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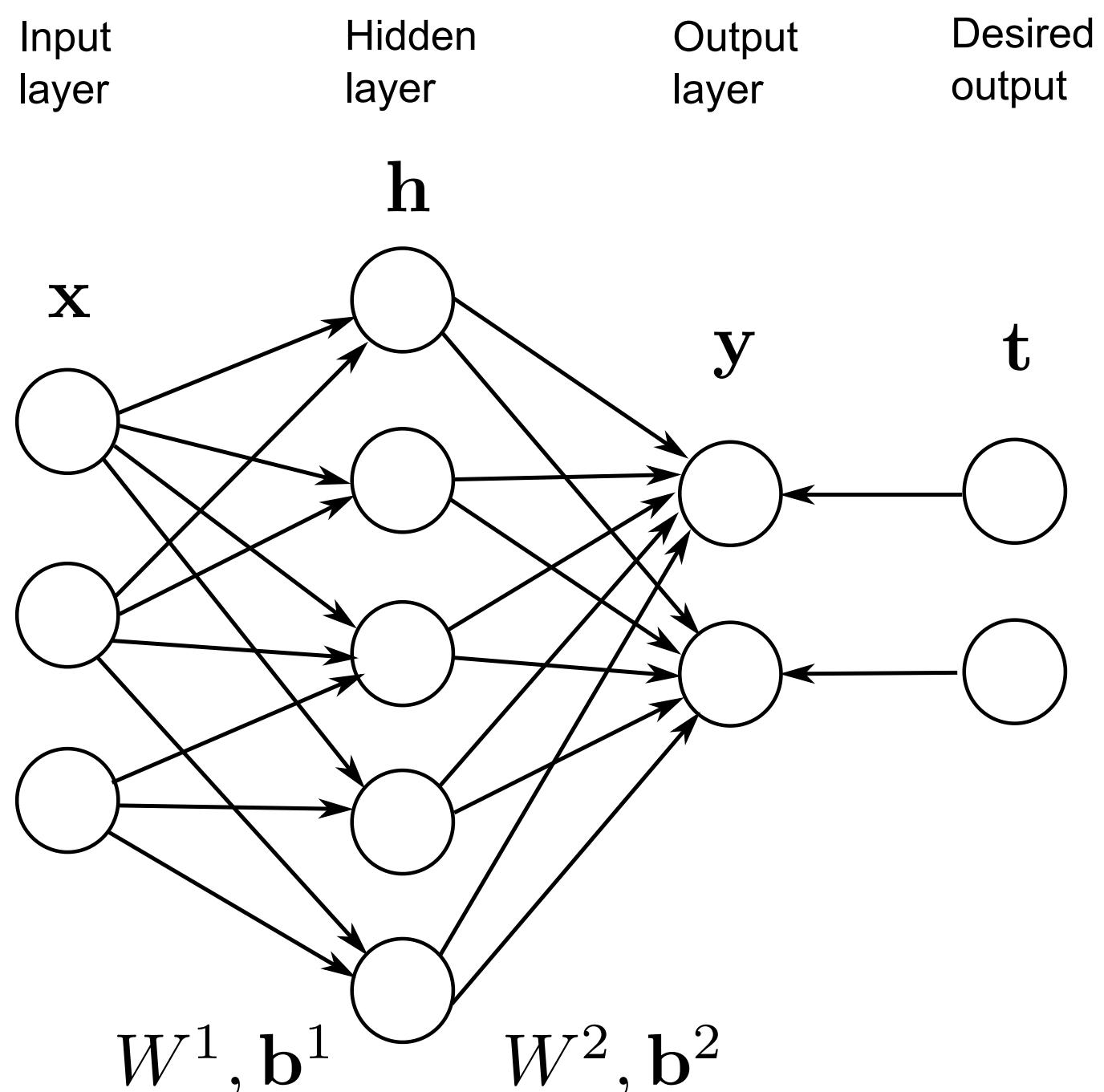
# Neurocomputing

Modern neural networks

Julien Vitay

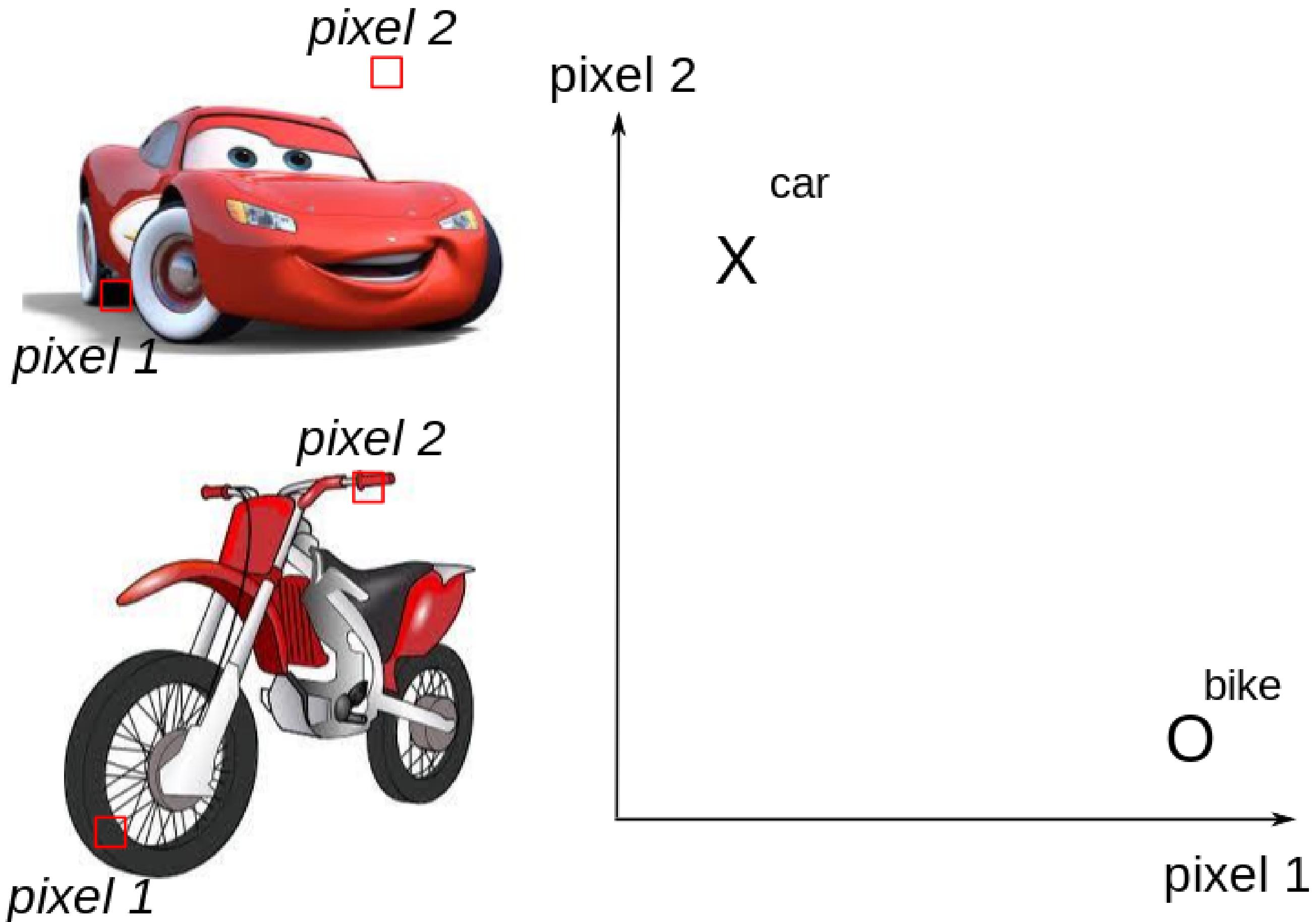
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# Shallow vs. deep networks



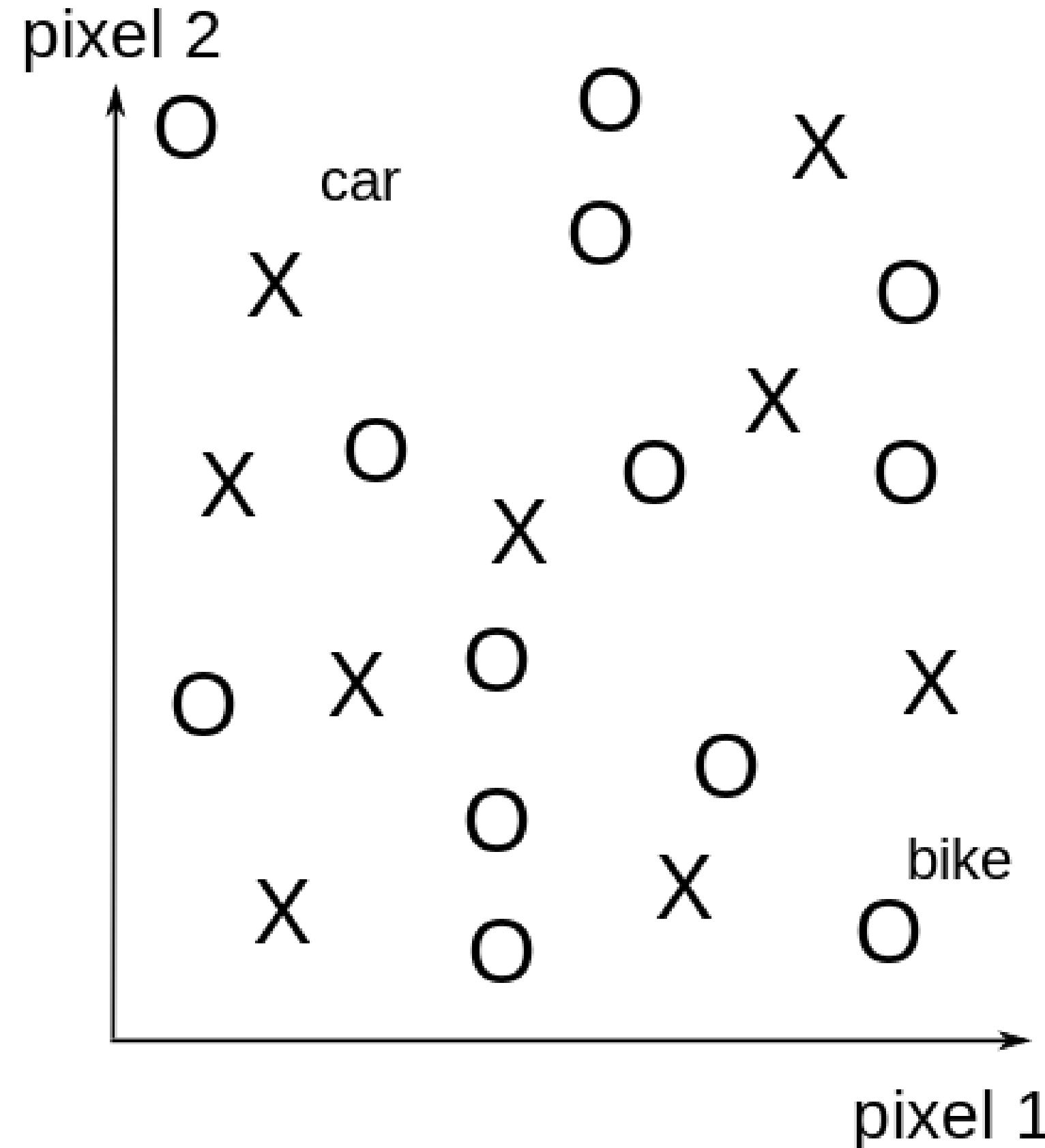
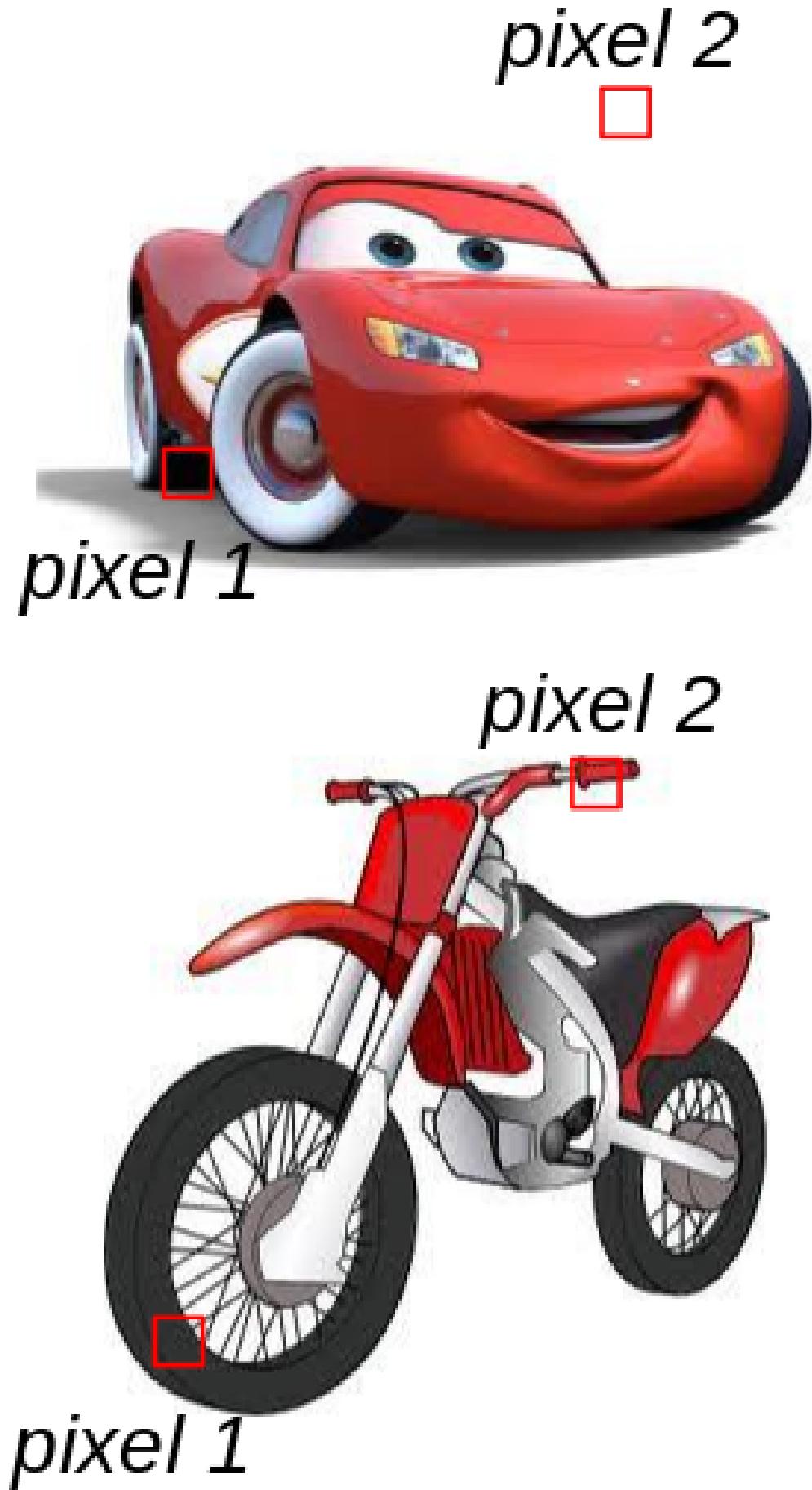
- Universal approximation theorem (Cybenko, 1989): a **shallow** network can approximate any mapping function between inputs and outputs.
- If the mapping function is too complex, a shallow network may need too many hidden neurons.
- The hidden neurons extract **features** in the input space: typical characteristics of the input which, when combined by the output neurons, allow to solve the classification task.
- Problem: the features are not hierarchically organized and cannot become complex enough.

## Feature selection



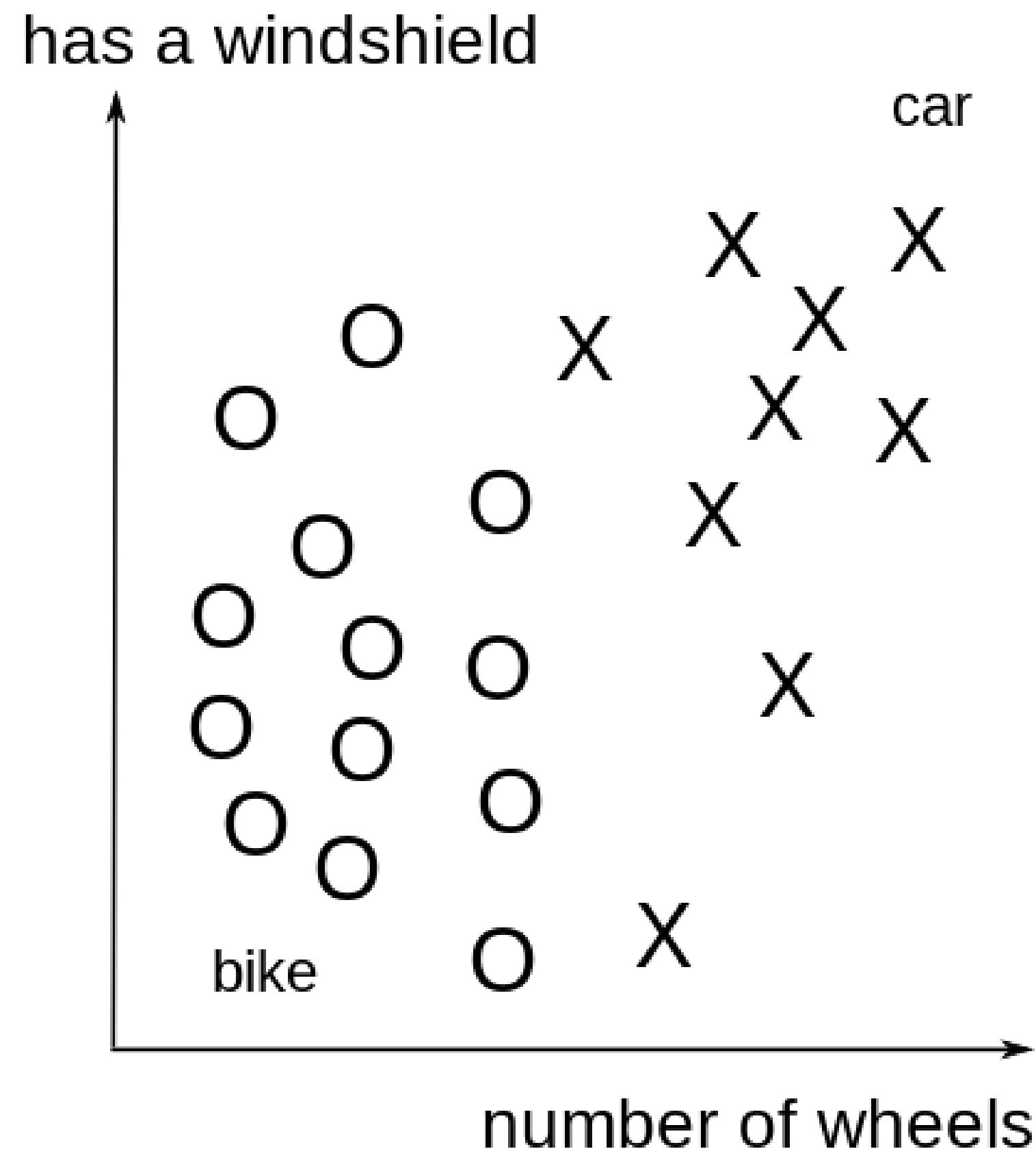
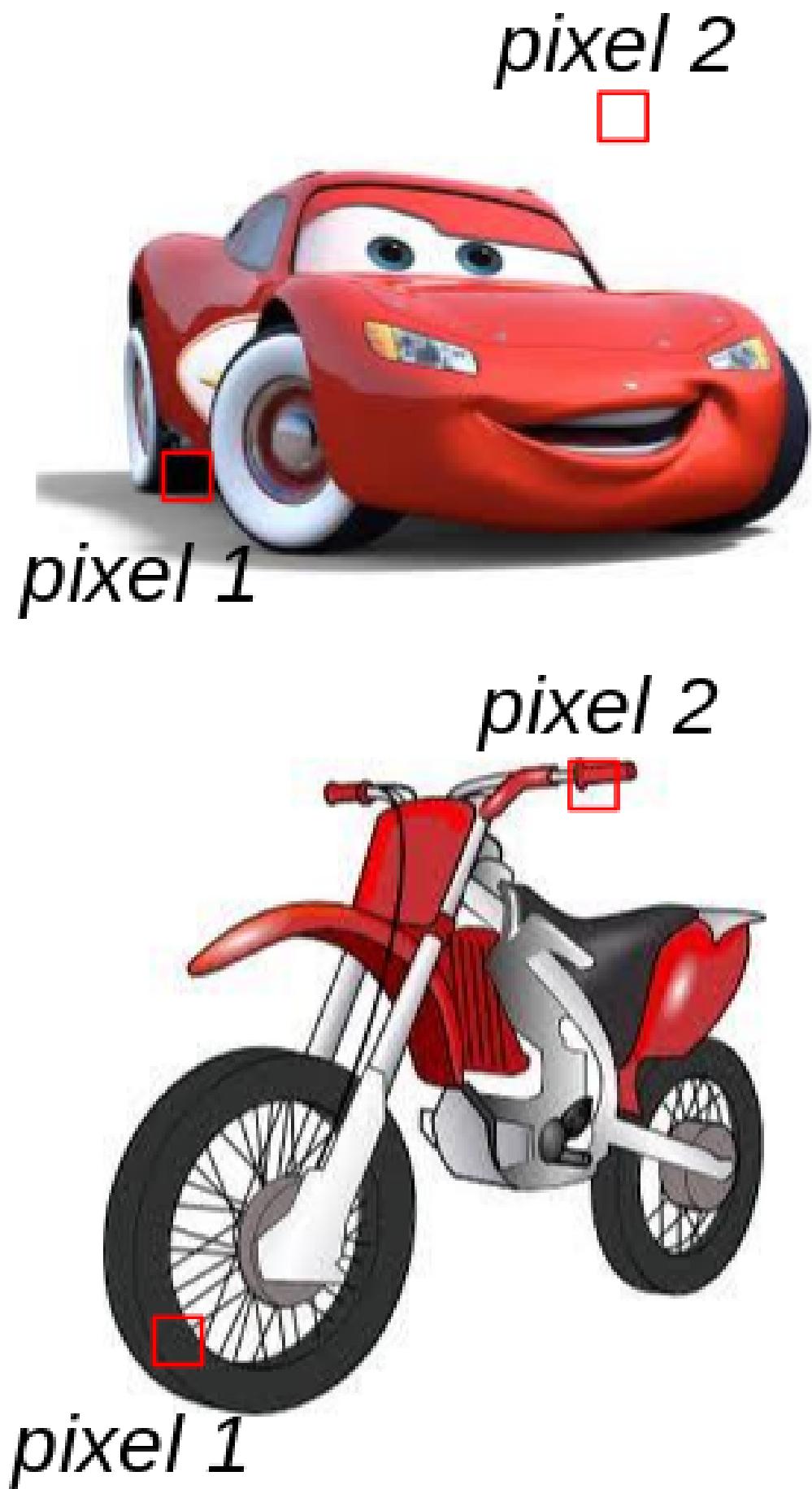
- Shallow networks can not work directly with raw images: noise, translation, rotation, scaling...
- One needs first to extract complex and useful features from the input images in order to classify them correctly.

