# Deep learning:
# tips and tricks for getting it right

Istituto Nazionale di Fisica Nucleare

SCUOLA NORMALE SUPERIORE

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tCSC Machine Learning 2024, Split, Croatia

# What Pisa can teach us about Deep Learning

People tried to make a very tall tower

Turns out it’s not enough to stack one floor on the other if the foundations are not solid

It’s the same thing with Deep Learning:

*Simply stacking many neurons is not enough!*

# Outline

A few things you may already know, motivated and trying to understand why we do them that way

- Bias-variance tradeoff
- Basic ML recipe
- Training and Bias
- Testing and Variance
- Different architectures

# Bias-variance tradeoff

Encountered in most statistical models

We have a bias when the model is too simple and it is not capturing the true relationship between x and y = h*(x)

e.g. a linear model cannot reproduce a quadratic one

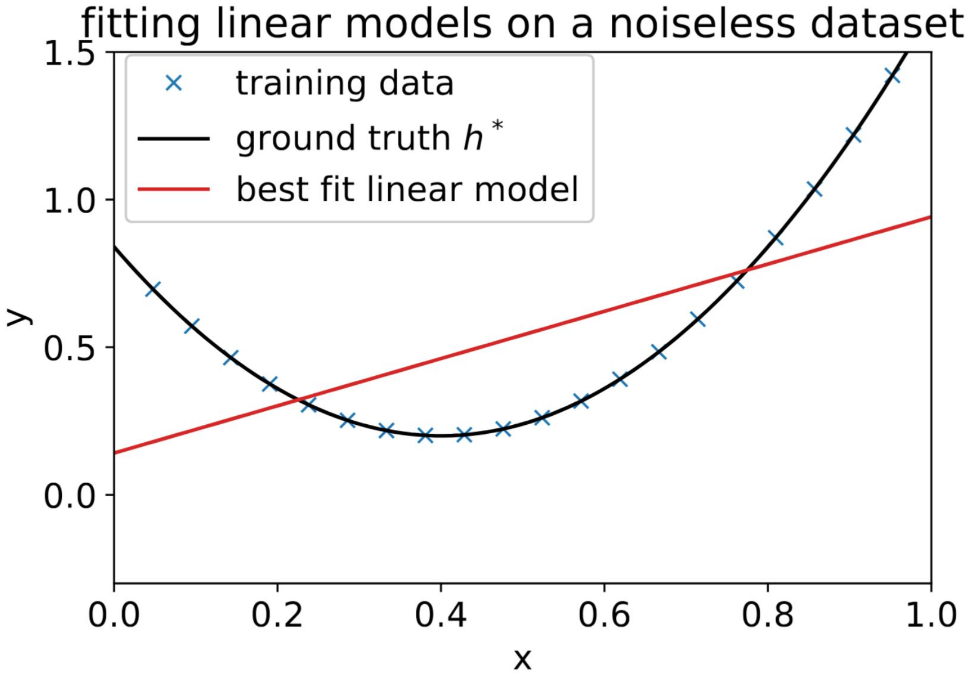


Image credit: https://cs229.stanford.edu/main_notes.pdf

# Bias-variance tradeoff

Encountered in most statistical models

When the model is too expressive, we risk fitting patterns of our small, finite training sample -- variance part of the error

e.g. a 5th-degree polynomial will overfit a small sample from a quadratic model

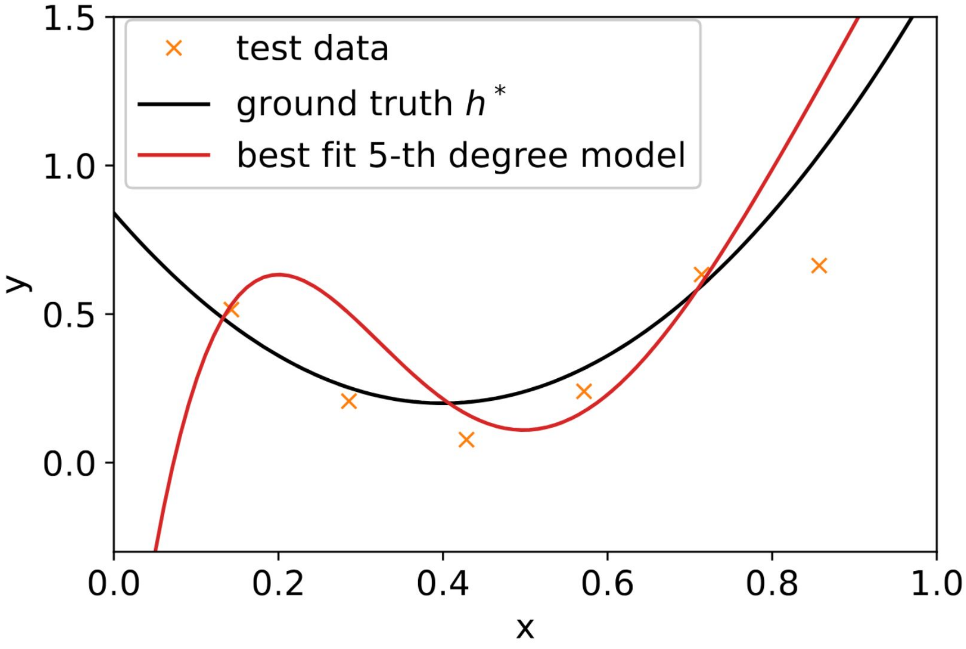
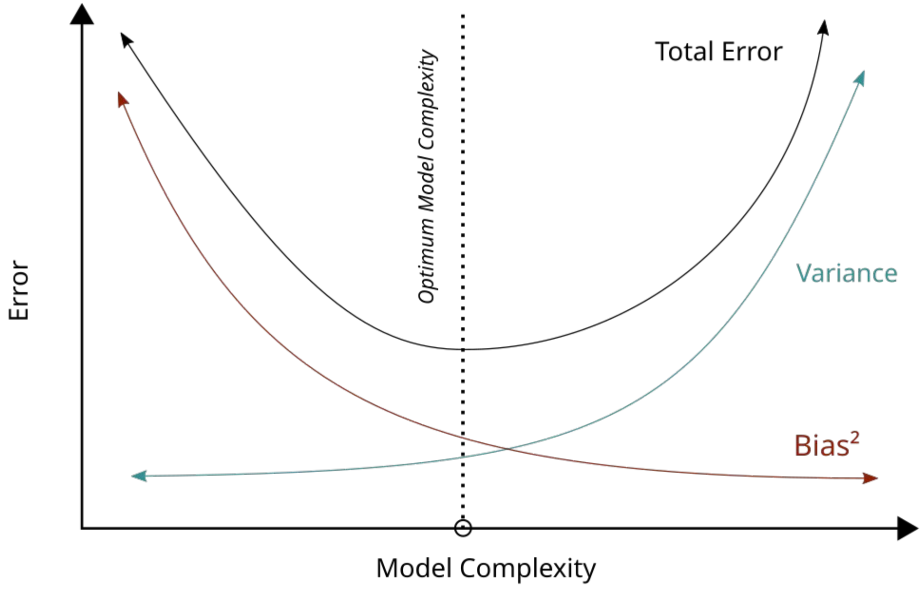


Image credit: https://cs229.stanford.edu/main_notes.pdf

# Bias-variance tradeoff defines an optimal complexity

We must strike the right balance between a simple, highly biased model and a complex, variance sensitive one

Deep learning requires careful tuning and experimentation!



# How do we address this? Basic ML recipe

Training dataset

How well I am modelling the process producing the training data

Checks for bias

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Test dataset

How well we generalize to previously unseen instances of the data

Checks for variance

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Deploy!

# Data matters!!

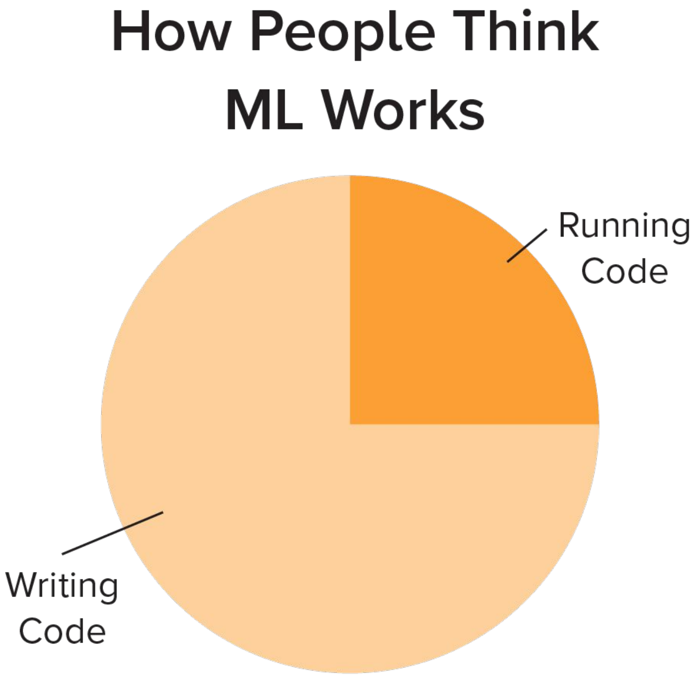


Image credit: https://www.benchling.com/blog/building-a-strong-data-foundation-to-get-machine-learning-and-automation-right

