MAI

Deep Learning

THEORY
Feed-forward and convolutional neural networks

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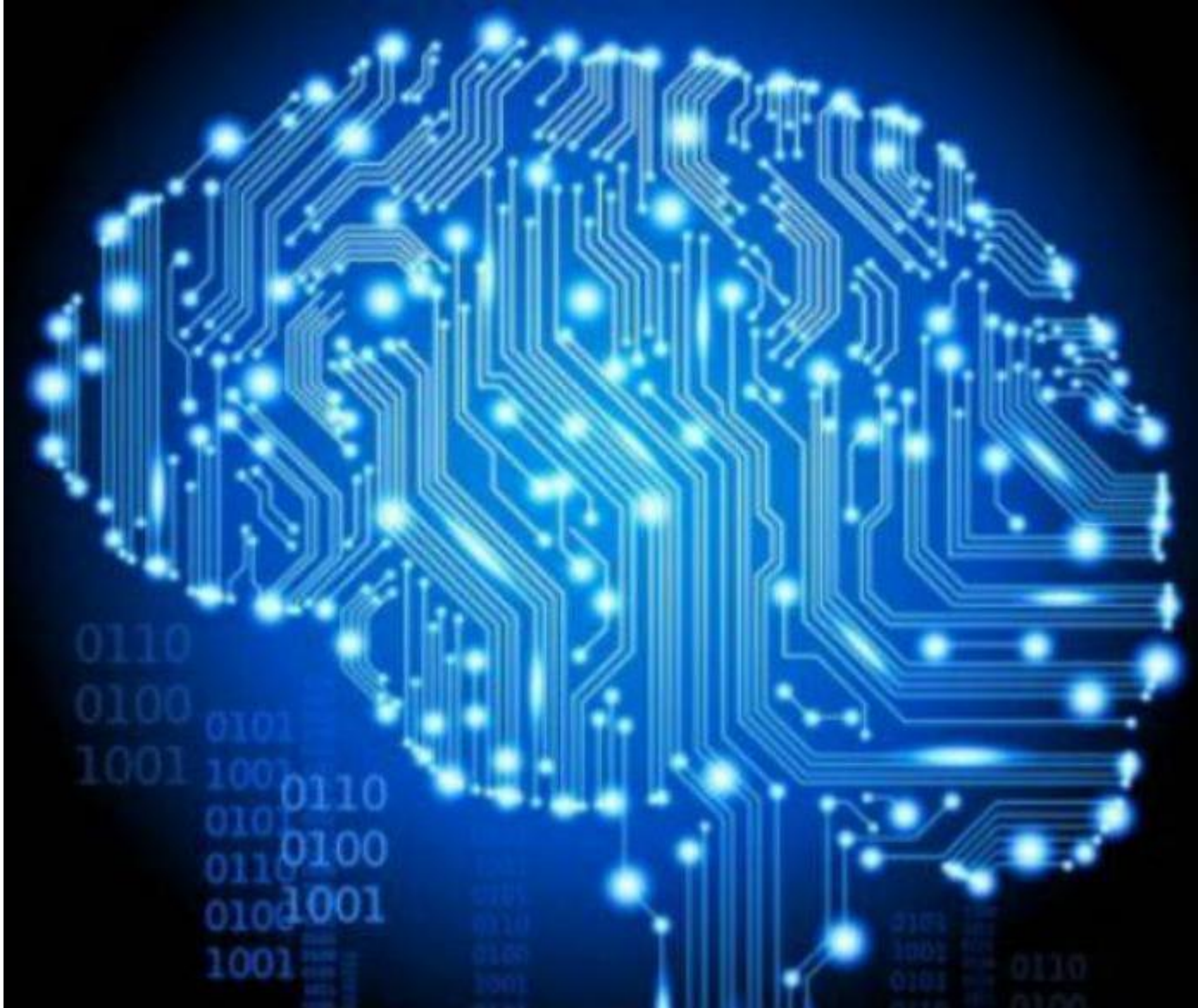
A bit of History



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A bit of History

McCullock & Pitts / Hebb

Rosenblatt's Perceptron

Minsky & Papert - XOR

Backpropagation Algorithm

- 1943 Warren McCulloch & Walter Pitts:
  - How To: From neurons to complex thought
  - Binary threshold activations
- 1949 Howard Hebb:
  - Neurons that fire together wire together
  - Weights: Learning and memory

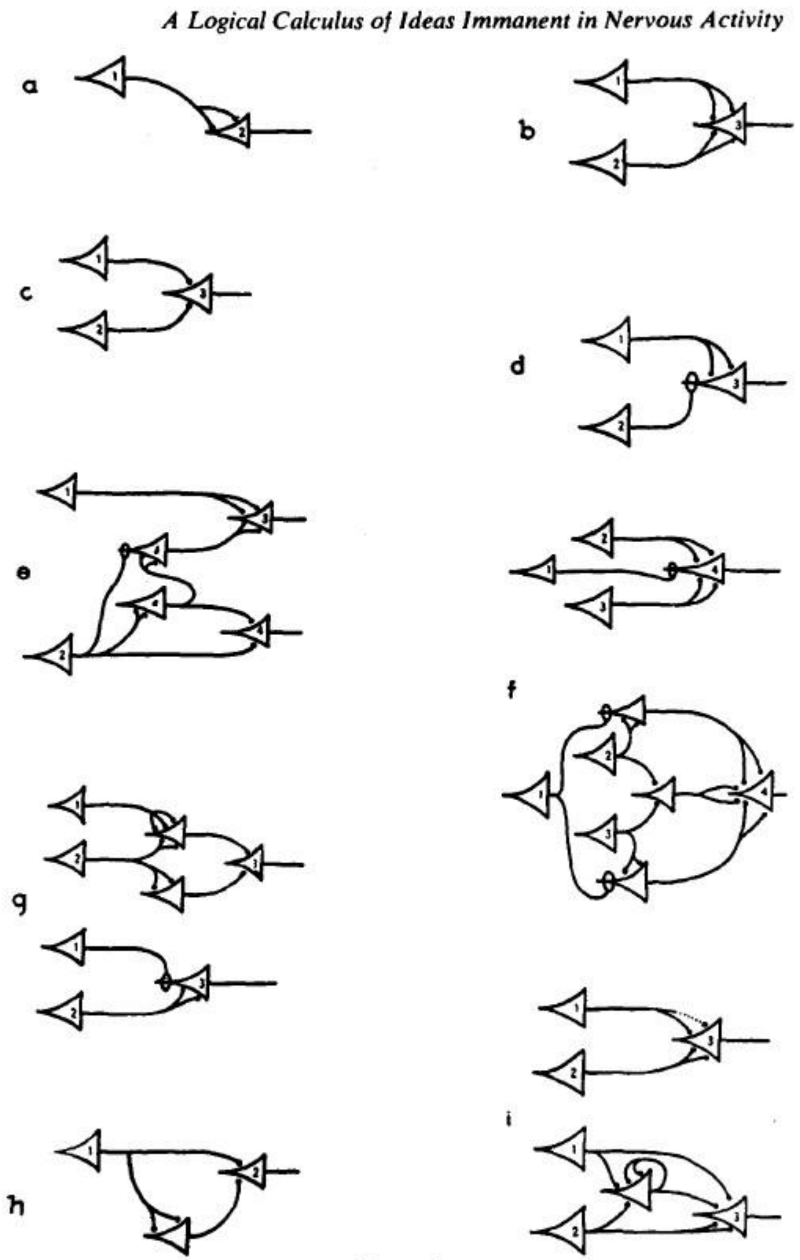


FIGURE 1

[McCullock, 43]

A bit of History

McCullock & Pitts / Hebb
Rosenblatt's Perceptron
Minsky & Papert - XOR
Backpropagation Algorithm

[Rosenblatt, 58] [Mark I Perceptron] [Perceptrons] [1]

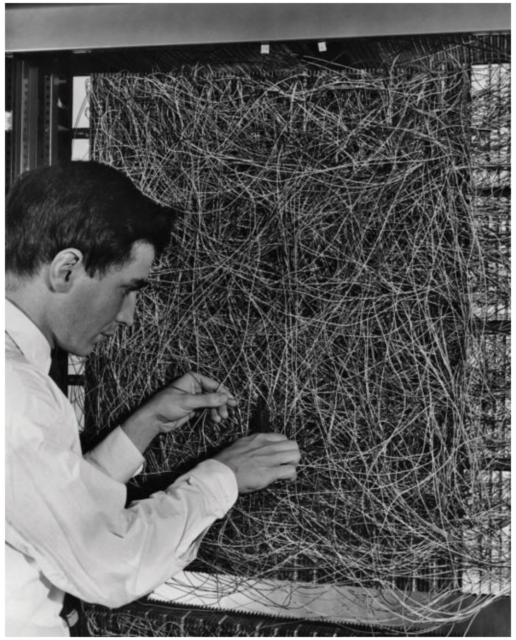
1948, Rosenblatt applied *Hebb's* learning to *McCulloch & Pitts* design

$$f(x) = \begin{cases} 1 \text{ if } w \cdot x + b > 0 \\ 0 \text{ otherwise} \end{cases}$$

w real-valued weights
· dot product
b real scalar constant

The Mark I Perceptron. A visual classifier with:

- 400 photosensitive receptors (sensory units)
- 512 stepping motors (association units, trainable)
- 8 output neurons (response units)



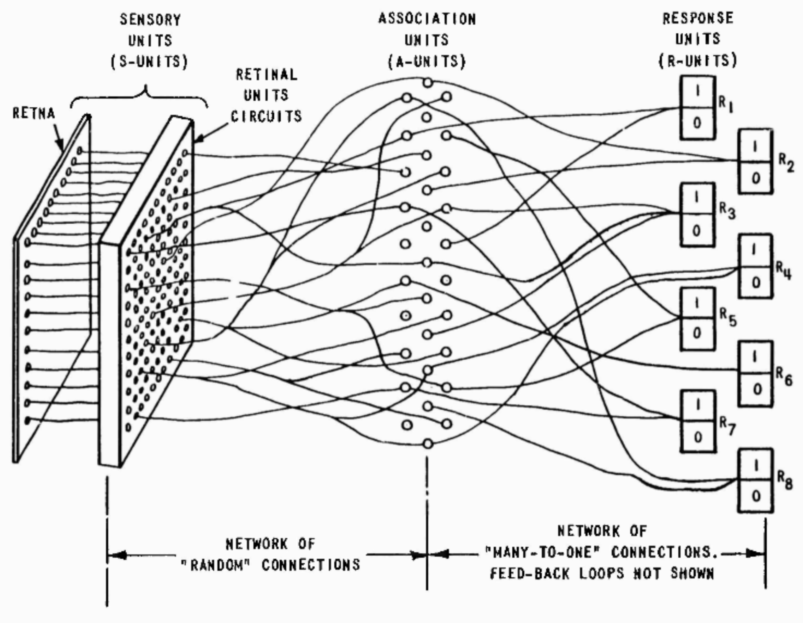


Figure I ORGANIZATION OF THE MARK I PERCEPTRON

A bit of History

McCullock & Pitts / Hebb
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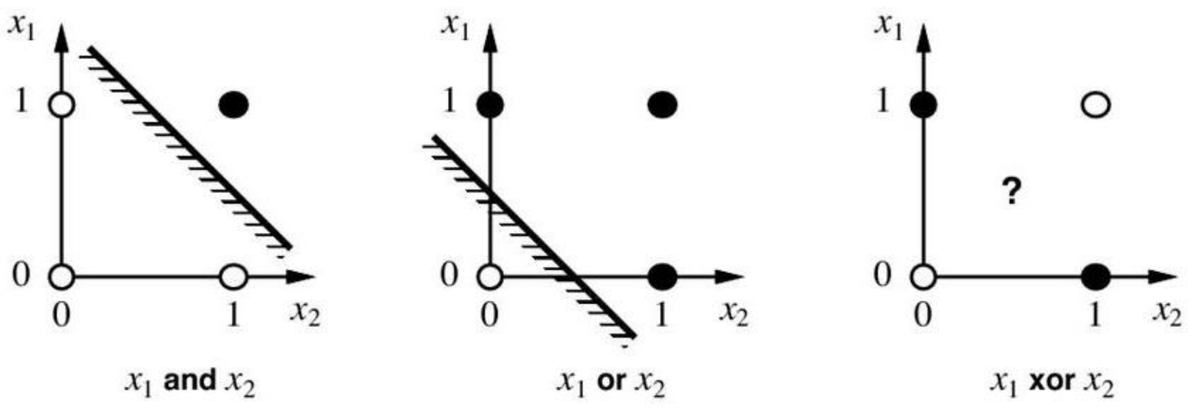
Rosenblatt acknowledged a set of limitations in the Perceptron machine.

Minsky & Papert did too in “*Perceptrons: an introduction to computational geometry*”, including:

- A multilayer perceptron (MLP) is needed for learning basic functions like XOR
- MLP cannot be trained.



This had a huge impact on the public, resulting in a drastic cut in funding of NNs until the mid 80s

1st AI WINTER

[Minsky, 69]

A bit of History

McCullock & Pitts / Hebb
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[Werbos,74]
[Rumelhard,85]

How can we optimize neuron weights which are not directly connected to the error measure?

Backpropagation algorithm:
Use the chain rule to find the derivative of cost with respect to any variable.

In other words, find the contribution of each weight to the overall error.

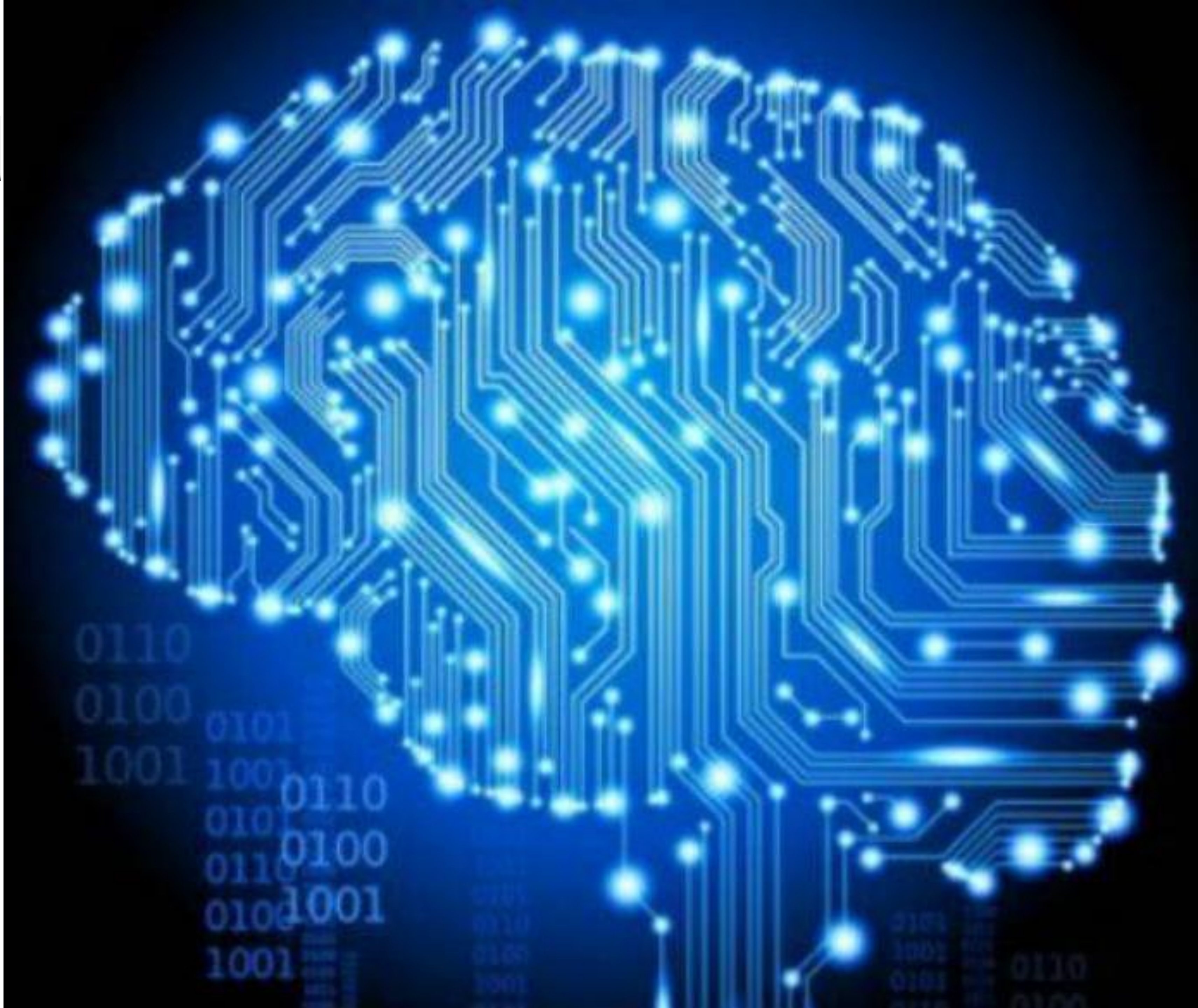
First proposed for training MLPs by *Werbos* in '74.
Rediscovered by *Rumelhart, Hinton and Williams* in '85.

End of NNs Winter

Training with backprop

1. Forward pass from input to output
2. Error measurement (loss function)
3. Find gradients towards minimizing error layer by layer (backward pass)

Feedforward Neural Networks



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Feedforward Neural Networks

SGD, Epochs, Batches and Steps
Activation functions
SGD learning rate
Other optimization methods
Regularization
Normalizing inputs
Vanishing/Exploding Gradients
Weights initialization

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Computing the gradients using all available training data would require huge amounts of memory.

Stochastic Gradient Descent: Iteratively update weights using random samples (hence, *stochastic*)

Each feedforward/backward cycle (a **step**) processes a random **batch** of images.

- Typical batch sizes: Powers of 2.
- Batch size = 1 --> Full stochastic (slower)
- Batch size = dataset_size --> Deterministic (bad generalization)

An **epoch** is the processing of the whole dataset once. It corresponds to processing as many batches as:

```
dataset_size / batch_size
```

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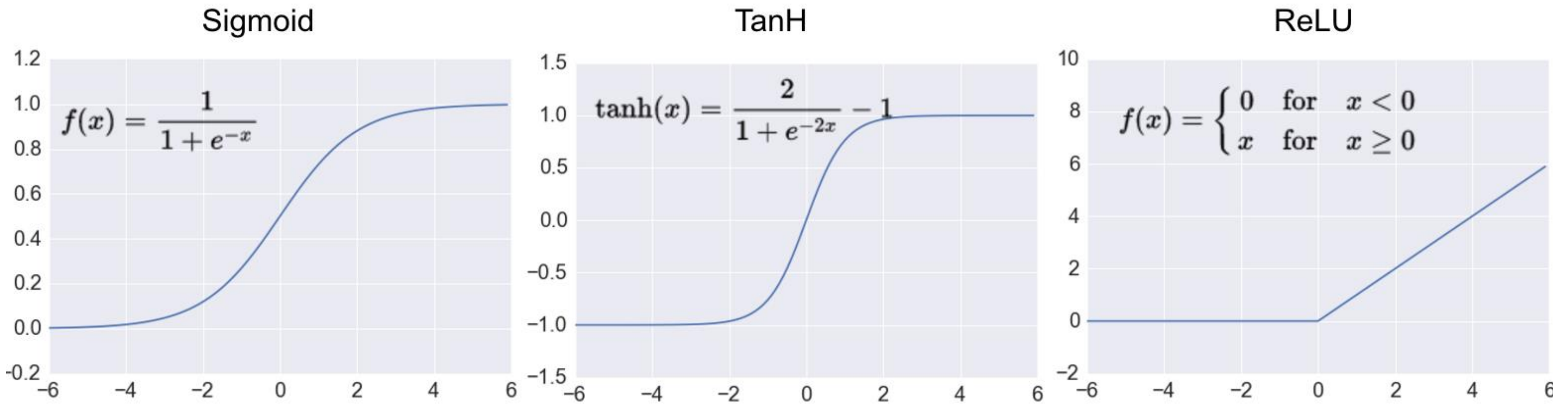
Activation functions transform the output of a layer to a given range. If the function is non-linear, the net can learn non-linear patterns (e.g., XOR).



- Zero gradient in most of f(x). Saturates!
- Max gradient is 0.25 or 1. Vanishing!

- Does not saturate
- Does not vanish
- Faster
- May die

ReLU is a safe choice in most cases

Undying alternatives: Leaky ReLU, ELU, ...

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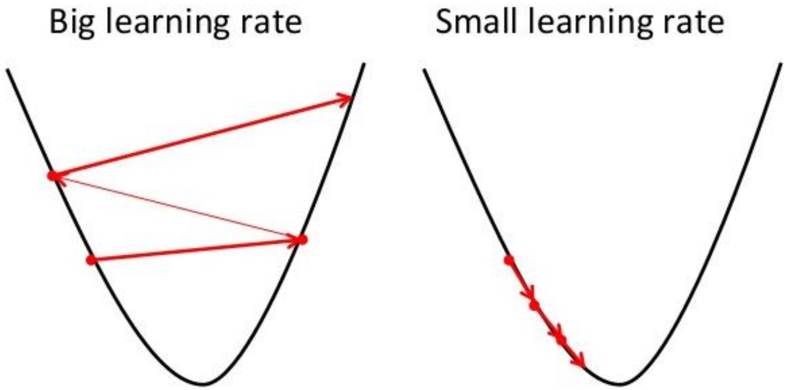
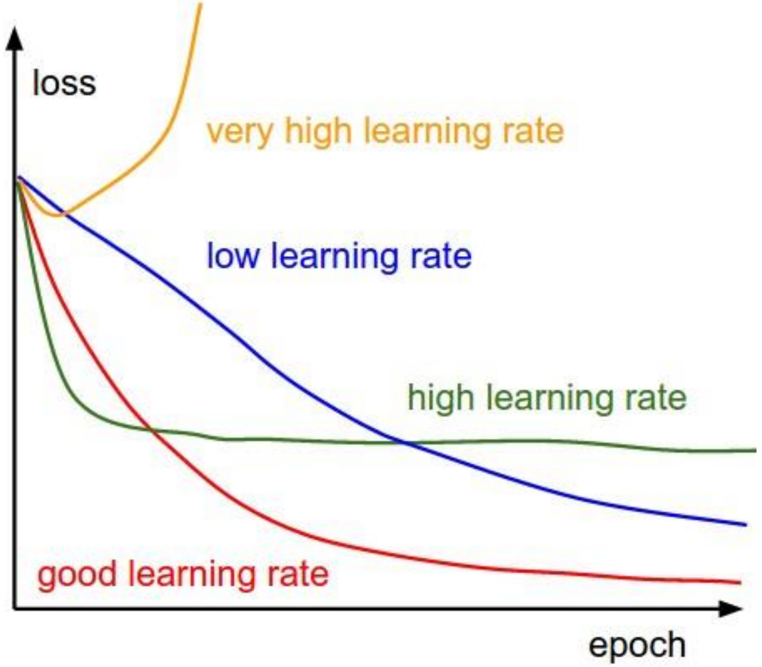
[Dauphin, 14]

Gradient descent is a simple and straight-forward optimization algorithm to update weights towards a min.

Learning rate determines how much we move in that direction. With the wrong LR you may end up in local minima or saddle points, or be too slow.

SGD will overshoot unless we keep decreasing the LR.





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[Dauphin, 14]
[Ruder,www]

Momentum: Include a fraction of the previous gradient. Keeps the general direction so far.

Nesterov: Compute current gradient considering where the previous gradient took you. (RNNs?)

Adagrad: Parameter-wise LR considering past updates. Good for infrequent patterns (GloVe). Vanishing LR due to growing history.

Adadelta: Adagrad with a decaying average over history. Typically set around 0.9.

Adam: Adadelta + Momentum

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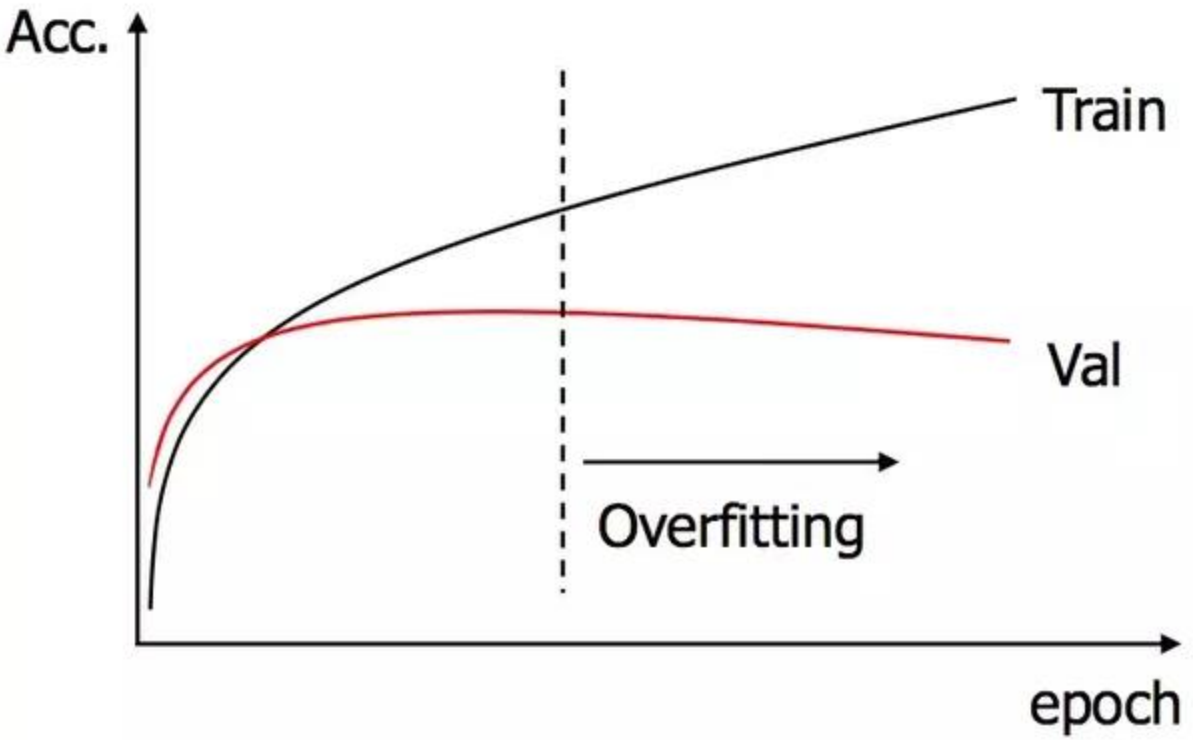
Why do we need regularization?

