Deep learning
3. Loss functions, optimization, regularization

A course @EDHEC
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Optimization in general

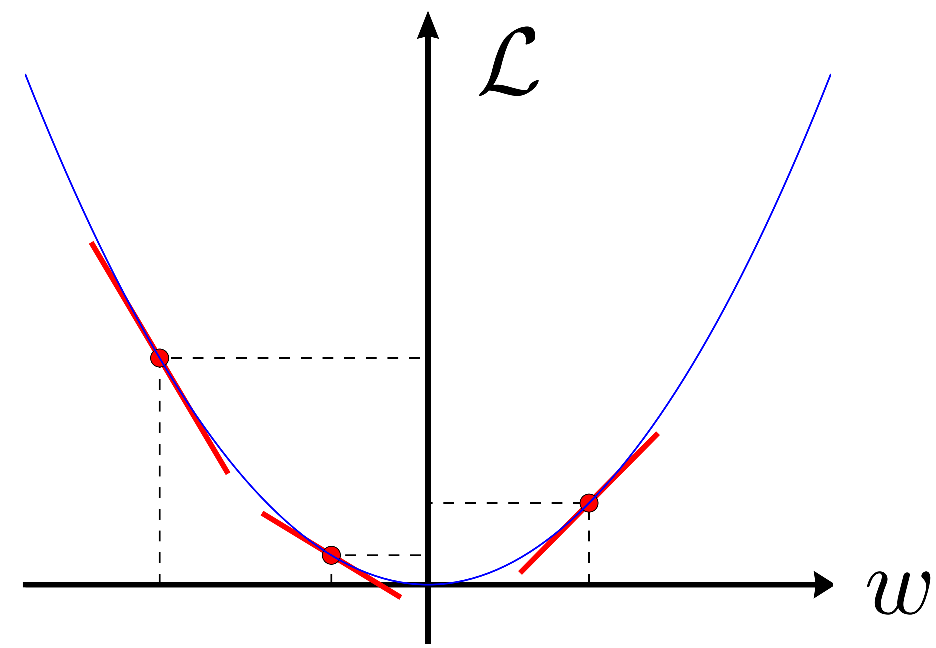
- **Goal:** Tune model parameters so as to minimize error