# Data matters!!

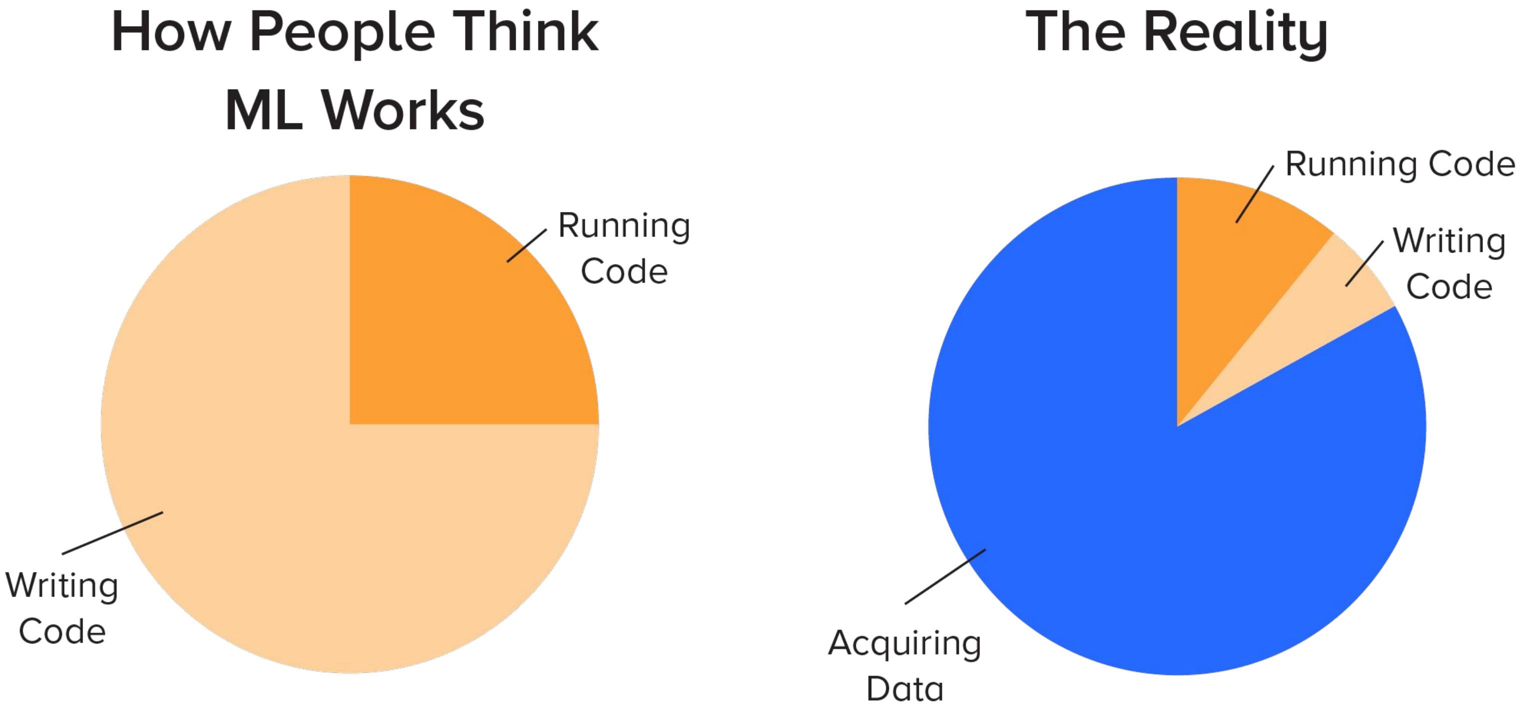
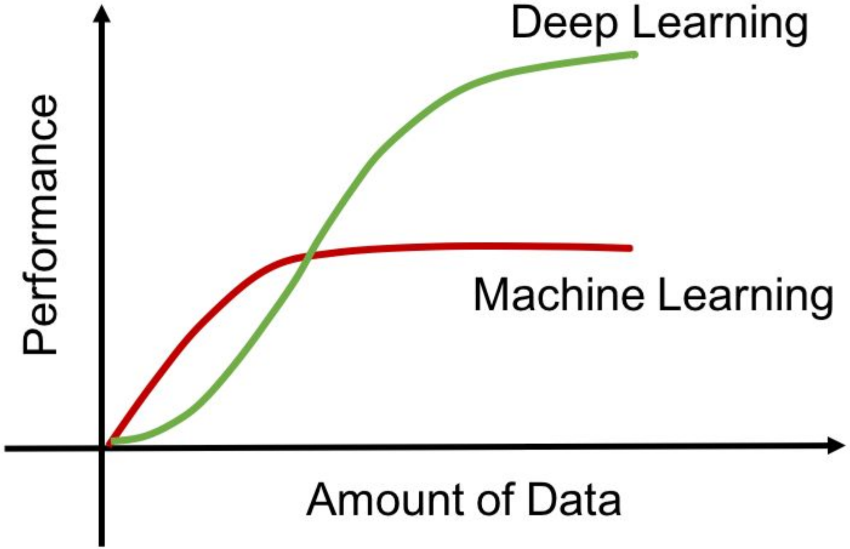


Image credit: https://www.benchling.com/blog/building-a-strong-data-foundation-to-get-machine-learning-and-automation-right

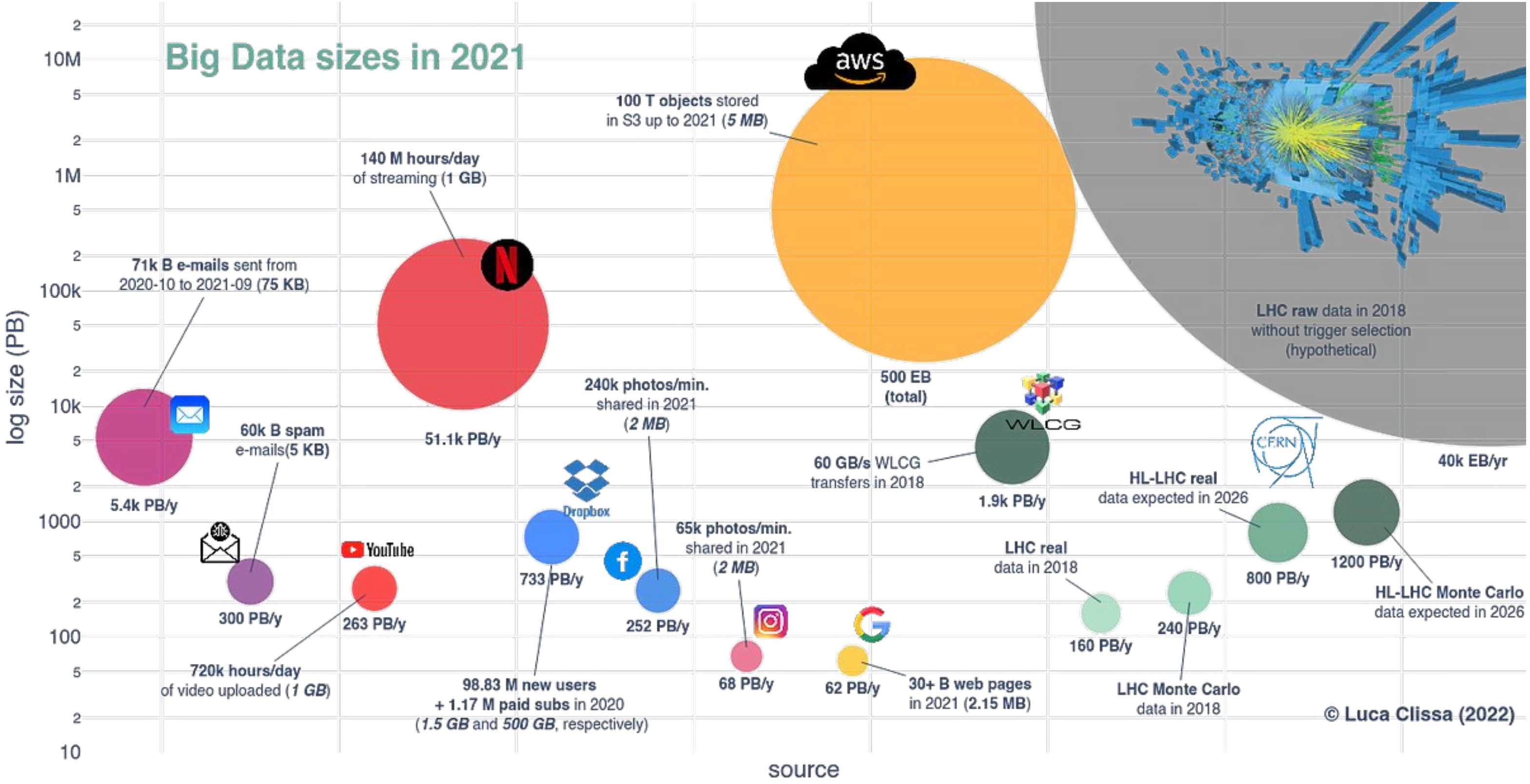
# Scale drives deep learning progress!

Assuming:

1. You can fit the training set pretty well.
2. The training set performance generalizes pretty well to the test set.



# Fortunately, we have an abundance of data!



# We still need to be careful in how we handle them

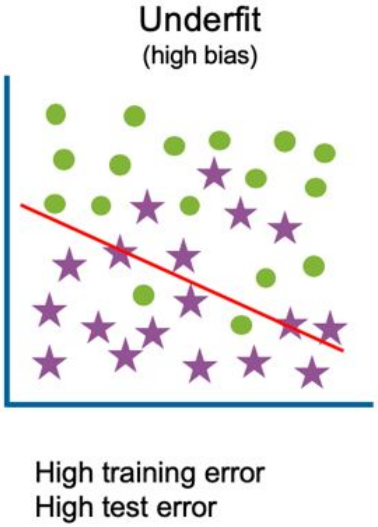
Understand your data

- Why is it relevant to your problem?
- Is some important physical information missing?
- Is the data correctly labelled?
- Is the data introducing some unwanted correlations?
- Is the data still relevant to my problem?

# The art of Training

What can I do if the training performance is lacking?

It means that we are not learning the underlying statistical model



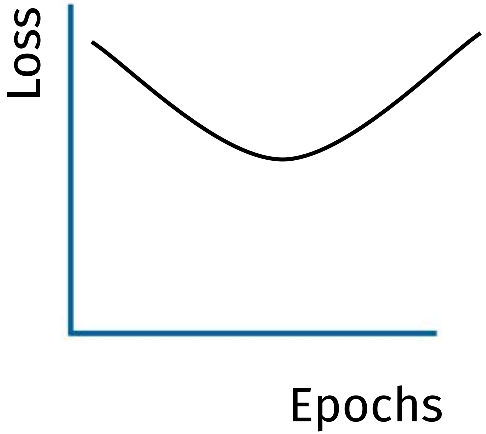


Image credit: https://www.javatpoint.com/overfitting-in-machine-learning

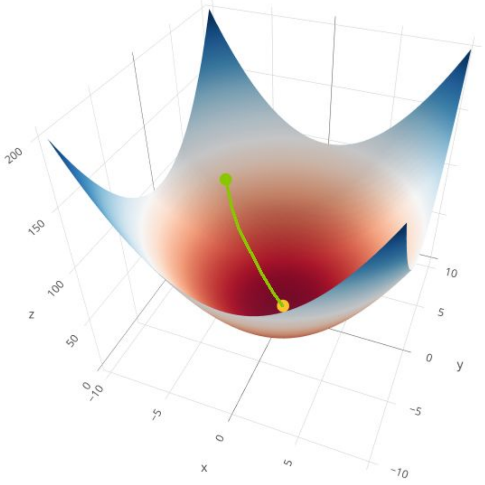
# The art of Training

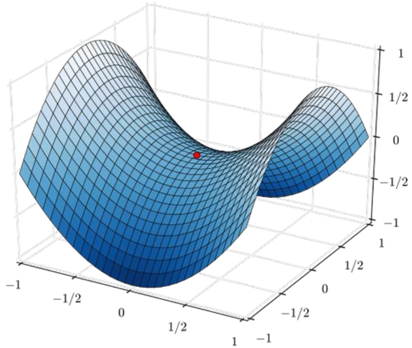
What can I do if the training performance is lacking?

