Deep learning
3. Loss functions, optimization, regularization

A course @EDHEC
by Romain Tavenard (Prof. @Univ. Rennes 2)

Optimization in general

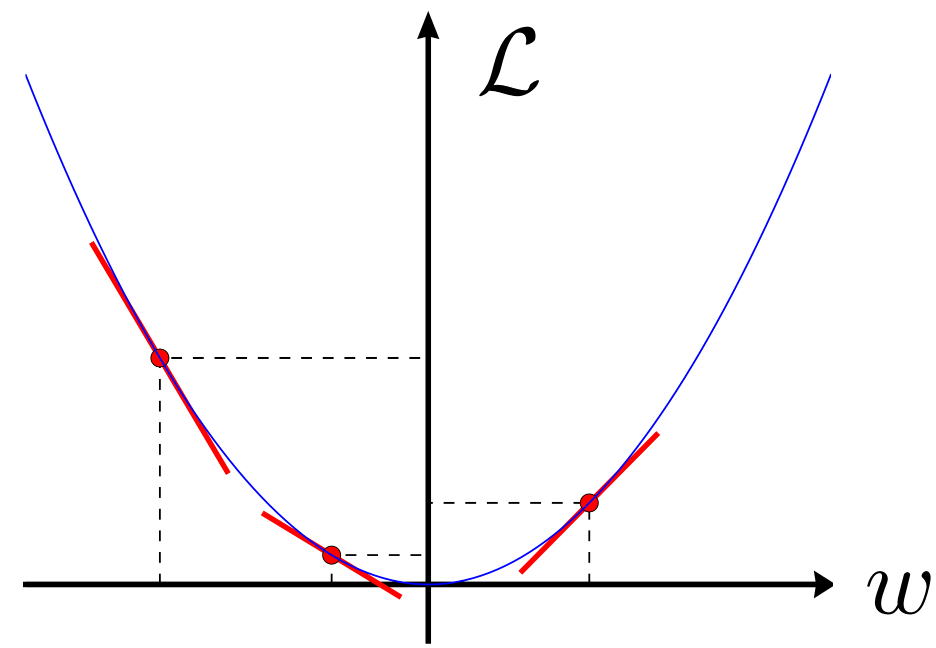
- **Goal:** Tune model parameters so as to minimize error

- Measuring error
    - Through a cost function / loss function
    - Typical example: Mean Squared Error in regression settings

