Deep Learning

Romain Tavenard (Université de Rennes 2)
A course @UR2

Contents

- Intro to deep learning
- Fully-connected models
- Images & ConvNets
- (Generative models, …)

Some slides are more important than others…

- Slides marked with this symbol:

  Are considered basic knowledge required to pass the exams

An introduction to deep learning

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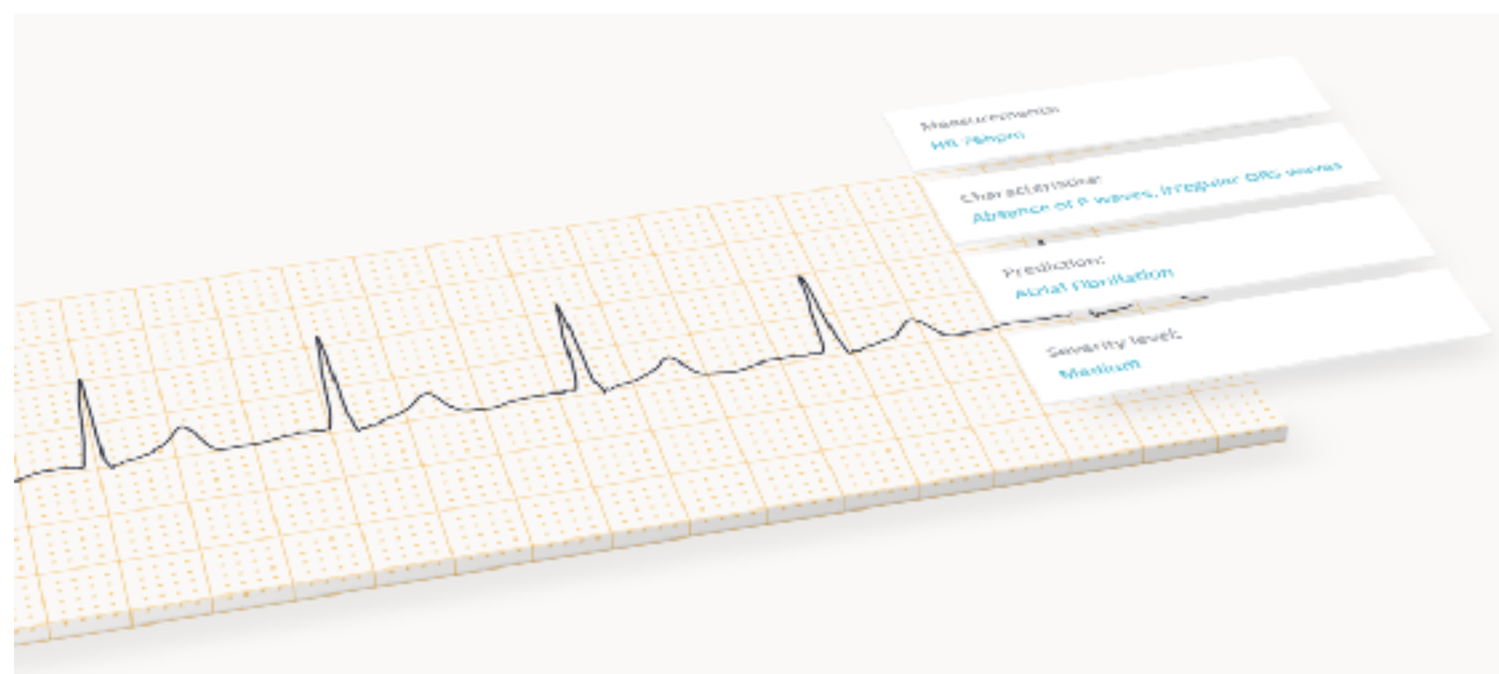
What can deep learning do?

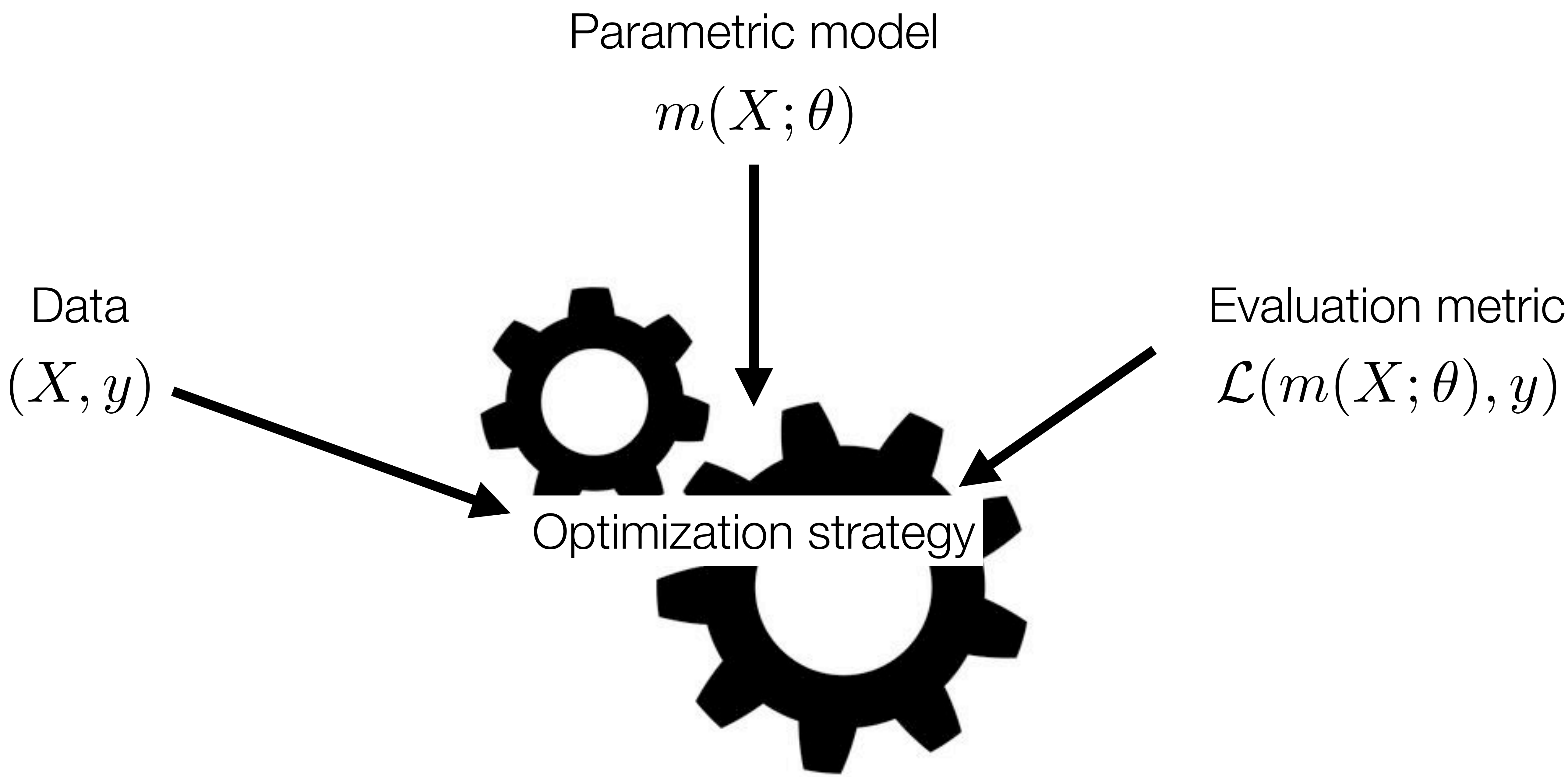
- Skin cancer image classification
  130 000 images
  Error rate : 28 % (human expert 34 %)

- ECG signal classification
  500 000 ECG
  Precision 92.6 %
  (human expert 80.0 %)



