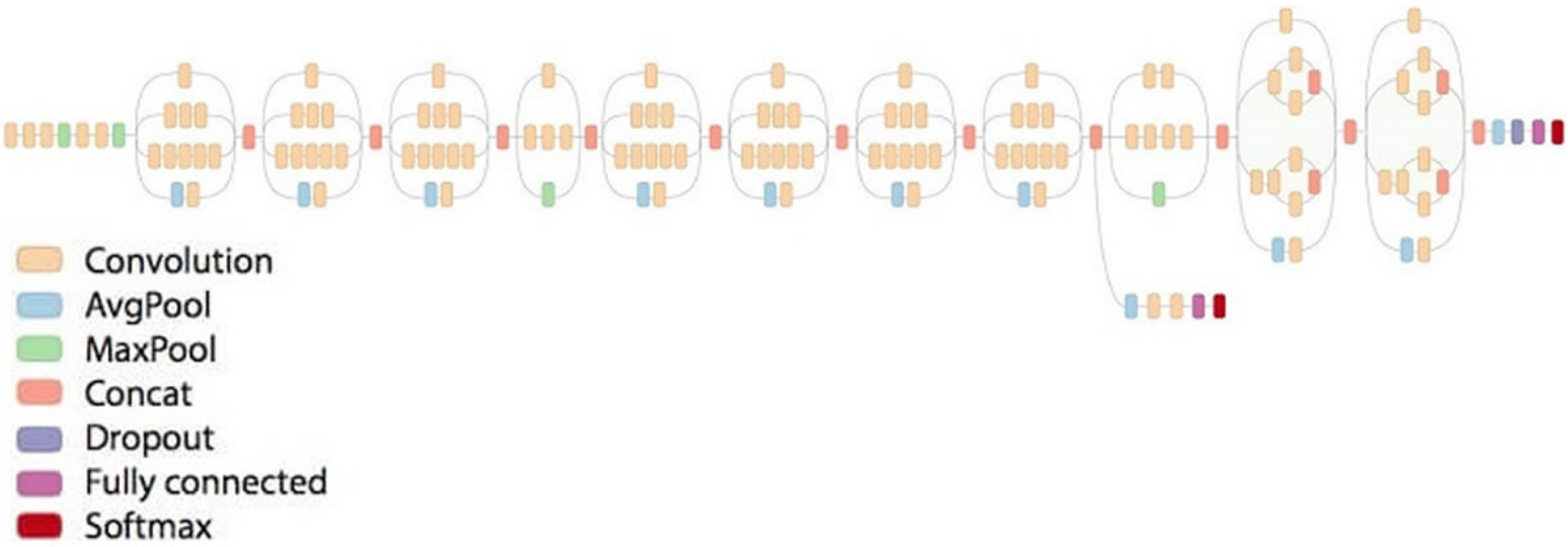


Real-world CNN



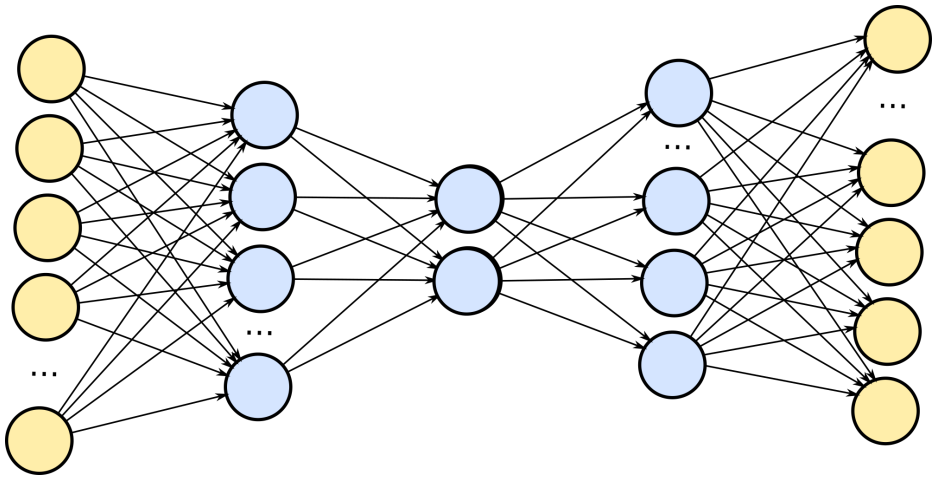
Source: InceptionV3

Applications: image recognition, segmentation [Minaee et al. 20] , etc.

