UNIVERSITY OF TECHNOLOGY
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Neurocomputing

Modern neural networks

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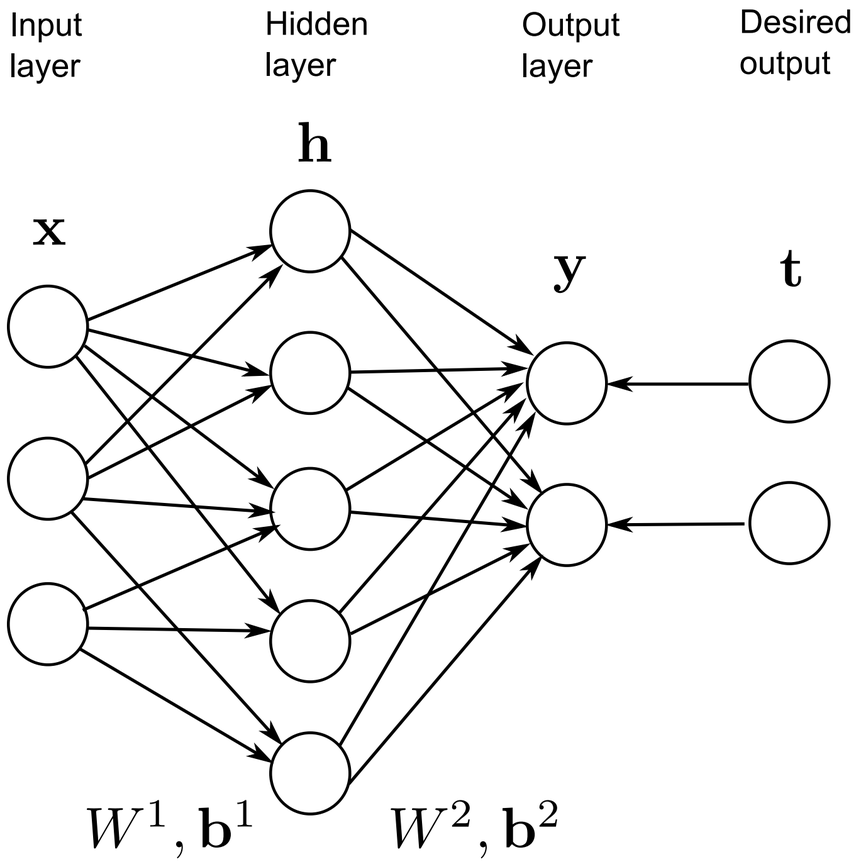
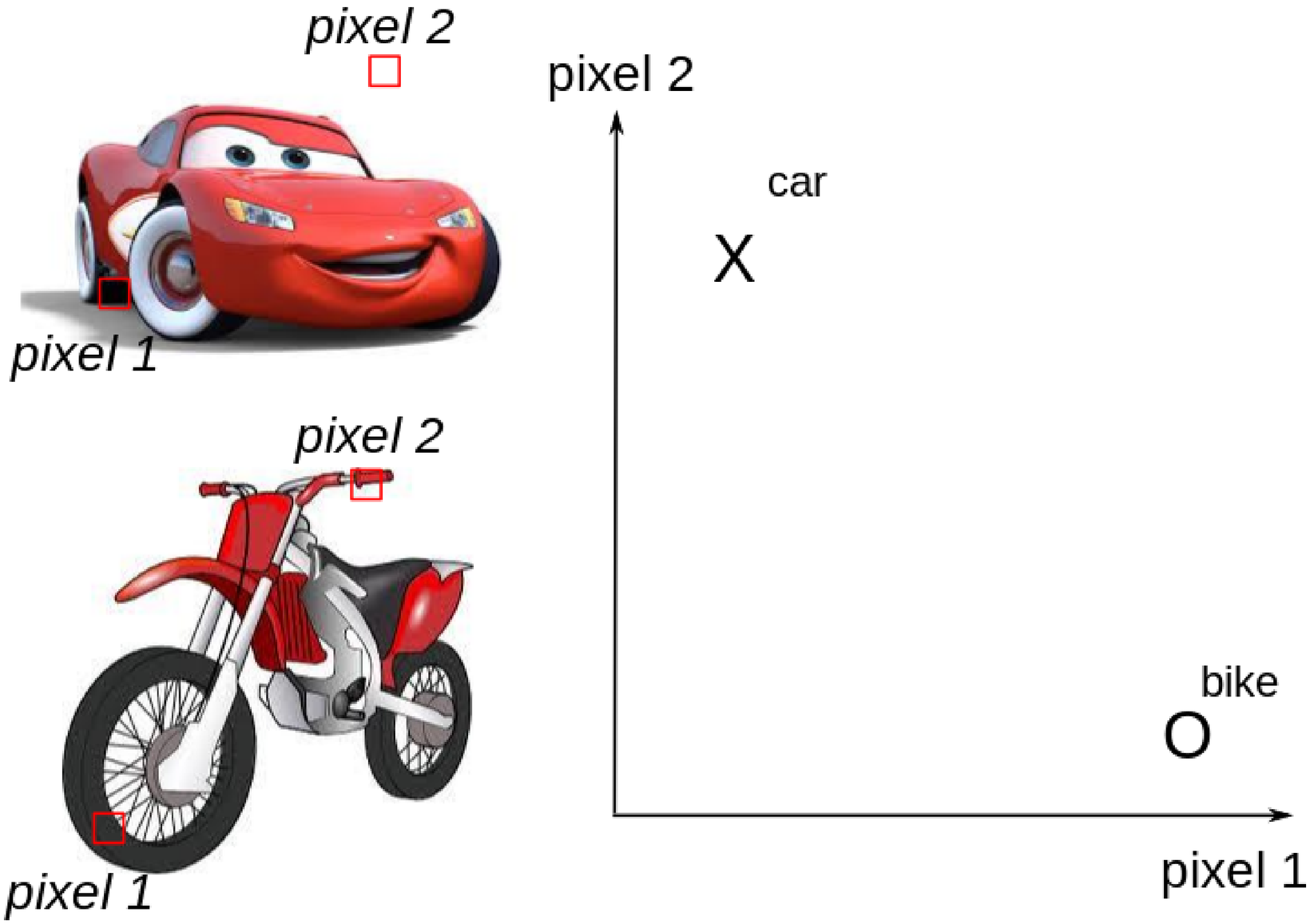
https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

Shallow vs. deep networks



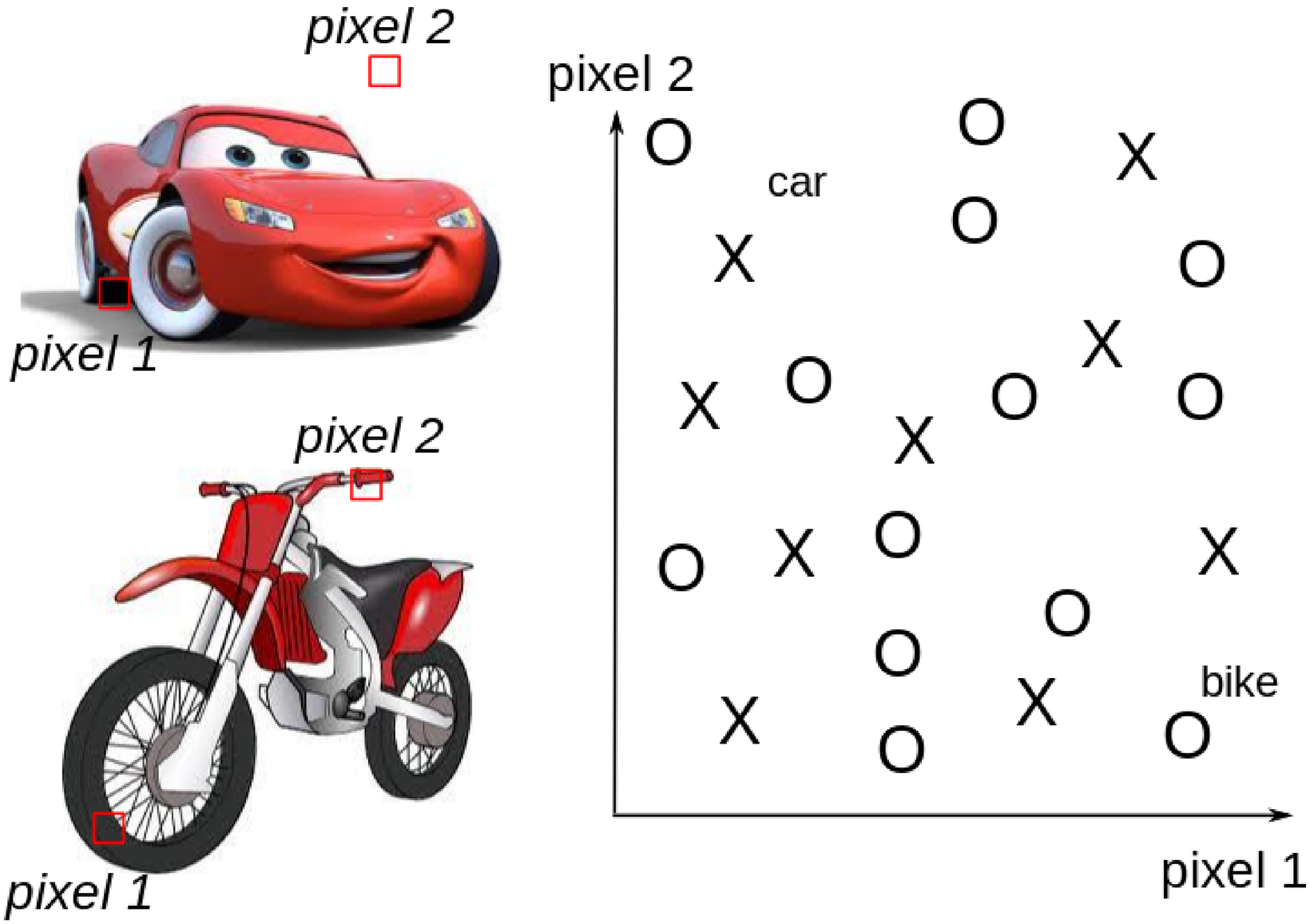
- Universal approximation theorem (Cybenko, 1989): a **shallow** network can approximate any mapping function between inputs and outputs.
- If the mapping function is too complex, a shallow network may need too many hidden neurons.
- The hidden neurons extract **features** in the input space: typical 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.

Feature selection



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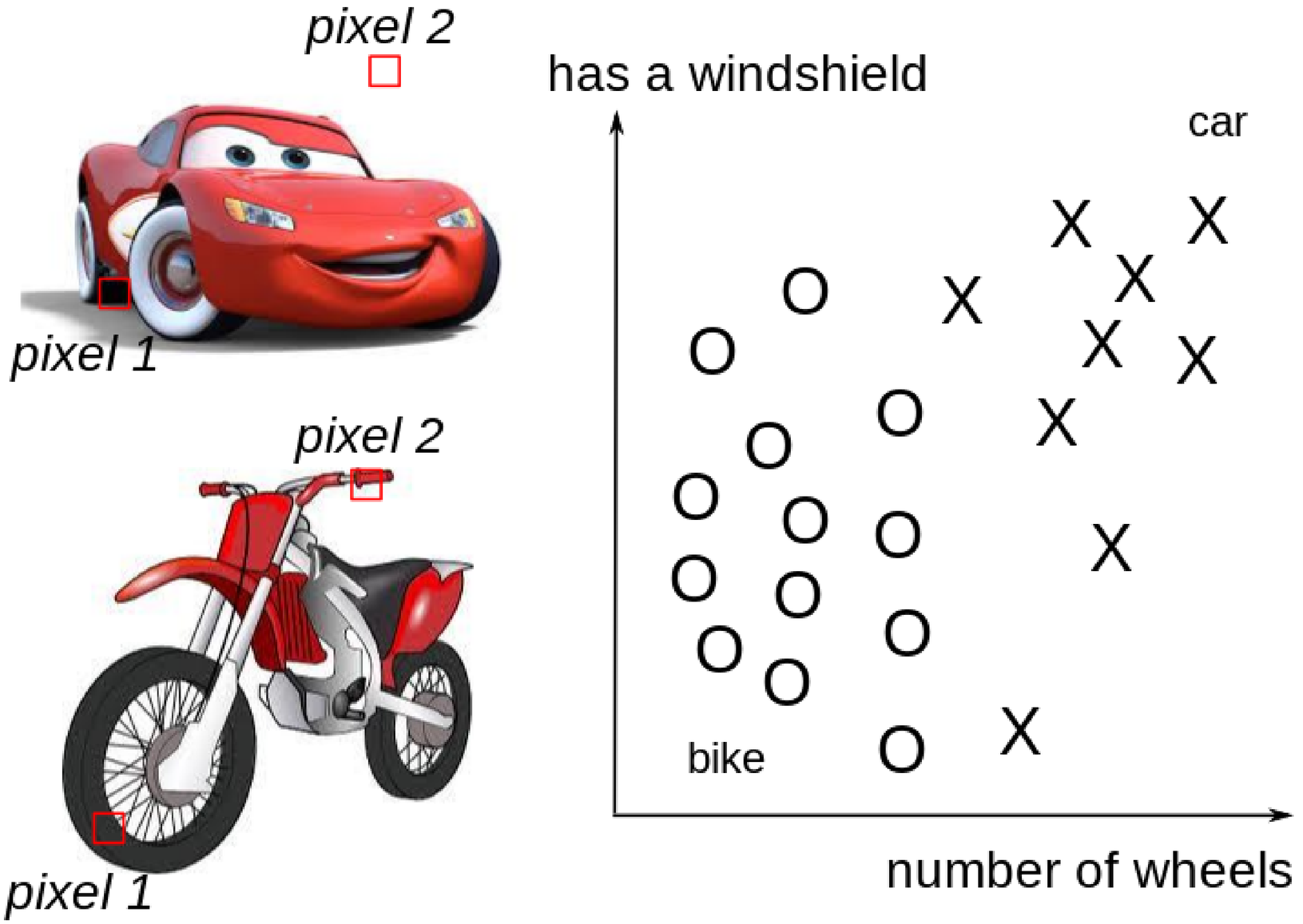
Feature selection



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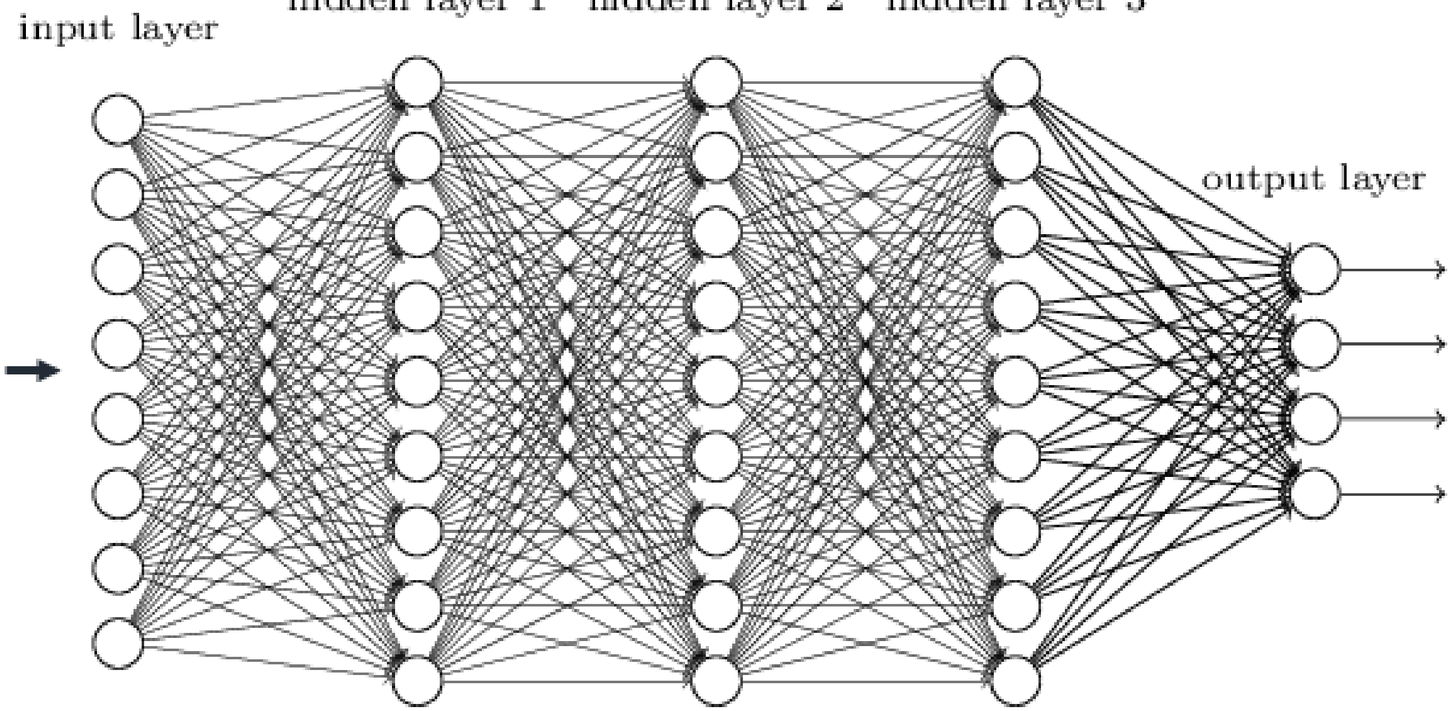
Deep Neural Network