Optimization
Gradient descent

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

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



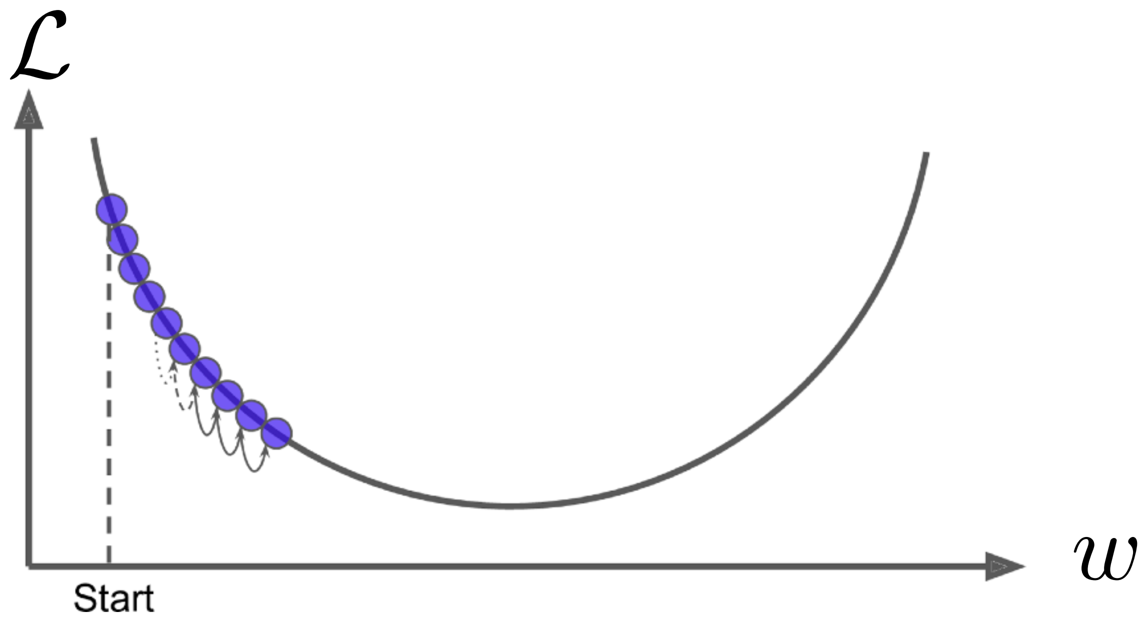
2. Use gradient descent

$$w^{(t+1)} \leftarrow w^{(t)} - \rho \nabla_w \mathcal{L}(w^{(t)})$$

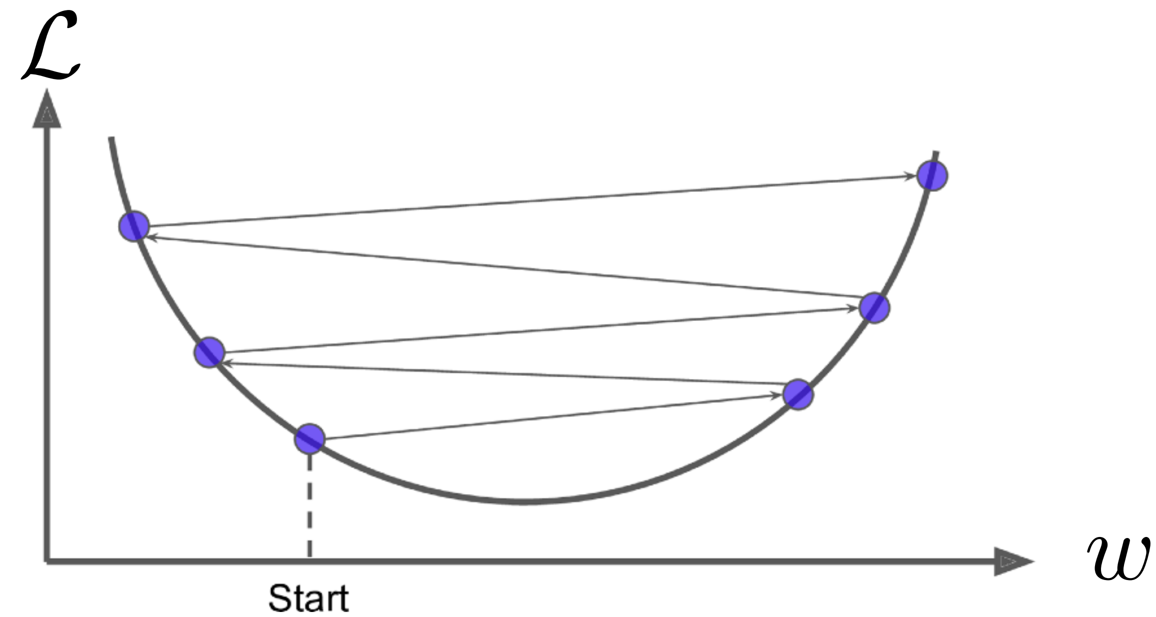
Algorithm 1: Gradient Descent

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

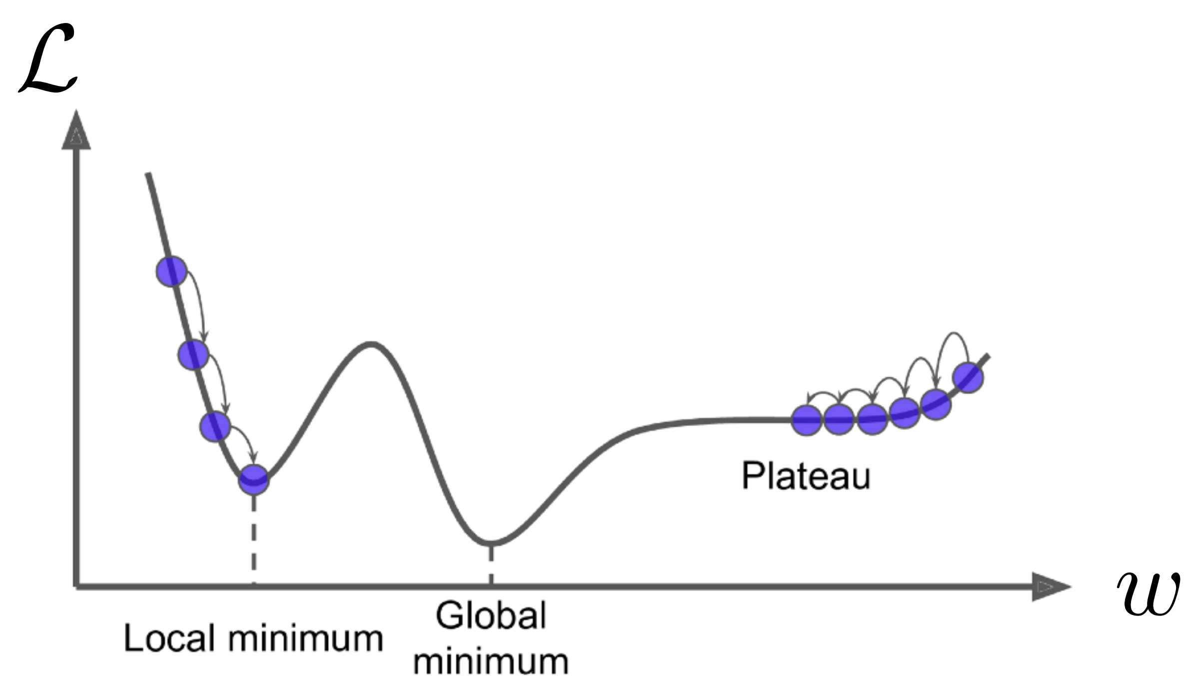
Optimization
Gradient descent in Real Life