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



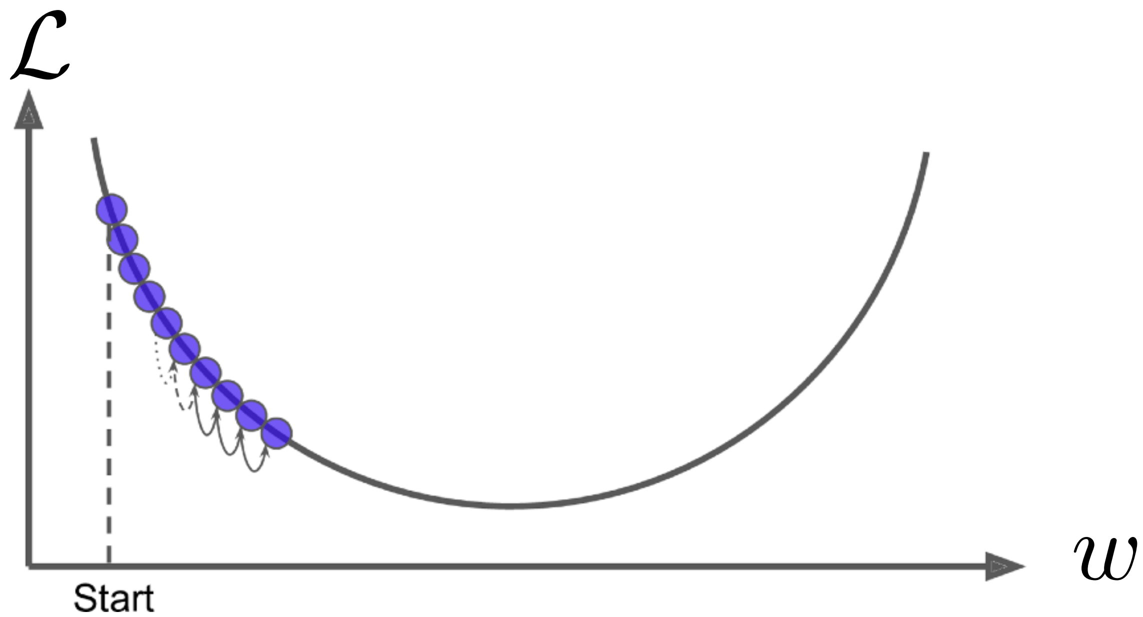
2. Use gradient descent

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

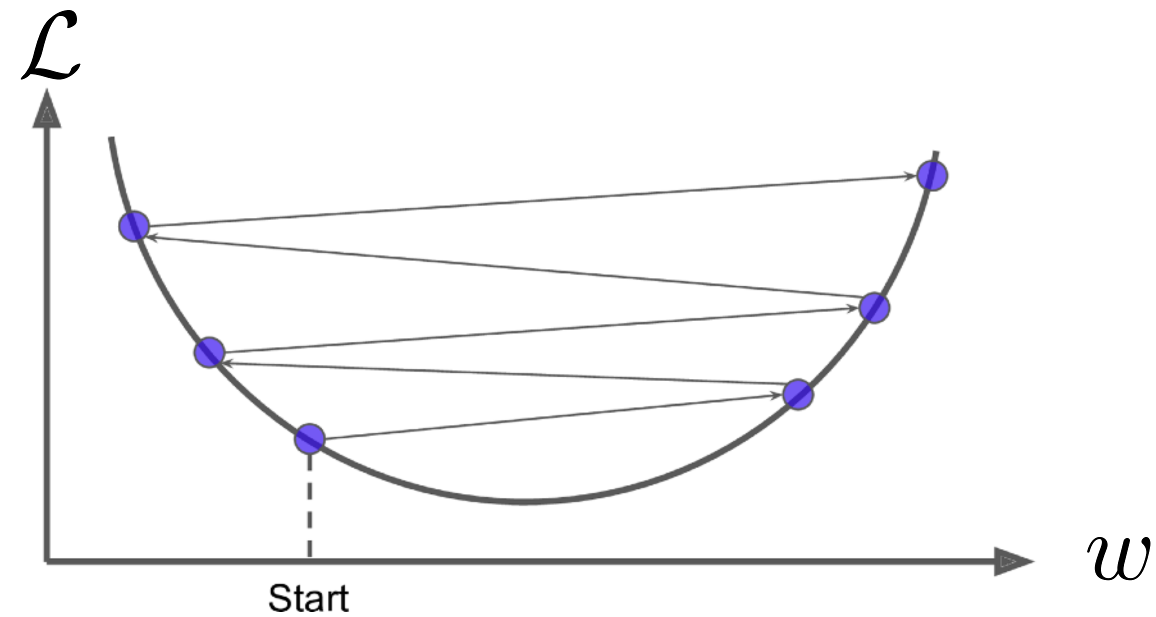
Algorithm 1: Gradient Descent

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

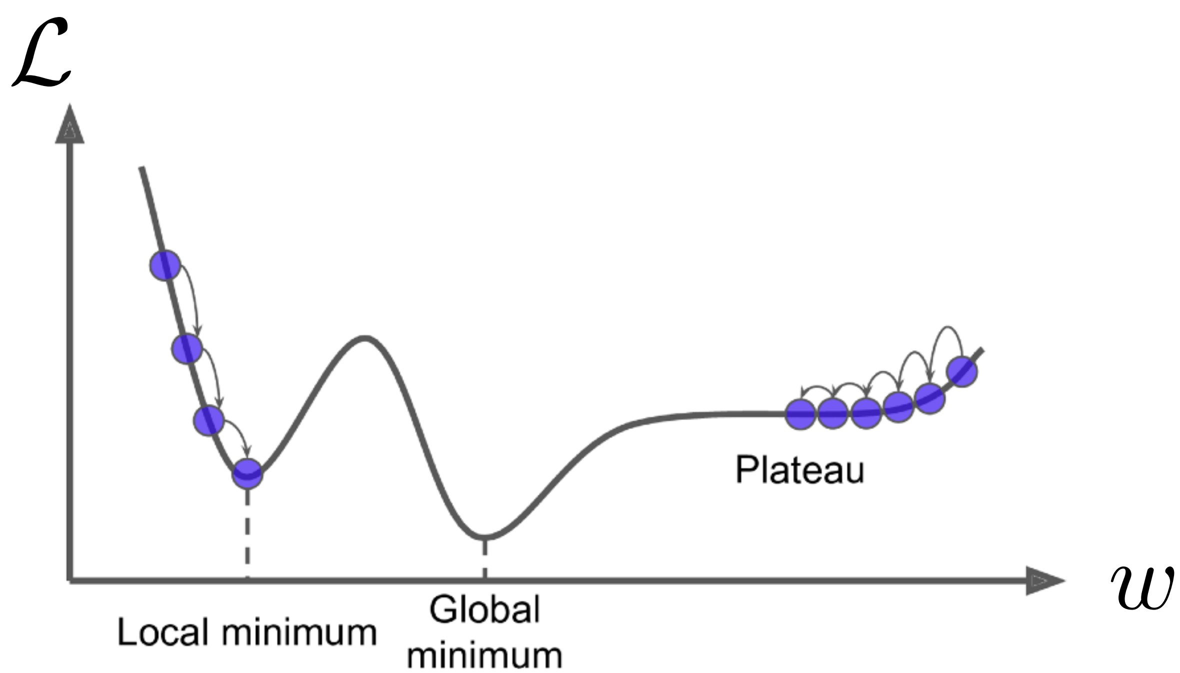
Optimization
Gradient descent in Real Life