It means that we are not learning the underlying statistical model:

- Train longer
- Bigger network (more capacity)
- Gradients spaces and learning algorithms
- Vanishing/exploding gradients

# Moving around the loss space can be tricky!





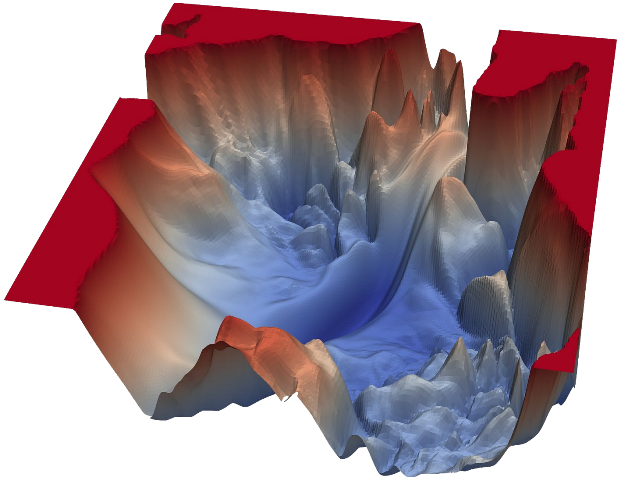


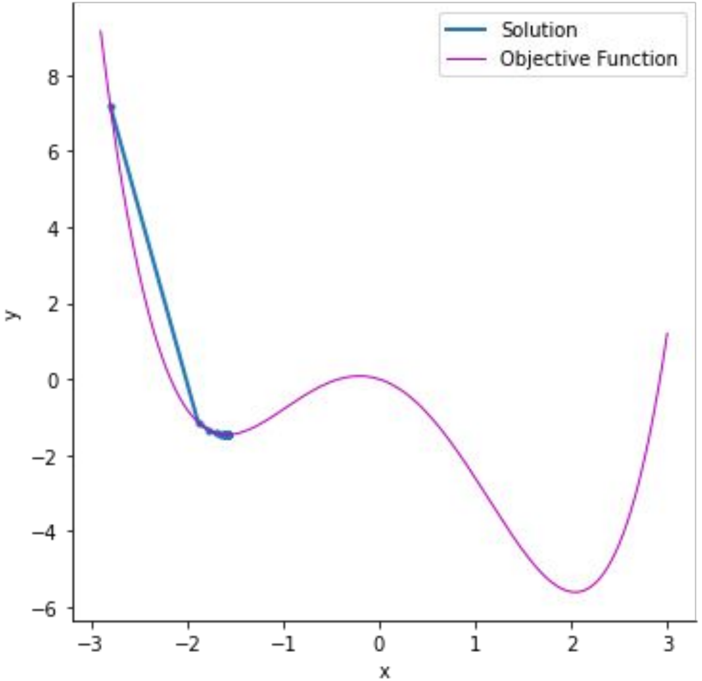
Image credit https://www.cs.umd.edu/~tomg/projects/landscapes

# Basic gradient descent is limited

The naive stochastic/batch gradient descent has many limitations in how it navigates complex loss spaces:

- sensitive to noise in current sample/batch
- easy to get trapped in local minimum

$$\theta_i = \theta_{i-1} - \gamma * g_i$$



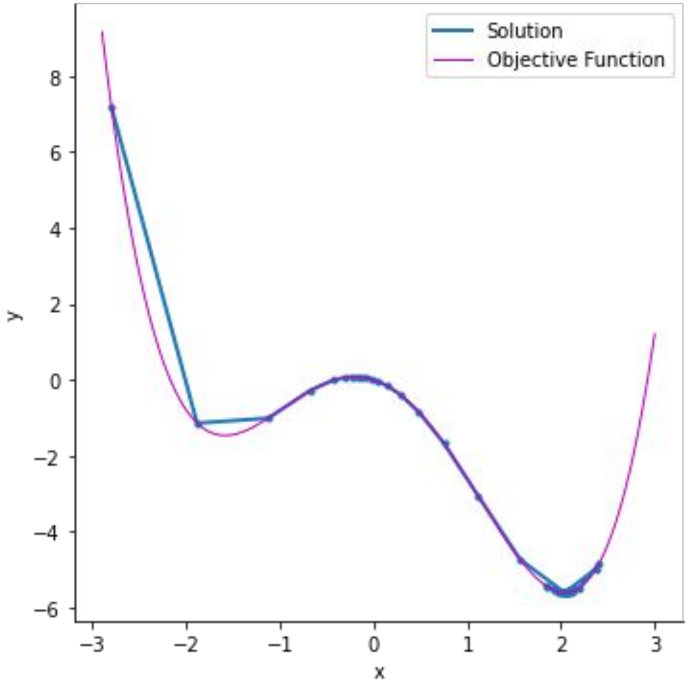
https://optimization.cbe.cornell.edu/index.php?title=Momentum

# Momentum helps overcoming these limitations

Momentum is an extension to the algorithm that builds inertia in a search direction to overcome local minima and oscillation of noisy gradients.

$$b_i = \mu * b_{i-1} + g_i$$

$$\theta_i = \theta_{i-1} - \gamma * b_i$$



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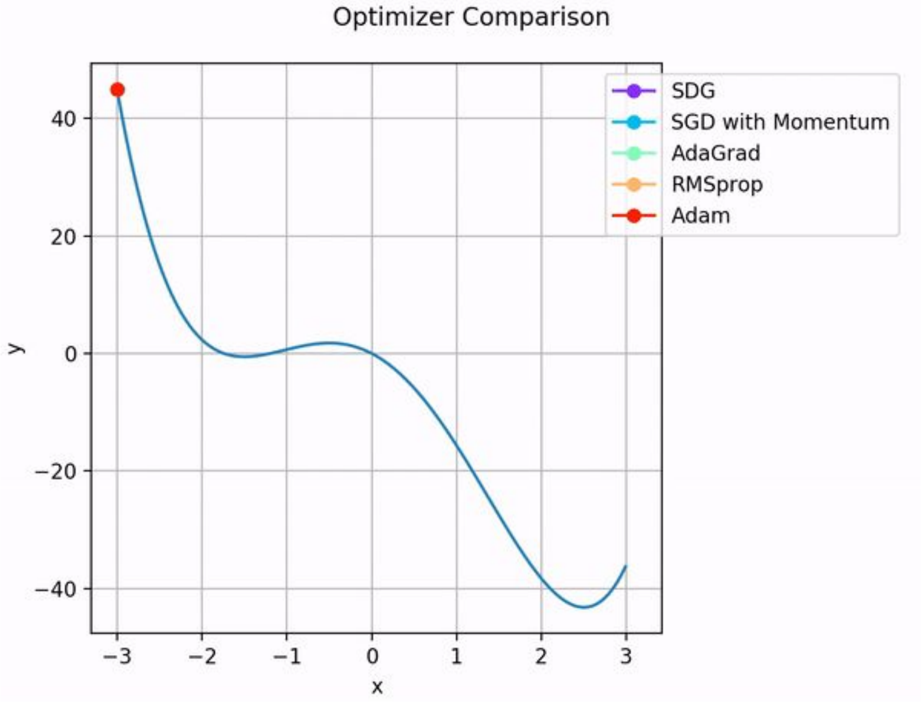
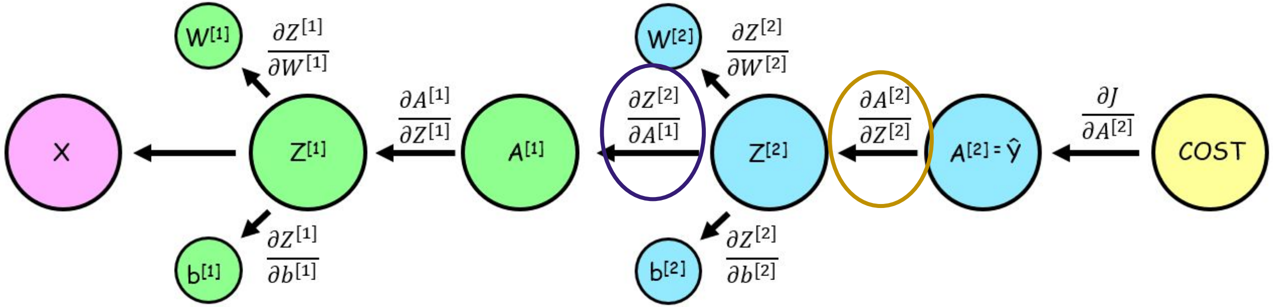
# State-of-the-art: Adaptive Moment Estimation (Adam)

Adam is an adaptive learning rate algorithm:

- It uses momentum
- It dynamically adjusts the learning rate for each individual parameter within a model, rather than using a single global learning rate



# Vanishing/Exploding gradients


X
Z[1]
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W[1]
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$\frac{\partial Z^{[1]}}{\partial b^{[1]}}$
$\frac{\partial A^{[1]}}{\partial Z^{[1]}}$
$\frac{\partial Z^{[2]}}{\partial A^{[1]}}$
$\frac{\partial Z^{[2]}}{\partial W^{[2]}}$
$\frac{\partial Z^{[2]}}{\partial b^{[2]}}$
$\frac{\partial A^{[2]}}{\partial Z^{[2]}}$
$\frac{\partial J}{\partial A^{[2]}}$

Remember that the gradients of the loss depend on:

- the derivative of the activation functions
- the derivative of the outputs (i.e. the weights)

Image credits: https://towardsdatascience.com/neural-networks-backpropagation-by-dr-lihi-gur-arie-27be67d8fdce

# The gradients can vanish for small derivatives

Some choices of activation functions have small derivatives

This can lead to chain multiplication of small numbers!

