Perceptron, neural network, and the back-propagation algorithm

Pavlo Mozharovskyi[1]

[1]LTCI, Télécom Paris, Institut Polytechnique de Paris

Machine learning

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Today

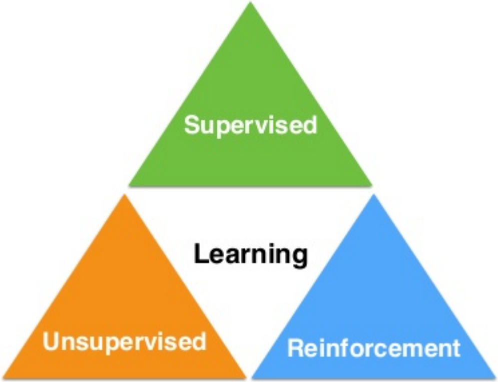
Literature

Supplementary **learning materials** include but are not limited to:

- Haykin, S. (2009).
  Neural Networks and Learning Machines (Third Edition).
  Pearson.
  - Introduction sections 3, 4, 6.
  - Sections 1.1–1.3.
  - Sections 3.3 (steepest descent), 3.5.
  - Sections 4.1–4.4.
- Vapnik, V. N. (1998).
  Statistical Learning Theory.
  John Wiley & Sons.
  - Section 9.1.
  - Section 9.6.
- Goodfellow, J., Bengio, Y., and Courville, A. (2016).
  Deep Learning.
  MIT Press.
- Bertsekas, D. P. (2016).
  Nonlinear programming (Third Edition).
  Athena Scientific.

Types of machine leaning

- Labeled data
- Direct feedback
- Predict outcome/future



- No labels
- No feedback
- “Find hidden structure”

- Decision process
- Reward system
- Learn series of actions

Binary supervised classification (reminder)

Notation:

- **Given:** for the random pair (X, Y) in $\mathbb{R}^d \times \{0, 1\}$ consisting of a random observation X and its random binary label Y (class), a sample of n i.i.d.: $(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_n, y_n)$.
- **Goal:** predict the label of the new (unseen before) observation $\boldsymbol{x}$.
- **Method:** construct a classification rule:

$$g \,:\, \mathbb{R}^d \to \{0, 1\}\,,\ \boldsymbol{x} \mapsto g(\boldsymbol{x})\,,$$

  so $g(\boldsymbol{x})$ is the prediction of the label for observation $\boldsymbol{x}$.
- **Criterion:** of the performance of g is the **error probability**:

$$R(g) = \mathbb{P}[g(X) \neq Y] = \mathbb{E}[\mathbb{1}\big(g(X) \neq Y\big)]\,.$$

- **The best solution:** is to know the distribution of (X,Y):

$$g(\boldsymbol{x}) = \mathbb{1}\big(\mathbb{E}[Y|X = \boldsymbol{x}] > 0.5\big)\,.$$

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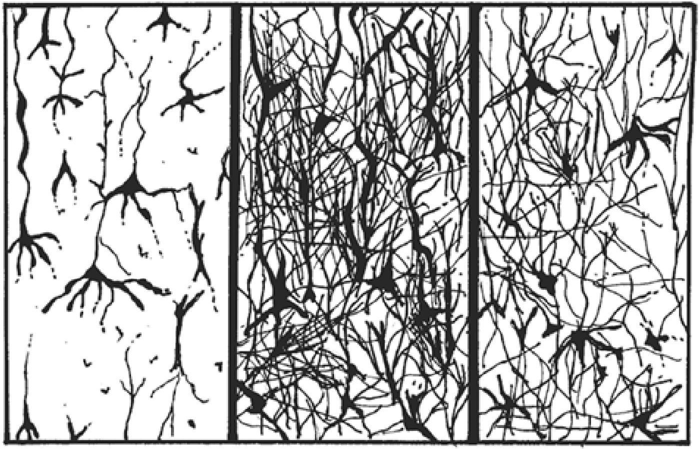
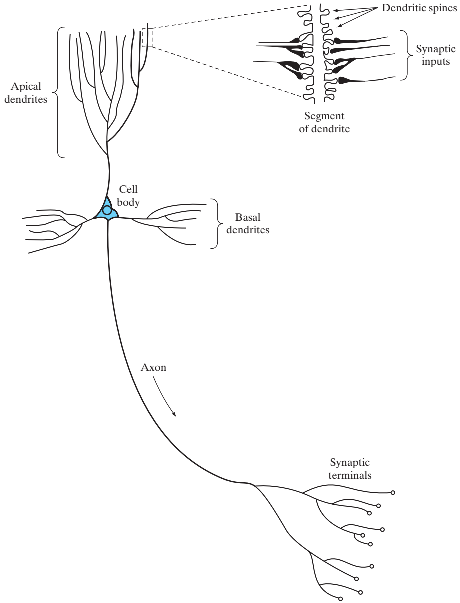
Neurons in the human body