Sources : Nature, cardiologs.com, talk by S. Canu

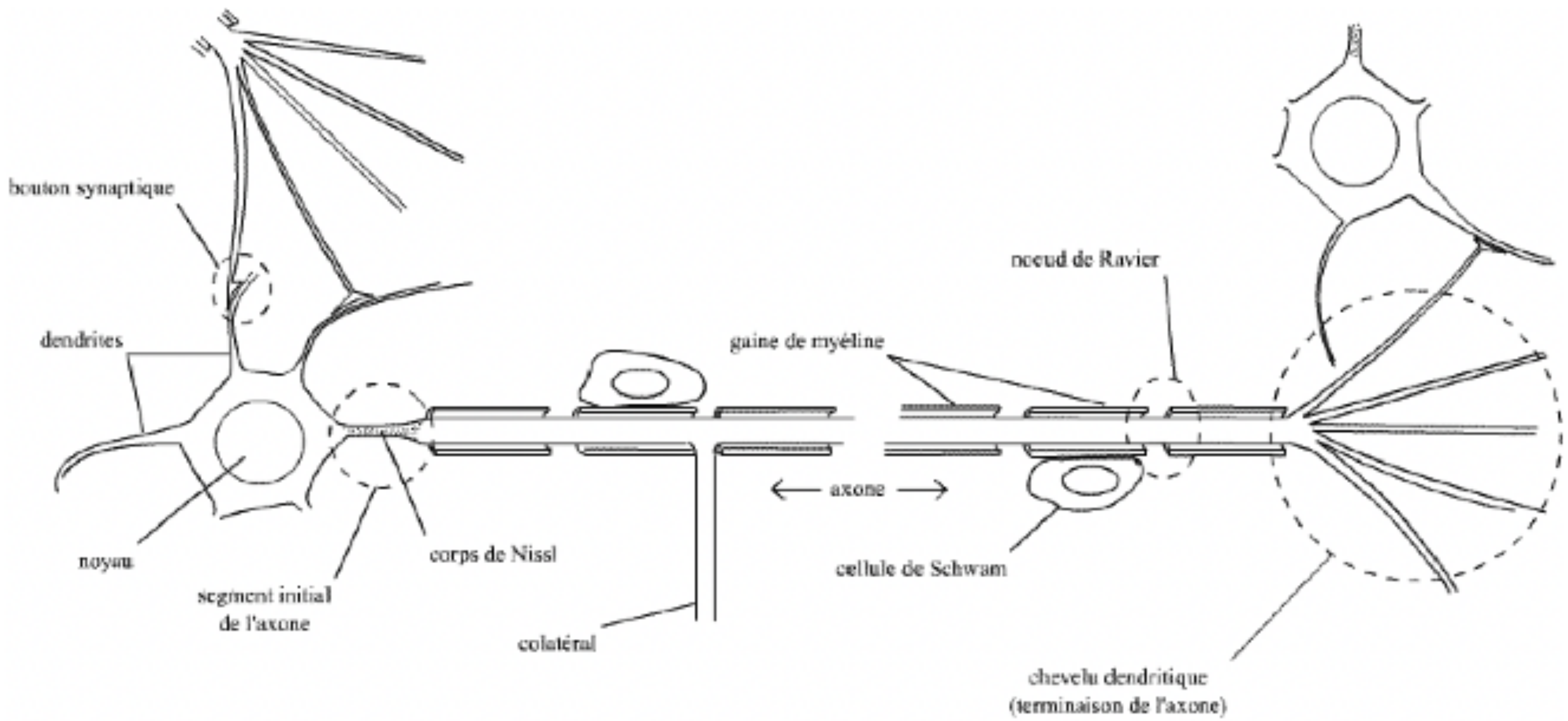
Deep learning in a nutshell

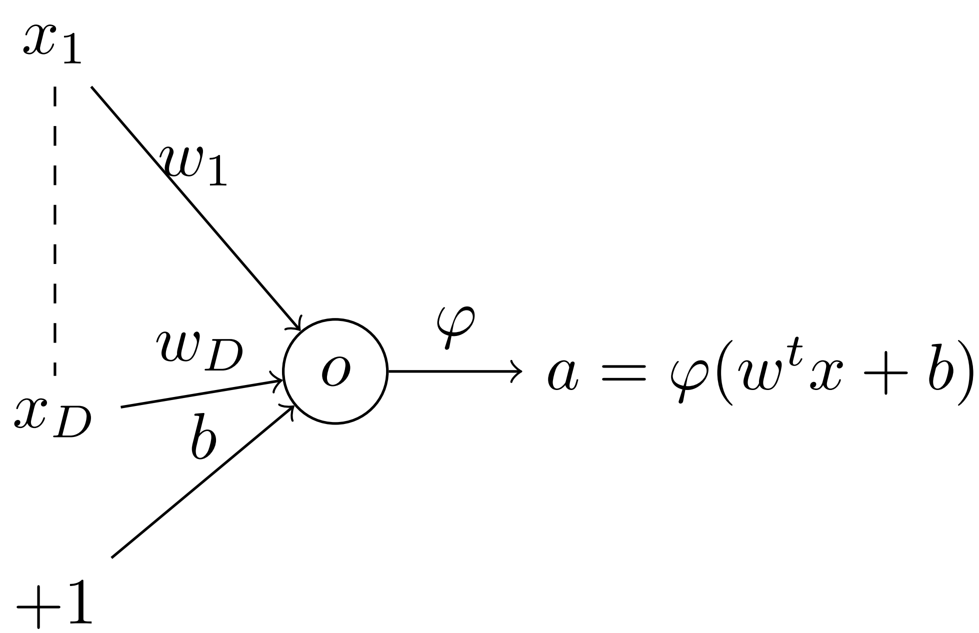


A first example: Linear / logistic regression

- Linear regression
  - **Data:** tabular data with features and targets
  - **Model:** predict output as linear combination of inputs
  - **Loss:** Mean Squared Error
- Logistic regression
  - **Data:** categorical targets
  - **Model:** linear + activation function
  - **Loss:** Cross-entropy (aka logistic loss)

Our first model: the Perceptron
Formal neuron by (McCulloch & Pitts, 1943)





φ activation function

a neuron response

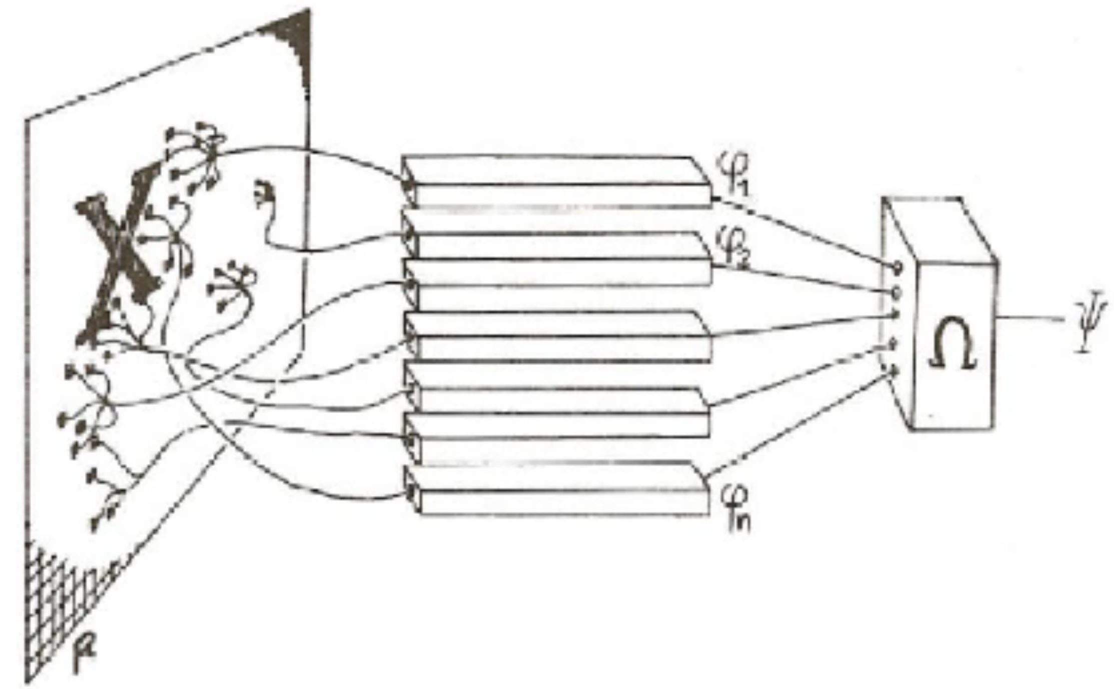
w, b weight, bias

Learning with the Perceptron (Rosenblatt, 1957)

- Problem statement
  - Given pairs of input-output data x_i, y_i
  - Find w such that:

$$\forall i,\ \varphi(w^t x_i) \approx y_i$$

  - To do so:
    - Gradient descent

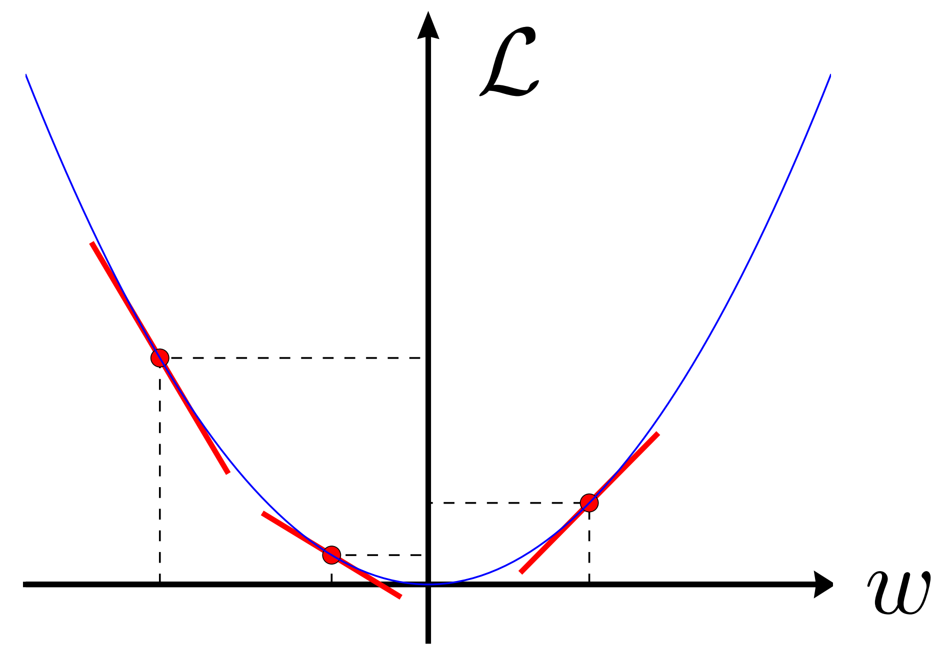


Source : (Minsky & Papert, 1969)

General optimization strategy: Gradient descent

1. Pick a (differentiable) loss function to be minimized

   eg. $$\mathcal{L}(w, \{x_i, y_i\}) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}_i(w, x_i, y_i) = \frac{1}{n}\sum_{i=1}^{n} (\varphi(w^t x_i) - y_i)^2$$

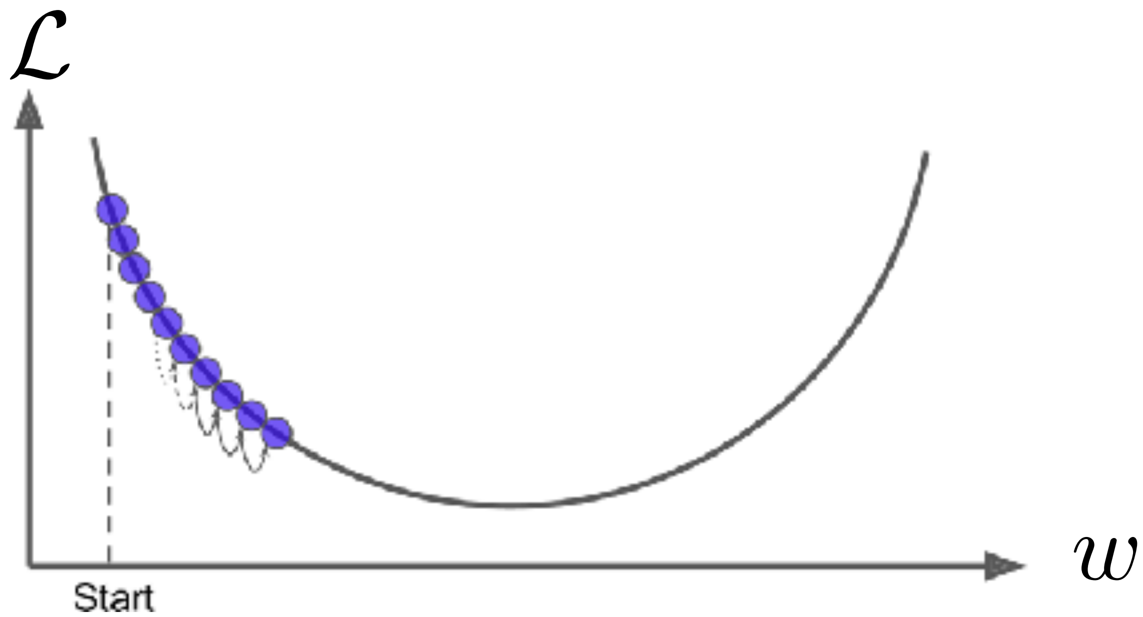


2. Use gradient descent

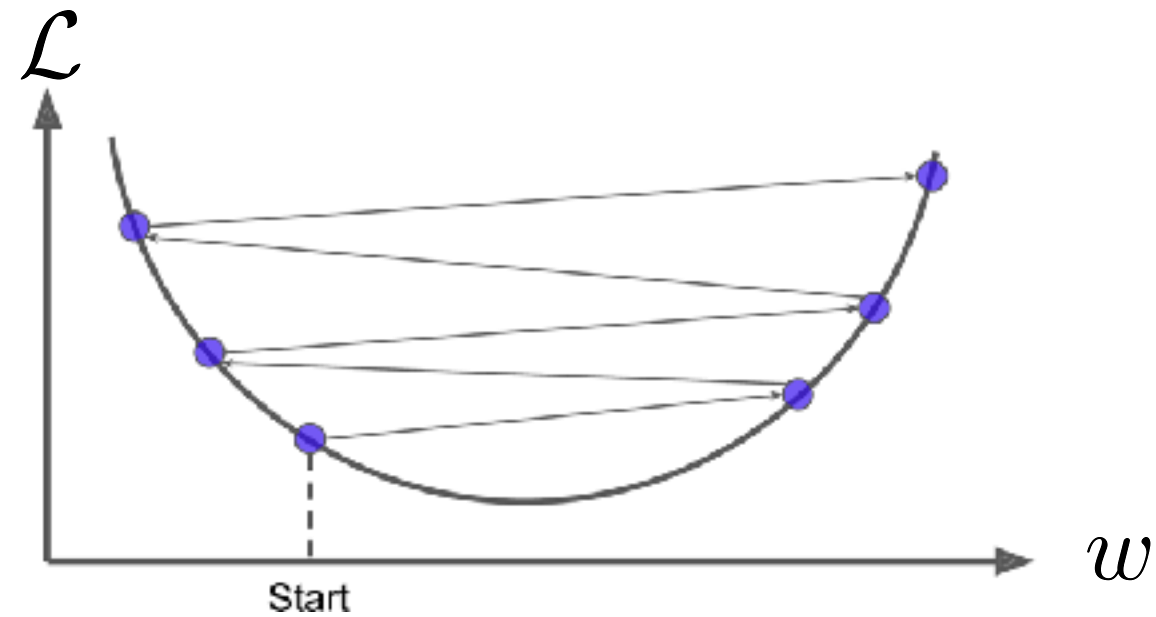
Algorithm 1: Gradient Descent

Data: $\mathcal{D}$: a dataset
Initialize weights
for e = *1..E* **do**
  `// e is called an epoch`
  for $(x_i, y_i) \in \mathcal{D}$ **do**
    Compute prediction $\hat{y}_i = h(x_i)$
    Compute gradient $\nabla_w \mathcal{L}_i$
  end
  Compute overall gradient $\nabla_w \mathcal{L} = \frac{1}{n}\sum_i \nabla_w \mathcal{L}_i$
  Update parameter w using $\nabla_w \mathcal{L}$
end

