

Why deep learning?

Some technical and practical aspects

Clovis Galiez



Grenoble

Statistiques pour les sciences du Vivant et de l'Homme

February 24, 2021

AI? What is it?
What for?
What types?

Our scope of AI today

Long-standing dream (back to the anciant Greeks)¹ of having intelligent artificial creatures.

¹See [The Quest for Artificial Intelligence, Nils J. Nilsson]

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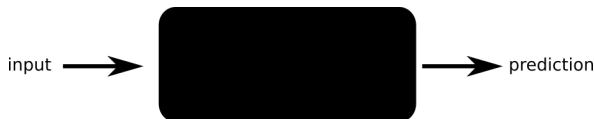
We focus here on the modern acceptation of AI: a computer program able to autonomously react to a context to achieve a goal.

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In particular, we will focus on (the distinction between):

- machine learning
- neural networks
- deep learning

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Controversies

In the media:

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

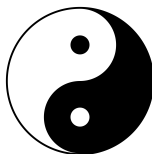
Interesting article about biases in [The Conversation](#).

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.

Be fair but critical



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 **good**, one as **bad**. Try to think in particular what would be the **societal impacts** if the examples you chose were generalized in the world.
Let's check 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
- Applications
- Timeline and future of AI
 - Biases
 - Ethics
 - Open problems

AI what for?

Any idea?

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- Operational (automation of tasks)
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 - Indexing images, tagging
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 - Extraction of information
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We trust the human more than the AI.
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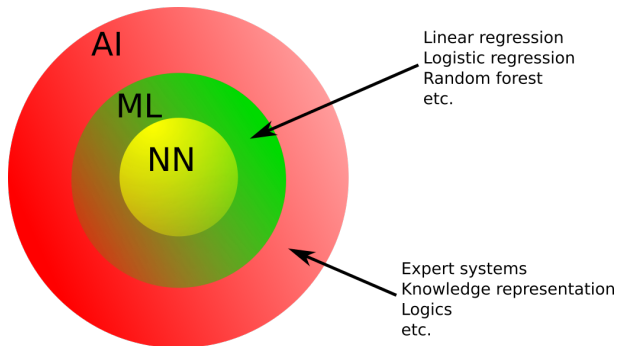
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In both cases we are interested by the quality of the prediction, but may be also interested by bound guarantees or explanation of the “black-box”.

AI taxonomy



We will focus on the *data science* part of artificial intelligence :
machine learning.

Some machine learning methods

What machine learning tool you already know?

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For classification tasks:

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

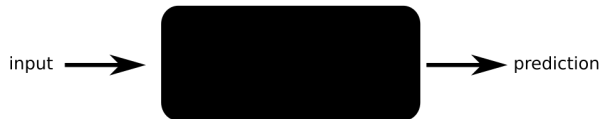
For regression tasks:

- Linear regression
- Regressive artificial neural networks

But also include parts of symbolic AI:

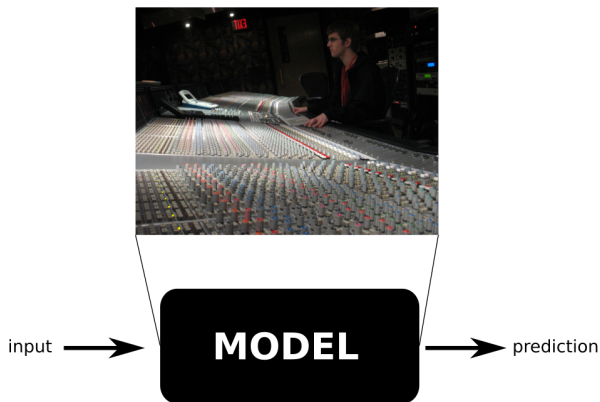
- Grammar inference
- Logic rule inference

Machine learning

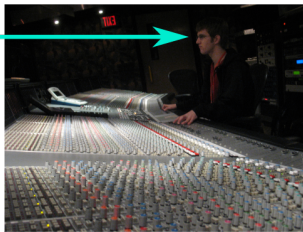




Machine learning



Machine learning



input

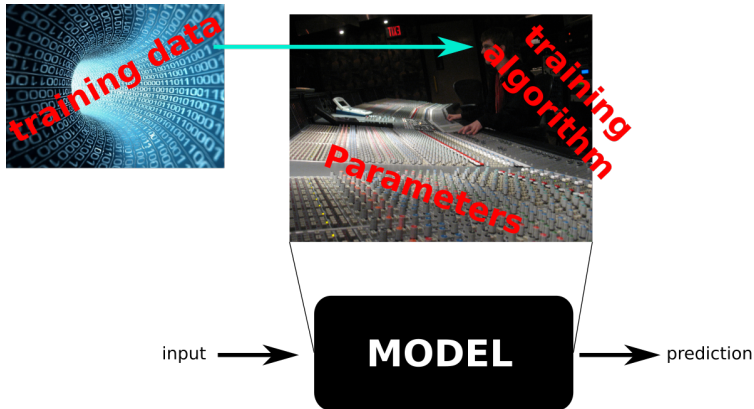


MODEL



prediction

Machine learning



Some order of magnitude: number of parameters

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

²[Brown et al. 20]

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Number of possible combinations:

$$2^{175.10^9}$$

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How it is possible to train such a model?

²[Brown et al. 20]

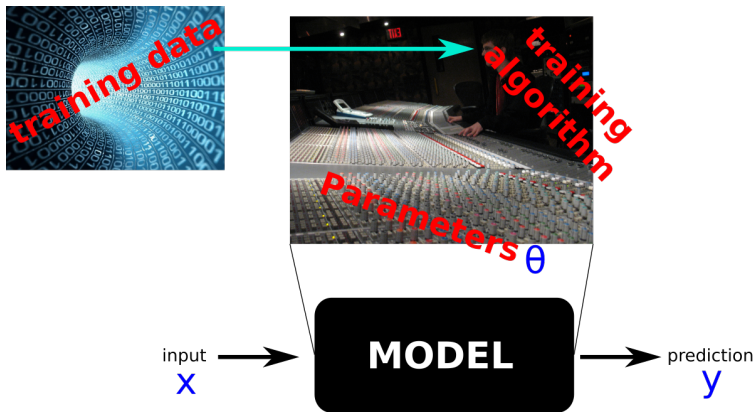
Some order of magnitude: training data

- 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

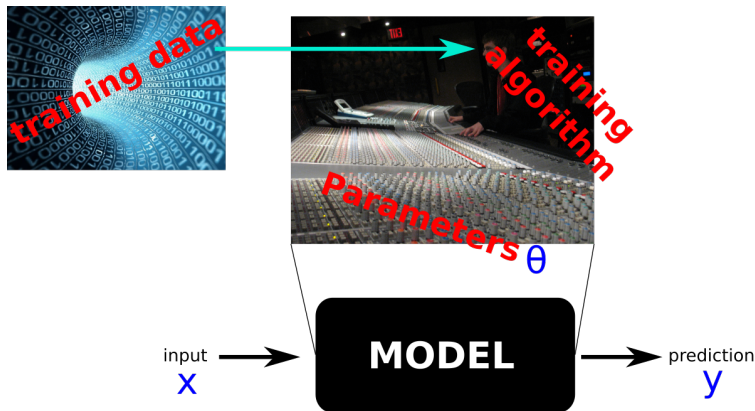
- Open Image Dataset V6 (18TB):
 - 9M images
 - 2M with labels from 600 classes

Training ML models



What training data?

Training ML models



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

Worked-out example



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

Worked-out example



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

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

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(operational)

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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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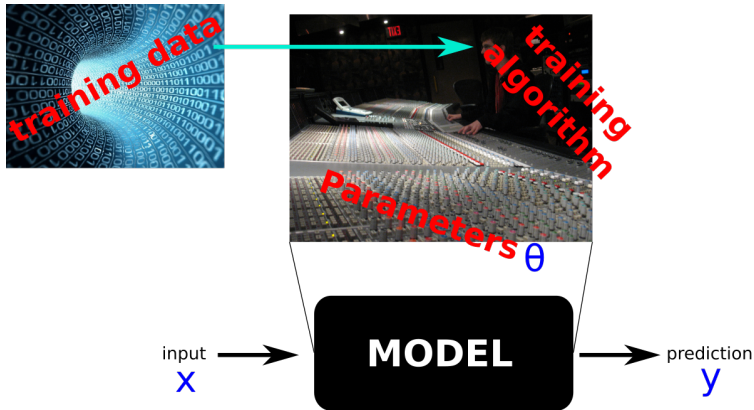
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Need to find the right θ_0 and θ_1 .