Density of neurons in the human brain at different ages



at a child's birth   at 7 years of age   at 15 years of age

Pyramidal neuron



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The three waves of machine learning

Wave 1 **1952–1974: The birth and the golden years**

- Biological analogy – McCulloch and Pitts model of neuron
- First try – Rosenblatt's perceptron
- Statistical foundations – Vapnik-Chervonenkis theory

Wave 2 **1980–1987: The boom**

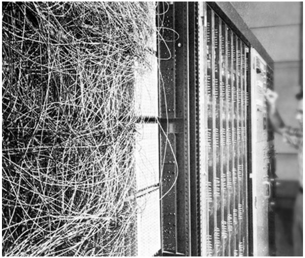
- Visual cortex model – neocognitron by Fukushima
- Expert systems
- Knowledge engineering
- Recurrent architectures – Hopfield net
- Learning algorithm – back-propagation by Hinton and Rumelhart

Wave 3 **1993–.......: Contemporary architectures**

- Convolutional networks (CNNs) – LeNet by LeCun
- CNNs with ReLU, drop-out, GPUs – AlexNet by Krizhevsky et al.
- Generative adversarial networks (GANs) – Goodfellow
- Big data deep learning (DL)
- Artificial general intelligence – full AI
- ...

Rosenblatt's perceptron

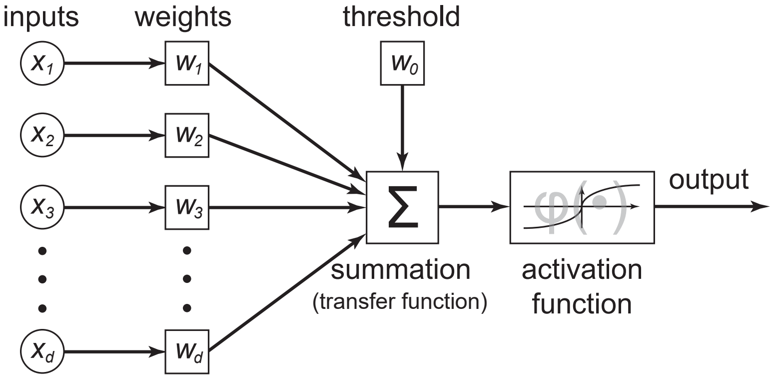
The **perceptron algorithm** was invented in 1957 at the Cornell Aeronautical Laboratory by **Frank Rosenblatt**.



(Photo downloaded from http://www.usbdata.co/rosenblatt-perceptron.html)

The **Mark I Perceptron** machine was the first implementation of the perceptron algorithm. The machine was connected to a **Camera** that used **20x20** cadmium sulfide **photocells** to produce a 400-pixel image. The main visible feature is a **Patchboard** that **allowed experimentation with** different combinations of **input features**. To the right of that are arrays of **Potentiometers** that **implemented the adaptive weights**.

Rosenblatt's perceptron



Let $\boldsymbol{w} = (w_1, w_2, ..., w_d)^T$ be the weight vector, then a new observation $\boldsymbol{x} = (x_1, x_2, ..., x_d)^T$ is classified as

$$g(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \phi\left(\sum_{k=1}^{d} w_k x_k + w_0\right) > 0\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

Rosenblatt's perceptron (training algorithm)

Initialize w_0 and $\boldsymbol{w}$ randomly or set $w_0 = 0$ and $\boldsymbol{w} = \boldsymbol{0}$.
Choose constant $\gamma \in (0, 1]$ controlling the learning speed.