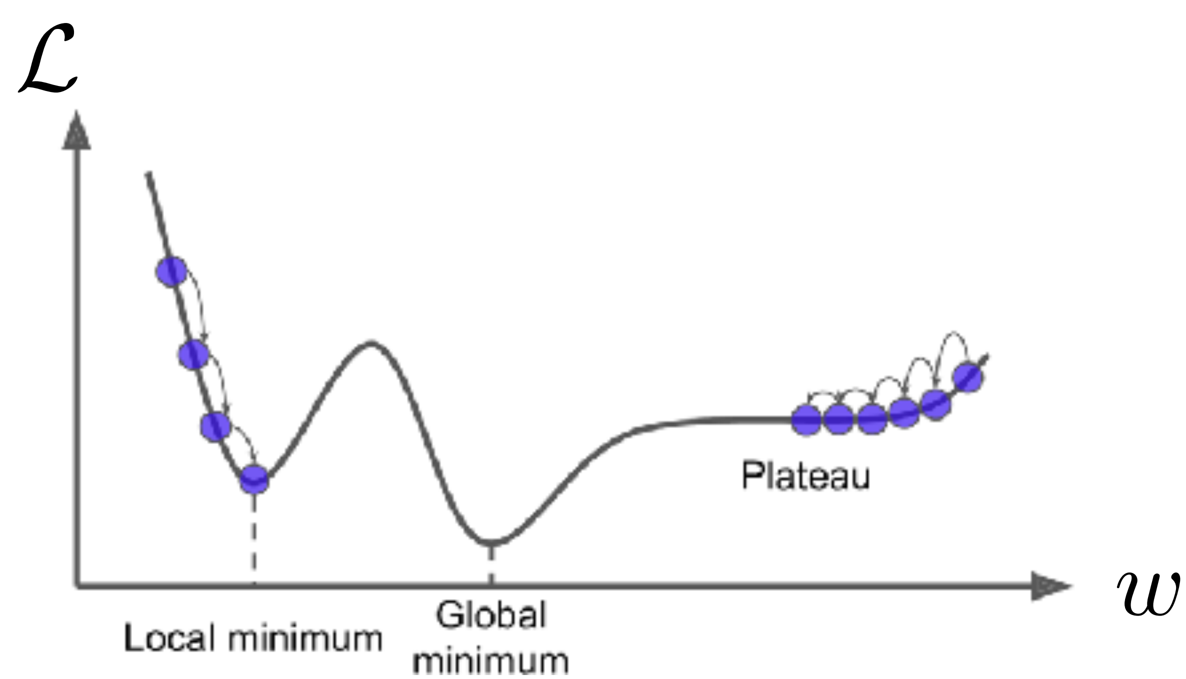
Optimization
Gradient descent in Real Life



Learning rate is too small



Learning rate is too large



Standard pitfalls

Source: "Hands-On Machine Learning with Scikit-Learn and TensorFlow", A. Géron

Optimization
Stochastic Gradient Descent

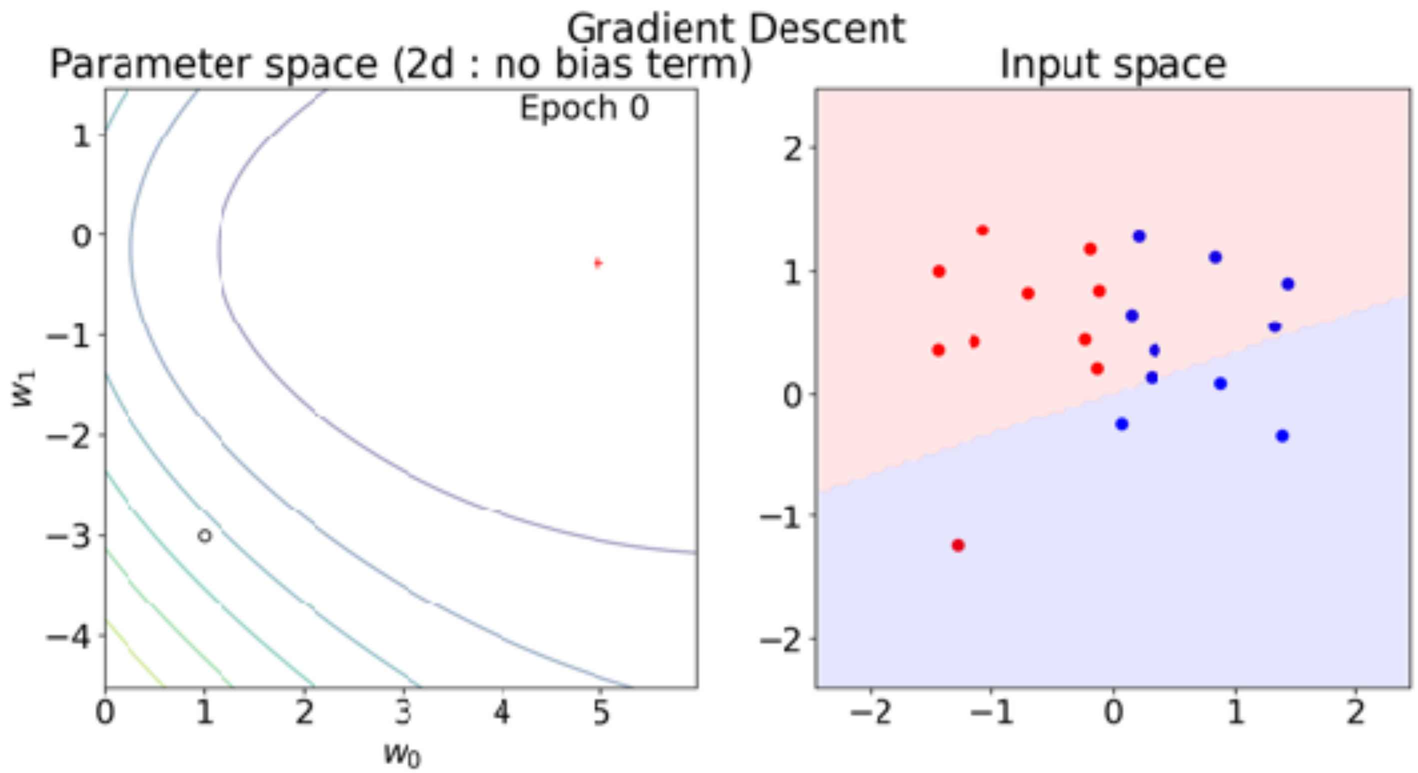
Algorithm 1: Gradient Descent

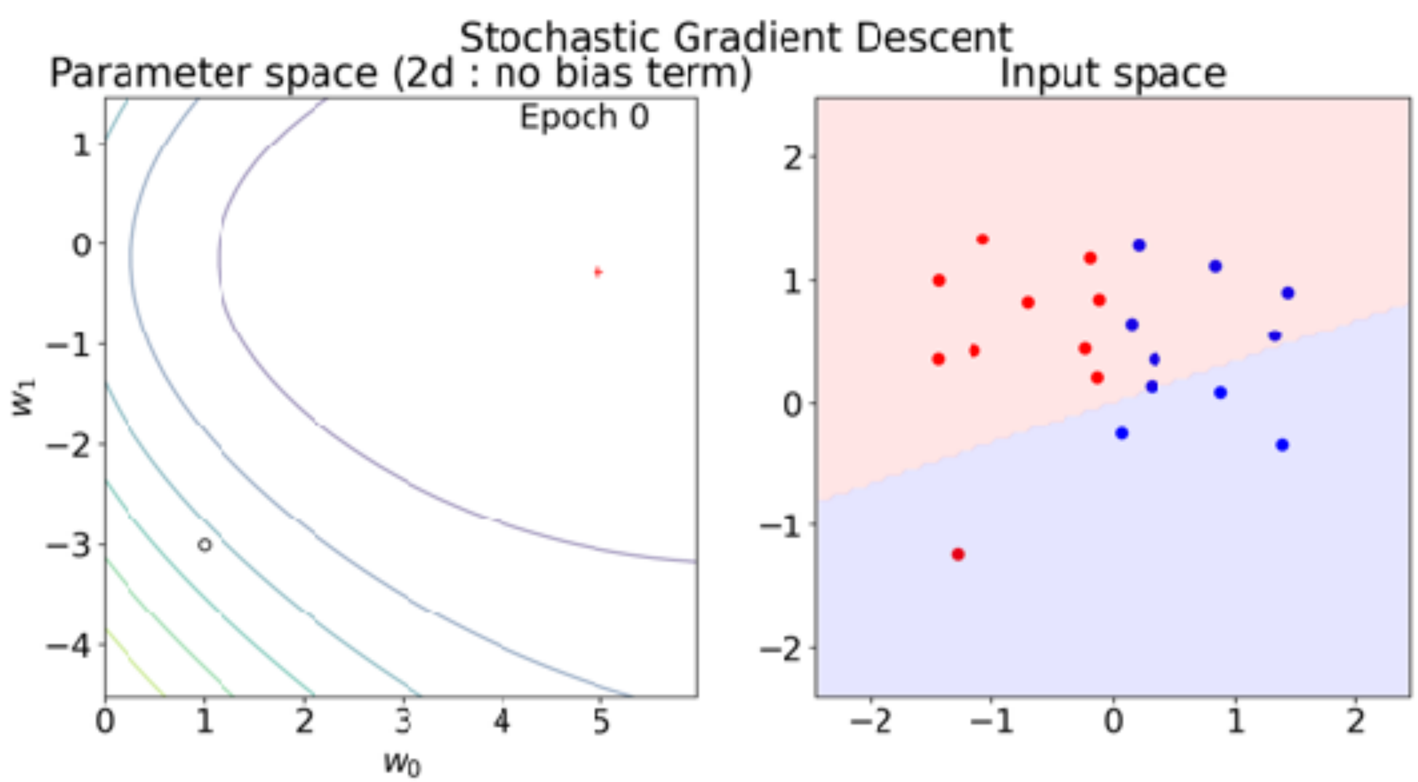
Data: $\mathcal{D}$: a dataset
Initialize weights
for $e = 1..E$ **do**
  `// e is called an epoch`
  for $(x_i, y_i) \in \mathcal{D}$ **do**
    Compute prediction $\hat{y}_i = h(x_i)$
    Compute gradient $\nabla_w \mathcal{L}_i$
  end
  Compute overall gradient $\nabla_w \mathcal{L} = \frac{1}{n} \sum_i \nabla_w \mathcal{L}_i$
  Update parameter w using $\nabla_w \mathcal{L}$
end