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

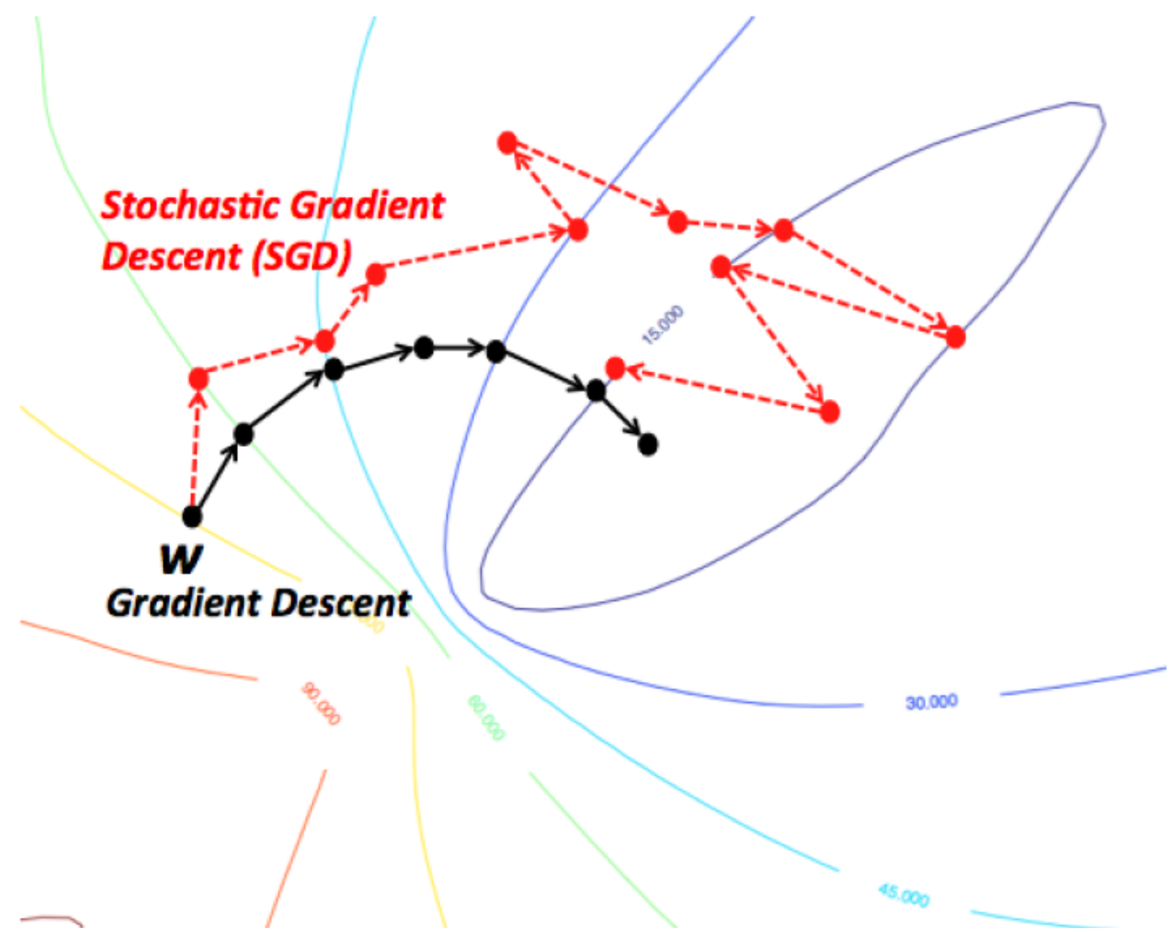
```
Data: D: a dataset
Initialize weights
for e = 1..E do
    // e is called an epoch
    for (x_i, y_i) ∈ D do
        Compute prediction ŷ_i = h(x_i)
        Compute gradient ∇_w L_i
    end
    Compute overall gradient ∇_w L = (1/n) Σ_i ∇_w L_i
    Update parameter w using ∇_w L
end
```