Time to play

Demo ResNet50.

Compressing data with NN: Autoencoders



Try to accurately reconstruct the input (unsupervised).

Analogy with the "Chinese Whispers"[9]*.* The mid-layer is called a latent and contains a compressed version of the input. Works when the data has an underlying structure.

[9] "Téléphone Arabe" in French

Compressing data: autoencoders

Example: predicting high altitude pollution from satellite images

Problem

- Cannot generate a lot of training data: only few ballon can be sent per year.
- hourly acquisition of 2000x2000px satellite images

What will happen if we learn the pollution from the raw sattelite images?

—

Compressing data: autoencoders

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You can: ___ the images of sattelite (trained on all unlabled data) and predict from the small ___ layer.

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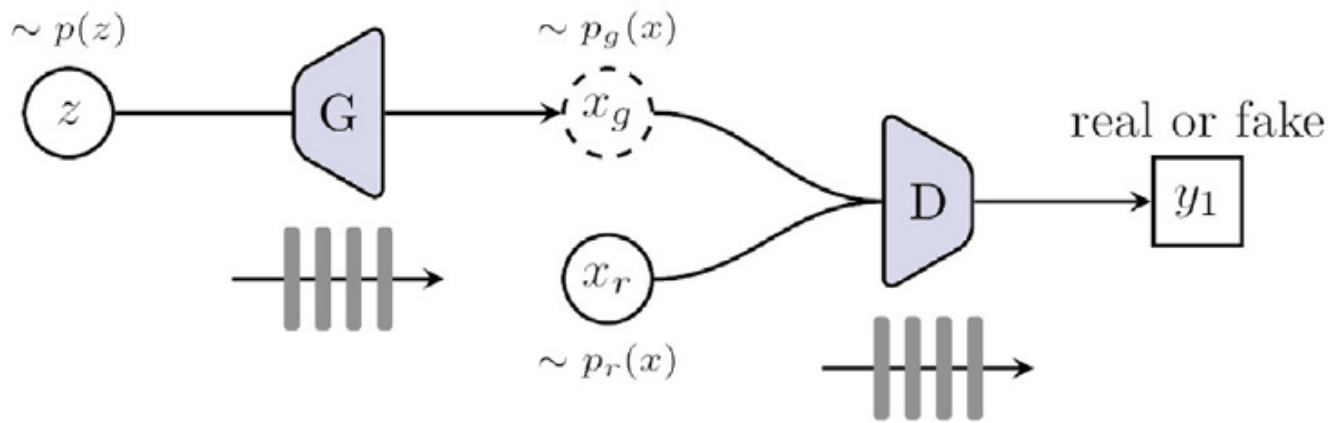
Overfitting
You can: **compress** the images of sattelite (trained on all unlabled data) and predict from the small **latent** layer.

It is very common to have **a lot** of **un**labled data and **few labeled** data.

Generative Adversial Networks (GAN)