Algorithm 2: Mini-Batch Stochastic Gradient Descent

Data: $\mathcal{D}$: a dataset
Initialize weights
for $e = 1..E$ **do**
  `// e is called an epoch`
  for $t = 1..n_b$ **do**
    `// t is called an iteration`
    for $i = 1..m$ **do**
      Draw (x_i, y_i) without replacement from t-th minibatch of $\mathcal{D}$
      Compute prediction $\hat{y}_i = h(x_i)$
      Compute gradient $\nabla_w \mathcal{L}_i$
    end
    Compute gradient for the t-th minibatch $\nabla_w \mathcal{L}_{(t)} = \frac{1}{m} \sum_i \nabla_w \mathcal{L}_i$
    Update parameter w using $\nabla_w \mathcal{L}_{(t)}$
  end
end

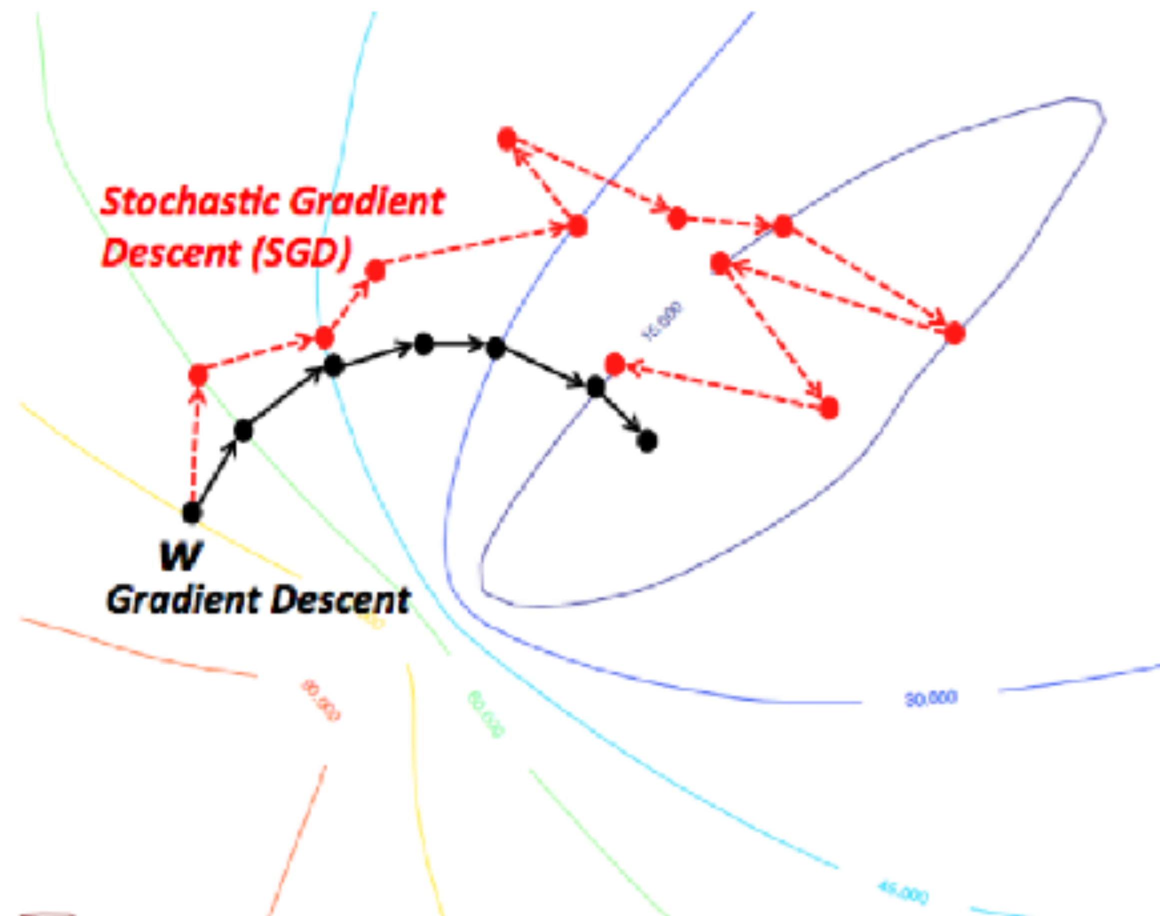
Optimization: Gradient Descent vs Stochastic Gradient Descent (1/2)





Optimization: Gradient Descent vs Stochastic Gradient Descent (2/2)

- Cons
  - Subject to high variance
- Pros
  - Faster weight update (each sample, or each mini batch)
  - Escape local minima in non-convex settings



Source: wikidocs.net/3413

Optimization
SGD variants: a focus on Adam

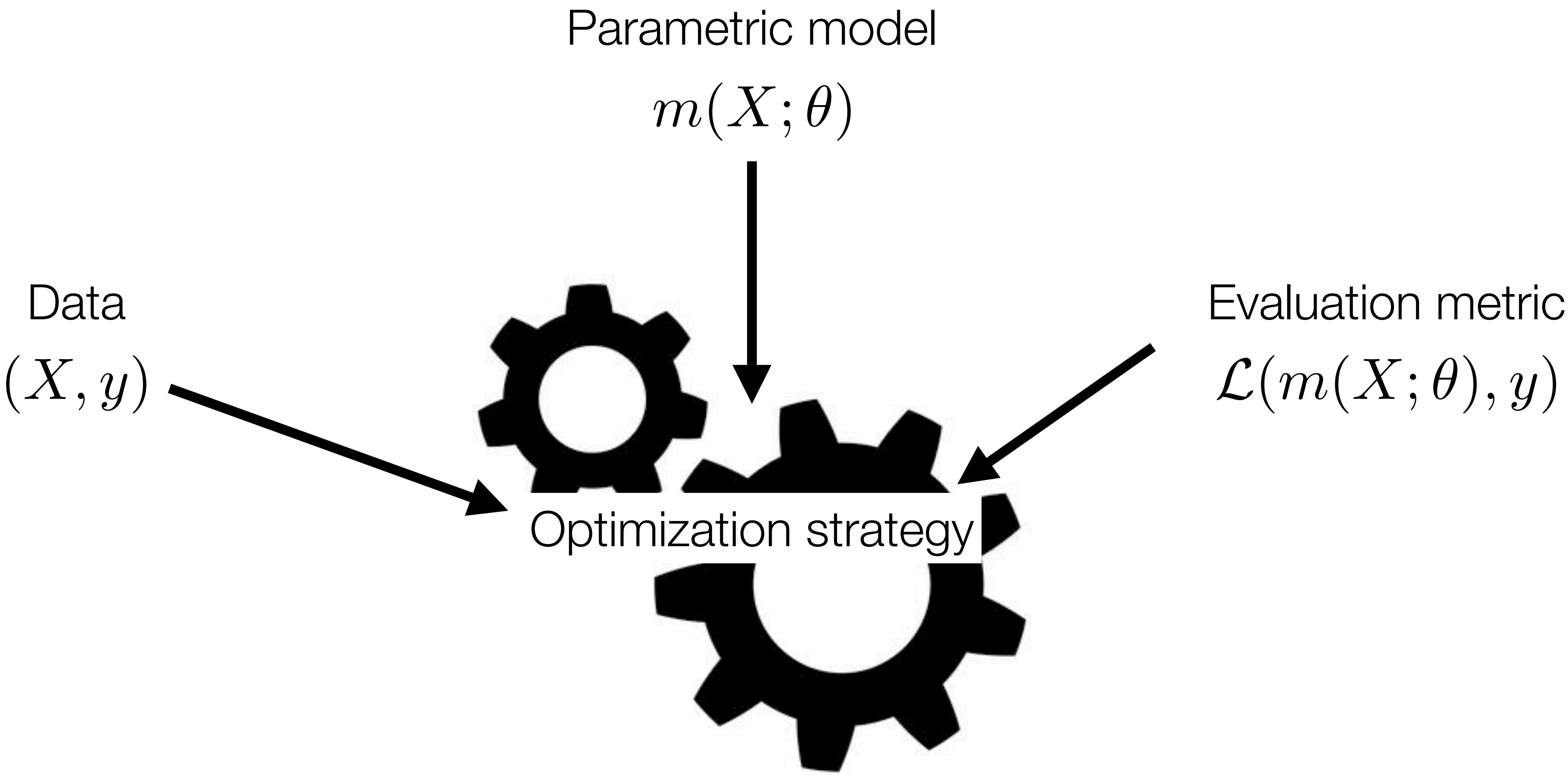
- Adam uses ideas from
  - Momentum [link to distill]
  - AdaGrad

$$\mathbf{m}^{(t+1)} \propto \beta_1 \mathbf{m}^{(t)} + (1 - \beta_1) \nabla_w \mathcal{L}$$

$$\mathbf{s}^{(t+1)} \propto \beta_2 \mathbf{s}^{(t)} + (1 - \beta_2) \nabla_w \mathcal{L} \otimes \nabla_w \mathcal{L}$$

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \rho \mathbf{m}^{(t+1)} \oslash \sqrt{\mathbf{s}^{(t+1)} + \epsilon}$$