Algorithm 2: Mini-Batch Stochastic Gradient Descent

```
Data: 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 D
            Compute prediction ŷ_i = h(x_i)
            Compute gradient ∇_w L_i
        end
        Compute gradient for the t-th minibatch ∇_w L_(t) = (1/m) Σ_i ∇_w L_i
        Update parameter w using ∇_w L_(t)
    end
end
```

Optimization:
Gradient Descent vs Stochastic Gradient Descent

- 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

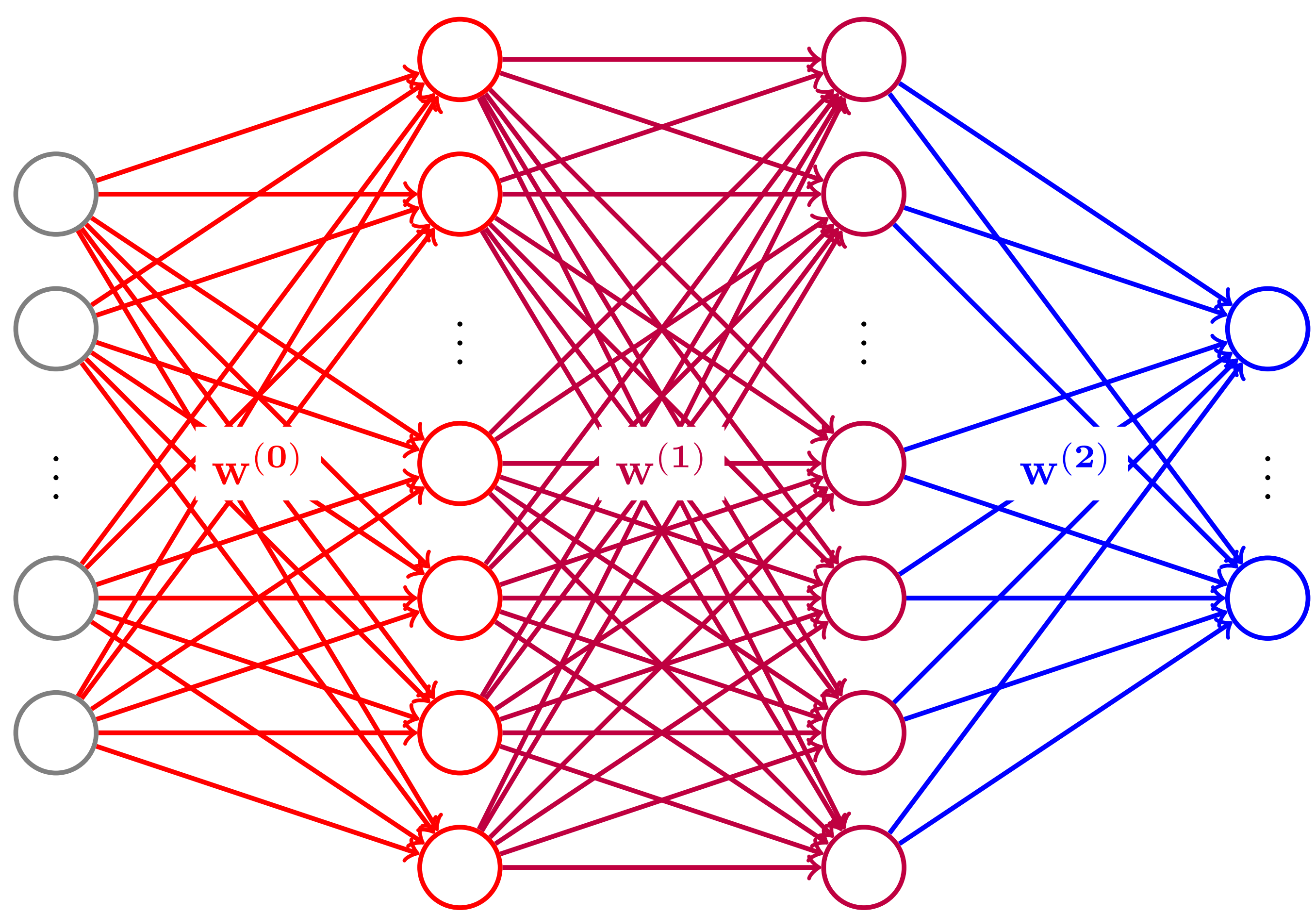
$$\mathbf{m}^{(t+1)} \propto \beta_1 \mathbf{m}^{(t)} + (1-\beta_1)\nabla_w \mathcal{L}$$