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

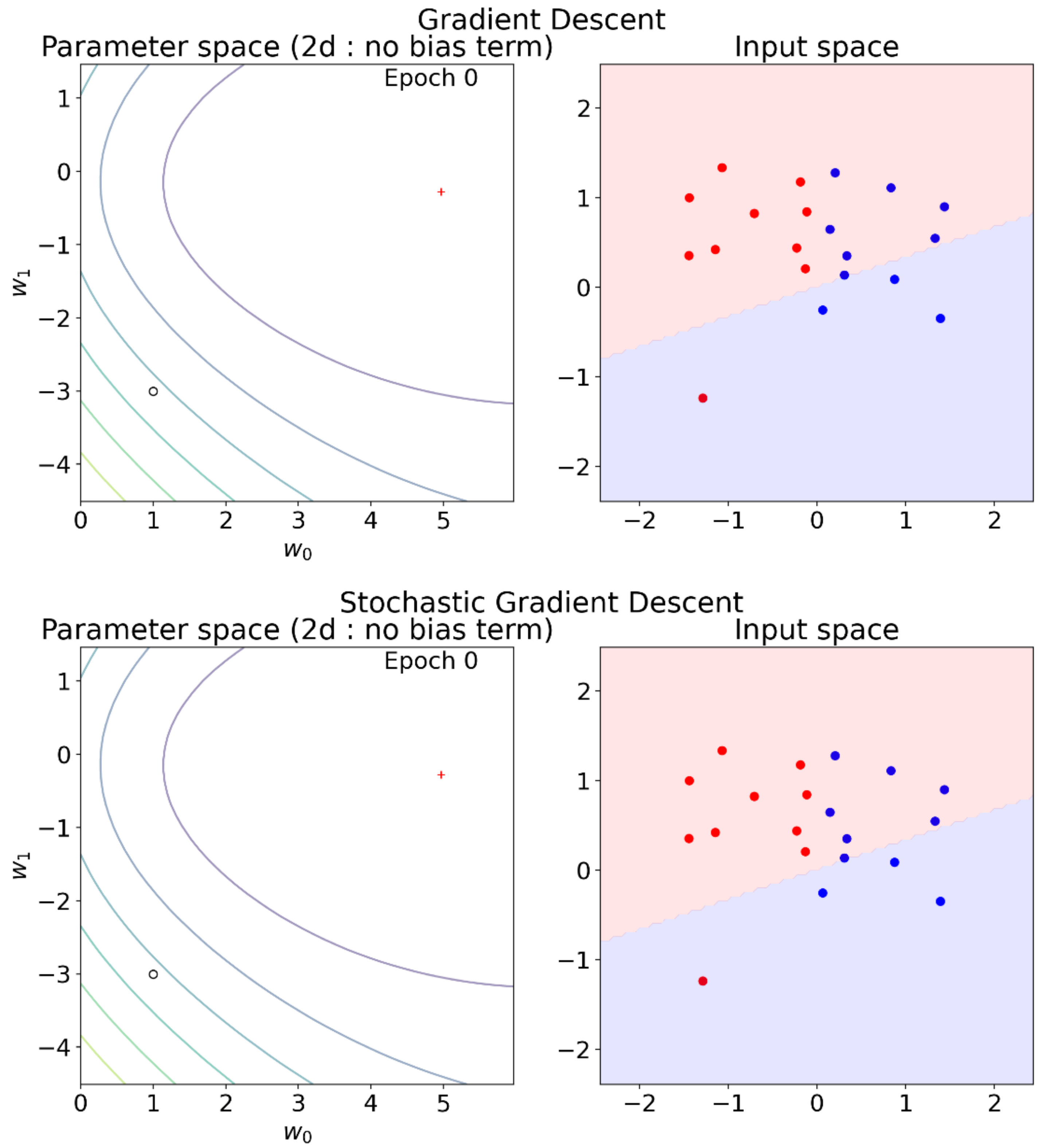
Algorithm 1: Gradient Descent

Data: $\mathcal{D}$: 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

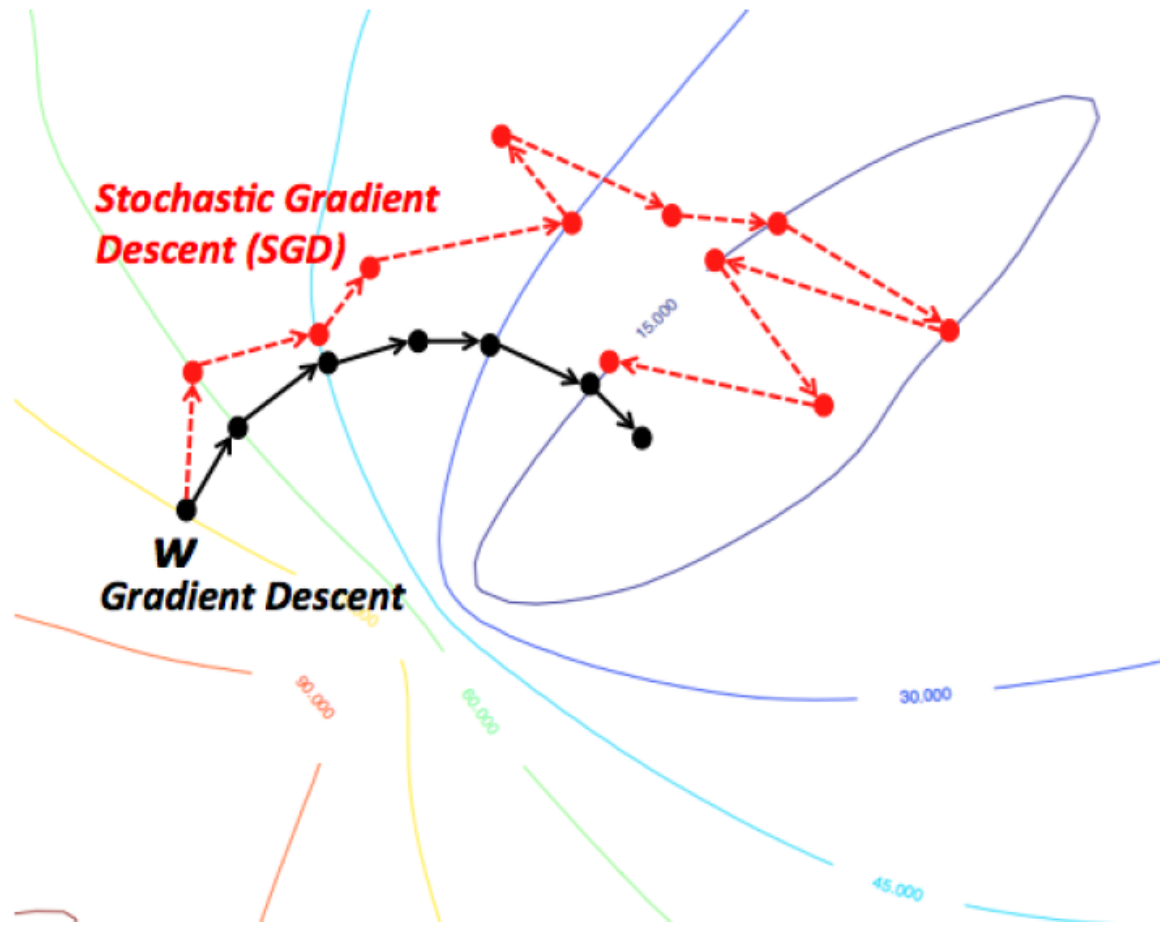
Data: $\mathcal{D}$: a dataset
Initialize weights
for $e = 1..E$ **do**
  `// e is called an epoch`
  for $t = 1..n_b$ **do**
    `// t is called an iteration`
    for $i = 1..m$ **do**
      Draw (x_i, y_i) without replacement from t-th minibatch of $\mathcal{D}$
      Compute prediction $\hat{y}_i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