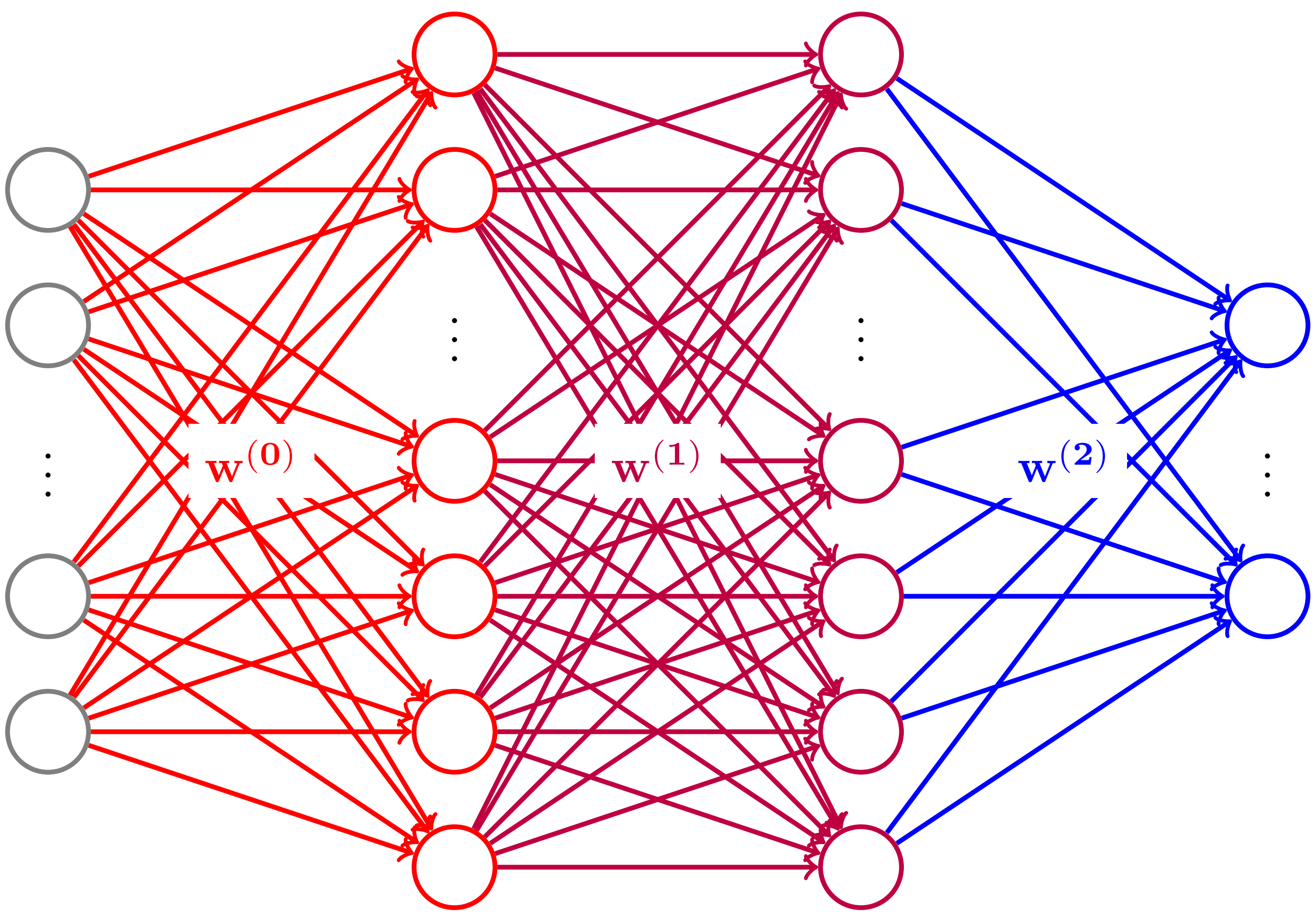
Deep learning in a nutshell



Multi-Layer Perceptron (MLP) model (Rumelhart, Hinton & Williams, 1985)

Definition

A Multilayer perceptron is an acyclic graph of neurons, where neurons are structured in successive layers, beginning by an input layer and finishing with an output layer.



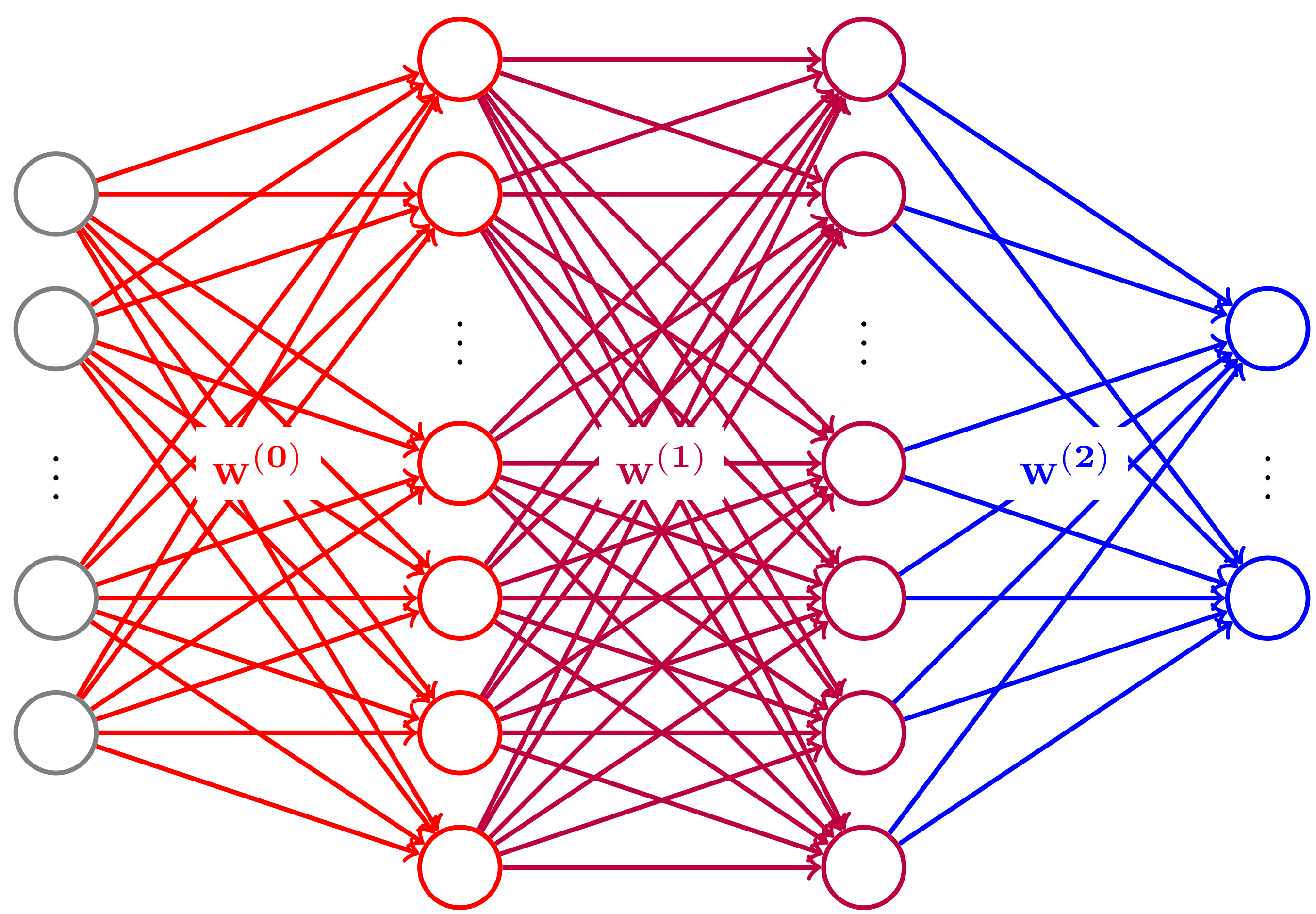
Universal approximation theorem (Cybenko, 1989)

- Under reasonable assumptions on the activation function to be used*
- For any continuous function on a compact g and any precision threshold ε
- There exists a 1-hidden-layer MLP with a finite number of neurons that can approximate g at level ε

*Non-constant, bounded, monotonically increasing, continuous
also holds for some unbounded functions like ReLU, cf. [Somoda & Murata, 2015]

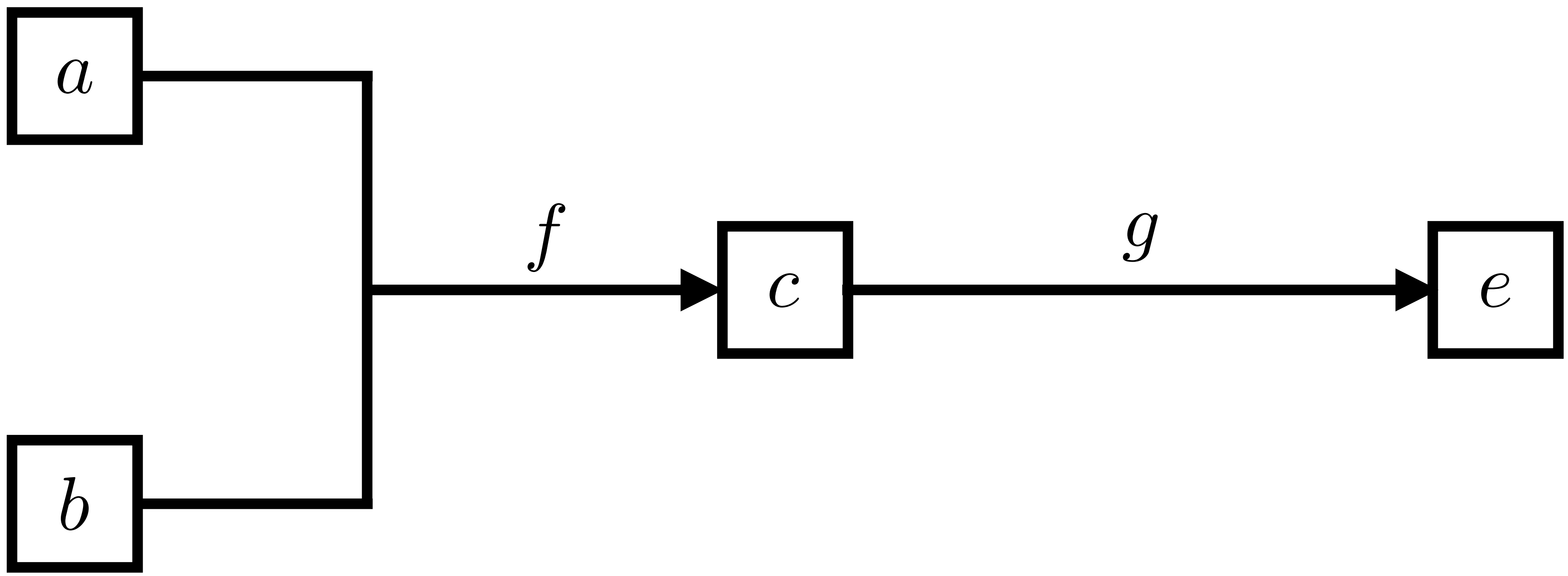
Optimizing multi-layer perceptron parameters

- Who wants to compute gradients by hand for such networks (and deeper ones)?



$$\hat{\mathbf{y}} = \varphi\left[\mathbf{w}^{(\mathbf{2})}\varphi\left(\mathbf{w}^{(\mathbf{1})}\varphi(\mathbf{w}^{(\mathbf{0})}\mathbf{x} + b^{(0)}) + b^{(1)}\right) + b^{(2)}\right]$$