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

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

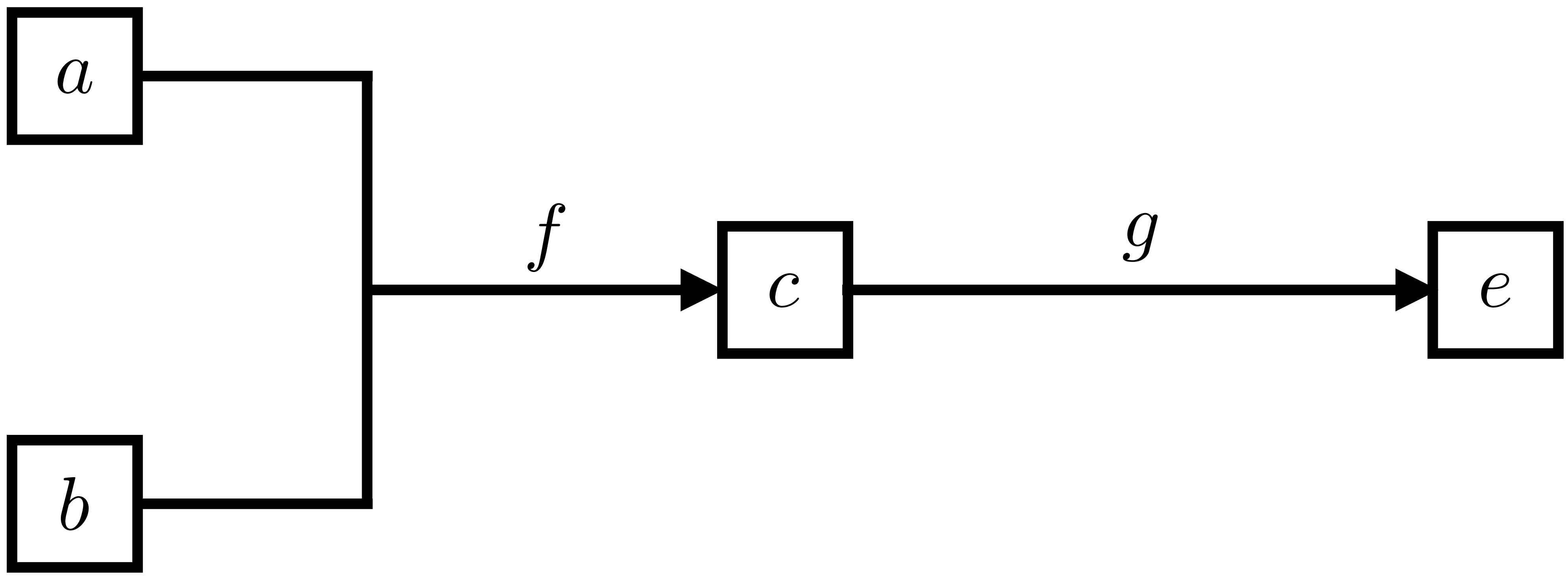
Optimizing multi-layer perceptron parameters