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## Feature selection

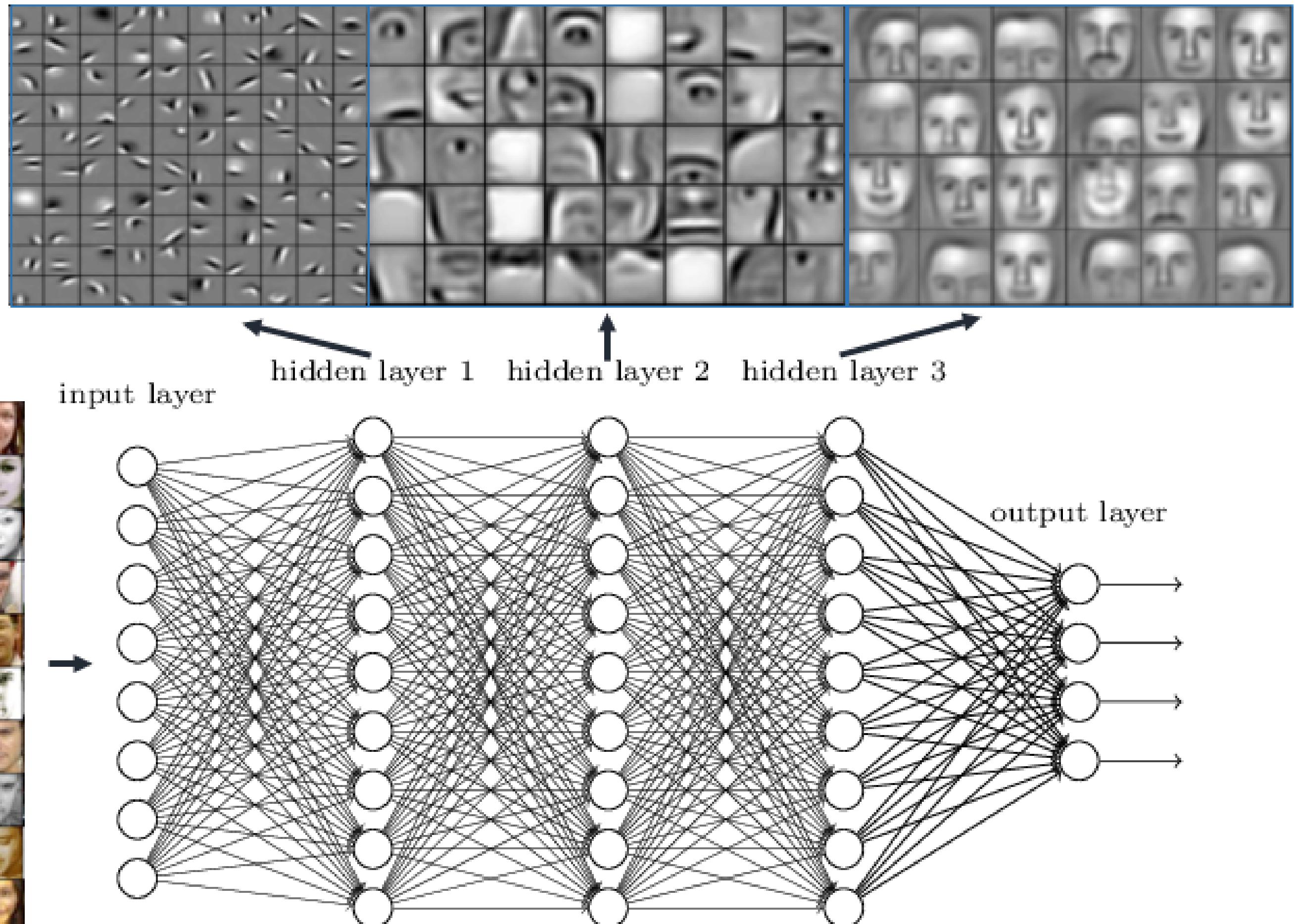
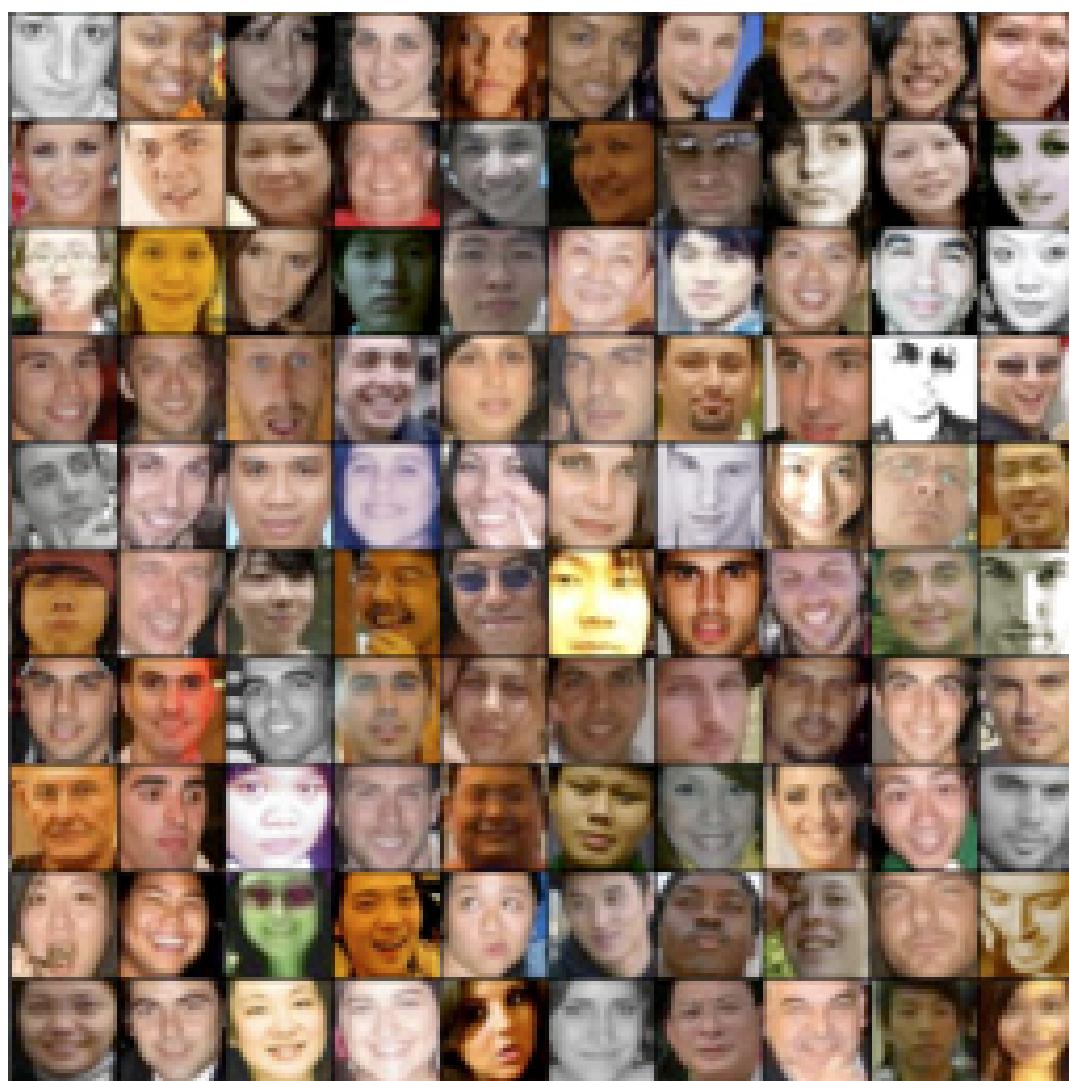


- Shallow networks can not work directly with raw images: noise, translation, rotation, scaling...
- One needs first to extract complex and useful features from the input images in order to classify them correctly.

# Deep Neural Network

- A MLP with more than one hidden layer is a **deep neural network**.
- The different layers extract increasingly complex features.

Deep neural networks learn hierarchical feature representations



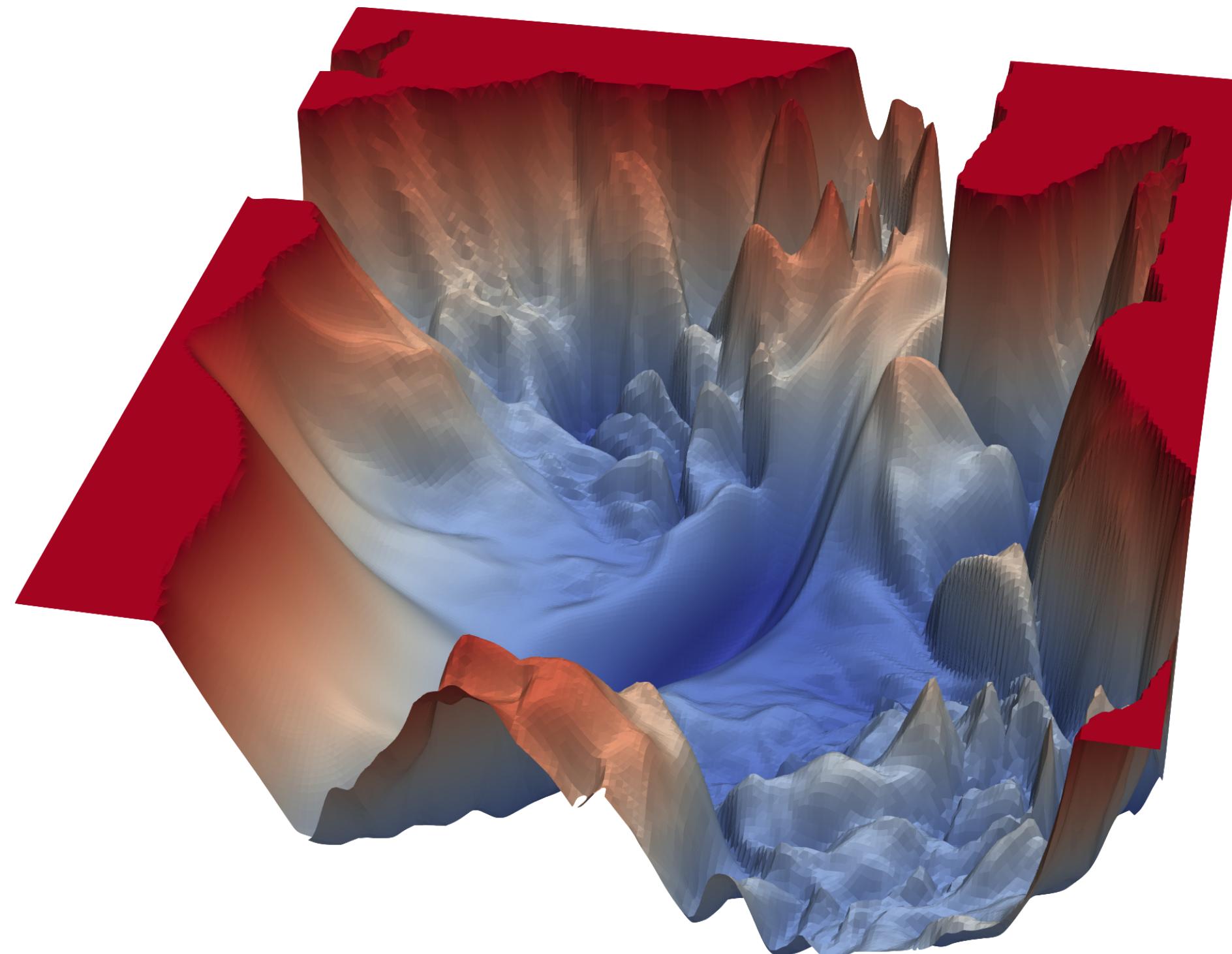
# Problems with deep networks

- In practice, training a deep network is not as easy as the theory would suggest.
- Four main problems have to be solved:
  1. **Bad convergence**: the loss function has many local minima.
    - Momentum, adaptive optimizers, annealing...
  2. **Long training time**: deep networks use gradient descent-like optimizers, an iterative method whose speed depends on initialization.
    - Normalized initialization, batch normalization...
  3. **Overfitting**: deep networks have a lot of free parameters, so they tend to learn by heart the training set.
    - Regularisation, dropout, data augmentation, early-stopping...
  4. **Vanishing gradient**: the first layers may not receive sufficient gradients early in training.
    - ReLU activation function, unsupervised pre-training, residual networks...

# 1 - Bad convergence

# Local minima

- The loss function  $\mathcal{L}(\theta)$  of a deep neural network has usually not a single global minimum, but many local minima: irregular **loss landscape**.



- Gradient descent gets stuck in local minima by design.
- One could perform different weight initializations, in order to find per chance an initial position close enough from the global minimum. → **inefficient**.

# Stochastic gradient descent

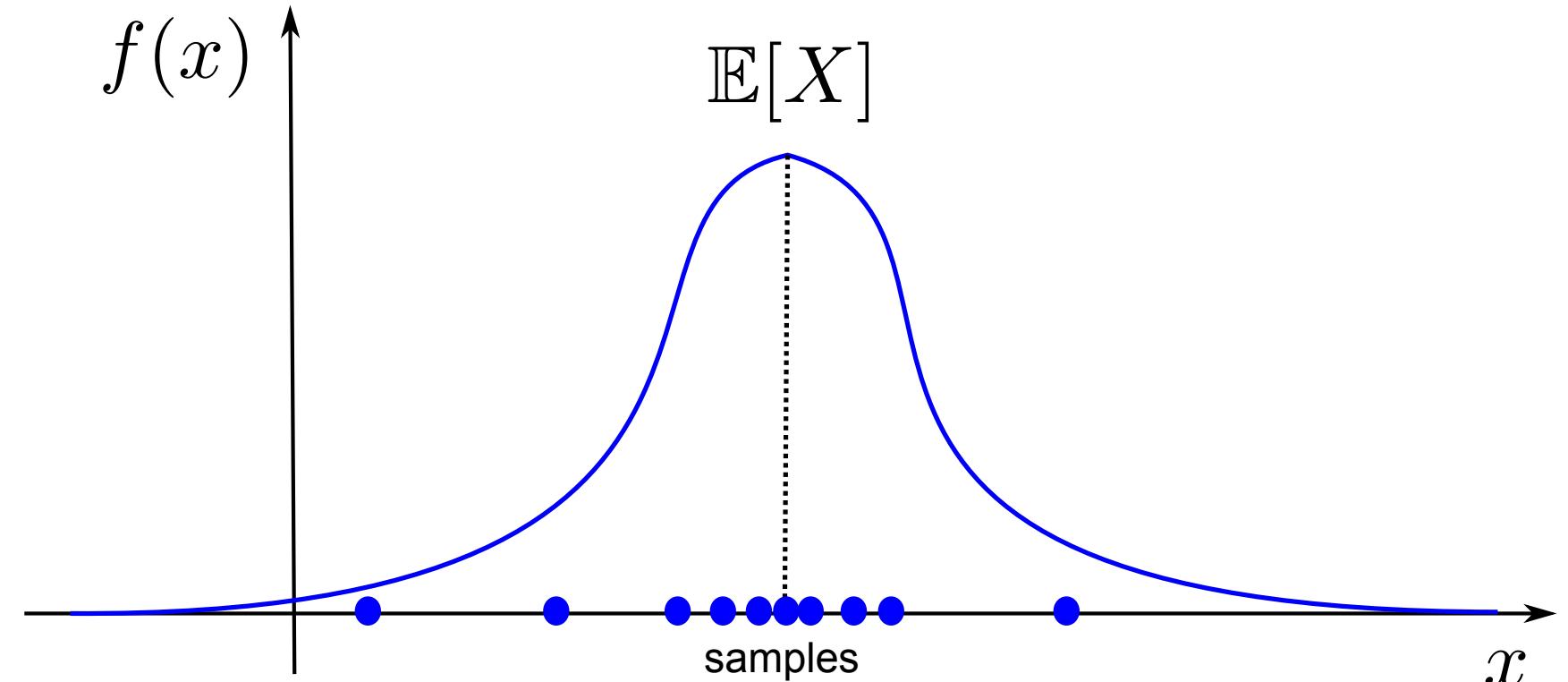
- What we actually want to minimize is the **mathematical expectation** of the square error (or any other loss) on the distribution of the data.

$$\mathcal{L}(\theta) = \mathbb{E}_{\mathcal{D}}(||\mathbf{t} - \mathbf{y}||^2)$$

- We do not have access to the true distribution of the data, so we have to estimate it through sampling.
- **Batch gradient descent** estimates the loss function by sampling the whole training set:

$$\mathcal{L}(\theta) \approx \frac{1}{N} \sum_{i=1}^N ||\mathbf{t}_i - \mathbf{y}_i||^2$$

- The estimated gradient is then unbiased (exact) and has no variance.
- Batch GD gets stuck in local minima.



- **Online gradient descent** estimates the loss function by sampling a single example:

$$\mathcal{L}(\theta) \approx ||\mathbf{t}_i - \mathbf{y}_i||^2$$

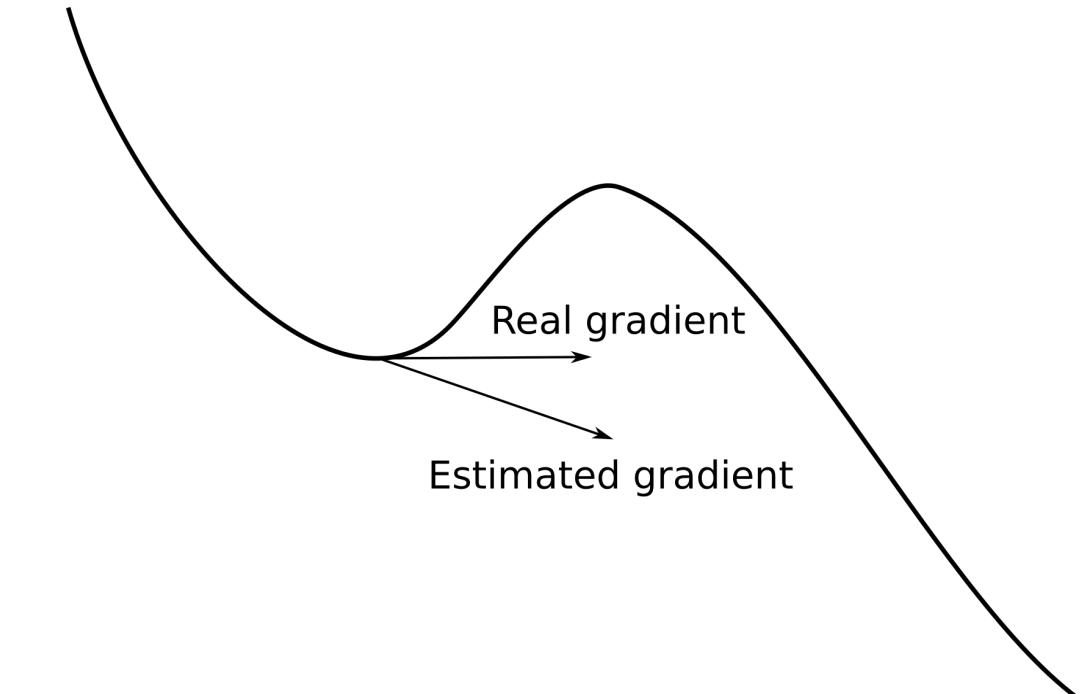
- The estimated gradient has a high variance (never right) but is unbiased on average.
- Online GD avoids local minima, but also global minima (unstable)...

# Stochastic gradient descent

- **Stochastic gradient descent** samples **minibatches** of  $K \sim 100$  examples to approximate the mathematical expectation.

$$\mathcal{L}(\theta) = E_{\mathcal{D}}(||\mathbf{t} - \mathbf{y}||^2) \approx \frac{1}{K} \sum_{i=1}^K ||\mathbf{t}_i - \mathbf{y}_i||^2$$

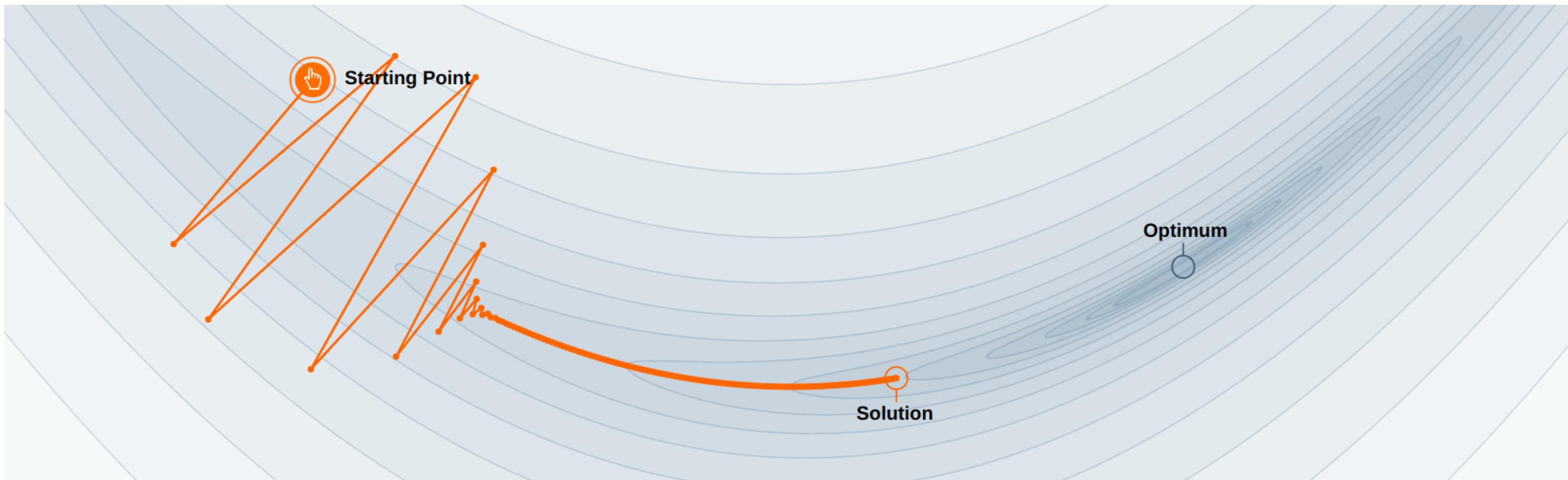
$$\Delta\theta = -\eta \nabla_{\theta} \mathcal{L}(\theta)$$



- This sampled loss has a high **variance**: take another minibatch and the gradient of the loss function will likely be very different.
- If the **batch size** is big enough, the estimated gradient is wrong, but usable on average (unbiased).
- The **high variance** of the estimated gradient helps getting out of local minimum: because our estimation of the gradient is often **wrong**, we get out of the local minima although we should have stayed in it.
  - The *true* gradient is 0 for a local minimum, but its sampled value may not, so the parameters will be updated and hopefully get out of the local minimum.
- Which **batch size** works the best for my data? **Cross-validation**, but beware that big batch sizes increase memory consumption, what can be a problem on GPUs.

# Parameter-dependent optimization

- Another issue with stochastic gradient descent is that it uses the same learning rate for all parameters. In **ravines** (which are common around minima), some parameters (or directions) have a higher influence on the loss function than others.



Source: <https://distill.pub/2017/momentum/>

- In the example above, you may want to go faster in the “horizontal” direction than in the “vertical” one, although the gradient is very small in the horizontal direction.
- With a fixed high learning rate for all parameters, SGD would start oscillating for the steep parameters, while being still very slow for the flat ones.
- The high variance of the sampled gradient is detrimental to performance as it can lead to oscillations.
- Most modern optimizers have a **parameter-dependent adaptive learning rate**.

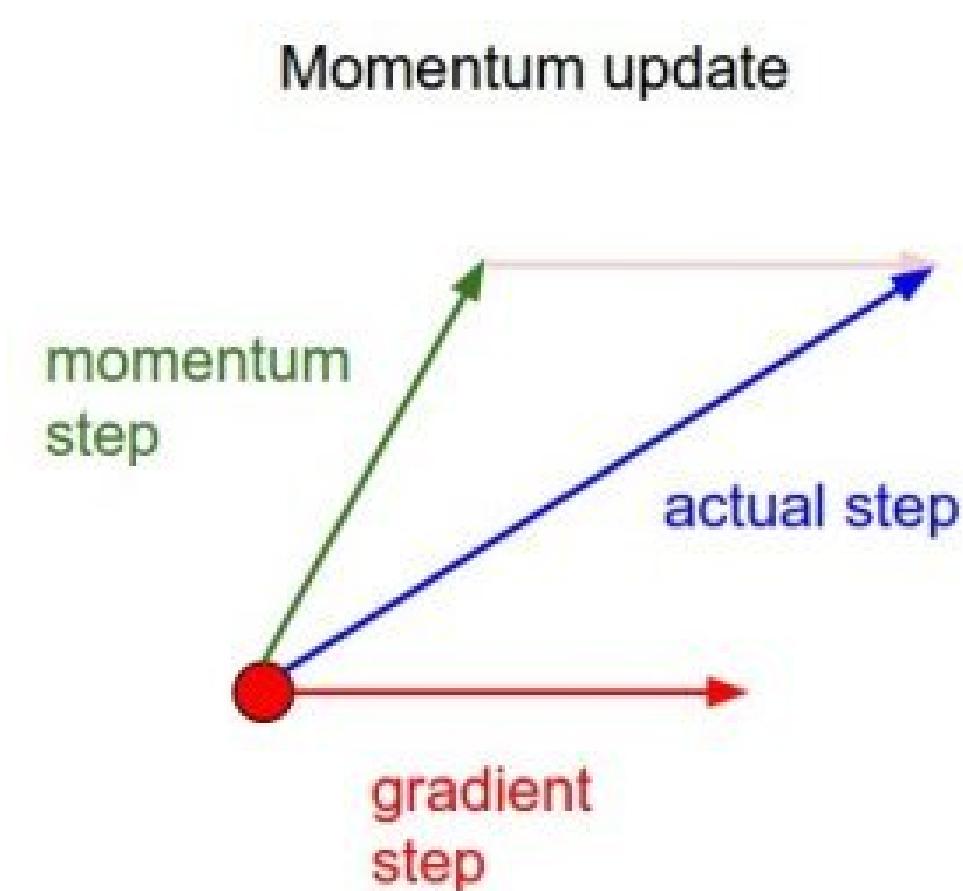
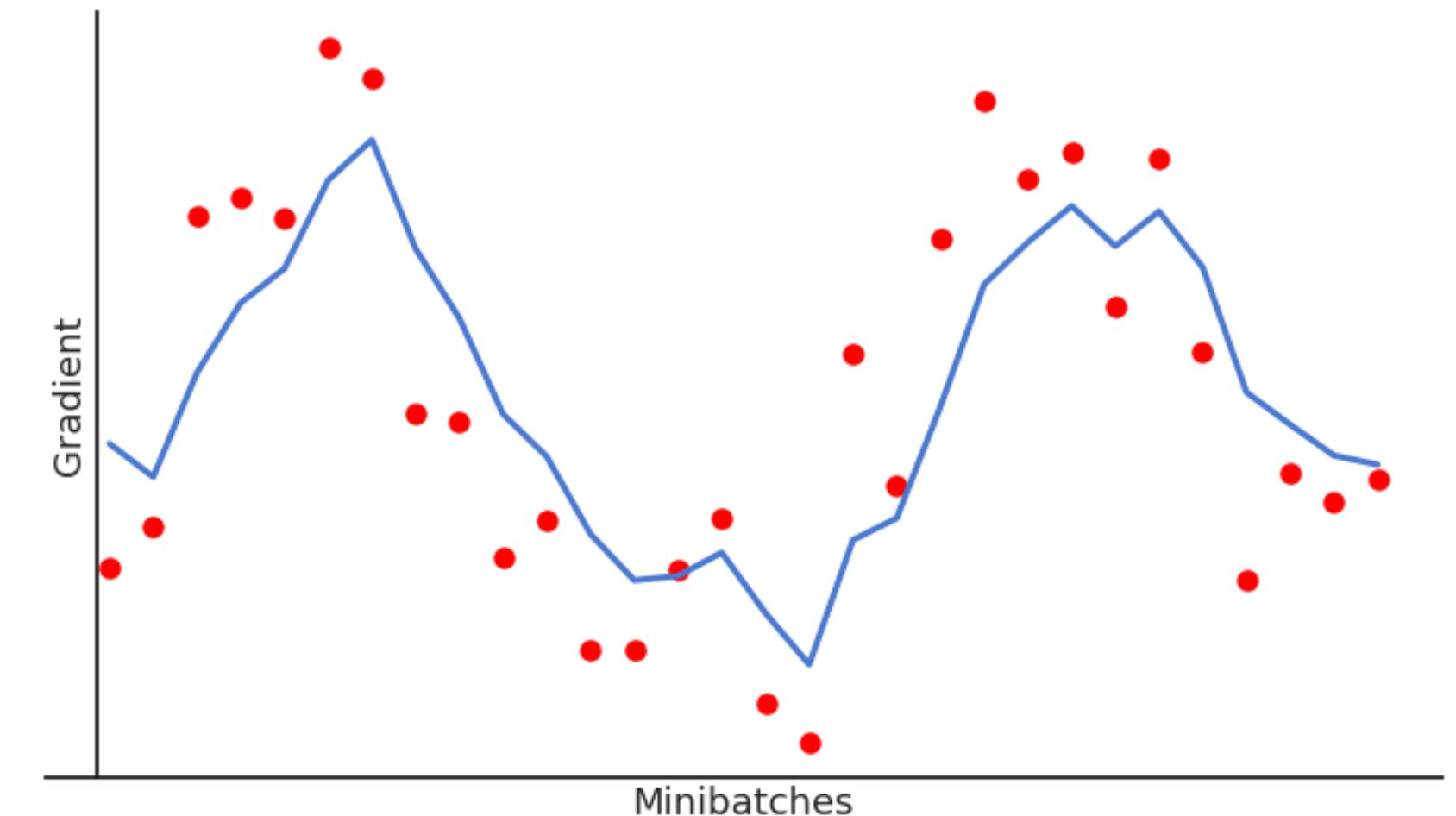
# SGD with momentum