Feed training pairs $(\boldsymbol{x}, y)$, and for each of them update current threshold and weights $w_0^{(i)}$ and $\boldsymbol{w}^{(i)}$ to $w_0^{(i+1)}$ and $\boldsymbol{w}^{(i+1)}$ as follows:

1. Classify current observation $\boldsymbol{x}$:

$$o^{(i)} = \begin{cases} 1 & \text{if } \sum_{k=1}^{d} w_k x_k + w_0 > 0\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

2. Calculate correction:

$$\delta^{(i)} = \begin{cases} 0 & \text{if } o^{(i)} = y\,, \\ 1 & \text{if } o^{(i)} = 0 \text{ but } y = 1\,, \\ -1 & \textit{if } o^{(i)} = 1 \text{ but } y = 0\,. \end{cases}$$

3. Update threshold and weights:

$$\begin{aligned} \boldsymbol{w}^{(i+1)} &= \boldsymbol{w}^{(i)} + \gamma \delta^{(i)} \boldsymbol{x}\,, \\ w_0^{(i+1)} &= w_0^{(i)} + \gamma \delta^{(i)}\,. \end{aligned}$$

Iris data

Fisher's iris data: is this the same flower?

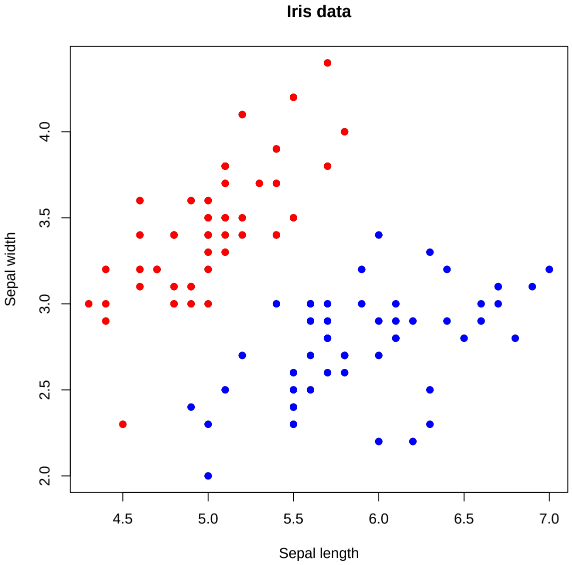
Iris **setosa**

Iris **versicolor**

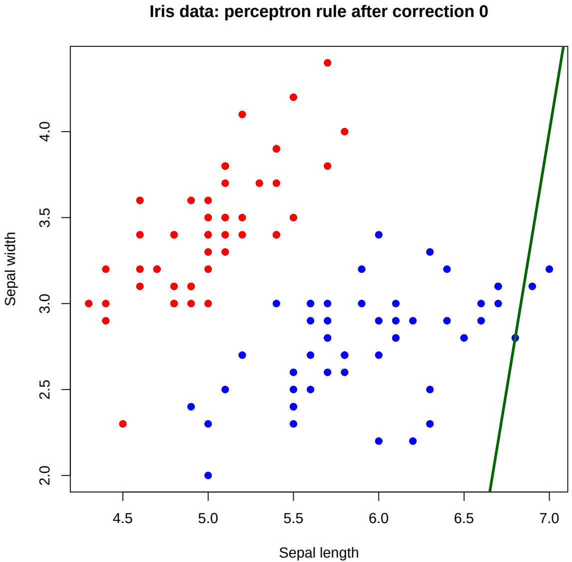
Iris data

Iris **setosa**		Iris **versicolor**	
Sepal length (cm)	Sepal width (cm)	Sepal length (cm)	Sepal width (cm)
5.1	3.5	7	3.2
4.9	3	6.4	3.2
4.7	3.2	6.9	3.1
4.6	3.1	5.5	2.3
5	3.6	6.5	2.8
5.4	3.9	5.7	2.8
4.6	3.4	6.3	3.3
5	3.4	4.9	2.4
4.4	2.9	6.6	2.9
...	...	...	...
...	...	...	...
...	...	...	...
4.6	3.2	6.2	2.9
5.3	3.7	5.1	2.5
5	3.3	5.7	2.8