- 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

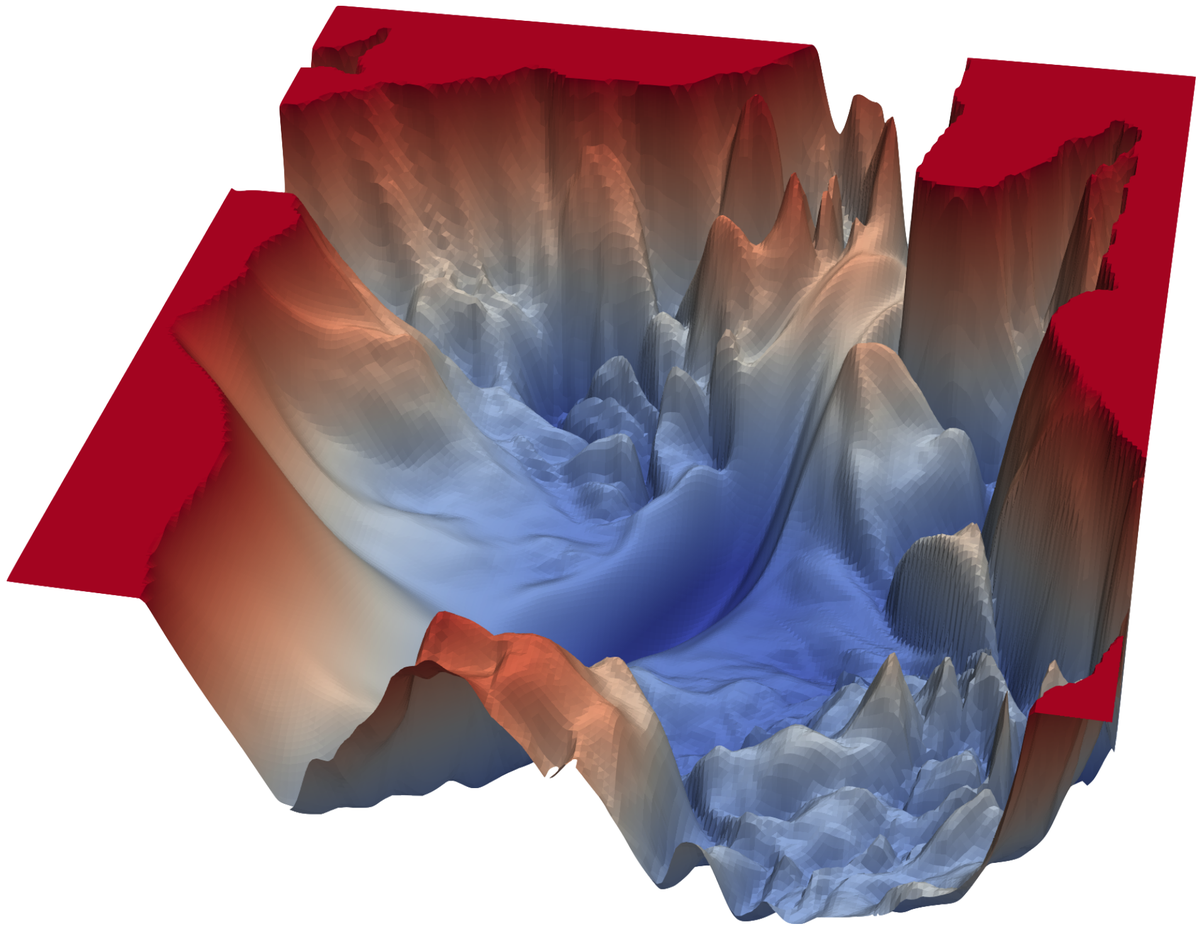
- In practice, training a deep network is not as easy as the theory would suggest.
- Four main problems have to be solved:

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. $\rightarrow$ **inefficient**.

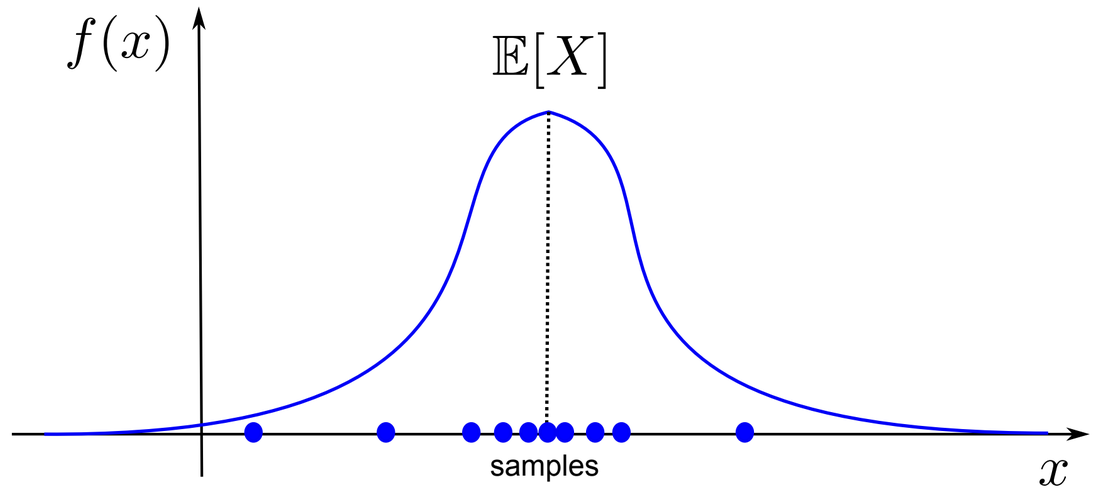
Li H, Xu Z, Taylor G, Studer C, Goldstein T. (2018). Visualizing the Loss Landscape of Neural Nets. arXiv:171209913

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.

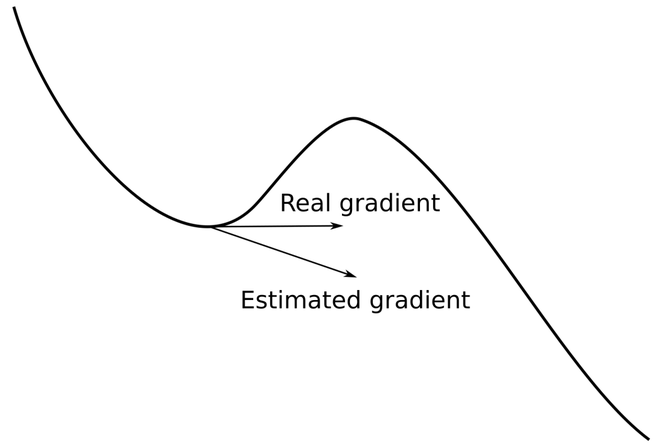
- **Online gradient descent** estimates the loss function by sampling a single example:

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

- 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 ~ 100 examples to approximate the mathematical expectation.



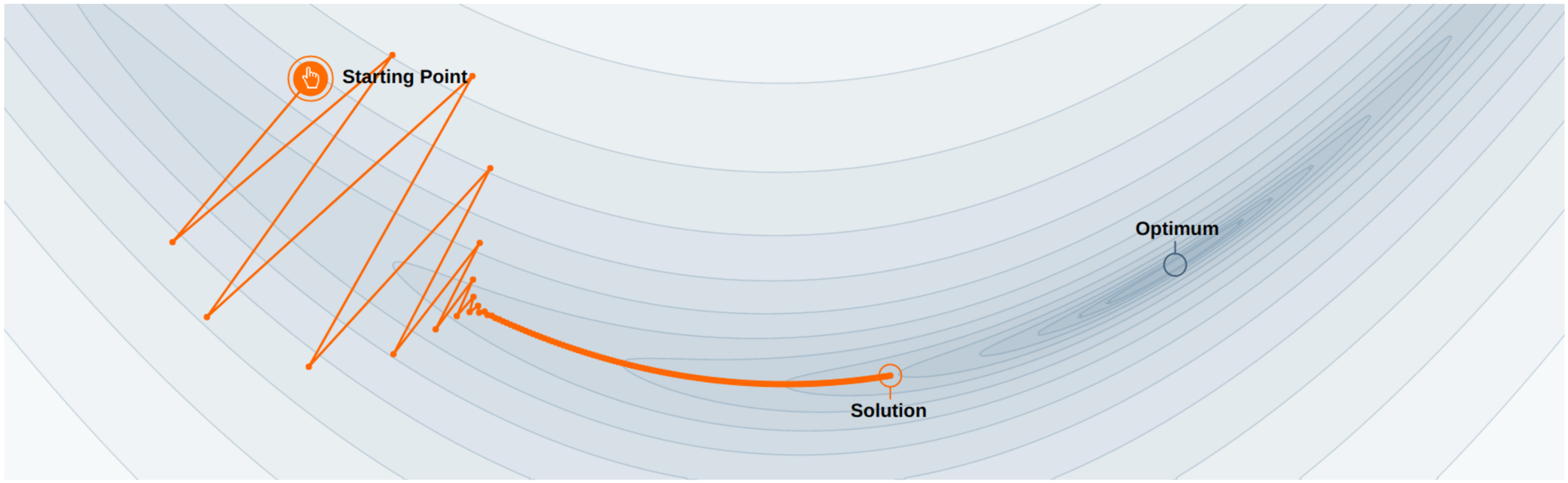
$$\mathcal{L}(\theta) = E_{\mathcal{D}}(||\mathbf{t} - \mathbf{y}||^2) \approx \frac{1}{K} \sum_{i=1}^{K} ||\mathbf{t}_i - \mathbf{y}_i||^2$$

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

- 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**.

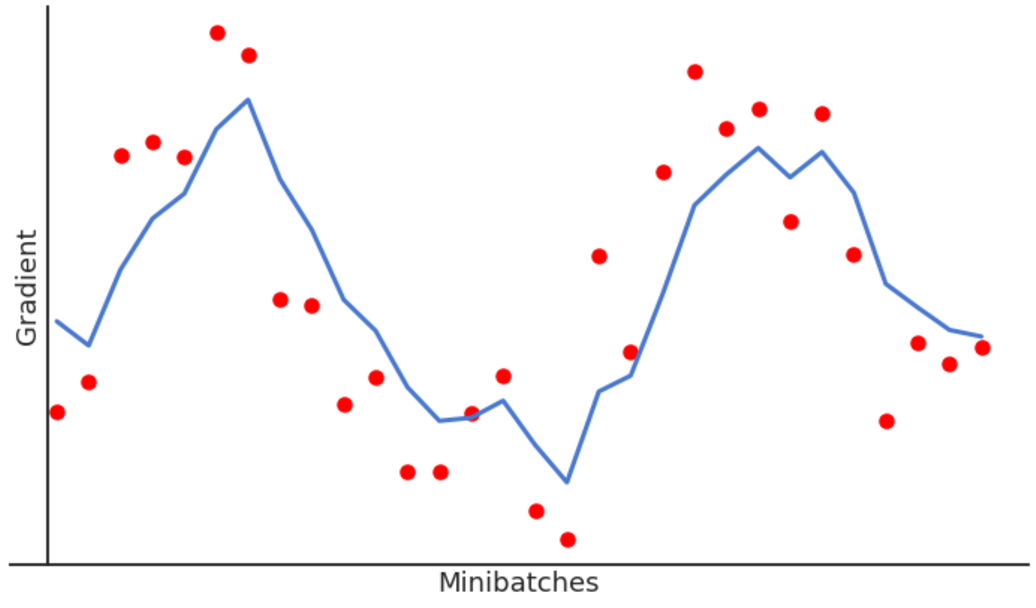
SGD with momentum

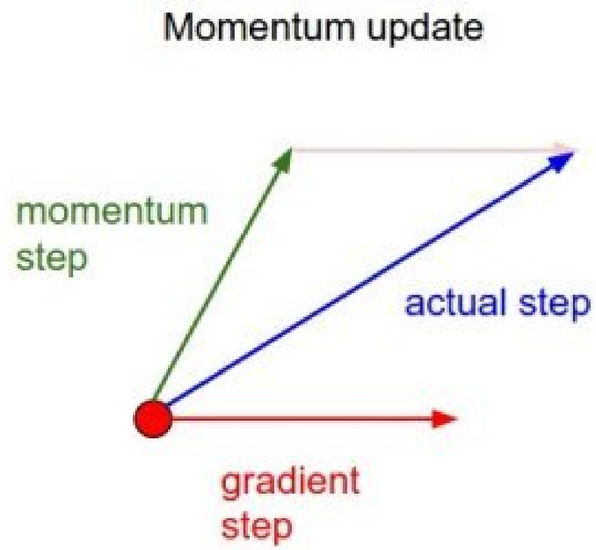
- One solution is to **smooth** the gradients over time (i.e. between minibatches), in order to avoid that one parameter is increased by one minibatch and decreased by the next one.
- The momentum method uses a **moving average** of the gradient (momentum step) to update the parameters:

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

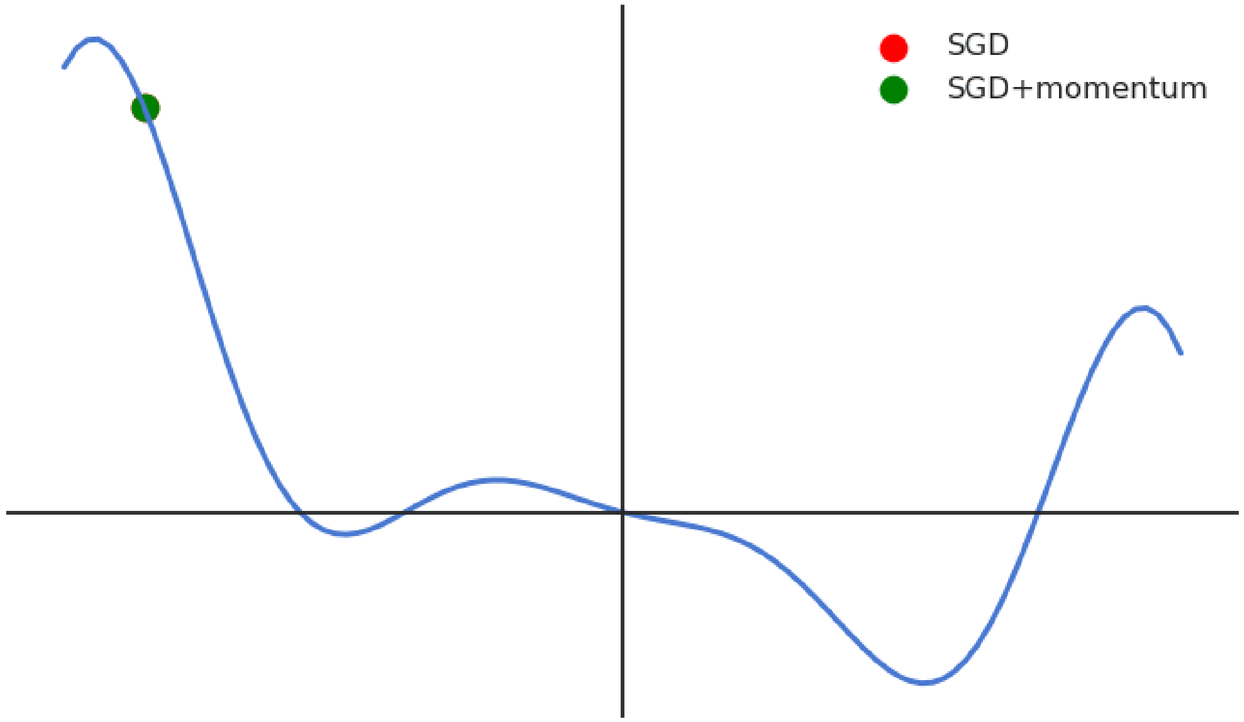
$$\Delta\theta = \eta\, v(\theta)$$

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





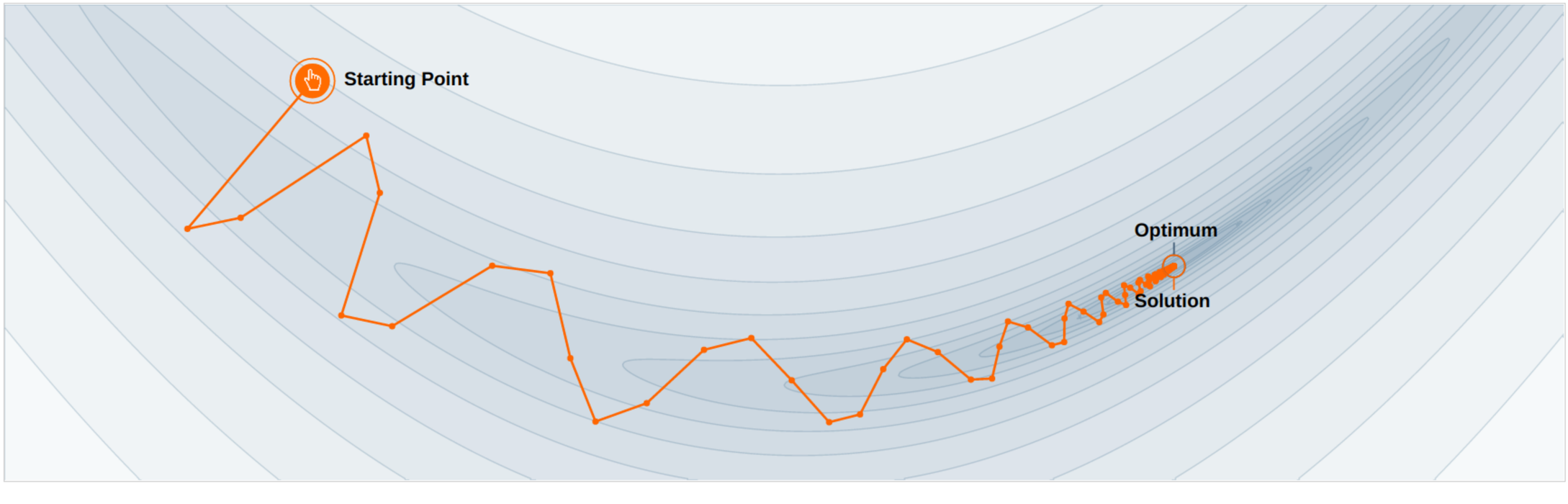
SGD with momentum



- 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 implictly higher when the gradient does not reverse its sign (the estimate “accelerates”).