- One solution is to **smooth** the gradients over time (i.e. between minibatches), in order to avoid that one parameter is increased by one minibatch and decreased by the next one.
- The momentum method uses a **moving average** of the gradient (momentum step) to update the parameters:

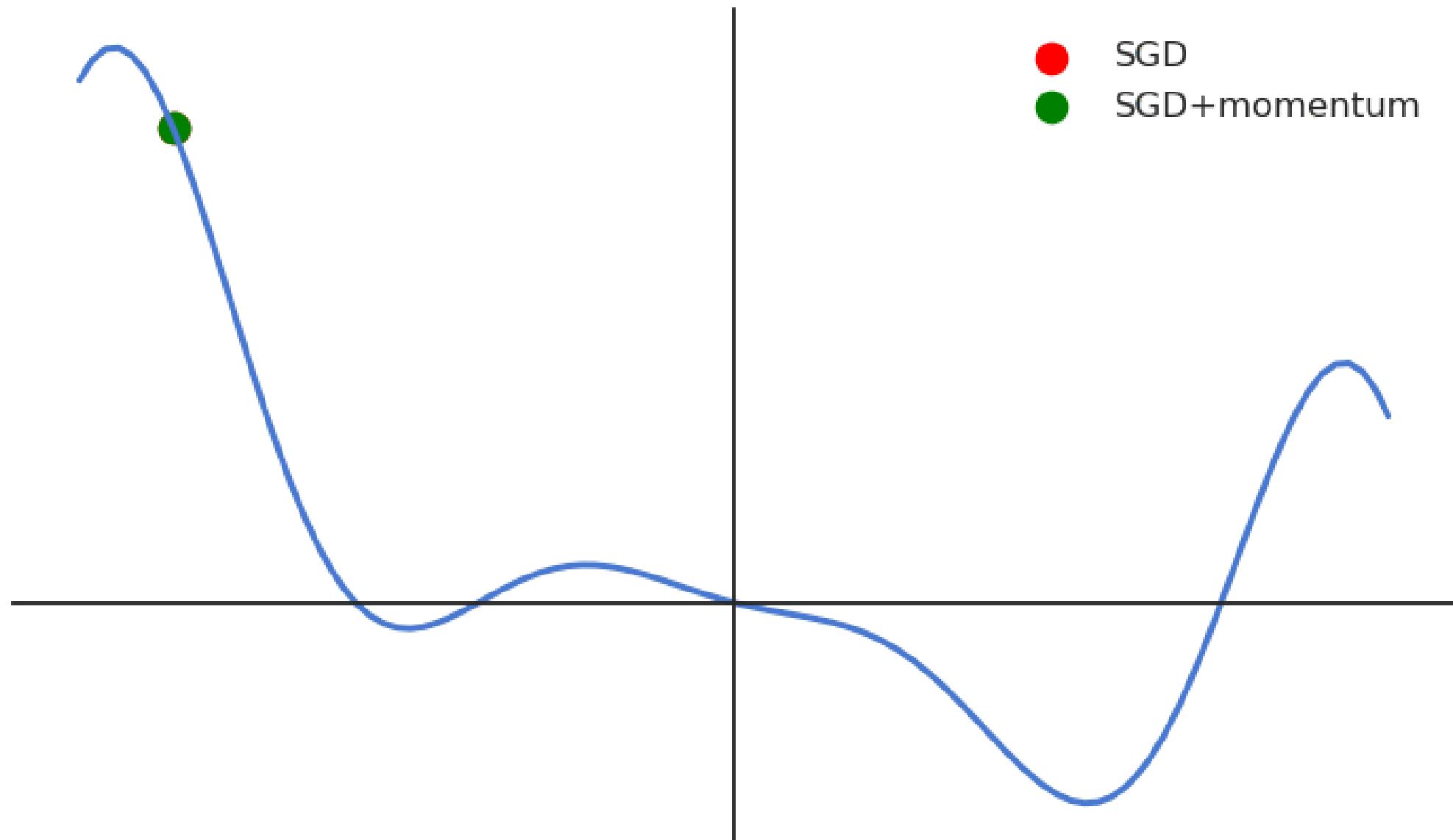
$$v(\theta) = \alpha v(\theta) - (1 - \alpha) \nabla_{\theta} \mathcal{L}(\theta)$$

$$\Delta\theta = \eta v(\theta)$$

- $0 \leq \alpha < 1$  controls how much of the gradient we use for the parameter update (usually around 0.9)
- $\alpha = 0$  is the vanilla SGD.

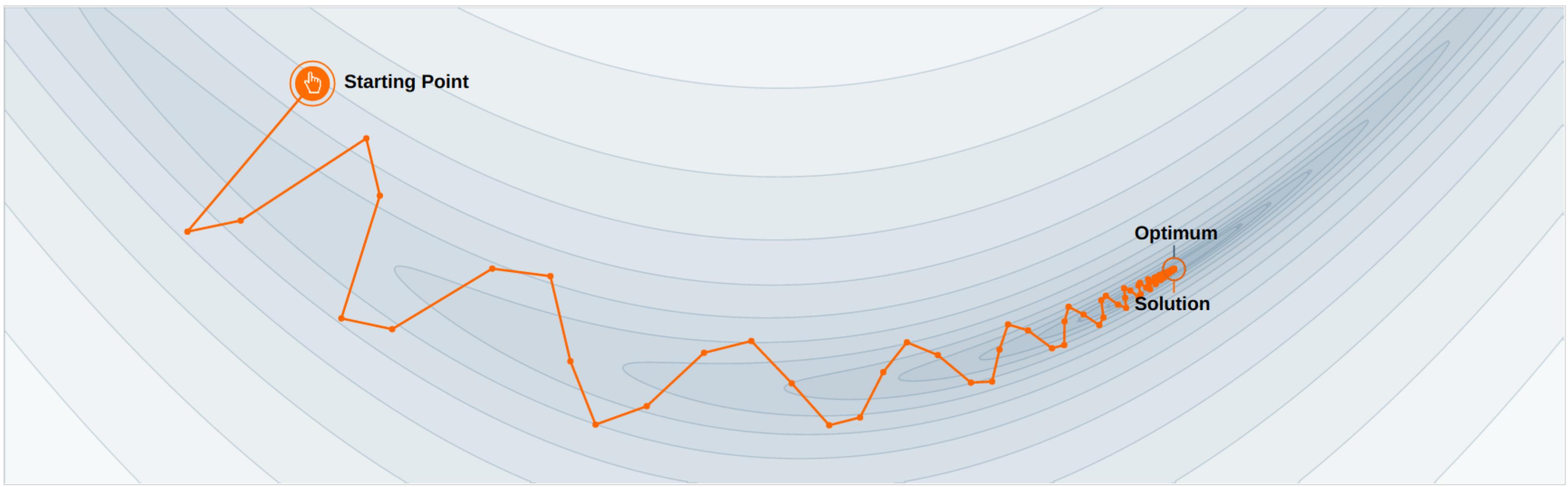


## SGD with momentum



- When the gradient for a single parameter has always the same direction between successive examples, gradient descent accelerates (bigger steps).
  - When its sign changes, the weight changes continue in the same direction for while, allowing to “jump” over small local minima if the speed is sufficient.
  - If the gradient keeps being in the opposite direction, the weight changes will finally reverse their direction.
- 
- SGD with momentum uses an **adaptive learning rate**: the learning is implicitly higher when the gradient does not reverse its sign (the estimate “accelerates”).

# SGD with momentum



Step-size  $\alpha = 0.0032$

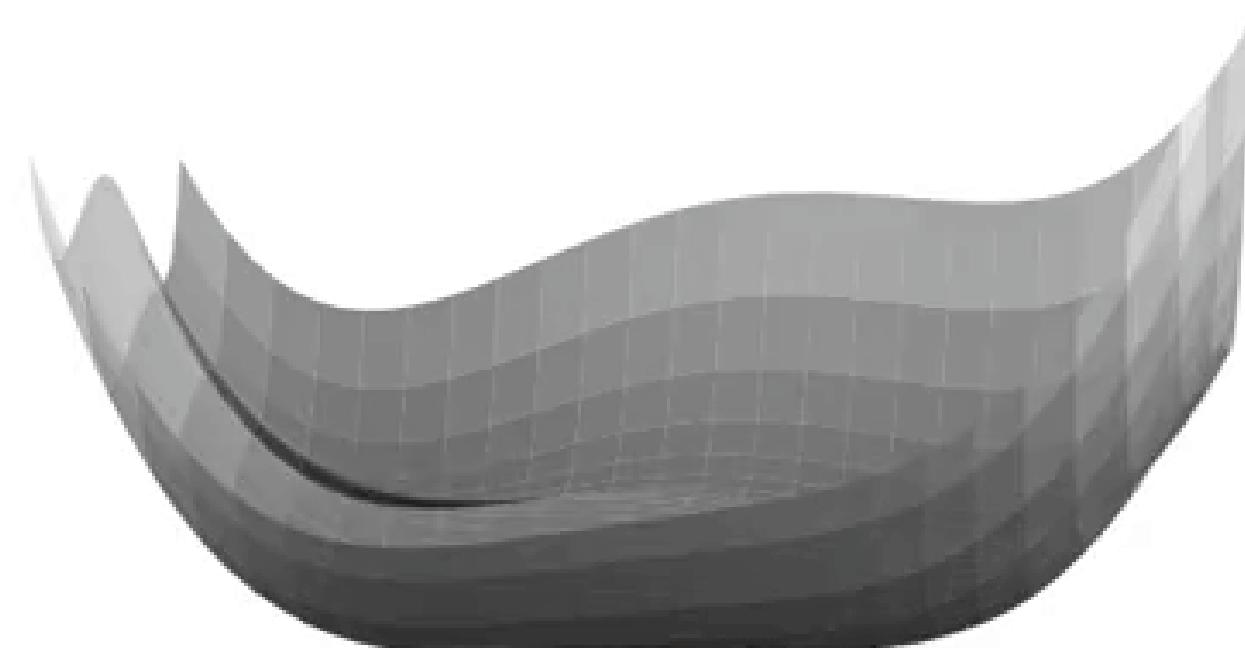
Momentum  $\beta = 0.86$

We often think of Momentum as a means of dampening oscillations and speeding up the iterations, leading to faster convergence. But it has other interesting behavior. It allows a larger range of step-sizes to be used, and creates its own oscillations. What is going on?

- With momentum, the flat parameters keep increasing their update speed, while the steep ones slow down.
- SGD with momentum gets rid of oscillations at higher learning rates.
- The momentum method benefits a lot from the variance of SGD: noisy gradients are used to escape local minima but are averaged around the global minimum.
- See the great visualization by Gabriel Goh on <https://distill.pub/2017/momentum/>.

# SGD with Nesterov momentum

Standard Momentum (black) vs Nesterov Momentum (red)

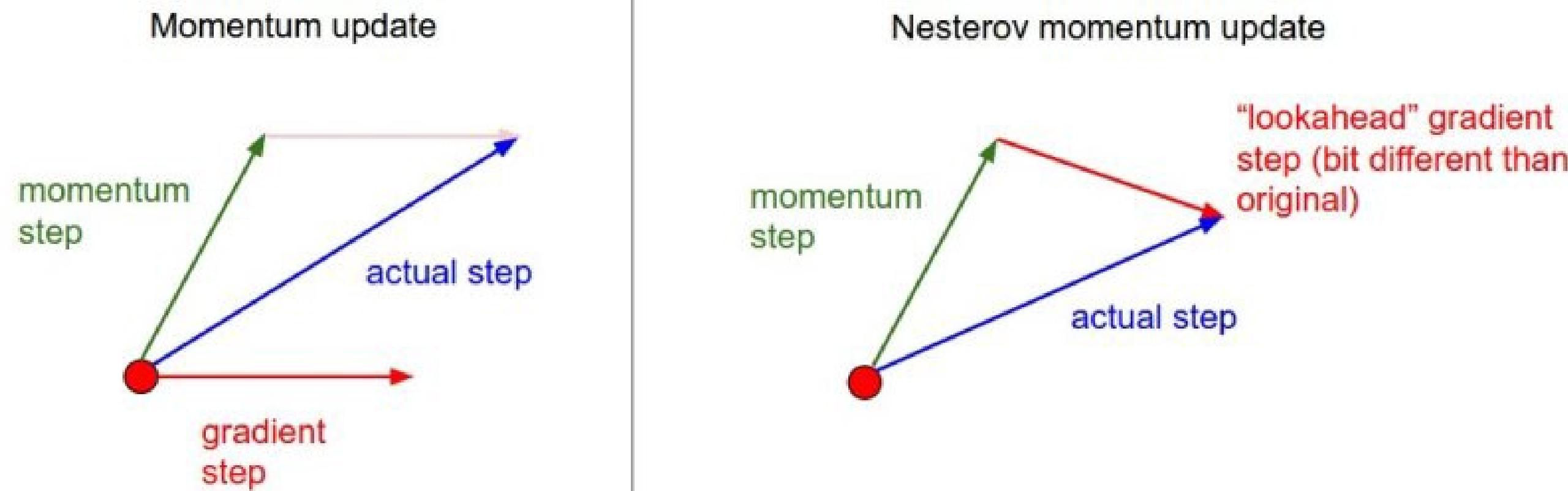


- SGD with momentum tends to oscillate around the minimum.
- The Nesterov momentum **corrects** these oscillations by estimating the gradient **after** the momentum update:

$$v(\theta) = \alpha v(\theta) - (1 - \alpha) \nabla_{\theta} \mathcal{L}(\theta + \alpha v(\theta))$$

$$\Delta\theta = \eta v(\theta)$$

Source: <https://ikocabiyik.com/blog/en/visualizing-ml-optimizers/>



Source: <https://cs231n.github.io/neural-networks-3/>

## RMSprop

- Instead of smoothing the gradient, what destroys information, one could adapt the learning rate to the **curvature** of the loss function:
  - put the **brakes** on when the function is steep (high gradient).
  - **accelerate** when the loss function is flat (plateau).
- RMSprop (Root Mean Square Propagation) scales the learning rate by a running average of the squared gradient (second moment  $\approx$  variance).

$$v(\theta) = \alpha v(\theta) + (1 - \alpha) (\nabla_{\theta} \mathcal{L}(\theta))^2$$

$$\Delta\theta = -\frac{\eta}{\epsilon + \sqrt{v(\theta)}} \nabla_{\theta} \mathcal{L}(\theta)$$

- If the gradients vary a lot between two minibatches, the learning rate is reduced.
- If the gradients do not vary much, the learning rate is increased.

## Adam

- Adam (Adaptive Moment Estimation) builds on the idea of RMSprop, but uses also a moving average of the gradient.

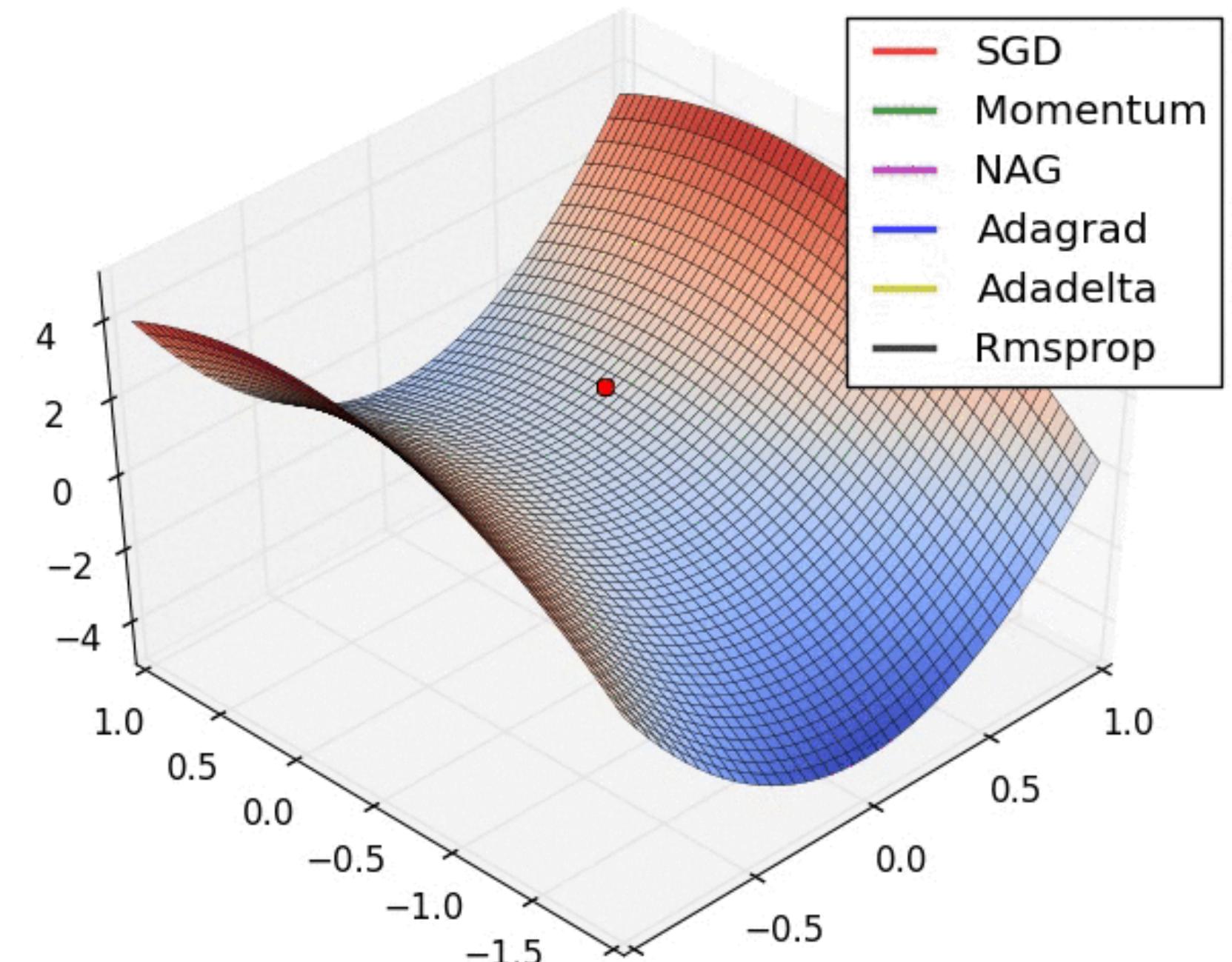
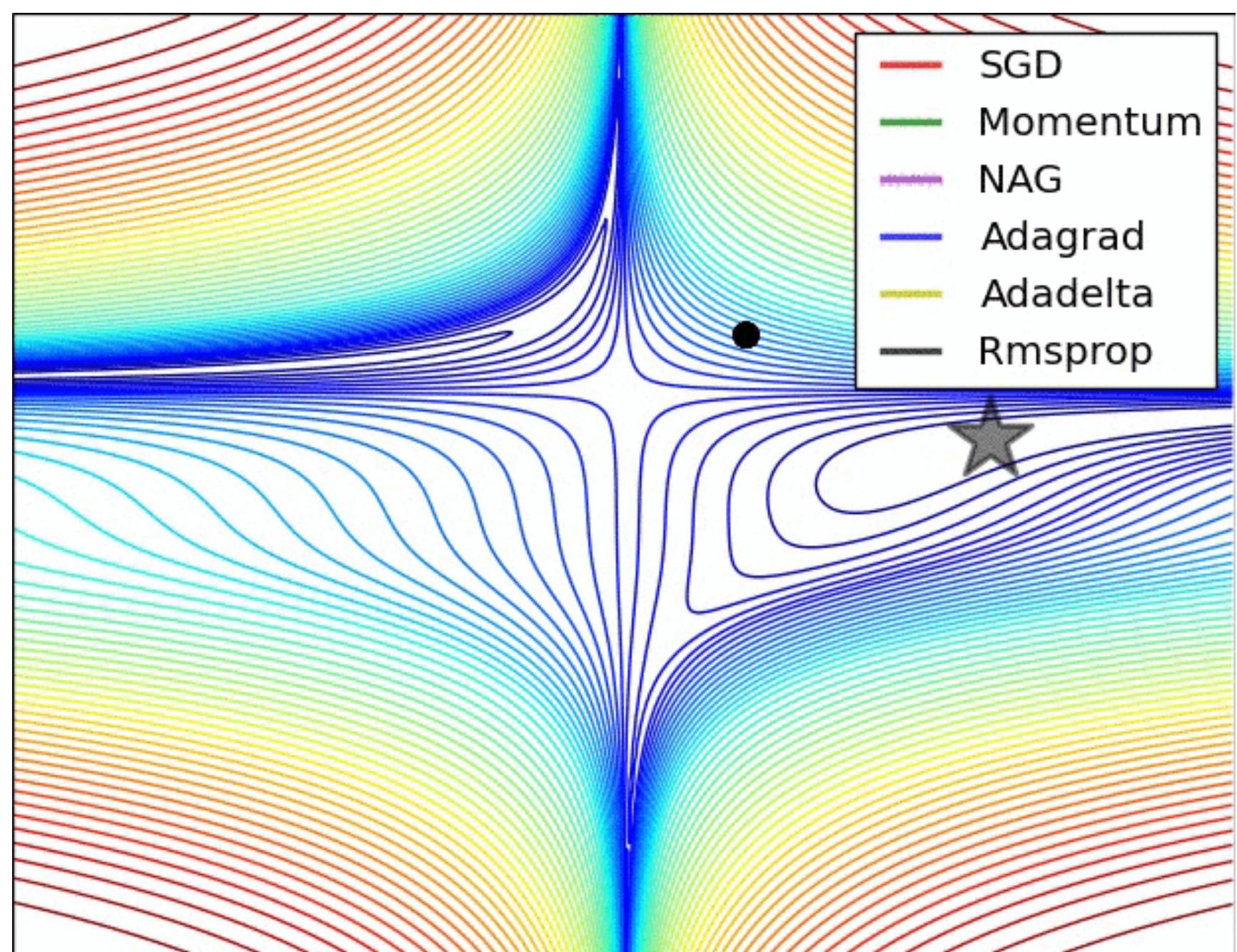
$$m(\theta) = \beta_1 m(\theta) + (1 - \beta_1) \nabla_{\theta} \mathcal{L}(\theta)$$

$$v(\theta) = \beta_2 v(\theta) + (1 - \beta_2) \nabla_{\theta} \mathcal{L}(\theta)^2$$

$$\Delta\theta = -\eta \frac{m(\theta)}{\epsilon + \sqrt{v(\theta)}}$$

- Adam = RMSprop + momentum.
- Other possible optimizers: Adagrad, Adadelta, AdaMax, Nadam...
- In practice, SGD with momentum allows to find better solutions, but the meta-parameters are harder to find (cross-validation).
- Adam finds slightly poorer solutions, but the parameters  $\beta_1$ ,  $\beta_2$  and  $\epsilon$  can usually be kept at default.