Because the difference between **Machine Learning** and **Optimization** is called **Generalization**



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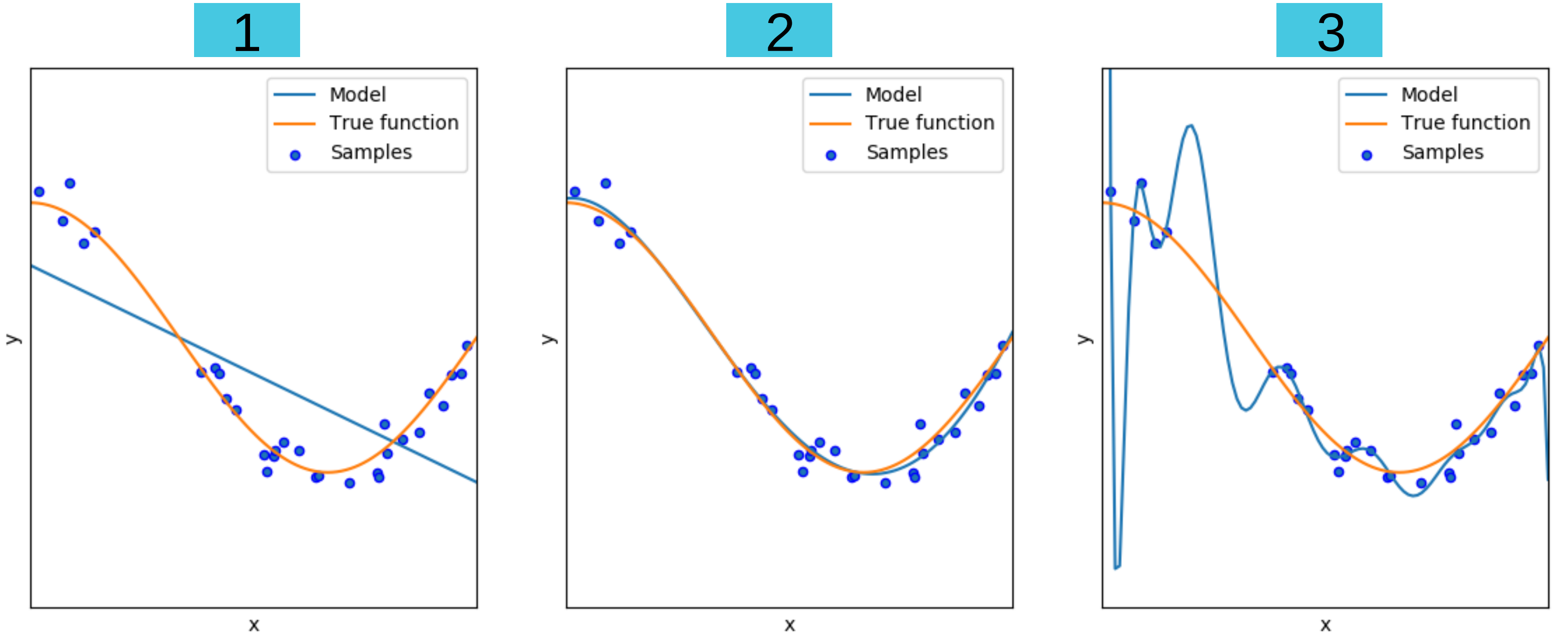
Generalization

Polynomial regression

1 $h(x) = w_1 x + b$

2 $h(x) = w_3 x^3 + w_2 x^2 + w_1 x + b$

3 $h(x) = w_{14} x^{14} + w_{13} x^{13} + \cdots + w_1 x + b$



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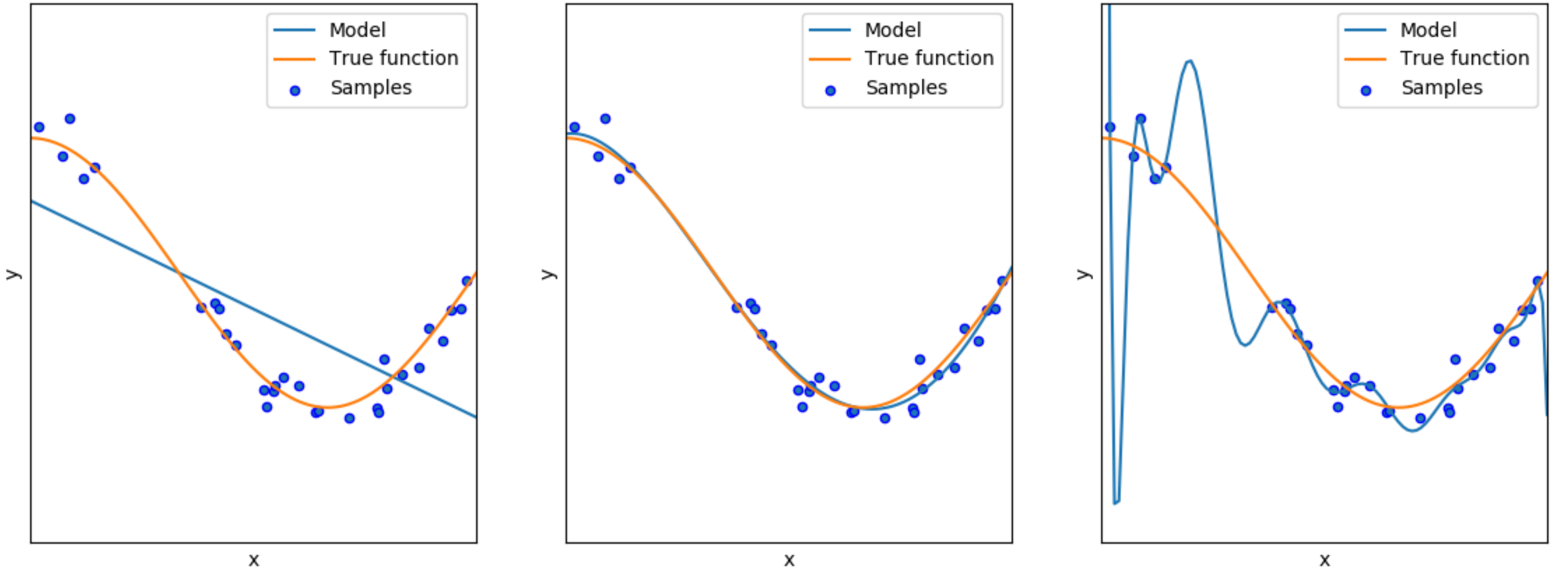
Generalization

Polynomial regression

Training Error		
Huge	Small	Tiny

Model Generalization		
Bad	Good	Horrible



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Generalization

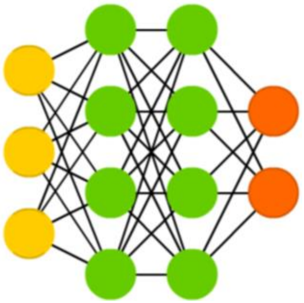
What **policy** can we use to **improve model generalization**?

Occam's Razor

when you have **two competing hypotheses**

that make the **same predictions**,

the **simpler one is the better**



Machine Learning

given **two models**

that have a **similar performance**,

It's better to **choose the simpler one**

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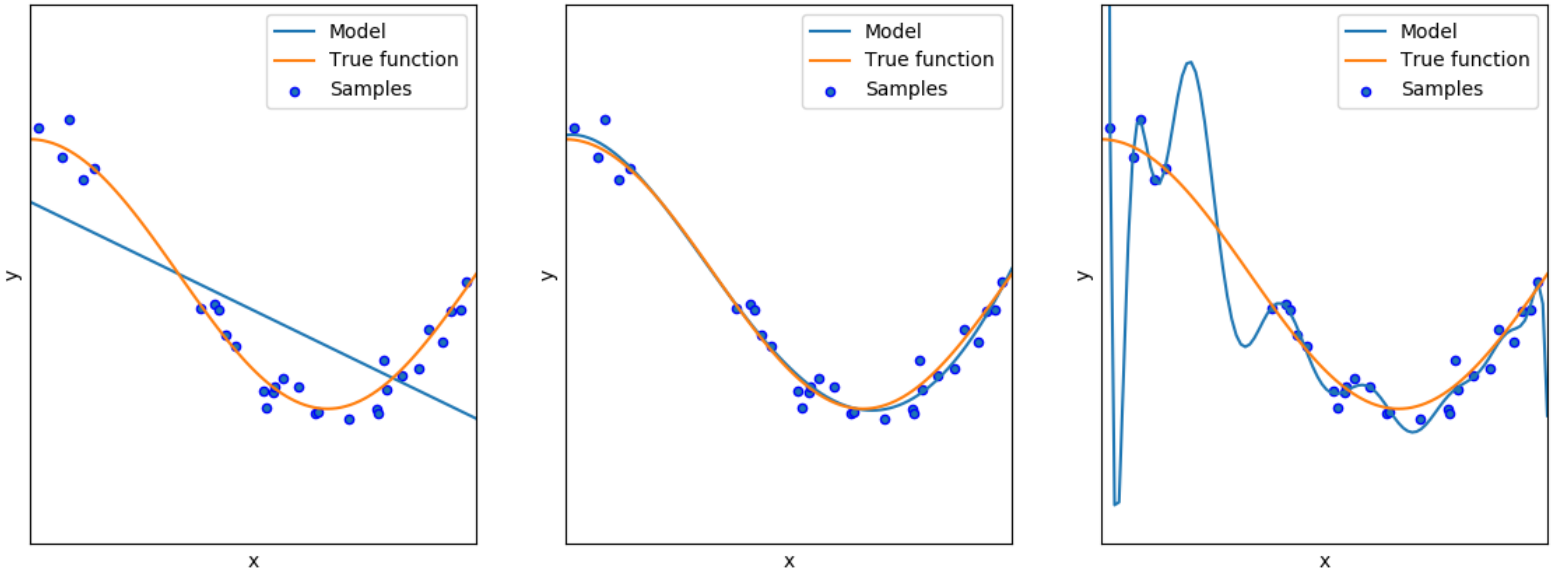
Model Complexity

What policy can we use to improve model generalization?

$$\text{Cost function} = \text{Training Error} + \textbf{Model Complexity}$$



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Model Complexity

$$h(x) = w_3x^3 + w_2x^2 + w_1x + w_0 \quad \text{VS} \quad h(x) = 0x^3 + 0x^2 + w_1x + w_0$$

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Model Complexity

$h(x) = w_3x^3 + w_2x^2 + w_1x + w_0$ VS $h(x) = 0x^3 + 0x^2 + w_1x + w_0$

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? ? ?

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Model Complexity

$h(x) = 0x^3 + 0x^2 + w_1 x + w_0$ **VS** $h(x) = 0x^3 + w_2 x^2 + 0x + 0$

ℓ_0 complexity: Number of non-zero coefficients

ℓ_1 "lasso" complexity: $\sum_{i=0}^{d} |w_i|$, for coefficients $w_0, ..., w_d$

ℓ_2 "ridge" complexity: $\sum_{i=0}^{d} w_i^2$, for coefficients $w_0, ..., w_d$

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Model Complexity

$h(x) = 0x^3 + 0x^2 + w_1 x + w_0$ VS $h(x) = 0x^3 + w_2 x^2 + 0x + 0$

$w_0 = 1.3 \quad w_1 = -1.2$ | $w_2 = 2.2$

ℓ_0 complexity

$|\{w_1, w_0\}| = 2$ VS $|\{w_2\}| = 1$

ℓ_1 complexity

$|1.3| + |-1.2| = 2.5$ VS $|2.2| = 2.2$

ℓ_2 complexity

$1.3^2 + (-1.2)^2 = 3.13$ VS $2.2^2 = 4.84$

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L1 / L2 Regularization

$$\text{Cost function} = \text{Loss} + \boxed{\frac{\lambda}{m}\sum_{i=0}^{m}|w_i|}$$

$$\text{Cost function} = \text{Loss} + \boxed{\frac{\lambda}{2m}\sum_{i=0}^{m}w_i^2}$$

$$\text{Regularization parameter} \rightarrow \lambda$$

What **complexities** do these methods use?

ℓ_1 "lasso" complexity: $\sum_{i=0}^{d}|w_i|$, for coefficients $w_0, \ldots, w_d$

ℓ_2 "ridge" complexity: $\sum_{i=0}^{d}w_i^2$, for coefficients $w_0, \ldots, w_d$

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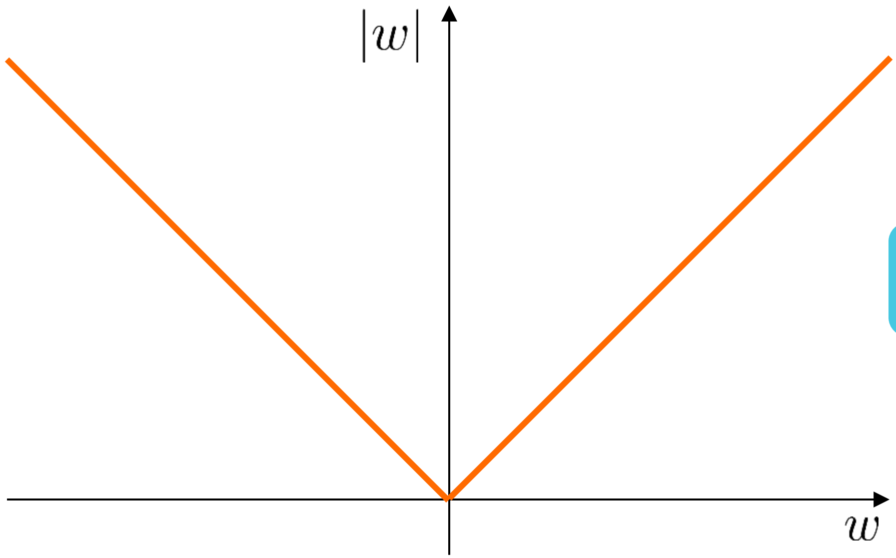
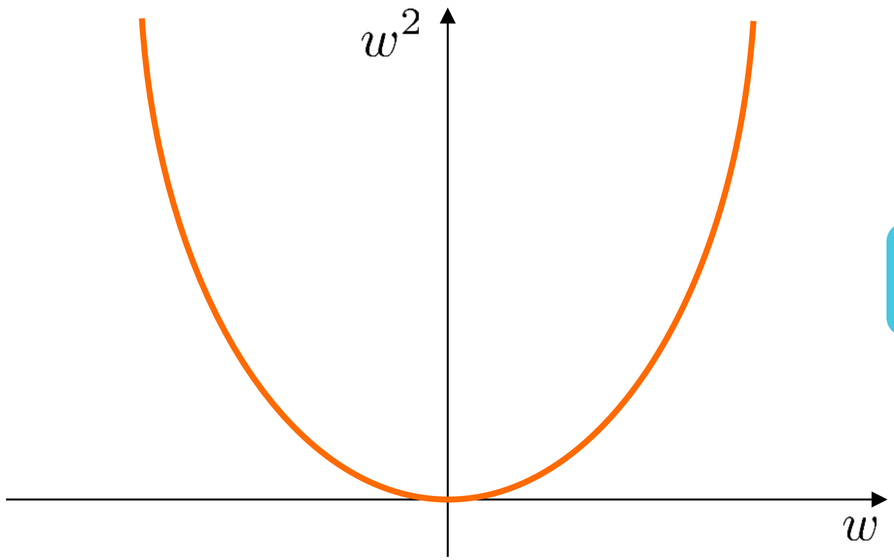
L1 / L2 Regularization



L1 Penalty



L2 Penalty

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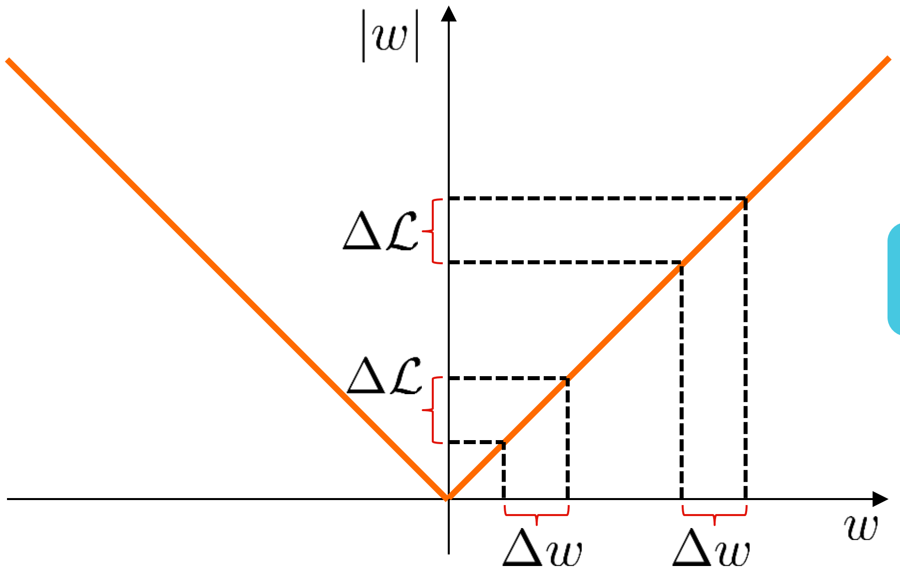
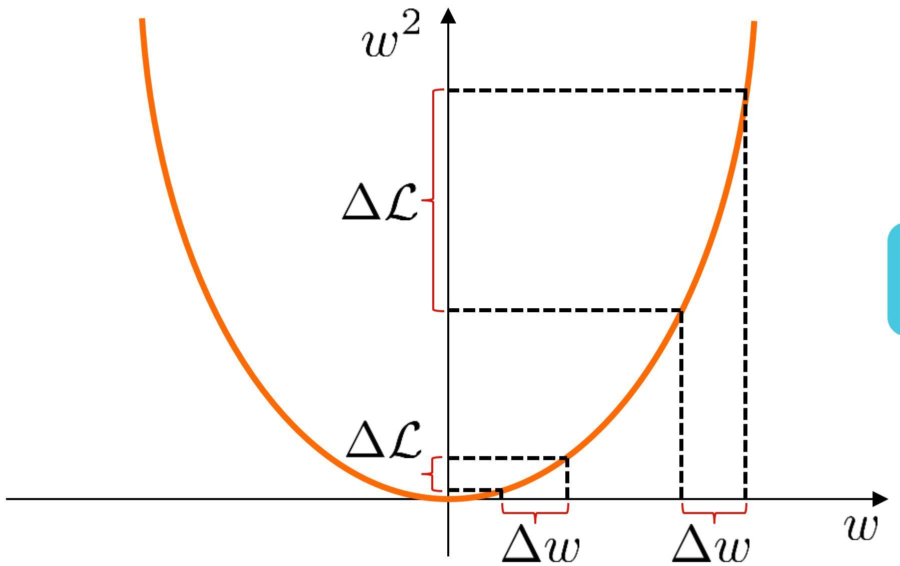


L1 Penalty



L2 Penalty

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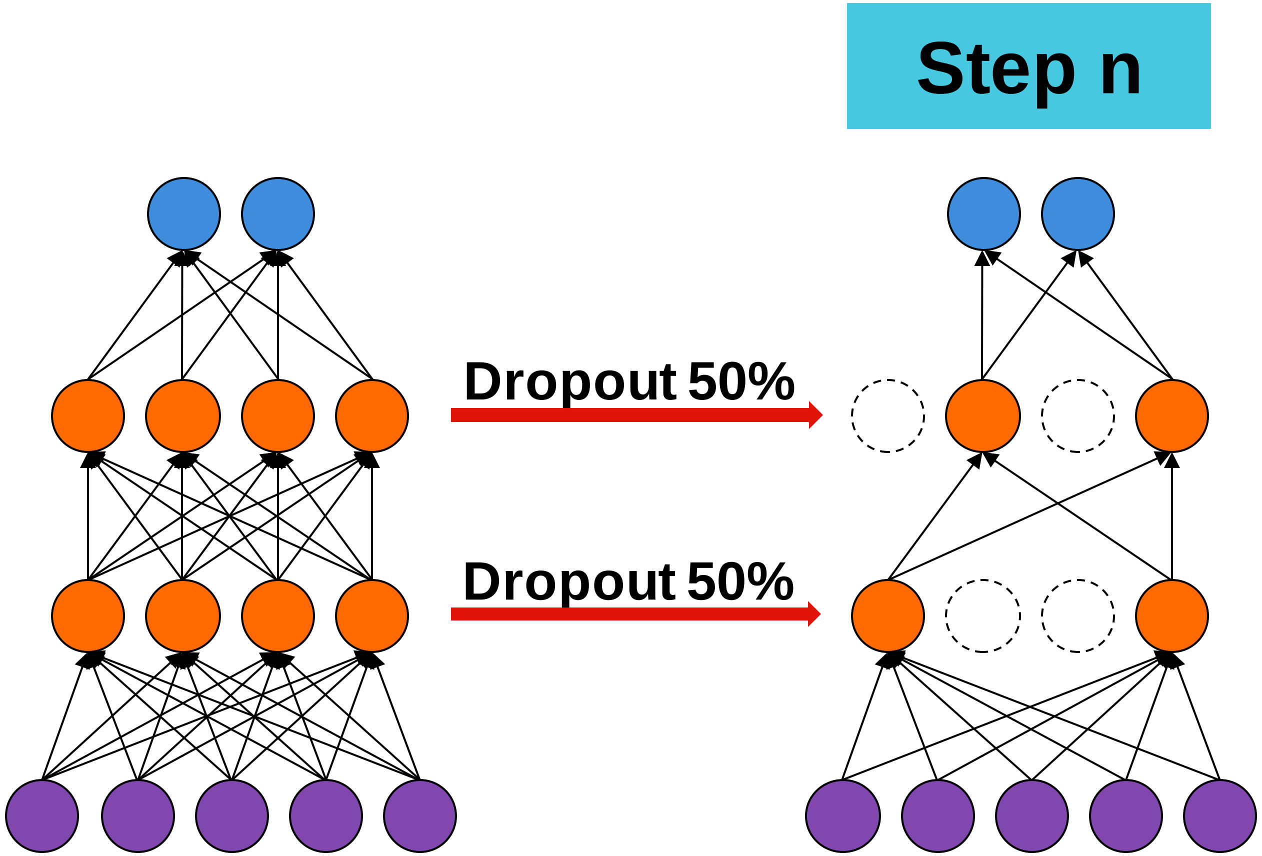
Dropout



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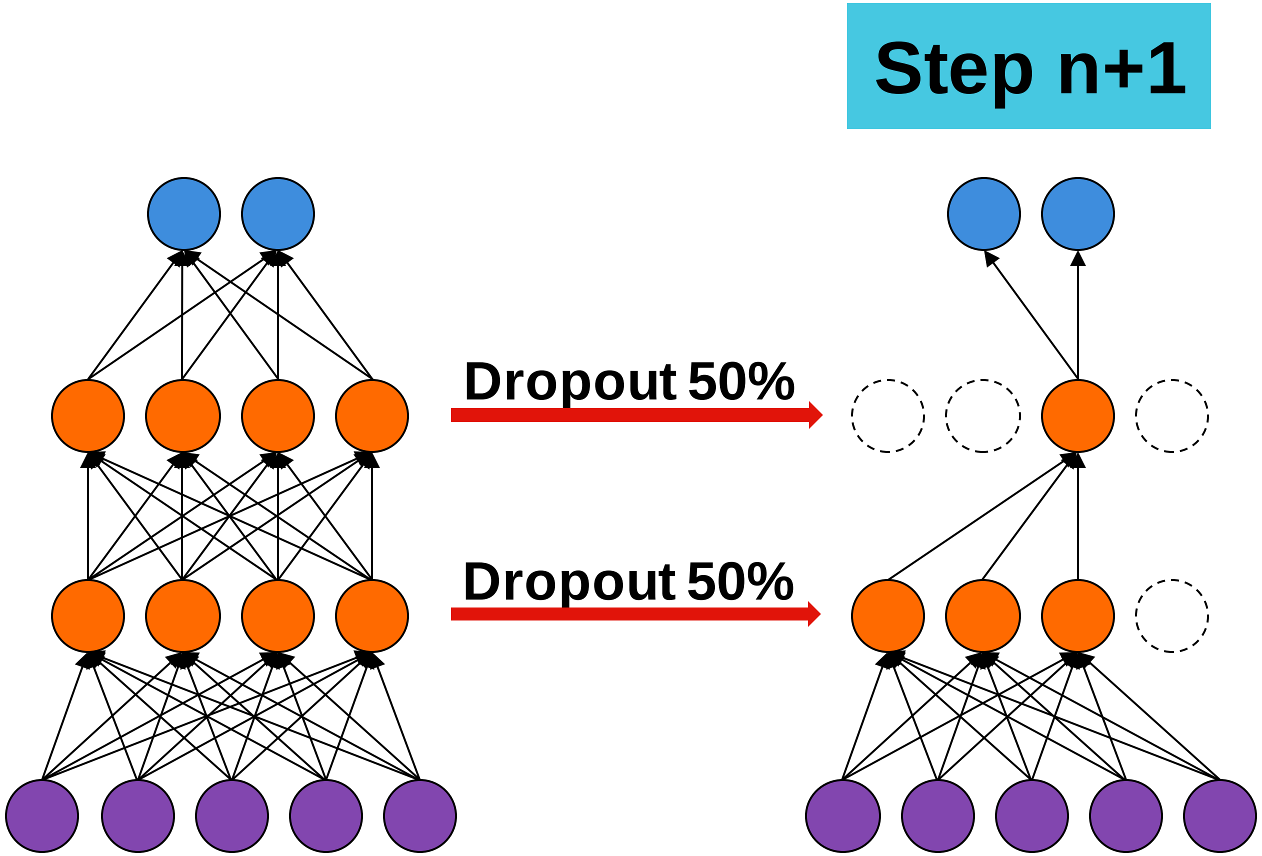

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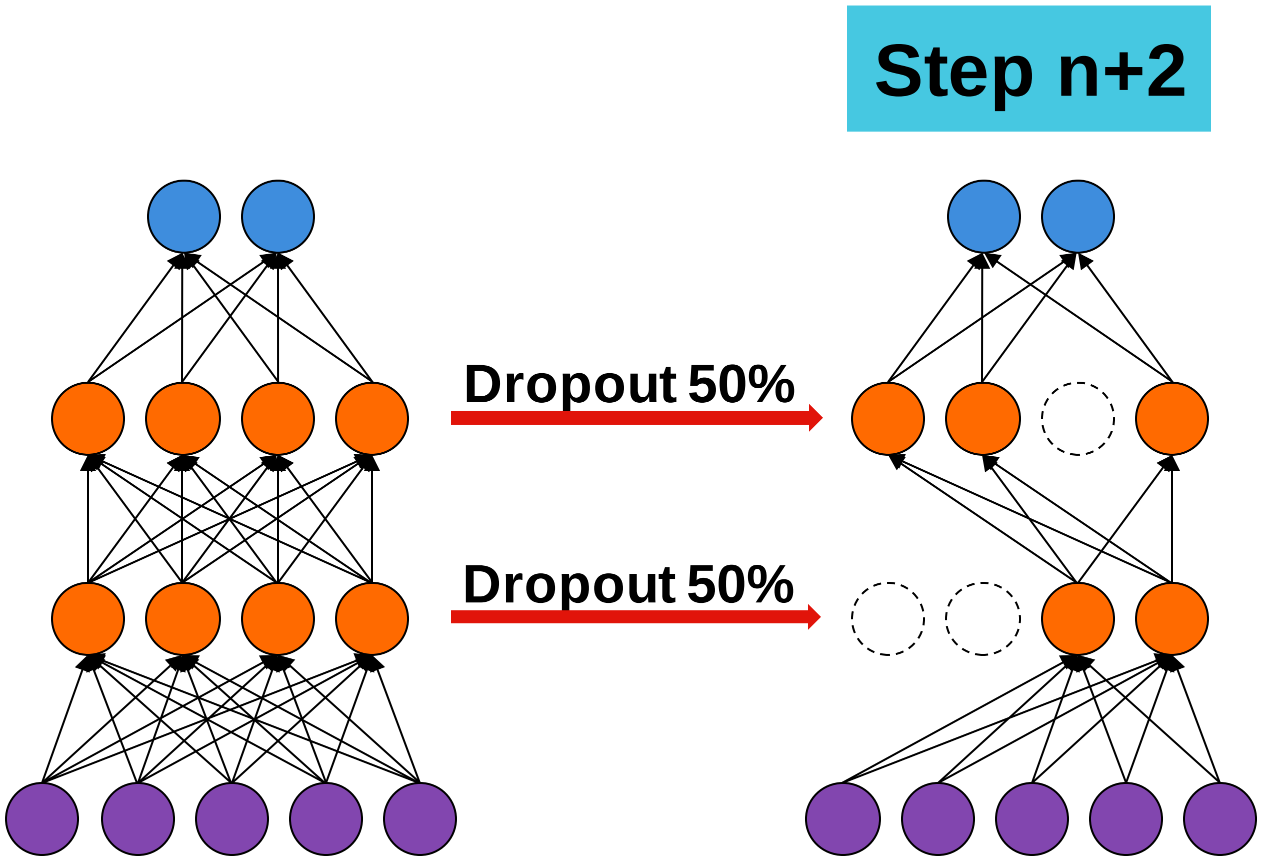

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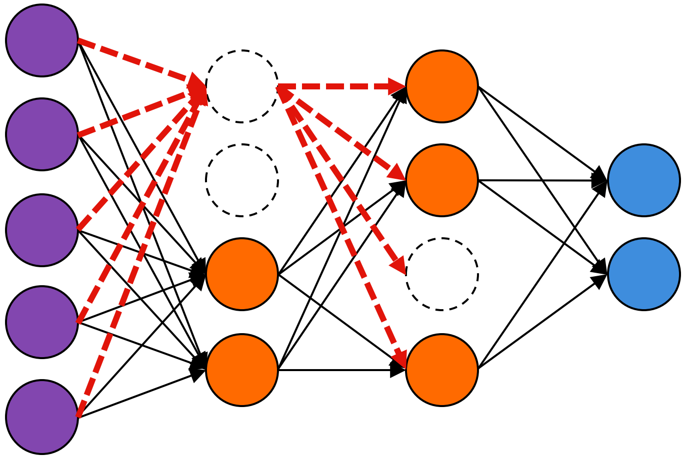

Before drop-out:

$$a_0^{[0]} = g\left(w_{00}^{[0]}x_0 + w_{10}^{[0]}x_1 + w_{20}^{[0]}x_2 + w_{30}^{[0]}x_3 + w_{40}^{[0]}x_4 + b_0^{[0]}\right)$$

After drop-out: $a_0^{[0]} = 0$

What **complexity** does this method use?