Rosenblatt's perceptron (iris data)



Rosenblatt's perceptron (iris data)



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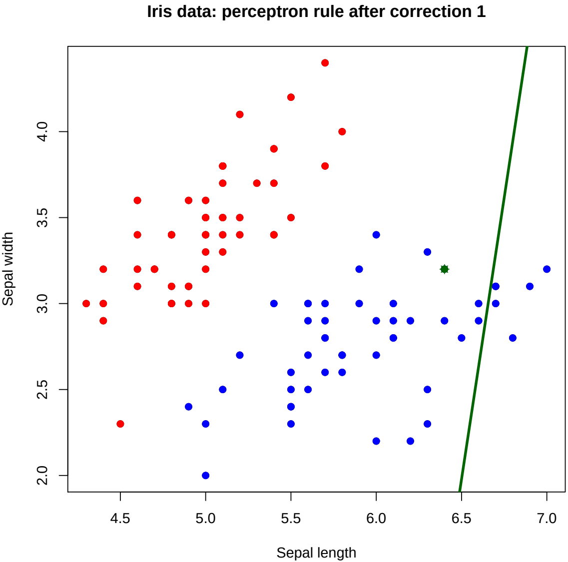

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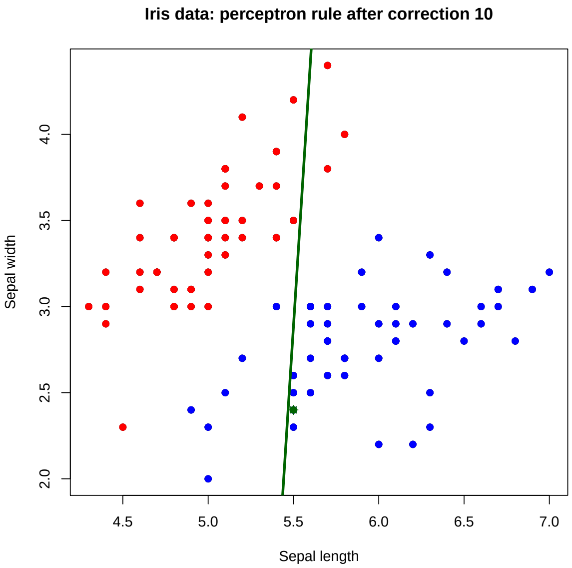

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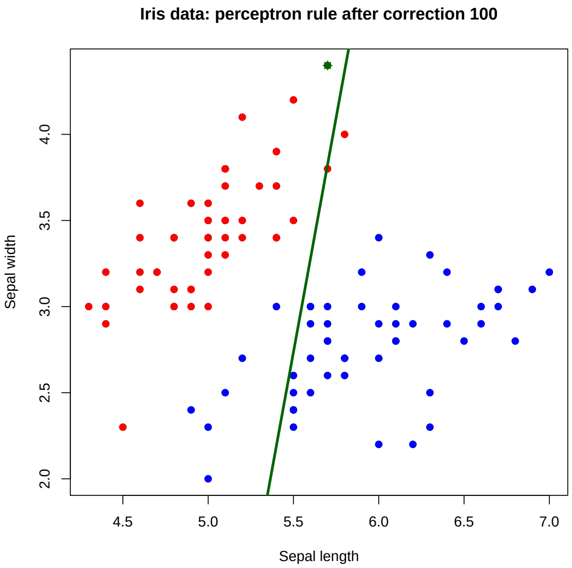