SGD with momentum



Step-size α = 0.0032

0 0.003 0.006

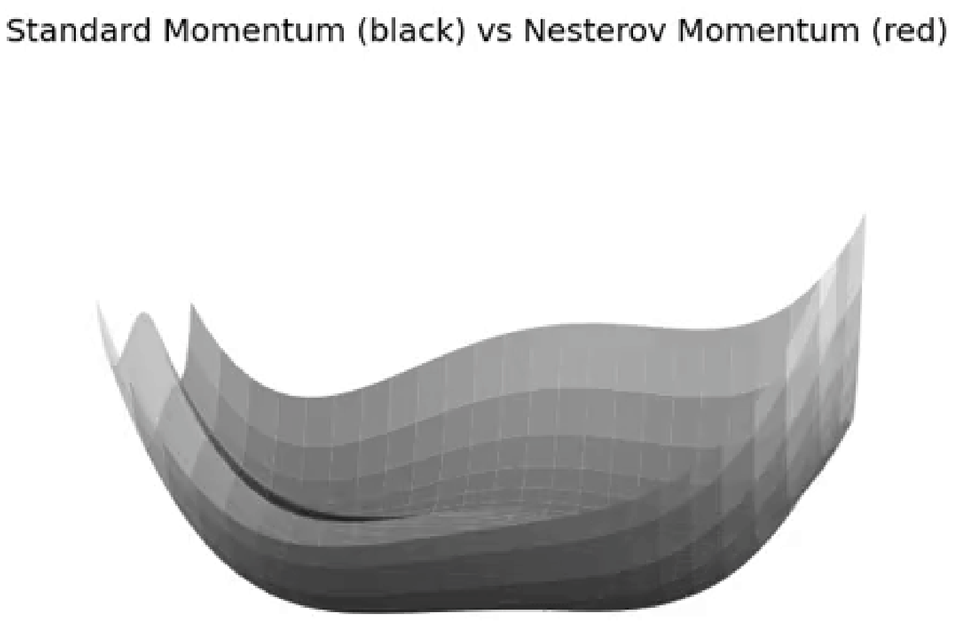
Momentum β = 0.86

0.00 0.500 0.990

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

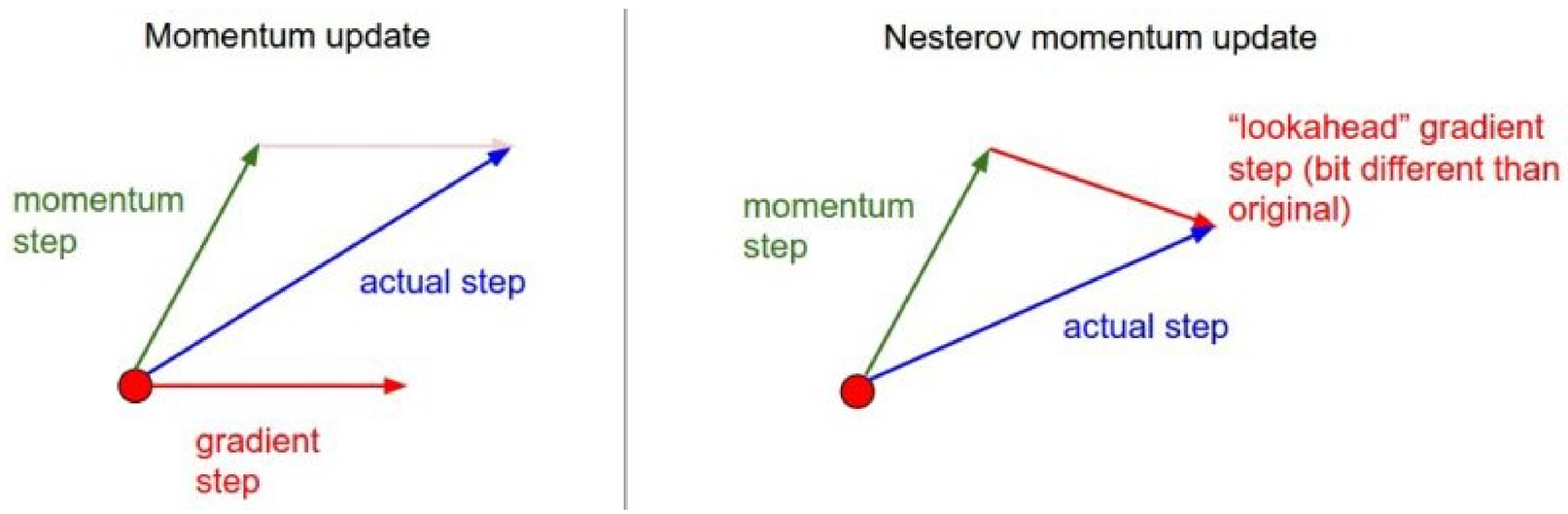


- SGD with momentum tends to oscillate around the minimum.
- The Nesterov momentum **corrects** these oscillations by estimating the gradient **after** the momentum update:

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

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

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).

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

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

- 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.

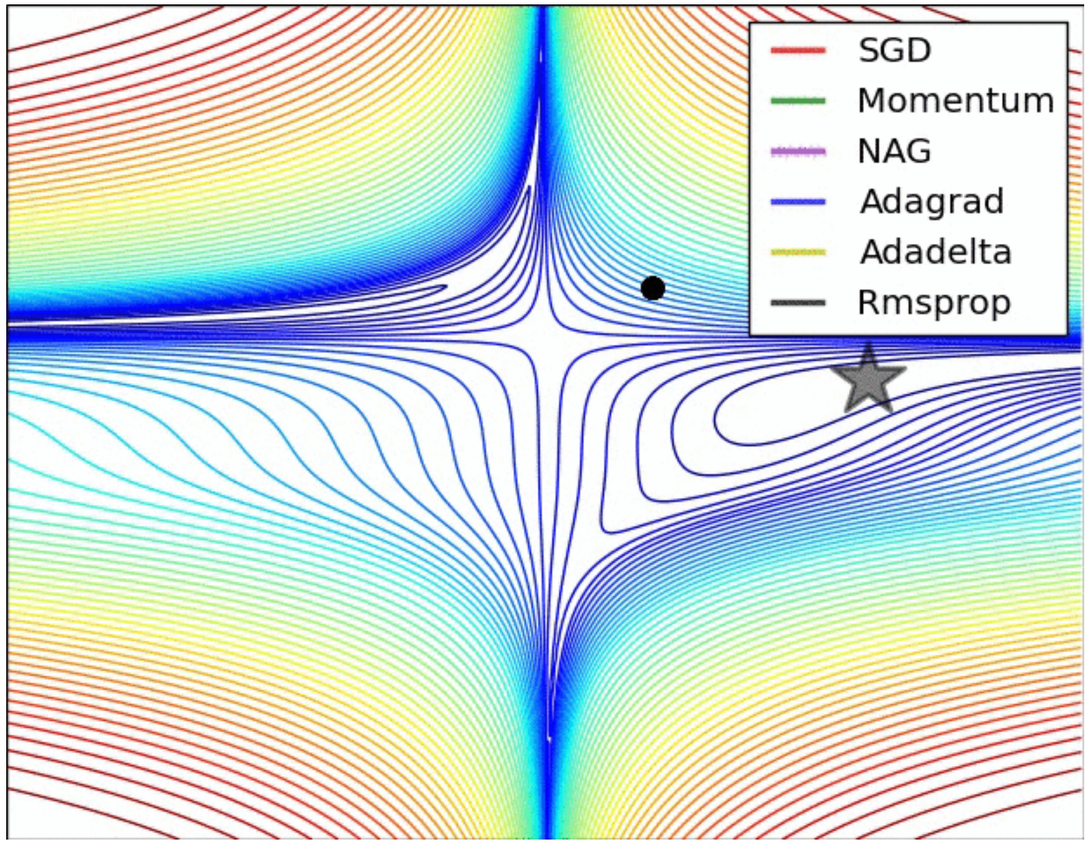
$$m(\theta) = \beta_1 m(\theta) + (1 - \beta_1) \nabla_\theta \mathcal{L}(\theta)$$

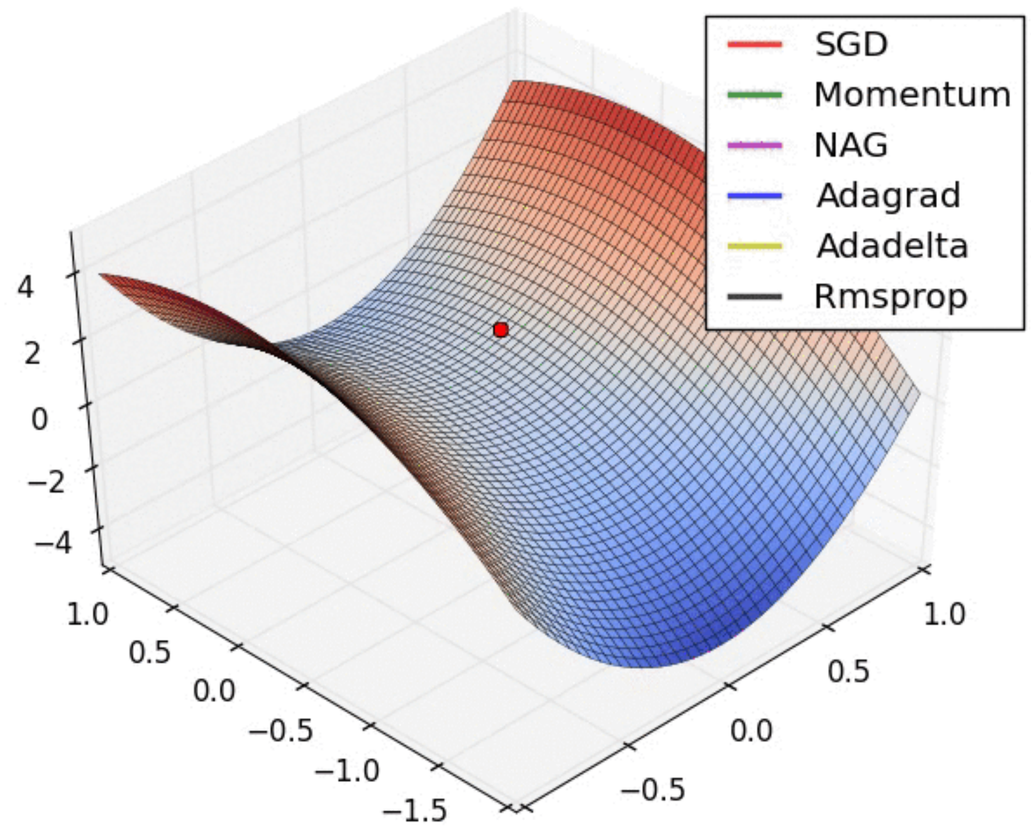
$$v(\theta) = \beta_2 v(\theta) + (1 - \beta_2) \nabla_\theta \mathcal{L}(\theta)^2$$

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

- 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 β_1, β_2 and ϵ 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
)
```

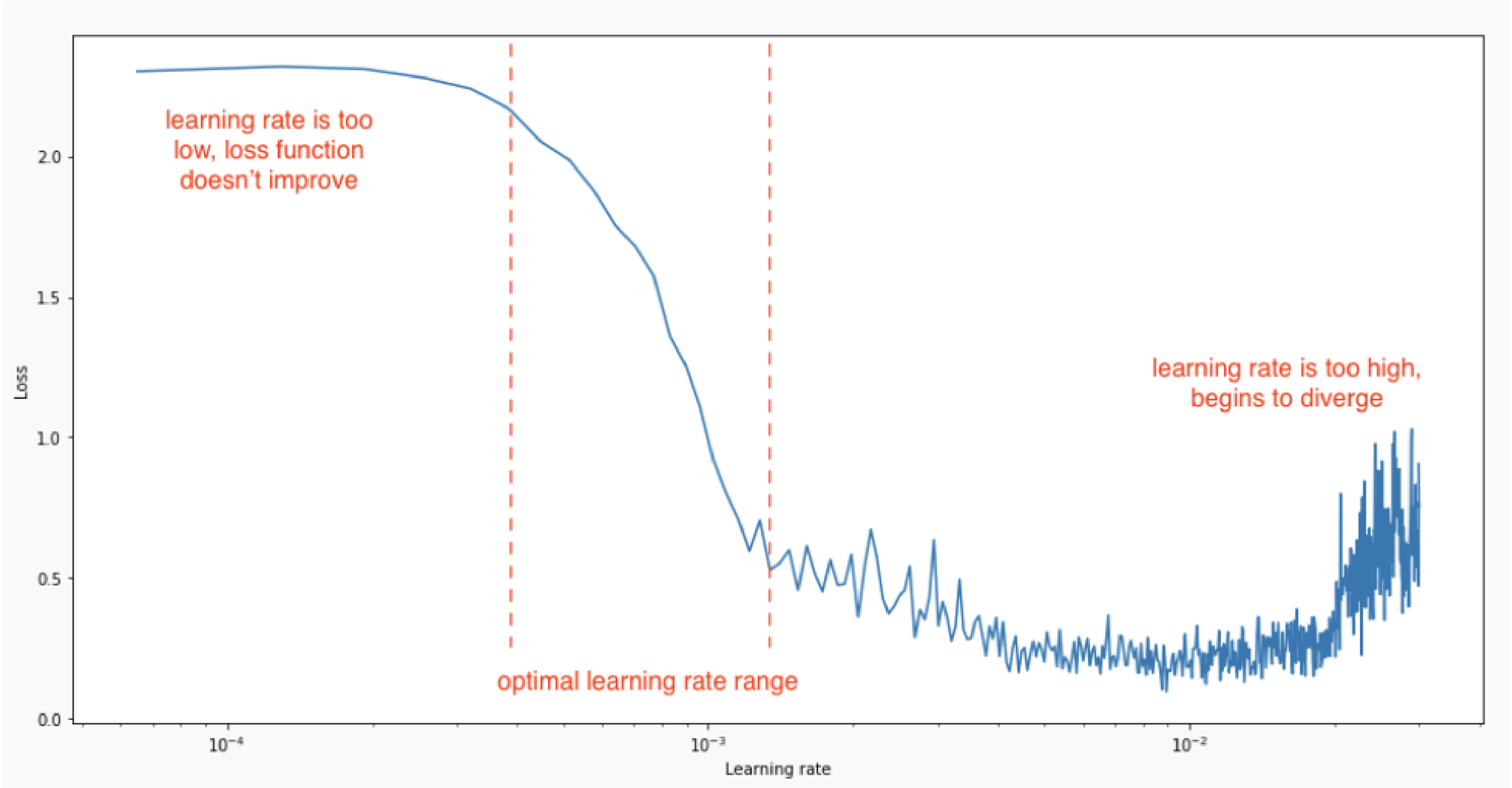
- Adam:

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

Hyperparameters annealing

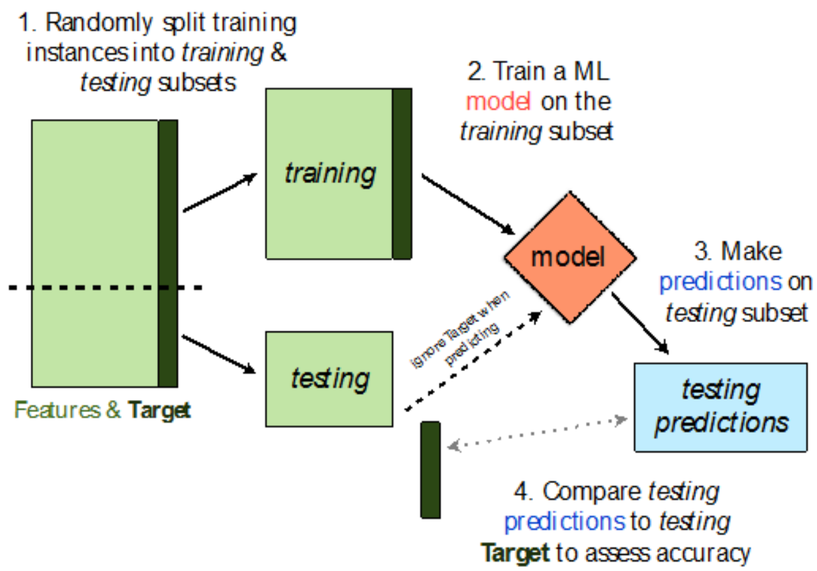
Finding a good range for the learning rate

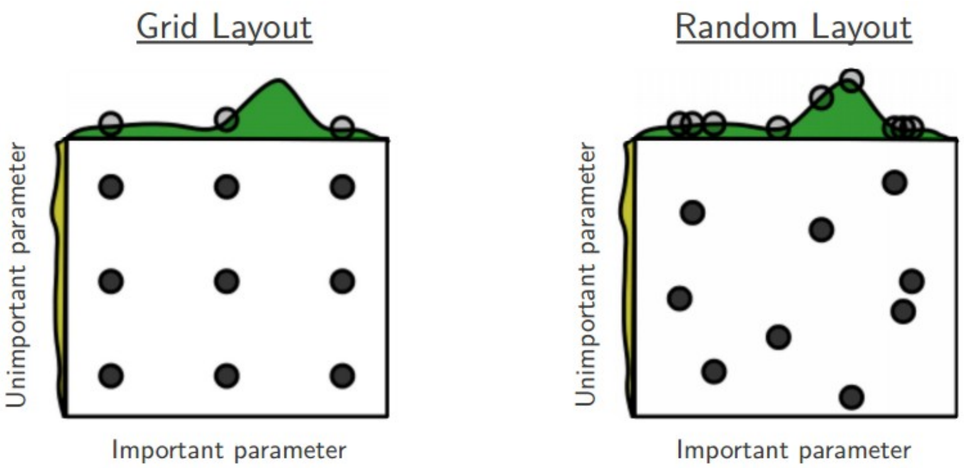
- A simple trick to find a good estimate of the learning rate (or its start/stop value) is to increase its value exponentially **for each minibatch** at the beginning of learning.
- The “good” region for the learning rate is the one where the validation loss decreases, but does not oscillate.



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

Hyperparameter search





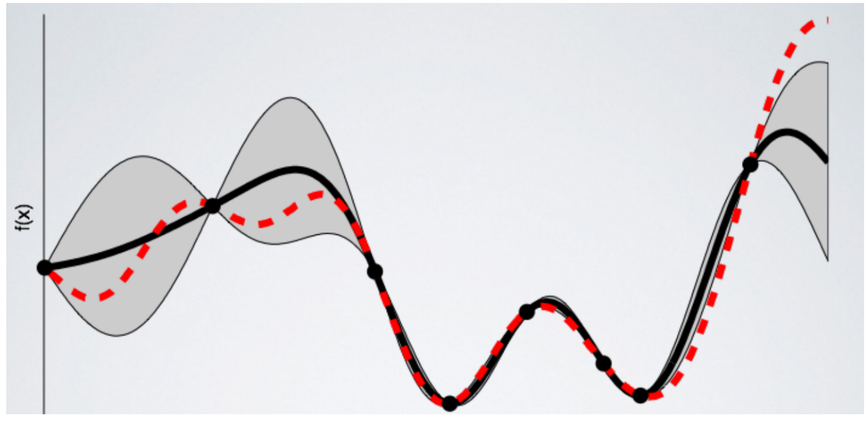
Source: http://cs231n.github.io/neural-networks-3/

- 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 ($[0.1, 0.2, \ldots, 0.9]$) or logarithmically ($[10^{-6}, 10^{-5}, \ldots, 10^{-1}]$).
  - **Random search**: the value 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**).

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` Python library https://github.com/hyperopt/hyperopt is extremely simple to use:

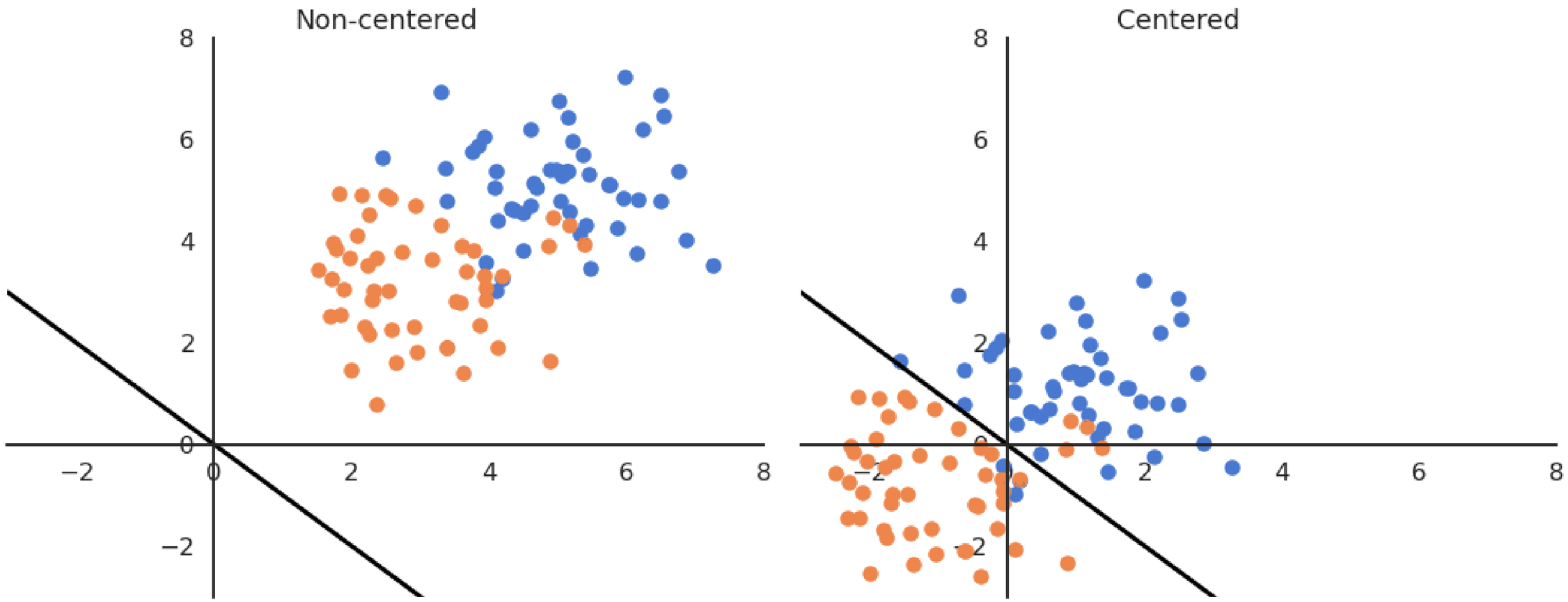
```
from hyperopt import fmin, tpe, hp, STATUS_OK