ℓ_0 complexity: Number of non-zero coefficients

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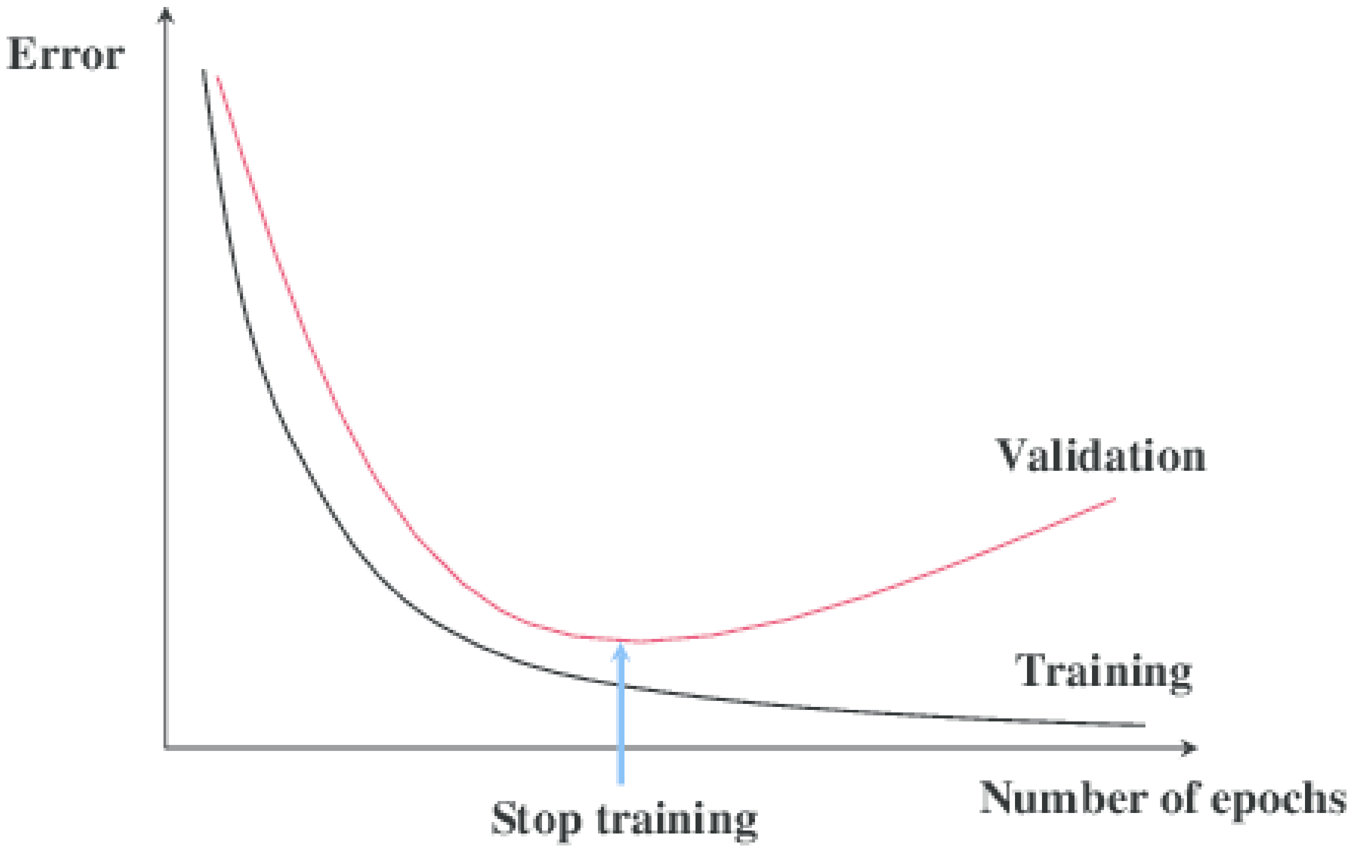
Early Stopping



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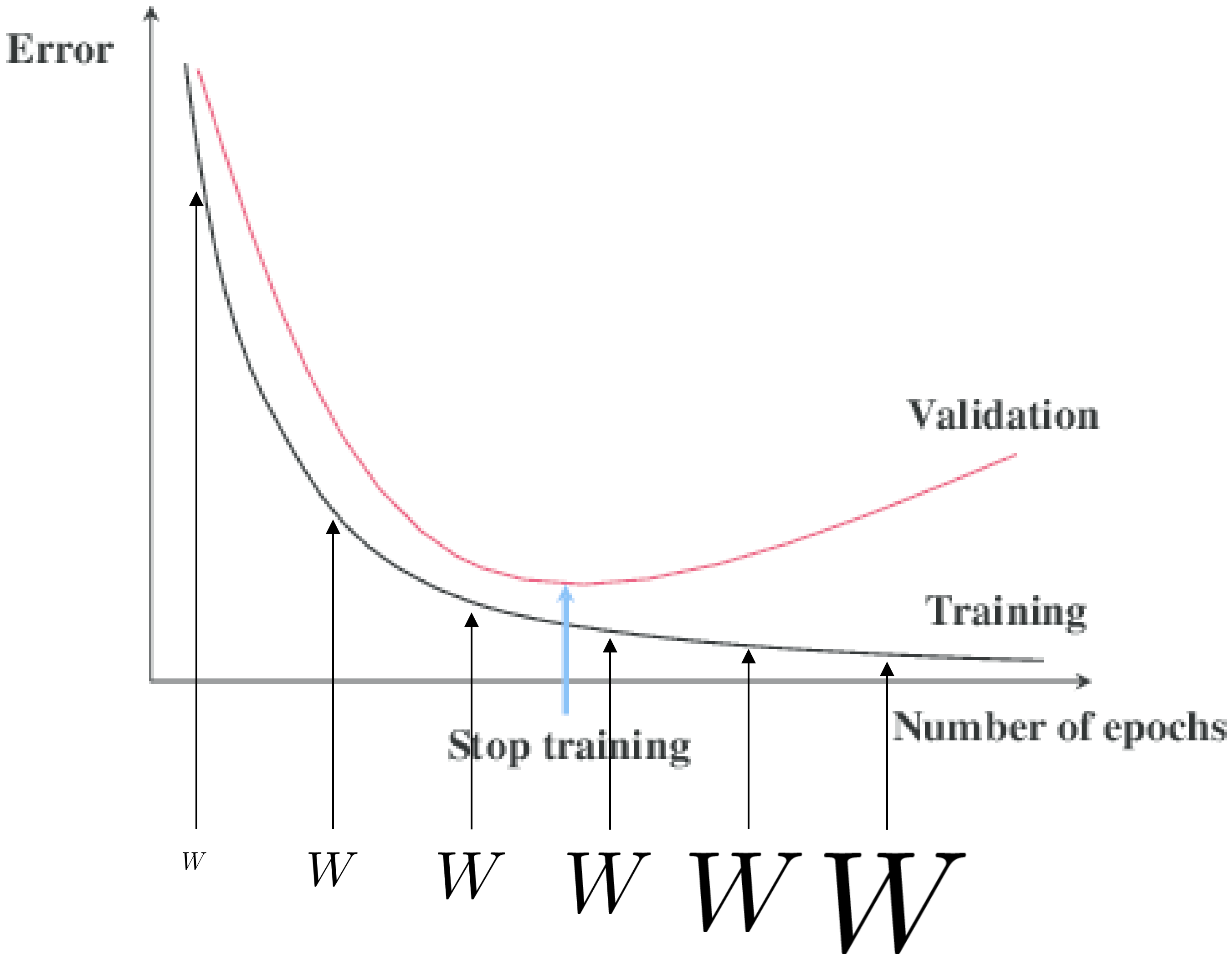

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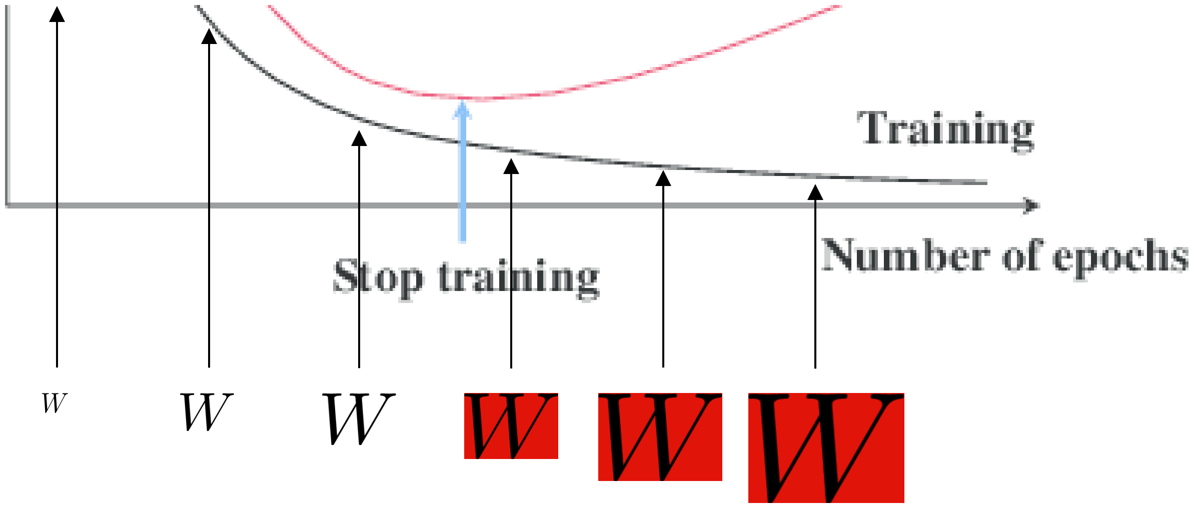

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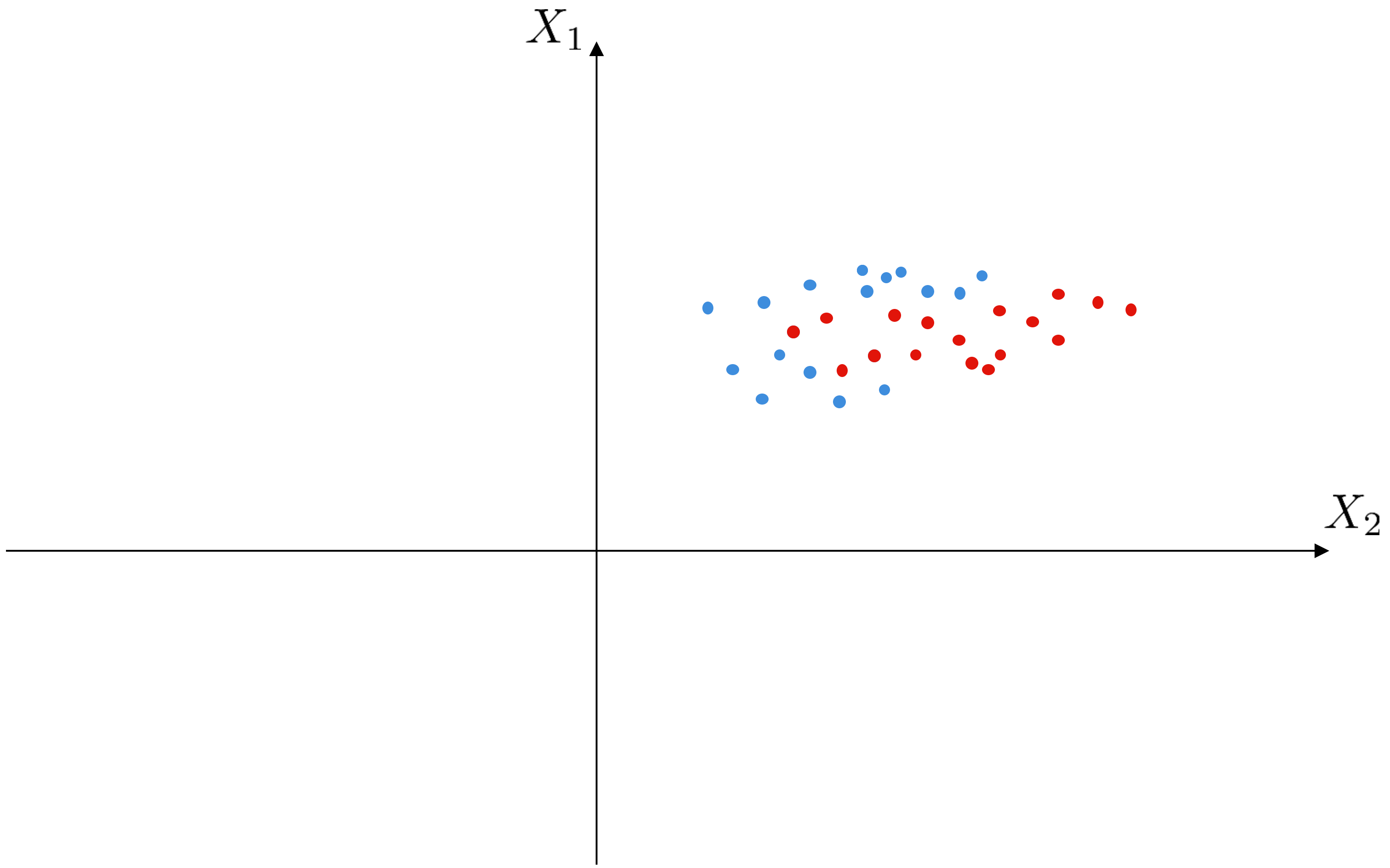

$$x = \frac{x - \mu}{\sigma^2}$$

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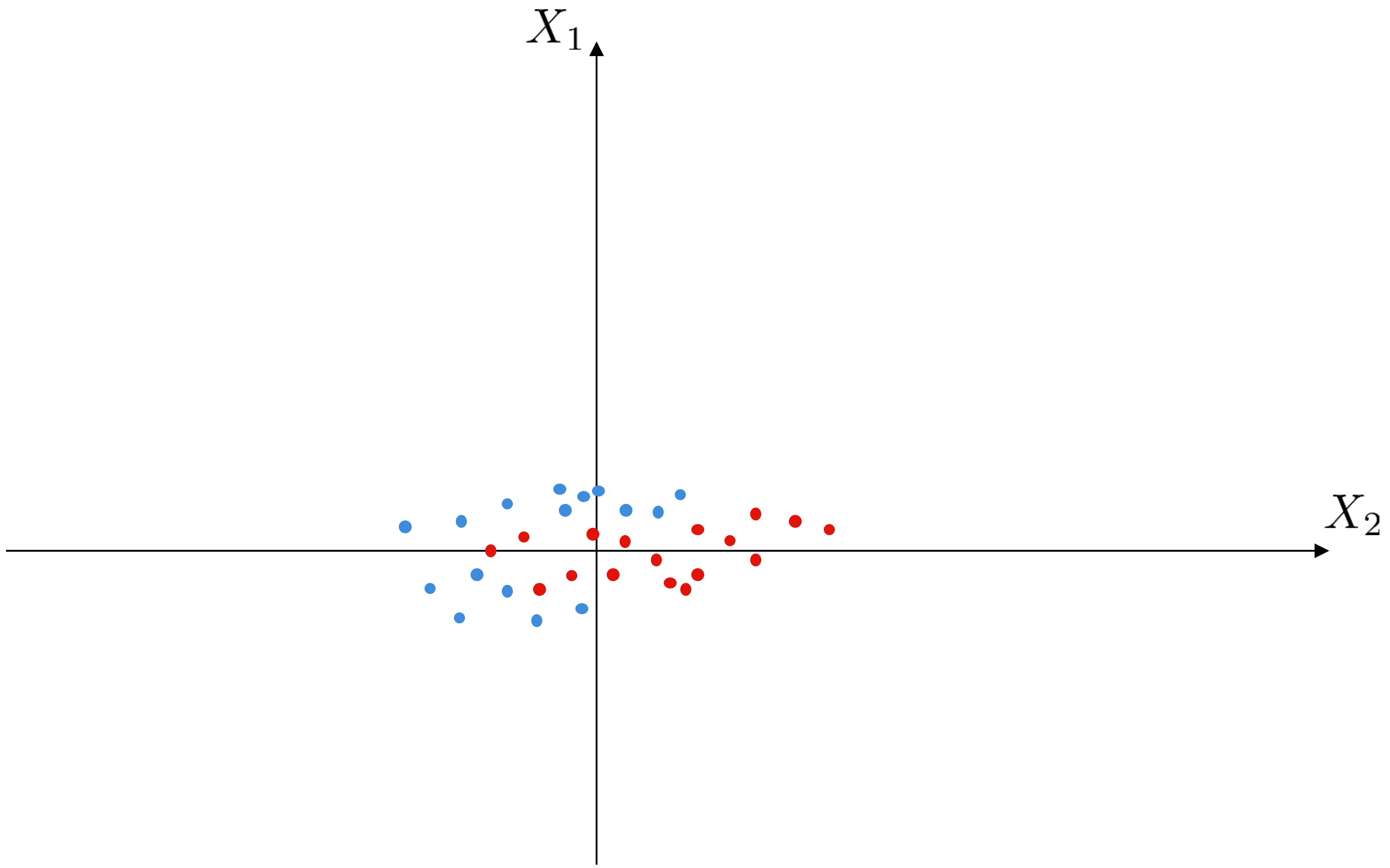

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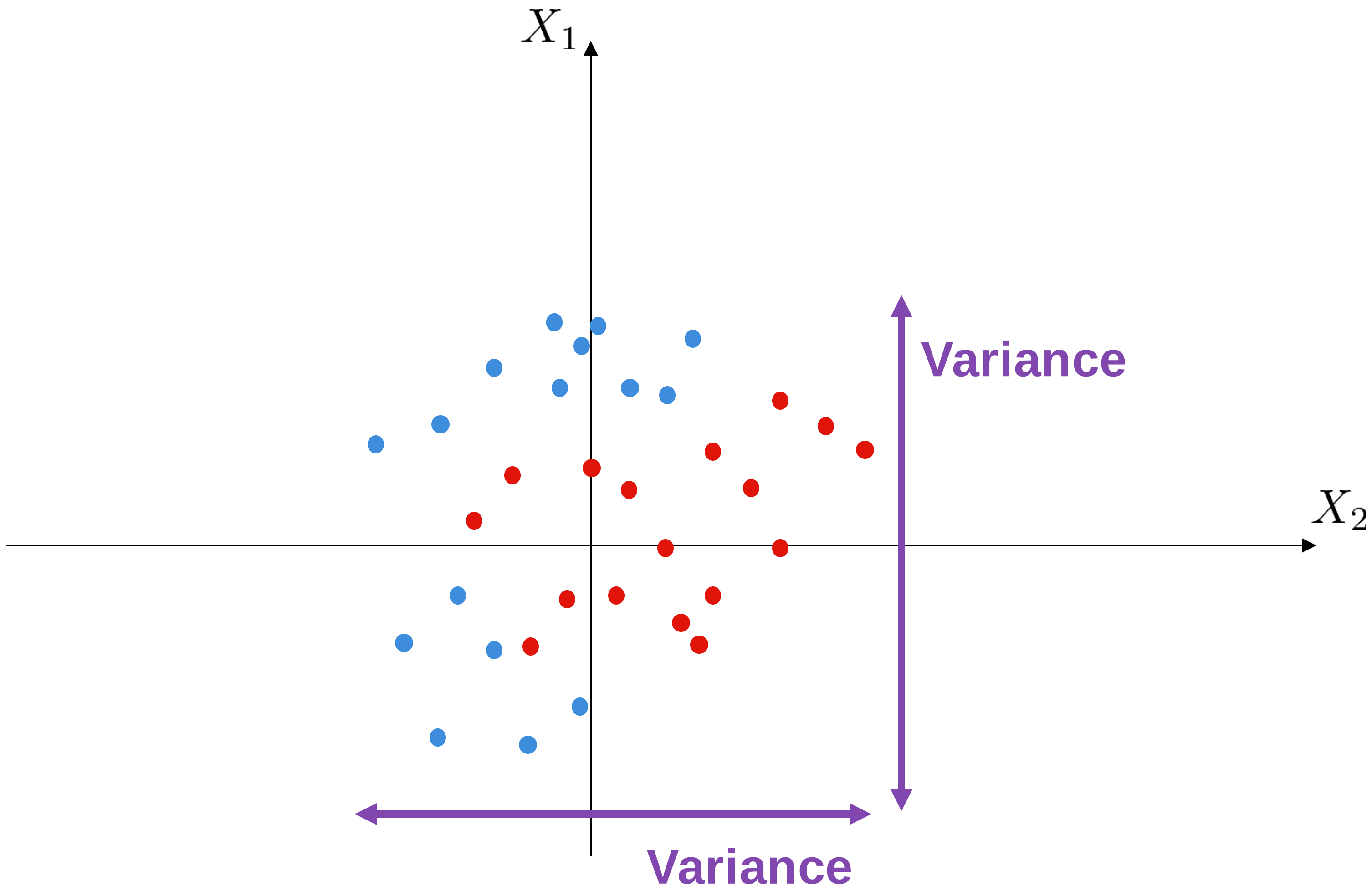

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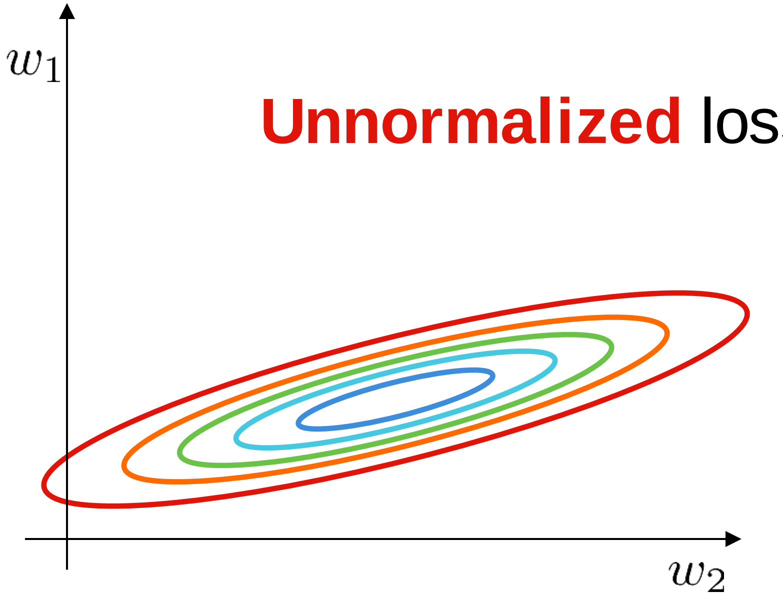
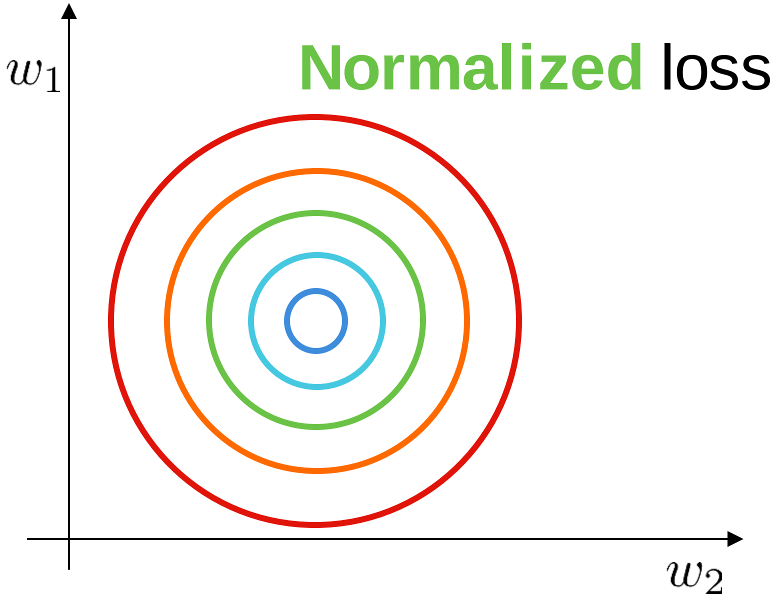
Why **input normalization** matters?