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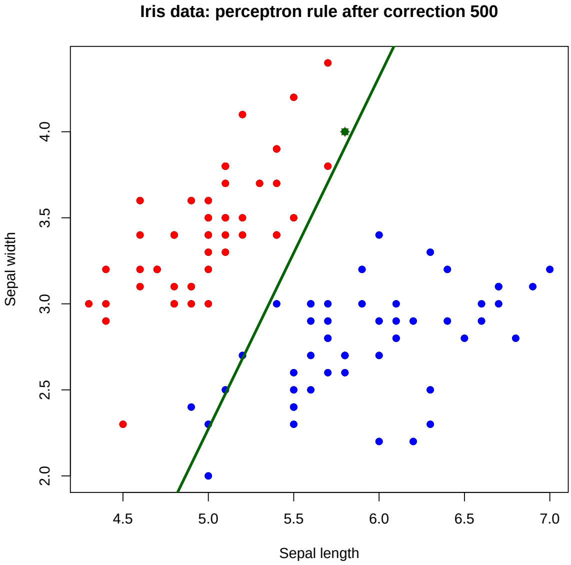
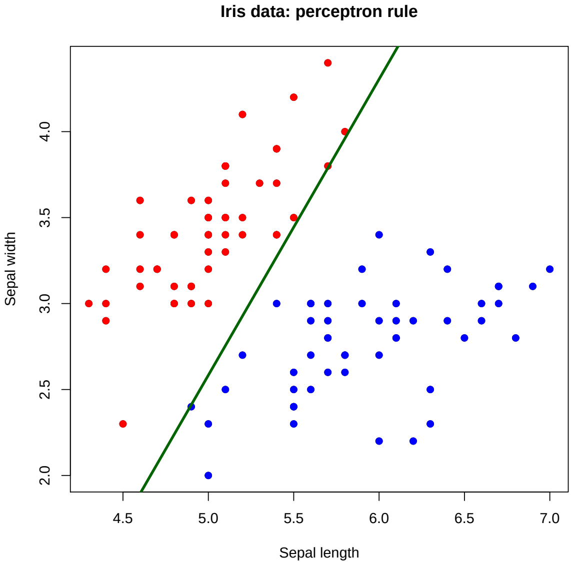


Rosenblatt's perceptron (iris data)



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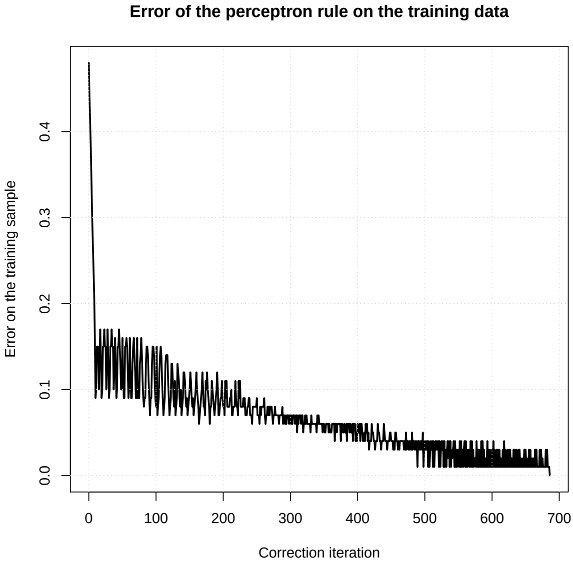
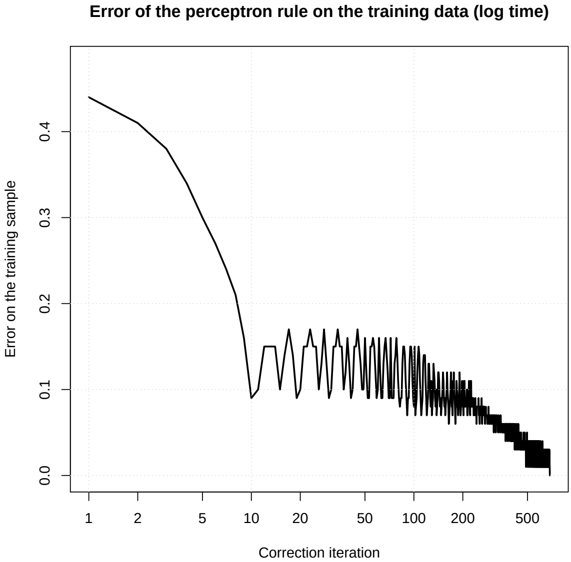


Rosenblatt's perceptron (iris data)