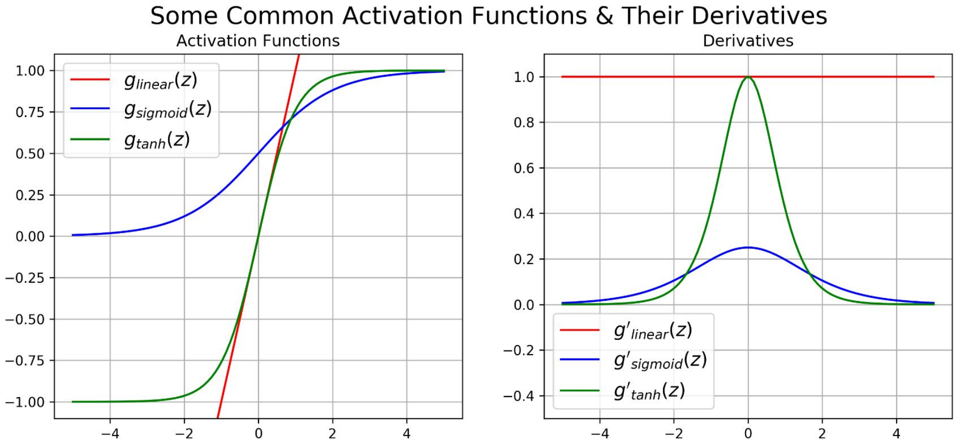


Image 1 credits https://dustinstansbury.github.io/theclevermachine/derivation-common-neural-network-activation-functions

# The gradients can vanish for small derivatives

This can lead to chain multiplication of small numbers, making the gradients of the initial layers effectively 0 and preventing learning

Mitigated through initialization and change of activation functions

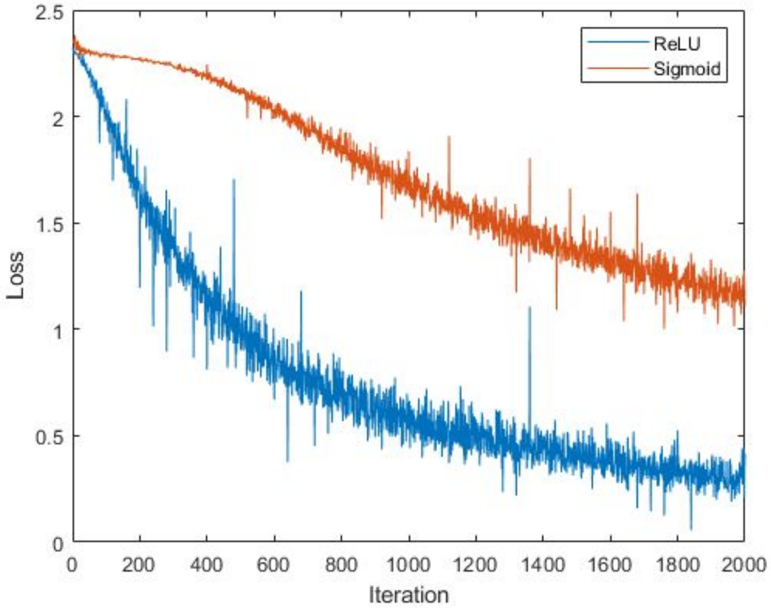


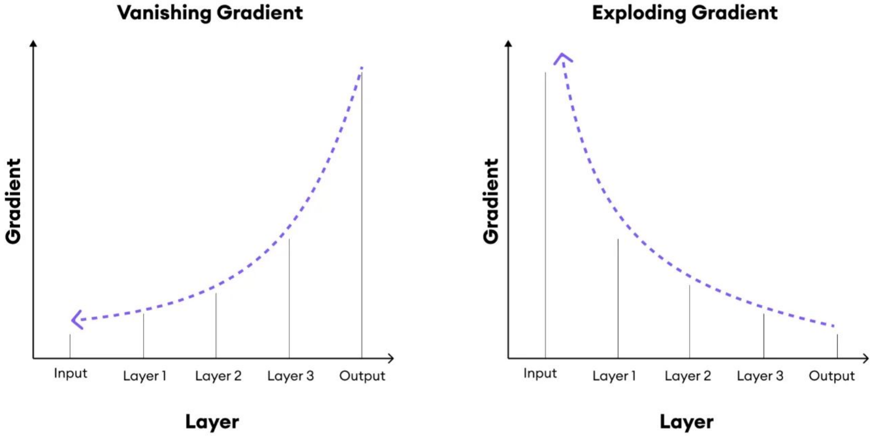
Image 2 credits https://www.jefkine.com/general/2018/05/21/2018-05-21-vanishing-and-exploding-gradient-problems/

# The gradients can explode for large weights

The weights can have a norm >>1

Multiplication of large numbers will result in exploding gradients for first weights

Can be mitigated with regularization and clipping of weights



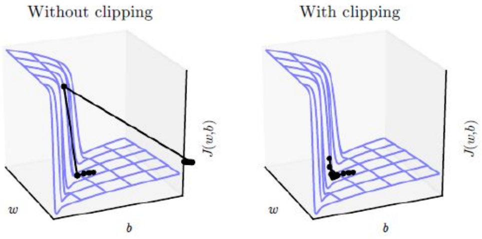
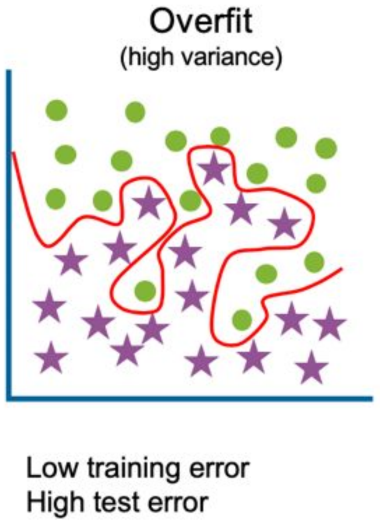


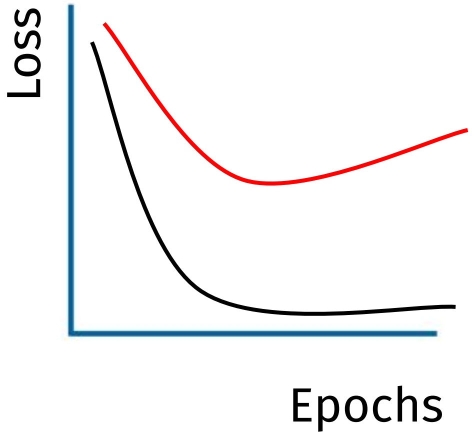
Image 1 credit
[https://www.superannotate.com/blog/activation-functions-in-neural-networks](https://www.superannotate.com/blog/activation-functions-in-neural-networks)
Image 2 credit
Deep Learning, Goodfellow et al

# The art of Testing or *Regularization*

What if the testing performance is poor after training?

It means that we are modelling a specific variance of our train dataset





# The art of Testing or *Regularization*

What if the testing performance is poor after training?

It means that we are modelling a specific variance of our train dataset:

- Use more training data
- Regularization techniques
- Preprocessing of data

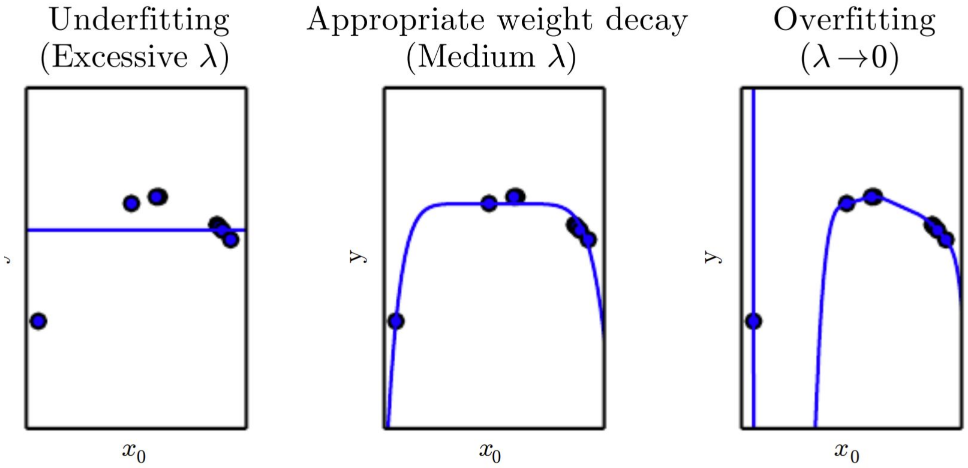
# Regularization I: Weight decay

$$L_{new}(w) = L_{original}(w) + \lambda w^T w$$

We add a term in the loss function proportional to the L2-norm of the weights

Penalizes large weights

But why do smaller weights correspond to simpler models?



Underfitting (Excessive $\lambda$)

Appropriate weight decay (Medium $\lambda$)

Overfitting ($\lambda \rightarrow 0$)

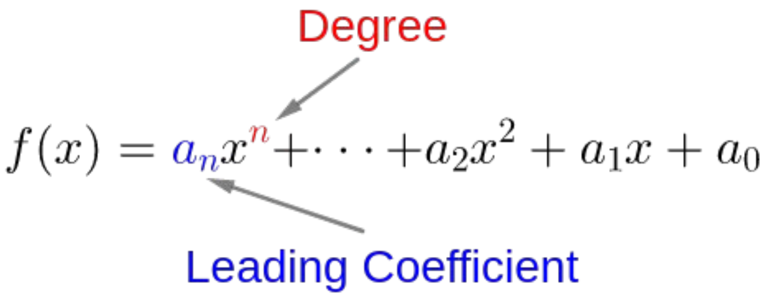
from: Deep Learning, Goodfellow et al

# Regularization I: Weight decay

Limits model complexity and non-linearity: think of an N-layer network as a Nth degree polynomial for one input feature when the others are fixed.

y = f_n(W_n * ...f_1(W*x + b)...)