$f_1 \in [1, 1000]$
$f_2 \in [0, 1]$



$f_1 \in [-0.5, 0.5]$
$f_2 \in [-0.5, 0.5]$

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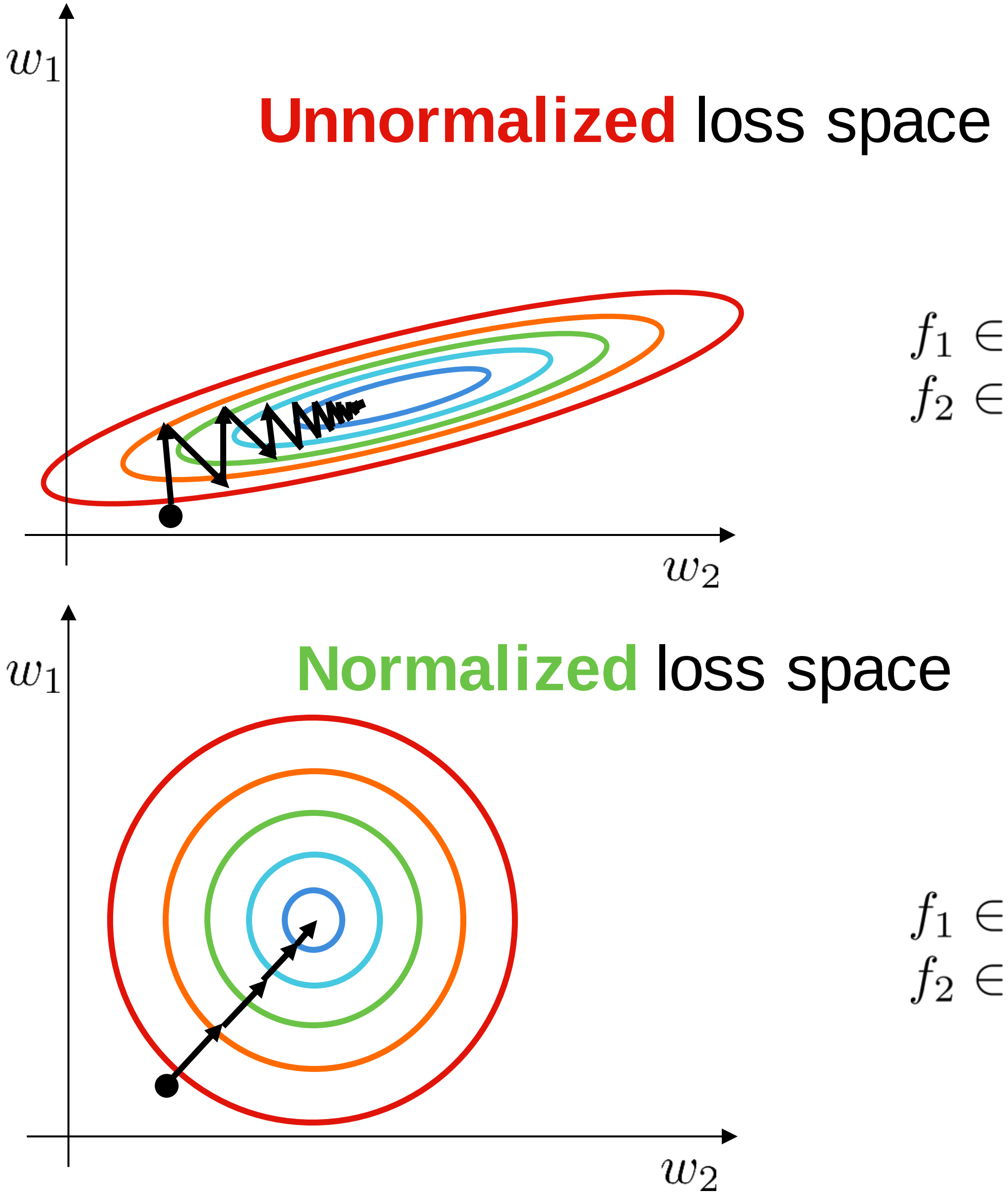

$f_1 \in [1, 1000]$
$f_2 \in [0, 1]$

$f_1 \in [-0.5, 0.5]$
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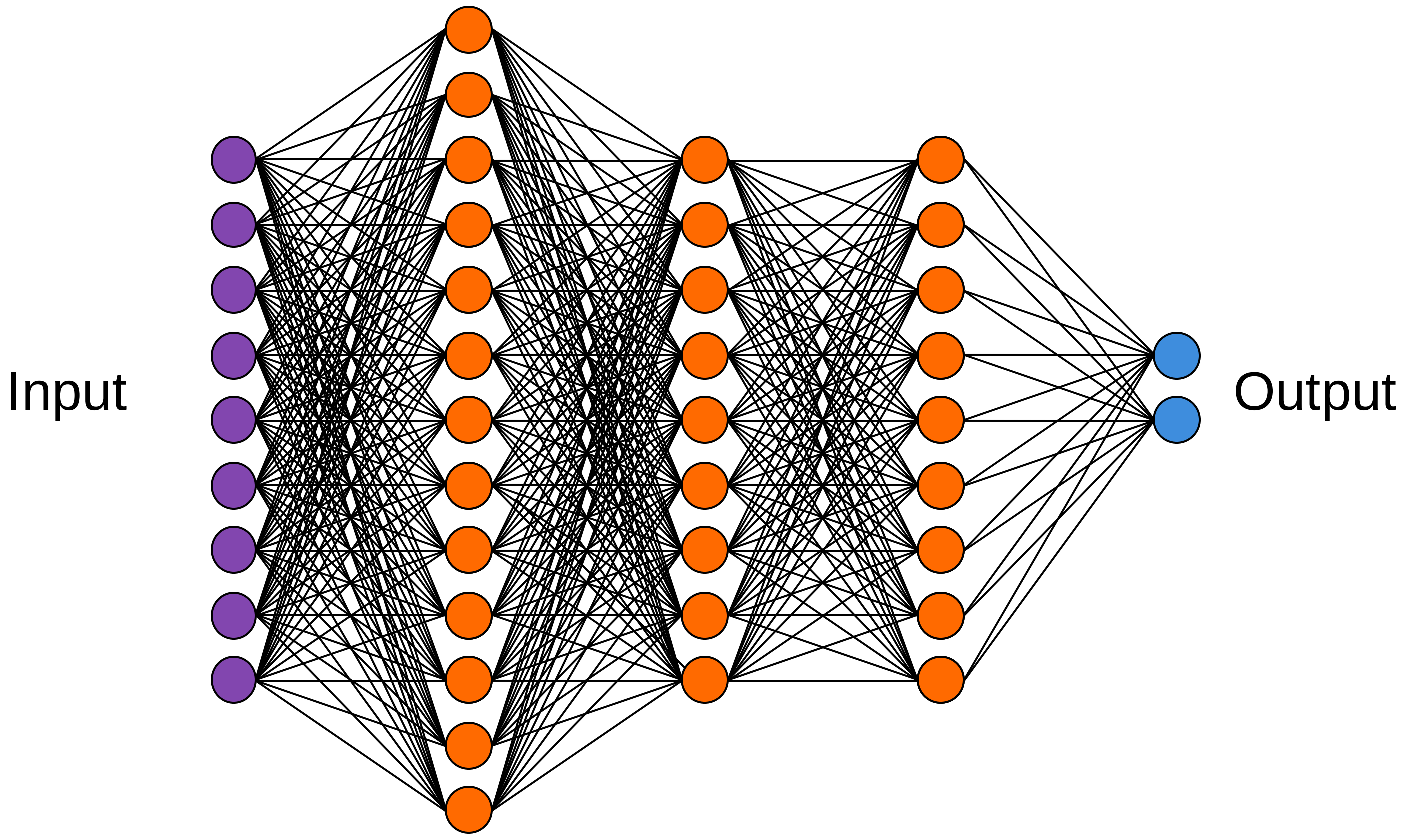

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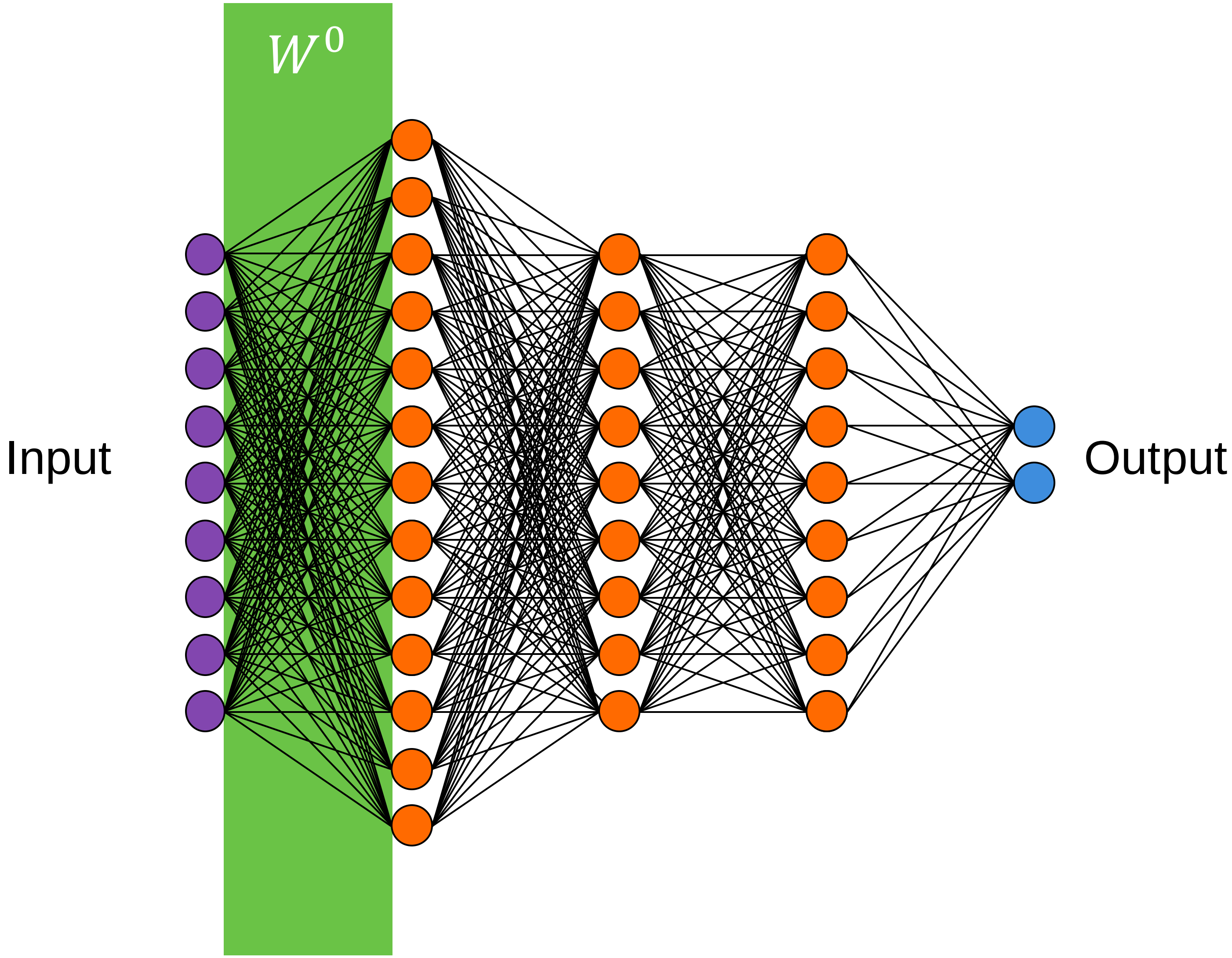

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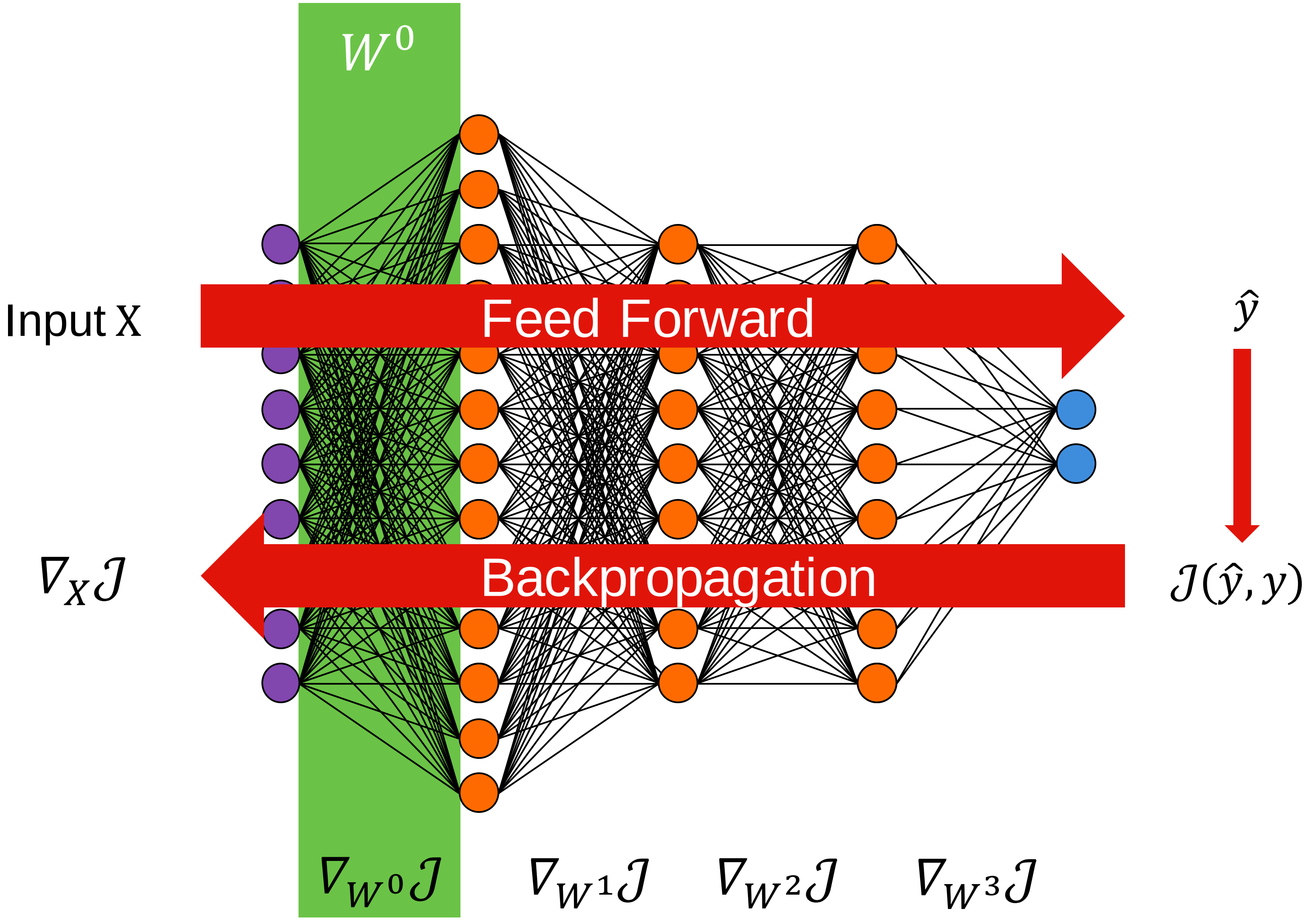

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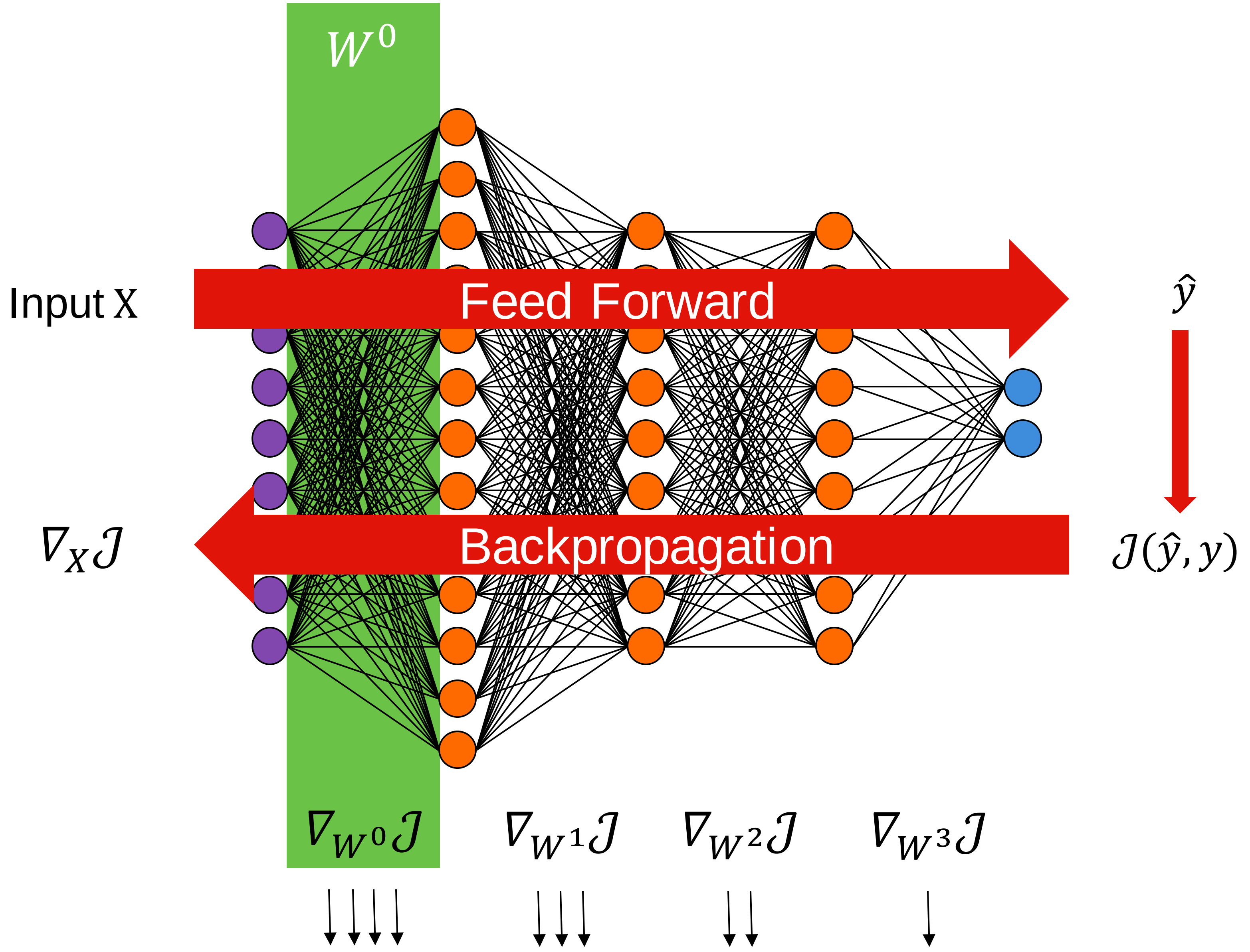

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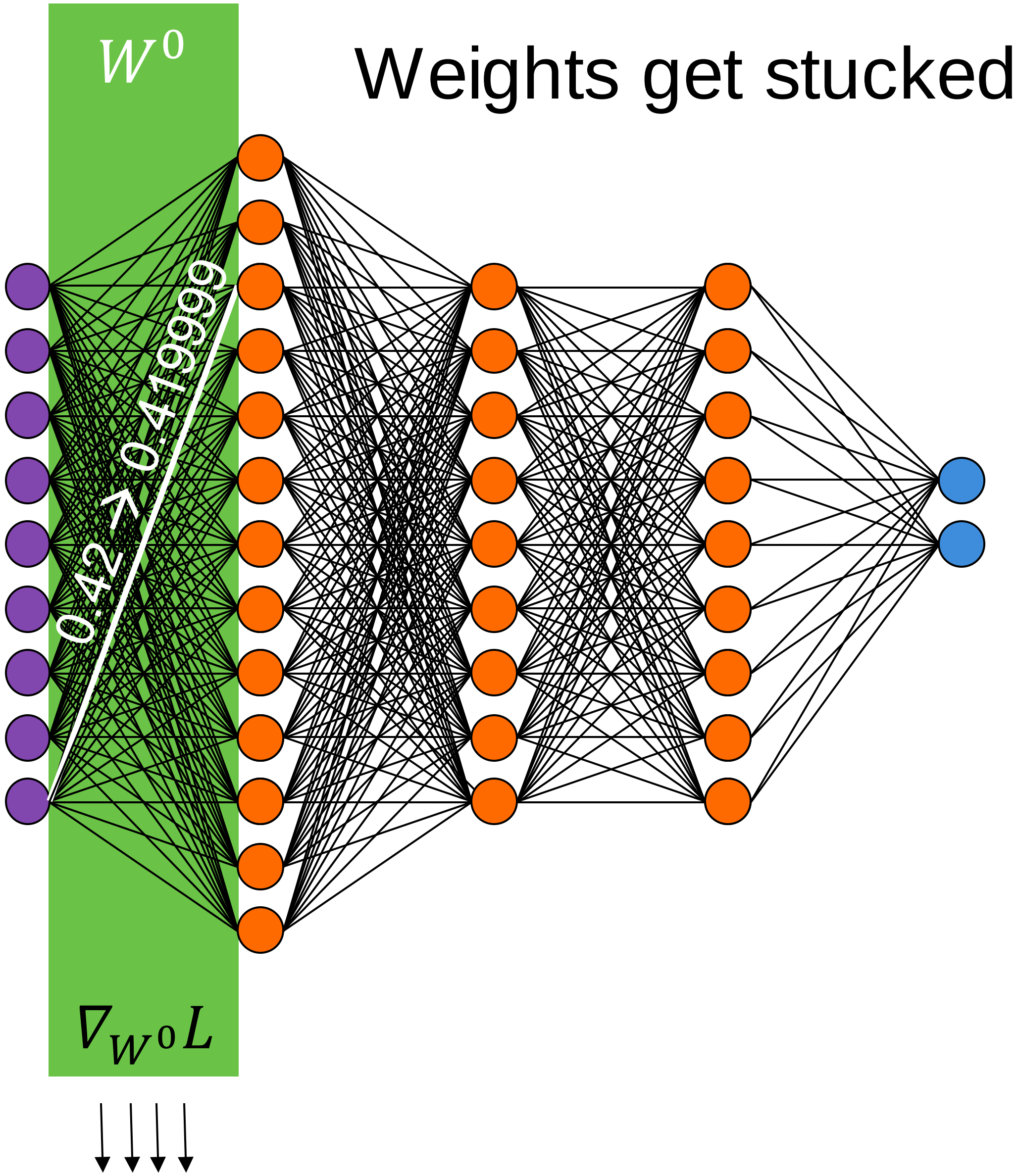

Weights get stucked!

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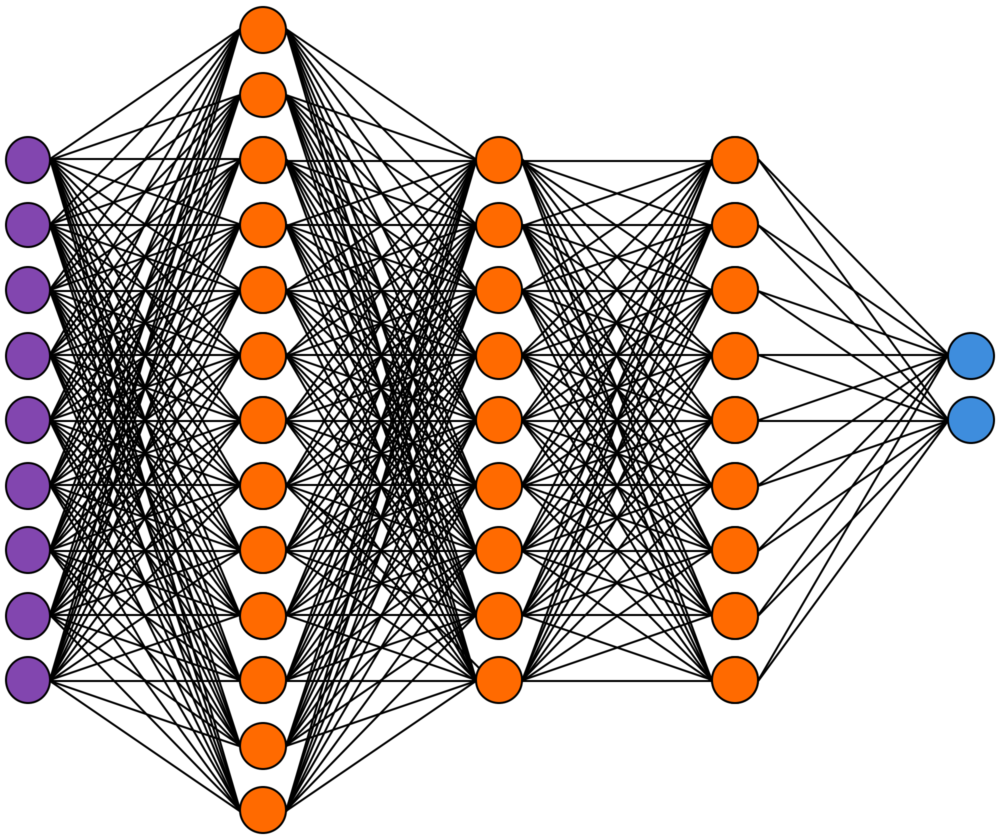
Why **gradients** get **smaller and smaller** at each layer on backpropagation?