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
```



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

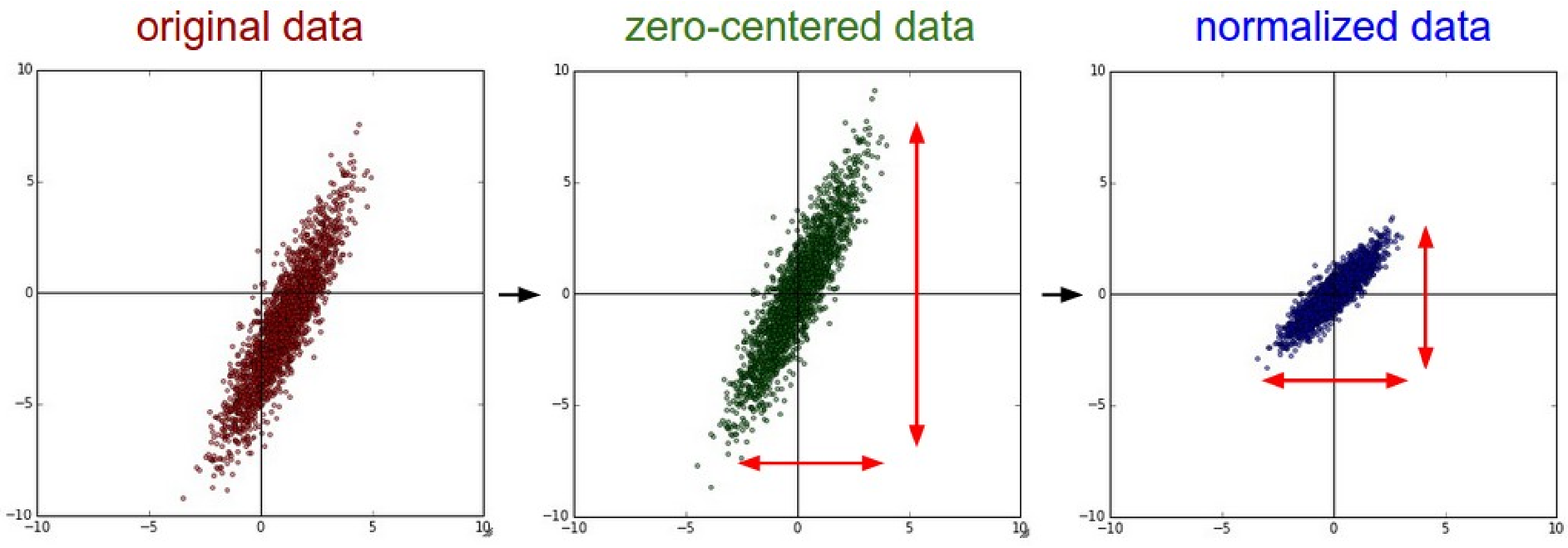
2 - Long training times

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/

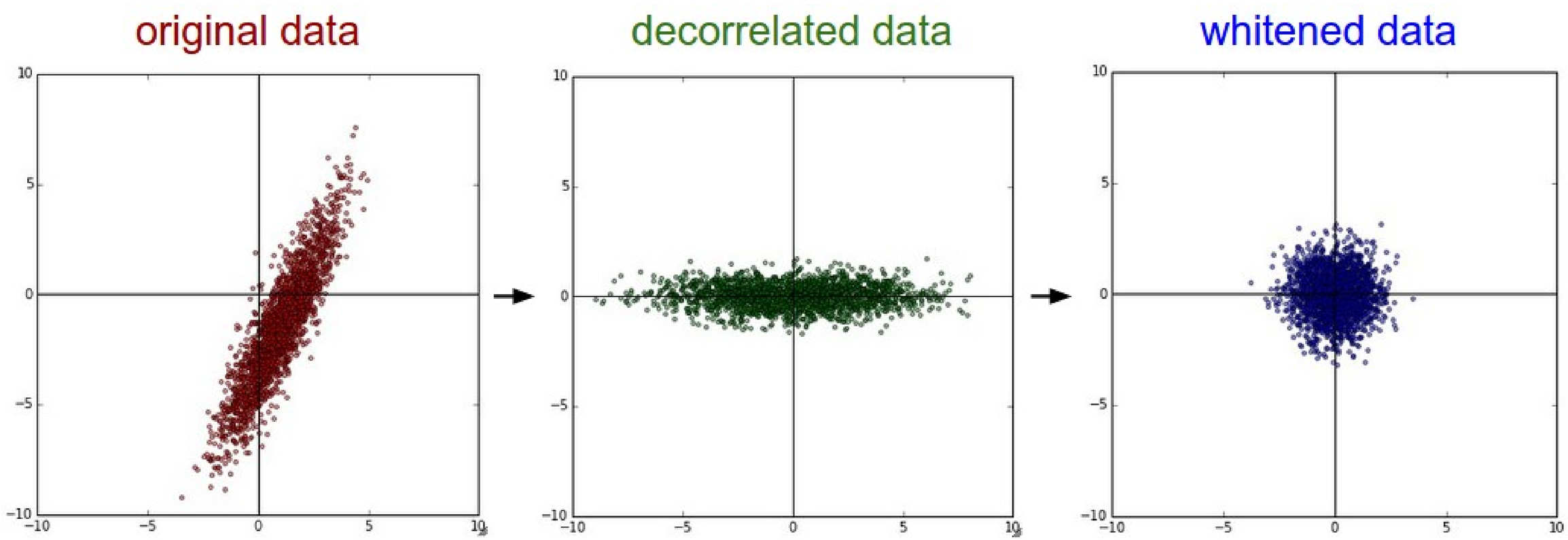
- In practice, the input data X **must** be normalized before training, in order to improve the training time:
  - **Mean removal** or **zero-centering**:

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

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

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

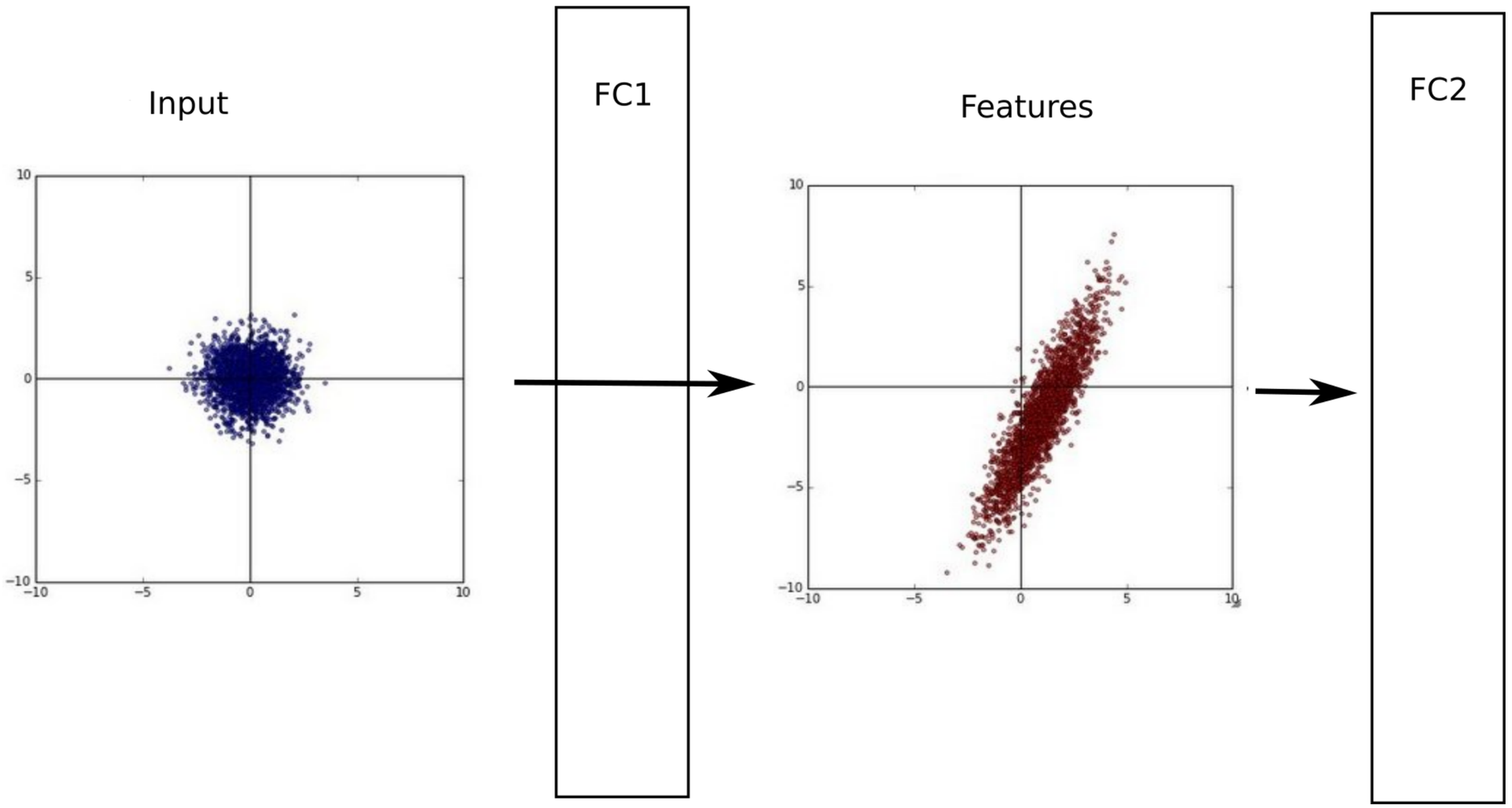
Data whitening



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: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

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

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

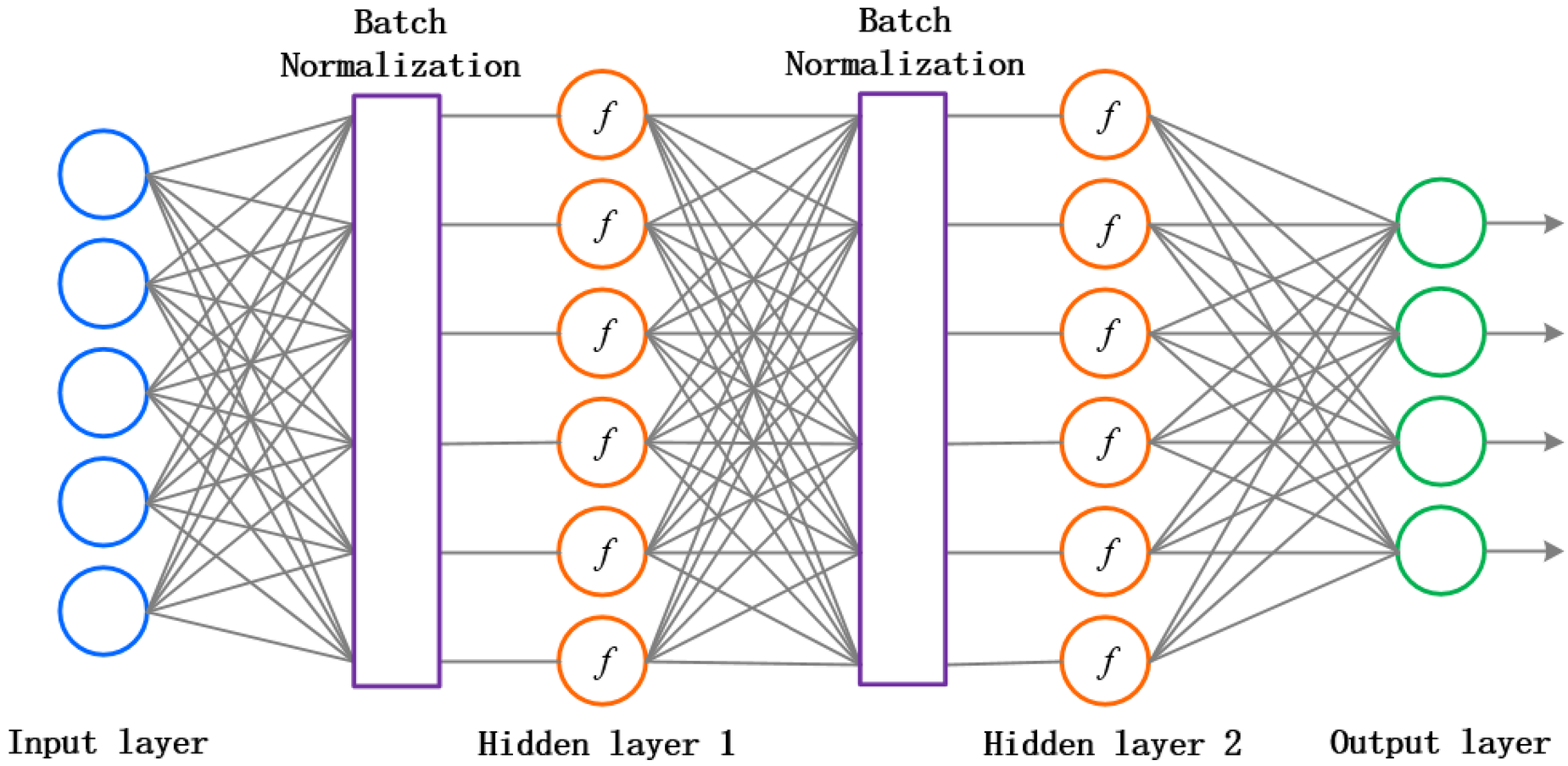
Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

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

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

- 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_{in} and N_{out} neurons.
  - **Xavier**: Uniform initialization (when using logistic or tanh, Glorot and Bengio, 2010):

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

  - **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.

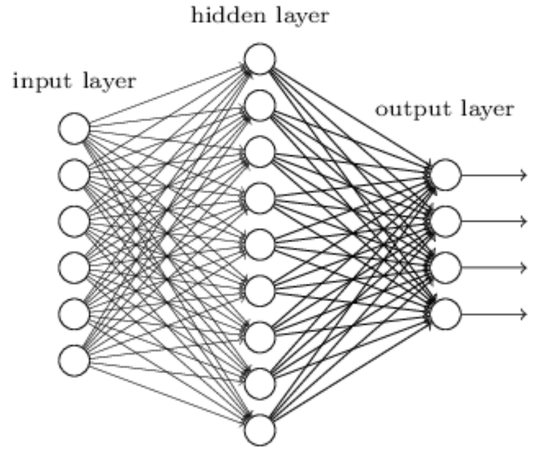