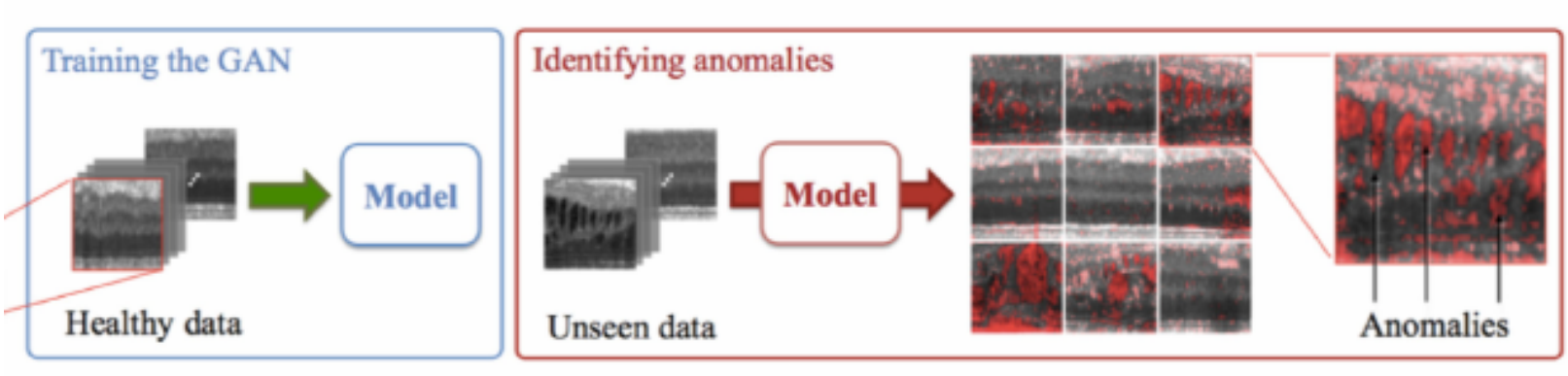


Equilibrium reached when $p_g = p_r$

Generative Adversial Networks (GAN)

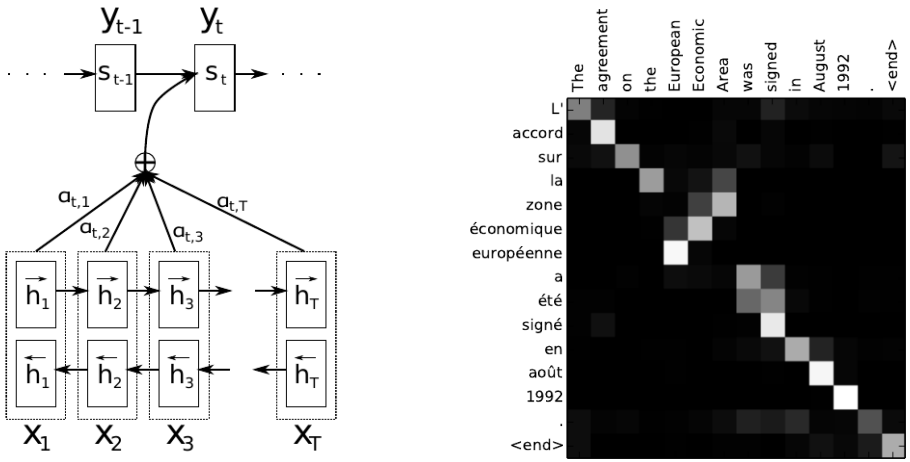
Can be use as a generative process

Generative Adversial Networks (GAN)



or as a classifier [Yi et al. 20]

Text processing: attention mechanism

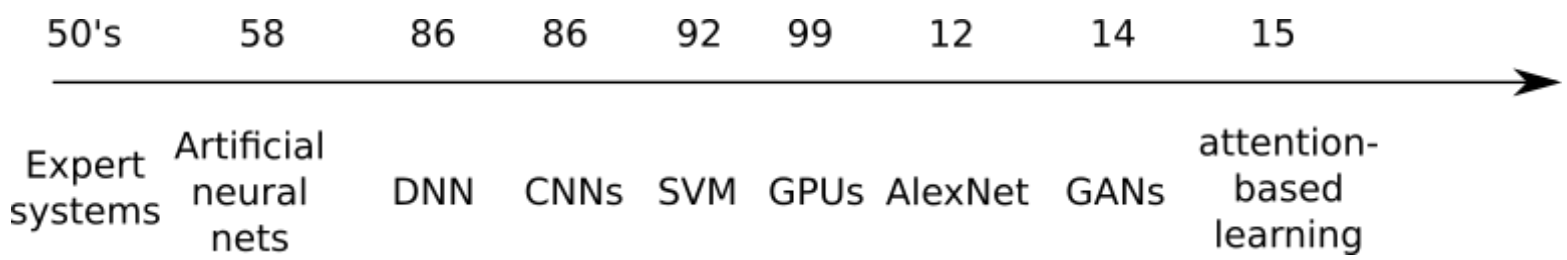


[Bahdanau et al. ICLR'15]

Improvement of the same idea: the Transformer architecture [Vaswani et al. 17] ,[Brown et al. 20]

Past and future

Timeline


50's
58
86
86
92
99
12
14
15
Expert systems
Artificial neural nets
DNN
CNNs
SVM
GPUs
AlexNet
GANs
attention-based learning

Biases

- Correlation $\neq$ causality
  - Pneumonia and asthma example [Crawford and Calo 16]
- Minorities in training data
  - less accurate for minorities [demo: beard-face on ResNet50]
- Models can increase biases
  - Underfitting and overfitting
  - preceptron for bonus attribution

AI, equality and environment

- Generalizing AI pushes forward development of microelectronics, energy consumption, mining of rare elements, etc. having a strong environmental impact (especially in mining countries).
- Hardware producers / cloud computing providers are mainly based in economically developed countries, which further digs the economic gap between nations.