$\nabla_{W^0}\mathcal{J}$ $\quad \nabla_{W^1}\mathcal{J}$ $\quad \nabla_{W^2}\mathcal{J}$ $\quad \nabla_{W^3}\mathcal{J}$

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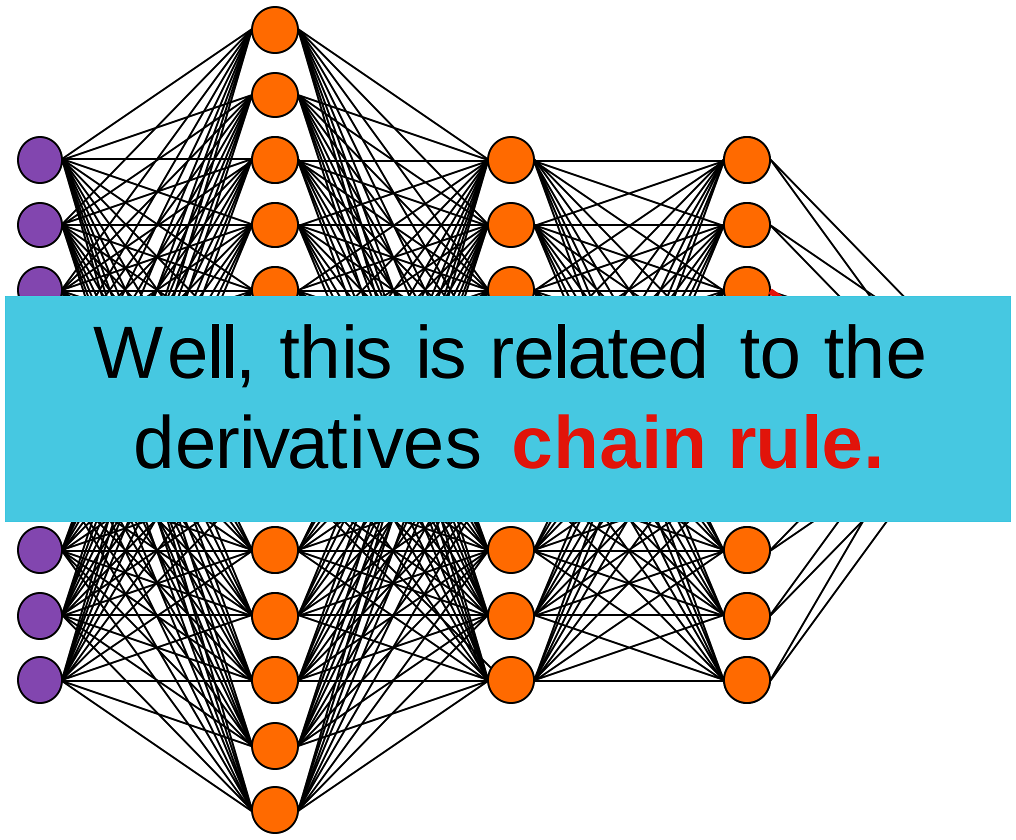

Well, this is related to the derivatives **chain rule.**

$\nabla_{W^0}\mathcal{J}$ $\nabla_{W^1}\mathcal{J}$ $\nabla_{W^2}\mathcal{J}$ $\nabla_{W^3}\mathcal{J}$

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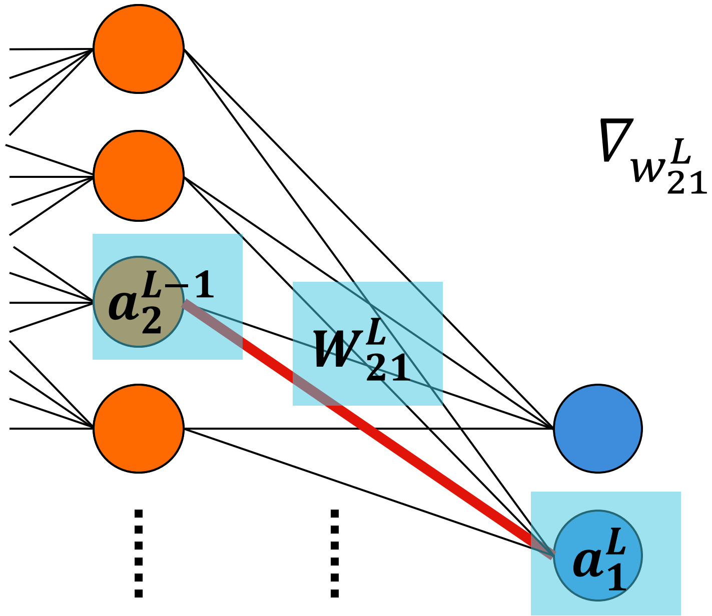

$$\nabla_{w_{21}^L}\mathcal{J} = \frac{\partial \mathcal{J}}{\partial w_{21}^L} = \frac{\partial \mathcal{J}}{\partial a_1^L} \times \frac{\partial a_1^L}{\partial z_1^L} \times \frac{\partial z_1^L}{\partial w_{21}^L}$$

$$\nabla_{w_{ij}^L}\mathcal{J} = a \times b \times c$$

$$\nabla_{w_{ij}^{L-1}}\mathcal{J} = a \times b \times c \times d \times e \times f$$

$$\nabla_{w_{ij}^{L-2}}\mathcal{J} = a \times b \times c \times d \times e \times f \times g \cdots$$

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Why **gradients** get **smaller and smaller** at each layer on backpropagation?

$$\nabla_{w_{ij}^{L}} \mathcal{J} = a \times b \times c$$

$$\nabla_{w_{ij}^{L-1}} \mathcal{J} = a \times b \times c \times d \times e \times f$$

$$\nabla_{w_{ij}^{L-2}} \mathcal{J} = a \times b \times c \times d \times e \times f \times g \cdots$$

Terms values < 1.0

+

#Multypling terms $\uparrow\uparrow\uparrow$

=

$\nabla_{W^0} \mathcal{J}$ $\downarrow\downarrow\downarrow\downarrow$ $\quad$ $\nabla_{W^1} \mathcal{J}$ $\downarrow\downarrow\downarrow$ $\quad$ $\nabla_{W^2} \mathcal{J}$ $\downarrow\downarrow$ $\quad$ $\nabla_{W^3} \mathcal{J}$ $\downarrow$

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What about **exploding gradients**?

$$\nabla_{w_{ij}^{L}}\mathcal{J} = a \times b \times c$$

$$\nabla_{w_{ij}^{L-1}}\mathcal{J} = a \times b \times c \times d \times e \times f$$

$$\nabla_{w_{ij}^{L-2}}\mathcal{J} = a \times b \times c \times d \times e \times f \times g \cdots$$

Terms values > 1.0

+

#Multypling terms $\uparrow\uparrow\uparrow$

=

$\nabla_{W^0}\mathcal{J}$ $\uparrow\uparrow\uparrow\uparrow$ $\nabla_{W^1}\mathcal{J}$ $\uparrow\uparrow\uparrow$ $\nabla_{W^2}\mathcal{J}$ $\uparrow\uparrow$ $\nabla_{W^3}\mathcal{J}$ $\uparrow$

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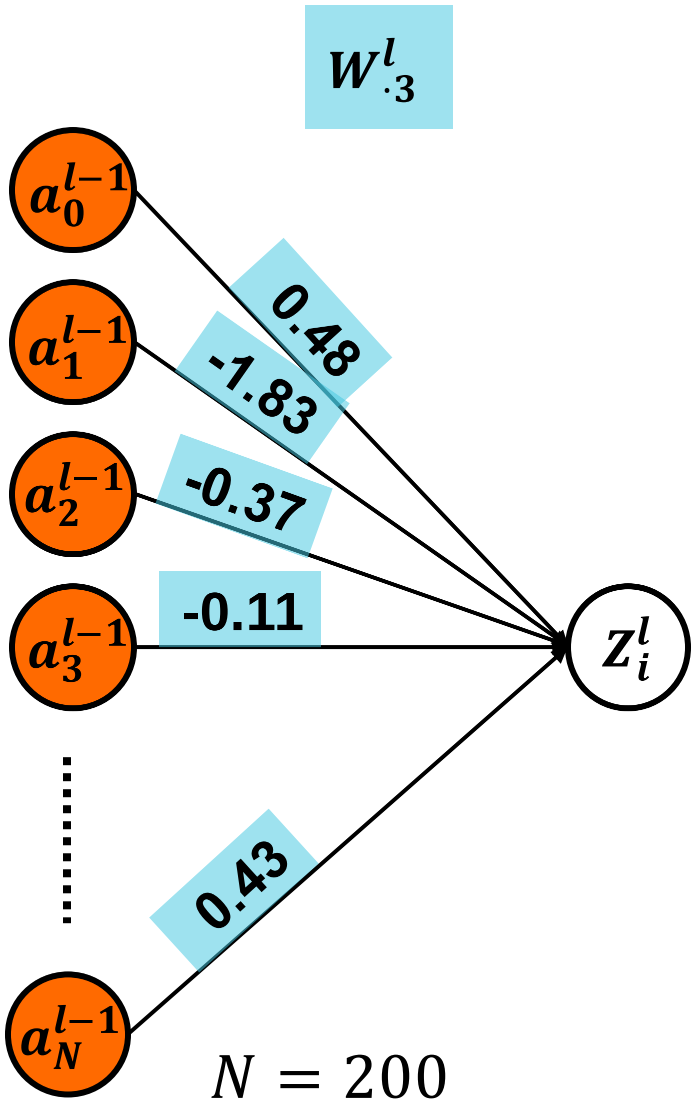
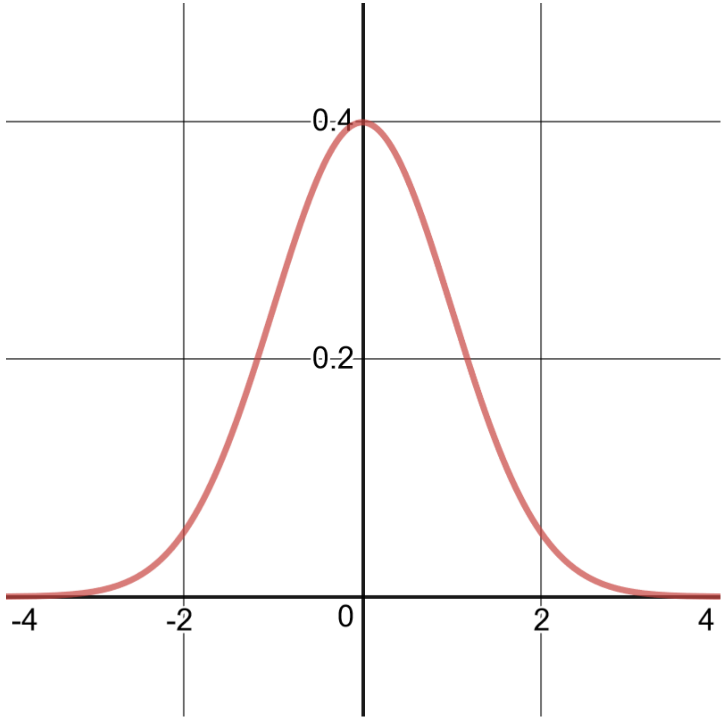


Normal Distribution
$N(\mu = 0, \sigma^2 = 1)$



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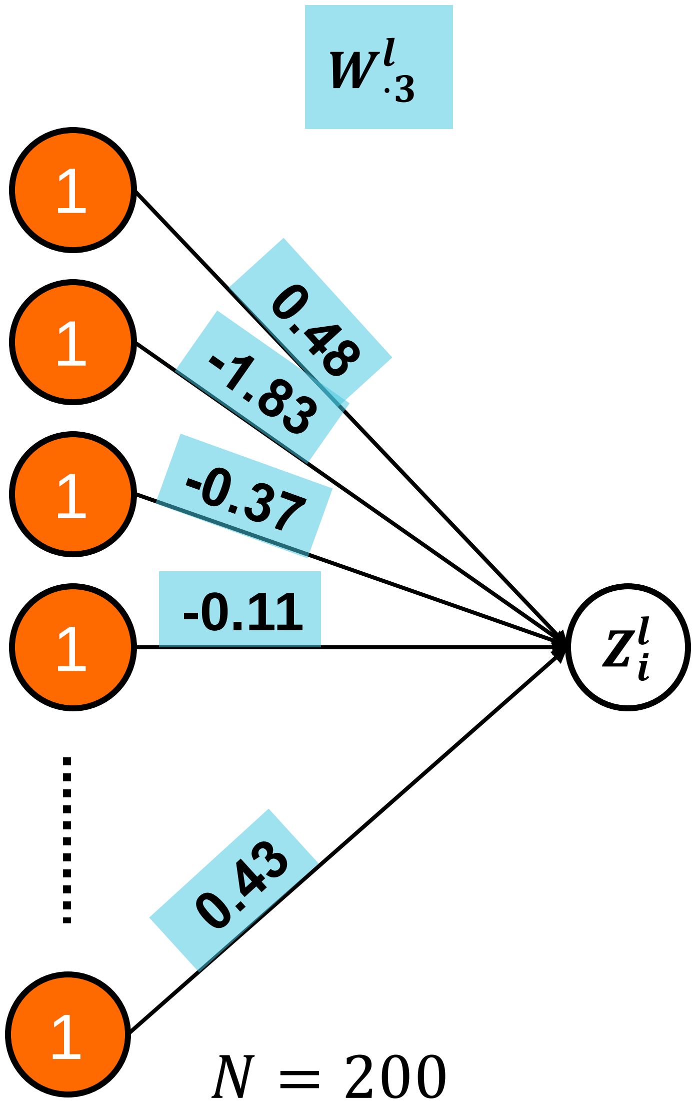

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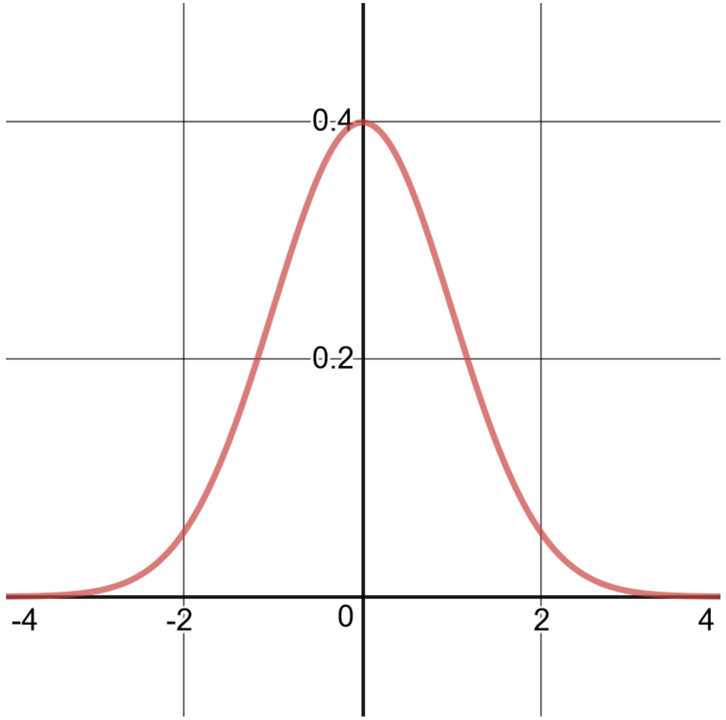

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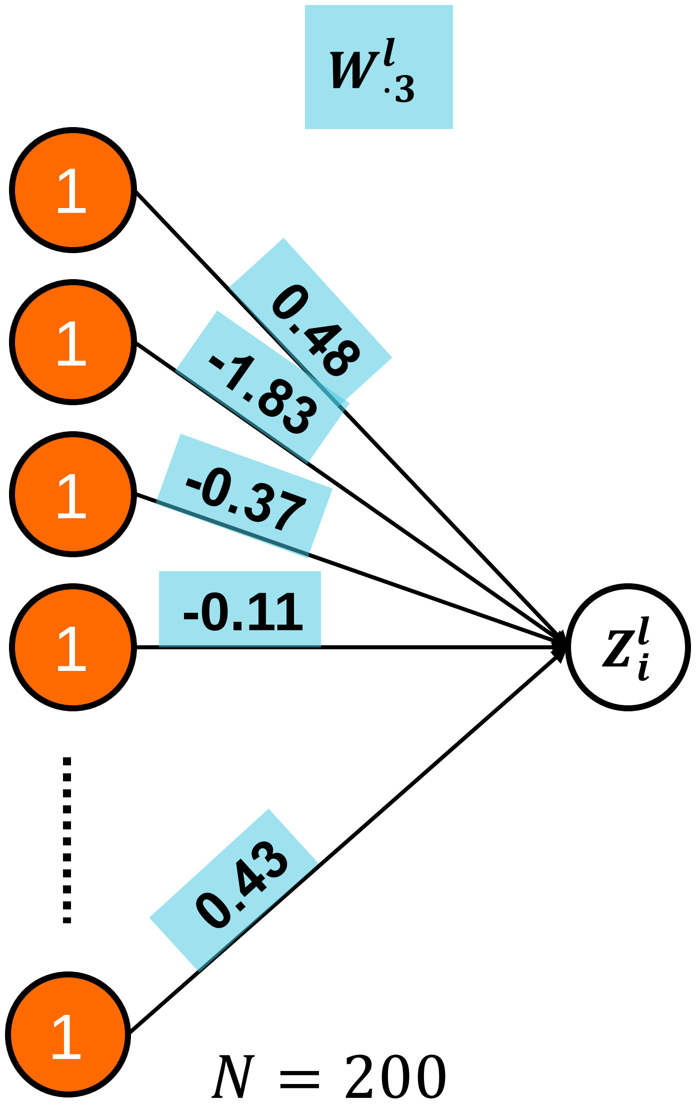


Sum of **independent random variables** that are **normally distributed**:

$$X \sim N(\mu_X, {\sigma^2}_X)$$

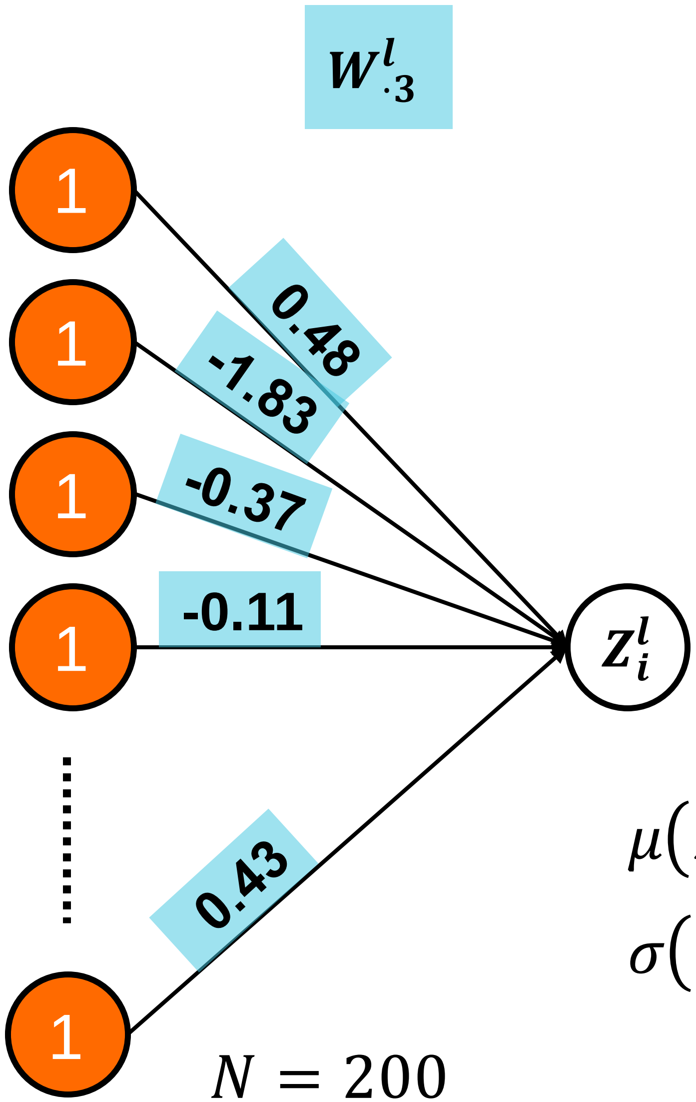
$$Y \sim N(\mu_Y, {\sigma^2}_Y)$$

$$Z = X + Y$$

$$Z \sim N(\mu_X + \mu_Y, {\sigma^2}_X + {\sigma^2}_Y)$$

Feedforward Neural Networks

- **SGD, Epochs, Batches and Steps**
- **Activation functions**
- **SGD learning rate**
- **Other optimization methods**
- **Regularization**
- **Normalizing inputs**
- **Vanishing/Exploding Gradients**
- **Weights initialization**



$$N = 200$$

Sum of **independent random variables** that are **normally distributed**:

$$X \sim N(\mu_X, \sigma^2{}_X)$$
$$Y \sim N(\mu_Y, \sigma^2{}_Y)$$
$$Z = X + Y$$

$$Z \sim N(\mu_X + \mu_Y, \sigma^2{}_X + \sigma^2{}_Y)$$

$$\mu(z^l_i) = 0.0$$
$$\sigma(z^l_i) = \sqrt{200} \approx 14.14$$

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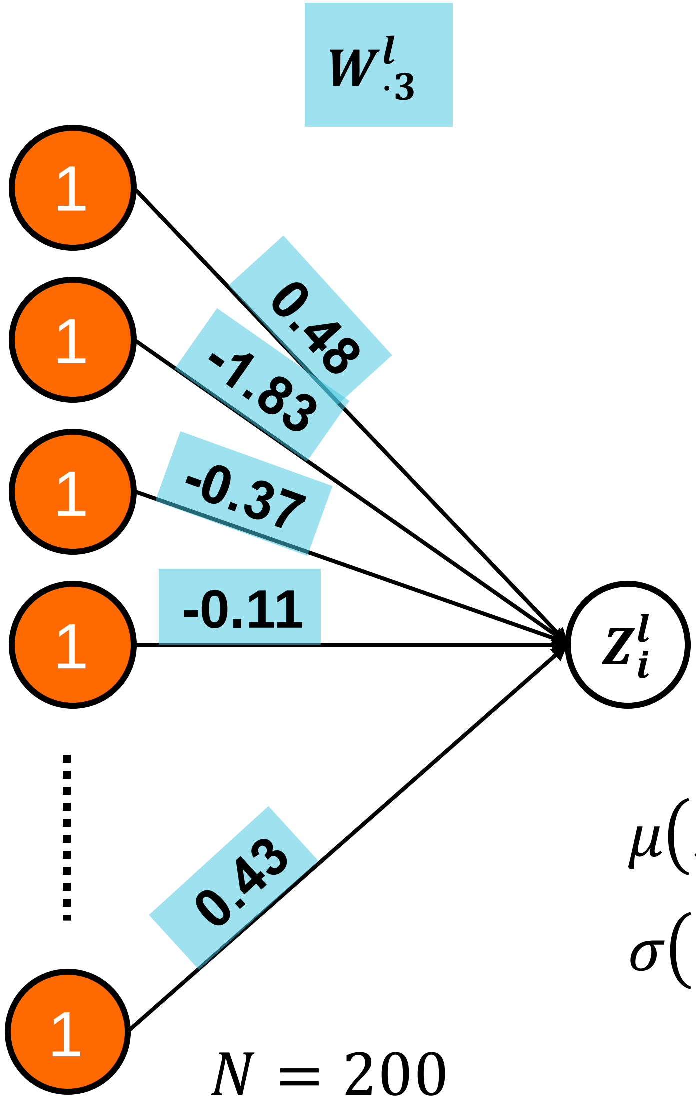
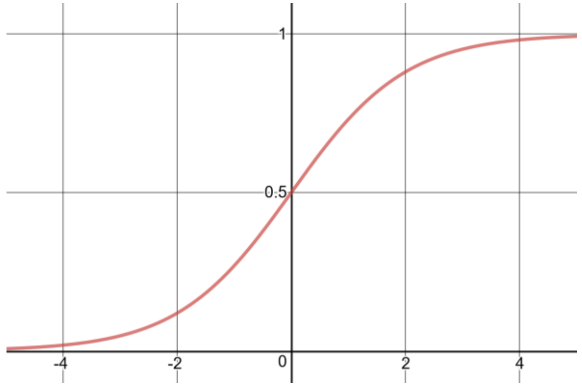


$N = 200$

$$sigmoid(x) = \frac{e^x}{e^x + 1}$$



$$\mu(z^l_i) = 0.0$$

$$\sigma(z^l_i) = \sqrt{200} \approx 14.14$$

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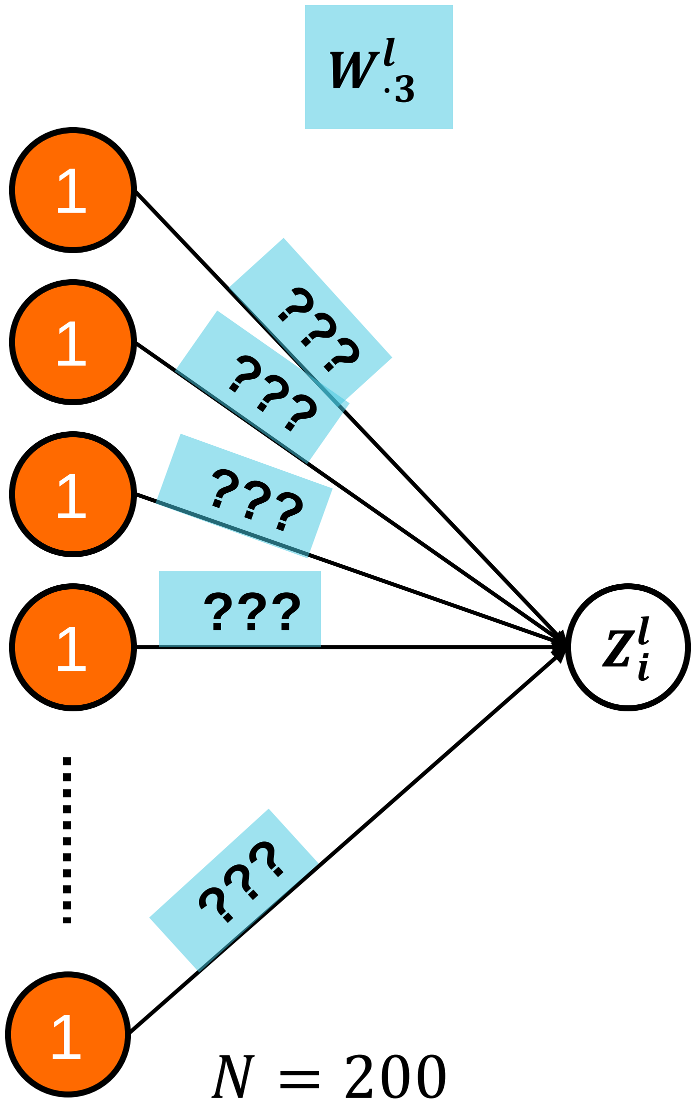

Alternative weights initializations?