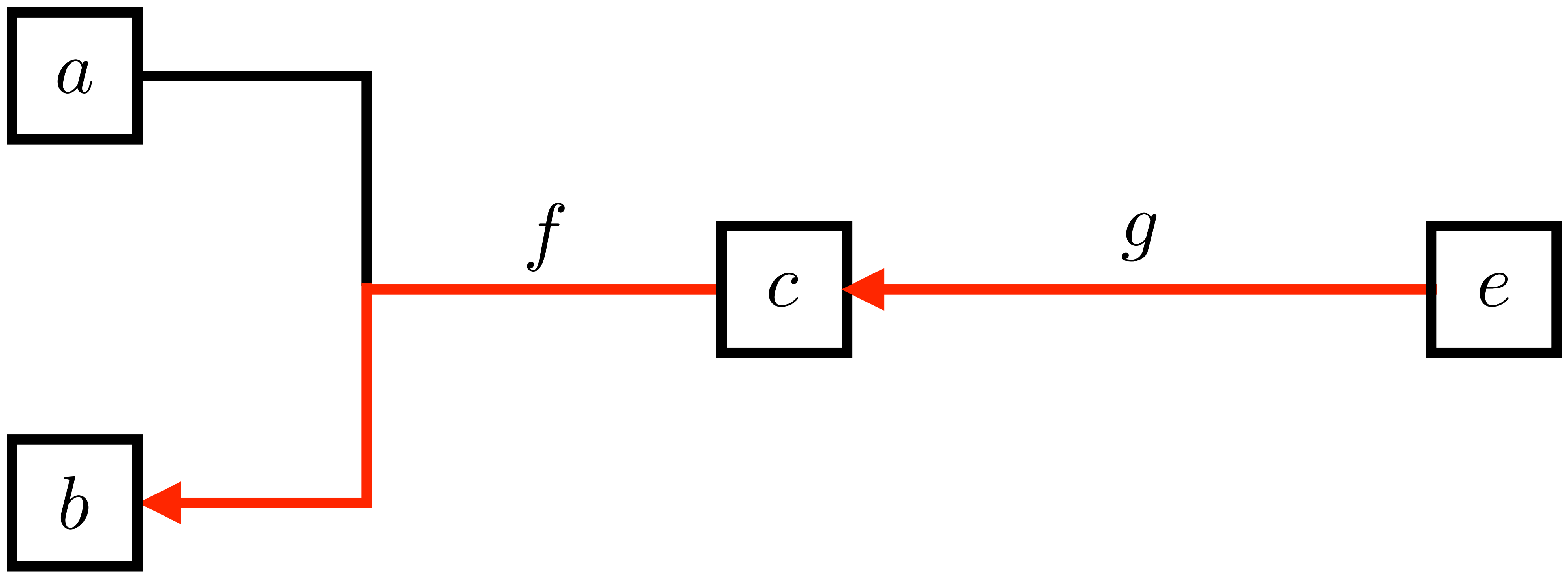
Optimizing multi-layer perceptron parameters
Automatic differentiation to the rescue!



$$c = f(a, b)$$

$$e = g(c)$$

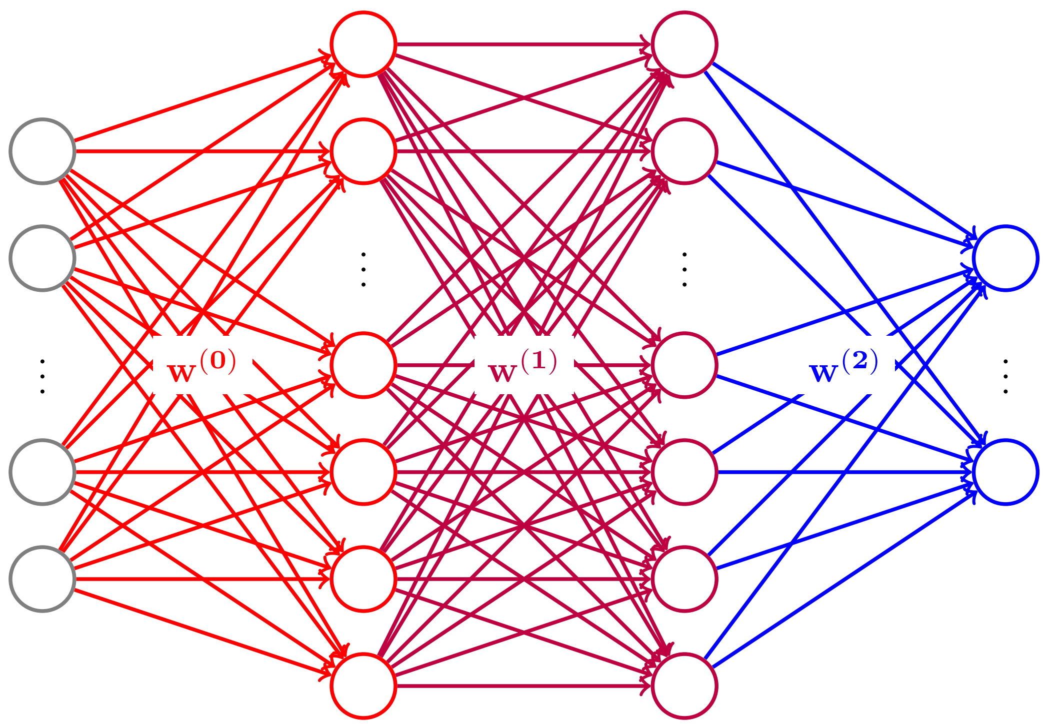
Optimizing multi-layer perceptron parameters
Automatic differentiation to the rescue!

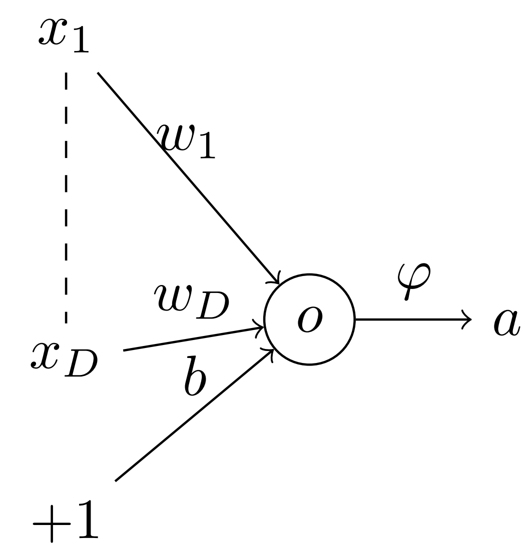


$$c = f(a, b)$$
$$e = g(c)$$

$$\frac{\partial e}{\partial b} = \underbrace{\left.\frac{\partial e}{\partial c}\right|_{c=c_0}}_{g'(c_0)} \cdot \left.\frac{\partial c}{\partial b}\right|_{b=b_0}$$

Optimization
Neural networks and back-propagation





$$\frac{\partial \mathcal{L}}{\partial w^{(2)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial w^{(2)}}$$

$$\frac{\partial \mathcal{L}}{\partial w^{(1)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial o^{(2)}} \frac{\partial o^{(2)}}{\partial w^{(1)}}$$

$$\frac{\partial \mathcal{L}}{\partial w^{(0)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial o^{(2)}} \frac{\partial o^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial o^{(1)}} \frac{\partial o^{(1)}}{\partial w^{(0)}}$$

$$\frac{\partial a^{(l)}}{\partial o^{(l)}} = \varphi'(o^{(l)})$$

$$\frac{\partial o^{(l)}}{\partial a^{(l-1)}} = w^{(l-1)}$$

Neural networks and back-propagation: Losses

$$\frac{\partial \mathcal{L}}{\partial w^{(0)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial o^{(2)}} \frac{\partial o^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial o^{(1)}} \frac{\partial o^{(1)}}{\partial w^{(0)}}$$

- Requirement
  - $\mathcal{L}$ should be differentiable wrt. to the net's output
- Standard losses
  - Mean Squared Error (MSE) for regression

$$\mathcal{L}(x_i, y_i; \theta) = (m(x_i; \theta) - y_i)^2$$

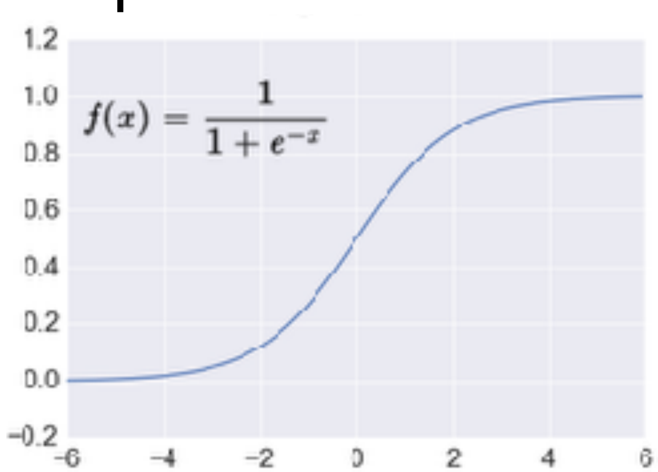
  - Cross-entropy for classification

$$\mathcal{L}(x_i, y_i; \theta) = -\log P_\theta(y = y_i | x_i)$$

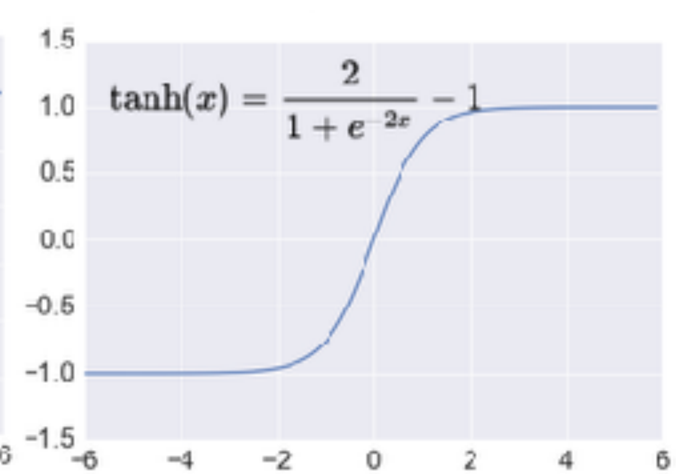
Neural networks and back-propagation: Activation functions

$$\frac{\partial \mathcal{L}}{\partial w^{(0)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial o^{(2)}} \frac{\partial o^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial o^{(1)}} \frac{\partial o^{(1)}}{\partial w^{(0)}} \qquad \frac{\partial a^{(l)}}{\partial o^{(l)}} = \varphi'(o^{(l)})$$

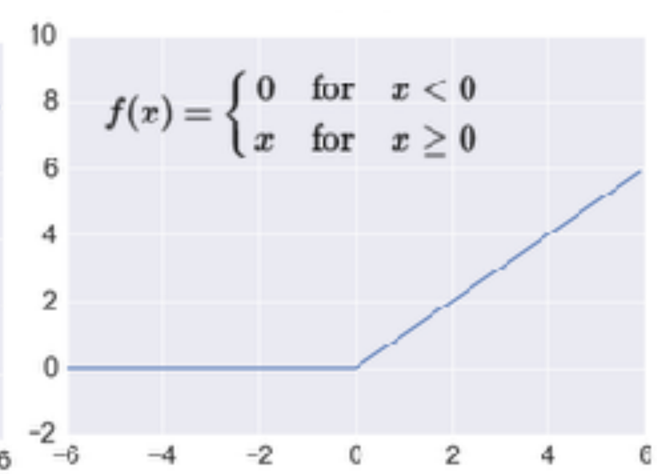
- Important features
  - φ should be differentiable almost everywhere
  - Non-linearities
  - Some linear regime
- Examples



sigmoid



tanh

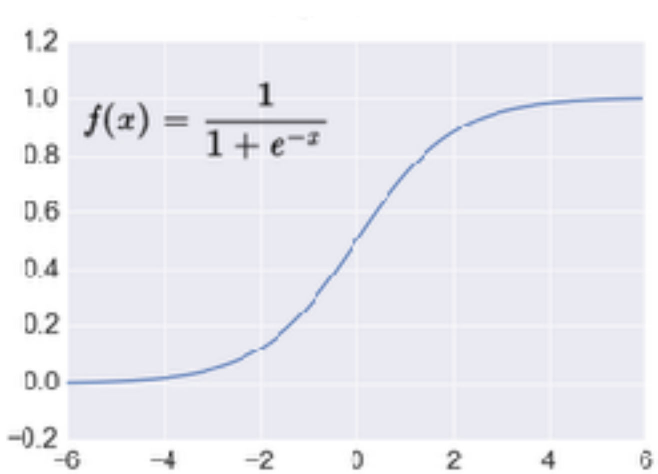


ReLU

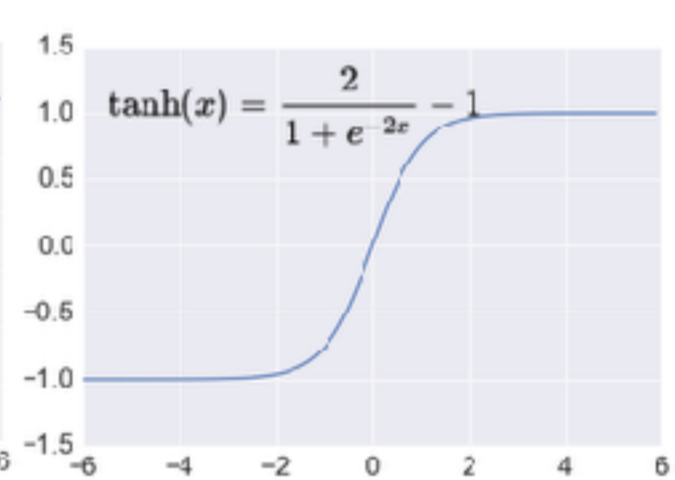
Neural networks and back-propagation: Activation functions: the reign of ReLU

$$\frac{\partial \mathcal{L}}{\partial w^{(0)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial o^{(2)}} \frac{\partial o^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial o^{(1)}} \frac{\partial o^{(1)}}{\partial w^{(0)}} \qquad \frac{\partial a^{(l)}}{\partial o^{(l)}} = \varphi'(o^{(l)})$$