# Comparison of modern optimizers



Source: Alec Radford <https://imgur.com/a/Hqolp>

# Optimizers in keras <https://keras.io/api/optimizers>

- SGD:

```
optimizer = tf.keras.optimizers.SGD(learning_rate=0.01)
```

- SGD with Nesterov momentum:

```
optimizer = tf.keras.optimizers.SGD(learning_rate=0.01, momentum=0.9, nesterov=True)
```

- RMSprop:

```
optimizer = tf.keras.optimizers.RMSprop(  
    learning_rate=0.001, rho=0.9, momentum=0.0, epsilon=1e-07  
)
```

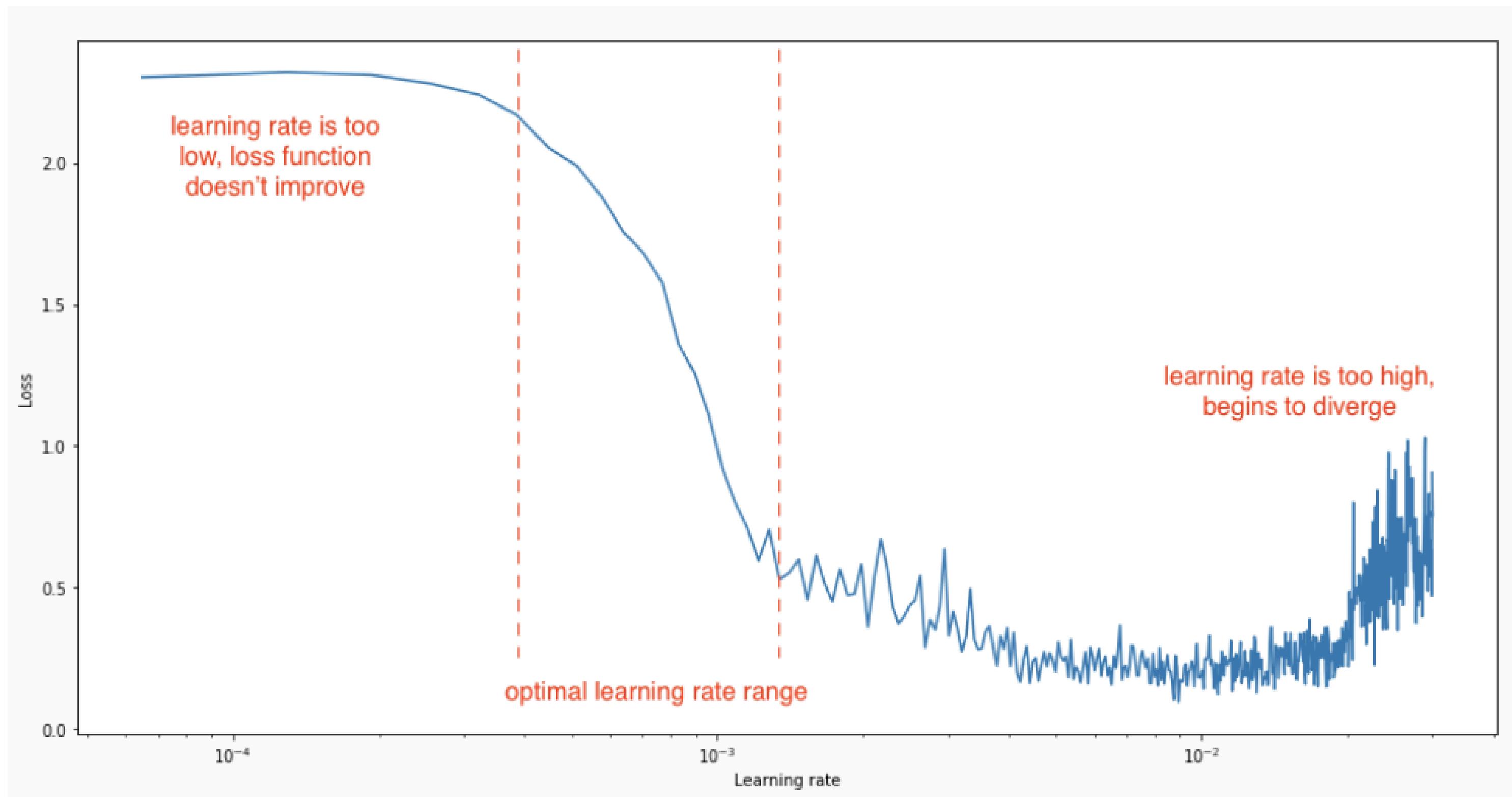
- Adam:

```
optimizer = tf.keras.optimizers.Adam(  
    learning_rate=0.001, beta_1=0.9, beta_2=0.999, epsilon=1e-07)
```

# Hyperparameters annealing

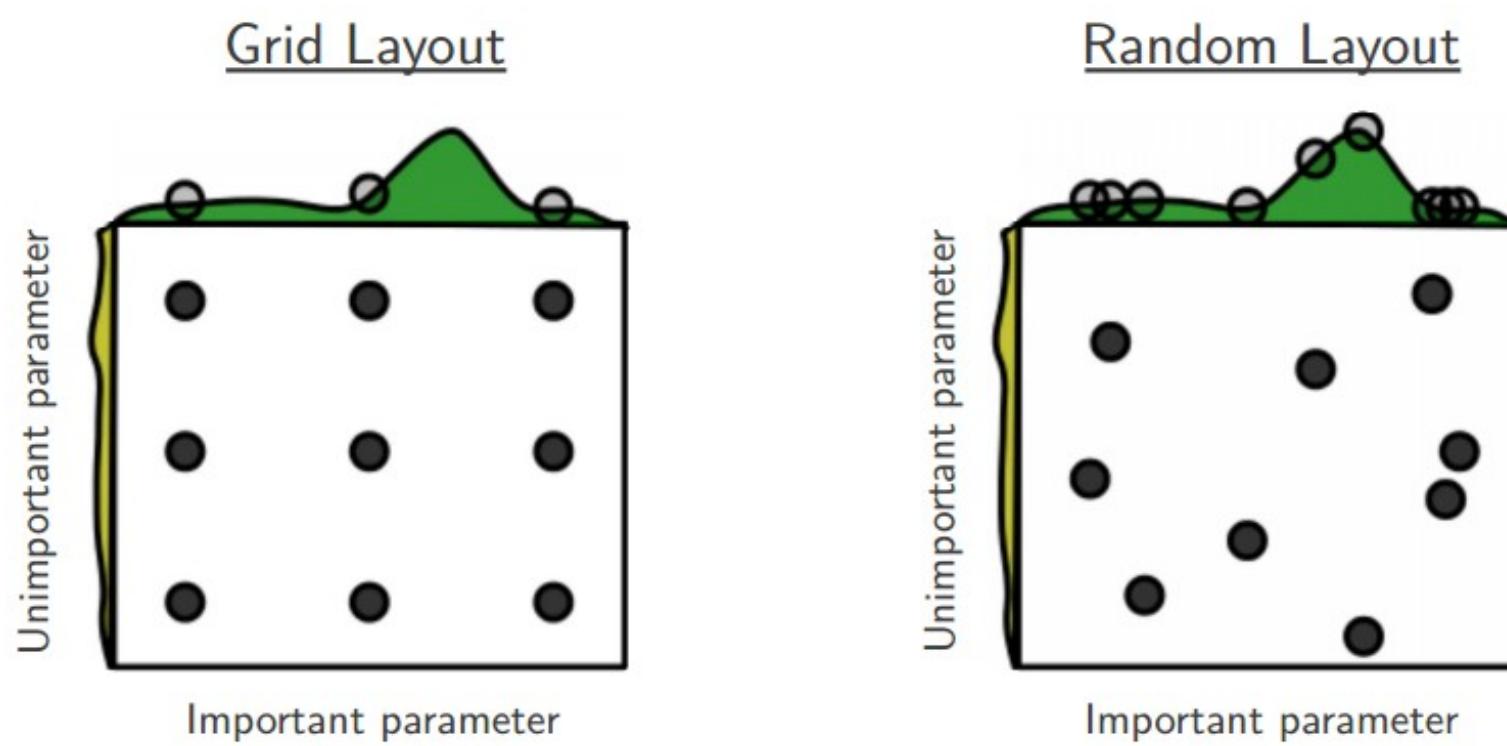
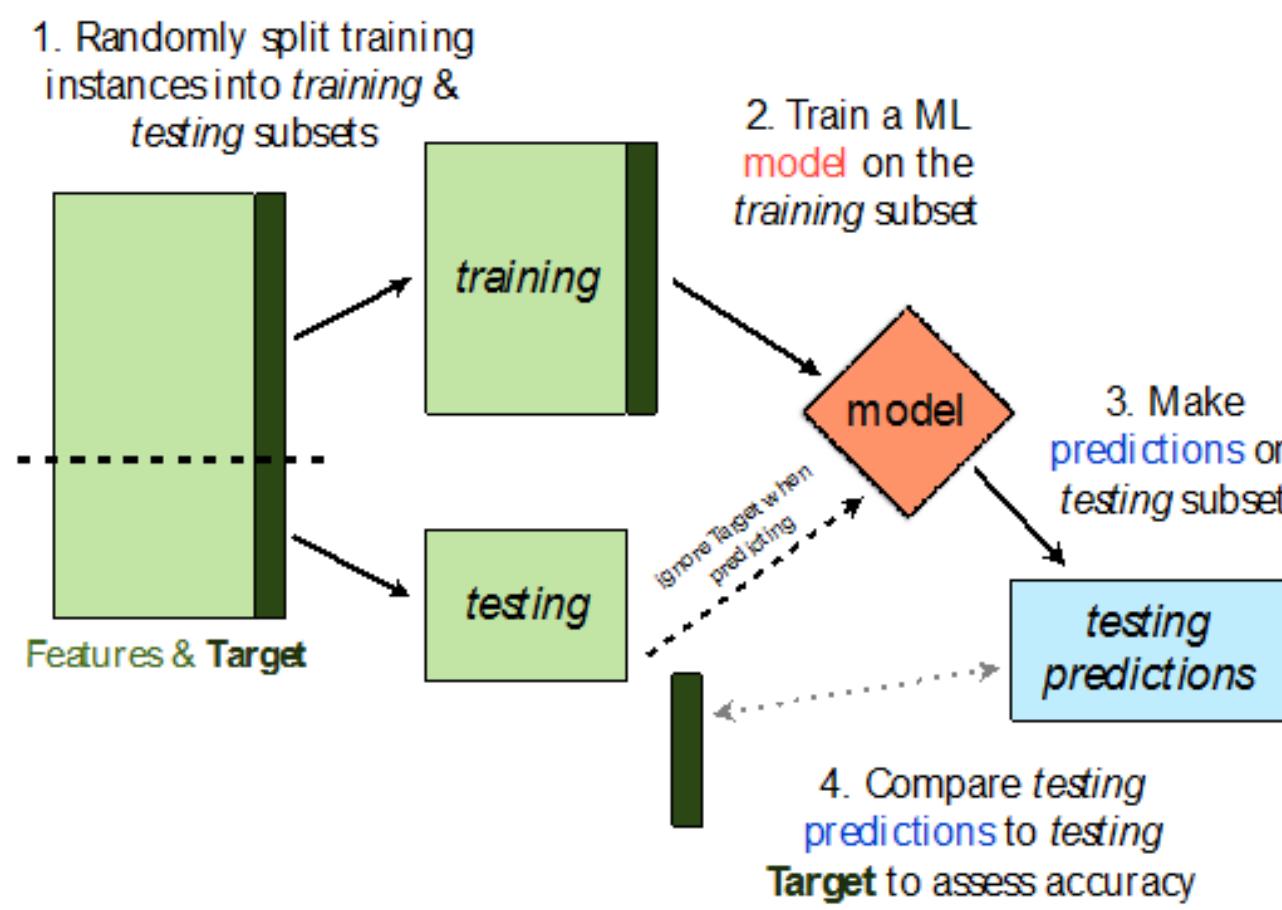
# Finding a good range for the learning rate

- A simple trick to find a good estimate of the learning rate (or its start/stop value) is to increase its value exponentially **for each minibatch** at the beginning of learning.
- The “good” region for the learning rate is the one where the validation loss decreases, but does not oscillate.



Source: <https://towardsdatascience.com/advanced-topics-in-neural-networks-f27fbcc638ae>

# Hyperparameter search



- Even with annealing, it is tricky to find the optimal value of the hyperparameters.
- The only option is to perform **cross-validation**, by varying the hyperparameters systematically and initializing the weights randomly every time.
- There are two basic methods:
  - **Grid search:** different values of each parameter are chosen linearly ( $[0.1, 0.2, \dots, 0.9]$ ) or logarithmically ( $[10^{-6}, 10^{-5}, \dots, 10^{-1}]$ ).
  - **Random search:** the values are randomly chosen each time from some distribution (uniform, normal, lognormal).
- The advantage of random search is that you can stop it anytime if you can not wait any longer.
- Very time-consuming, but easy to perform in parallel if you have clusters of CPUs or GPUs (**data-parallel**).

Source: <http://cs231n.github.io/neural-networks-3/>

# Bayesian hyperparameter optimization

- A more advanced and efficient technique is **Bayesian hyperparameter optimization**, for example the **Tree Parzen Estimator** (TPE) algorithm.
- The idea is to build a probability model of the objective function and use it to select the most promising hyperparameters to evaluate in the true objective function.
- Roughly speaking, it focuses parameter sampling on the interesting regions.
- The [hyperopt](https://github.com/hyperopt/hyperopt) Python library <https://github.com/hyperopt/hyperopt> is extremely simple to use:

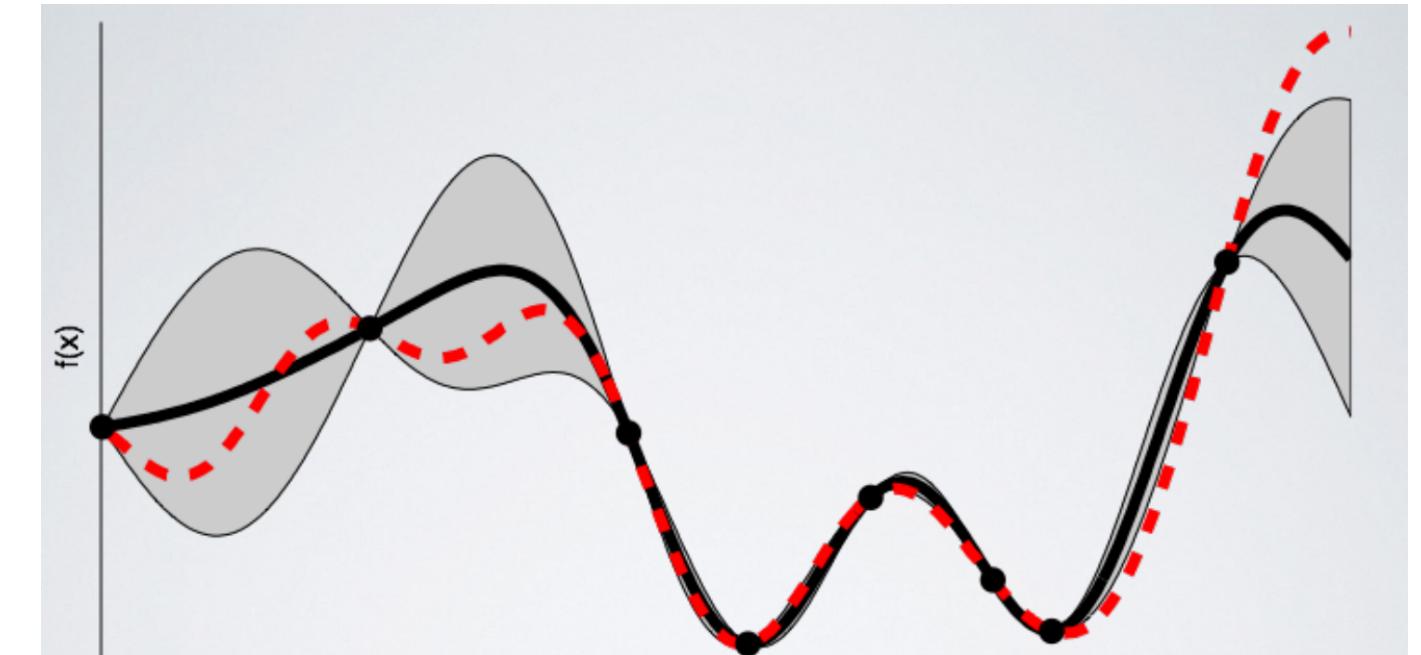
```
from hyperopt import fmin, tpe, hp, STATUS_OK

def objective(eta):
    # Train model with:
    optimizer = tf.keras.optimizers.SGD(eta)
    return {'loss': test_loss, 'status': STATUS_OK }

best = fmin(objective,
            space=hp.loguniform('eta', -6, -1),
            algo=tpe.suggest,
            max_evals=100)

print(best)
```

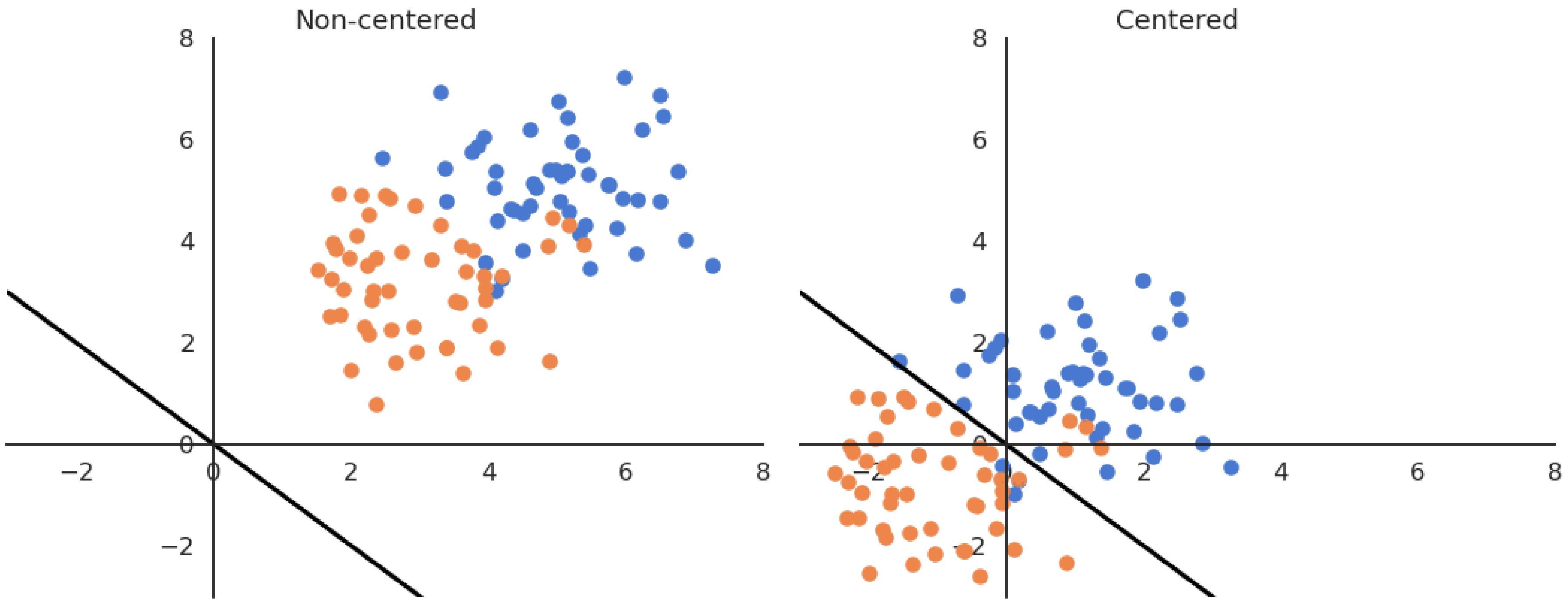
- Other library: [optuna](https://optuna.org) <https://optuna.org>



Source: <https://towardsdatascience.com/a-conceptual-explanation-of-bayesian-model-based-hyperparameter-optimization-for-machine-learning-b8172278050f>

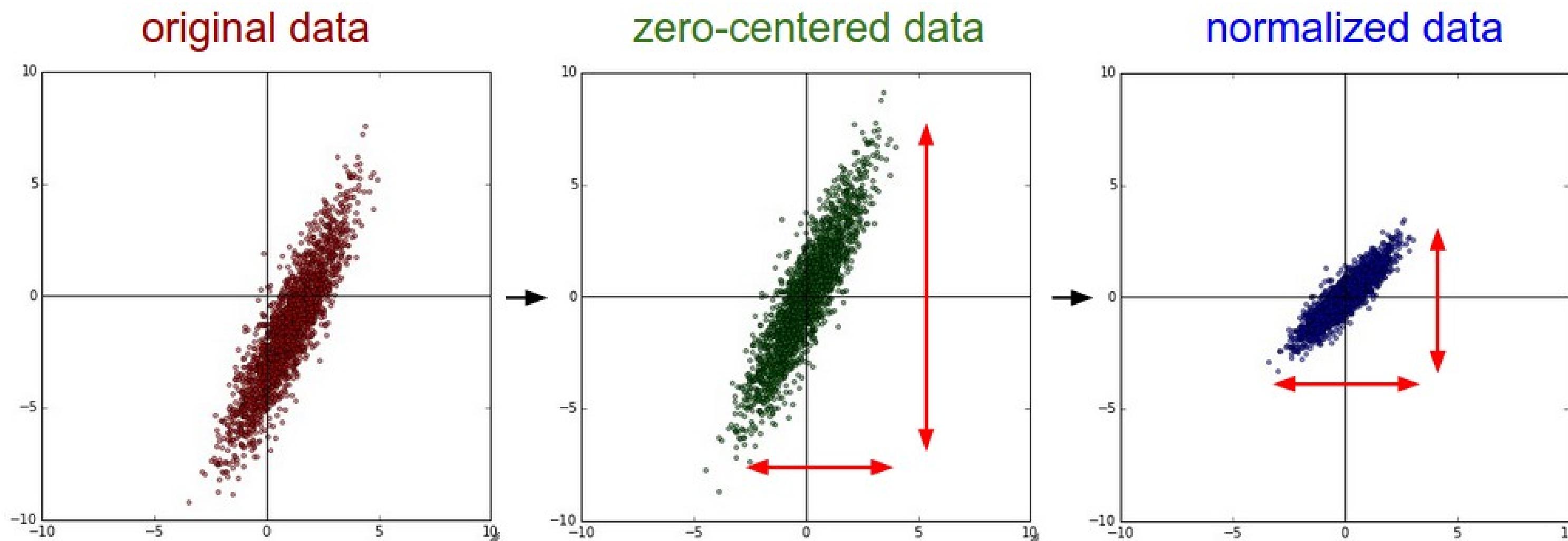
## **2 - Long training times**

# Importance of weight initialization



- If the data is not centered in the input space, the hyperplane (i.e. each neuron) may need a lot of iterations to “move” to the correct position using gradient descent. The initialization of the weights will matter a lot: if you start too far away from the solution, you will need many iterations.
- If the data is normalized (zero mean, unit variance), the bias can be initialized to 0 and will converge much faster. Only the **direction** of the weight vector matters, not its norm, so it will be able to classify the data much faster.

# Data normalization



Source : <http://cs231n.github.io/neural-networks-2/>

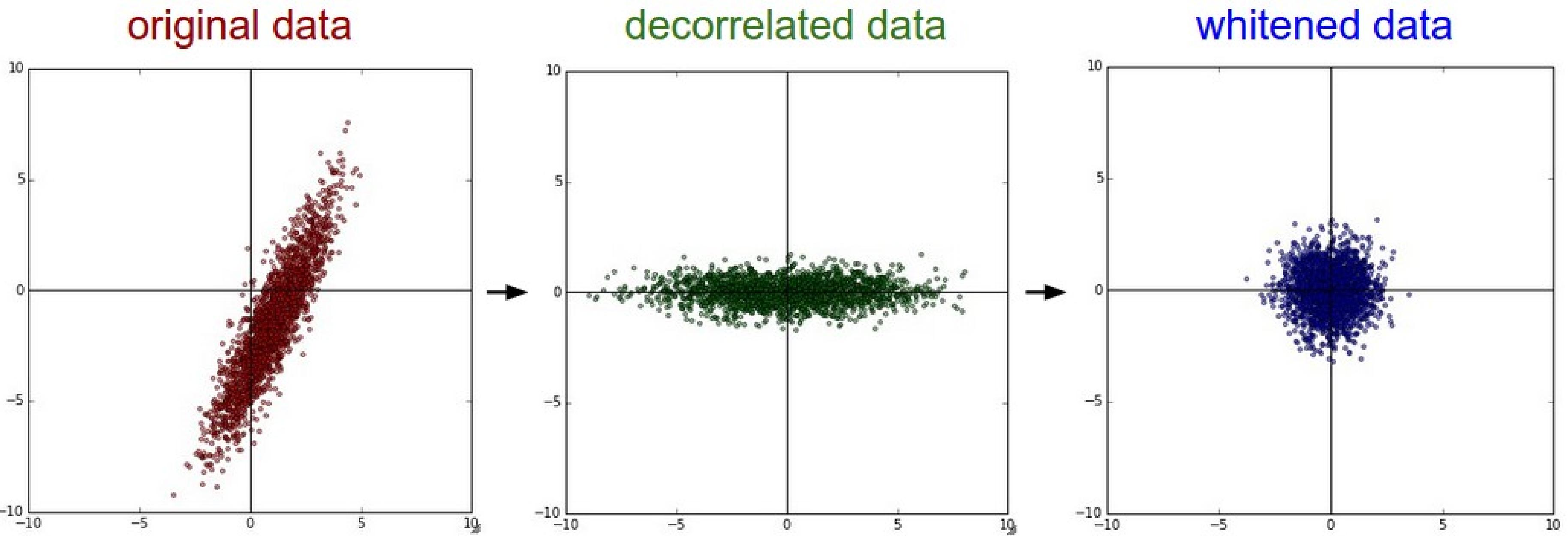
- In practice, the input data  $X$  **must** be normalized before training, in order to improve the training time:
  - **Mean removal or zero-centering:**

$$X' = X - \mathbb{E}(X)$$

- **Normalization** : mean removal + **unit variance**:

$$X' = \frac{X - \mathbb{E}(X)}{\text{Std}(X)}$$

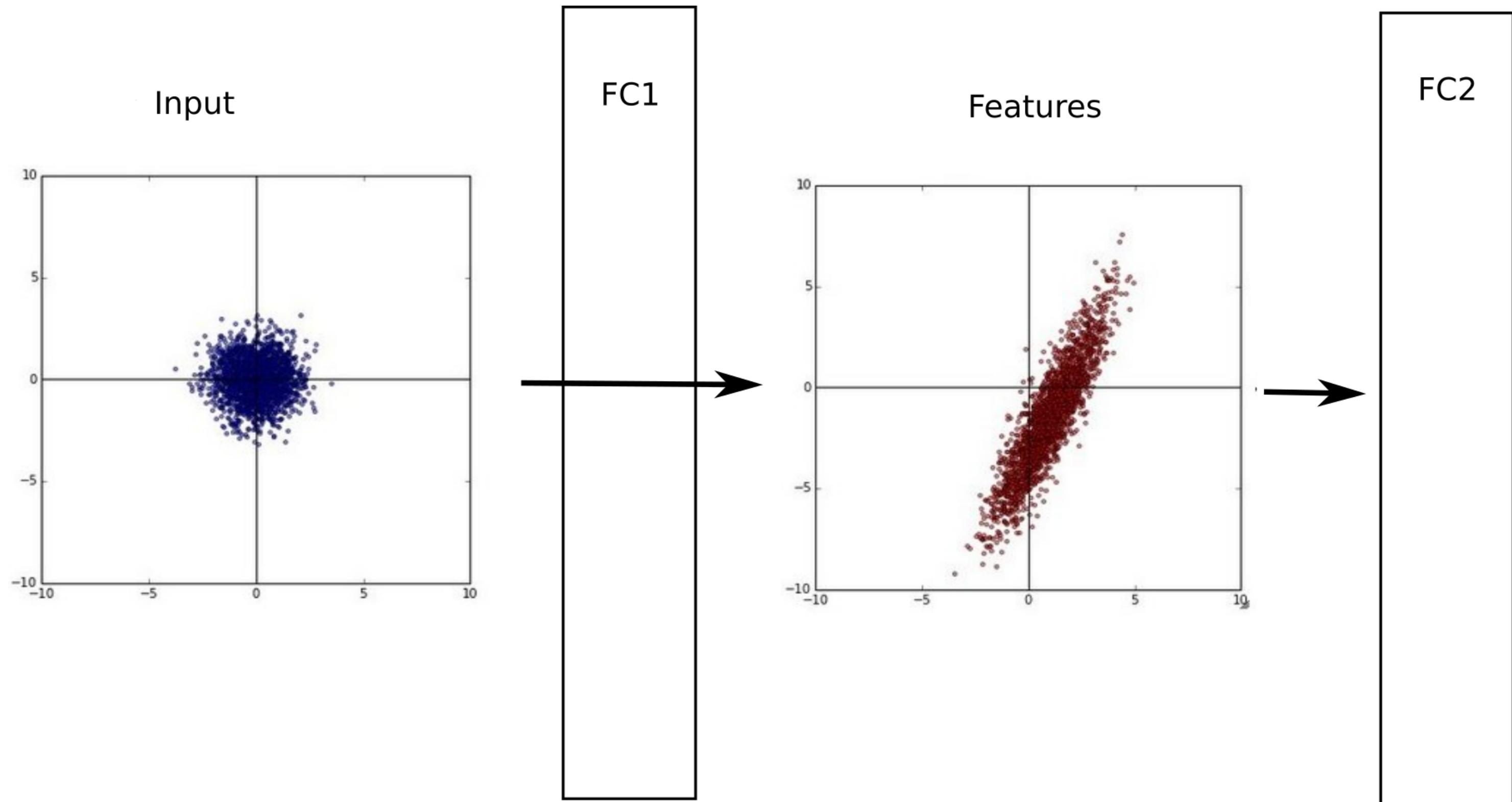
# Data whitening



Source : <http://cs231n.github.io/neural-networks-2/>

- Whitening goes one step further by first decorrelating the input dimensions (using **Principal Component Analysis** - PCA) and then scaling them so that the data lies in the unit sphere.
- Better method than simple data normalization, but computationally expensive.
- When predicting on new data, do not forget to normalize/whiten them too!