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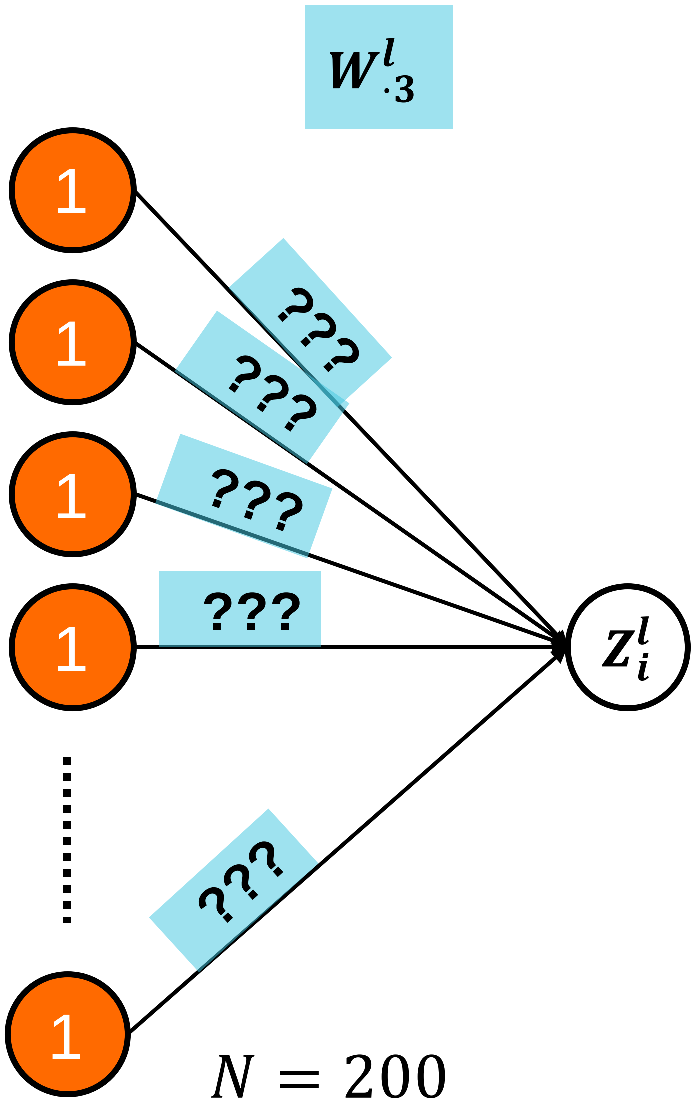
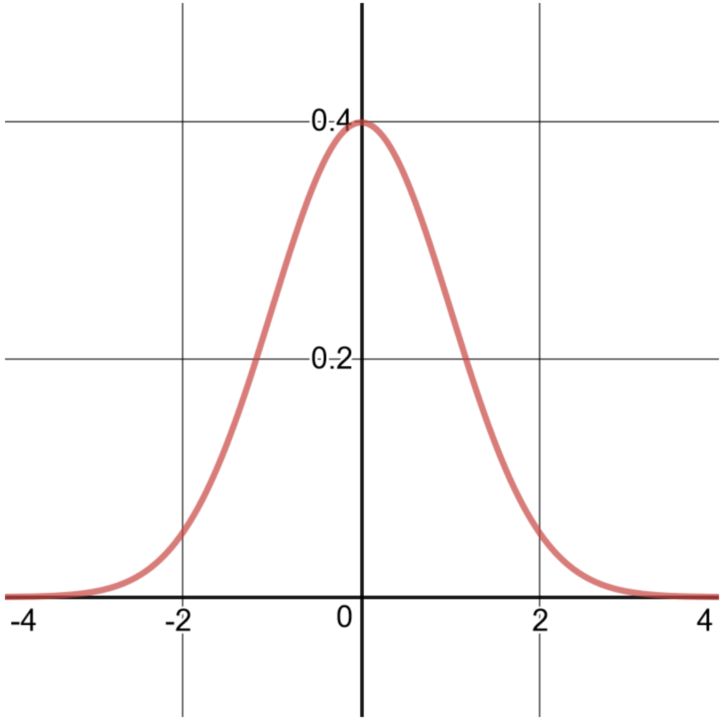


Truncated Normal Initialization

Normal Distribution
$N(\mu = 0, \sigma^2 = 1)$



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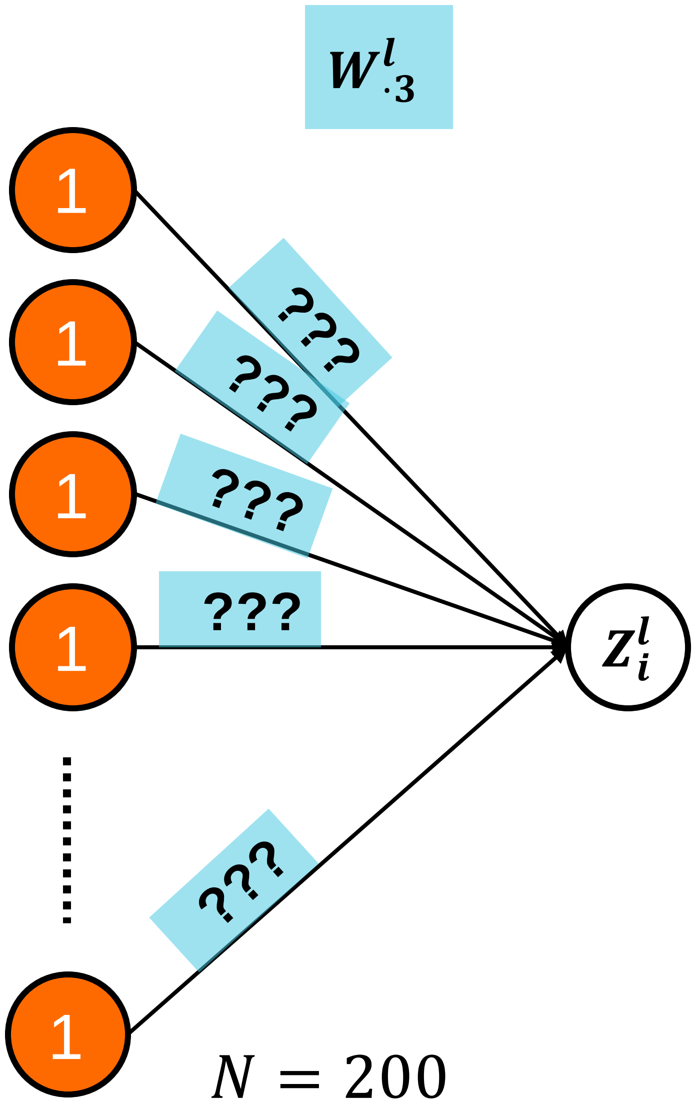

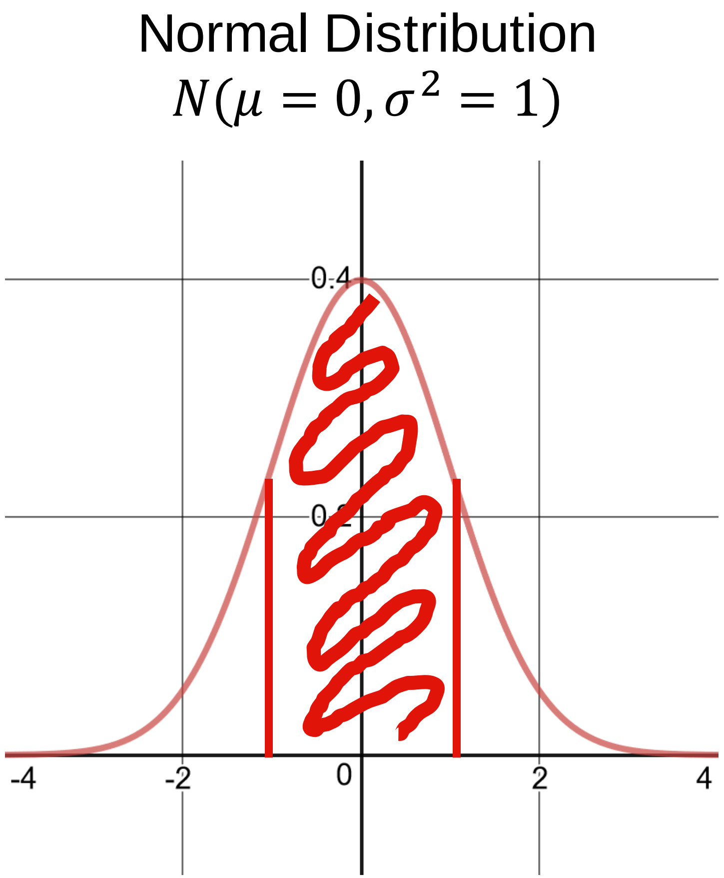

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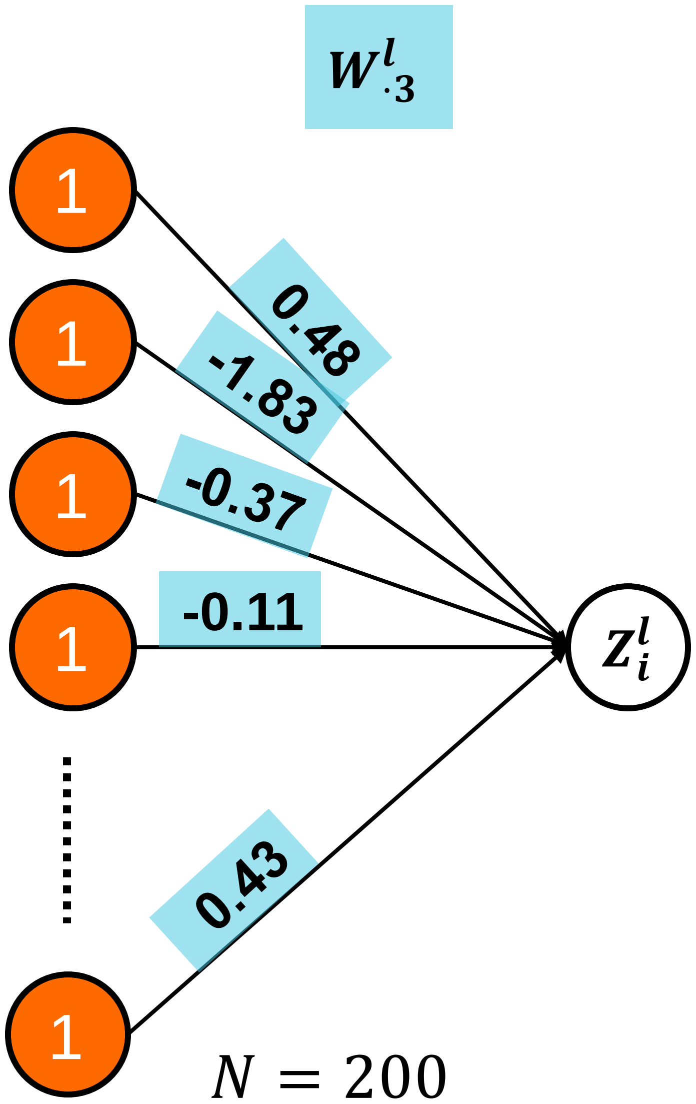

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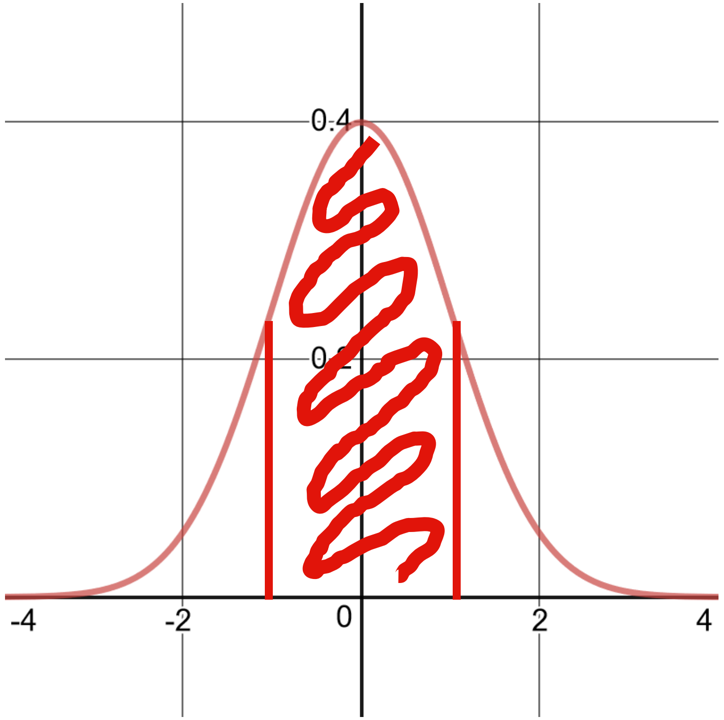

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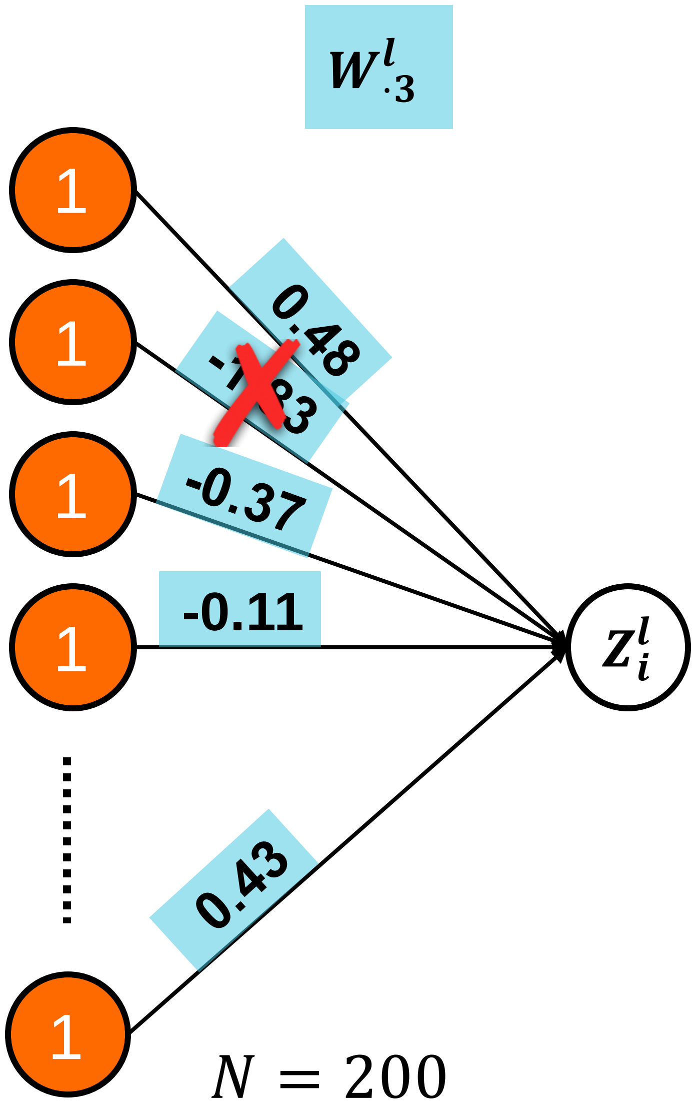

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Normal Distribution
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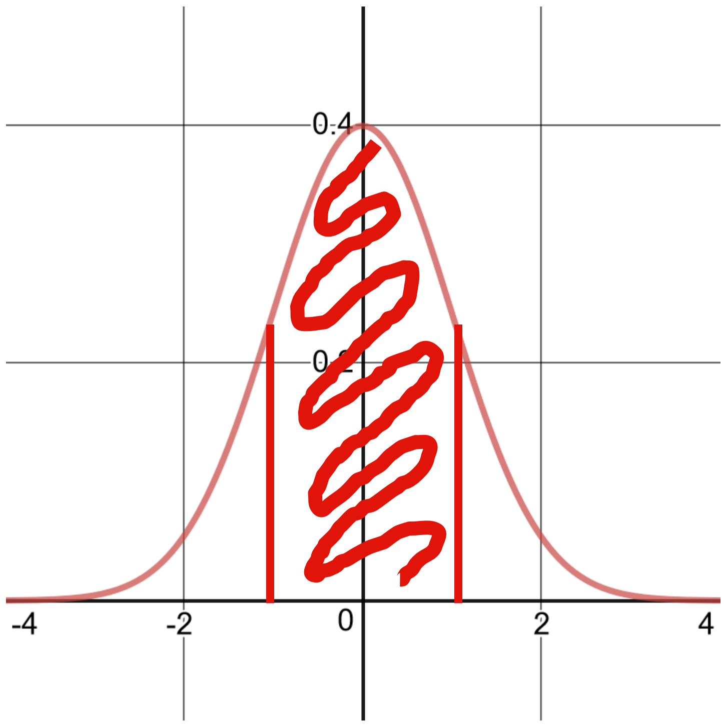

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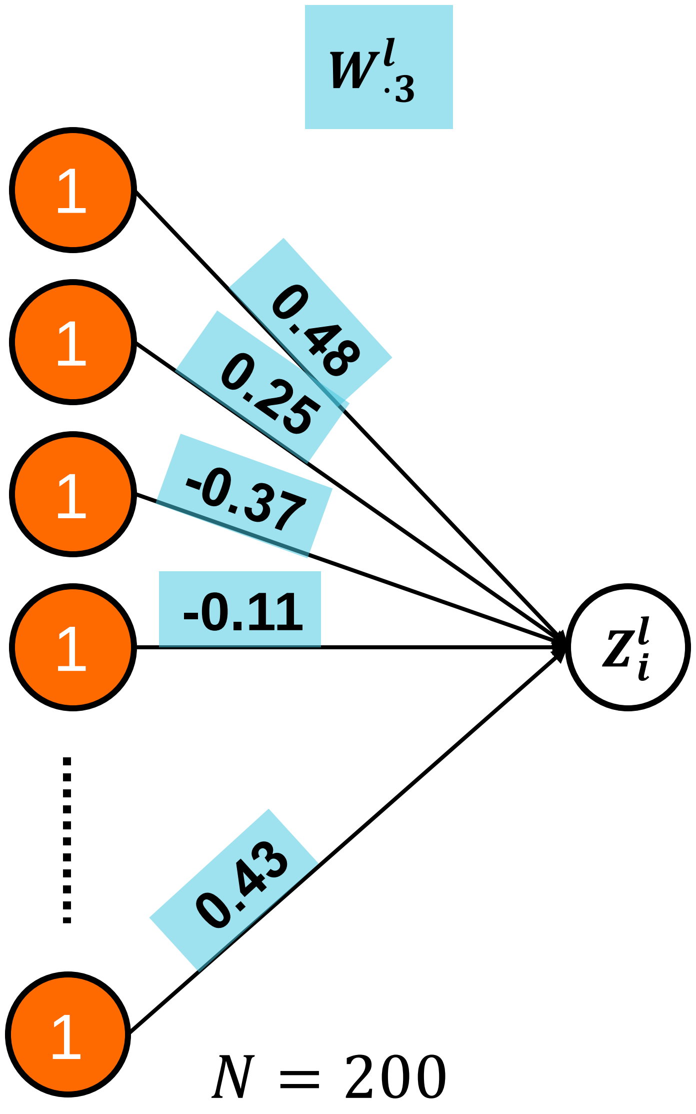

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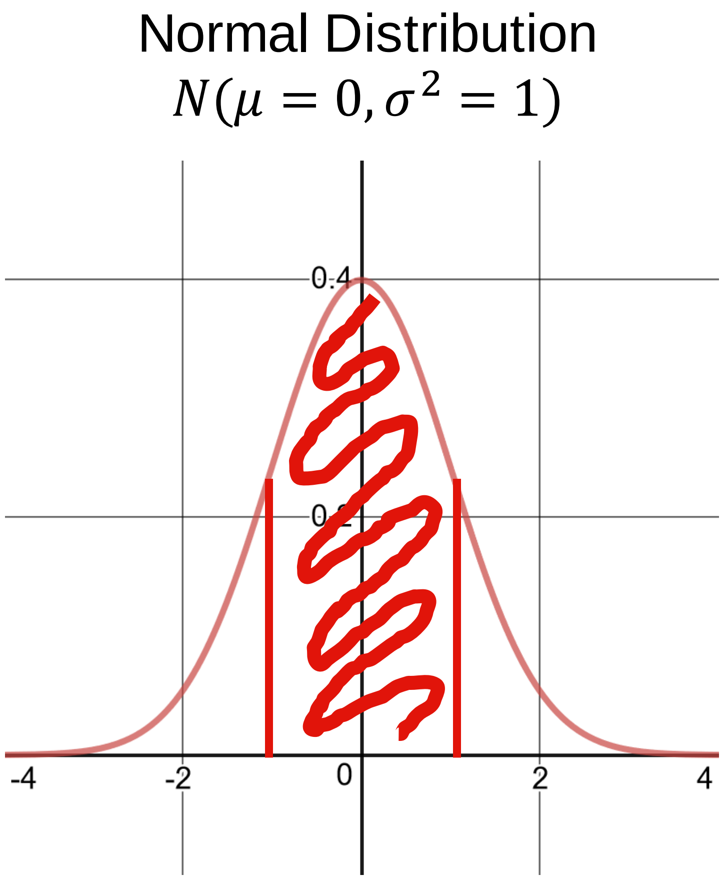

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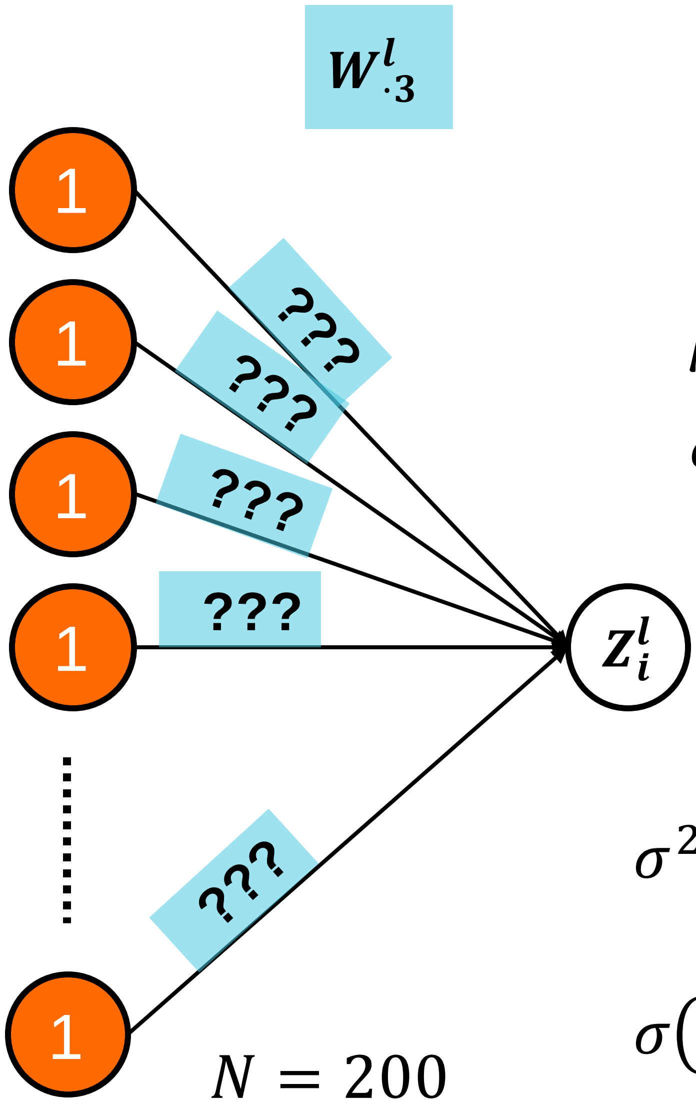
Xavier / Glorot Initialization