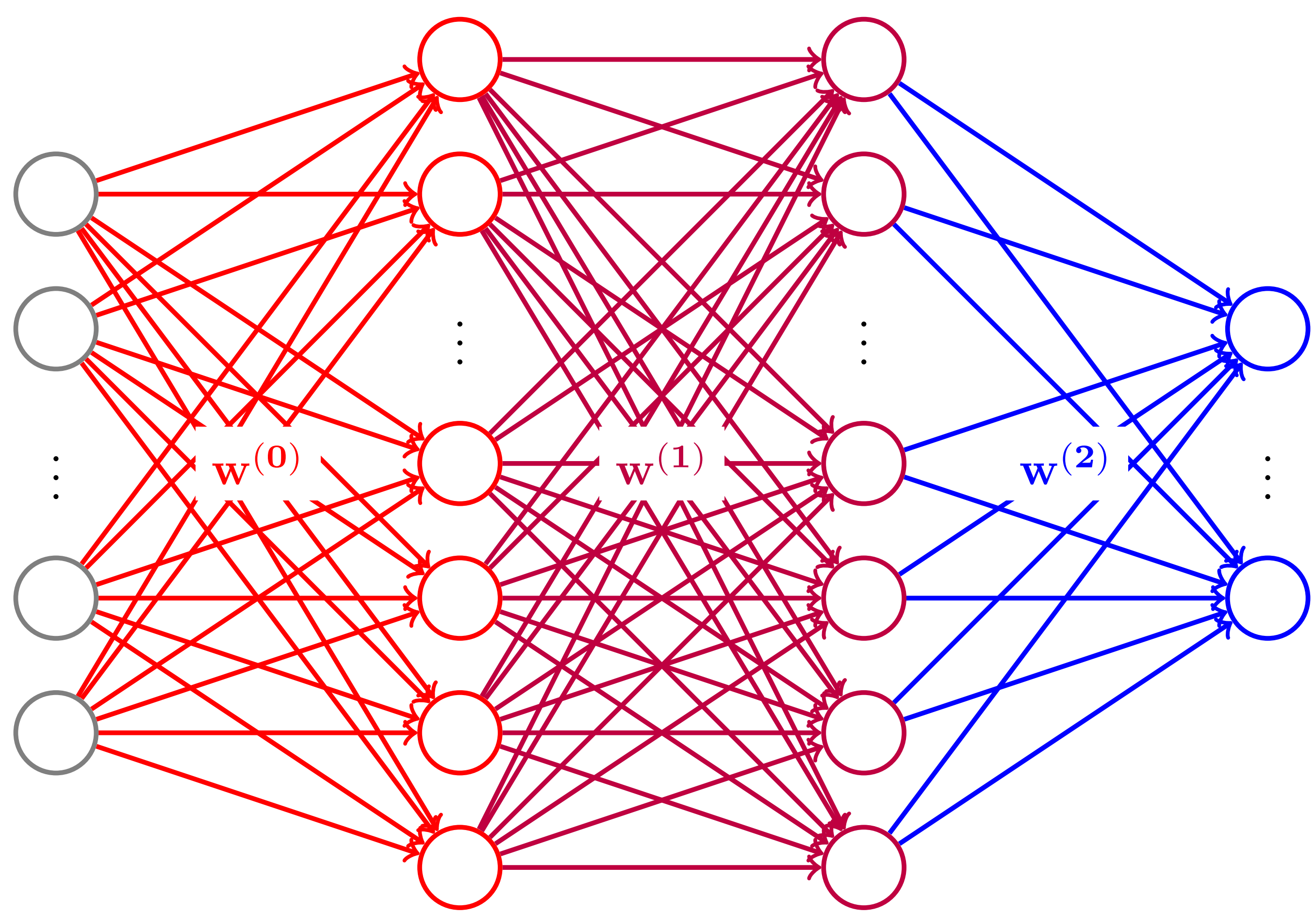
$$\mathbf{m}^{(t+1)} \propto \beta_1 \mathbf{m}^{(t)} + (1 - \beta_1) \nabla_w \mathcal{L}$$