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



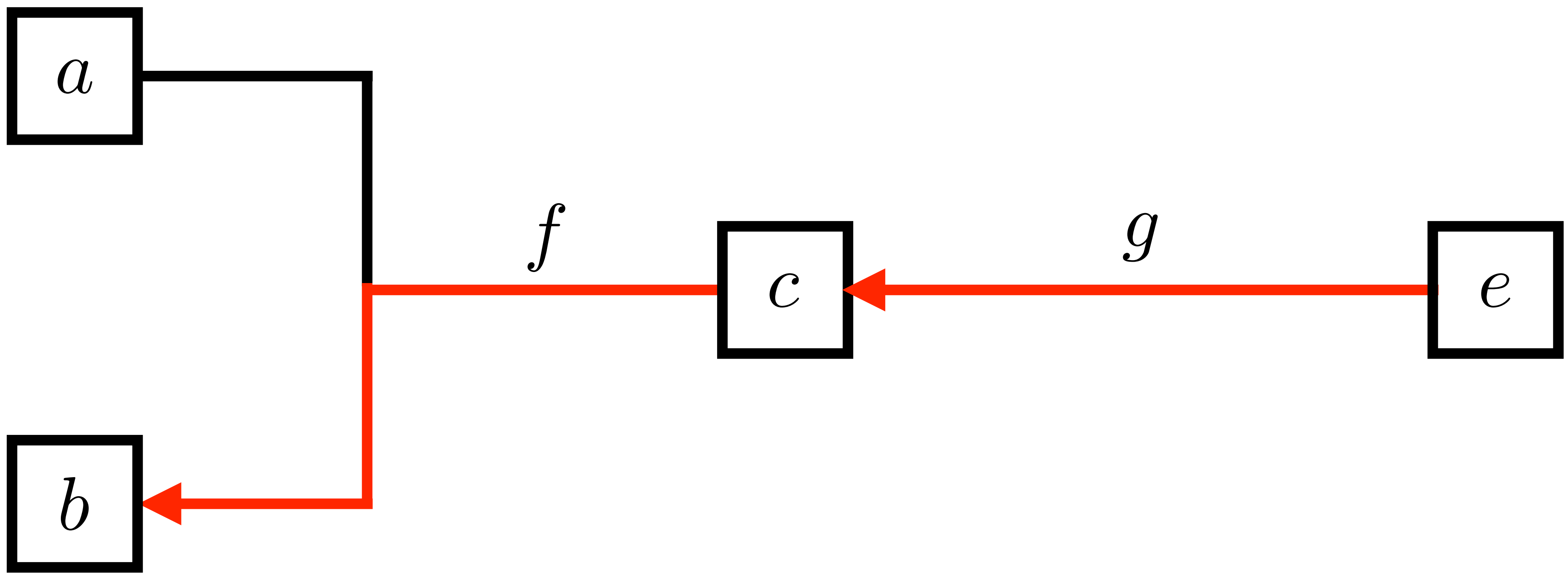
$$\hat{\mathbf{y}} = \varphi\left[\mathbf{w}^{(\mathbf{2})}\varphi\left(\mathbf{w}^{(\mathbf{1})}\varphi(\mathbf{w}^{(\mathbf{0})}\mathbf{x} + b^{(0)}) + b^{(1)}\right) + b^{(2)}\right]$$

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



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

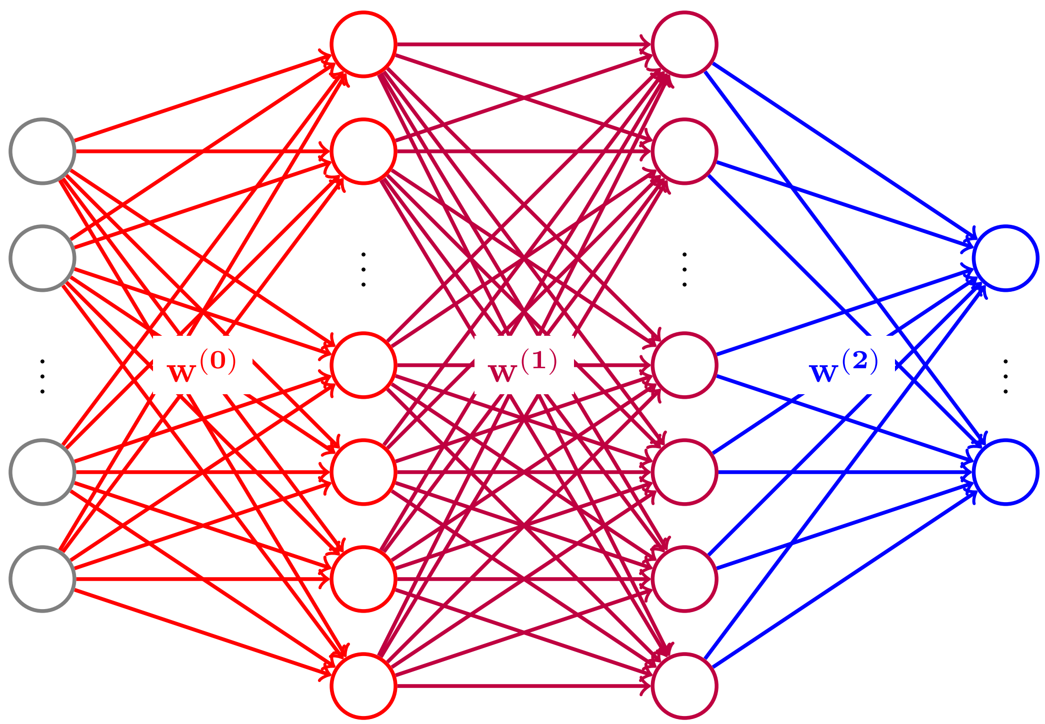
Optimizing multi-layer perceptron parameters
Automatic differentiation to the rescue!