$$\mu(z_i^l) = 0.0$$

$$\sigma(z_i^l) = 1.0$$

$$\sigma^2(W^l_{\cdot 3}) = \frac{1}{N} = 0.005$$

$$\sigma(W^l_{\cdot 3}) = \sqrt{{}^{1}/_{N}} \approx 0.0707$$

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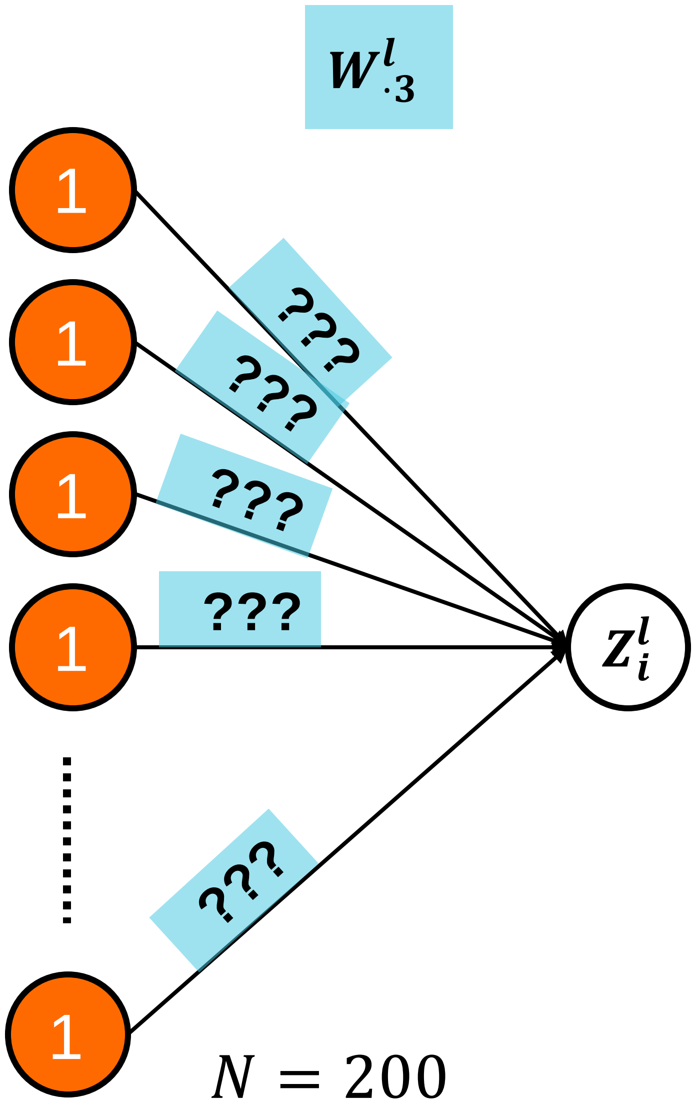
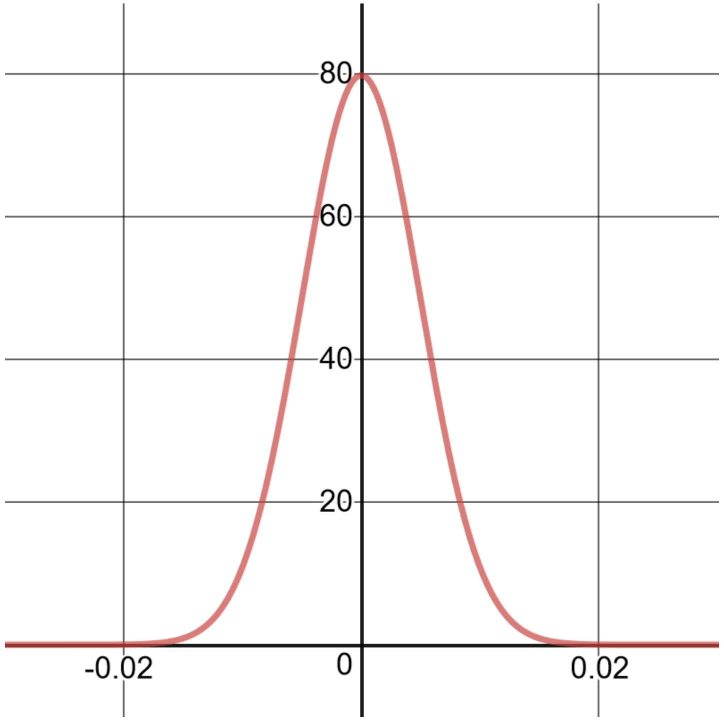
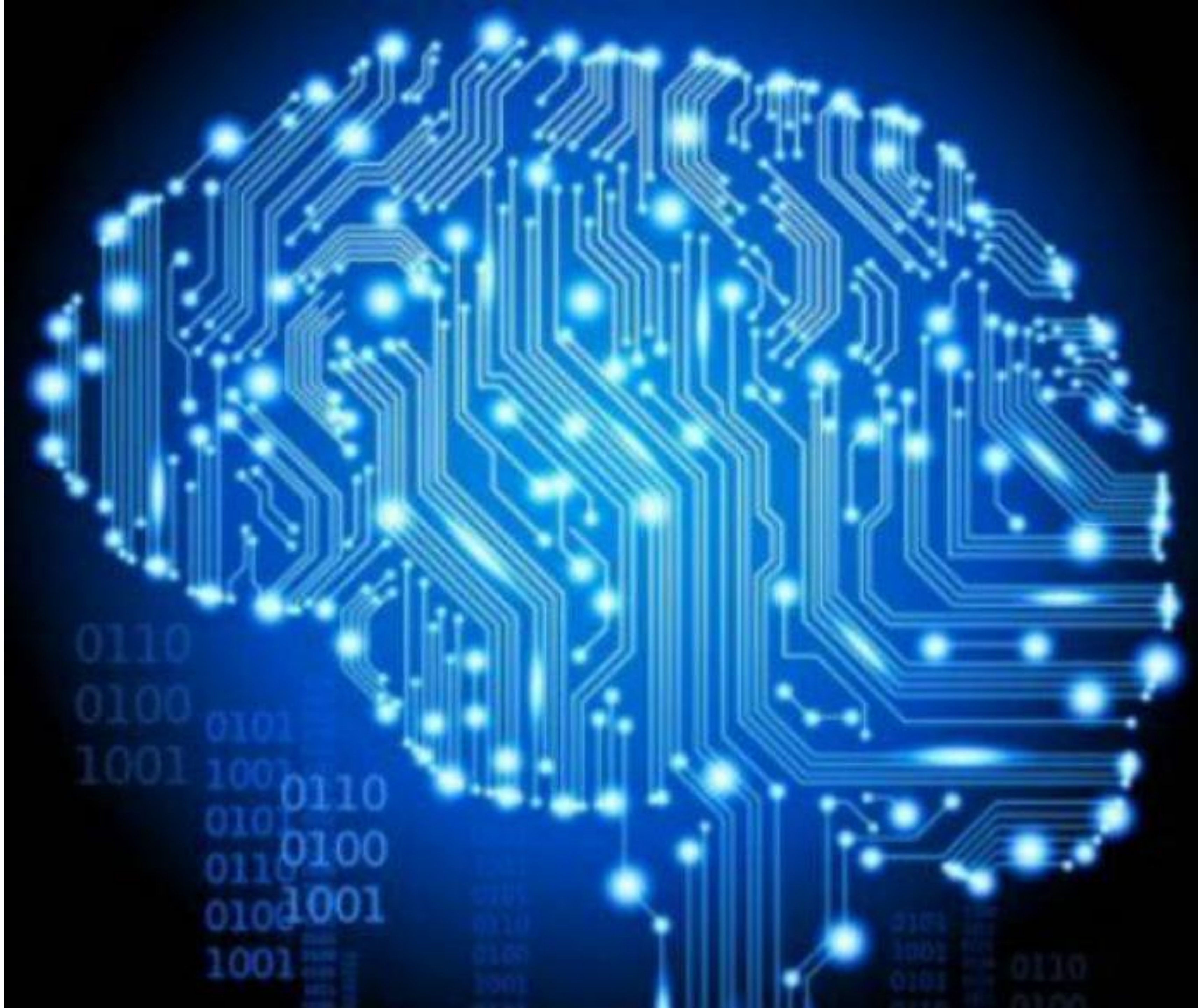


Xavier / Glorot Initialization

Normal Distribution
$N(\mu = 0, \sigma^2 = 0.005)$



Practical Aspects



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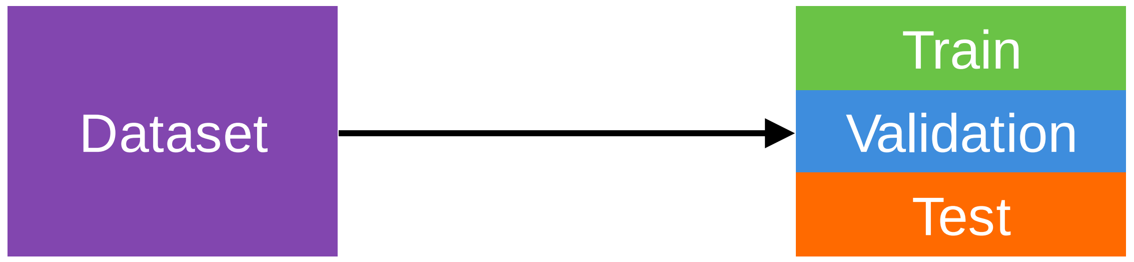
Practical Aspects

Train / Validation / Test

Workflow



Train	Set used to **train & control bias**
Validation	Set used to **control variance**
Test	Set used to **estimate** the **generalization error** of the final model

Practical Aspects

Train / Validation / Test

Workflow

Dataset → Train / Validation / Test

Train — Set used to **train & control bias**

Validation — Set used to **control variance**

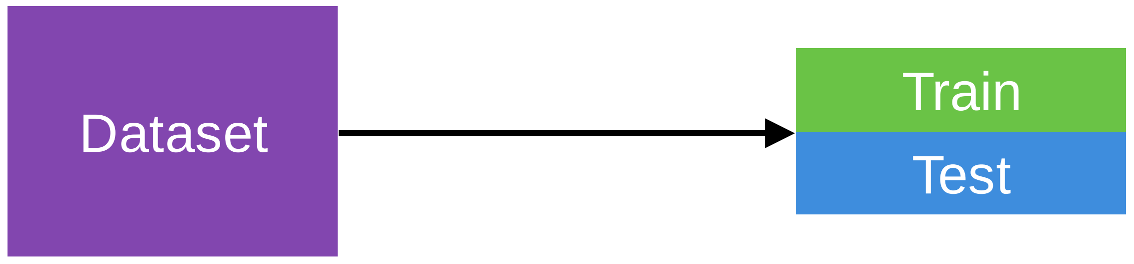
OPTIONAL

Test — Set used to **estimate** the **generalization error** of the final model

Practical Aspects

Train / Validation / Test

Workflow



Train — Set used to **train & control bias**

Test — Set used to **control variance**

OPTIONAL — Set used to **estimate** the **generalization error** of the final model

Practical Aspects

Train / Validation / Test

Workflow

Machine Learning

80%	10%	10%

How many **images** do we **need** for each set?

Train — **As many as possible**

Validation — The **minimum** amount to appropriately **represent each class**

Test — The **minimum** amount to appropriately **represent each class**

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Practical Aspects

Train / Validation / Test

Workflow

Machine Learning

Typical dataset size: 1.000 - 30.000

Deep Learning

Typical dataset size: 30.000 - 10.000.000

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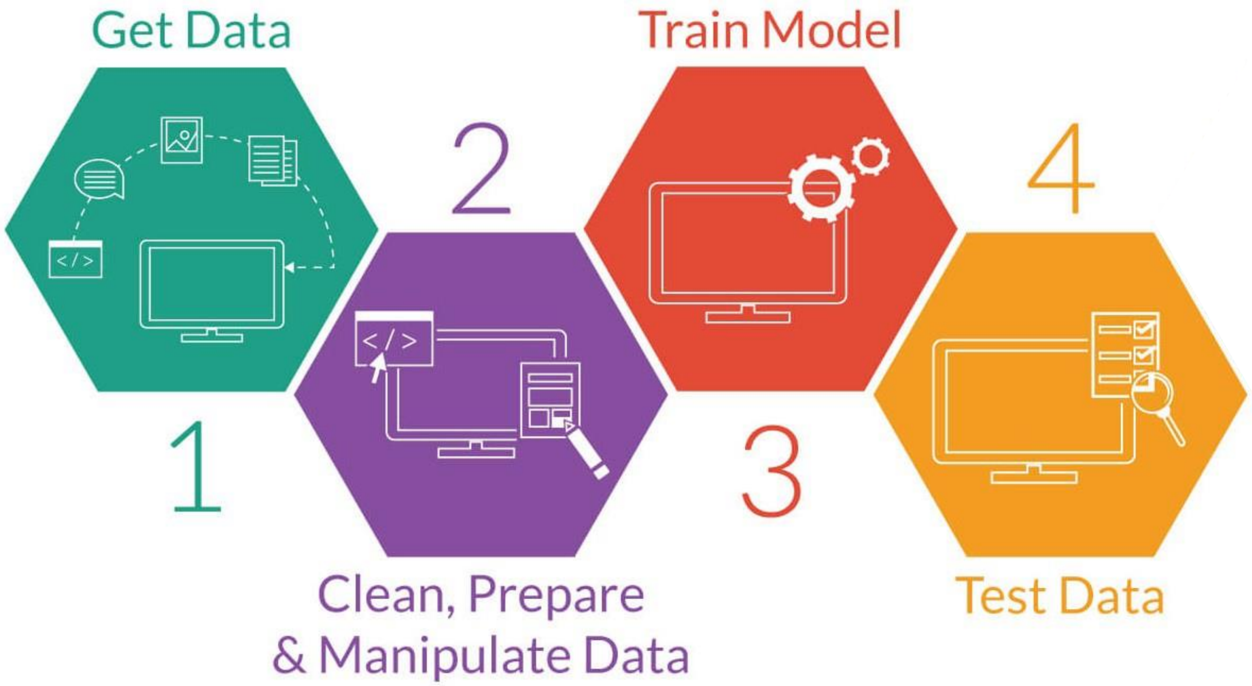
Practical Aspects

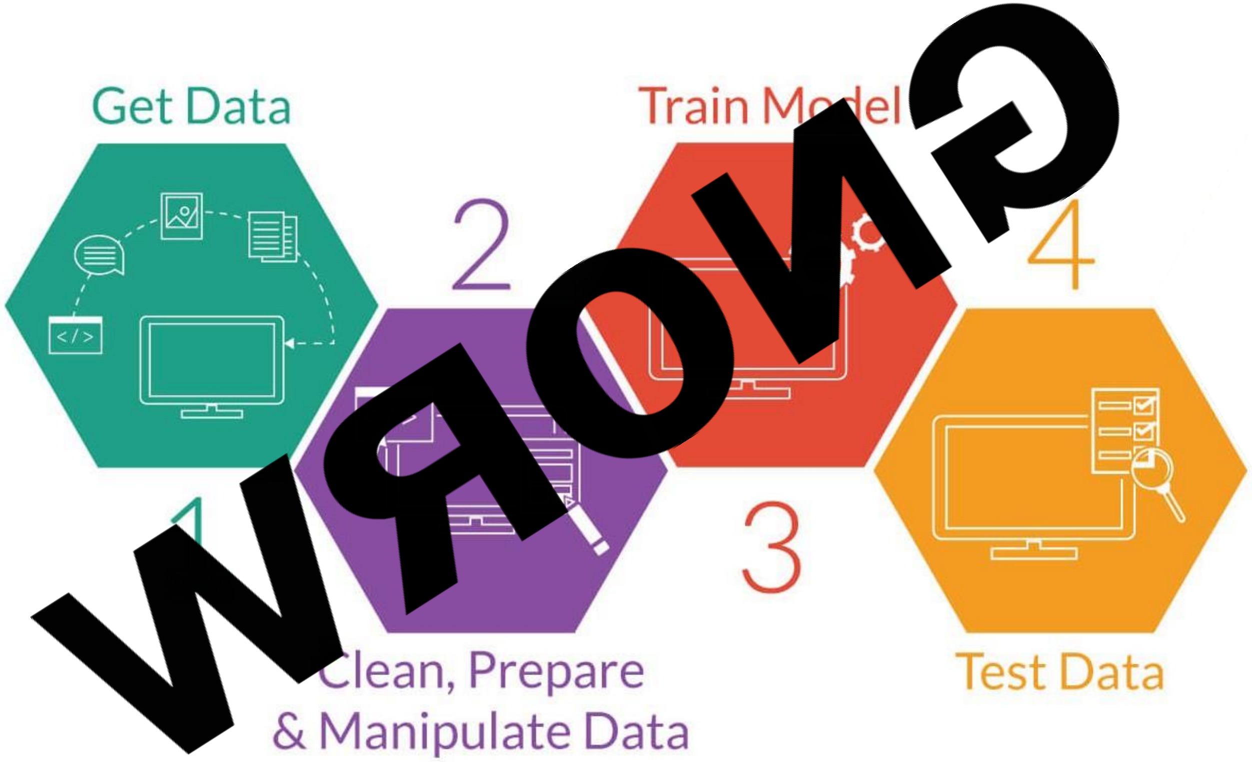
Train / Validation / Test
Workflow



Practical Aspects

Train / Validation / Test

Workflow



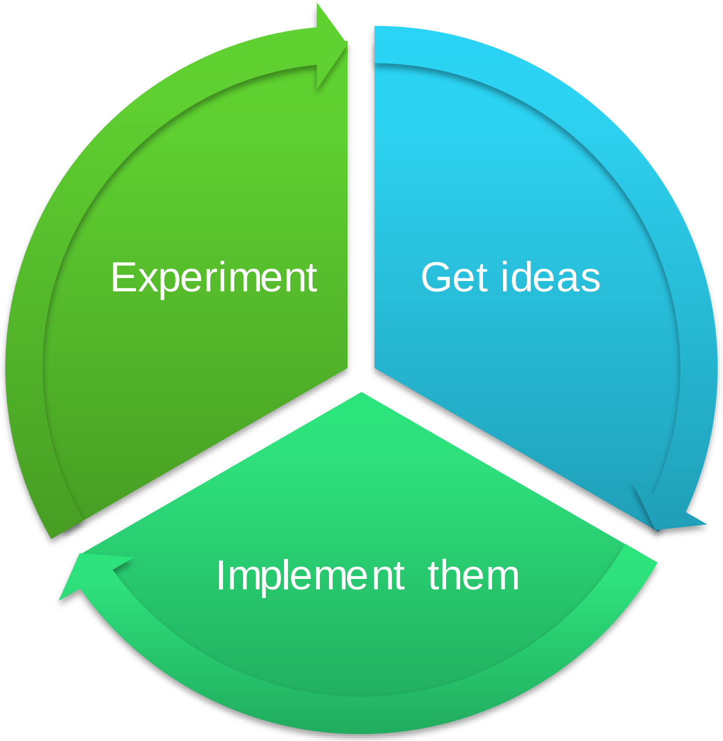
Practical Aspects

Train / Validation / Test

Workflow

Lots of hyper-parameters:

- Network architecture:
  - # layers
  - # neurons
  - Activation function
- Learning rate
- Optimization algorithm
- ...



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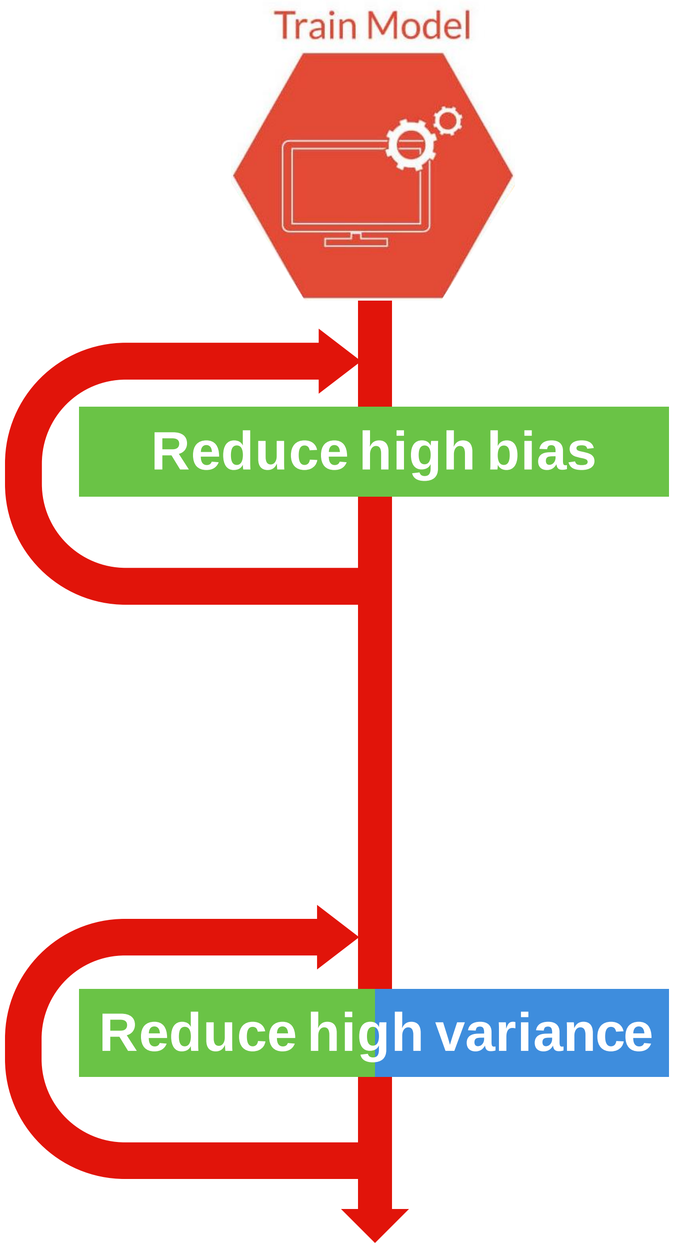
Practical Aspects

Train / Validation / Test

Workflow



- Train longer
- Increase model's capacity:
  - More layers
  - More hidden neurons
- Search for architecture suitable for your data structure
- Preprocessing data to simplify the task

- More data
- Data Augmentation
- Regularization
- Search for architecture suitable for your data structure

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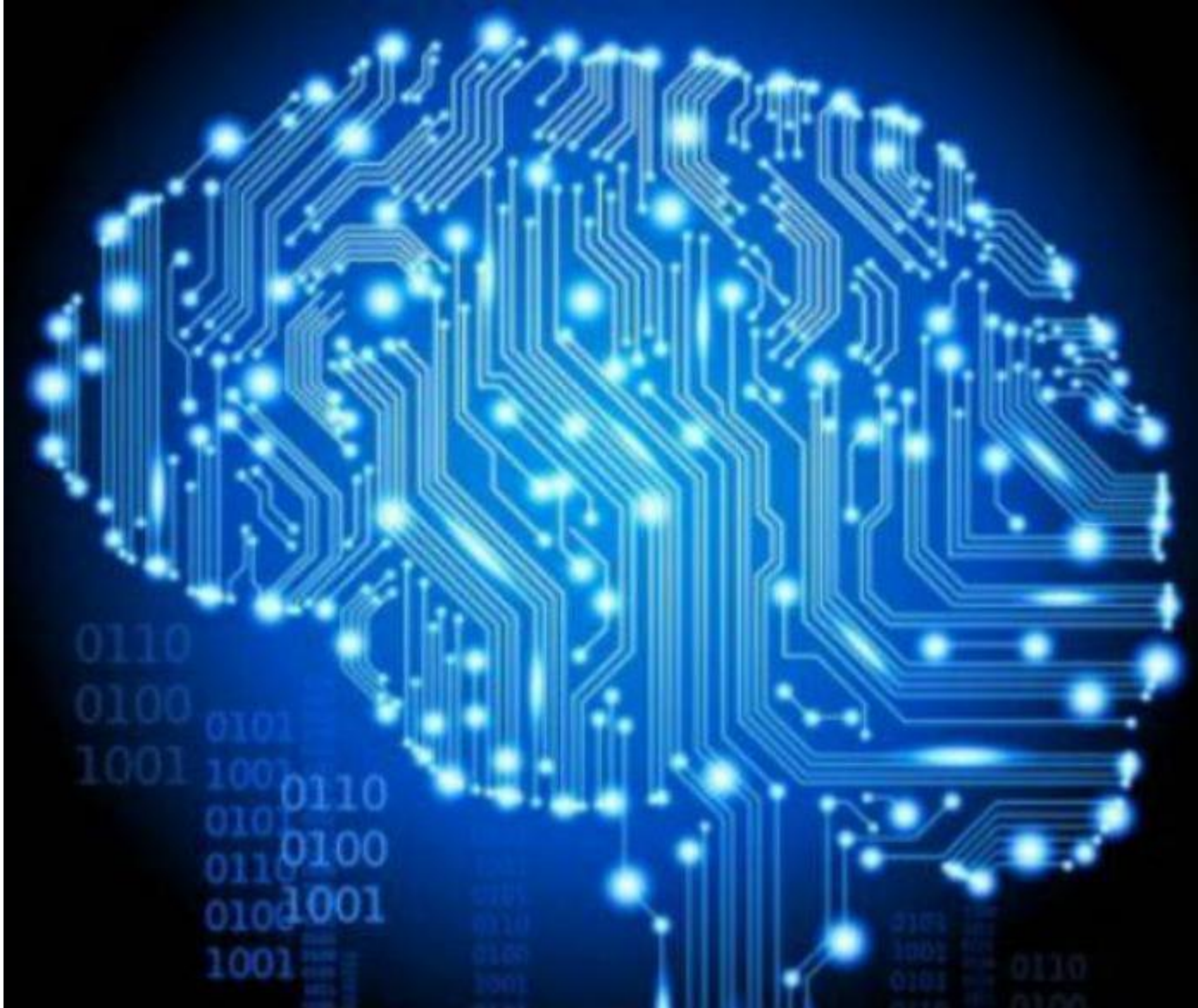
Convolutional Neural Networks



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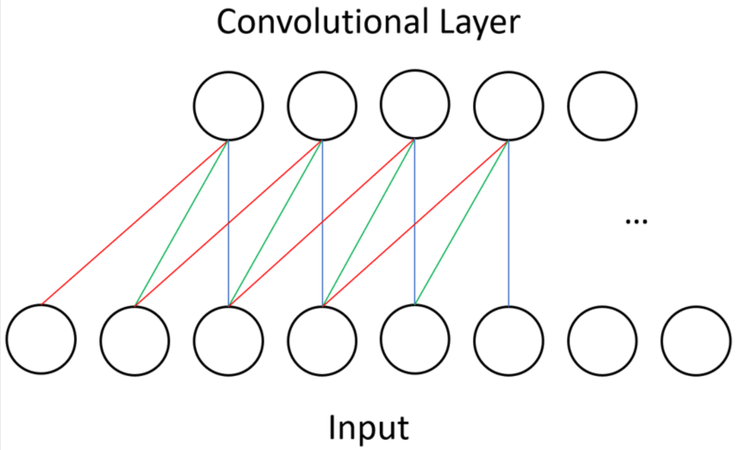
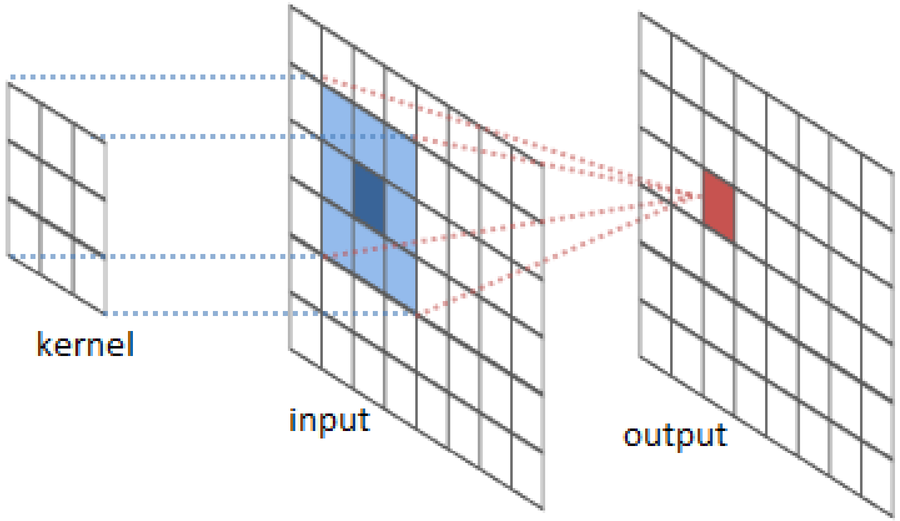
Convolutional Neural Networks

Some data has spatial correlations that could be exploited (in 1D, 2D, 3D, ...):

- *Near-by* data points are more relevant than *far-away.*

If we sparsify connectivity with a consistent purpose, we may **reduce complexity** and ease the learning of **more coherent patterns**





Convolutional Neural Networks

Limited connectivity

Convolution & weight sharing

Filters

Kernel size, stride and padding

Convolutional volumes

Pooling layers

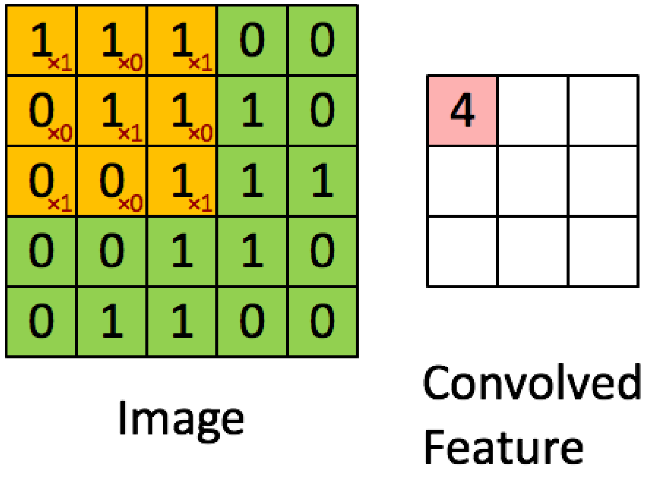
Convolutional architectures

CNNs from the inside

CNN Applications

Sparse connectivity is nice, but we still want to apply filters everywhere.

Each limited connectivity pattern (a **kernel**) will get **convolved** all over the image, generating a number of values.
Notice each kernel generates a 2D matrix of values.