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

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

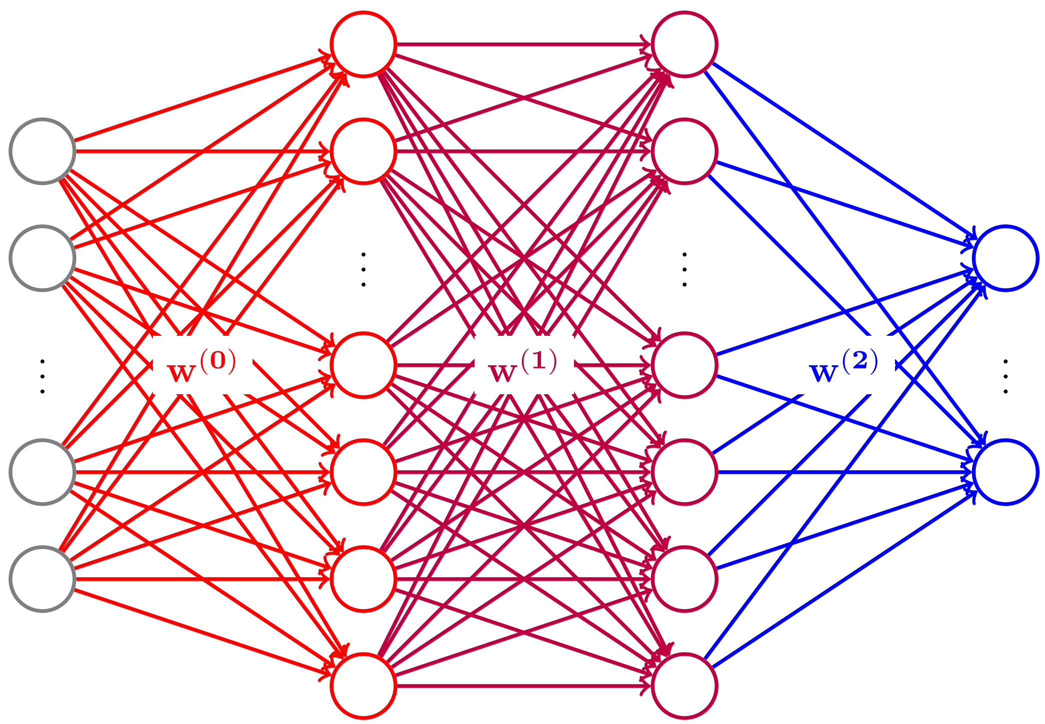
Optimizing multi-layer perceptron parameters