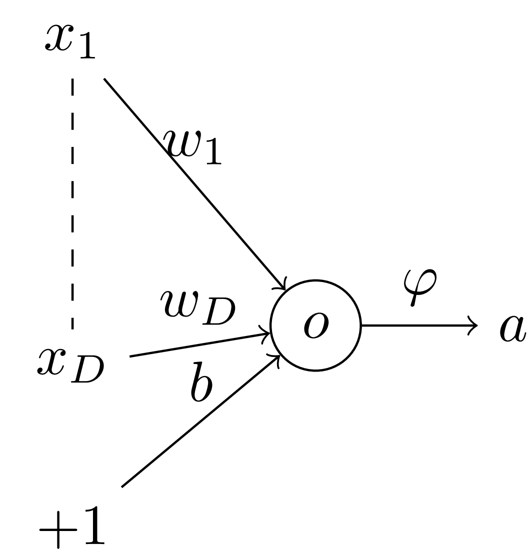


$$c = f(a, b)$$
$$e = g(c)$$

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

Optimization
Neural networks and back-propagation





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

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

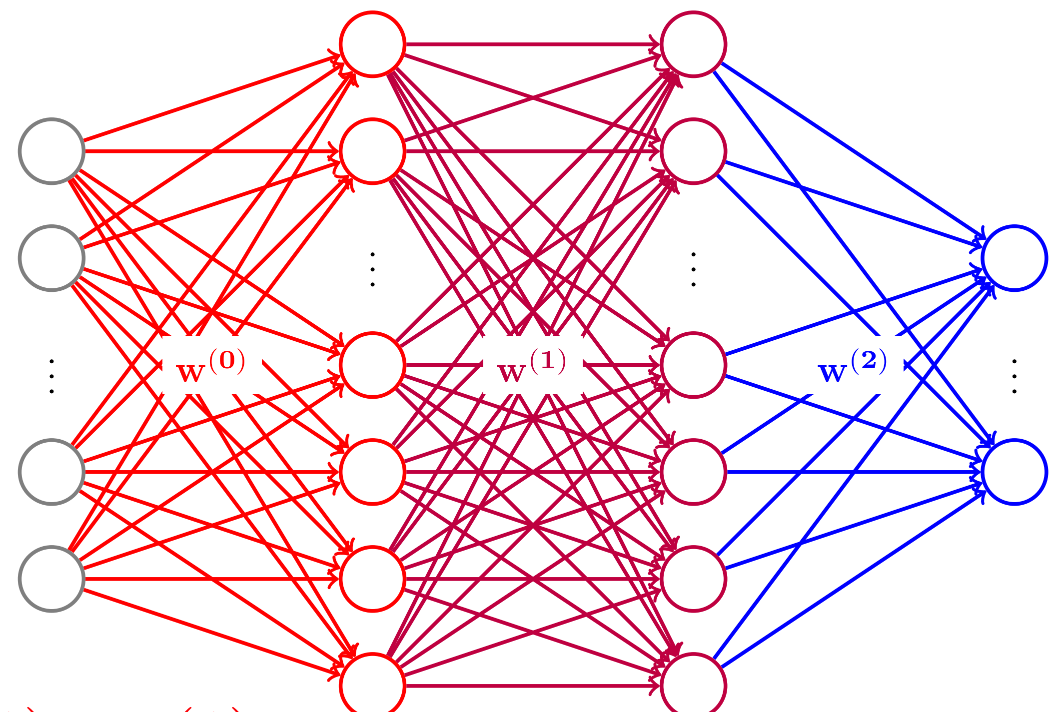
$$\frac{\partial \mathcal{L}}{\partial w^{(0)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial o^{(2)}} \frac{\partial o^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial o^{(1)}}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

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

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

A history of Convolutional neural networks (CNN)
Deeper and deeper networks

- Deeper networks = higher-level understanding
- Main limitation: vanishing gradients