We say we need to **fit** the model.

Worked-out example: fitting

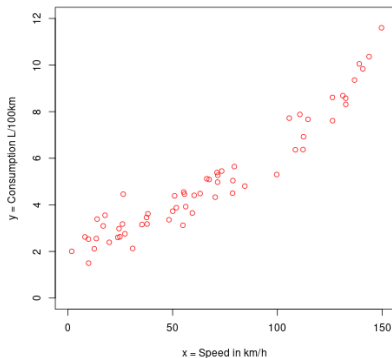


Worked-out example: the training data



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:

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

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Goal: find optimal θ_0, θ_1 such that:

$$\forall i = 1, \dots, 60, y_i \approx \theta_0 + \theta_1 \cdot x_i$$

Worked-out example: fitting the model

Goal: find optimal θ_0, θ_1 such that:
 $\forall i = 1, \dots, 60, |y_i - (\theta_0 + \theta_1 \cdot x_i)|$ is small

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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

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

is **minimal**.

Worked-out example: fitting the model

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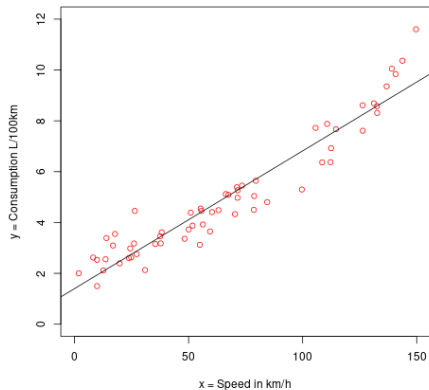
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Definition

\mathcal{L} is called a **loss function** for the model^a.

^aThis one in particular is called the *mean squared error*

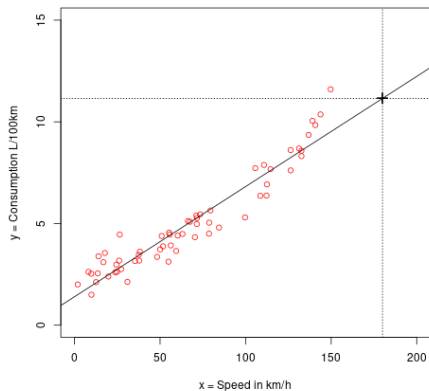
Worked-out example: the fit



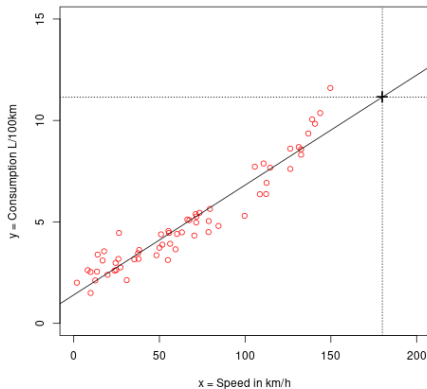
Worked-out example: the prediction



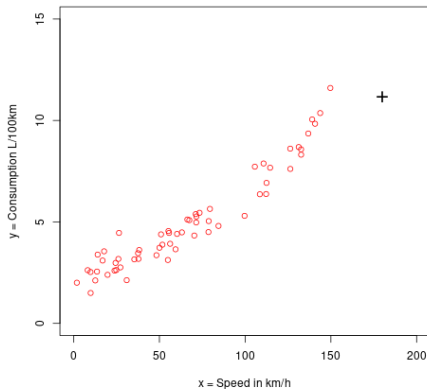
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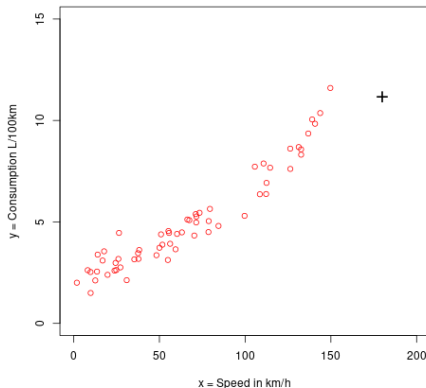
Worked-out example: toward more complex models



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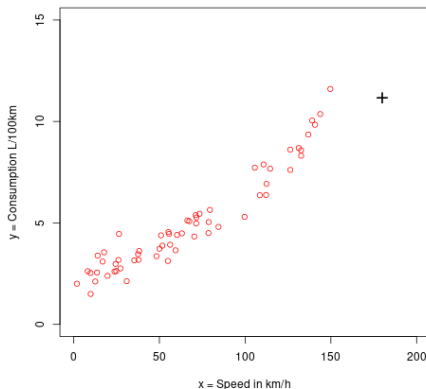


Worked-out example: toward more complex models



Any comment?

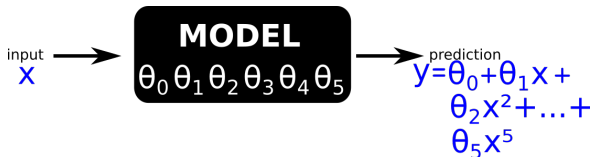
Worked-out example: toward more complex models



Any comment?

This phenomenon is known as **underfitting**

Worked-out example: toward more complex models



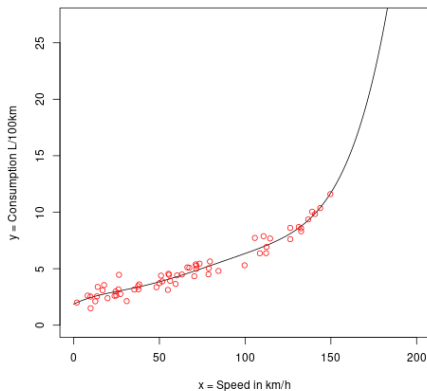
Worked-out example: toward more complex models

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

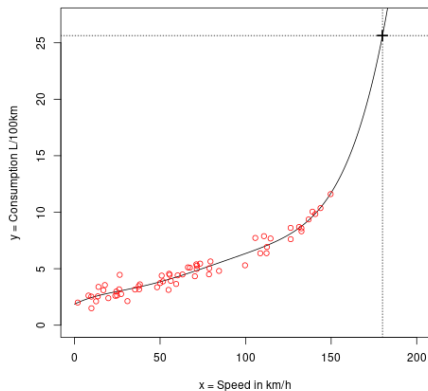
$$\mathcal{L}(\theta_0, \dots, \theta_5) = \frac{1}{60} \sum_{i=1}^{60} [y_i - (\sum_{j=0}^5 \theta_j \cdot x_i^j)]^2 \quad (2)$$

is **minimal**.

Worked-out example: toward more complex models



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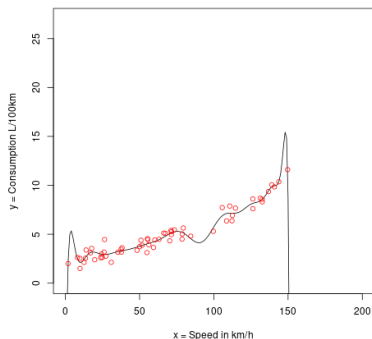
Worked-out example: toward more complex models

Informal definition

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

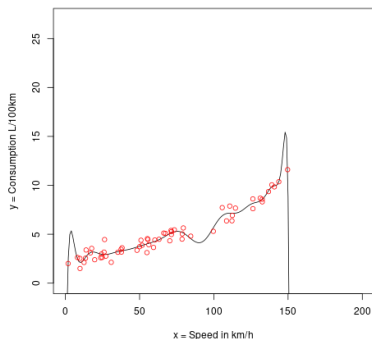
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With 30 parameters: $\theta_0, \dots, \theta_{29}$

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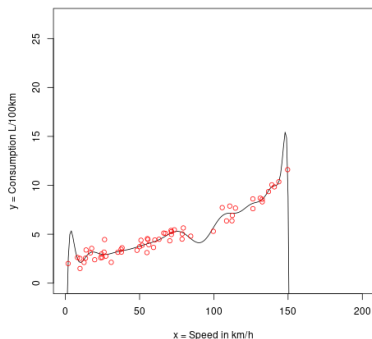


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Definition

The phenomenon is called **overfitting**.