We are reducing the coefficients of such a polynomial, hence making it less expressive!



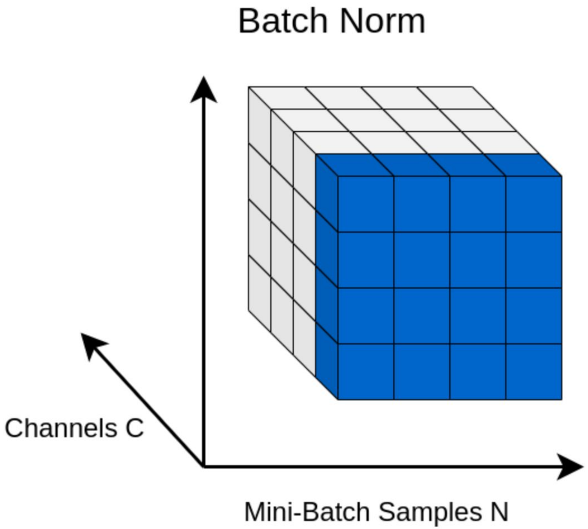
Degree

$$f(x) = a_n x^n + \cdots + a_2 x^2 + a_1 x + a_0$$

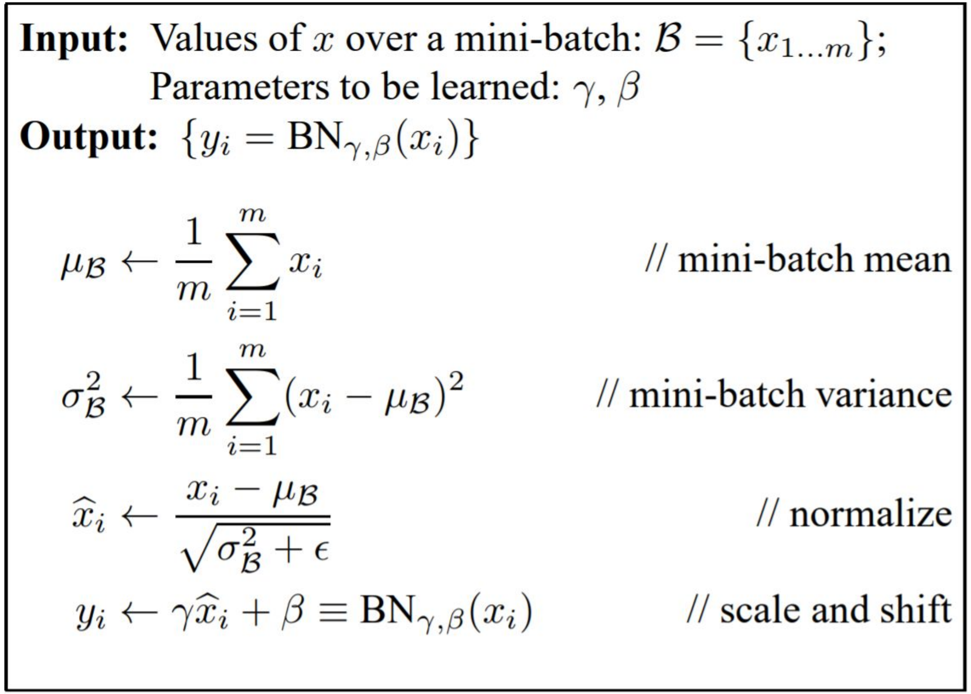
Leading Coefficient

from: Deep Learning, Goodfellow et al

# Regularization II: Batch Normalization



Increases robustness by subtraction of “batch-random” mean and variance



**Input:** Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1 \ldots m}\}$;
Parameters to be learned: $\gamma$, $\beta$

**Output:** $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

# Batch Normalization may help in the following case

Train:

Dog, y=1

Not Dog, y=0

# Batch Normalization may help in the following case

Train:

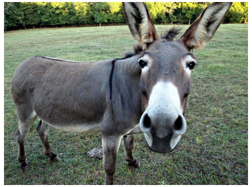
Dog, y=1

Not Dog, y=0

Test:

Dog, y=1

Not Dog, y=0



# Batch Normalization may reduce covariance shift

Covariance shift refers to changes in the data distribution between training and testing, affecting model performance.

Batch normalization helps by normalizing input features across mini-batches, reducing internal covariate shift and stabilizing learning, thus improving generalization across varying distributions.

Train:

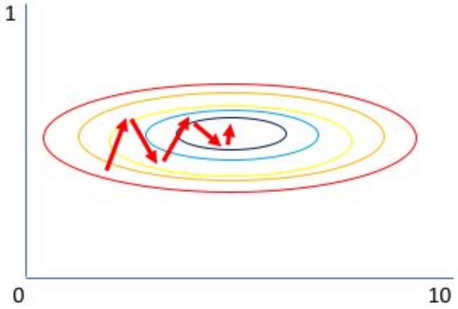
Test:

BatchNorm??

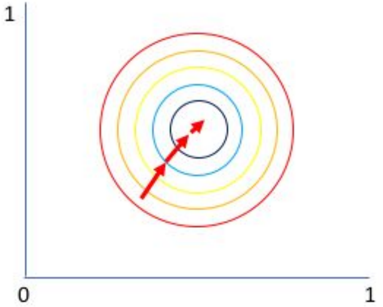
# (Data) Regularization III: Normalization of Inputs

It’s standard practice to normalize the input of the network to have mean 0 and variance 1

This helps to make the gradients space more regular and speed up training



Gradient of larger parameter dominates the update



Both parameters can be updated in equal proportions

Image credits: https://heytech.tistory.com/

# Regularization IV: Dropout

We don’t want to relay on single input features, so we spread out the information through many “sub-networks”

At inference time, all of the sub-networks are activated and contribute to the output (“wisdom of the crowd”)

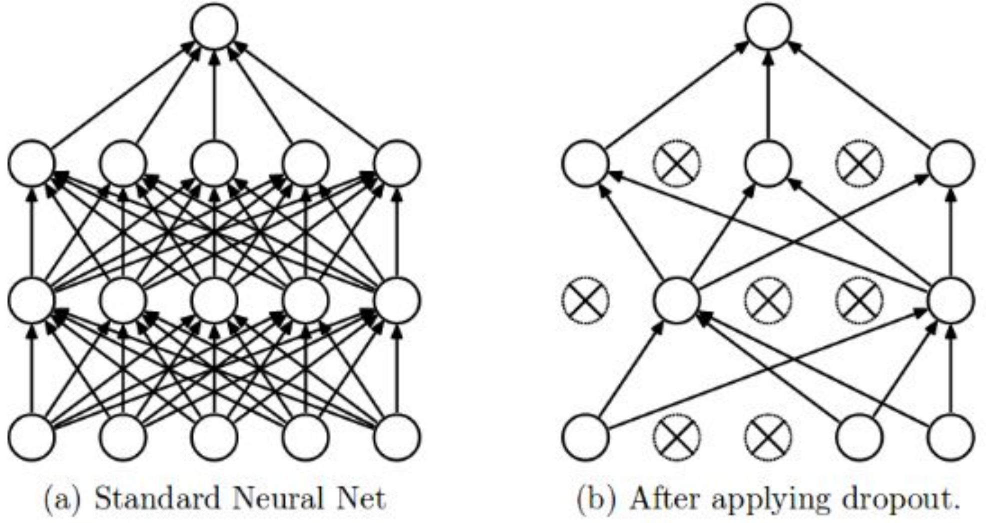


Image credit https://towardsdatascience.com/dropout-in-neural-networks-47a162d621d9

# Data preprocessing can help with generalization

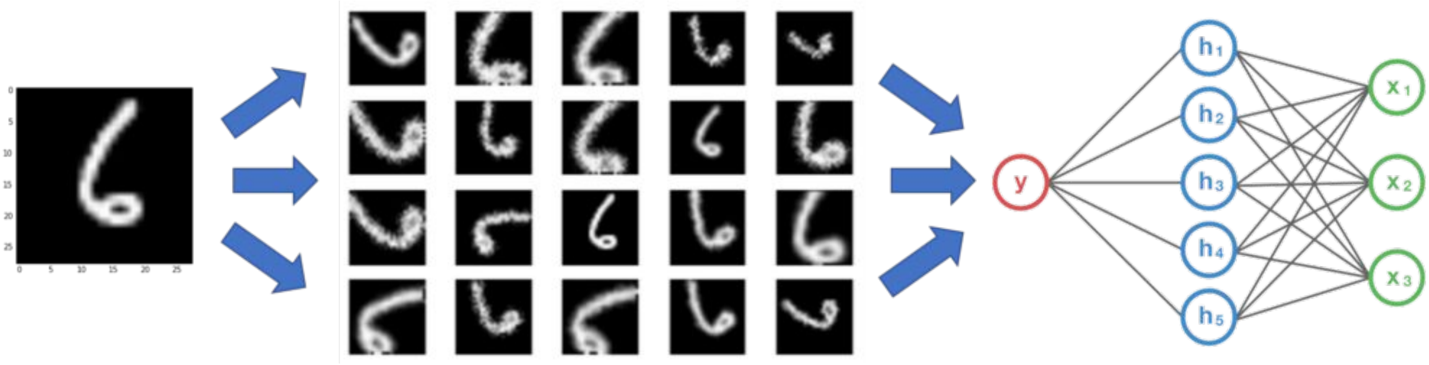
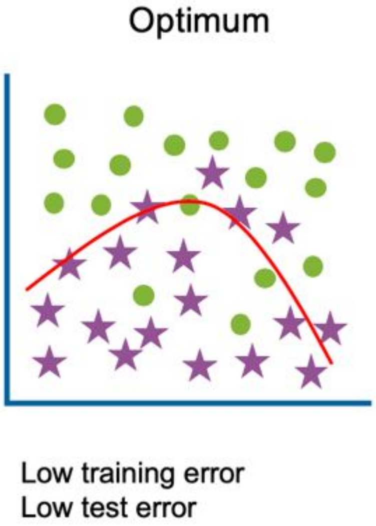


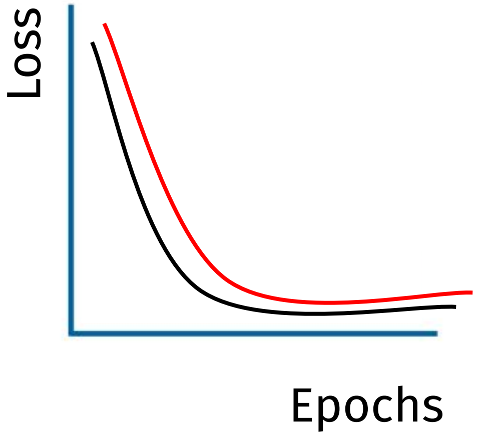
Image credits:
https://learnai1.home.blog/2020/08/15/data-preprocessing-for-neural-networks/

# Now hopefully things work ok!

Both the train and test errors are reasonable

We can deploy our models in the wild!