In practice we have sets of neurons **sharing weights**

Convolutional Neural Networks

- Limited connectivity
- Convolution & weight sharing
- **Filters**
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Convolution kernels can do all sorts of things on an image:

Input image

Edge detection	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Gaussian blur 3 × 3	$\frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$	

Let's let the model learn them

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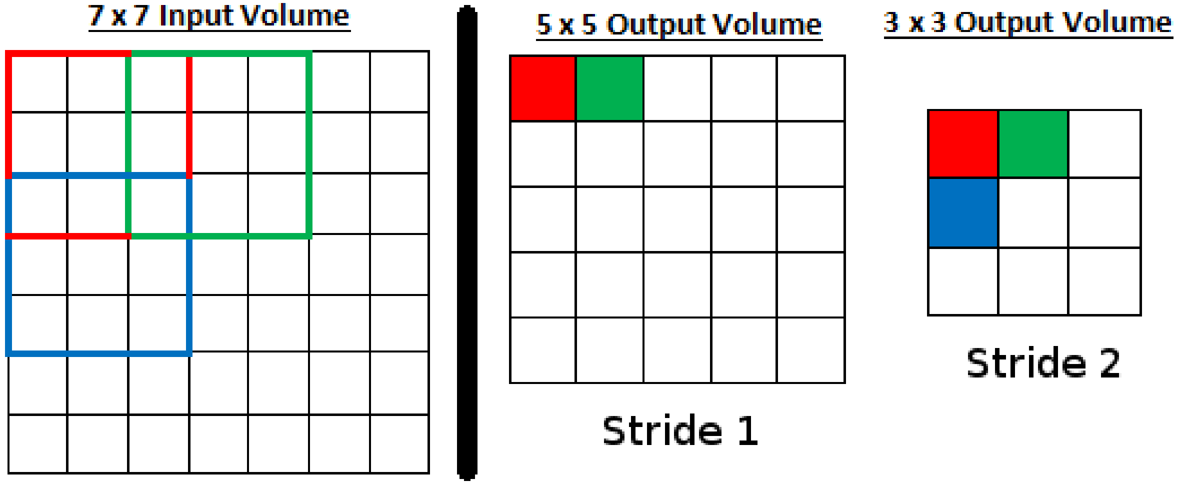
Kernel size: Size of the receptive field of convolutional neurons. Typically 3x3, 5x5, 7x7

Stride: Number of steps while convolving filter.



Stride 1 the most common. Larger strides can replace pooling.

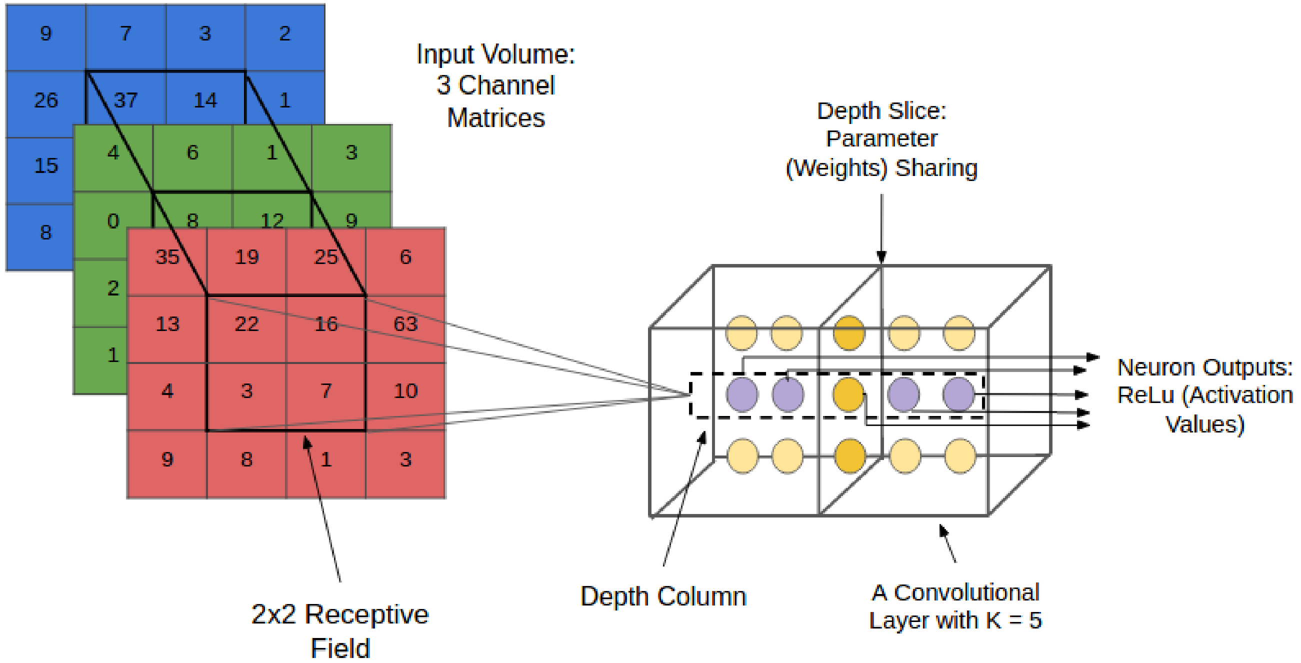
Padding: Border added to center conv. everywhere

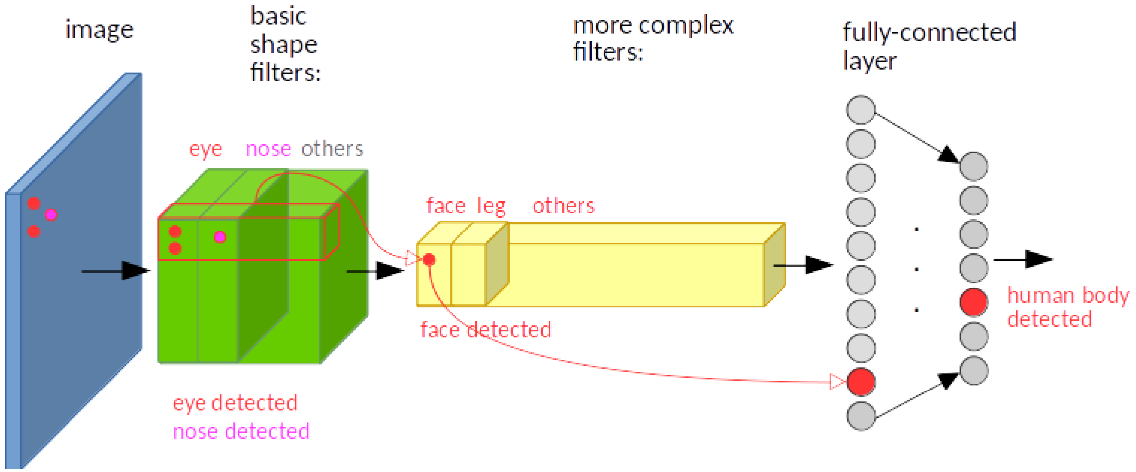
- No padding: Dimensionality reduced
- Most common, zero equal/same padding

$$OutputSize = \frac{InputSize - KernelSize + 2 * Padding}{Stride} + 1$$

Convolutional Neural Networks

- In a typical 2D CNN, conv filters are 3D (full depth).
- Each filter convolved generates a 2D plane of data.
- Depth provides all the neural views on a part of data





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Convolutional Neural Networks

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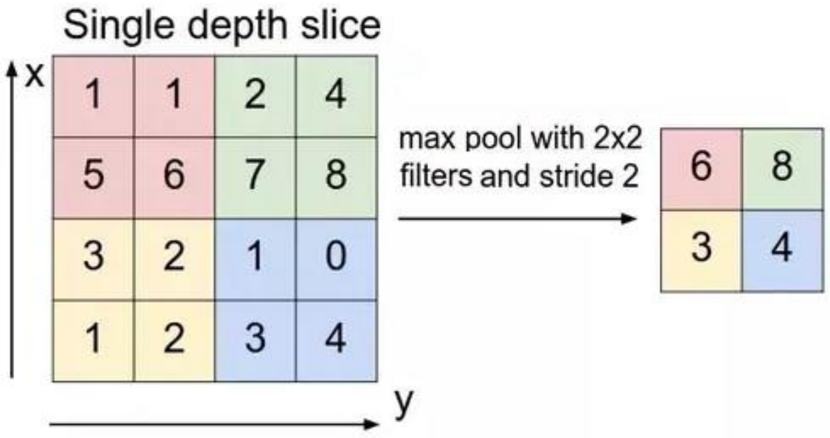
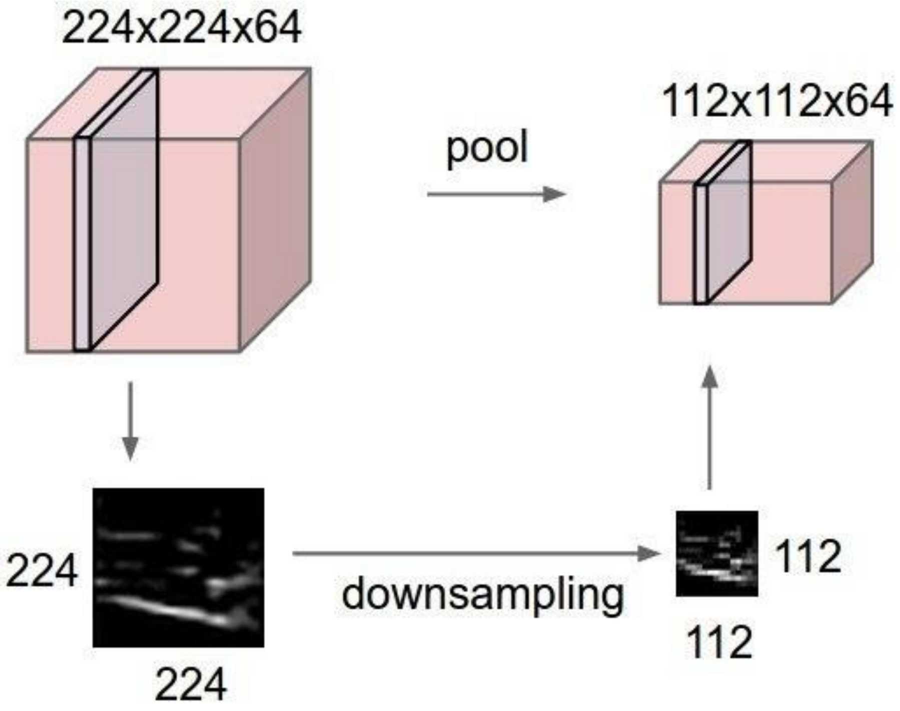
Pooling:

- Small spatial invariance
- Dimensionality reduction (along *x* and *y* only)
- Never applied full depth!
- Parameter free layer
- Hyperparams:
  - Size & Stride
- Loss in precision
- Max >> Avg





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[AlexNet,12]
[VGG,14]

The first influential architecture was **AlexNet**:

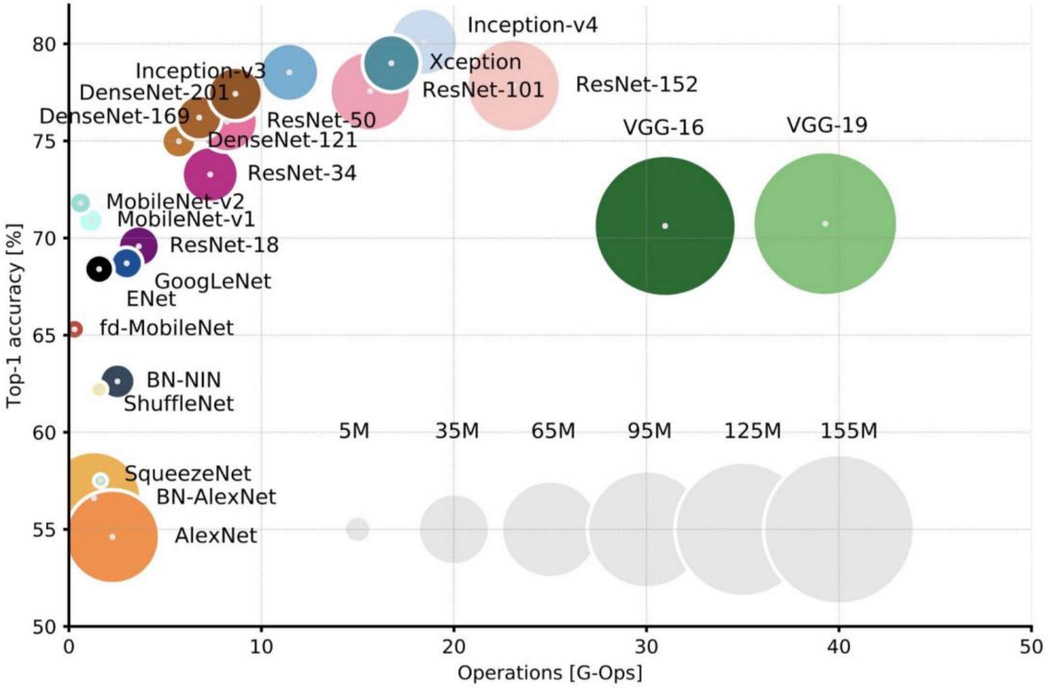
- 5 layers using convs, pools, *ReLU*, 2 dense, and *dropout*.
- 62M parameters

VGG16/19 extends the (conv-pool)*dense design:

- Smaller, 3x3 filters, but more
- 138M parameters

Some design principles: KISS, be repetitive & pyramidal

Bigger is not better!



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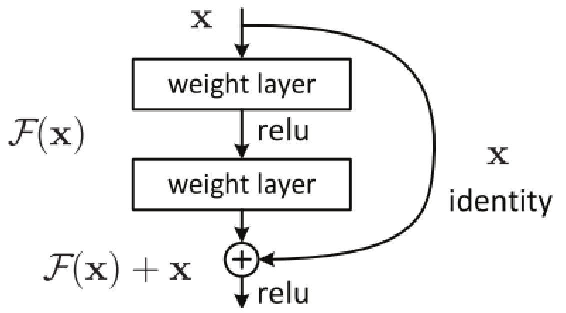
[Inception,15]
[ResNet,16]
[Huang,16]
[Xu,WWW]

But deeper should never be worse!

- In theory, yes. In practice, identity is hard to learn

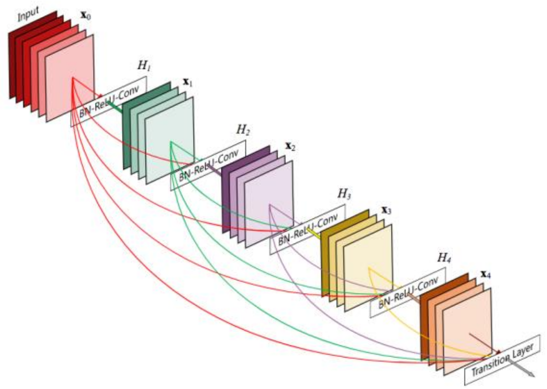
ResNet: Learning zero is easier than learning id.

- We can now train a 1K layer net



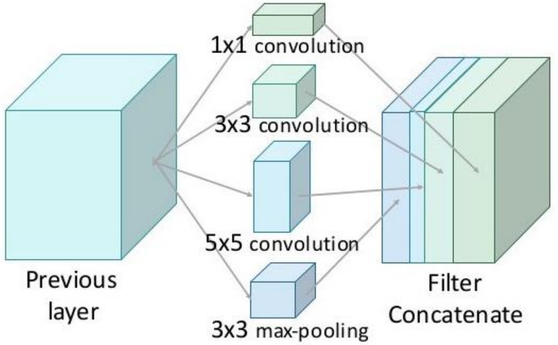
DenseNet: link all to all

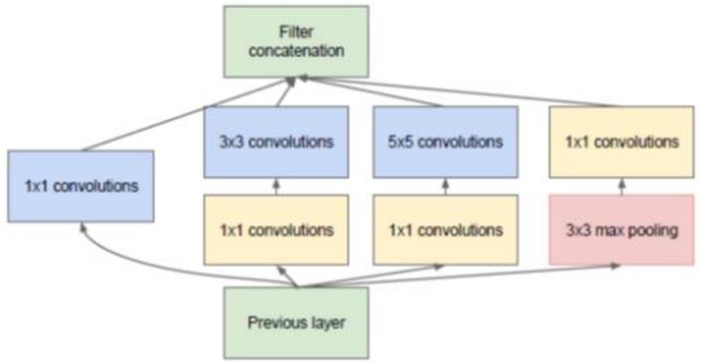
- Use depth concats
- 1x1 convs to make it feasible



Inception: how to fix filter size?

- Let the net decide which is best
- Avg. Pooling instead of dense





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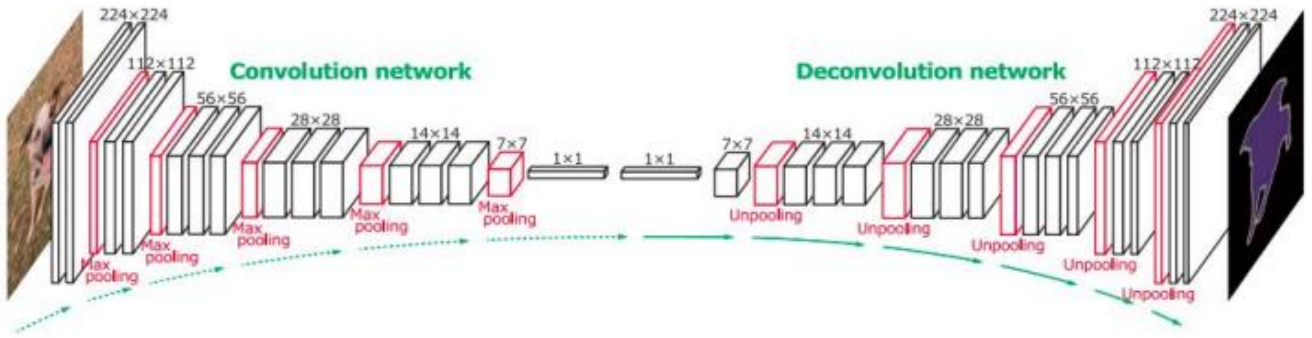
Different architectures that can be done...

- Convolution – Transposed convolution (pixel-wise)



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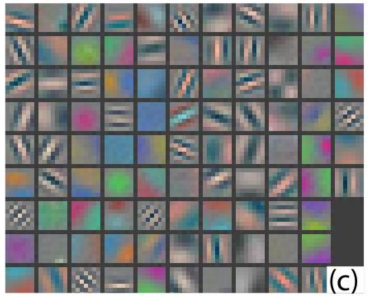
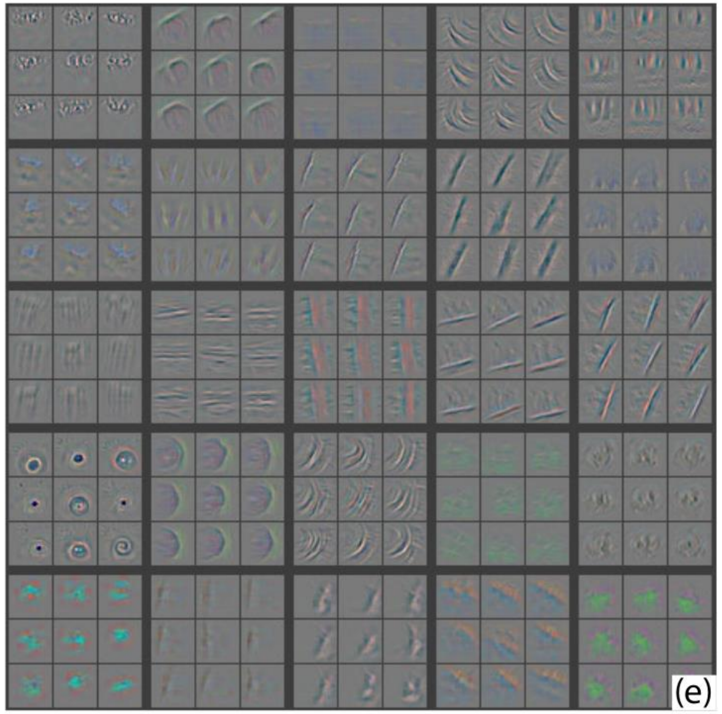
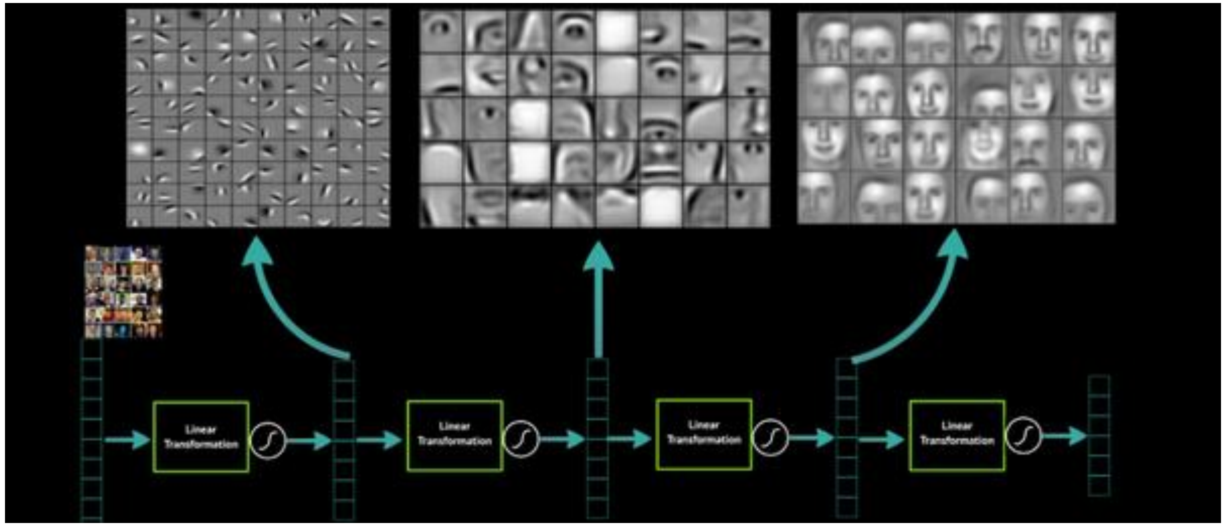
What do filters learn?







Convolutional Neural Networks

- **Limited connectivity**
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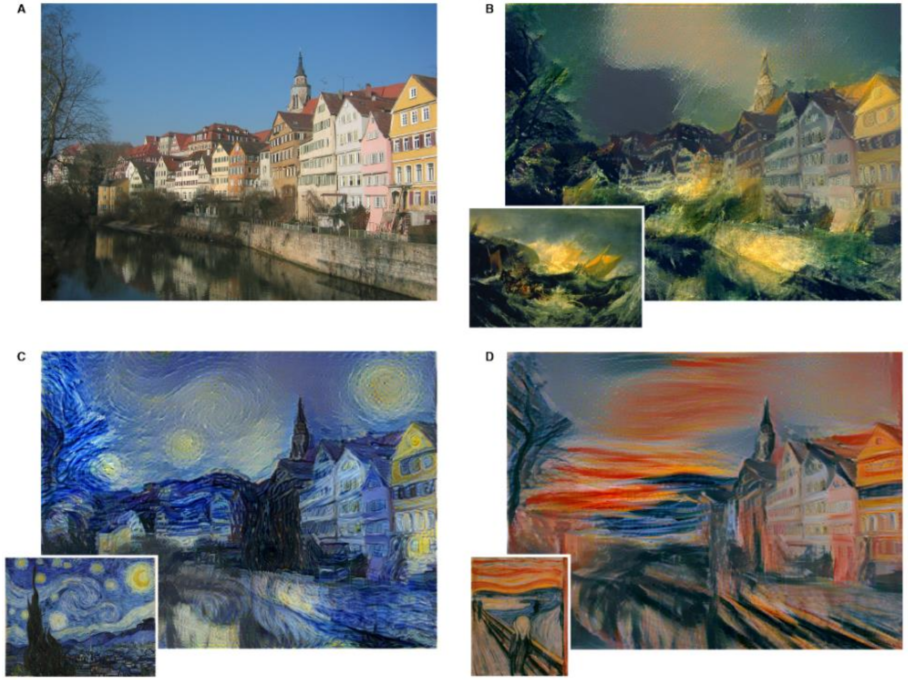
Style transfer



Multimodal pipelines

[Gatys,15]
[Kiros,14]

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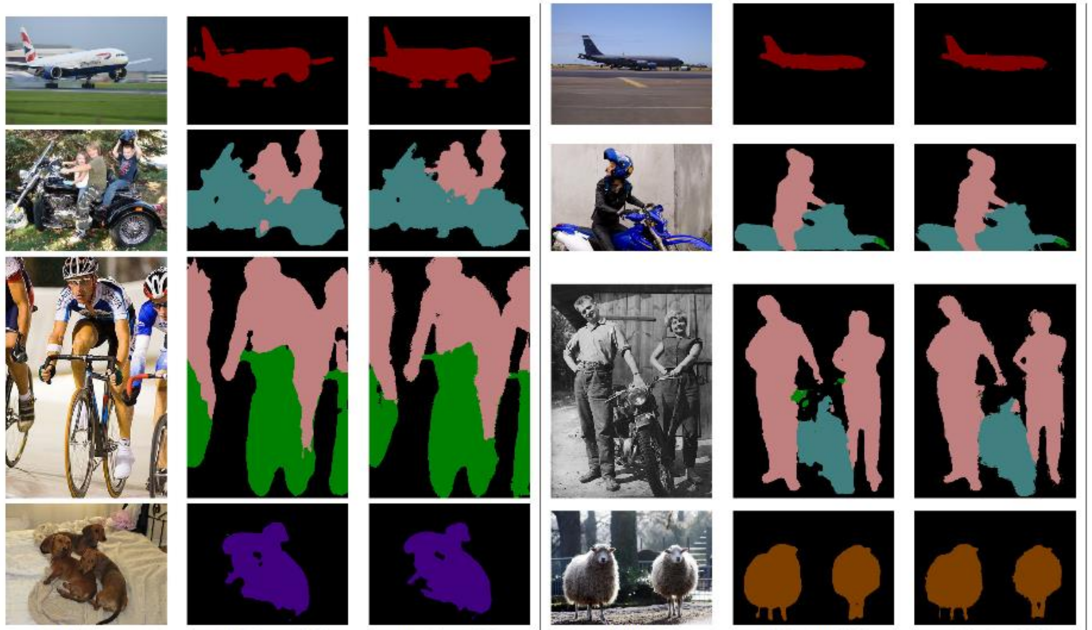
Image colorization

(a) Colorado National Park, 1941 (b) Textile Mill, June 1937 (c) Berry Field, June 1909 (d) Hamilton, 1936

Image segmentation



(a) Image (b) Before CRF (c) After CRF (a) Image (b) Before CRF (c) After CRF

[Zhang,16]
[Iizuka,16]
[Chen,16]