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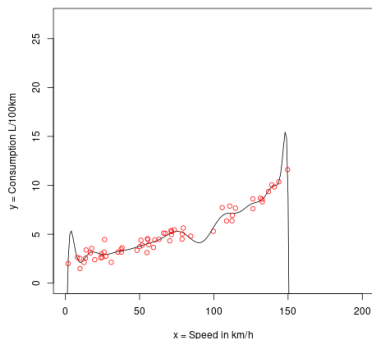


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The phenomenon is called **overfitting**. Mainly happens because of **hyperparametrization**.

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Cross-validation to control overfitting



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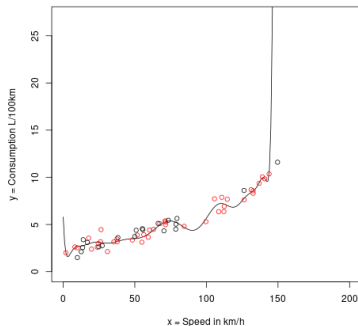


Cross-validation to control overfitting



Cross-validation example: 30 parameters

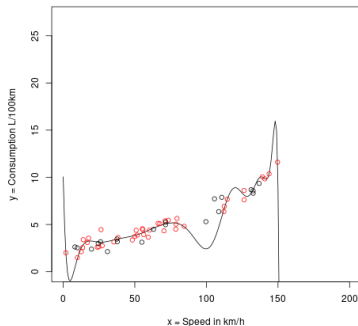
Red: training set Black: validation set



30 parameters, fold 1

Cross-validation example: 30 parameters

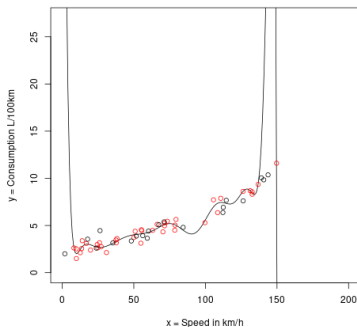
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30 parameters, fold 2

Cross-validation example: 30 parameters

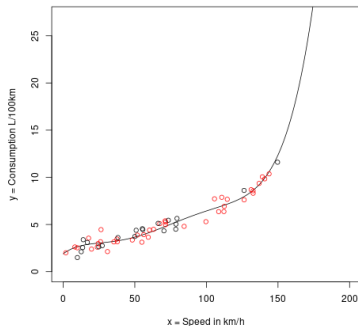
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30 parameters, fold 3

Cross-validation example: 6 parameters

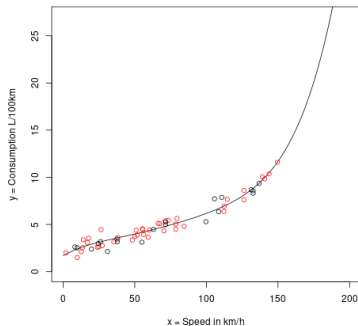
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6 parameters, fold 1

Cross-validation example: 6 parameters

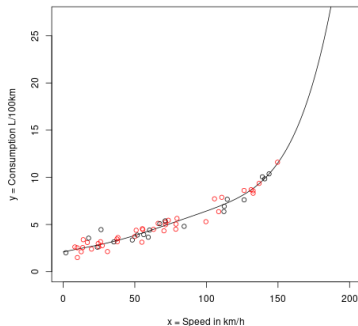
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6 parameters, fold 2

Cross-validation example: 6 parameters

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6 parameters, fold 3

What do you observe?

- Lower error on training with ___parameters
- If the error on the validation is much higher than on training set, it means that the model ____.
- More variance among fits with ___parameters³

³As we will see, things are different with neural nets

What do you observe?

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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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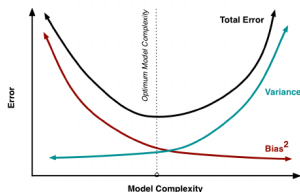
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- More variance among fits with **more** parameters³

More specifically, one can decompose the error of the model as:

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

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



³As we will see, things are different with neural nets

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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Quizz - Checkpoint

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

Quizz - Checkpoint

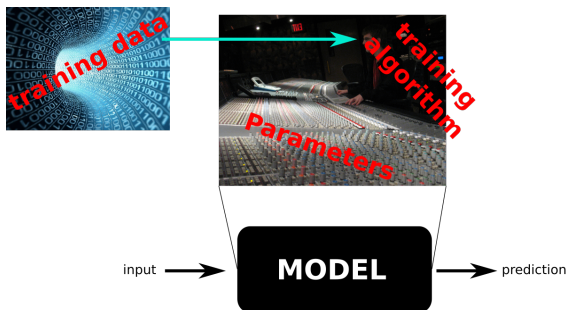
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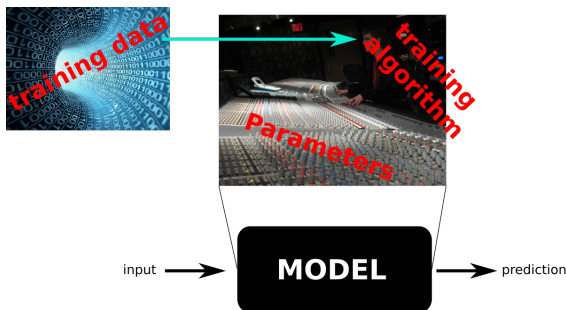
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Remaining questions:

- 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.

Learning algorithms

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

Learning algorithms

Of course...

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

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 $\theta_0, \theta_1, \dots, \theta_p$ such that

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

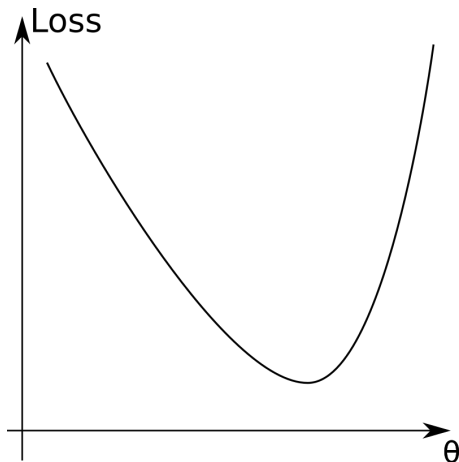
is **minimal**.

One would like to find the minimum of this loss.