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

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

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

ReLU
as default
activation function

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

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

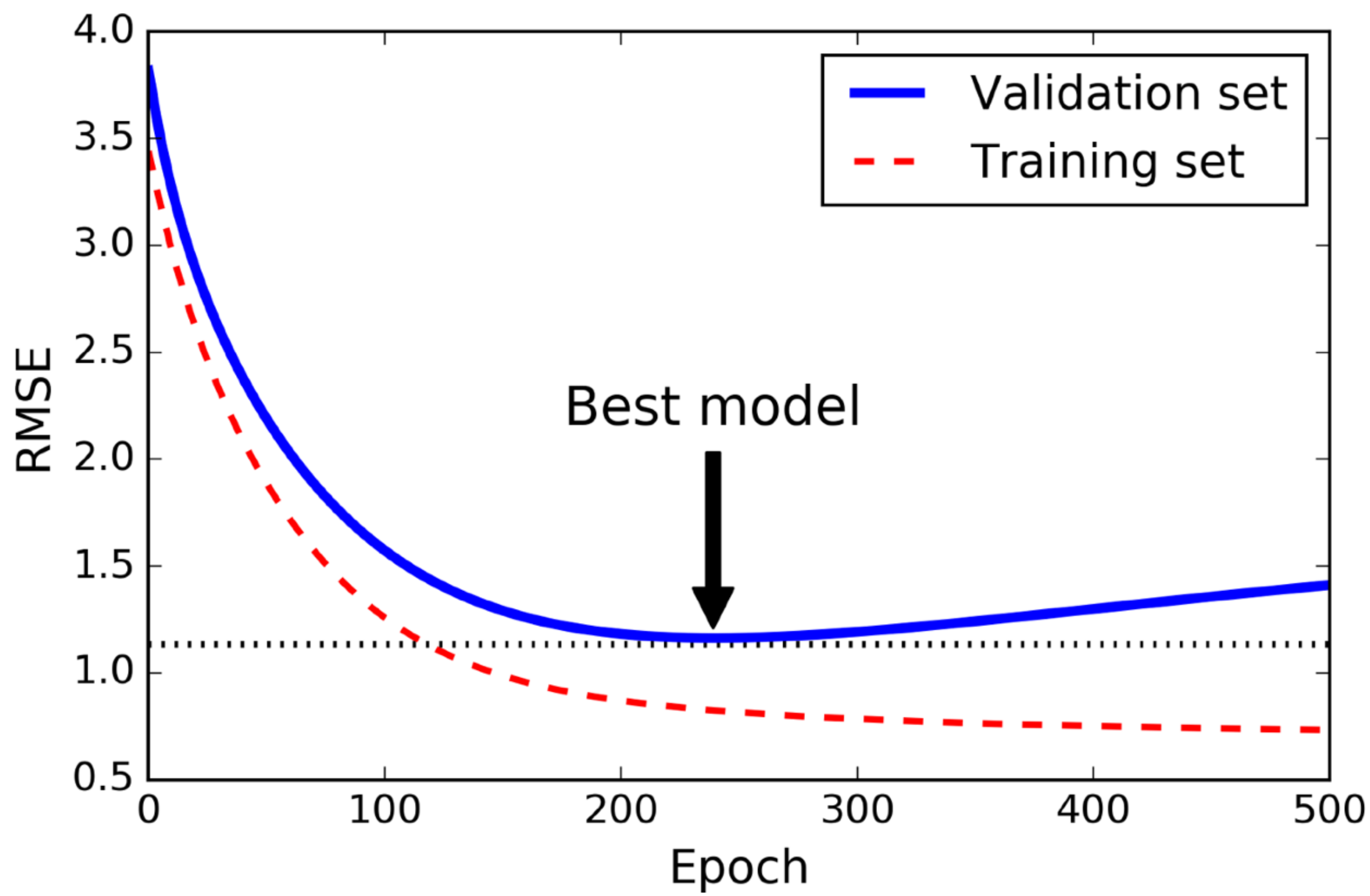
Optimization
Over-parametrization in deep learning

- 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

Conclusion

- Stochastic Gradient Descent
  - Gradient estimates computed on mini-batches
  - More frequent updates
  - Adam is an extremely powerful variant
- Loss functions
  - Mean Squared Error for regression
  - Logistic loss for classification
- Neural networks are usually used in over-parametrized mode
  - Need regularization
  - Need to check performance on hold-out data (validation set)