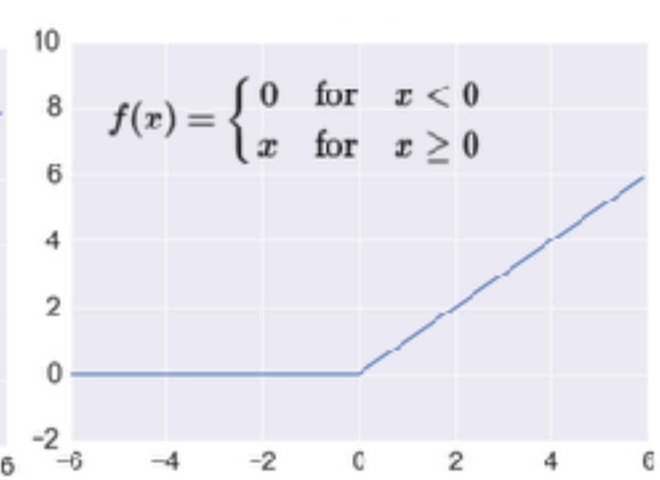
- ReLU has become the default choice over time
- 2 main reasons:
  - cheap to compute (both ReLU and its derivative)
  - vanishing gradients phenomenon (more on that later)



sigmoid



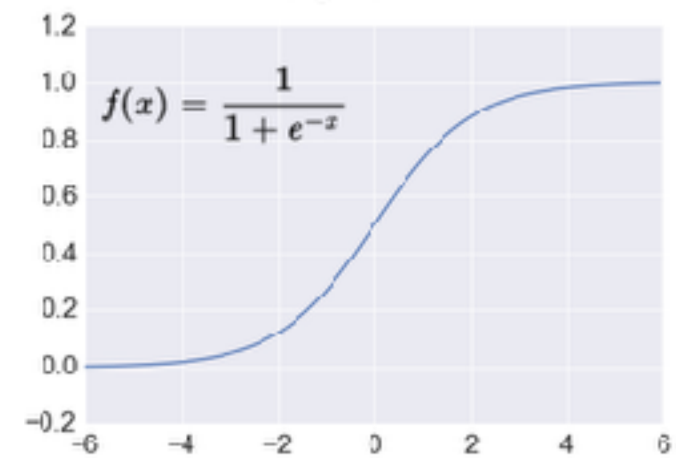
tanh



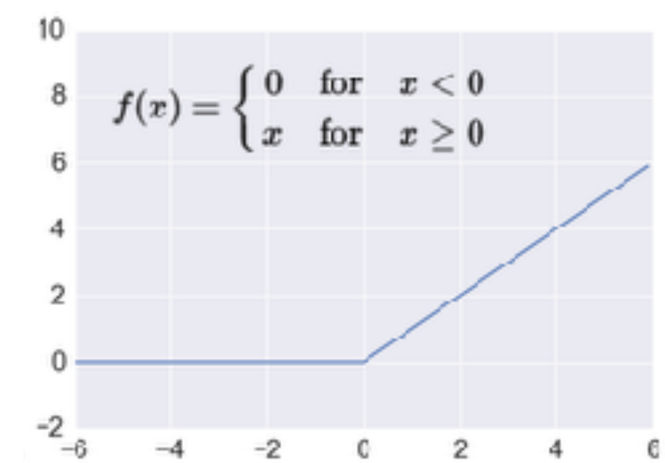
ReLU

Neural networks and back-propagation: activation functions: the case of the output layer

- Output activation functions drive the possible output values:
  - identity ("linear" in keras): any real value
  - ReLU: any positive value
  - sigmoid: any value in [0, 1]
  - softmax: >0 and sums to 1 (across output neurons)



sigmoid



ReLU

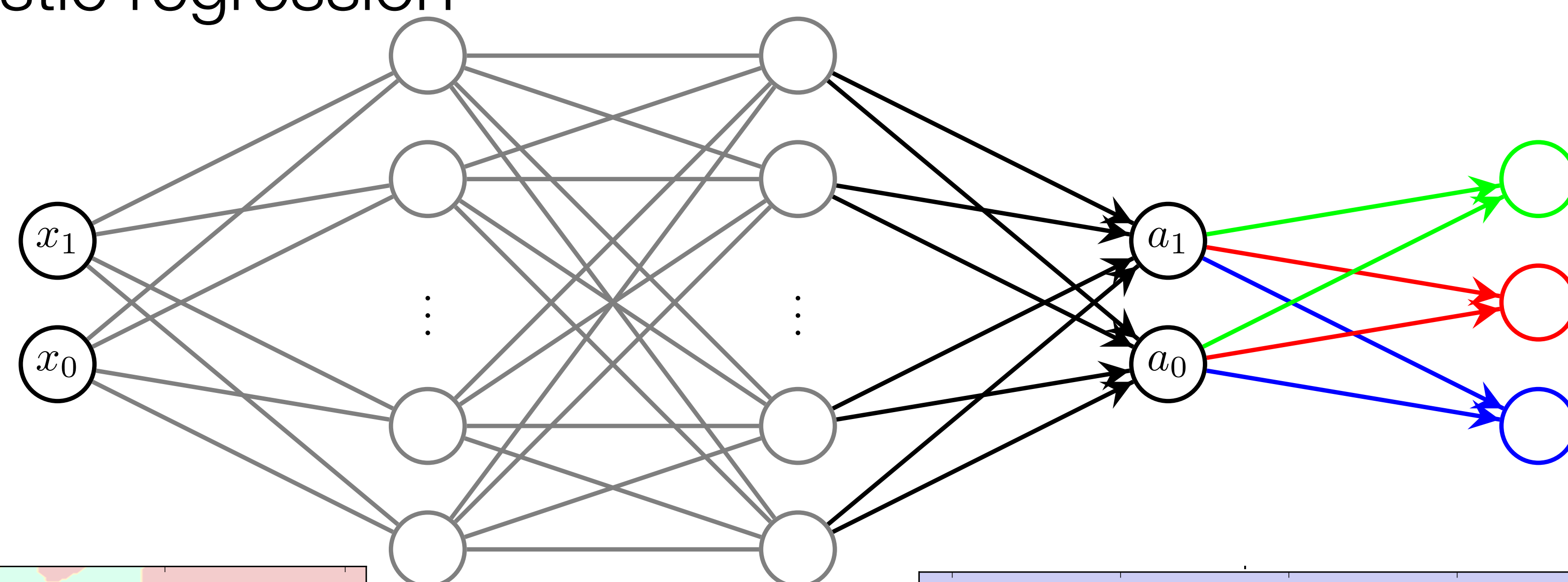
$$\text{soft-max}(o)_i = \frac{e^{o_i}}{\sum_j e^{o_j}}$$

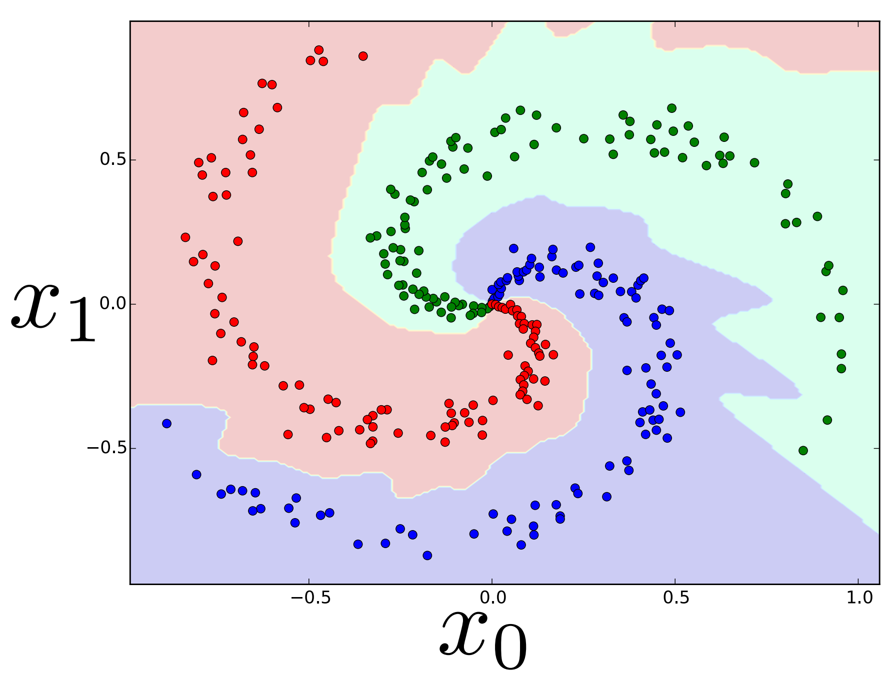
Neural networks and back-propagation: link with keras implementation