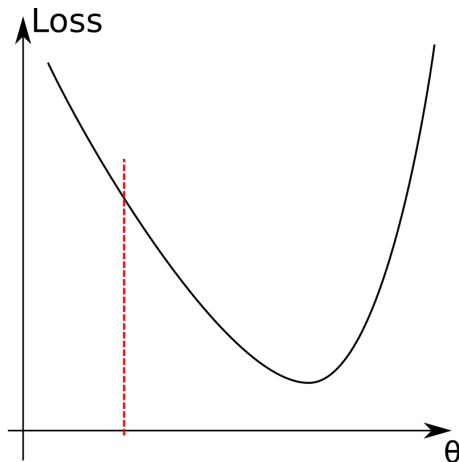
Issue: $p, n \sim 10^9$

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

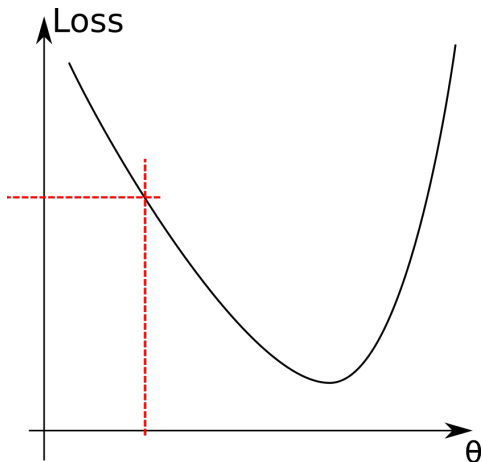
Gradient descent for convex loss



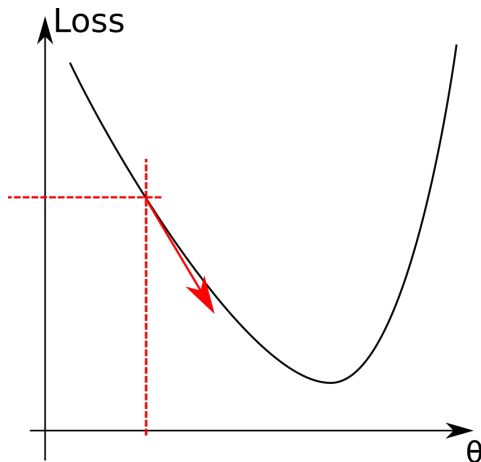
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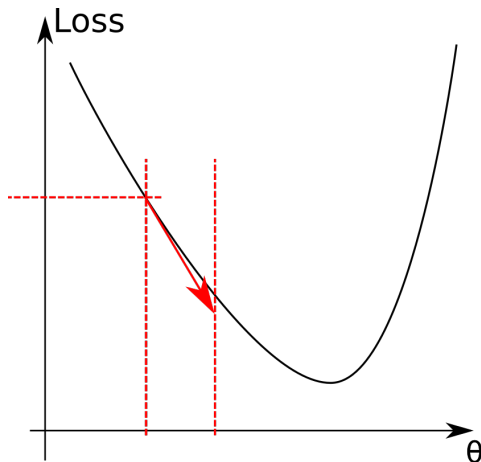
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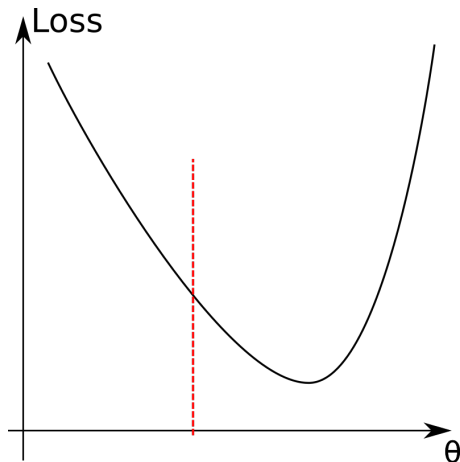
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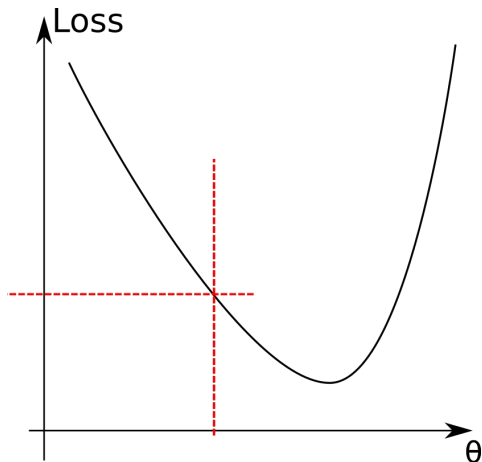
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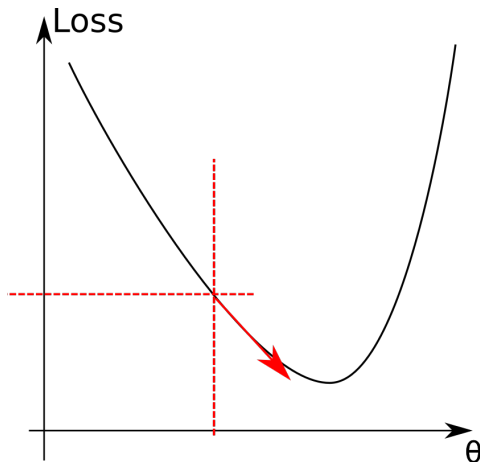
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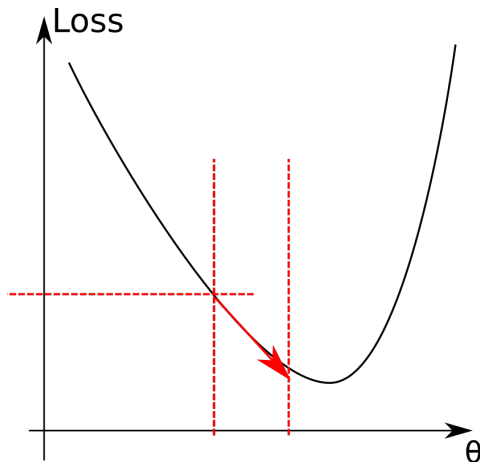
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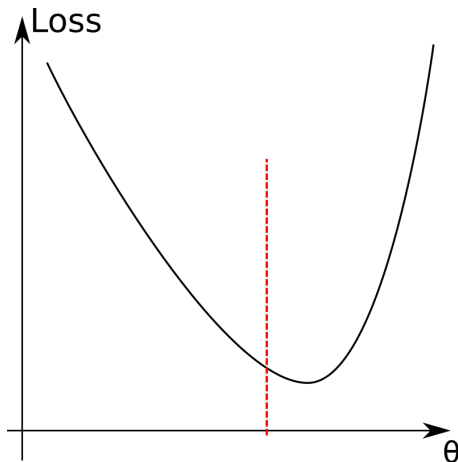
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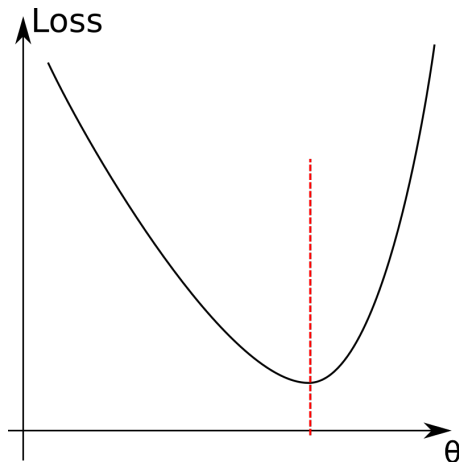
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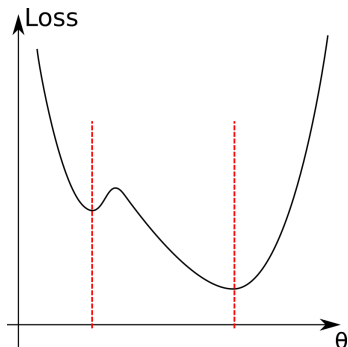
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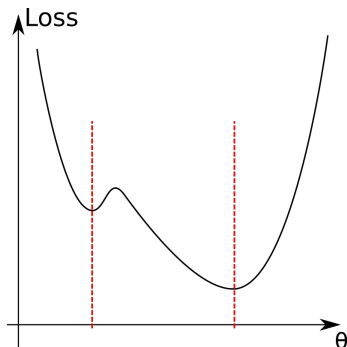


Gradient descent for **non-convex** loss



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

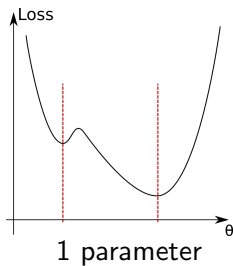
Gradient descent for **non-convex** loss



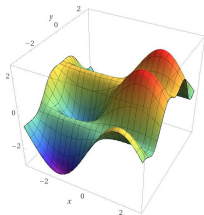
The gradient descent stops when it reaches a **critical point**: $\nabla \mathcal{L}(\theta_n) = \vec{0}$

What are the possible *types* of critical points?