# What if we were to work with images?

In a Feed-forward NN we need to *flatten* the image

For a 18*16 pixels image that’s already 288 input features

For a Whatsapp image ~800*800 -> 640k inputs!!

Additionally, no notion of *locality*

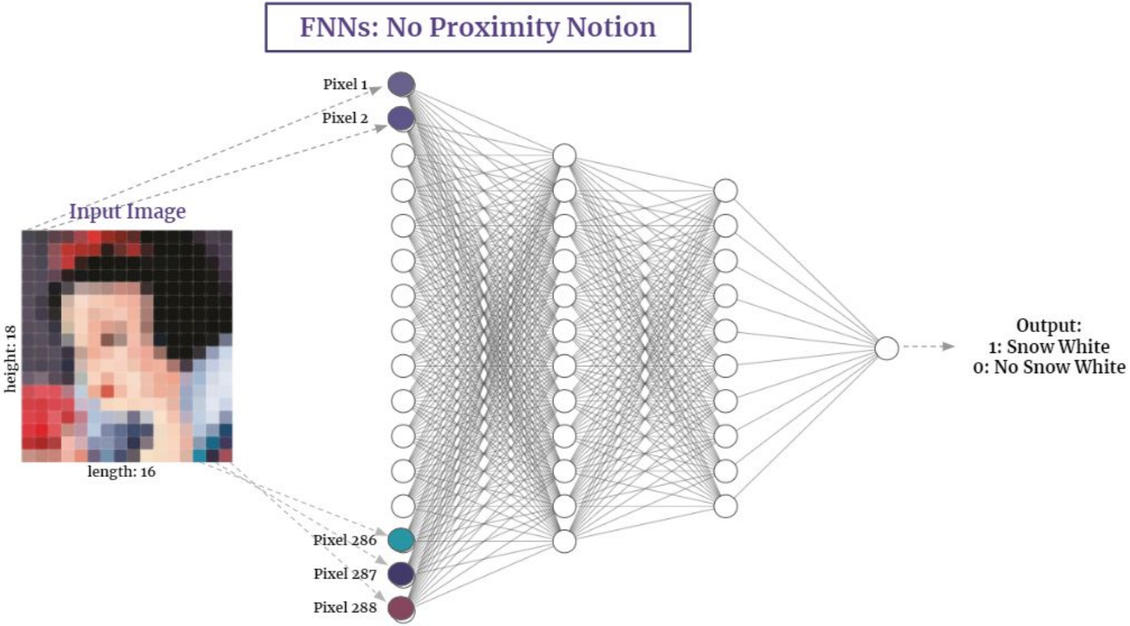


Image credit: https://www.kaggle.com/code/andradaolteanu/convolutional-neural-nets-cnns-explained

# Data symmetries matter! Can we account for them?

An eye is an eye, weather or not it's top or bottom, right or left, small or big, etc.

How can we build a network that is invariant under the shift of input features?

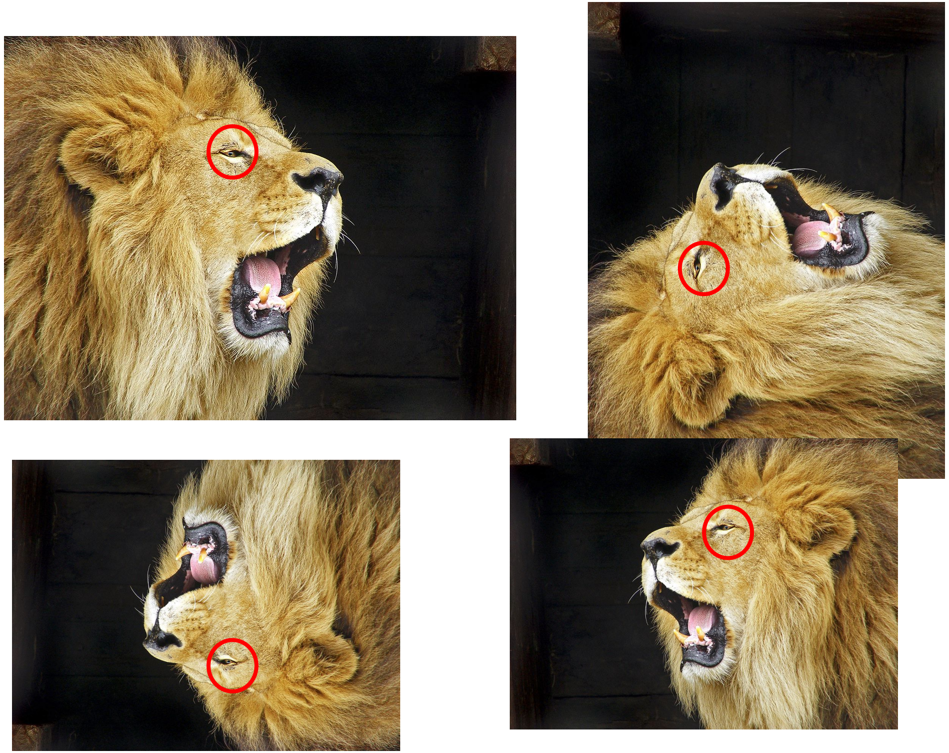
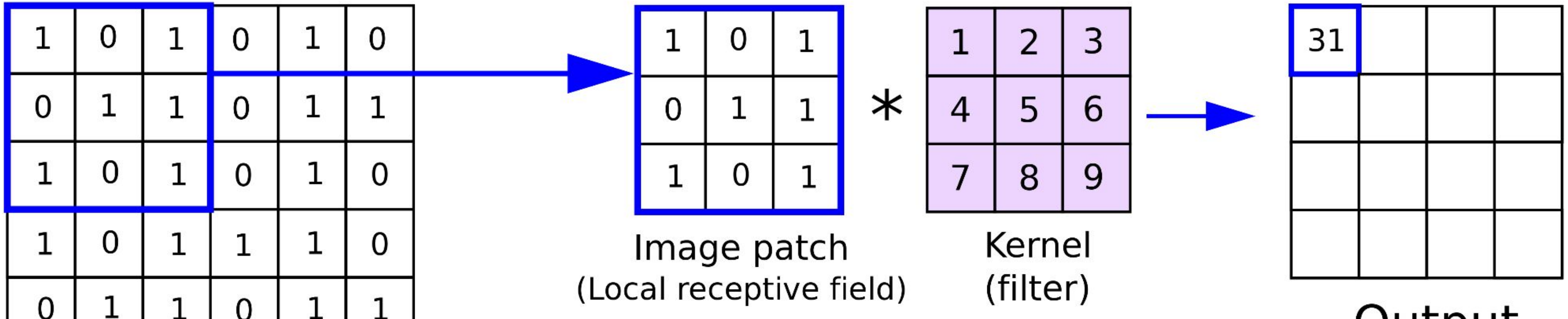


Image credit Tambako The Jaguar, Flickr

# Convolutional neural networks



|  |  |  |  |  |  |
|---|---|---|---|---|---|
| 1 | 0 | 1 | 0 | 1 | 0 |
| 0 | 1 | 1 | 0 | 1 | 1 |
| 1 | 0 | 1 | 0 | 1 | 0 |
| 1 | 0 | 1 | 1 | 1 | 0 |
| 0 | 1 | 1 | 0 | 1 | 1 |
| 1 | 0 | 1 | 0 | 1 | 0 |

|  |  |  |
|---|---|---|
| 1 | 0 | 1 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |

|  |  |  |
|---|---|---|
| 1 | 2 | 3 |
| 4 | 5 | 6 |
| 7 | 8 | 9 |

|  |  |  |  |
|---|---|---|---|
| 31 |  |  |  |
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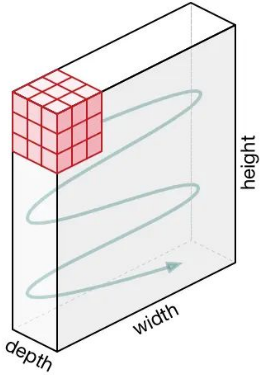


Image 1 credit
https://wikidocs.net/164365
Image 2 credit
https://saturncloud.io/blog/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way/

# Convolutional neural networks

Essentially

Filter == Learned matrix multiplication

By going over the image, each filter can focus on the local features

We will have filter specializing in recognizing the same element over multiple training images