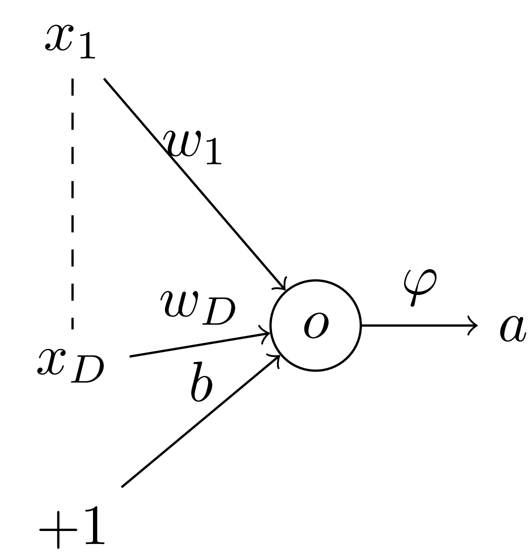
- Who wants to compute gradients by hand for such networks (and deeper ones)?



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

Optimization
Neural networks and back-propagation





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

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

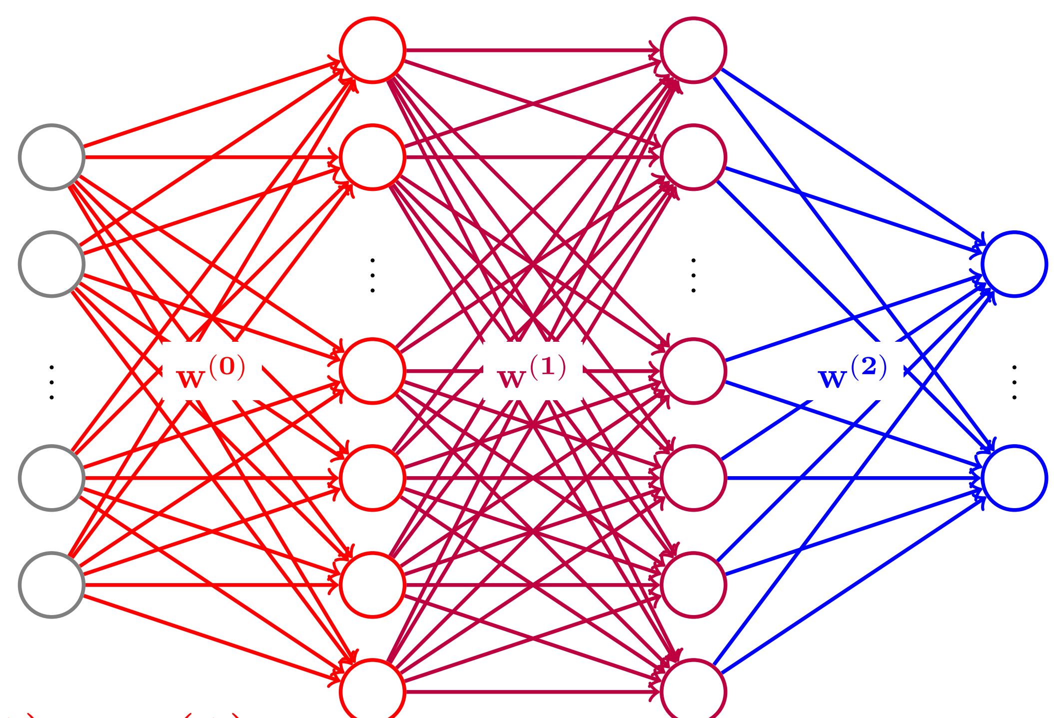
$$\frac{\partial \mathcal{L}}{\partial w^{(0)}} = \frac{\partial \mathcal{L}}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial o^{(3)}} \frac{\partial o^{(3)}}{\partial a^{(2)}} \frac{\partial a^{(2)}}{\partial o^{(2)}} \frac{\partial o^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial o^{(1)}}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