# Batch normalization (BN)



- A single layer can learn very fast if its inputs are normalized with zero mean and unit variance.
- This is easy to do for the first layer, as one only need to preprocess the inputs  $\mathbf{x}$ , but not the others.
- The outputs of the first layer are not normalized anymore, so learning in the second layer will be slow.

# Batch normalization (BN)

**Input:** Values of  $x$  over a mini-batch:  $\mathcal{B} = \{x_{1\dots m}\}$ ;

Parameters to be learned:  $\gamma, \beta$

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

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

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

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

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

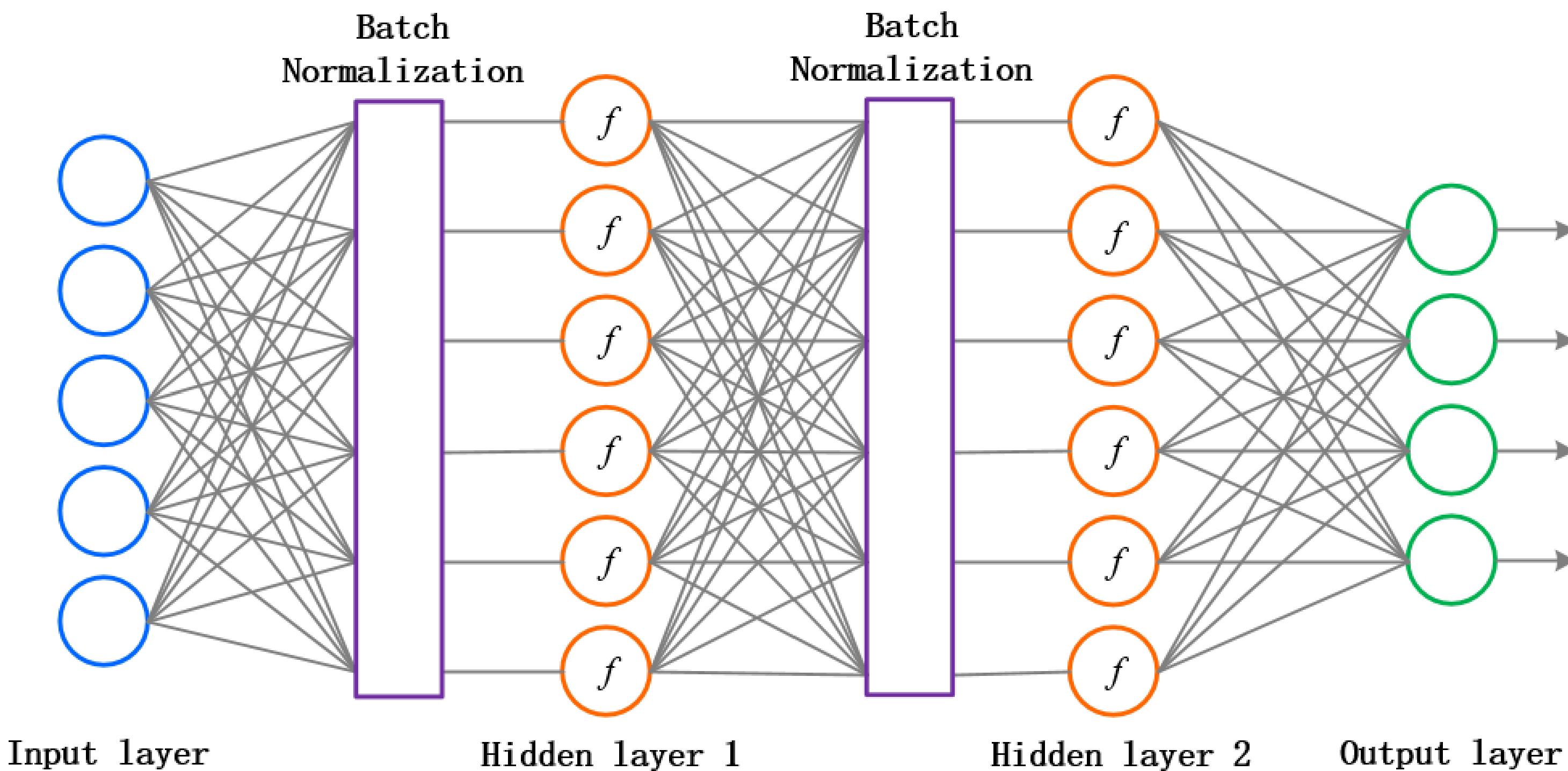
**Algorithm 1:** Batch Normalizing Transform, applied to activation  $x$  over a mini-batch.

- **Batch normalization** allows each layer to normalize its inputs on a **single minibatch**:

$$X'_{\mathcal{B}} = \frac{X_{\mathcal{B}} - E(X_{\mathcal{B}})}{\text{Std}(X_{\mathcal{B}})}$$

- The mean and variance will vary from one minibatch to another, but it does not matter.
- At the end of learning, the mean and variance over the whole training set is computed and stored.
- BN allows to more easily initialize the weights relative to the input strength and to use higher learning rates.

## Batch normalization (BN)



Source : <http://heimingx.cn/2016/08/18/cs231n-neural-networks-part-2-setting-up-the-Data-and-the-loss/>

- The **Batch Normalization** layer is usually placed between the FC layer and the activation function.
- It is differentiable w.r.t the input layer and the parameters, so backpropagation still works.

# Weight initialization

- Weight matrices are initialized randomly, but how they are initialized impacts performance a lot.
- There are empirical rules to initialize the weights between two layers with  $N_{\text{in}}$  and  $N_{\text{out}}$  neurons.
  - **Xavier:** Uniform initialization (when using logistic or tanh, Glorot and Bengio, 2010):

$$W \in \mathcal{U}\left(-\sqrt{\frac{6}{N_{\text{in}} + N_{\text{out}}}}, \sqrt{\frac{6}{N_{\text{in}} + N_{\text{out}}}}\right)$$

- **He:** Gaussian initialization (when using ReLU or PReLU, He et al. 2015):

$$W \in \mathcal{N}(0, \sqrt{\frac{2}{N_{\text{in}}}})$$

- When using BN, the bias  $b$  can be initialized to 0.
- Most frameworks (tensorflow, pytorch) initialize the weights correctly for you, but you can also control it.

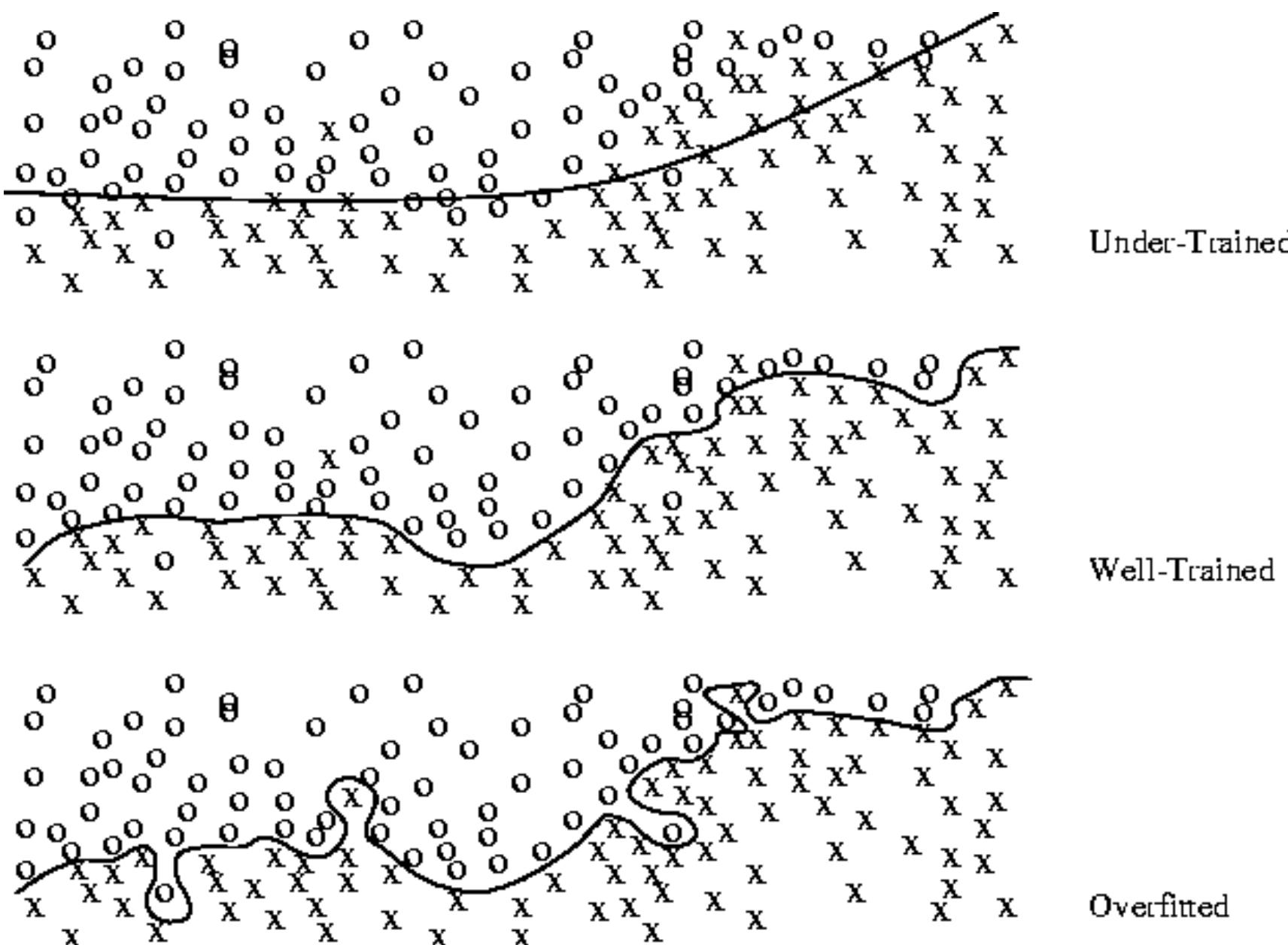
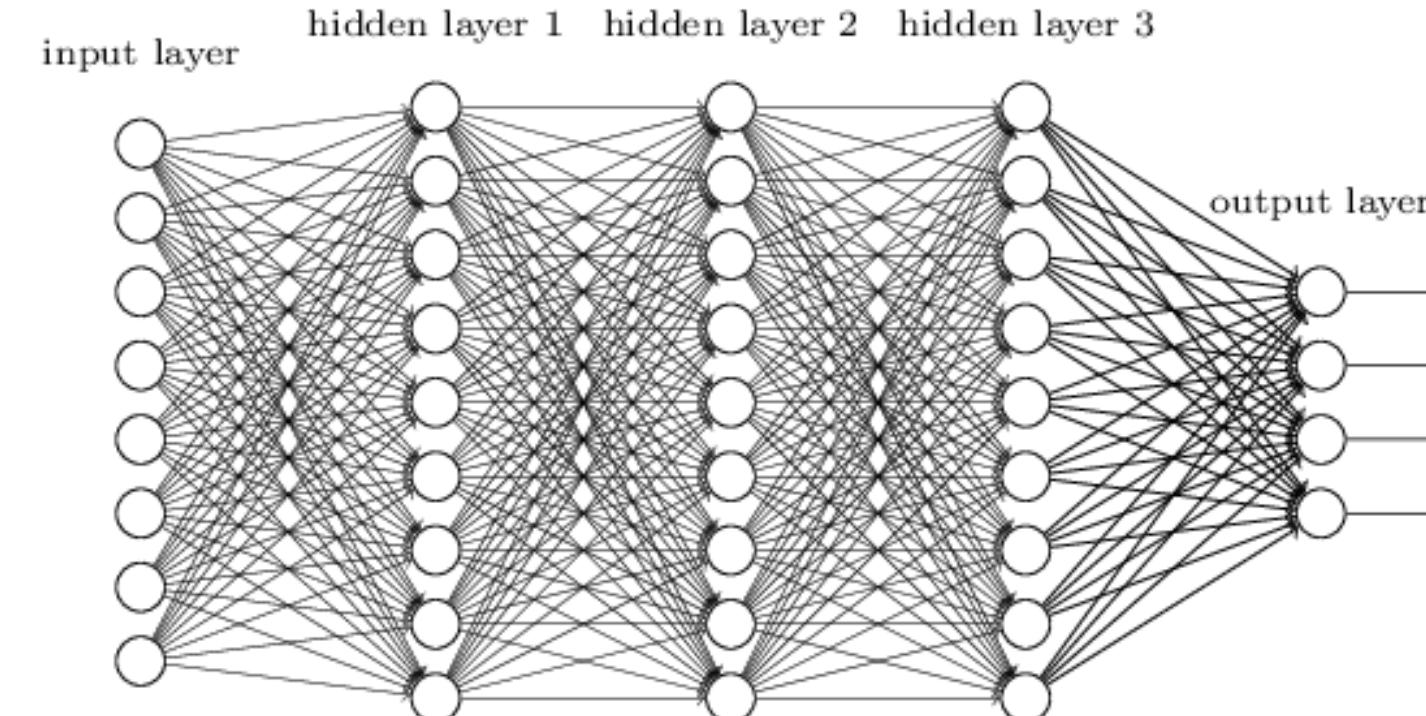
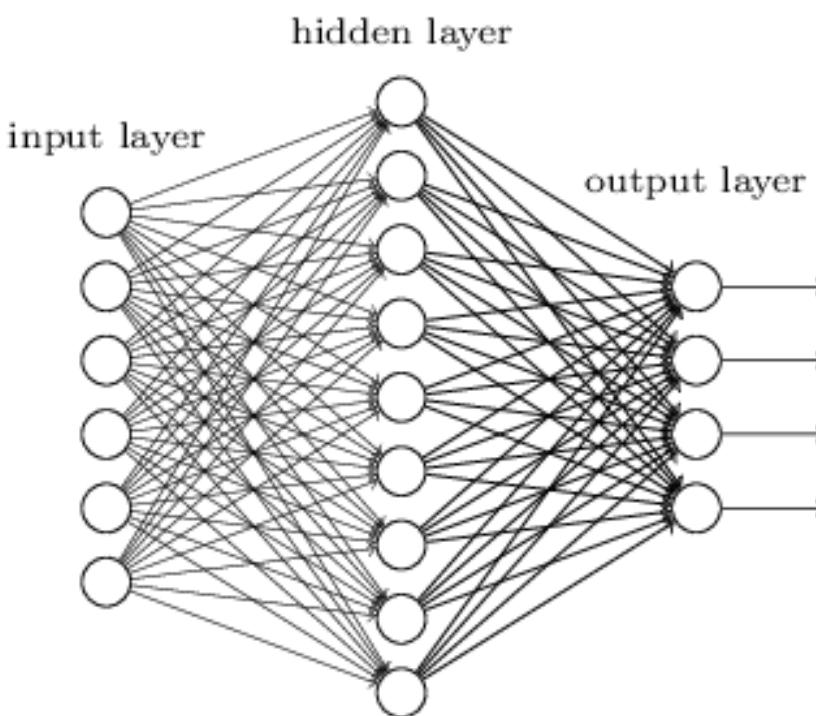
## References

Glorot and Bengio (2010). Understanding the difficulty of training deep feedforward neural networks. AISTATS.

He et al. (2015). Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification. arXiv:1502.01852

## **3 - Overfitting**

# Overfitting : Need for regularization



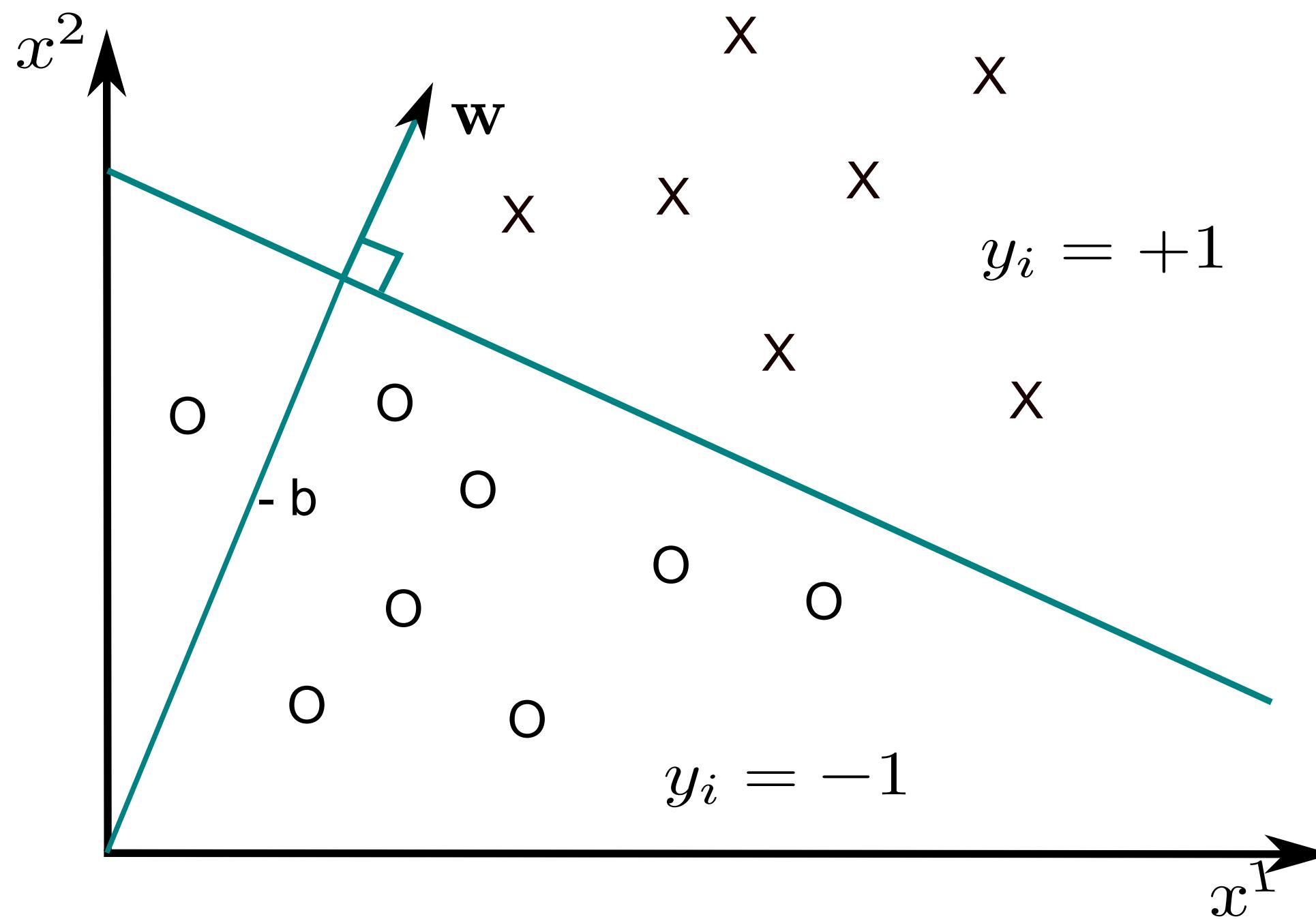
- The main problem with deep NN is **overfitting**.
- With increasing depth, the network has too many weights = free parameters, so its VC dimension is high.

$$\epsilon = \frac{\text{VC}_{\text{dim}}}{N}$$

- The training error will be very small, but the generalization error high.
- **The network learns the data, not the underlying function.**

# Overfitting : Need for regularization

- We need to put constraints on the weights to reduce the VC dimension.
  - If the weights move freely (i.e. can take any value), the VC dimension is equal to the number of free parameters.
  - If the weights cannot take any value they like, this implicitly reduces the VC dimension.
- In linear classification, the weights were unconstrained: the norm of the weight vector can take any value, as only its direction is important.

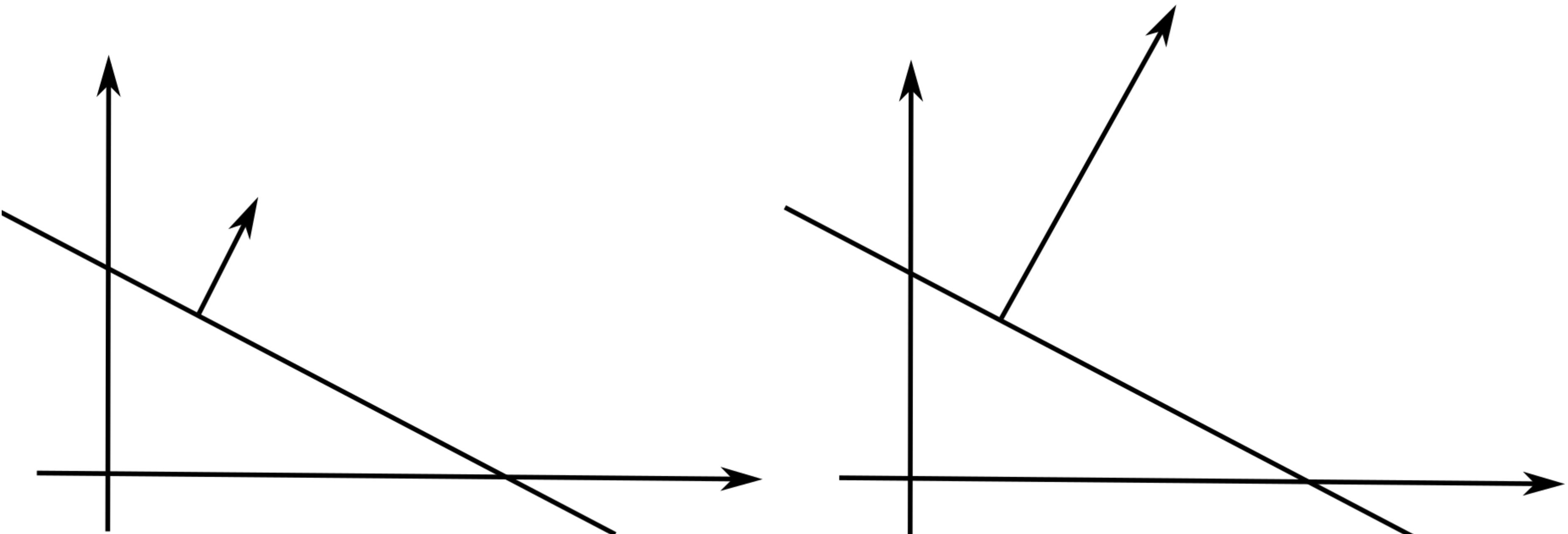


## Overfitting : Need for regularization

- **Intuition:** The norm of the weight vector influences the speed of learning in linear classification.
- A weight update on a strong weight has less influence than on a weak weight:

$$W \leftarrow W + \Delta W = W - \eta \frac{\partial l(\theta)}{\partial W}$$

as the gradient  $\frac{\partial l(\theta)}{\partial W}$  does not depend on the norm of the weights, only the output error.

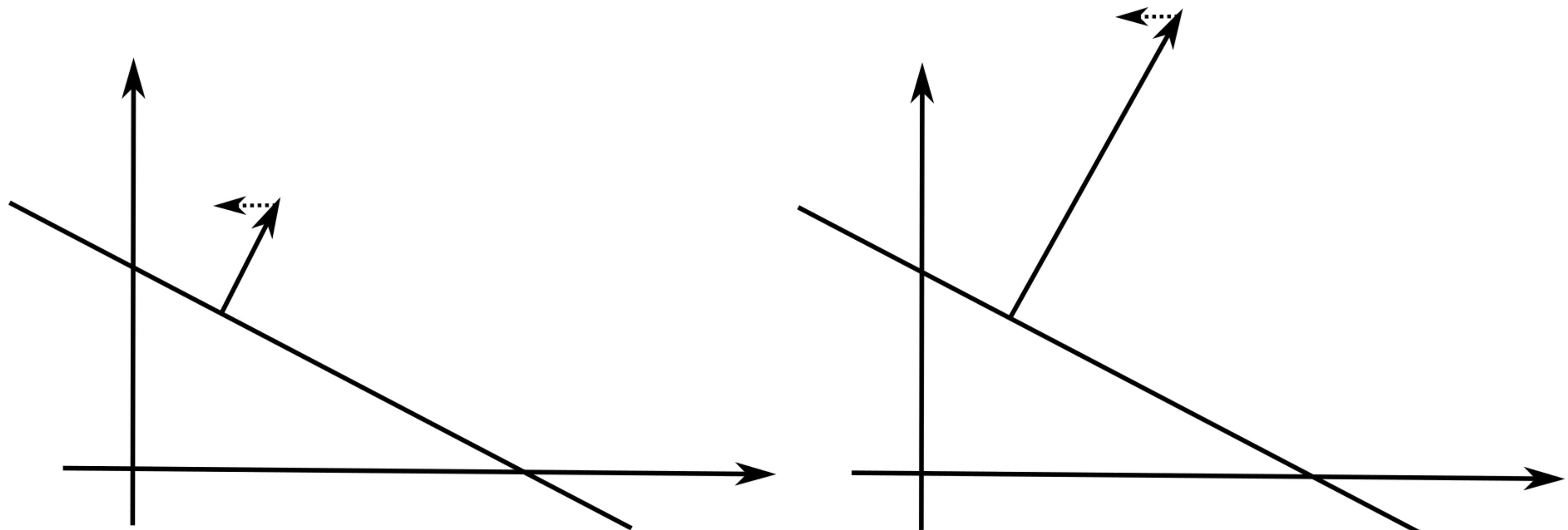


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$$W \leftarrow W + \Delta W = W - \eta \frac{\partial l(\theta)}{\partial W}$$

as the gradient  $\frac{\partial l(\theta)}{\partial W}$  does not depend on the norm of the weights, only the output error.