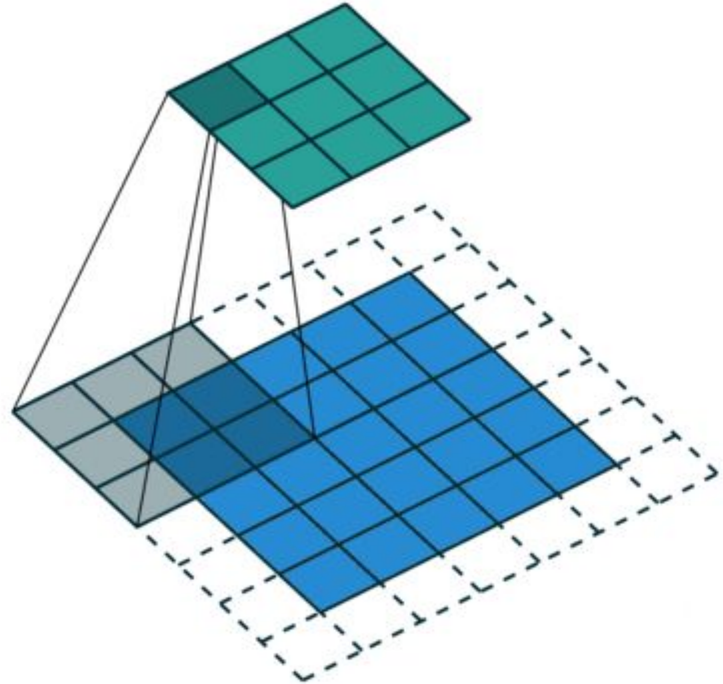
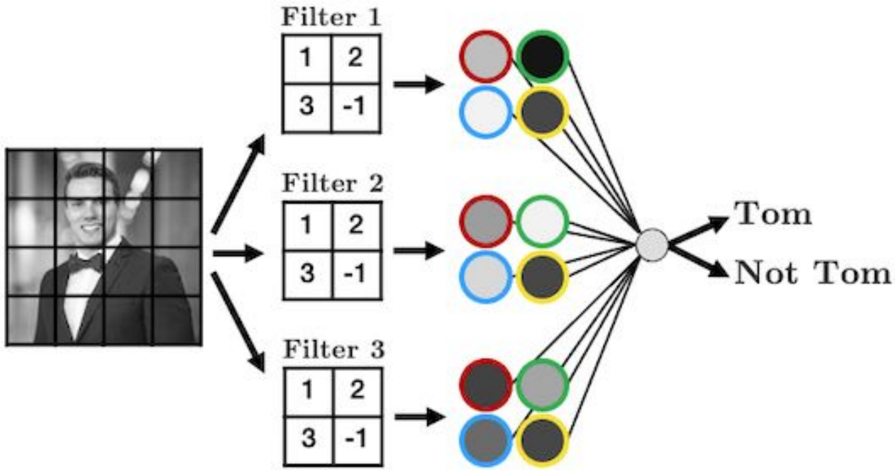


Image credit https://saturncloud.io/blog/a-comprehensive-guide-to-convolutional-neural-networks-the-eli5-way/

# Filters in action

By going over the image, each filter can specialize on the extraction of single features and create an higher-level representation

The last part of the network is usually a feedforward NN which reasons on such a representation



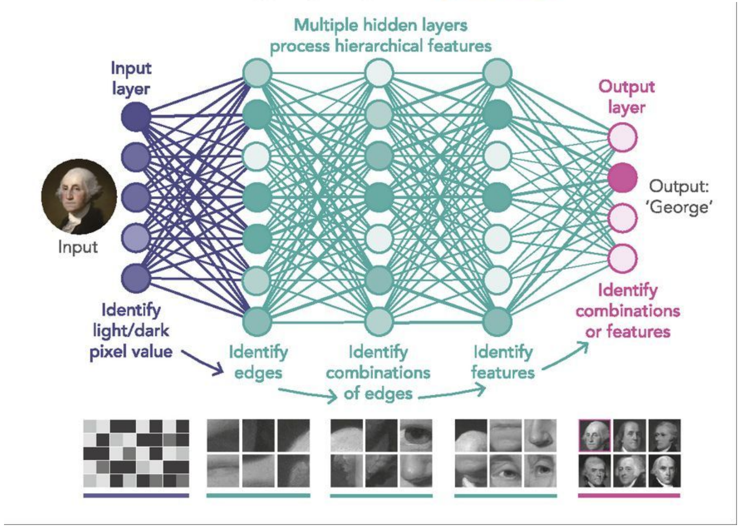
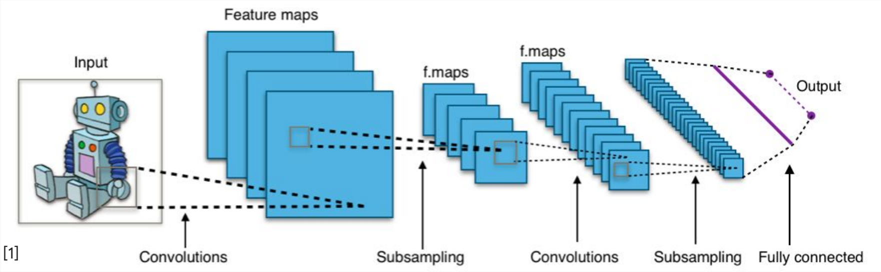

Multiple hidden layers process hierarchical features
Input layer
Input
Output layer
Output: 'George'
Identify light/dark pixel value
Identify edges
Identify combinations of edges
Identify features
Identify combinations or features

Image 1 credit
https://www.tomasbeuzen.com/deep-learning-with-pytorch/chapters/chapter5_cnns-pt1.html
Image 2 credit: Lucy Reading-Ikkanda (artist).

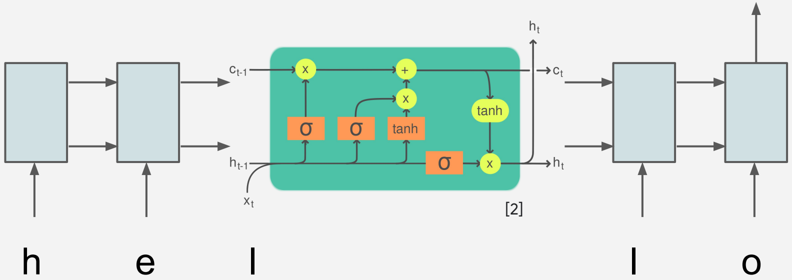
# Computer Vision

## Convolutional NNs (+ResNets)



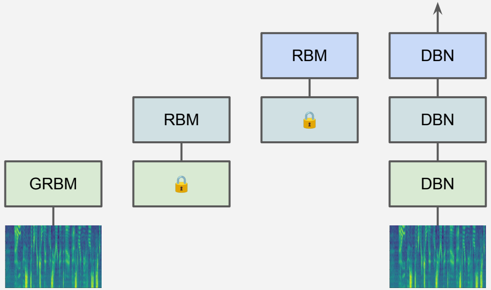
# Natural Lang. Proc.

## Recurrent NNs (+LSTMs)



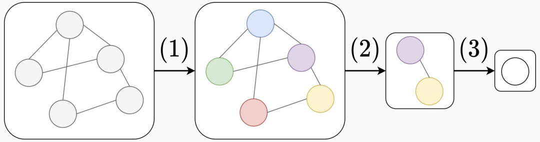
# Speech

## Deep Belief Nets (+non-DL)



# Science

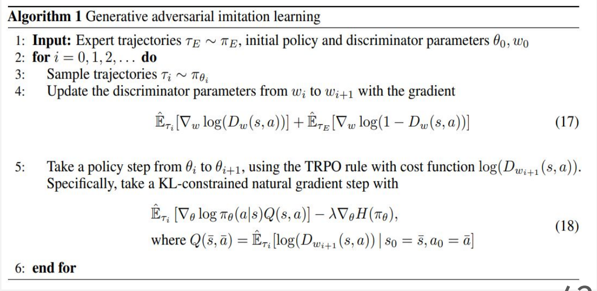
## Graph NNs



[3]

# RL

## BC/GAIL



**Algorithm 1** Generative adversarial imitation learning

```
Input: Expert trajectories $\tau_E \sim \pi_E$, initial policy and discriminator parameters $\theta_0, w_0$
for $i = 0, 1, 2, \ldots$ do
    Sample trajectories $\tau_i \sim \pi_{\theta_i}$
    Update the discriminator parameters from $w_i$ to $w_{i+1}$ with the gradient
        $\hat{\mathbb{E}}_{\tau_i}[\nabla_w \log(D_w(s,a))] + \hat{\mathbb{E}}_{\tau_E}[\nabla_w \log(1 - D_w(s,a))]$   (17)
    Take a policy step from $\theta_i$ to $\theta_{i+1}$, using the TRPO rule with cost function $\log(D_{w_{i+1}}(s,a))$.
    Specifically, take a KL-constrained natural gradient step with
        $\hat{\mathbb{E}}_{\tau_i}[\nabla_\theta \log \pi_\theta(a|s) Q(s,a)] - \lambda \nabla_\theta H(\pi_\theta)$,
        where $Q(\bar{s},\bar{a}) = \hat{\mathbb{E}}_{\tau_i}[\log(D_{w_{i+1}}(s,a)) \mid s_0 = \bar{s}, a_0 = \bar{a}]$   (18)
end for
```

Slide from Lucas Beyer lbeyer@google.com [1] CNN image CC-BY-SA by Aphex34 for Wikipedia https://commons.wikimedia.org/wiki/File:Typical_cnn.png
[2] RNN image CC-BY-SA by GChe for Wikipedia https://commons.wikimedia.org/wiki/File:The_LSTM_Cell.svg [3] By NickDiCicco - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=119932650

# The end?

# A new trend in frontier AI/DL: the “bitter lesson”

The biggest lesson that can be read from 70 years of AI research is that **general methods that leverage computation are ultimately the most effective**, and by a large margin. The ultimate reason for this is Moore's law, or rather its generalization of **continued exponentially falling cost per unit of computation.** [...]

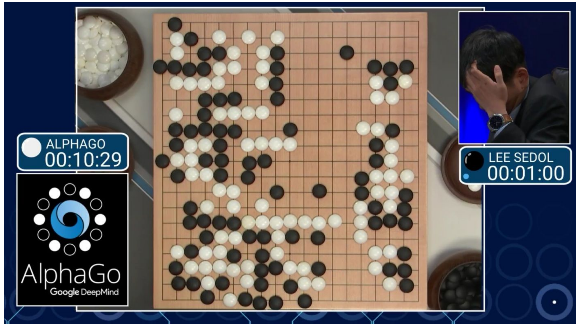
Seeking an improvement that makes a difference in the shorter term, **researchers seek to leverage their human knowledge of the domain, but the only thing that matters in the long run is the leveraging of computation**. These two need not run counter to each other, but in practice they tend to. Time spent on one is time not spent on the other. [...]

And the **human-knowledge approach tends to complicate methods** in ways that make them less suited to taking advantage of general methods leveraging computation. [...] --- **Rich Sutton**

# Tw famous examples

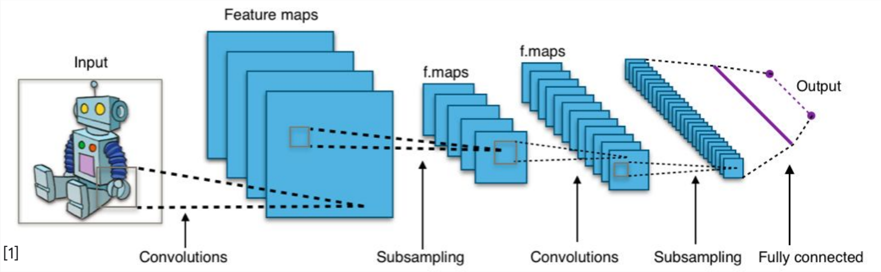
Deep Blue and AlphaGo leveraged massive, brute force search strategies and then self-play

At the time, this was looked upon with dismay by the majority of computer-chess/go researchers who had pursued methods that leveraged human understanding of the special structure of chess/go!