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Novikoff's convergence theorem

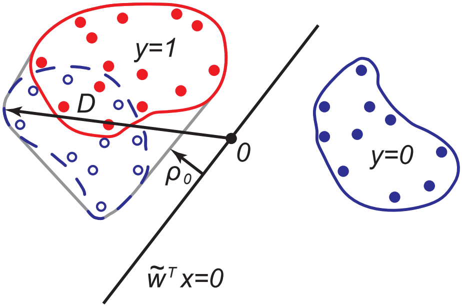
- Let $w_0 = 0$ and set $\gamma = 1$.
- Let $(\mathcal{X}, \mathcal{Y}) = (\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_i, y_i), \ldots$ be an infinite training sequence.
- In addition, let (construct) $\tilde{\mathcal{X}} = \{\boldsymbol{x} \mid (\boldsymbol{x}, y) \in (\mathcal{X}, \mathcal{Y}),\ y = 1\} \cup \{-\boldsymbol{x} \mid (\boldsymbol{x}, y) \in (\mathcal{X}, \mathcal{Y}),\ y = 0\}$.
- Let $\tilde{\boldsymbol{w}}$ exist such that for some $\rho_0 > 0$ it holds

  $$\min_{\tilde{\boldsymbol{x}} \in \tilde{\mathcal{X}}} \frac{\tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{x}}}{\|\tilde{\boldsymbol{w}}\|} \geq \rho_0 \,.$$

  i.e. the classes are **linearly separable via the origin** with margin ρ_0.
- Let $0 < D < \infty$ exist such that it holds

  $$\max_{\boldsymbol{x} \in \mathcal{X}} \|\boldsymbol{x}\| < D \,.$$

Novikoff's convergence theorem



Theorem (Novikoff, 1962)

The perceptron constructs a hyperplane that correctly separates all pairs $(\boldsymbol{x}, y) \in (\mathcal{X}, \mathcal{Y})$ *with the number of corrections at most*

$$\left\lfloor \frac{D^2}{\rho_0^2} \right\rfloor .$$

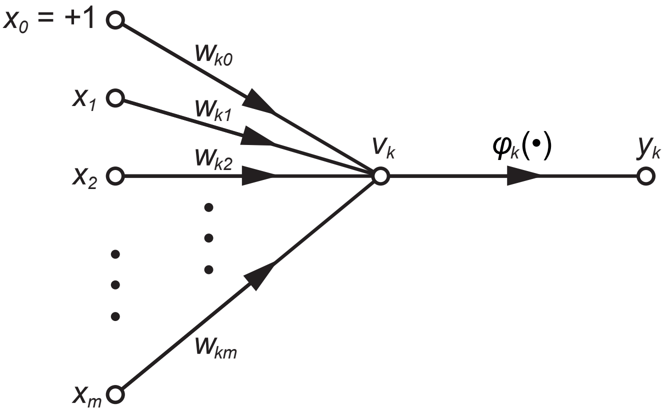
Contents

A signal-flow graph

A **signal-flaw graph** is a network of directed **links (branches)** that are interconnected at certain points called **nodes**.

1. A signal flows along a link only in the direction defined by the arrow on the link.
   There are two types of links:
   - **Synaptic links**: behavior is defined by a **linear** input-output relation. Specifically, the node signal x_j is multiplied with the synaptic weight w_{kj} to produce the node signal y_k.
   - **Activation links**: behavior is defined by a **nonlinear** input-output relation. The change of the signal is performed due to the activation function $\phi(\cdot)$.
2. A node signal equals the algebraic sum of all signals entering the pertinent node via the incoming links: **synaptic convergence** or **fan-in**.
3. The signal at node is transmitted to each outgoing link originating from that node, with the transmission entirely independent of the transfer functions of the outgoing links: **synaptic divergence** or **fan-out**.