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

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

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

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



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

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

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

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

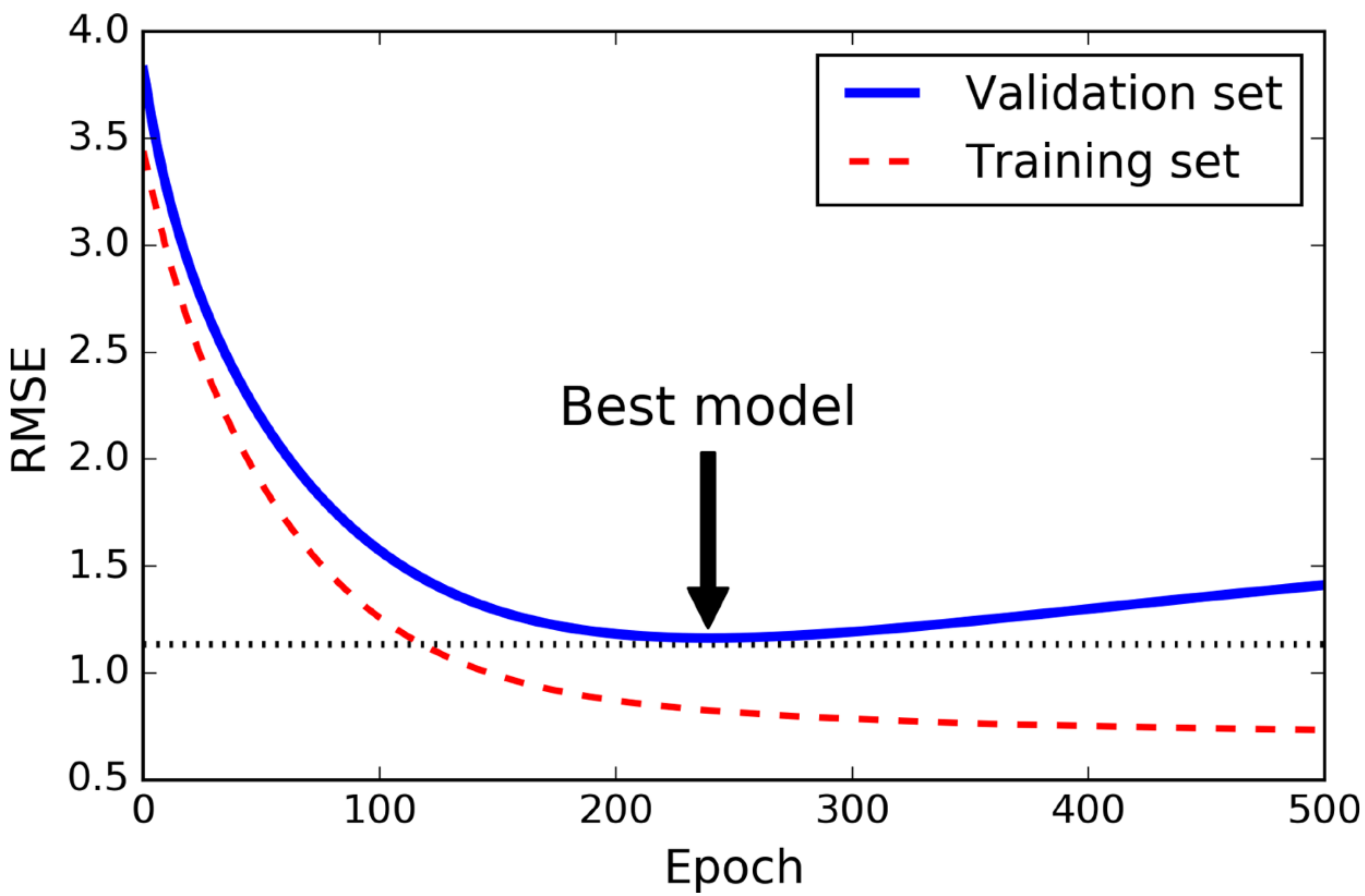
Optimization
Over-parametrization in deep learning

- 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)