Critical points in higher dimension

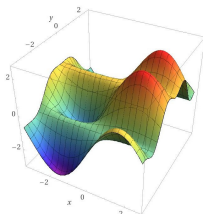


Critical points in higher dimension



≥ 2 parameters

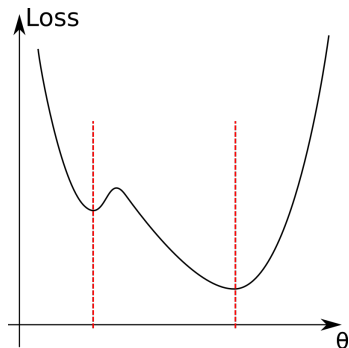
Critical points in higher dimension



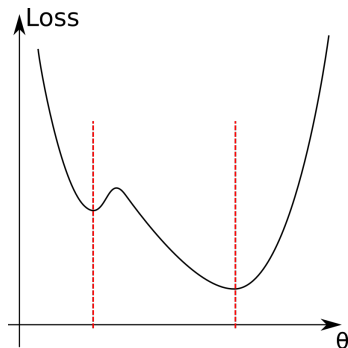
Type	Hessian ⁴
Local minimum	all eigenvalues > 0
Local maximum	all eigenvalues < 0
Saddle points	else

⁴ $\mathcal{H}_{ij} = \frac{\partial^2 \mathcal{L}}{\partial \theta_i \partial \theta_j}$

Escaping *easy* local minima



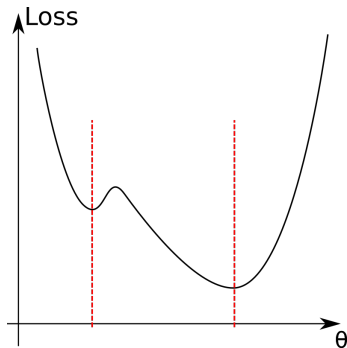
Escaping *easy* local minima



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

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

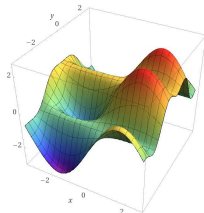
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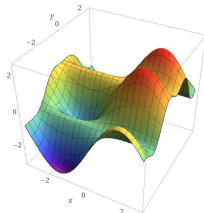
Escaping local non-minimal critical points



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

⁵Would need to invert a $175 \cdot 10^9$ dimensional matrix for GPT3... $\approx 5.3 \cdot 10^{33}$ operations :-/

Escaping local non-minimal critical points

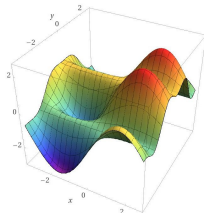


How is it possible to escape a critical point that is **not** a minimum?

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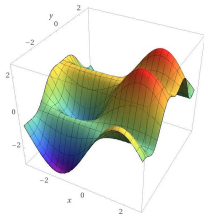


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Escaping local non-minimal critical points



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

- Compute the Hessian (too big if a lot of parameters⁵)
- **Add "noise" to the gradient !**

How to add some noise?

⁵Would need to invert a $175 \cdot 10^9$ dimensional matrix for GPT3... $\approx 5.3 \cdot 10^{33}$ operations :-/

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.

⁶By linearity of expectation: $\mathbb{E}_{\mathcal{B}}[\mathcal{L}_{\mathcal{B}}(\theta, X, Y)] = \mathcal{L}(\theta, X, Y)$

Stochastic gradient descent (SGD)

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

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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 unbiased⁶ **noisy** estimate of the gradient:

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

⁶By linearity of expectation: $\mathbb{E}_{\mathcal{B}}[\mathcal{L}_{\mathcal{B}}(\theta, X, Y)] = \mathcal{L}(\theta, X, Y)$

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)
- works very well in practice to find *good* local minima

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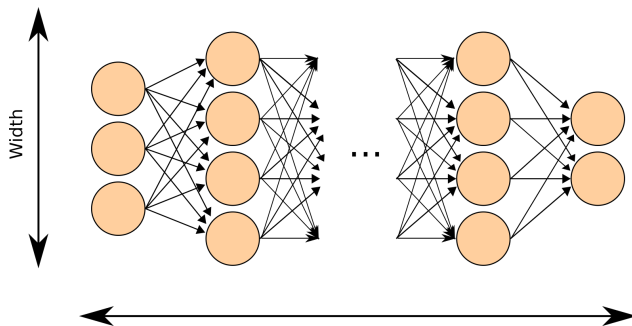
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It seems that we have a candidate to train a model with billions of parameters...

Neural Networks

Neural networks

Dense feed-forward neural network:



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

Parameters⁷: $w_{j,k}$'s.

σ_l : activation functions.

⁷GPT-3 has 96 layers and 175B parameters

Input and outputs

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

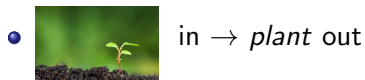
It can be:



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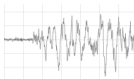
It can be:

-  in \rightarrow  out
-  in \rightarrow *plant* out
- *Draw me a plant* in \rightarrow  out

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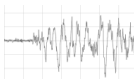
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It can be:

-  in \rightarrow  out
-  in \rightarrow *plant* out
- *Draw me a plant* in \rightarrow  out
-  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

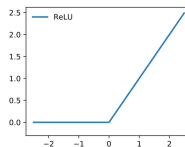
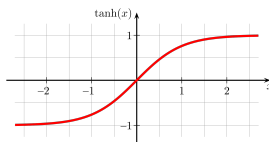
Let's see how an ANN looks like in practice:

<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 $f : \mathbb{R}^m \rightarrow \mathbb{R}$, there exists a ReLU neural network η such that:

$$\int |f(x) - \eta(x)| dx < \epsilon \quad (6)$$

Moreover, one can also restrict 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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Which training algorithm?

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Nevertheless...

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

$$f_w(x) = \sigma_d\left(\sum_{k_d} w_{d,1,k_d} \sigma_{d-1}\left(\sum \dots \sigma_1\left(\sum_{k_1} w_{1,i,k_1} x_{k_1}\right)\right)\right).$$

How to fit the parameters w_{jkl} ?

- Get a training set (x_s, y_s) , can range from kB to TB of data⁸.
- Define a loss function, for instance $\mathcal{L}(w) = \sum_s [y_s - f_w(x_s)]^2$.
- Then compute⁹ the derivatives $\frac{\partial \mathcal{L}}{\partial w_{i,j}}$
- Use your favorite variant of SGD, and find a good minimum of the loss.

⁸the more the better

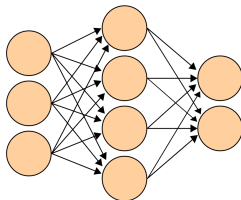
⁹An analytical formula can be obtained by a computer for well-chosen activation functions

Architecture matters for training: resNet example

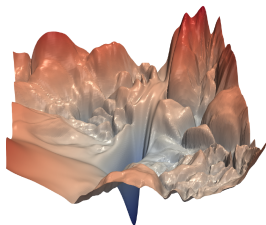
The loss function can change dramatically depending on the NN architecture.

Architecture

Dense



Loss landscape

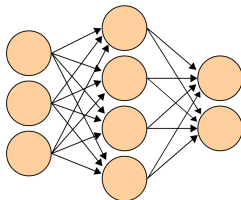


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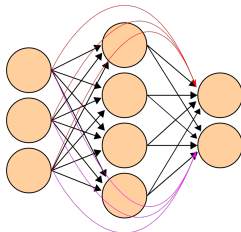
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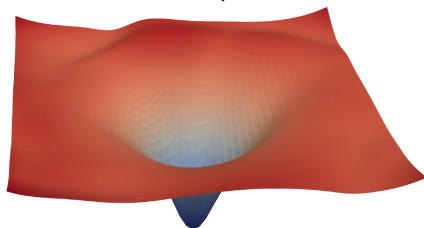
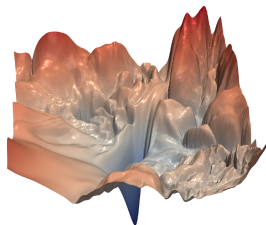
Dense



resNet



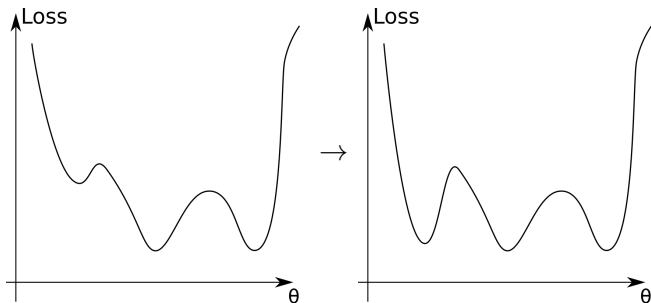
Loss landscape



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?!