References

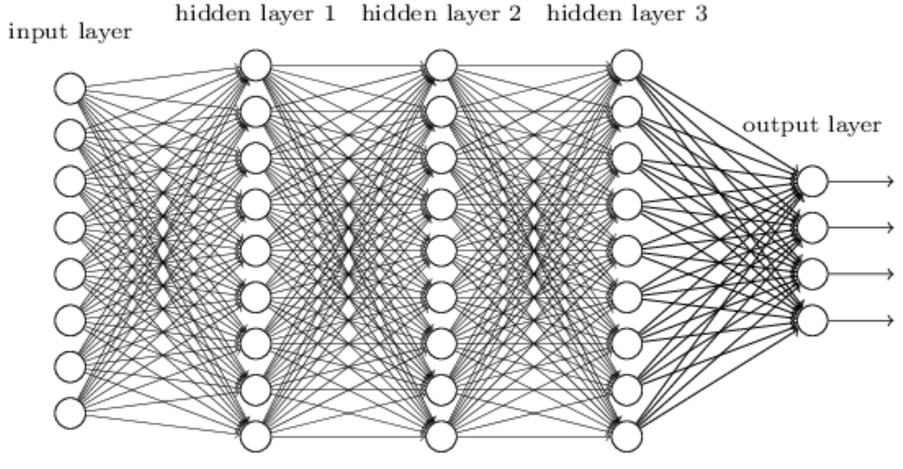
Glorot and Bengio (2010). Understanding the difficulty of training deep feedforward neural networks. AISTATS.

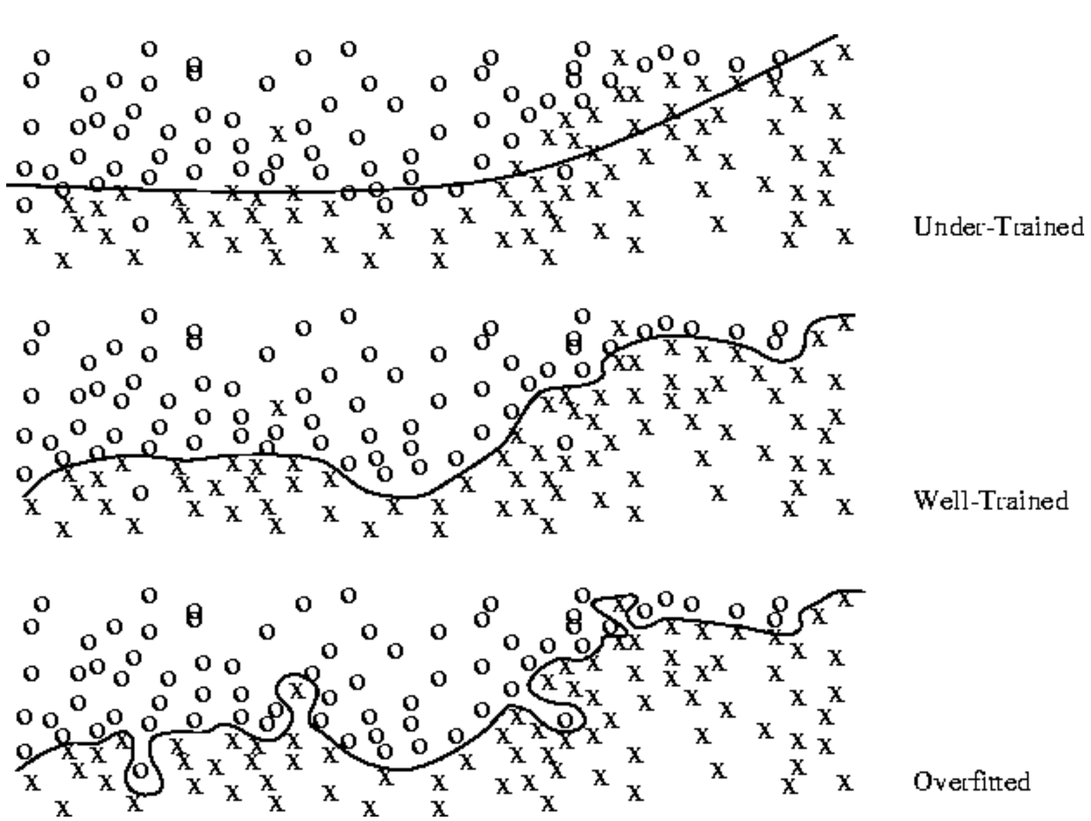
He et al. (2015). Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification. arXiv:1502.01852

3 - Overfitting

Overfitting : Need for regularization







Source : https://www.teco.edu/~albrecht/neuro/html/node10.html

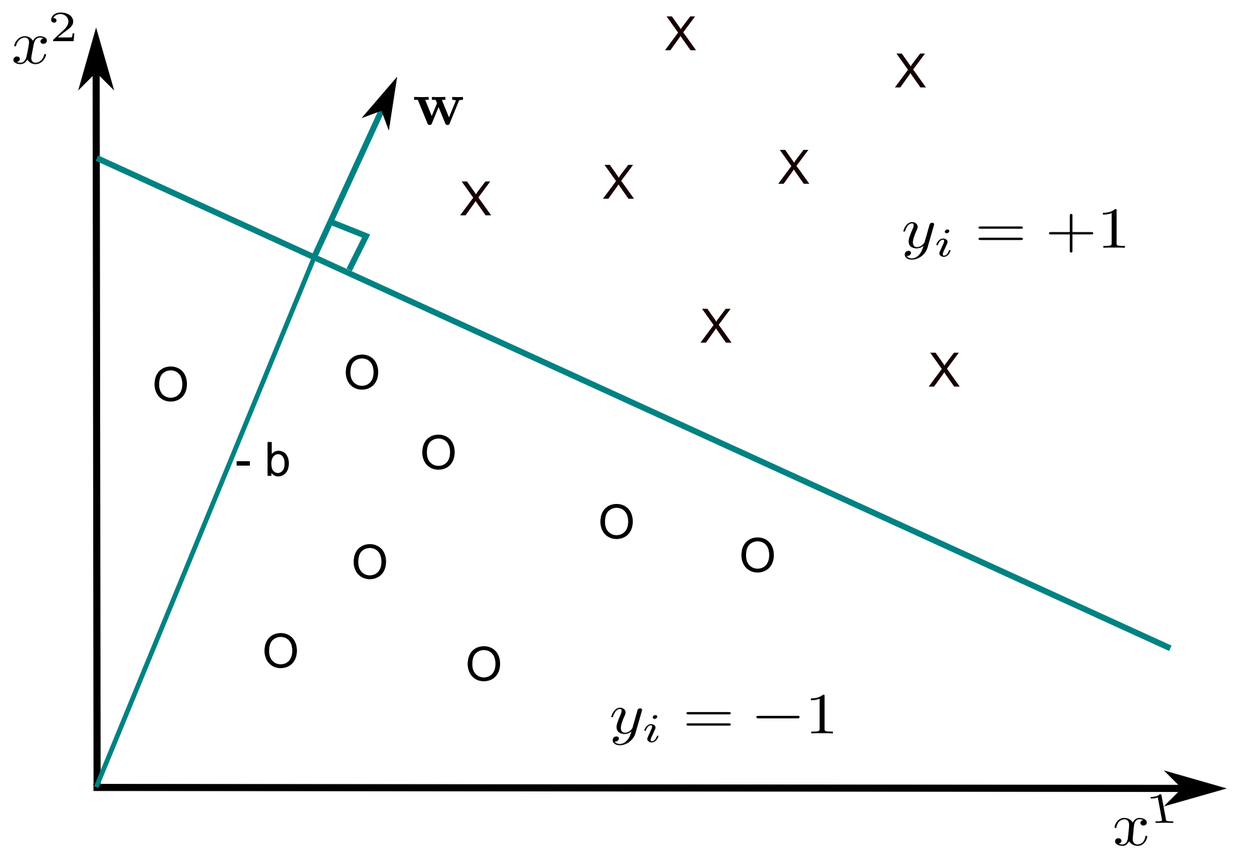
- The main problem with deep NN is **overfitting**.
- With increasing depth, the network has too many weights = free parameters, so its VC dimension is high.

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

- 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 implicitely 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.

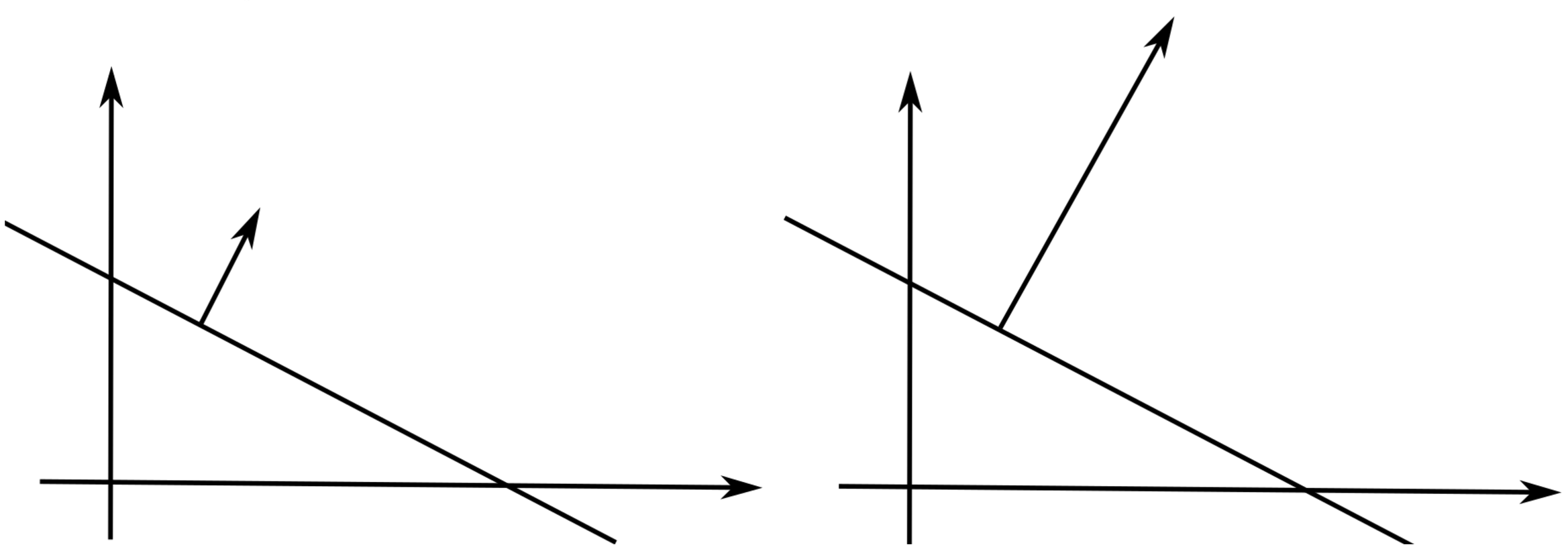


Overfitting : Need for regularization

- **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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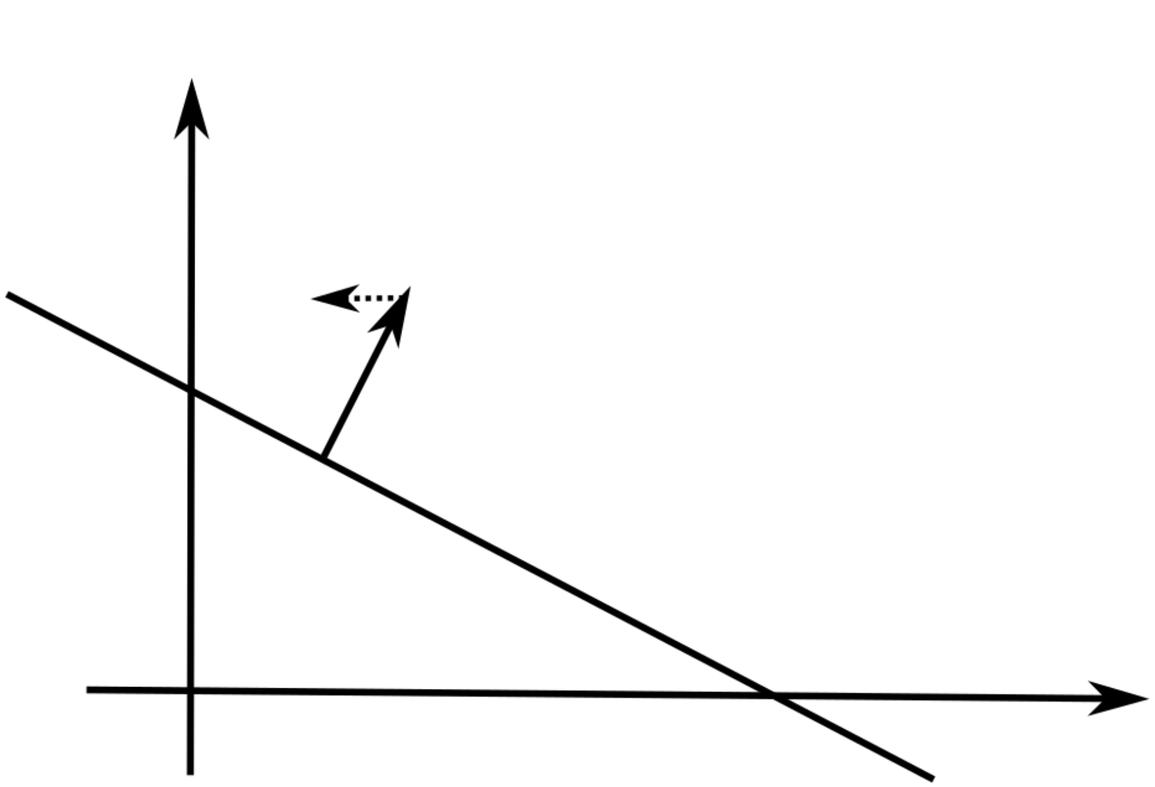

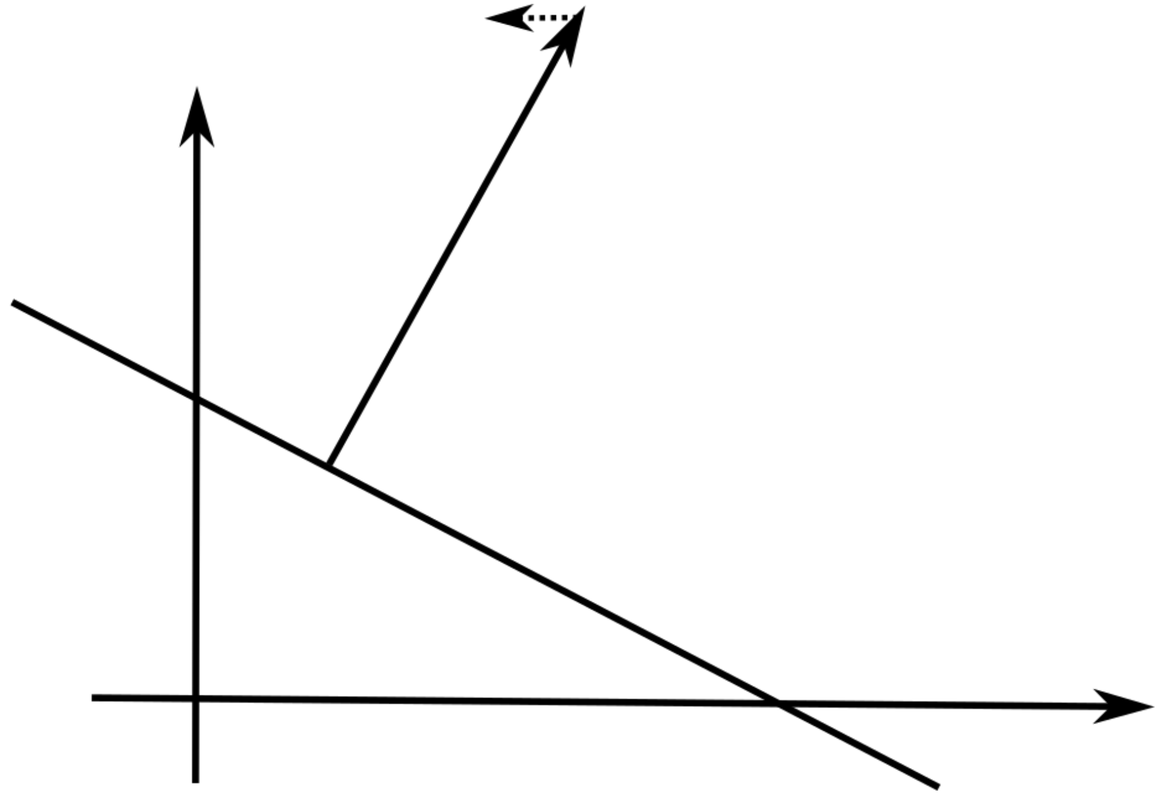

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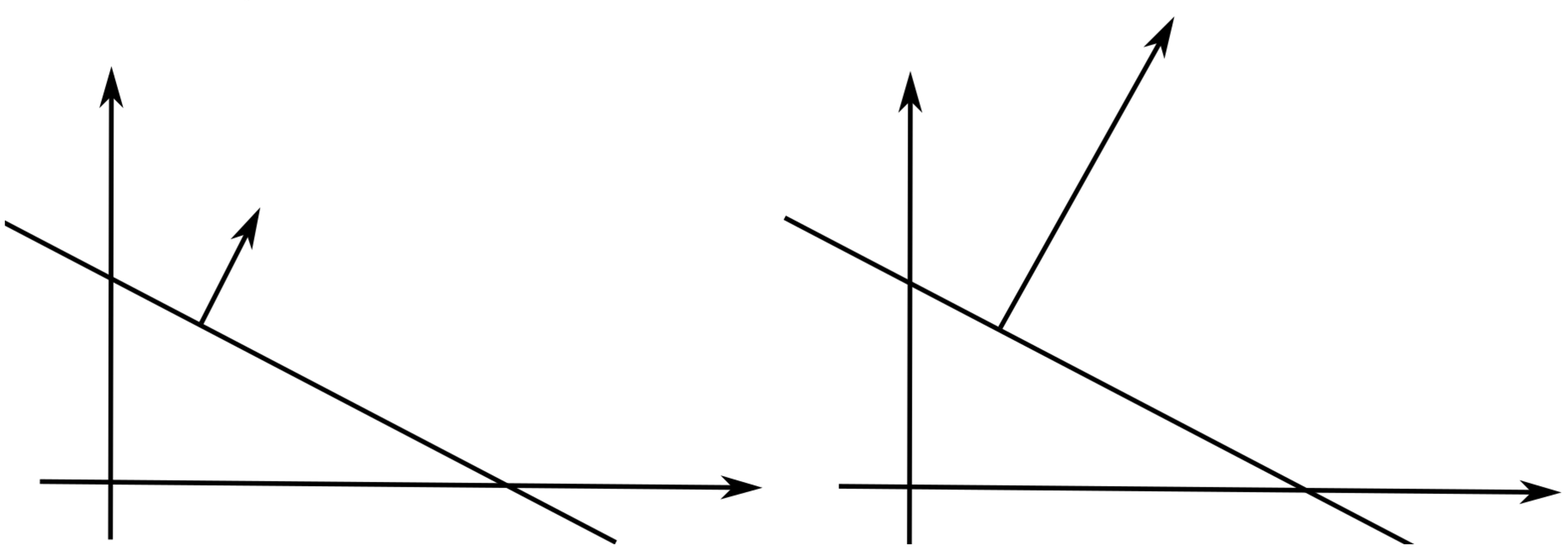


L2 Regularization

- **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 on 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** λ controls the strength of regularization:
  - if λ is small, there is only a small regularization, the weights can increase.
  - if λ 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:

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

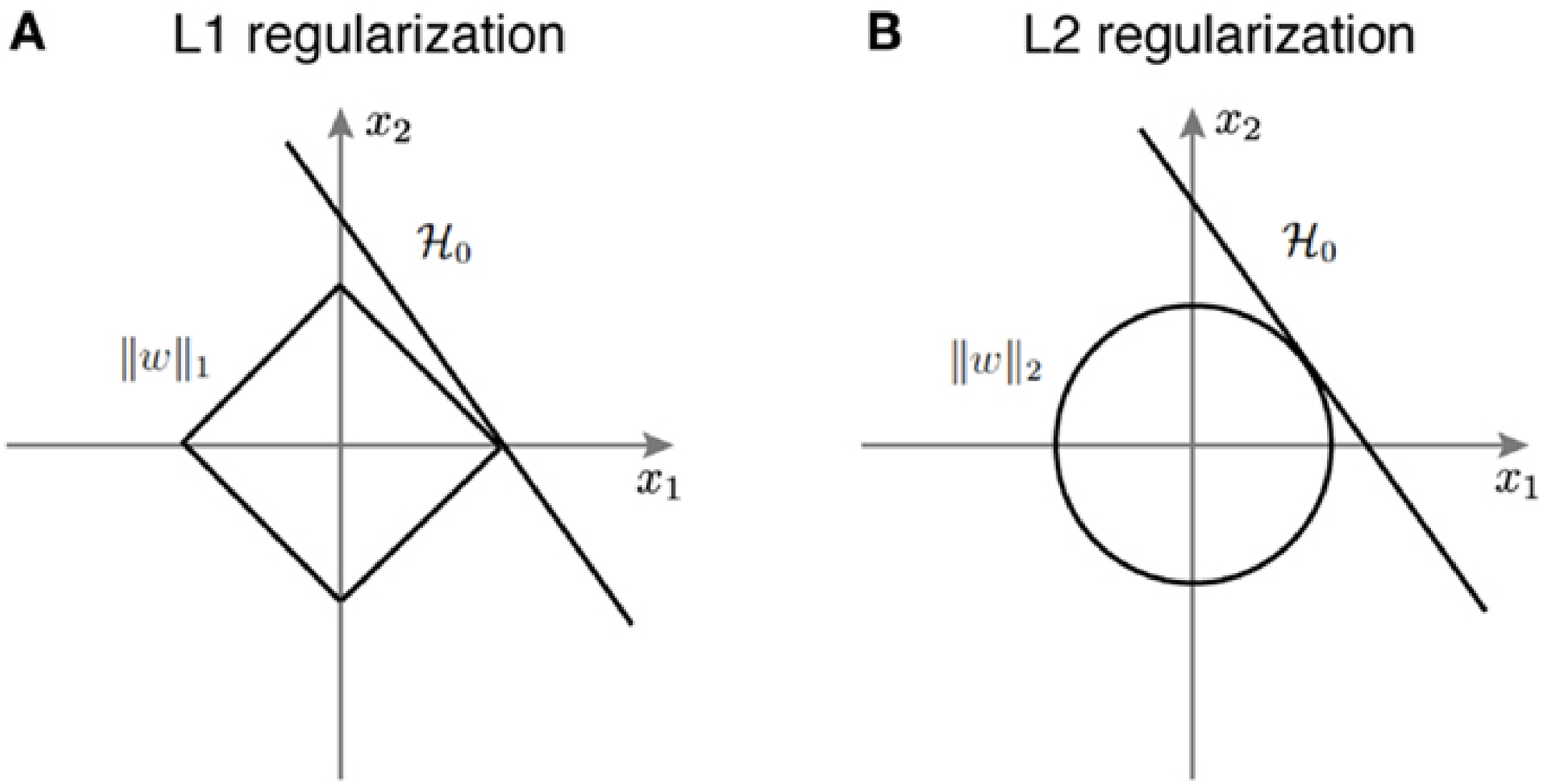
- L2 regularization leads to **weight decay**: even if there is no output error, the weight will converge to 0.
- This forces the weight to constantly learn: it can not specialize on a particular example anymore (overfitting) and is forced to generalize.

L1 Regularization

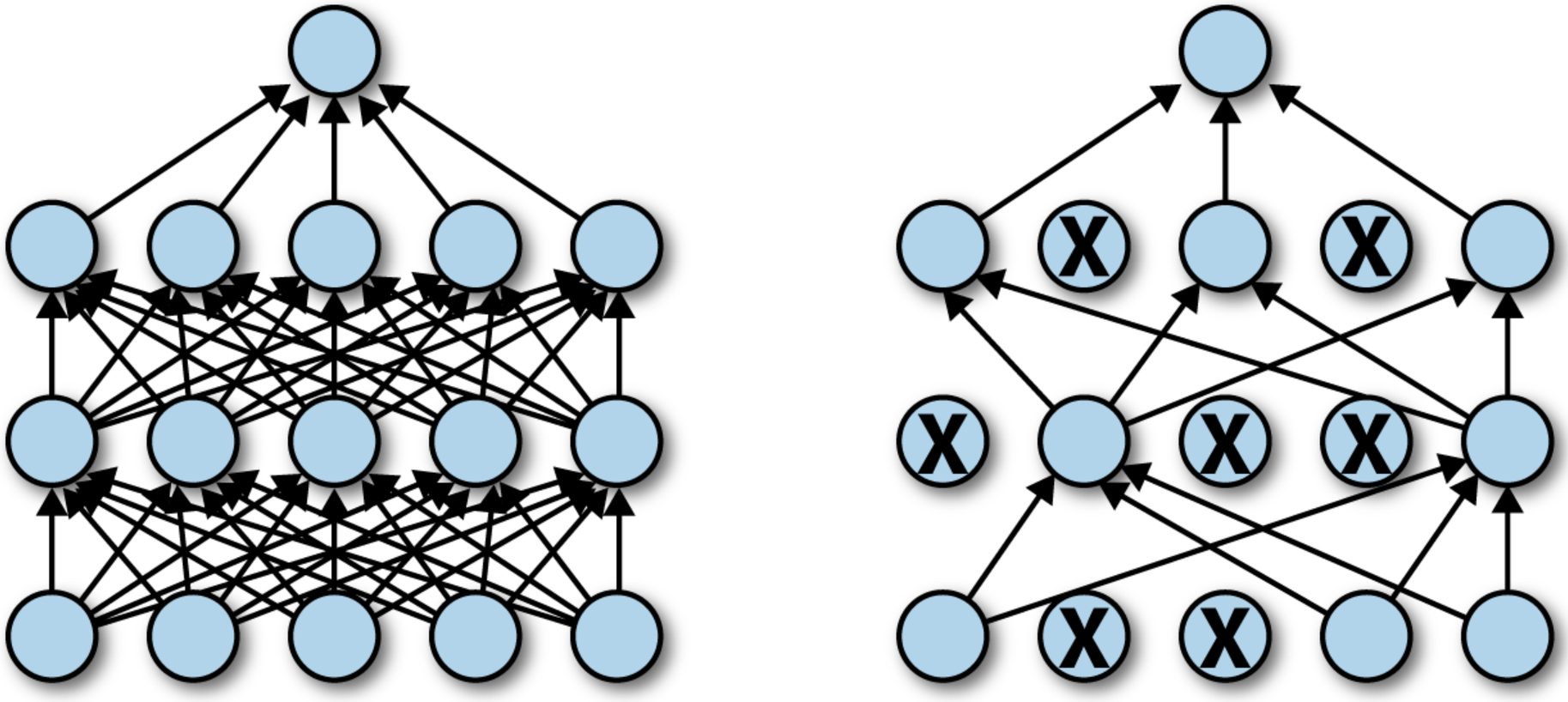
- **L1 regularization** penalizes the absolute value of the weights instead of their Euclidian norm:

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

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



Dropout



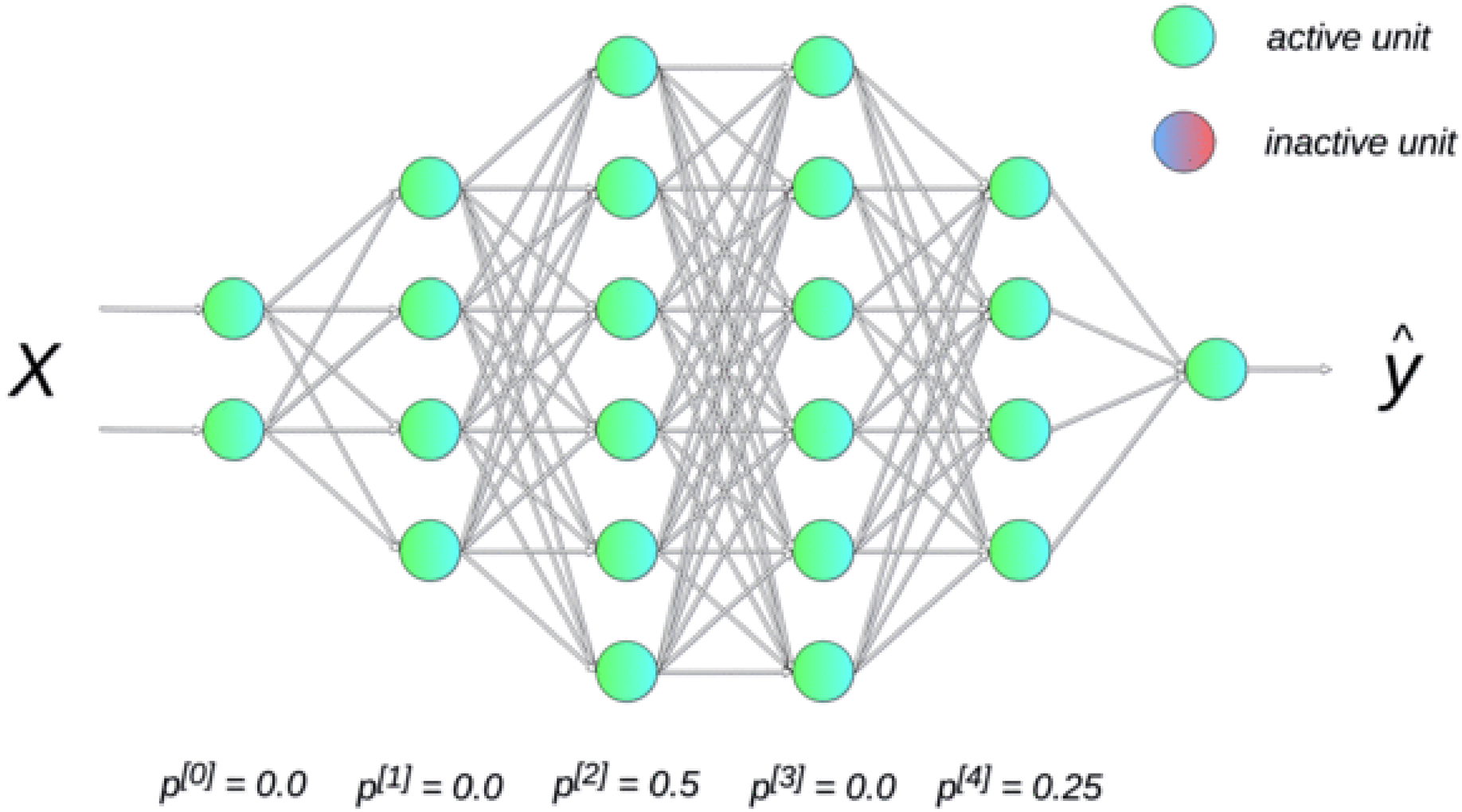
(a) Standard Neural Net

(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.

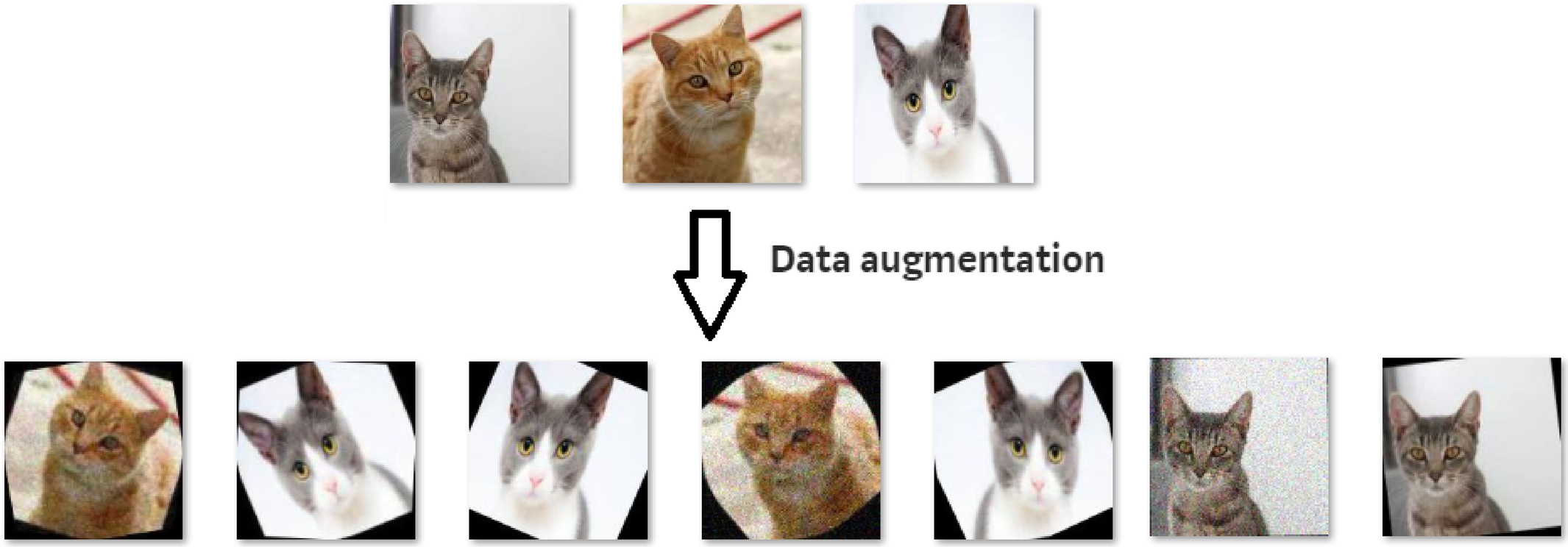
Dropout

- 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

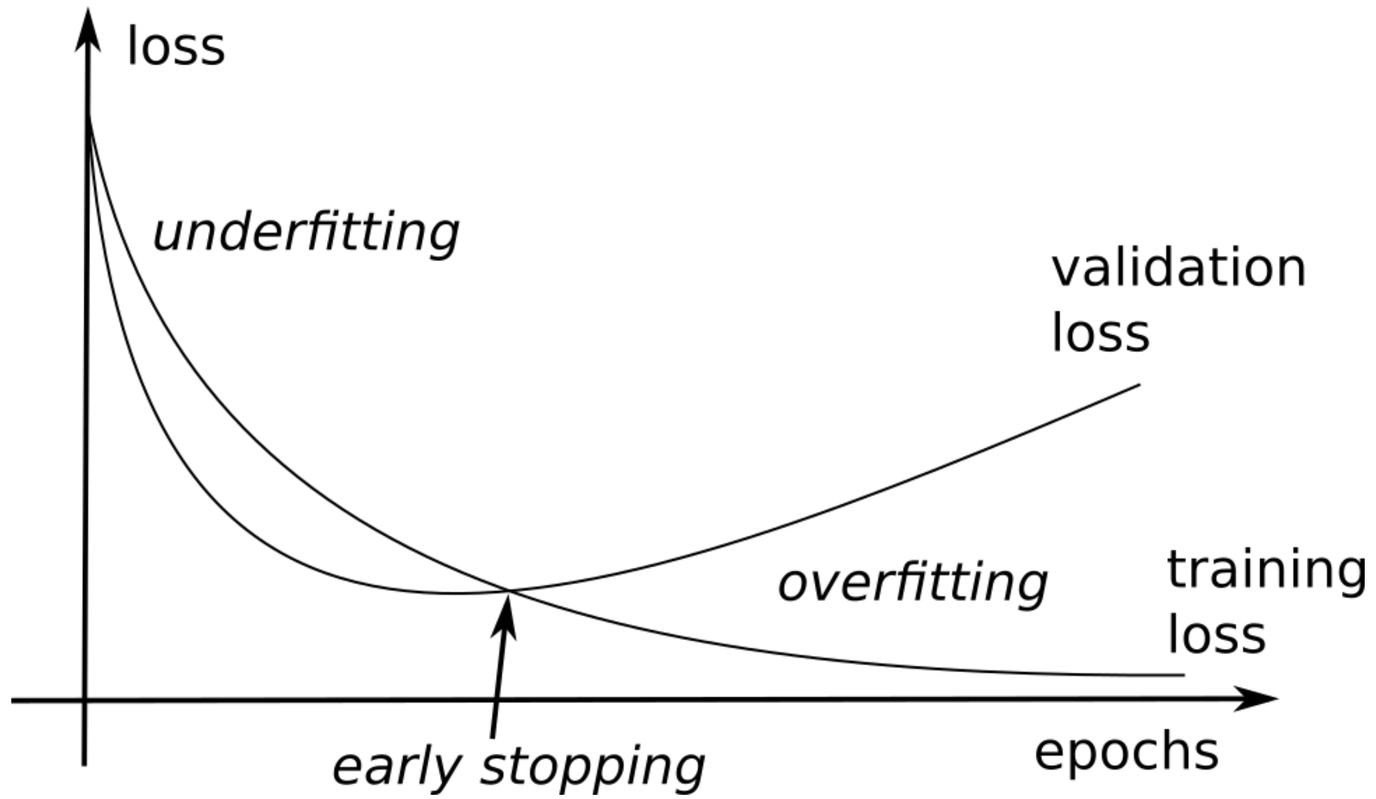
Data augmentation



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

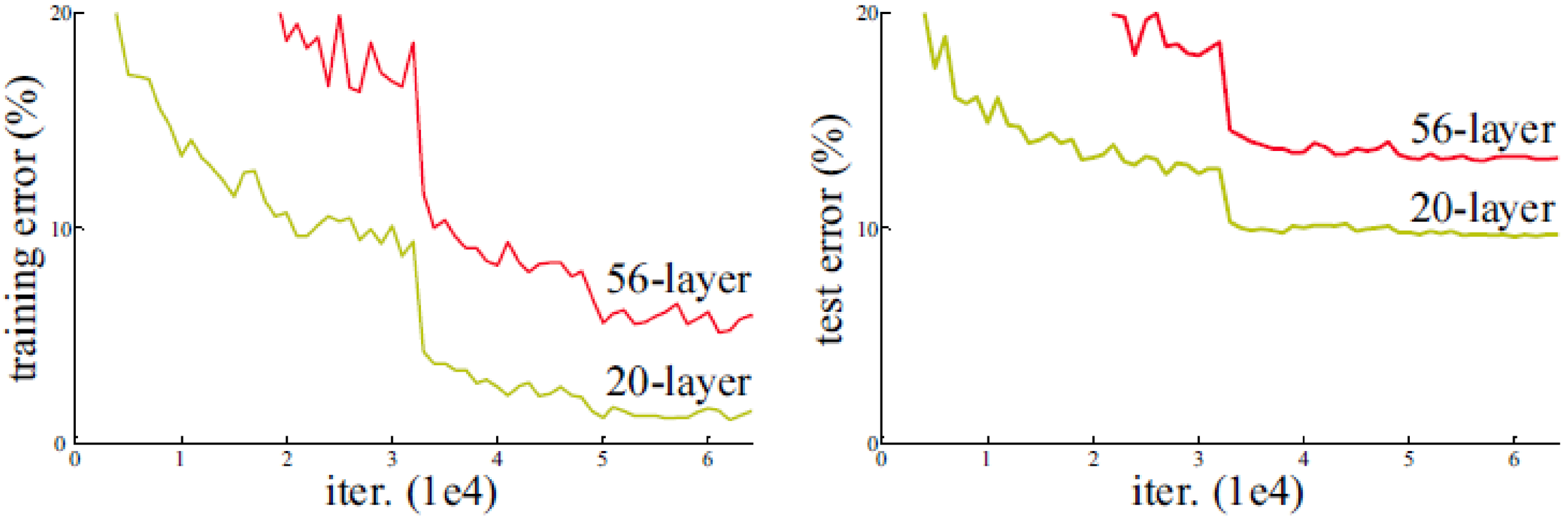


- Early-stopping fights overfitting by monitoring the model's performance on a validation set.
- A **validation set** is a set of examples that we never use for gradient descent, but which is also not a part of the test set.