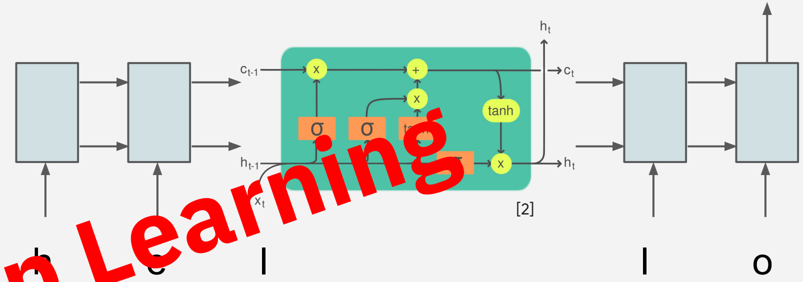
## Computer Vision

### Convolutional NNs (+ResNets)



## Natural Lang. Proc.

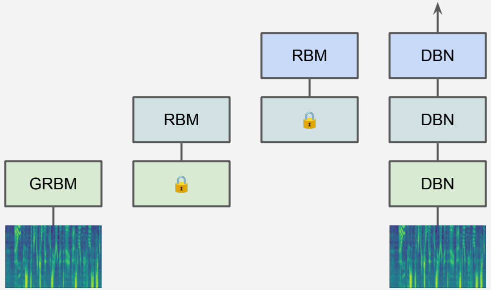
### Recurrent NNs (+LSTMs)



**Pre-2017 Deep Learning**

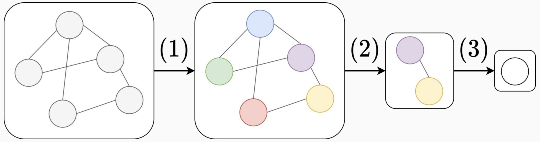
## Speech

### Deep Belief Nets (+non-DL)



## Science

### Graph NNs



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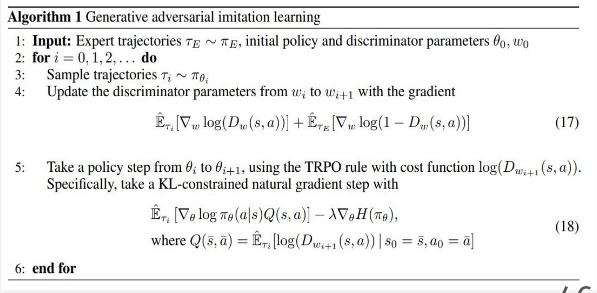
## RL

### BC/GAIL



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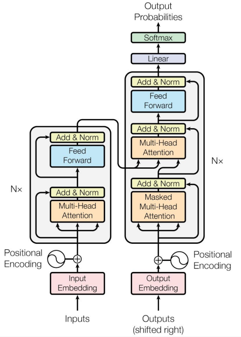
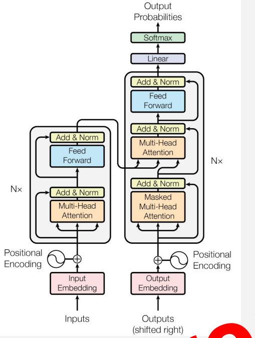
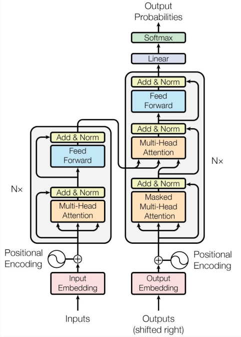
# Computer Vision



# Natural Lang. Proc.

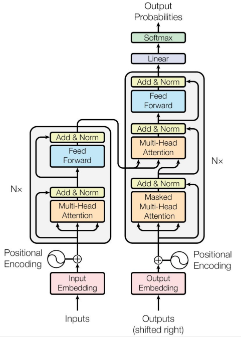


# Reinf. Learning

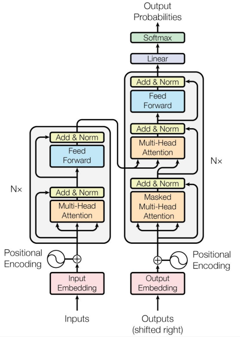


**Current trends**

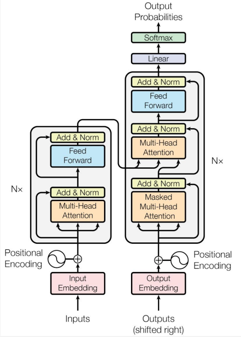
# Speech



# Translation



# Graphs/Science



Slide from Lucas Beyer lbeyer@google.com Transformer image source: "Attention Is All You Need" paper

# So in the end, we’re back to stacking layers??

Not quite!

Everything we’ve seen in this lecture is the backbone of scaling Deep(er) Networks and making them converge

Human/Physical knowledge is still extremely helpful and impactful in the short/medium term both for time and scale regimes

And most of the times we are dealing with finite resources to train/deploy

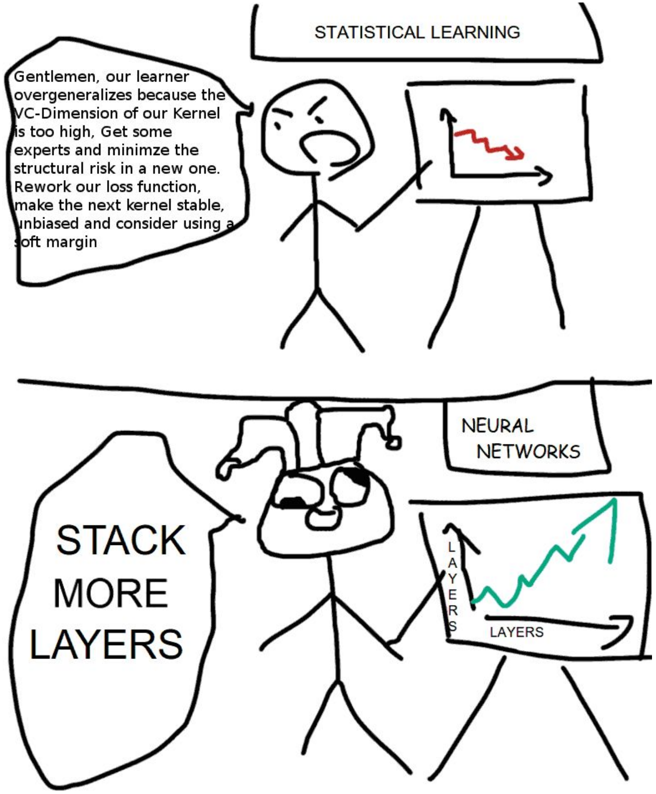

STATISTICAL LEARNING
Gentlemen, our learner overgeneralizes because the VC-Dimension of our Kernel is too high, Get some experts and minimze the structural risk in a new one. Rework our loss function, make the next kernel stable, unbiased and consider using a soft margin
NEURAL NETWORKS
STACK MORE LAYERS
LAYERS
LAYERS

Image credit: Ilya Sutskever

# Conclusions

From a simple set of linear algebra operations, we can construct incredible tools called Deep Neural Networks

Basic neurons are not enough! We need to introduce a set of algorithms and data preprocessing to make learning easier, more stable, and more generalizable

Different ways of combining neurons can result in optimized architectures for handling different data types… but who knows what the future holds!

# backup

# We can do the math if needed

$$\mathrm{MSE} \triangleq \mathrm{E}\left[(y-\hat{f})^2\right] = \mathrm{E}\left[y^2 - 2y\hat{f} + \hat{f}^2\right] = \mathrm{E}\left[y^2\right] - 2\,\mathrm{E}\left[y\hat{f}\right] + \mathrm{E}\left[\hat{f}^2\right]$$

$$\begin{aligned} \mathrm{E}\left[y^2\right] &= \mathrm{E}\left[(f+\varepsilon)^2\right] \\ &= \mathrm{E}[f^2] + 2\,\mathrm{E}[f\varepsilon] + \mathrm{E}[\varepsilon^2] && \text{by linearity of } \mathrm{E} \\ &= f^2 + 2f\,\mathrm{E}[\varepsilon] + \mathrm{E}[\varepsilon^2] && \text{since } f \text{ does not depend on the data} \\ &= f^2 + 2f\cdot 0 + \sigma^2 && \text{since } \varepsilon \text{ has zero mean and variance } \sigma^2 \end{aligned}$$

$$\begin{aligned} \mathrm{E}\left[y\hat{f}\right] &= \mathrm{E}\left[(f+\varepsilon)\hat{f}\right] \\ &= \mathrm{E}[f\hat{f}] + \mathrm{E}[\varepsilon\hat{f}] && \text{by linearity of } \mathrm{E} \\ &= \mathrm{E}[f\hat{f}] + \mathrm{E}[\varepsilon]\,\mathrm{E}[\hat{f}] && \text{since } \hat{f} \text{ and } \varepsilon \text{ are independent} \\ &= f\,\mathrm{E}[\hat{f}] && \text{since } \mathrm{E}[\varepsilon] = 0 \end{aligned}$$

$$\begin{aligned} \mathrm{MSE} &= f^2 + \sigma^2 - 2f\,\mathrm{E}[\hat{f}] + \mathrm{Var}[\hat{f}] + \mathrm{E}[\hat{f}]^2 \\ &= (f - \mathrm{E}[\hat{f}])^2 + \sigma^2 + \mathrm{Var}\left[\hat{f}\right] \\ &= \mathrm{Bias}[\hat{f}]^2 + \sigma^2 + \mathrm{Var}\left[\hat{f}\right] \end{aligned}$$

$$\mathrm{E}\left[\hat{f}^2\right] = \mathrm{Var}(\hat{f}) + \mathrm{E}[\hat{f}]^2 \qquad \text{since } \mathrm{Var}[X] \triangleq \mathrm{E}\left[(X - \mathrm{E}[X])^2\right] = \mathrm{E}[X^2] - \mathrm{E}[X]^2 \text{ for any random variable } X$$