ANN and optimization

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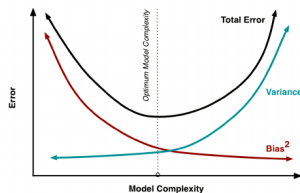
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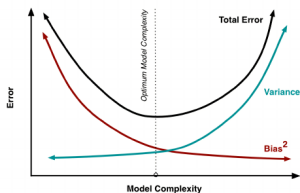
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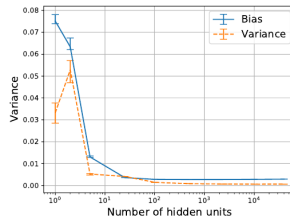
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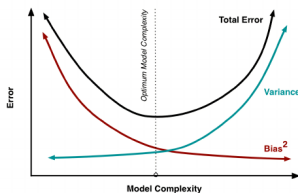
[Neal et al. 19]



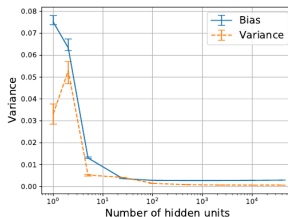
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Variance increasing with the nb of parameters is not true for SGD-learned ANN.



[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 transferred 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:

¹⁰Actually it may be also why biological neural nets have been selected by evolution

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- More data (better as for any ML, allows for more depth)
- Better optimization algorithms (SGD and its variants)
- Better hardware (GPUs for parallel computations)
- Some luck¹⁰: ANN tend *not* to overfit (but it has been noticed afterwards)



¹⁰Actually it may be also why biological neural nets have been selected by evolution

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: convolutional neural nets (CNN)

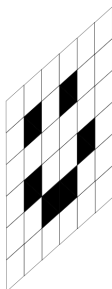


Image processing: convolutional neural nets (CNN)

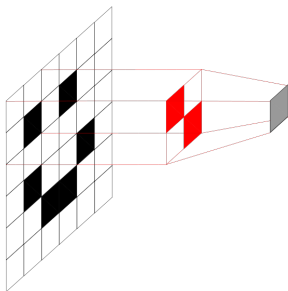


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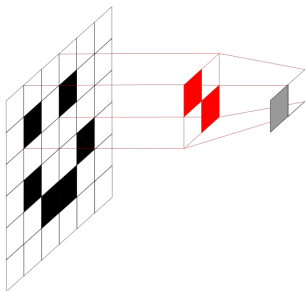


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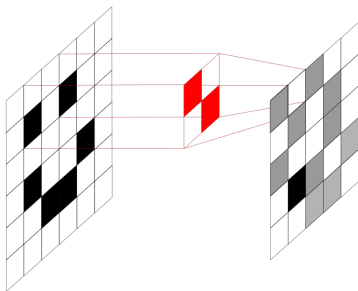


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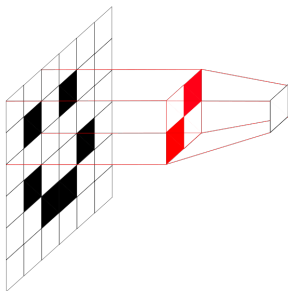


Image processing: convolutional neural nets (CNN)

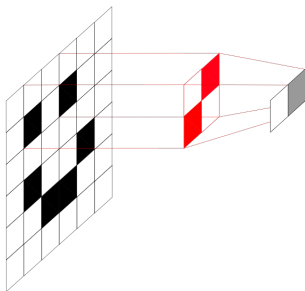


Image processing: convolutional neural nets (CNN)

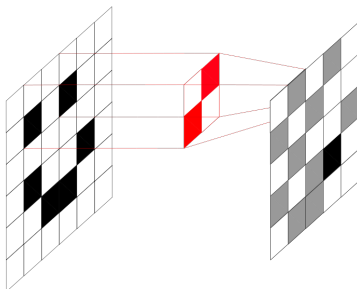


Image processing: convolutional neural nets (CNN)

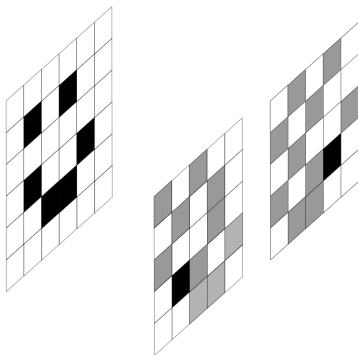
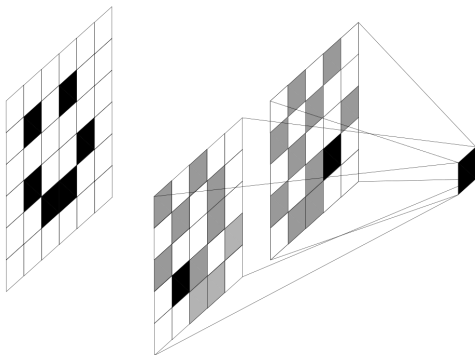
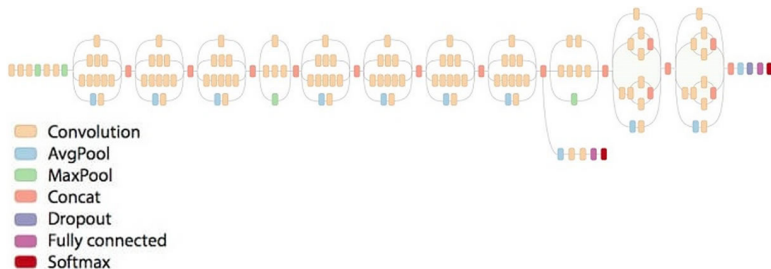


Image processing: convolutional neural nets (CNN)



Real-world CNN



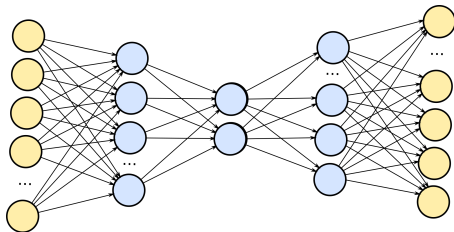
Source: InceptionV3

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”*¹¹. The mid-layer is called a latent and contains a compressed version of the input. Works when the data has an underlying structure.

¹¹ “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 balloons can be sent per year.
- hourly acquisition of 2000x2000px satellite images

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

—

Compressing data: autoencoders

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

Compressing data: autoencoders

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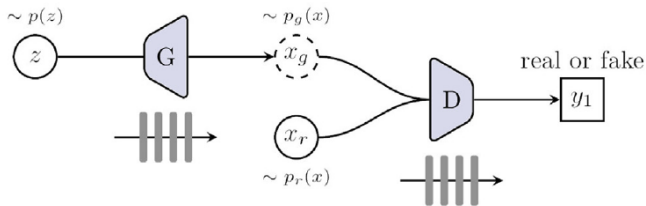
What will happen if we learn the pollution from the raw satellite images?

Overfitting

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

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

Generative Adversarial Networks (GAN)



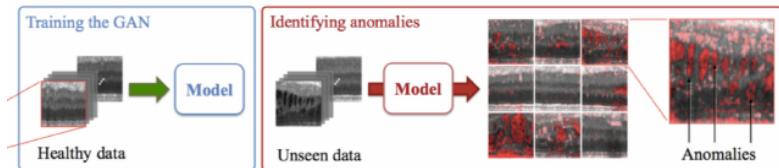
Equilibrium reached when $p_g = p_r$

Generative Adversarial Networks (GAN)



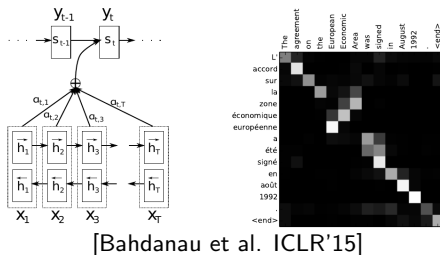
Can be use as a **generative** process

Generative Adversarial Networks (GAN)



or as a classifier [Yi et al. 20]

Text processing: attention mechanism

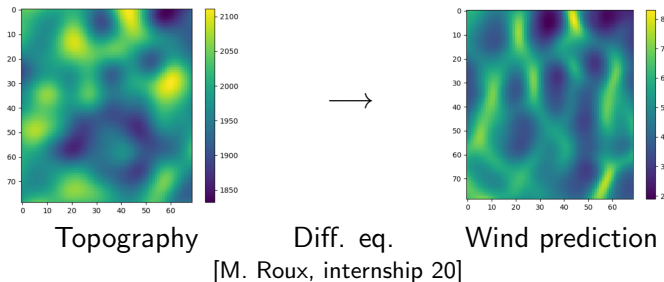


Improvement of the same idea: the Transformer architecture [Vaswani et al. 17] ,[Brown et al. 20]

Applications

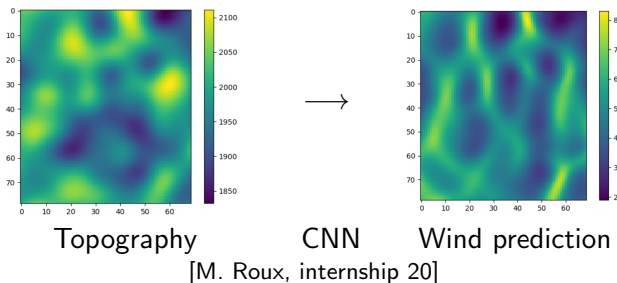
Surrogate models

Goal: use a neural network to approximate a costly model



Surrogate models

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Glaciers grow and melt



AI and glacier evolution prediction

The causes influencing the evolution of glacier are complex:

- temperature 
- solar radiation 
- albedo of the glacier
- wind
- ...