- If the model's performance ceases to improve sufficiently on the validation 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

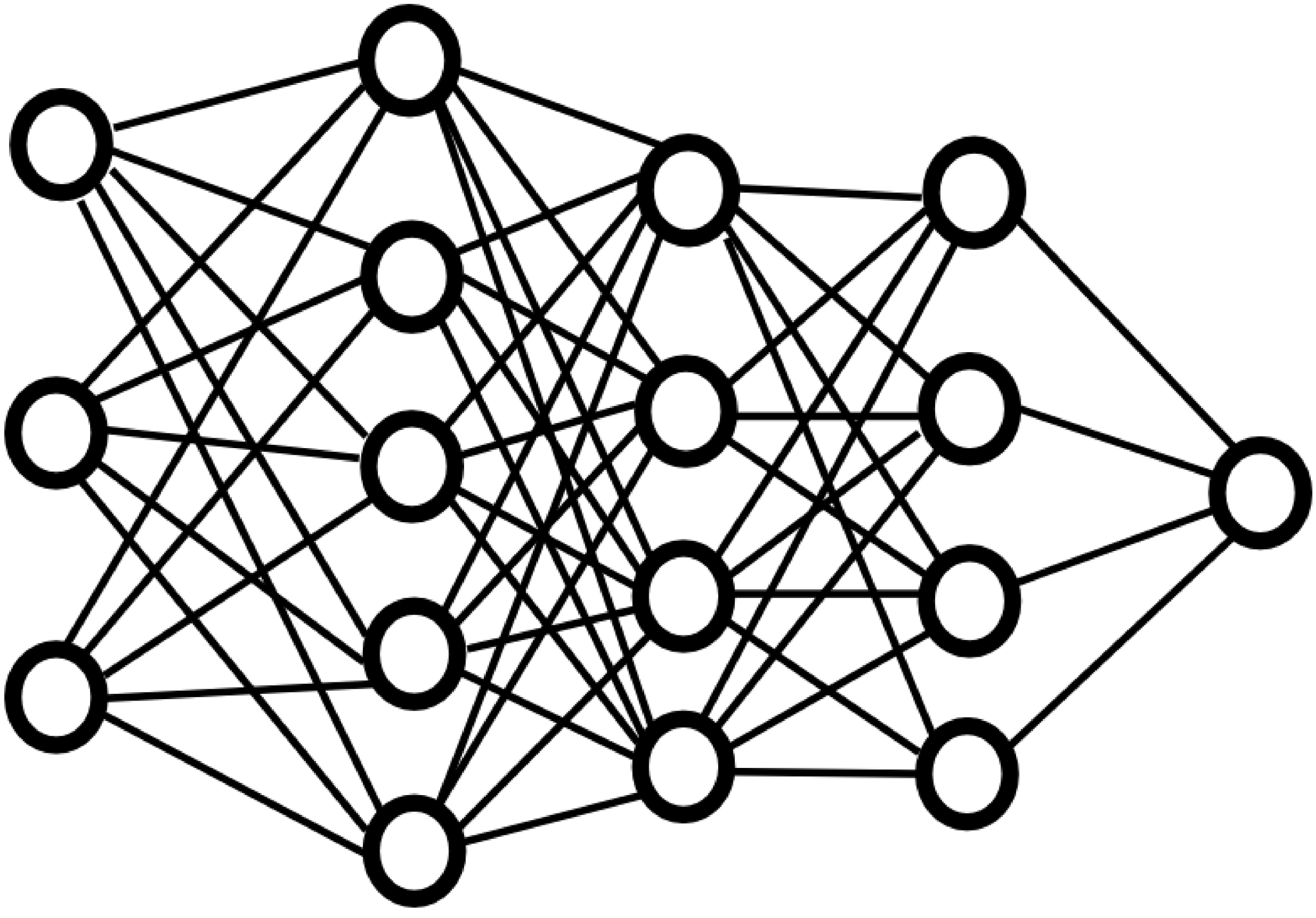
- Contrary to what we could think, adding more layers to a DNN does not necessarily lead to a better performance, both on the training and test set.
- Here is the performance of neural networks with 20 or 56 layers on **CIFAR-10**:



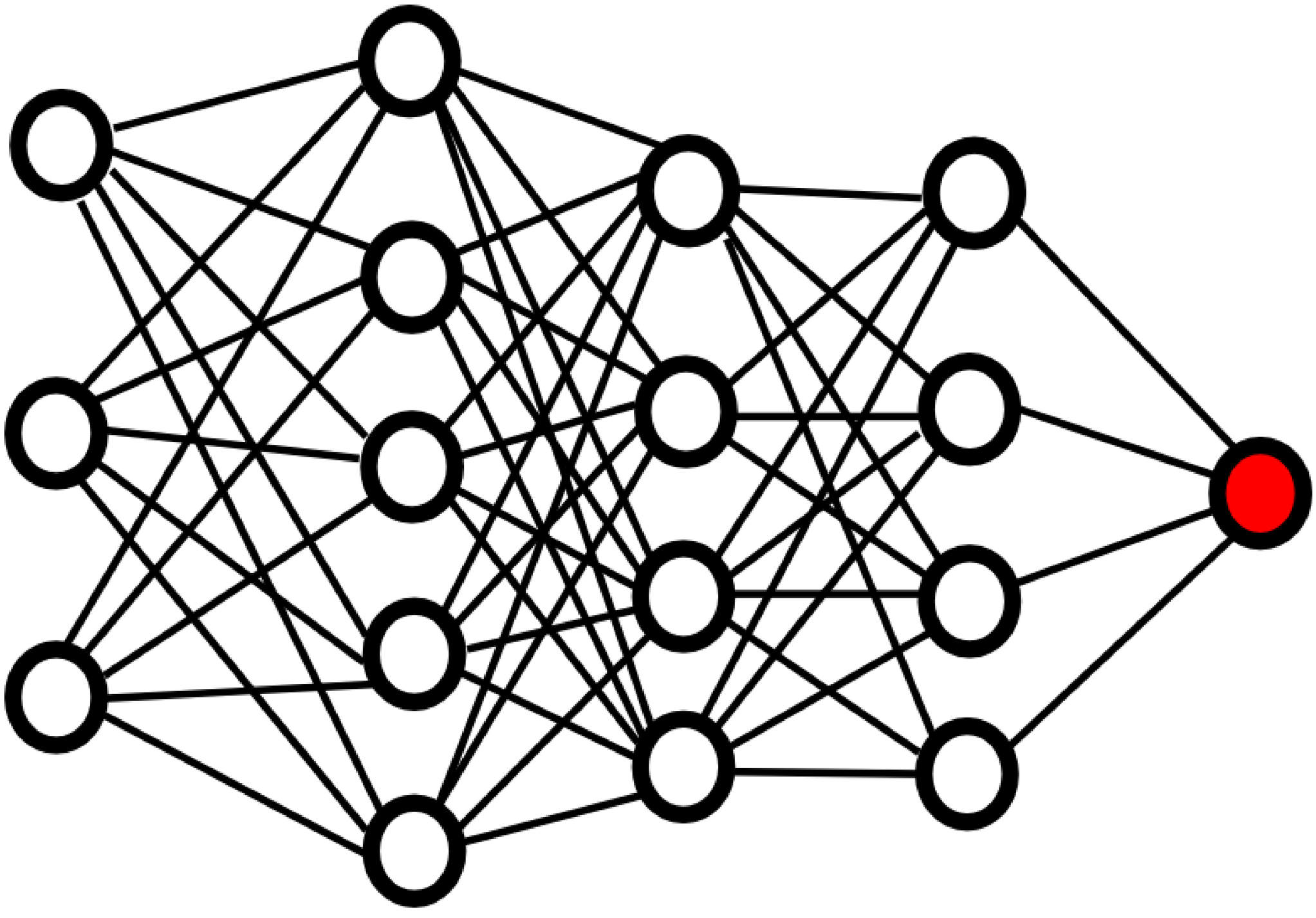
Source: https://towardsdatascience.com/review-resnet-winner-of-ilsvrc-2015-image-classification-localization-detection-e39402bfa5d8

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

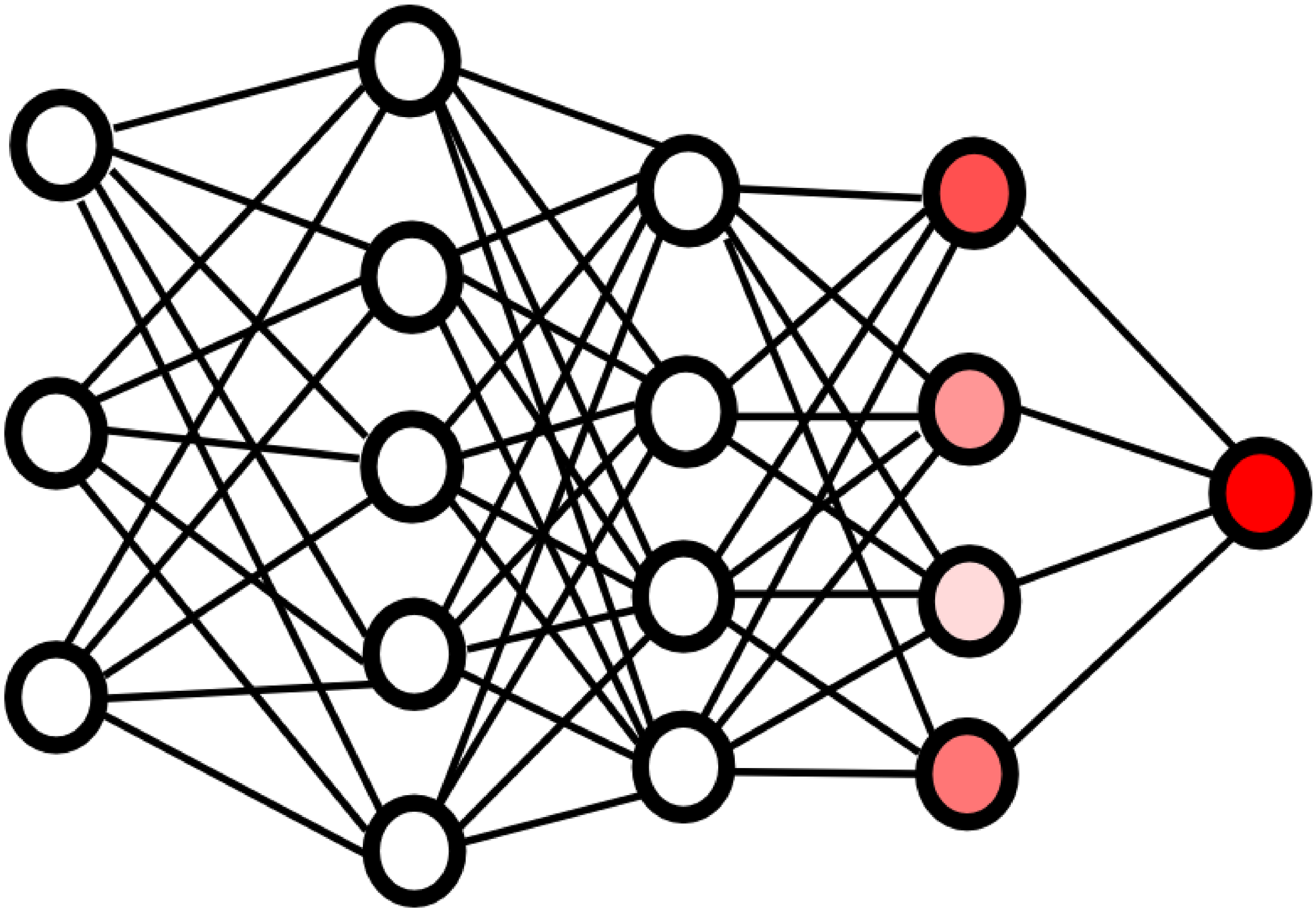
Vanishing Gradient problem



Vanishing Gradient problem



Vanishing Gradient problem



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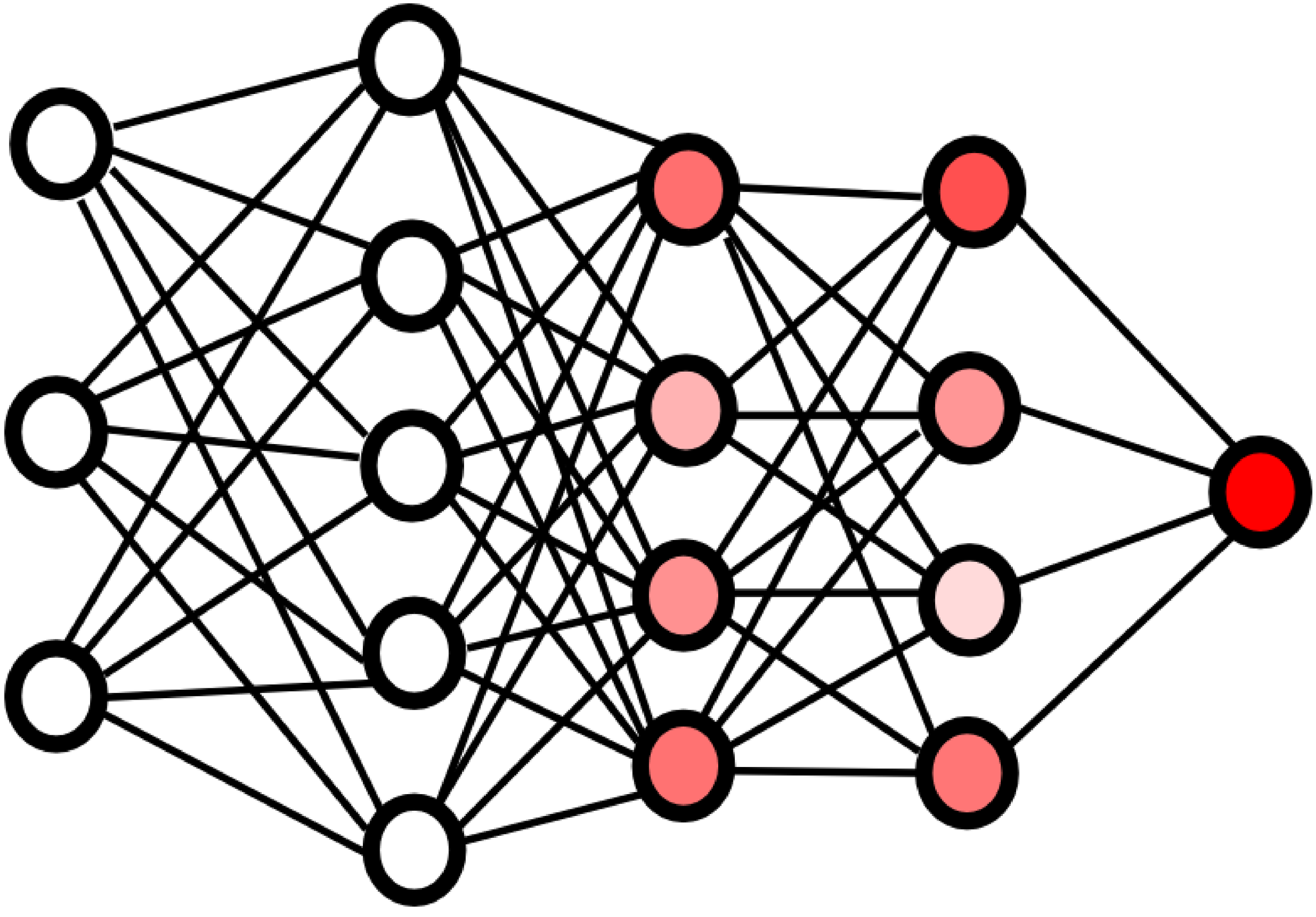

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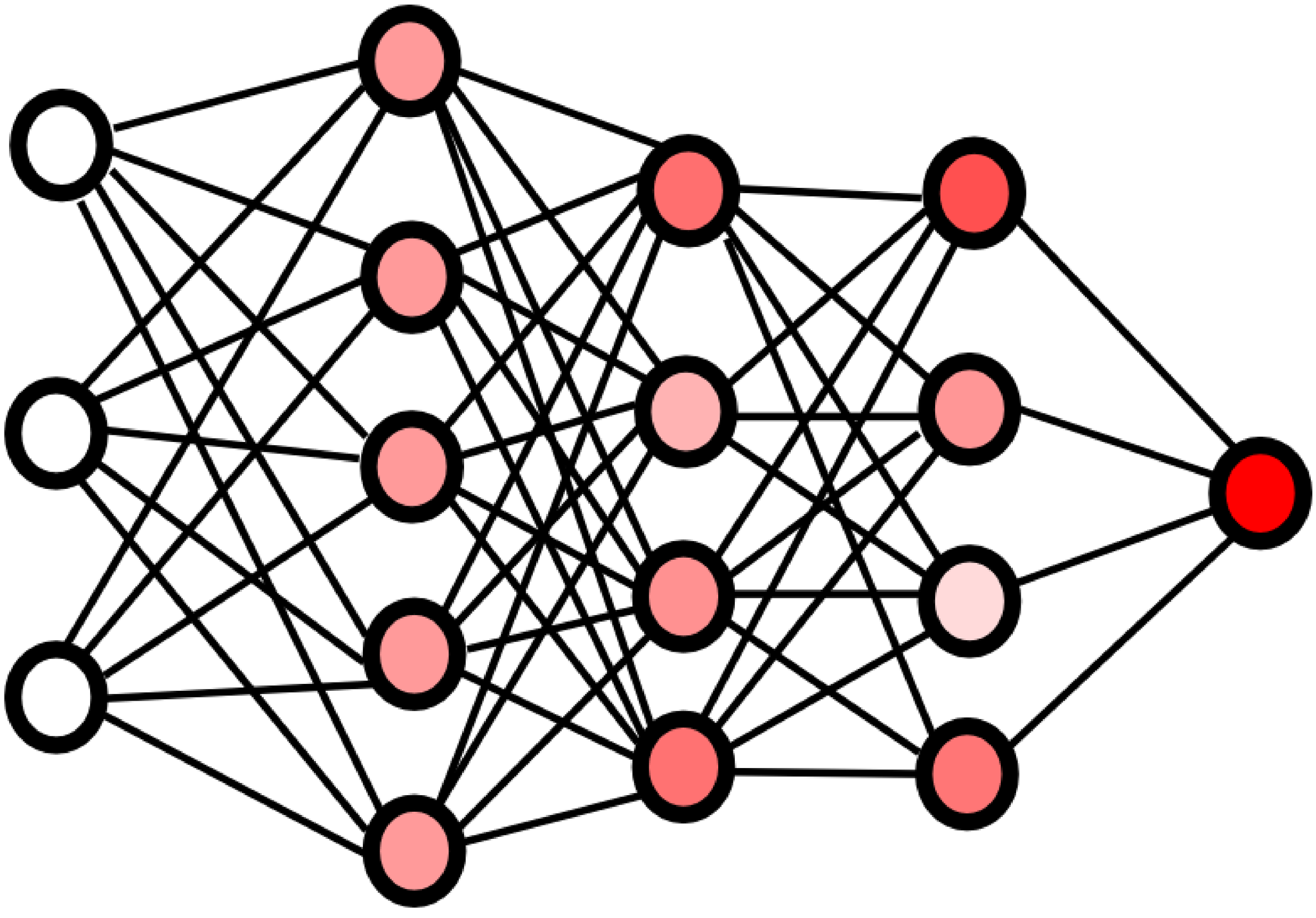

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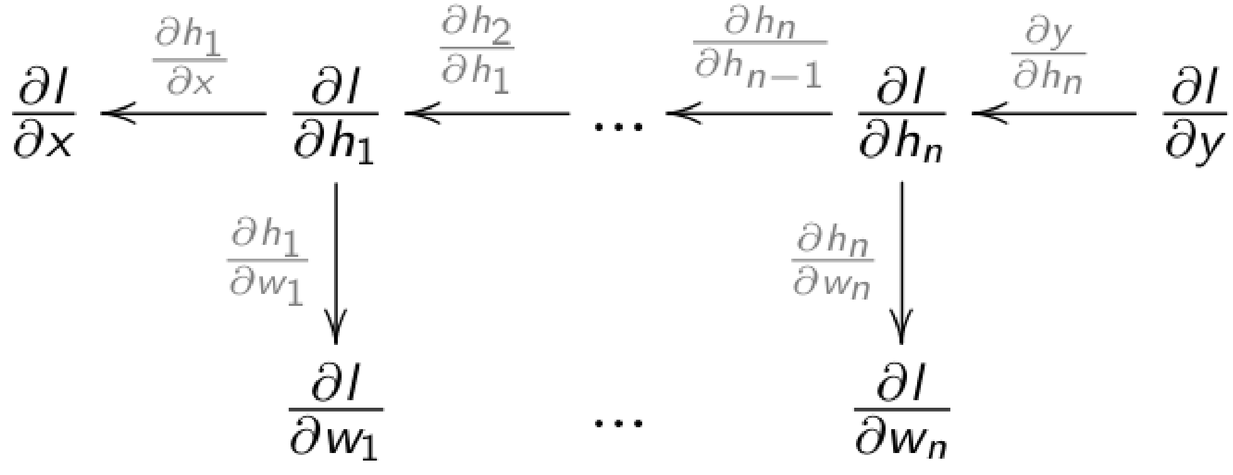


- The gradient of the loss function is repeatedly multiplied by a weight matrix W as it travels backwards in a deep network.

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

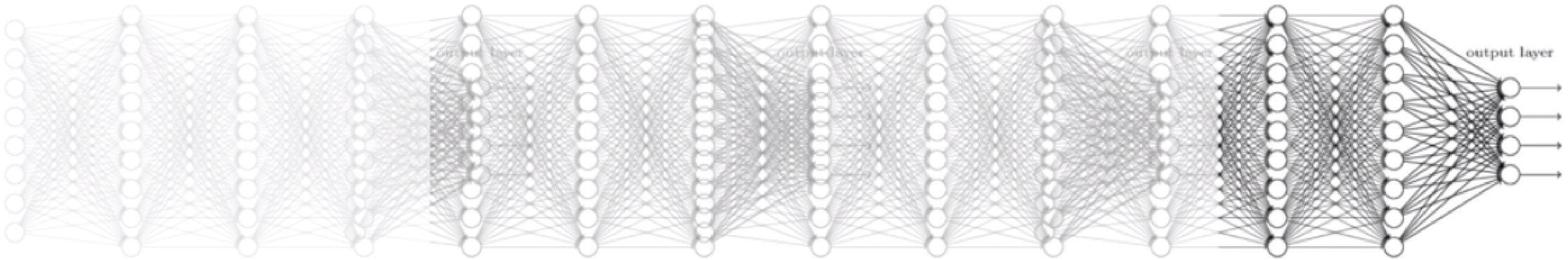
- When it arrives in the first FC layer, the contribution of the weight matrices is comprised between:

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