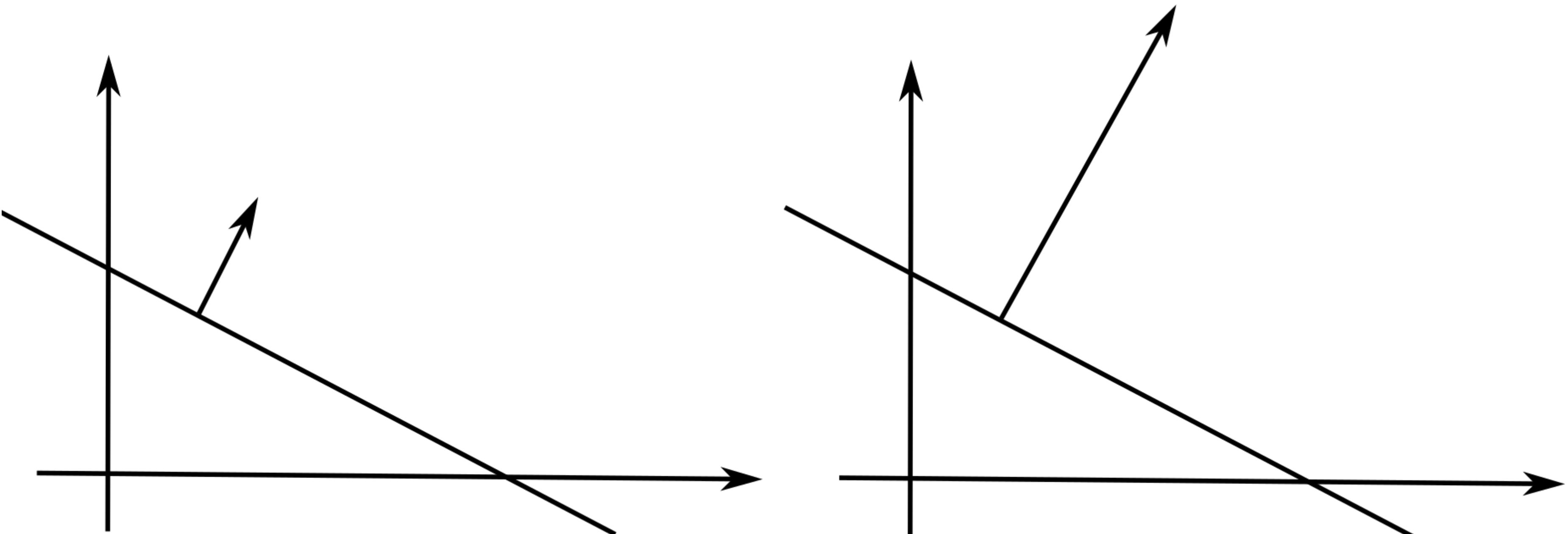


## Overfitting : Need for regularization

- **Intuition:** The norm of the weight vector influences the speed of learning in linear classification.
- A weight update on a strong weight has less influence than on a weak weight:

$$W \leftarrow W + \Delta W = W - \eta \frac{\partial l(\theta)}{\partial W}$$

as the gradient  $\frac{\partial l(\theta)}{\partial W}$  does not depend much on the norm of the weights, only the output error.



## L2 Regularization

- **L2 regularization** keeps the  $\mathcal{L}_2$  norm of the free parameters  $||\theta||$  as small as possible during learning.

$$||\theta||^2 = w_1^2 + w_2^2 + \cdots + w_M^2$$

- Each neuron will use all its inputs with small weights, instead of specializing on a small part with high weights.
- Two things have to be minimized at the same time: the training loss and a **penalty term** representing the norm of the weights:

$$\mathcal{L}(\theta) = \mathbb{E}_{\mathcal{D}}(||\mathbf{t} - \mathbf{y}||^2) + \lambda ||\theta||^2$$

- The **regularization parameter**  $\lambda$  controls the strength of regularization:
  - if  $\lambda$  is small, there is only a small regularization, the weights can increase.
  - if  $\lambda$  is high, the weights will be kept very small, but they may not minimize the training loss.

## L2 Regularization

- MSE loss with L2 regularization penalty term:

$$\mathcal{L}(\theta) = \mathbb{E}_{\mathcal{D}}[||\mathbf{t} - \mathbf{y}||^2] + \lambda ||\theta||^2$$

- The gradient of the new loss function is easy to find:

$$\nabla_{\theta} \mathcal{L}(\theta) = -2 (\mathbf{t} - \mathbf{y}) \nabla_{\theta} \mathbf{y} + 2 \lambda \theta$$

- Weight updates become:

$$\Delta \theta = \eta (\mathbf{t} - \mathbf{y}) \nabla_{\theta} \mathbf{y} - \eta \lambda \theta$$

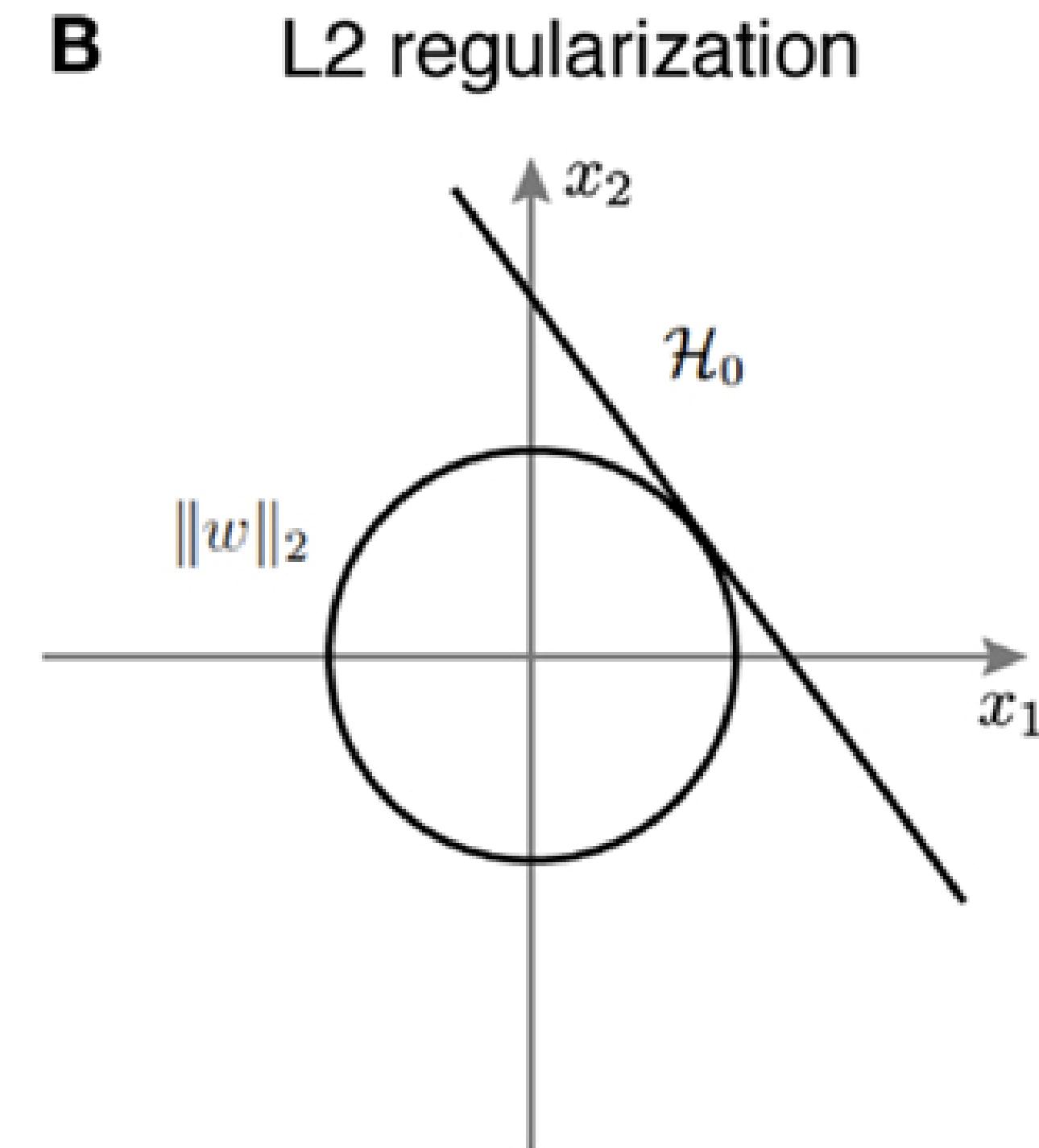
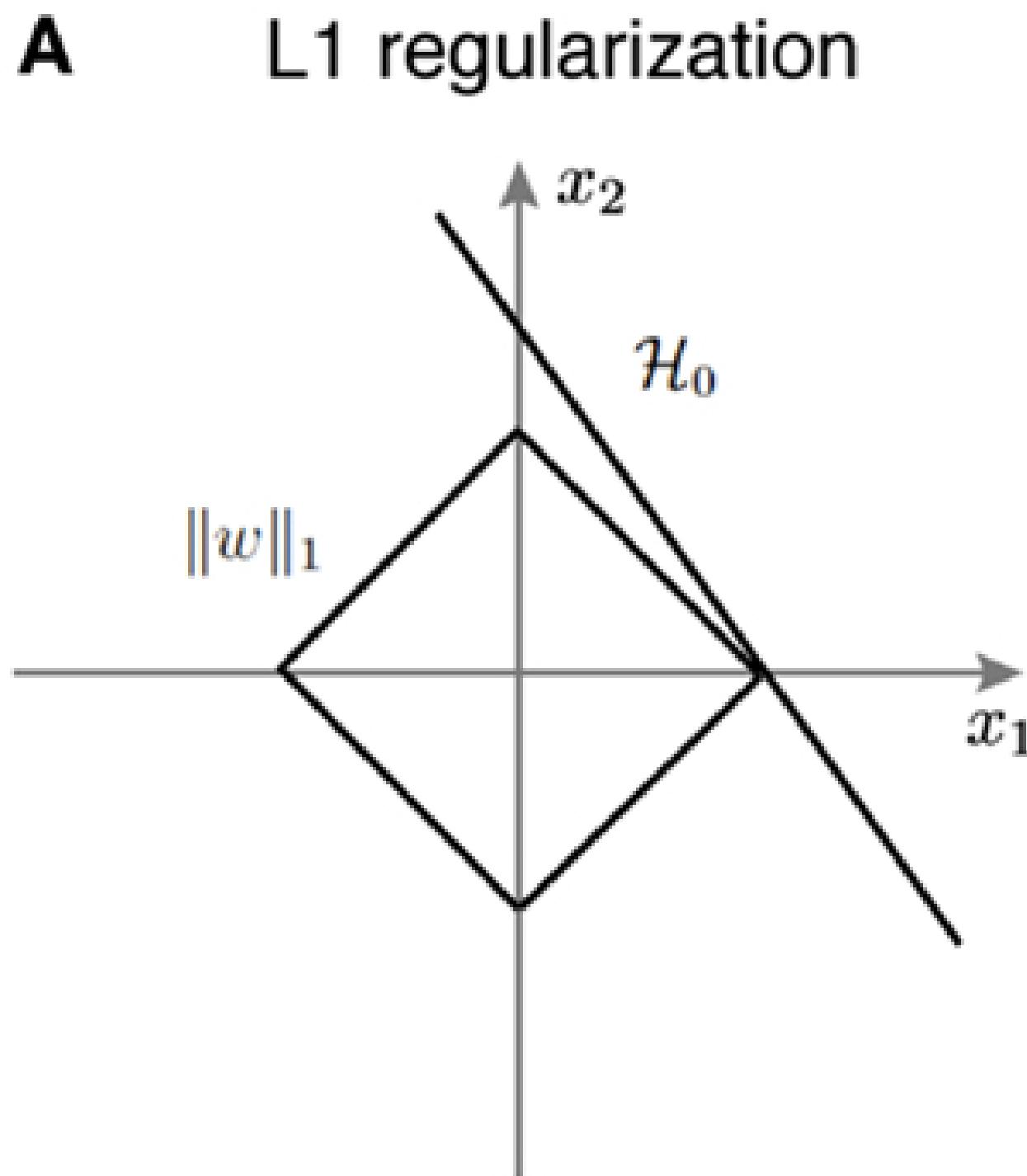
- L2 regularization leads to **weight decay**: even if there is no output error, the weight will converge to 0.
- This forces the weight to constantly learn: it can not specialize on a particular example anymore (overfitting) and is forced to generalize.

# L1 Regularization

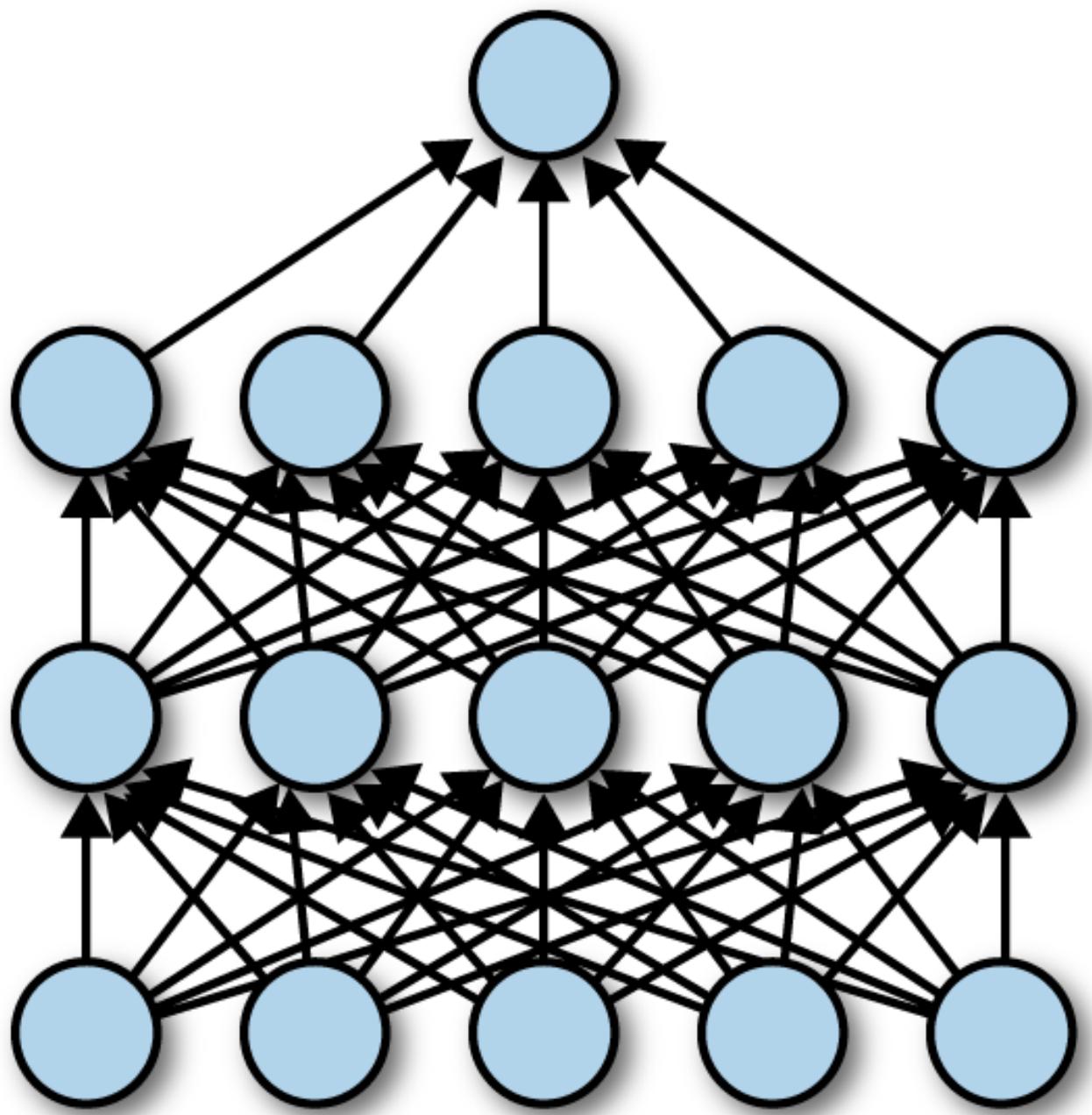
- **L1 regularization** penalizes the absolute value of the weights instead of their Euclidian norm:

$$\mathcal{L}(\theta) = \mathbb{E}_{\mathcal{D}}[||\mathbf{t} - \mathbf{y}||^2] + \lambda |\theta|$$

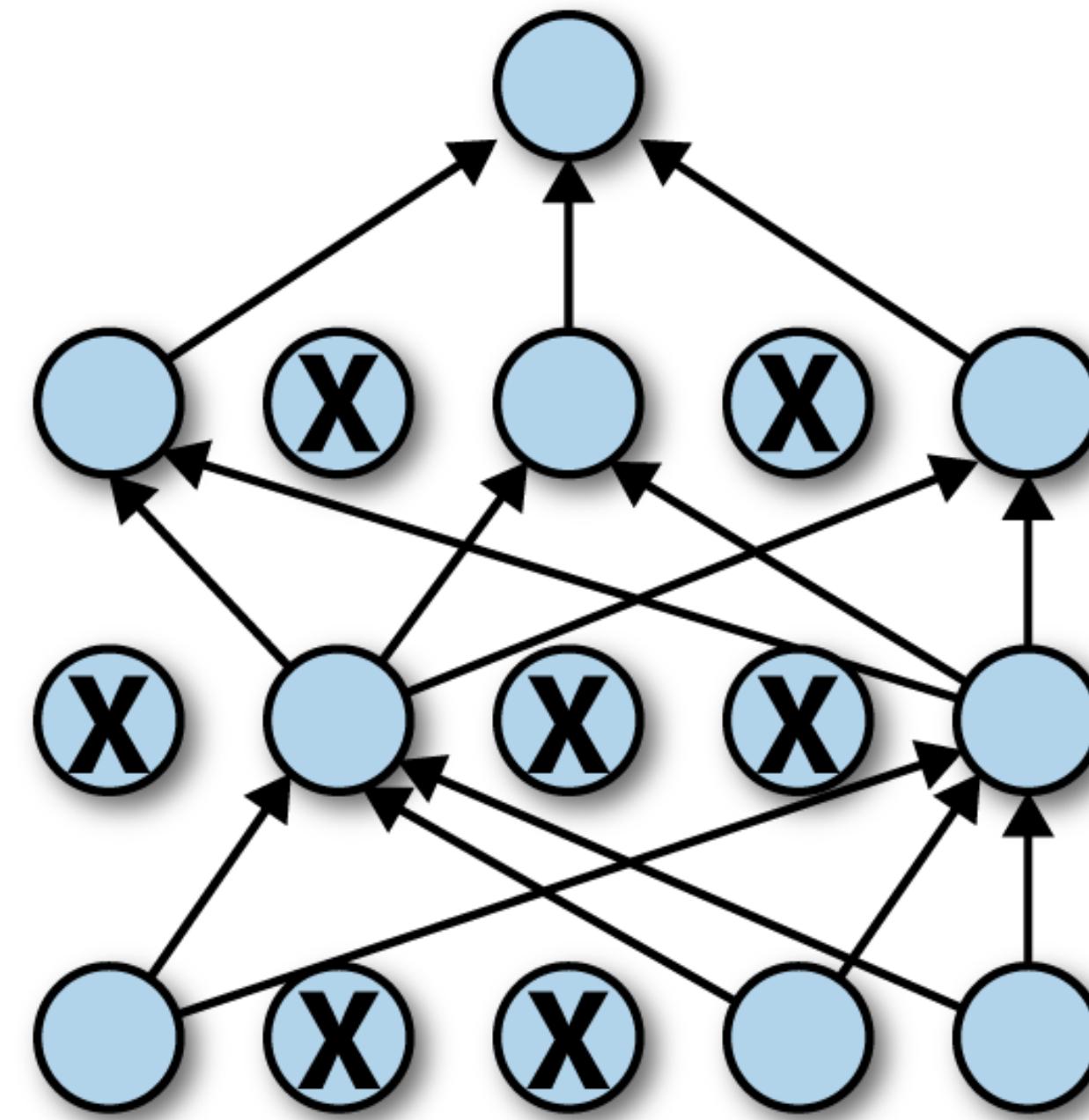
- It leads to very sparse representations: a lot of neurons will be inactive, and only a few will represent the input.



# Dropout



(a) Standard Neural Net

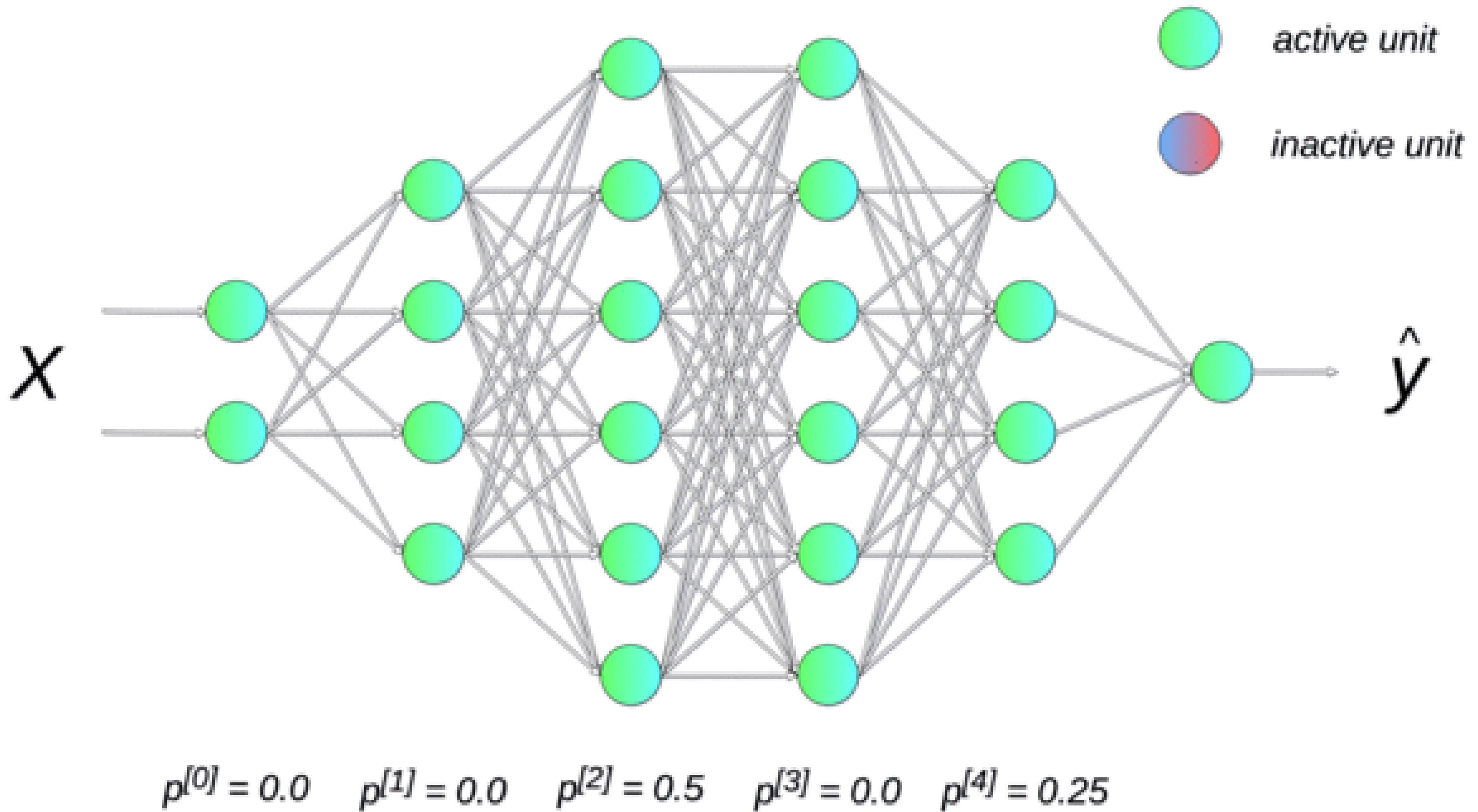


(b) After applying dropout

- Randomly dropping (inactivating) some neurons with a **probability  $p$**  between two input presentations reduces the number of free parameters available for each learning phase.
- Multiple smaller networks (smaller VC dimension) are in fact learned in parallel on different data, but they share some parameters.
- This method forces the network to generalize. It is a form of regularization (mathematically equivalent to L2), now preferred in deep networks.  $p$  is usually around 0.5.

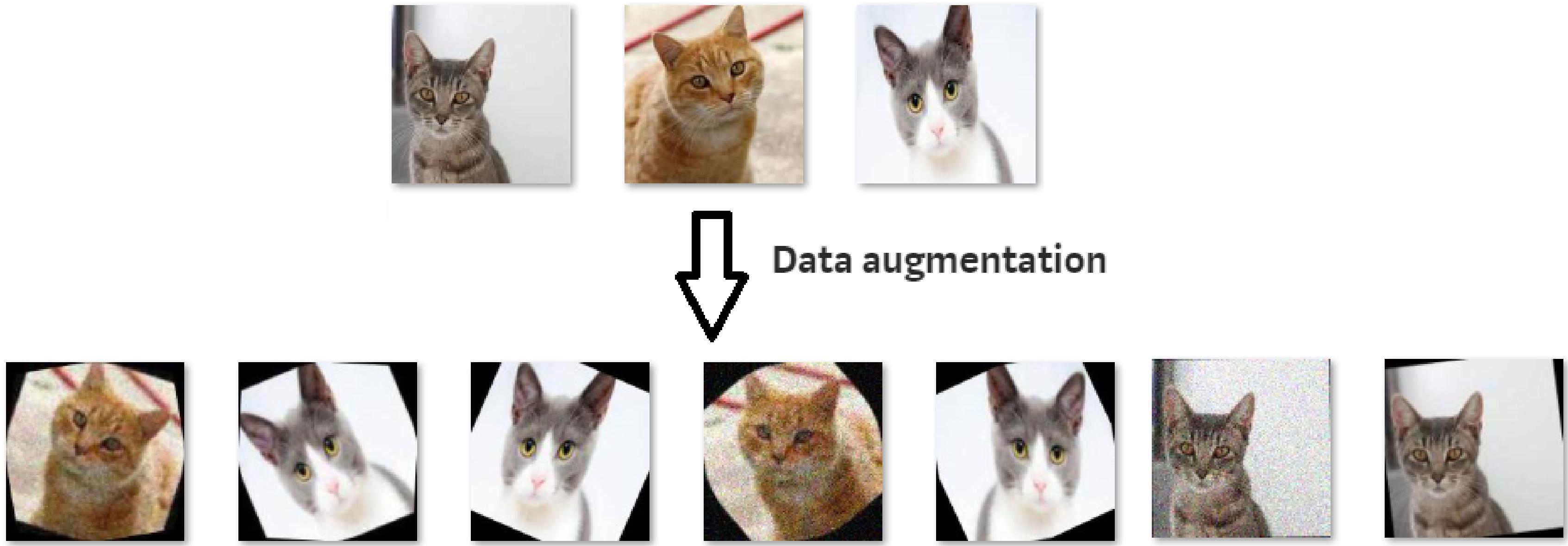
# Dropout

- Each new input  $\mathbf{x}$  (or minibatch of inputs) is learned by a different neural network.
- But **on average**, the big neural network has learned the whole dataset without overfitting.