Yearly mass balance can be estimated with physical models involving all these parameters.

Physical parameters are hard to get

Measuring the physical parameters can be cumbersome.

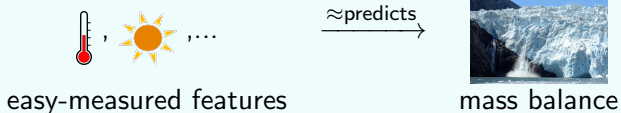


...sometimes hard to evaluate (e.g. measuring properties of the ice).

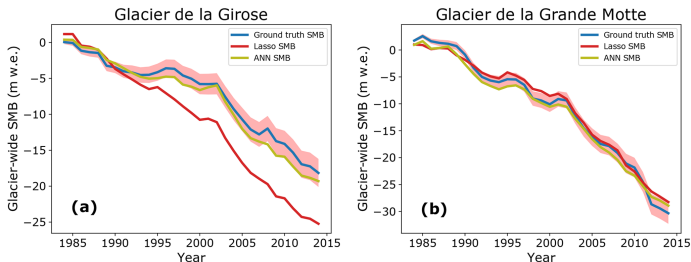
Even with the fanciest physical model (that can also be wrong), the results can't be totally accurate.

Use unbiased and easy to measure *proxy* parameters

We can design a regression NN model so that we predict the mass balance:

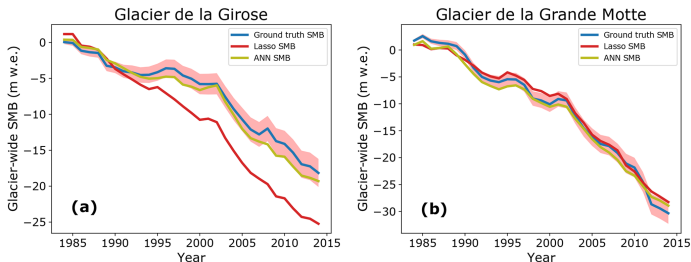


Regression glacier model: better than linear



[Bolibar et al. 2020]

Regression glacier model: better than linear

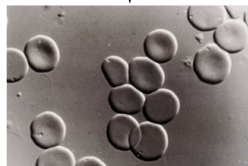
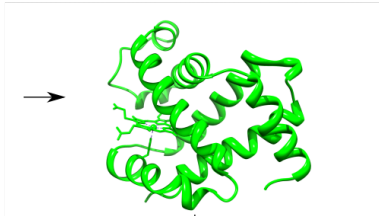
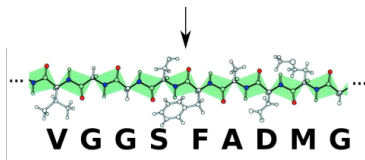


[Bolibar et al. 2020]

Why not done before? Overfitting was hard to get rid of!

Protein sequence and structure

ACG**ATGTATTCAGCGATTACGATAAAGCTACGTAGT**GGCA

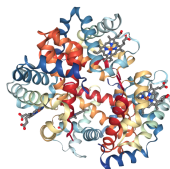


O₂ transport

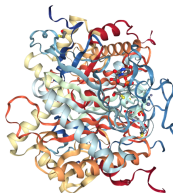
A recent big achievement: protein structure prediction

Goal: predict the structure from sequence

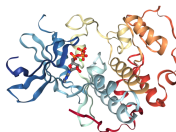
```
>1A3N:A|PDBID|CHAIN|SEQUENCE
VLSPADKTNVKAAGKVGAGHAGEYGAEALER
MFLSFPTTKTYFPHFDLSHGSAQVKGHGKKV
ADALTNAAVHVDDMPNALSALSDLHAHKLRV
DPVNFKLLSHCLLVTLAAHLPAEFTPAVHAS
LDKFLASVSTVLTSKYR
```



```
>1HXP:A|PDBID|CHAIN|SEQUENCE
MTQFPNPVDHPHRRYNPLTGQWILVSPHRAKRPW
EGAQETPAKVQLPAHDPDCLCAGNVRVTGDKN
PDVYTGTYVFTNDFALMSDTPDAPESHDPIMRC
QSARGTSRVICFSPDHSKTLPELSVAALTEIVK
TWQEQTAELGKTYFWQVFENKGAAMGCSNPHP
HGQIWANSFLPNEAEREDRLQKEYFAQKSPML
VDYVQRELADGSRVTEHMLAVVPYWAANPF
ETLLLPKHAHLRITDITDAQRSDLAALKLTS
RYDNLFCQSFPPSMGWHGAPFNGEENQHWQLHA
HFYPPLLRSATVRKFMVGYEMLAETQRDLTAEQ
AAERLRAVSDIHFRESGV
```



```
>1HCK:A|PDBID|CHAIN|SEQUENCE
MENPQKVEKIGEGTYGVVYKARNKLTGEVVAL
KKIRLDTEGVPSTAIREISLLKELNHPNIV
KLLDVIHTENKLYLVFEFLHQDLKKFMDASAL
TGIFPLPKSYLFQLLQGLAFCHSHRVLHRDL
KPNQLINTEGAIKLADPGLARAGVVPVRYT
HEVVTWYRAPEILLGCKYYSTAVDINSLGCI
FAEMVTRRALFPDGSEIDQLFRIFRTLGTPE
VVMFGVTSMPDYKFSFPKNARQDFSKVPPFD
EDGRSLLSQMDLHYDNPKRISAKAALAHPPFD
VTKFPVPHRL
```



CASP competition

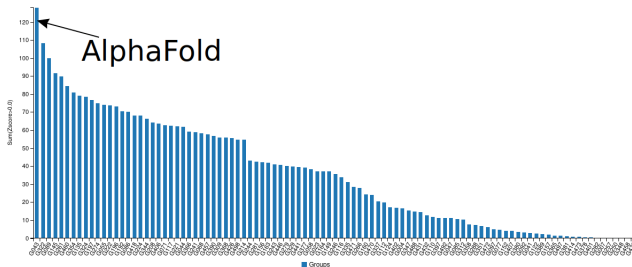
Blind competition. Simple principle:

- a sequence is given
- have to predict the structure.

Prior to 2018 it used to be (pseudo) physical models that were best performing.

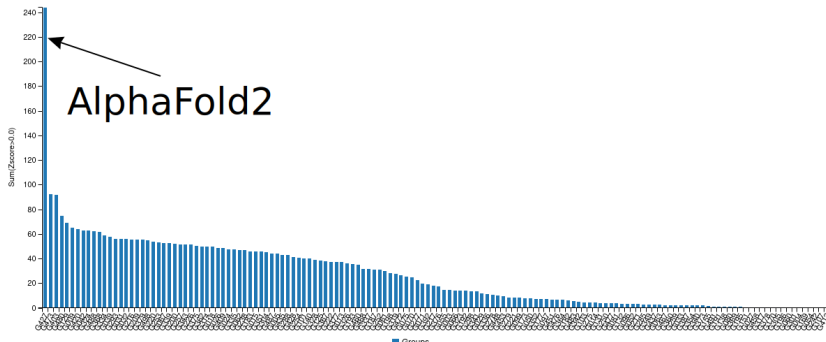
CASP13 (2018)

Al wins the challenge for the first time.