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

S. Hochreiter. Untersuchungen zu dynamischen neuronalen Netzen. Diploma thesis, Institut f. Informatik, Technische Univ. Munich, 1991.

Vanishing Gradient problem



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

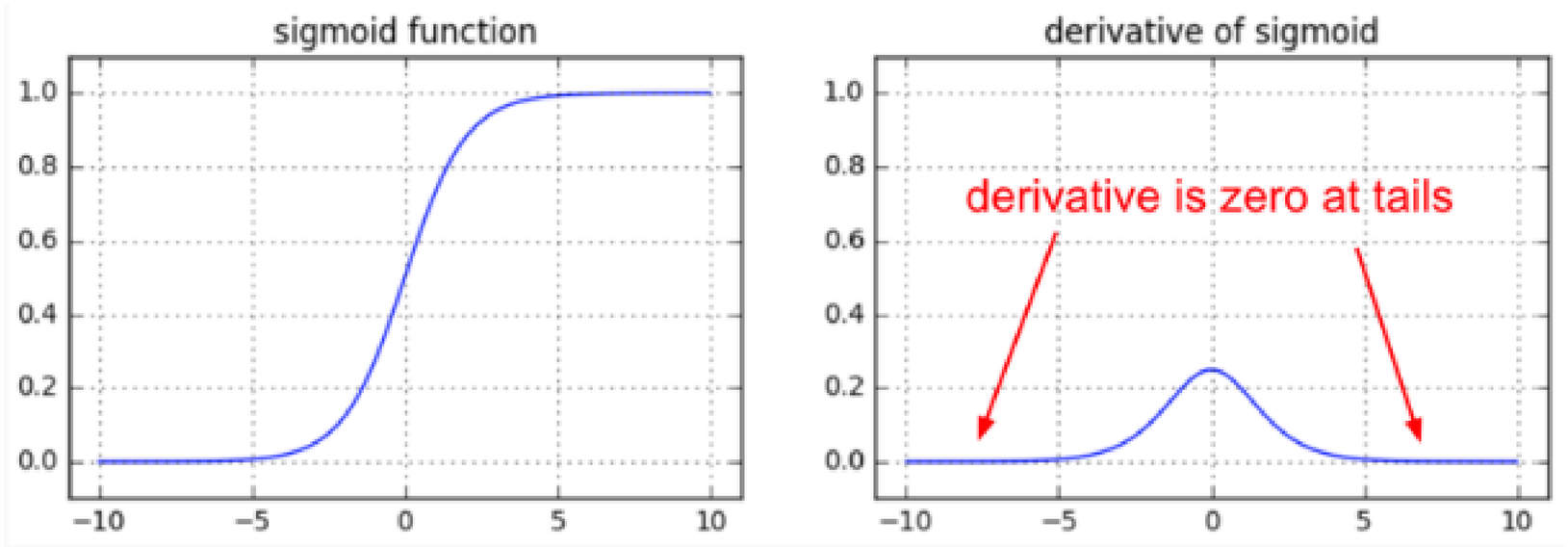
- If $\left|W_{\max}\right| < 1$, then $\left(W_{\max}\right)^d$ is very small for high values of d : **the gradient vanishes**.
- If $\left|W_{\min}\right| > 1$, then $\left(W_{\min}\right)^d$ is very high for high values of d : **the gradient explodes**.
- **Exploding gradients** can be solved by **gradient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

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

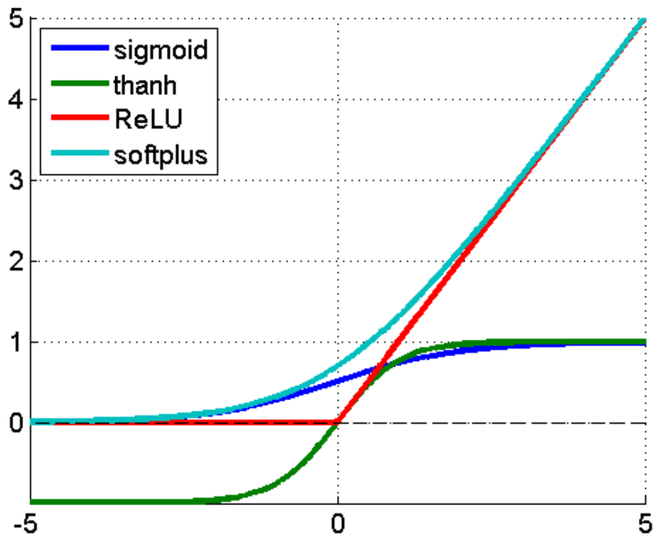
- **Vanishing gradients** are still the current limitation of deep networks.
- Solutions: ReLU, pre-training, batch normalization, **residual networks**…

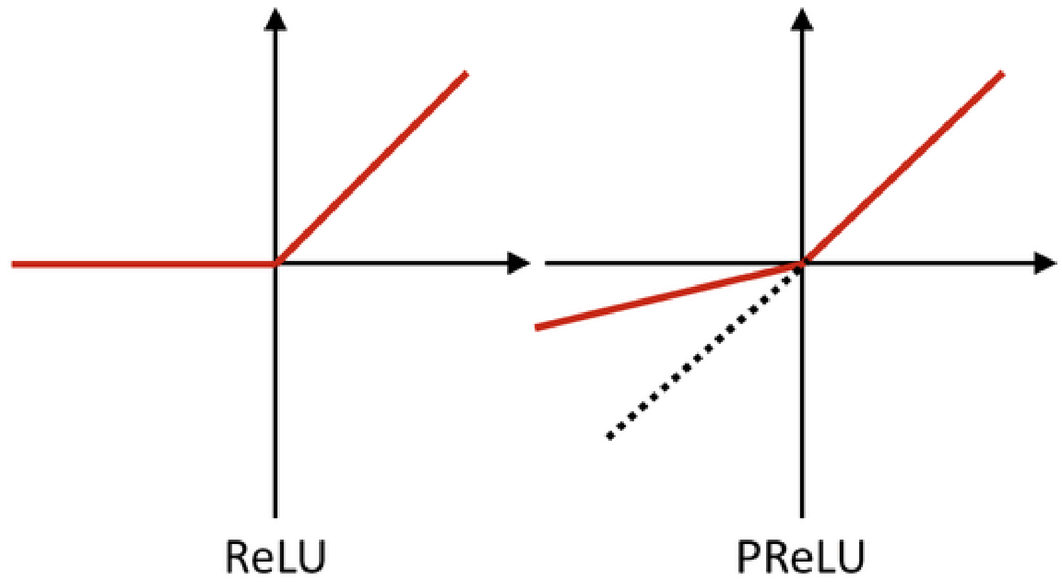
Derivative of the activation function

- 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.

Maas, Hannung, Ng (2013). Rectifier Nonlinearities Improve Neural Network Acoustic Models. ICML.

5 - Deep neural networks in practice

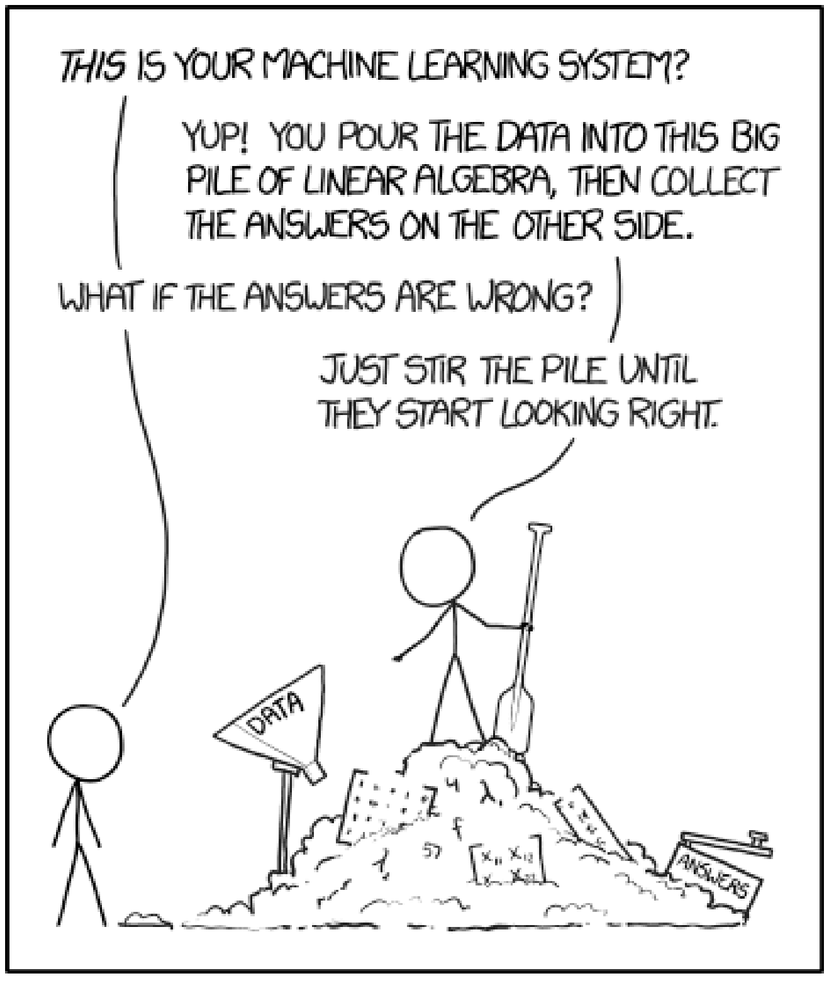
Deep NN in keras

```
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),
    metrics=['accuracy']
)
```

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/