Conclusion

Open problems

- (Fully) understand generalization ability of deep NN
- How to improve collaboration/reuse of models in AI?
  - Model distillation (big model $\rightarrow$ small model)
  - Transfer learning (application A $\rightarrow$ application B)
- How to reduce learning hassle?
  - Unsupervised learning
  - Few-shot learning
- How to have guarantees?
  - Explainable AI
- How to reduce/remove biases (disentangle correlation and causality)
- How to regulate the creations/usages of AI[10]?

[10] Cannot rely on companies for this. See here.

To sum up: what can I do with DL?

As soon as you have data, either labelled or unlabelled, you can learn a model.
If there is some *information*[11] in your training set, there is a good chance that the model will learn it.
You can use this model to predict on further data, to take decision, to estimate values, etc.

Beware

Although powerful in many situations, there is no magic in AI: it often involves a lot of architecture engineering, data science expertise and extensive benchmarking.

Pre-computed models

Many basic tasks (segmentation, image classification, etc.) can be achieved using pre-trained models. You can adapt your model to your specific dataset (few-shot learning).

[11]

The good, the bad, and the ugly

What applications would you consider as beneficial or detrimental in your field?

Discussion and questions?

Regularization

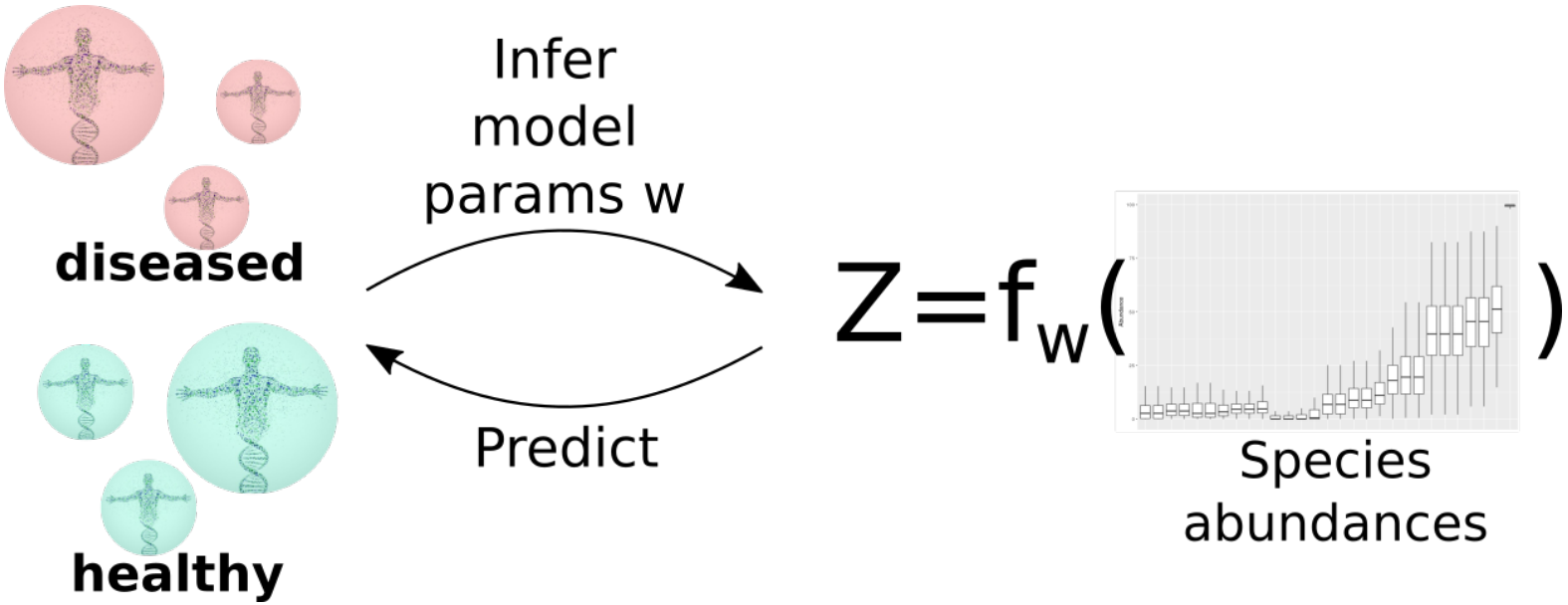
Regularization is an important technique that aims at excluding unrealistic parameter combinations.