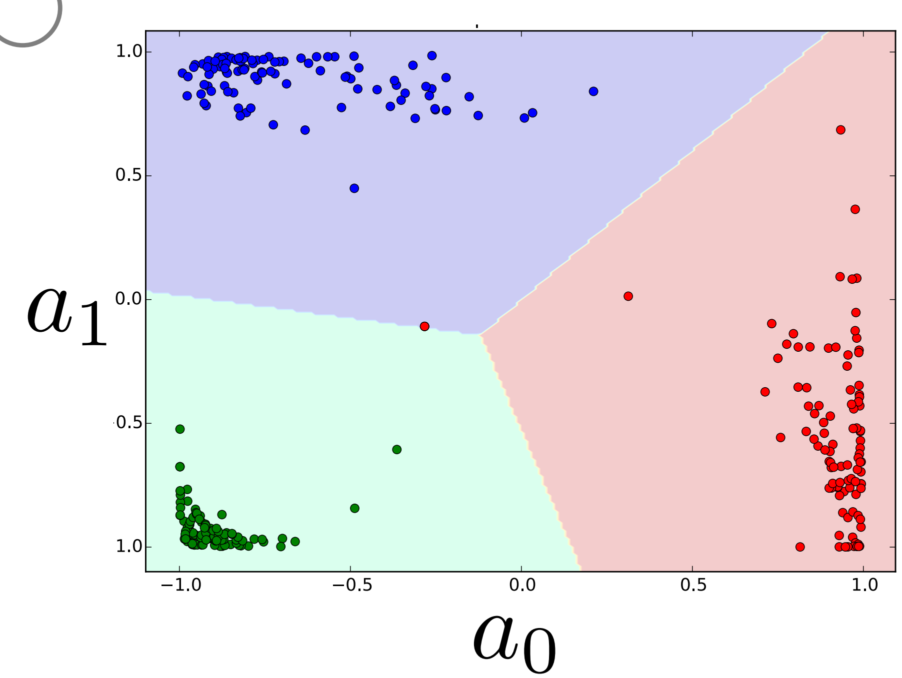
- In keras, these considerations have practical impact:
  - Model structure:
    - Input layer dimension is the number of features in the dataset
    - Output layer has as many units as columns in y
  - Output layer activation:
    - Binary classification: "sigmoid"
    - Multiclass classification: "softmax"
  - Loss function:
    - Binary classification: "binary_crossentropy"
    - Multiclass classification: "categorical_crossentropy"
    - Regression: "mse"

End-to-end learning

- Classification using MLP
  - Hidden layers: non-linear transformations
  - Last layer: logistic regression
- Example







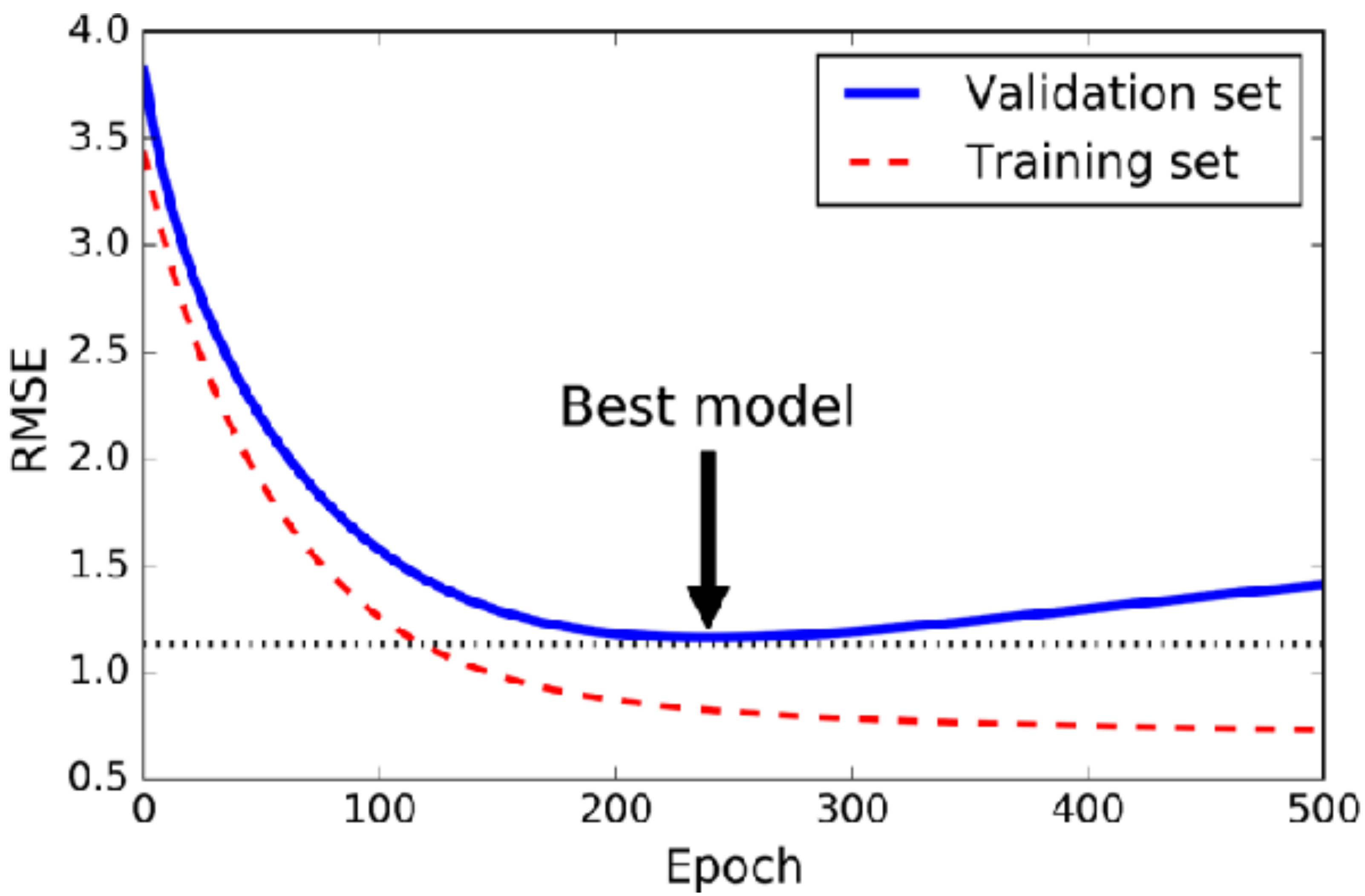
Optimization
Over-parametrization in deep learning

- Optimization (SGD) to minimize a loss function
  - Larger & deeper nets improve (training) performance
  - Risks over-fitting

$$\arg\min_{\theta} \sum_{(x_i, y_i) \in \mathcal{D}_t} \mathcal{L}(x_i, y_i; \theta) \neq \arg\min_{\theta} \mathbb{E}_{x,y \sim \mathcal{D}} \mathcal{L}(x, y; \theta)$$

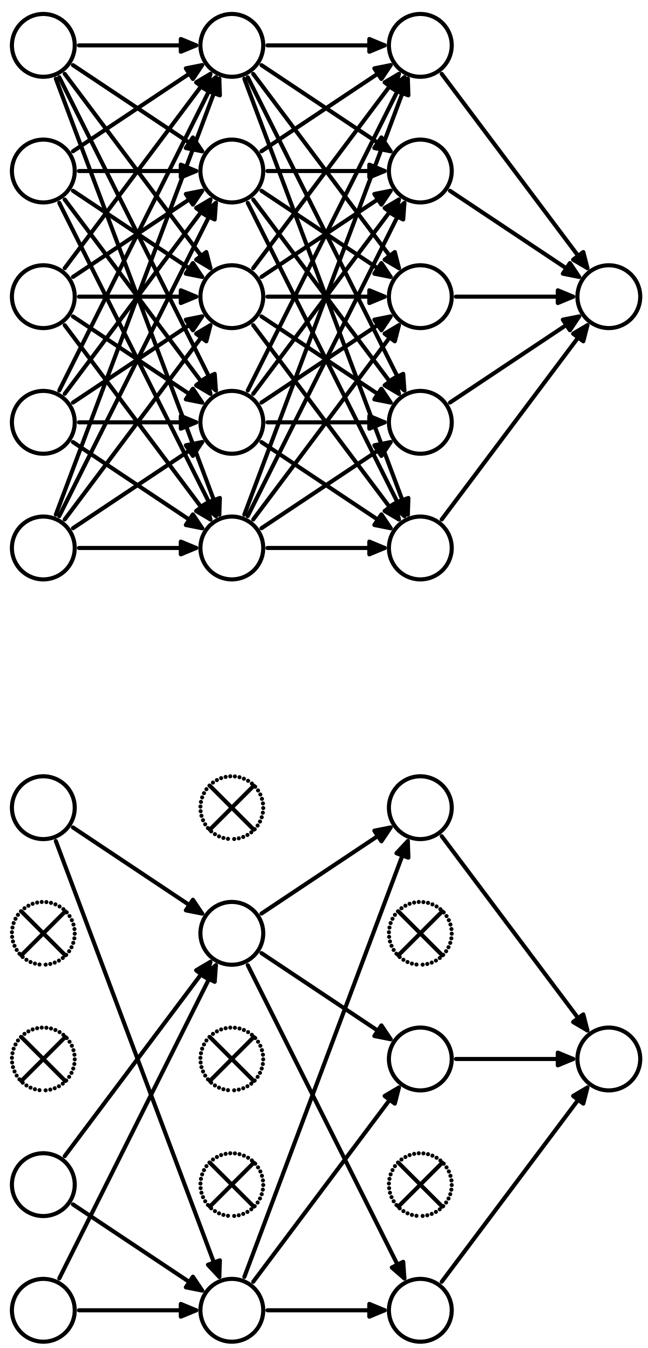
- Regularization tricks
  - L2 penalty on weights (cf. Ridge regression)
  - Early stopping (cf. Gradient boosting)
  - Dropout (relates to Random Forests)

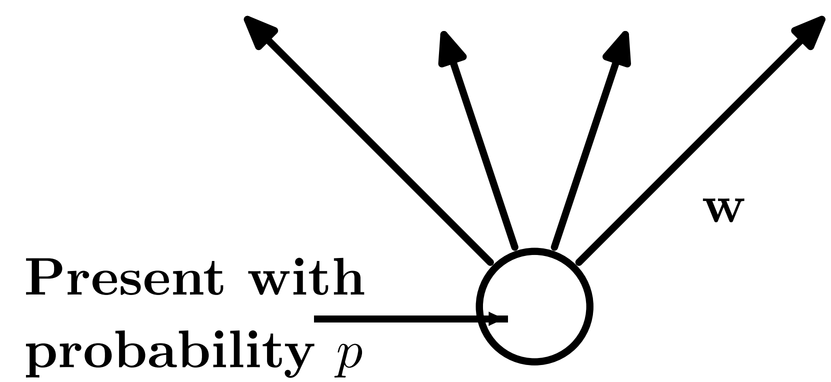
Optimization
Regularization: Early Stopping



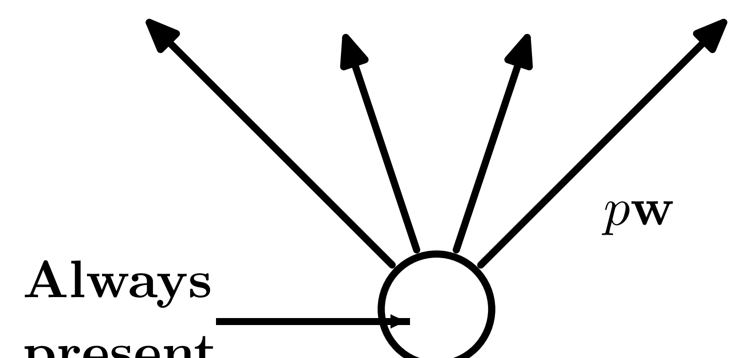
Source: "Hands-On Machine Learning with Scikit-Learn and TensorFlow", A. Géron

Optimization
Regularization: Dropout





(a) At training time



(b) At test time

Images from [Srivastava *et al.*, 2014]

Conclusion

- Early stage: 1943 - 1969
  - learning with stochastic gradient descent
- Back in the game: 1985 - 1995
  - NN are universal approximators
- A *de facto* standard in computer vision: 2009 - ?
  - deep nets can leverage on big data + high perf. computers