CASP14 (2020)

“The big leap forward”



Alphafold2: attention-based learning on protein sequence alignments

[Casp14.]

Nature's article.

Some fun and worrying examples: deepfake

[link to video](#)

Some useful and worrying examples: GPT3 examples

Poor English input: I eated the purple berries.

Good English output: I ate the purple berries.

Poor English input: Thank you for picking me as your designer. I'd appreciate it.

Good English output: Thank you for choosing me as your designer. I appreciate it.

Poor English input: The mentioned changes have done. or I did the alteration that you requested. or I changed things you wanted and did the modifications.

Good English output: The requested changes have been made. or I made the alteration that you requested. or I changed things you wanted and made the modifications.

Poor English input: I'd be more than happy to work with you in another project.

Good English output: I'd be more than happy to work with you on another project.

Poor English input: Please provide me with a short brief of the design you're looking for and that'd be nice if you could share some examples or project you did before.


Good English output: Please provide me with a brief description of the design you're looking for and that would be nice if you could share some examples or projects you have done before.

Poor English input: The patient was died.

Good English output: The patient died.

Poor English input: We think that Leslie likes ourselves.

Good English output: We think that Leslie likes us.

That's useful. 

Some useful and worrying examples: GPT3 examples

Helsinki is the capital and largest city of Finland. It is in the region of Uusimaa, in southern Finland, on the shore of the Gulf of Finland. Helsinki has a population of , an urban population of , and a metropolitan population of over 1.4 million, making it the most populous municipality and urban area in Finland. Helsinki is some north of Tallinn, Estonia, east of Stockholm, Sweden, and west of Saint Petersburg, Russia. Helsinki has close historical connections with these three cities.

The Helsinki metropolitan area includes the urban core of Helsinki, Espoo, Vantaa, Kauniaiainen, and surrounding commuter towns. It is the world's northernmost metro area of over one million people, and the city is the northernmost capital of an EU member state. The Helsinki metropolitan area is the third largest metropolitan area in the Nordic countries after Stockholm and Copenhagen, and the City of Helsinki is the third largest after Stockholm and Oslo. Helsinki is Finland's major political, educational, financial, cultural, and research center as well as one of northern Europe's major cities. Approximately 75% of foreign companies that operate in Finland have settled in the Helsinki region. The nearby municipality of Vantaa is the location of Helsinki Airport, with frequent service to various destinations in Europe and Asia.

Q: what is the most populous municipality in Finland?

A: Helsinki

Q: how many people live there?

A: 1.4 million in the metropolitan area

Q: what percent of the foreign companies that operate in Finland are in Helsinki?

A: 75%

That's impressive. 🤖

Some useful and worrying examples: GPT3 examples

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church has agreed to a historic split - one that is expected to end in the creation of a new denomination, one that will be "theologically and socially conservative," according to The Washington Post. The majority of delegates attending the church's annual General Conference in May voted to strengthen a ban on the ordination of LGBTQ clergy and to write new rules that will "discipline" clergy who officiate at same-sex weddings. But those who opposed these measures have a new plan: They say they will form a separate denomination by 2020, calling their church the Christian Methodist denomination.

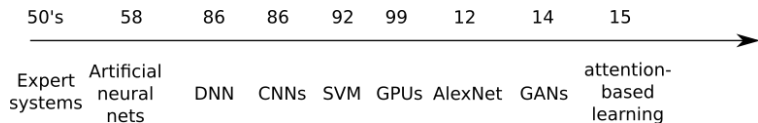
The Post notes that the denomination, which claims 12.5 million members, was in the early 20th century the "largest Protestant denomination in the U.S.," but that it has been shrinking in recent decades. The new split will be the second in the church's history. The first occurred in 1968, when roughly 10 percent of the denomination left to form the Evangelical United Brethren Church. The Post notes that the proposed split "comes at a critical time for the church, which has been losing members for years," which has been "pushed toward the brink of a schism over the role of LGBTQ people in the church." Gay marriage is not the only issue that has divided the church. In 2016, the denomination was split over ordination of transgender clergy, with the North Pacific regional conference voting to ban them from serving as clergy, and the South Pacific regional conference voting to allow them.

Figure 3.14: The GPT-3 generated news article that humans had the greatest difficulty distinguishing from a human written article (accuracy: 12%).

That's worrying! 🤔

Past and future

Timeline



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
 - preception for hiring

AI and CO₂

AI can consumes a lot of electrical energy, having a strong environmental impact. Here are some figures showing the equivalent CO₂ emission for creating some famous AI models for natural language processing:

Model	Hardware	Power (W)	Hours	kWh·PUE	CO ₂ e	Cloud compute cost
Transformer _{base}	P100x8	1415.78	12	27	26	\$41–\$140
Transformer _{big}	P100x8	1515.43	84	201	192	\$289–\$981
ELMo	P100x3	517.66	336	275	262	\$433–\$1472
BERT _{base}	V100x64	12,041.51	79	1507	1438	\$3751–\$12,571
BERT _{base}	TPUv2x16	—	96	—	—	\$2074–\$6912
NAS	P100x8	1515.43	274,120	656,347	626,155	\$942,973–\$3,201,722
NAS	TPUv2x1	—	32,623	—	—	\$44,055–\$146,848
GPT-2	TPUv3x32	—	168	—	—	\$12,902–\$43,008

Table 3: Estimated cost of training a model in terms of CO₂ emissions (lbs) and cloud compute cost (USD).⁷ Power and carbon footprint are omitted for TPUs due to lack of public information on power draw for this hardware.

[Strubell et al. 19]

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 AI¹²?

¹²Cannot rely on companies for this. See [here](#).

To sum up: what can I do with DL?

As soon as you have data, either labeled or unlabeled, you can learn a model (in particular a DNN).

If there is some *information*¹³ 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.

Note that now, most of the 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).

¹³for instance between the data and the labels, or a structure underlying the data

The good, the bad, and the ugly

What applications would you consider as beneficial or detrimental for the society?

The good, the bad, and the ugly

What applications would you consider as beneficial or detrimental for the society?

- Backfire effect/Jevons paradox



- Less humanistic considerations
- Biases
- “Unresponsibilizing”
- Pushes society toward technology
- Automation of (boring) tasks
- Prevents from human mistakes
- Allow extract (unseen) information from data

Discussion and questions?

Regularization

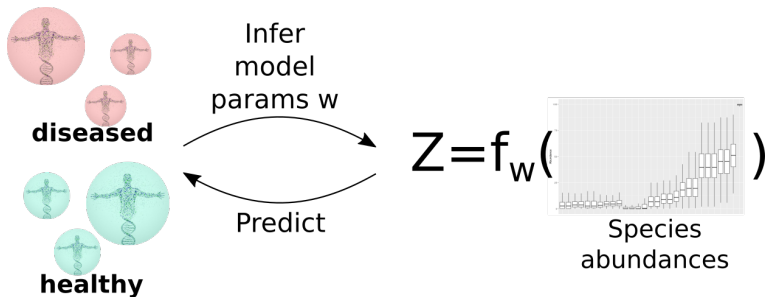
Regularization is an important technique that aims at excluding unrealistic parameter combinations.

- Ridge regularization: avoids big values of parameters
- Lasso regularization: favor nullity of parameters (parsimonious 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 $f : \mathbb{R}_+^M \rightarrow [0, 1]$ such that it minimizes a *loss* on a training set $(\vec{x}_1, z_1), \dots, (\vec{x}_N, z_N)$:

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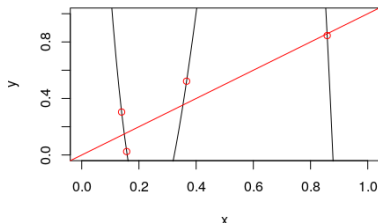
$$\min_f - \sum_{i=1}^N z_i \cdot \log f(\vec{x}_i) + (1 - z_i) \cdot \log(1 - f(\vec{x}_i))$$

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:



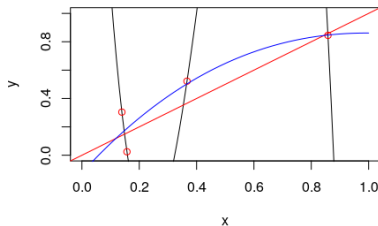
Maximum *likelihood* coefficients:

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

Overfitting depends on:

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