- Ridge regularization: avoids big values of parameters
- Lasso regularization: favor nullity of parameters (parcimonious model)
- Bayesian modeling: model a priori knowledge on each parameter

Application: example in health

MWAS: metagenome-wide association studies

We can build models to predict diseases from microbial abundances, a process known as MWAS:



MWAS as a classification problem

Let:

- $\vec{X}$ be an M-dimensional random vector of abundance of species,
- and Z binary (0/1) random variable describing the disease state of a human.

Define a predictor $f : \mathbb{R}_+^M \to [0, 1]$ such that it minimizes a *loss* on a training set $(\vec{x}_1, z_1), ..., (\vec{x}_N, z_N)$:

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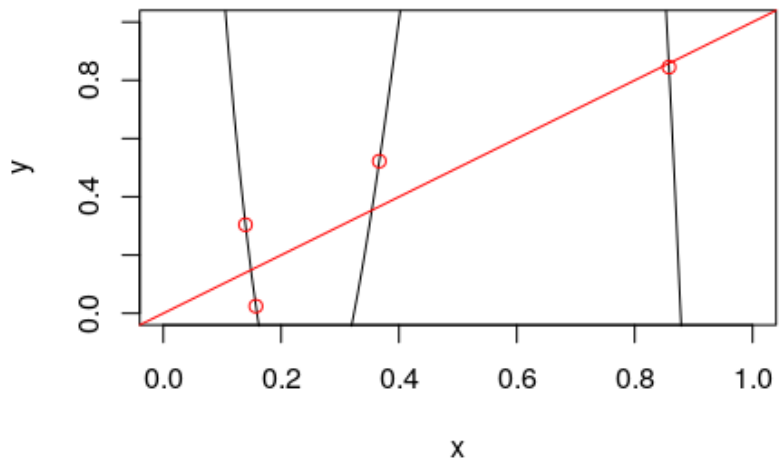
$$\min_f - \sum_{i=1}^{N} z_i . \log f(\vec{x}_i) + (1 - z_i) . \log(1 - f(\vec{x}_i))$$

Regularization

Ridge regularization example

Let's come back to the model $Y = \sum_{i=0}^{3} \beta_i x^i + \epsilon$.

The maximum likelihood with 4 points will give a $\vec{\beta}$ fitting perfectly the points:



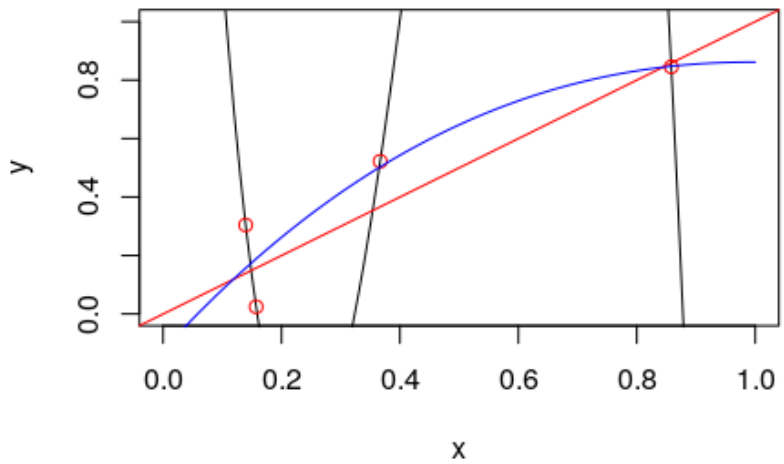
Maximum *likelihood* coefficients:

β_0	β_1	β_2	β_3
5.169	-54.388	155.755	-114.487

Ridge regularization example

Let's come back to the model $Y = \sum_{i=0}^{3} \beta_i x^i + \epsilon$.

With a prior $\mathcal{N}(0, \eta^2)$ the maximum a posteriori of the vector $\vec{\beta}$ corresponds to (blue curve):



Maximum *a posteriori* coefficients

β_0	β_1	β_2	β_3
-0.1279	2.2561	-1.5779	0.3180

Quizz

Overfitting depends on:

- Size of the training set
- Complexity of the problem
- The parametrization of the model
- The type of the model