Source: <https://towardsdatascience.com/preventing-deep-neural-network-from-overfitting-953458db800a>

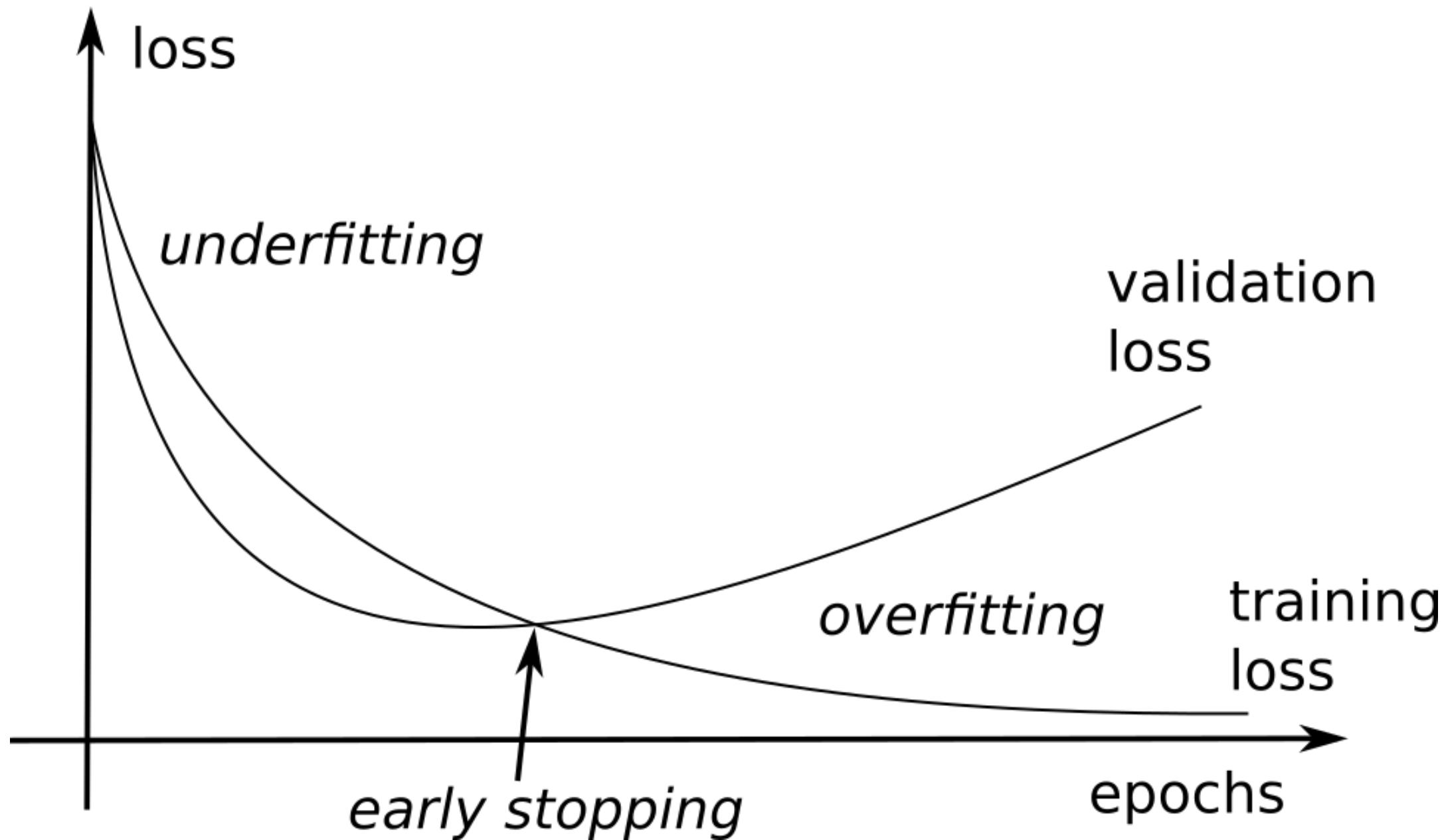
# Data augmentation



Source : <https://blog.keras.io/building-powerful-image-classification-models-using-very-little-data.html>

- The best way to avoid overfitting is to use more data (with variability), but this is not always possible.
- A simple trick to have more data is **data augmentation**, i.e. modifying the inputs while keeping the output constant.
- For object recognition, it consists of applying various affine transformations (translation, rotation, scaling) on each input image, while keeping the label constant.
- Allows virtually infinite training sets.

# Validation set and Early-Stopping

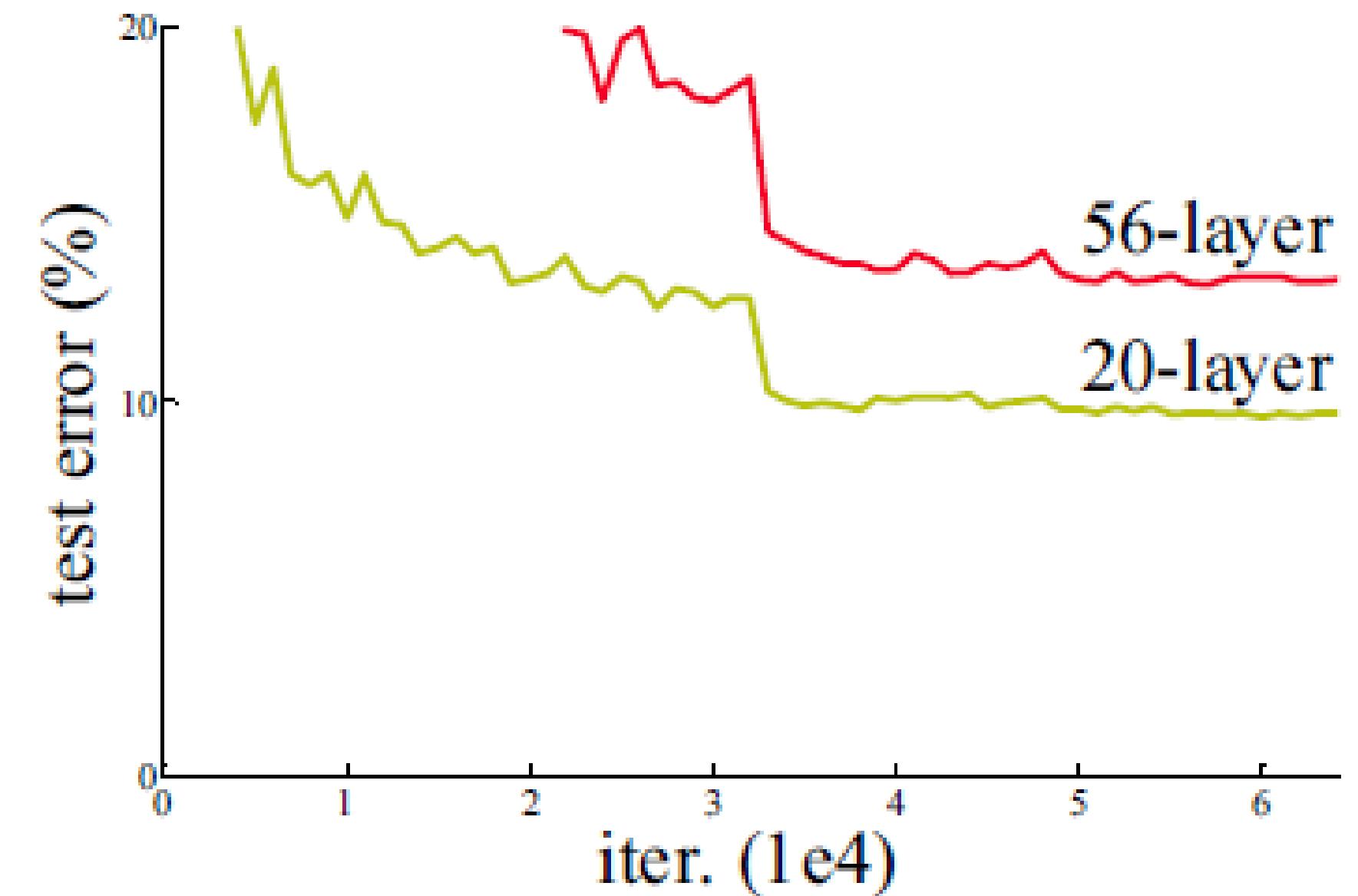
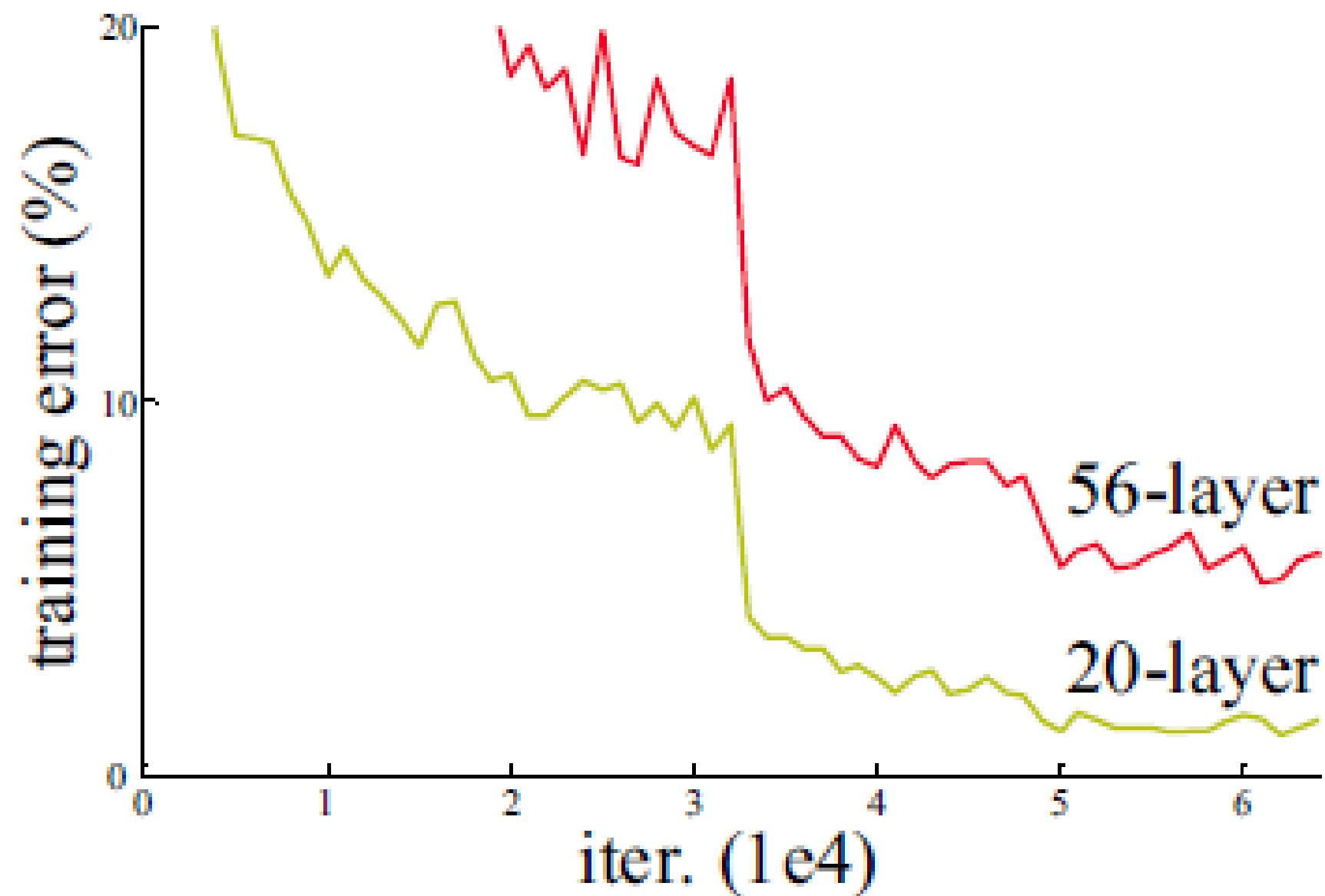


- Early-stopping fights overfitting by monitoring the model's performance on a validation set.
- A **validation set** is a set of examples that we never use for gradient descent, but which is also not a part of the test set.
- If the model's performance ceases to improve sufficiently on the validation set, or even degrades with further optimization, we can either stop learning or modify some meta-parameters (learning rate, momentum, regularization...).
- The validation loss is usually lower than the training loss at the beginning of learning (underfitting), but becomes higher when the network overfits.

## 4 - Vanishing gradient

# Vanishing Gradient problem

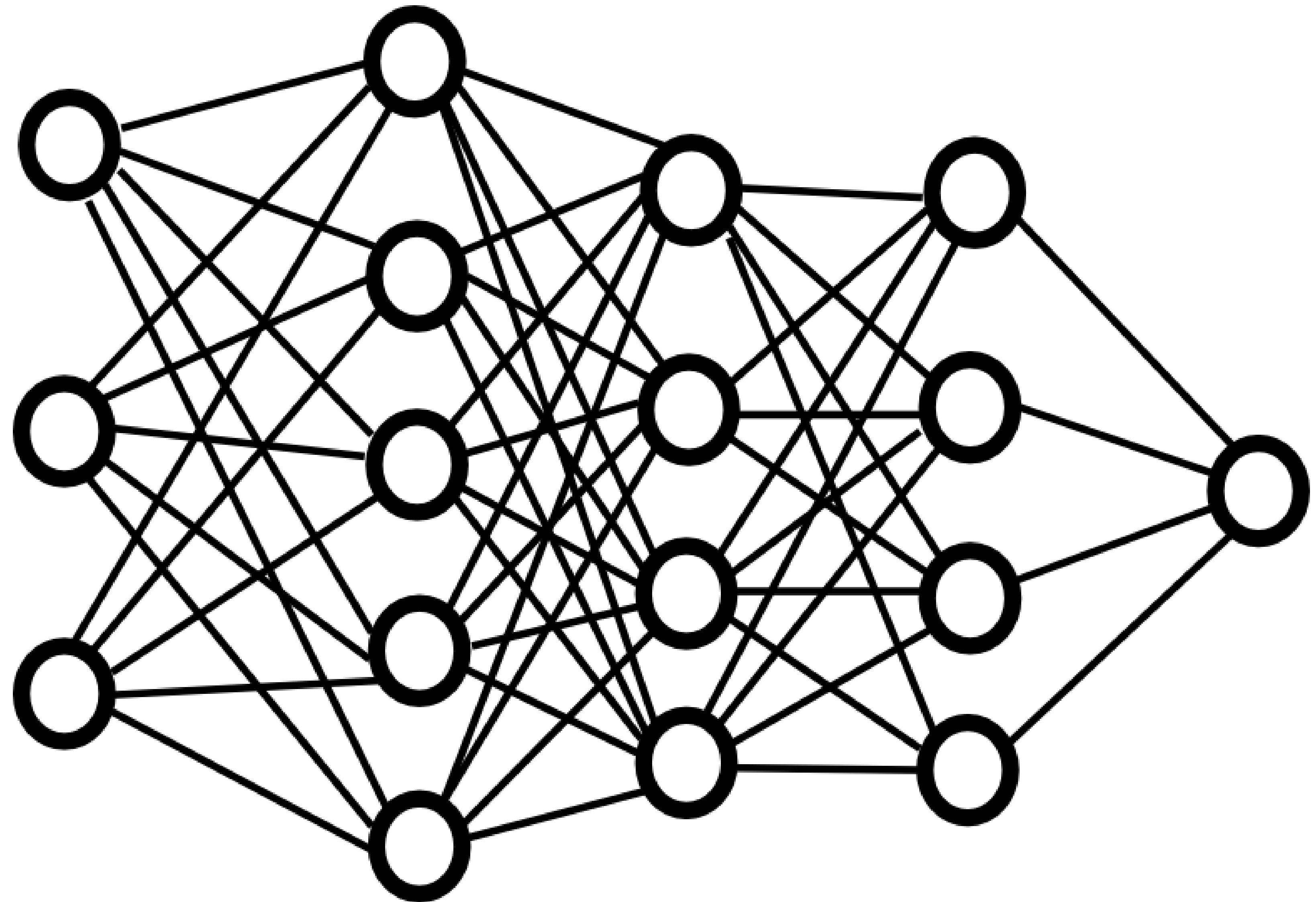
- Contrary to what we could think, adding more layers to a DNN does not necessarily lead to a better performance, both on the training and test set.
- Here is the performance of neural networks with 20 or 56 layers on **CIFAR-10**:



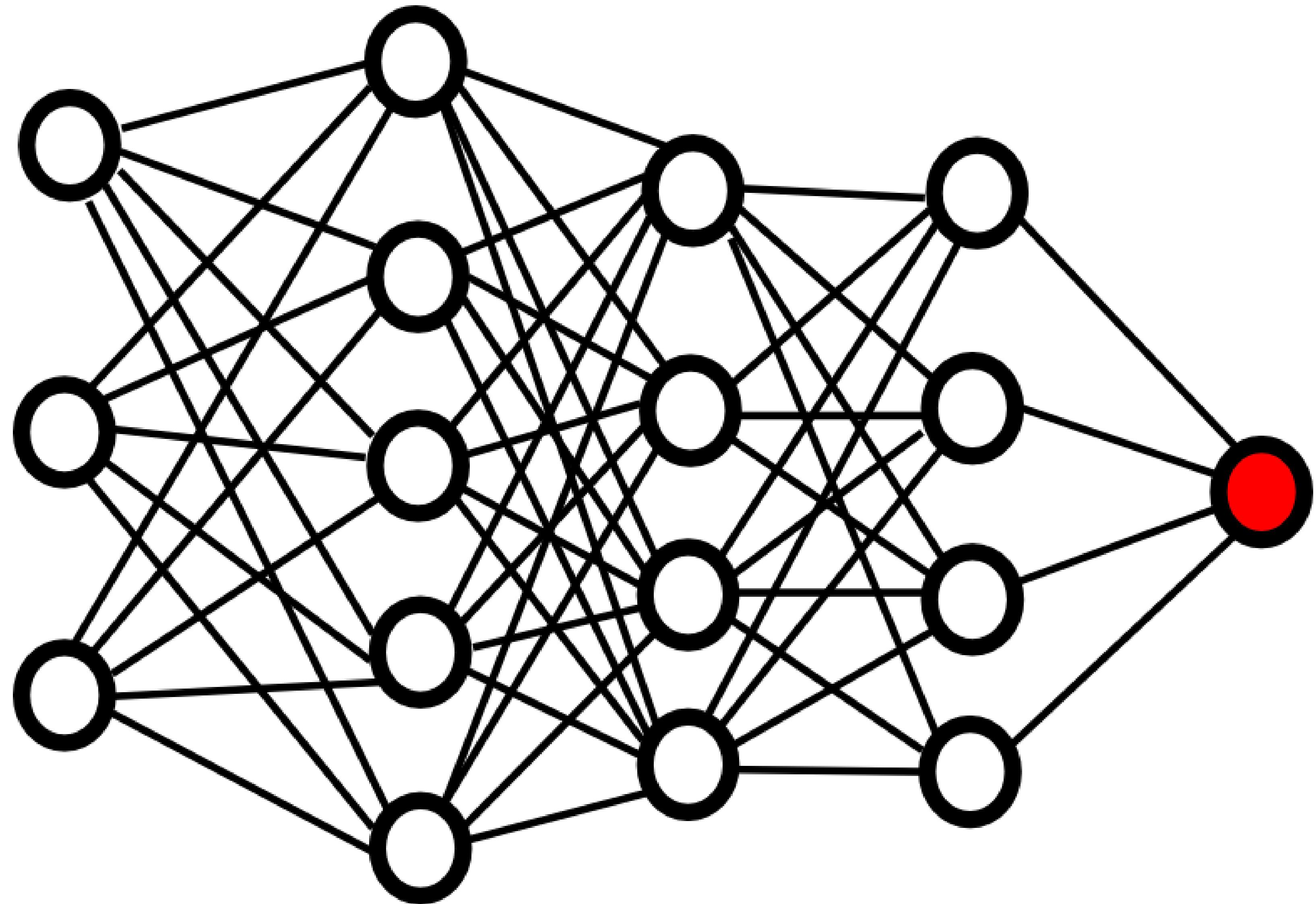
Source: <https://towardsdatascience.com/review-resnet-winner-of-ilsvrc-2015-image-classification-localization-detection-e39402bfa5d8>

- The main reason behind this is the **vanishing gradient problem**.

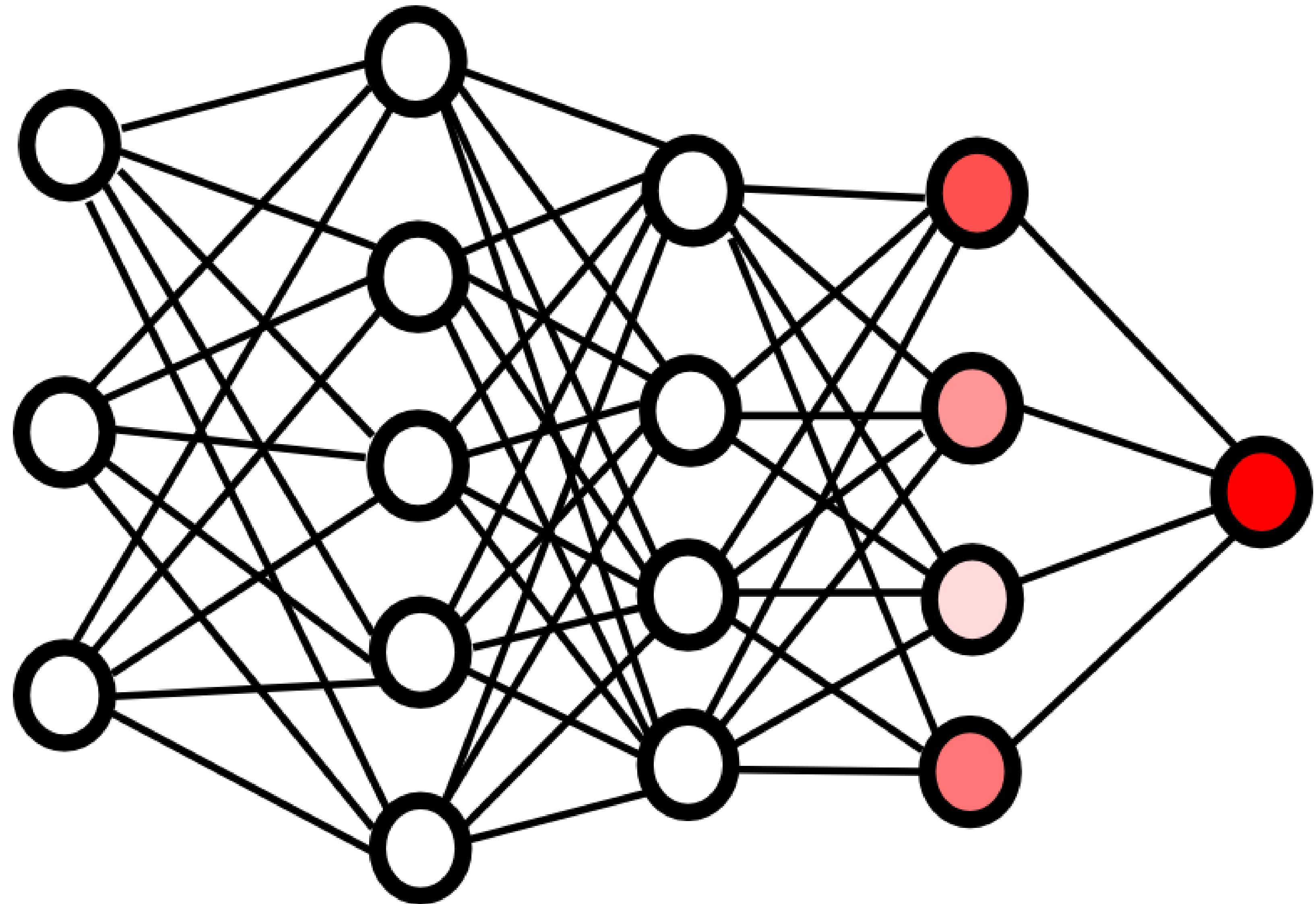
## Vanishing Gradient problem



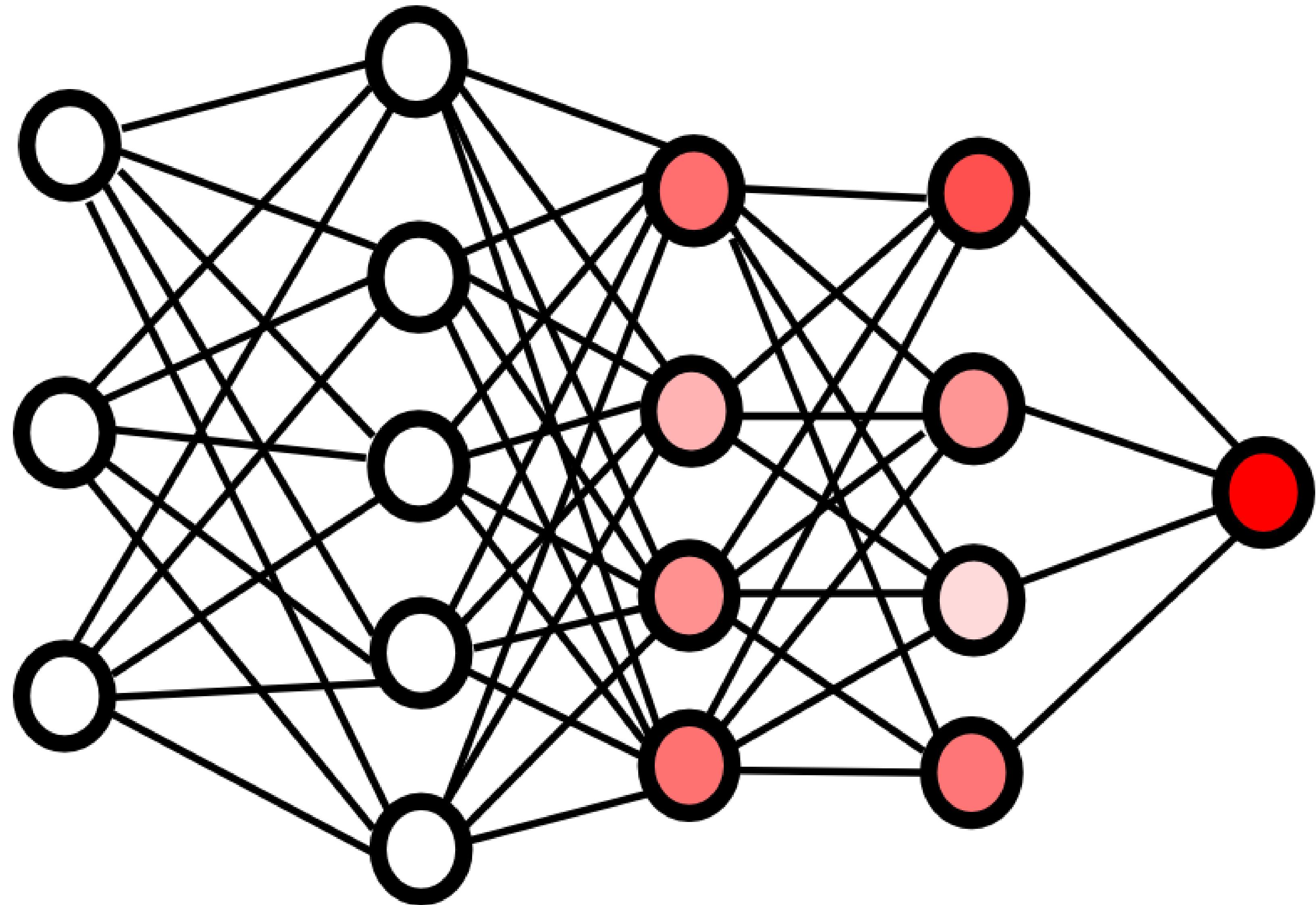
## Vanishing Gradient problem



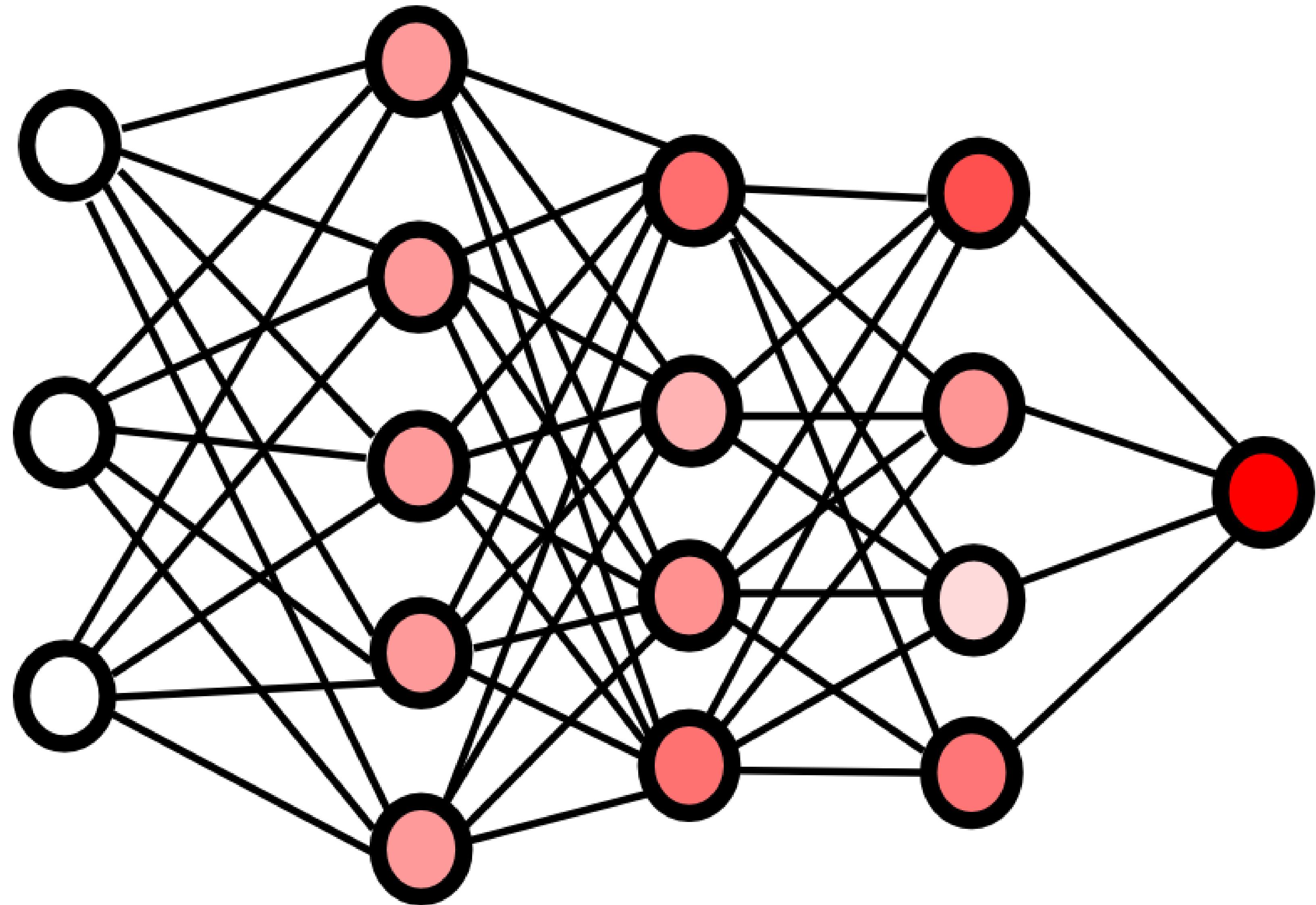
## Vanishing Gradient problem



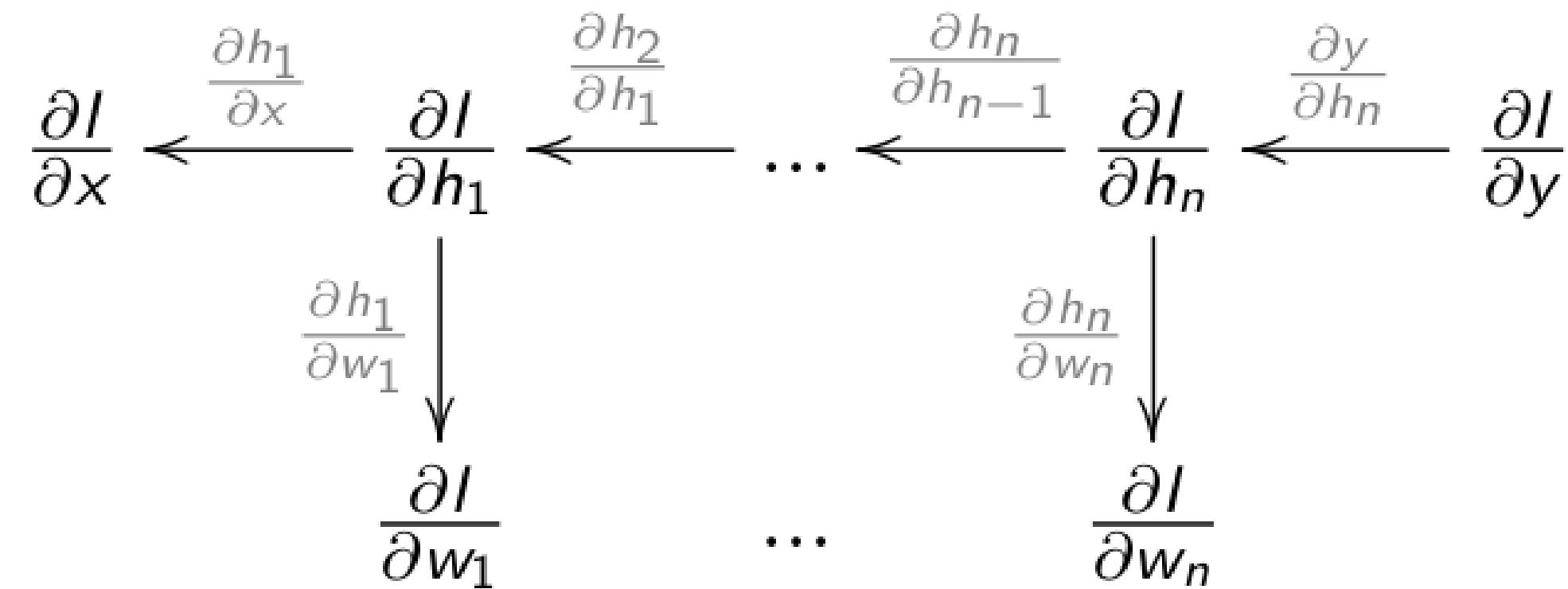
## Vanishing Gradient problem



## Vanishing Gradient problem



# Vanishing Gradient problem



- The gradient of the loss function is repeatedly multiplied by a weight matrix  $W$  as it travels backwards in a deep network.

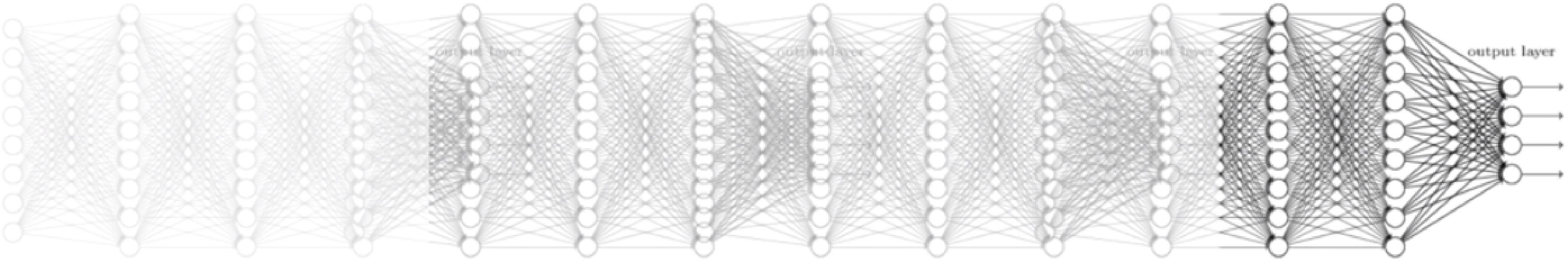
$$\frac{\partial \mathbf{h}_k}{\partial \mathbf{h}_{k-1}} = f'(W^k \mathbf{h}_{k-1} + \mathbf{b}^k) W^k$$

- When it arrives in the first FC layer, the contribution of the weight matrices is comprised between:

$$(W_{\min})^d \quad \text{and} \quad (W_{\max})^d$$

where  $W_{\max}$  (resp.  $W_{\min}$ ) is the weight matrix with the highest (resp. lowest) norm, and  $d$  is the depth of the network.

# Vanishing Gradient problem



Source: <https://smartstuartkim.wordpress.com/2019/02/09/vanishing-gradient-problem/>

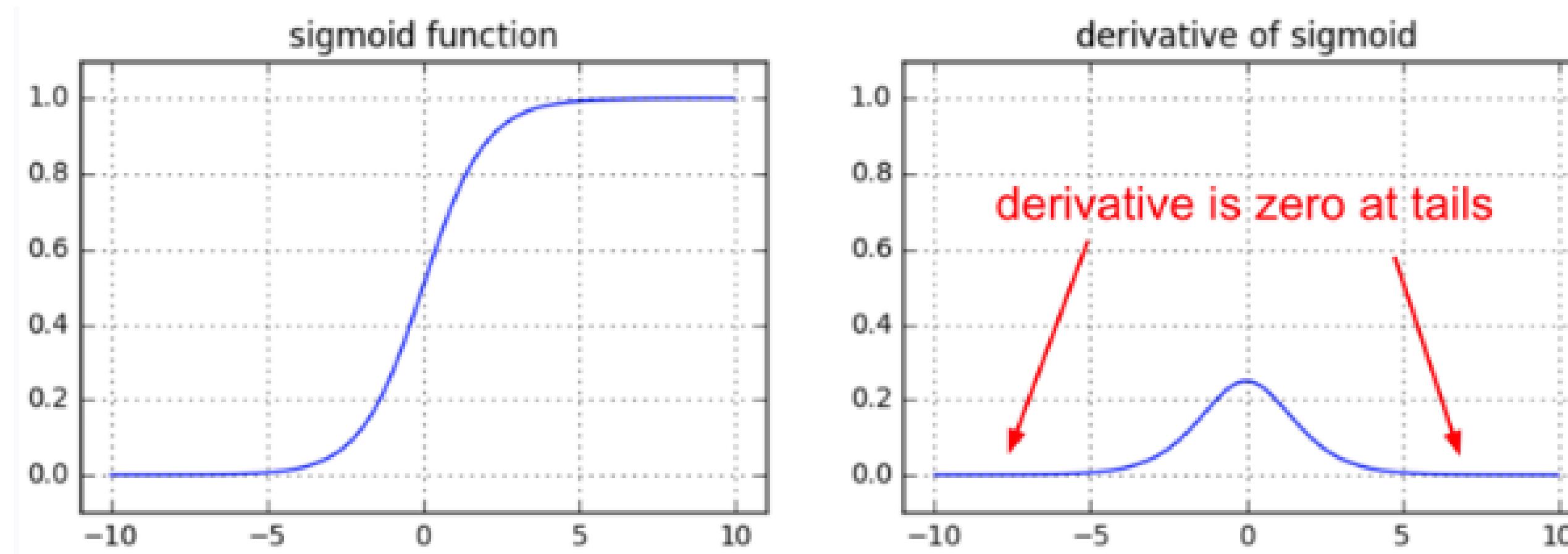
- If  $|W_{\max}| < 1$ , then  $(W_{\max})^d$  is very small for high values of  $d$  : **the gradient vanishes**.
- If  $|W_{\min}| > 1$ , then  $(W_{\min})^d$  is very high for high values of  $d$  : **the gradient explodes**.
- **Exploding gradients** can be solved by **gradient clipping**, i.e. normalizing the backpropagated gradient if its norm exceeds a threshold (only its direction actually matters).

$$\left\| \frac{\partial \mathcal{L}(\theta)}{\partial W^k} \right\| \leftarrow \min\left(\left\| \frac{\partial \mathcal{L}(\theta)}{\partial W^k} \right\|, K\right)$$

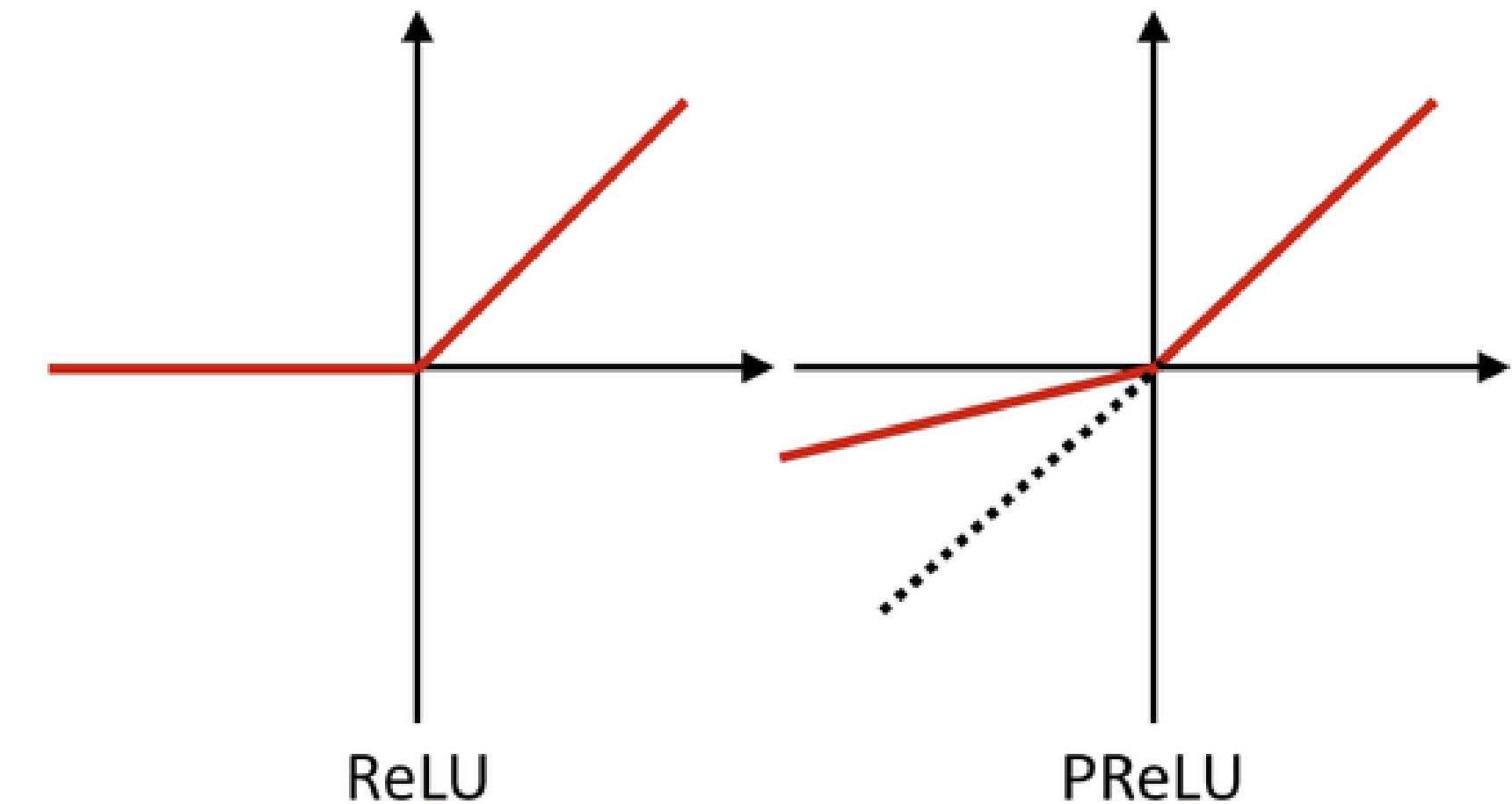
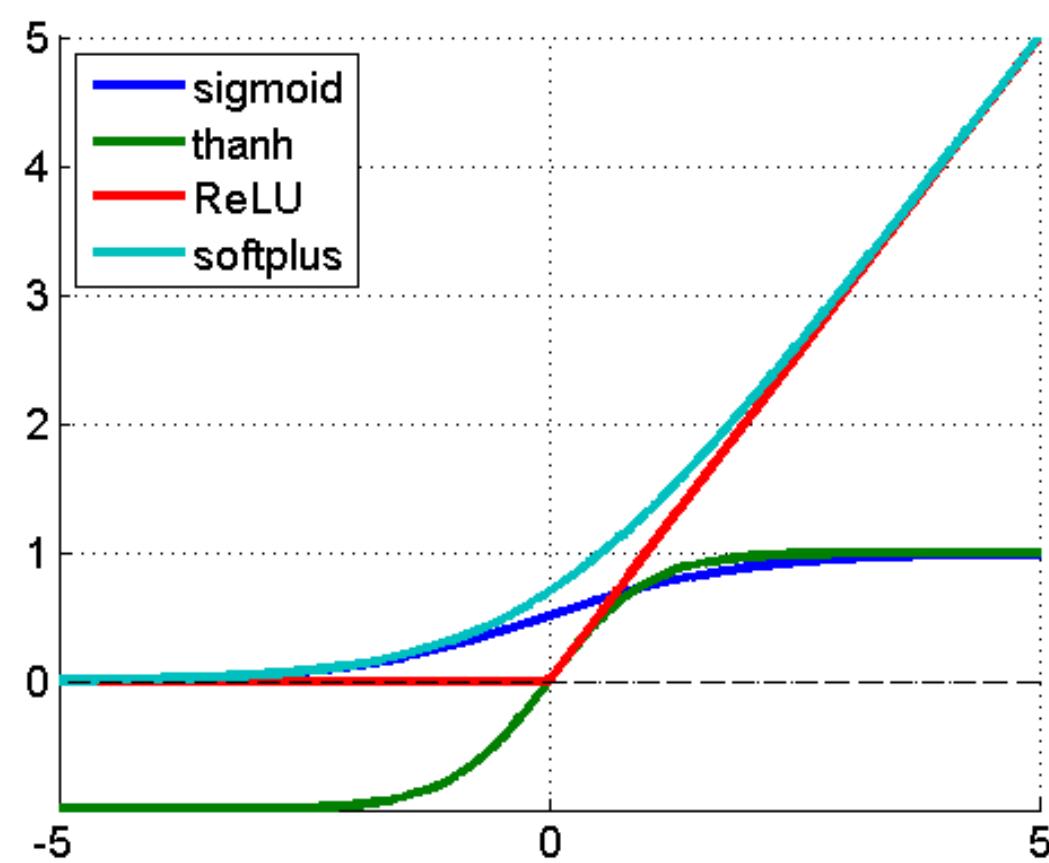
- **Vanishing gradients** are still the current limitation of deep networks.
- Solutions: ReLU, batch normalization + weight initialization, unsupervised pre-training, **residual networks**...

# Derivative of the activation function

- Old-school MLP used logistic or tanh transfer functions for the hidden neurons, but their gradient is zero for very high or low net activations.
- If a neuron is saturated, it won't transmit the gradient backwards, so the vanishing gradient is even worse.



# Choice of the activation function



- Deep networks now typically use the ReLU or PReLU activation functions to improve convergence.

$$f'(x) = \begin{cases} 1 & \text{if } x > 0 \\ \alpha & \text{if } x \leq 0 \end{cases}$$

- PReLU always backpropagates the gradient, so it helps fighting against vanishing gradient.

## **5 - Deep neural networks in practice**

# Deep NN in keras

```
from tf.keras.models import Sequential
from tf.keras.layers import Input, Dense, Dropout, Activation, BatchNormalization
from tf.keras.optimizers import Adam

model = Sequential()

model.add(Input(784))

model.add(Dense(200))
model.add(BatchNormalization())
model.add(Activation('relu'))
model.add(Dropout(0.5))

model.add(Dense(100))
model.add(BatchNormalization())
model.add(Activation('relu'))
model.add(Dropout(0.5))

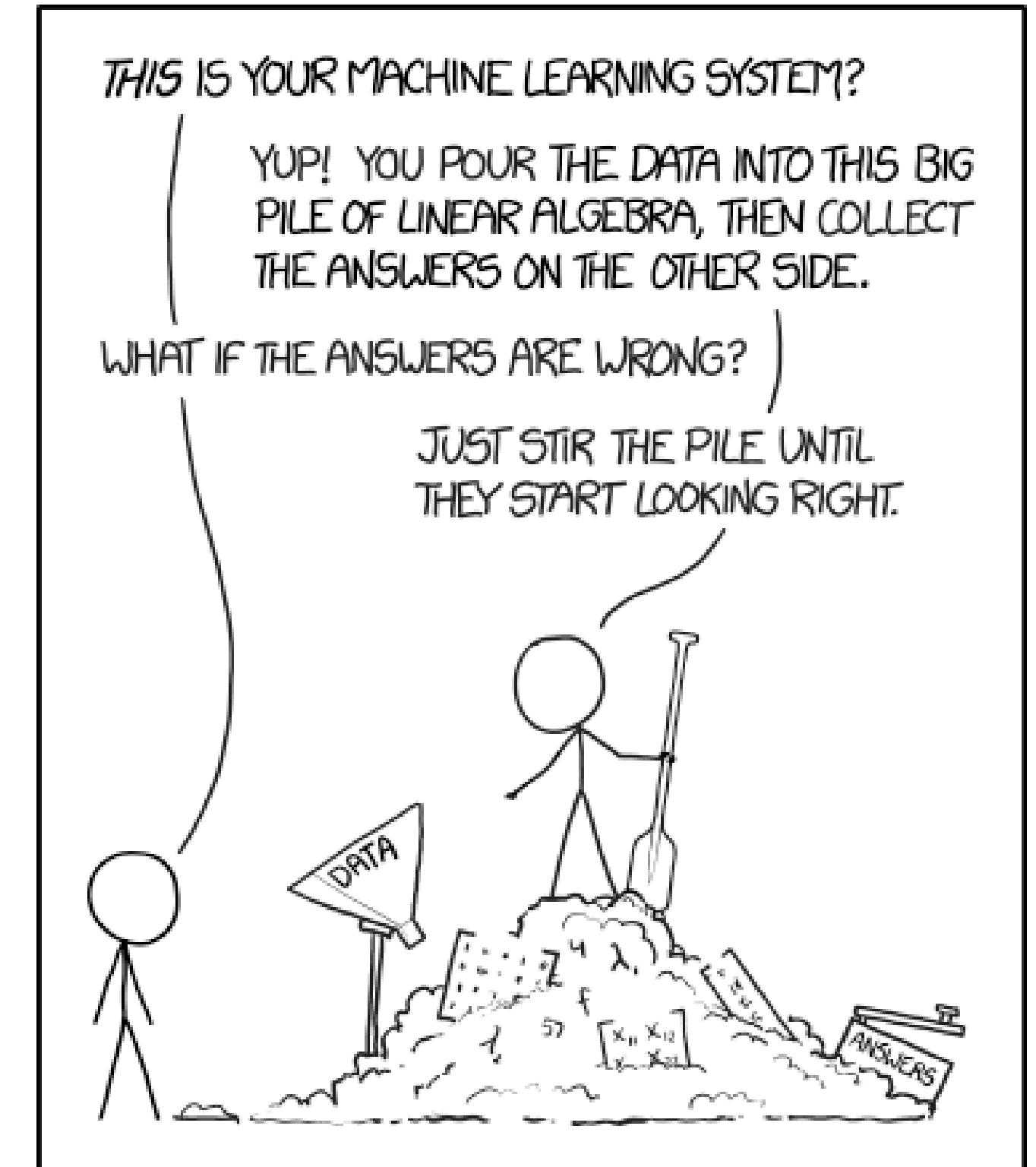
model.add(Dense(units=10, activation='softmax'))

model.compile(loss='categorical_crossentropy', optimizer=Adam(lr=0.01, decay=1e-6))
```

# Take-home messages

If you want to successfully train a deep neural network, you should:

- Use as much data as possible, with **data augmentation** if needed.
- **Normalize** the inputs.
- Use **batch normalization** in every layer and at least **ReLU**.
- Use a good **optimizer** (SGD with momentum, Adam).
- **Regularize** learning (L2, L1, dropout).
- Track overfitting on the validation set and use **early-stopping**.
- Search for the best **hyperparameters** using grid search or hyperopt:
  - Learning rate, schedule, momentum, dropout level, number of layers/neurons, transfer functions, etc.



Source: <https://xkcd.com/1838/>