A signal-flow graph of a neuron



Definition of a neural network

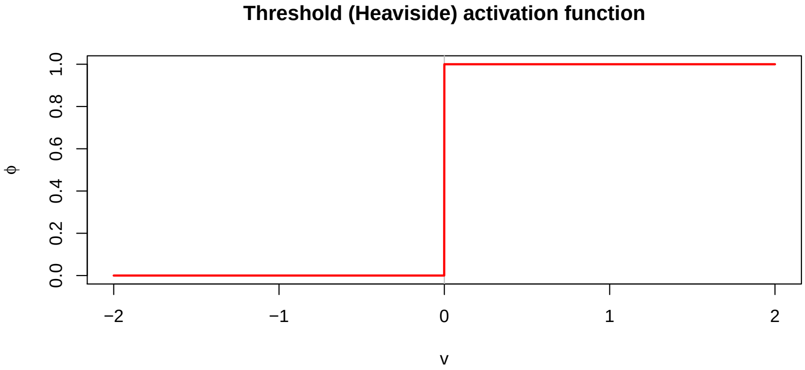
A **neural network is a directed graph** consisting of nodes with interconnecting synaptic and activation links and is characterized by four properties:

1. Each neuron is represented by a set of linear synaptic links, an externally applied bias, and a possibly nonlinear activation link. The bias is represented by a synaptic link connected to an input fixed at $+1$.
2. The **synaptic links** of a neuron weight their respective input signals.
3. The weighted sum of the input signals defines the **induced local field** of the neuron in question.
4. The **activation link** squashes the induced local field of the neuron to produce **output**.

Activation function $\phi(v)$

- **Threshold (Heaviside) function:**

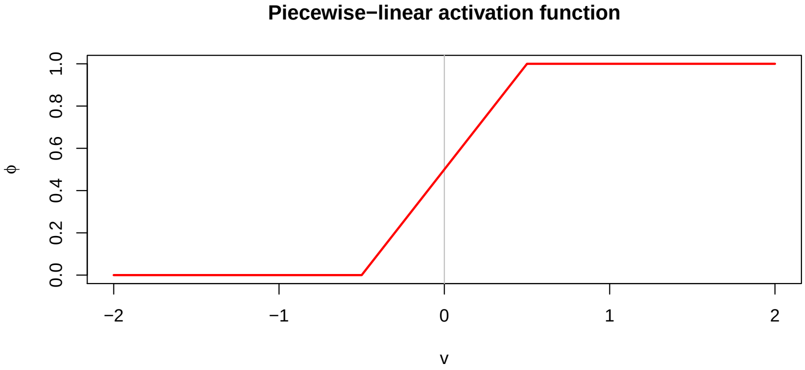
$$\phi(v) = \begin{cases} 1 & \text{if } v \geq 0\,, \\ 0 & \text{if } v < 0\,. \end{cases}$$



Activation function $\phi(v)$

- **Piecewise-linear function:**

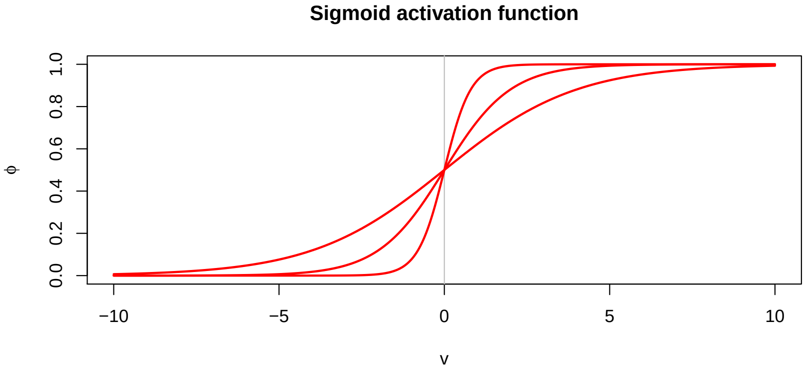
$$\phi(v) = \begin{cases} 1 & \text{if } v \geq \frac{1}{2}\,, \\ v + \frac{1}{2} & \text{if } -\frac{1}{2} < v < \frac{1}{2}\,, \\ 0 & \text{if } v \leq -\frac{1}{2}\,. \end{cases}$$



Activation function $\phi(v)$

- **Sigmoid function:**

$$\phi(v) = \frac{1}{1 + exp(-av)} .$$



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Minimization of the empirical risk: a reminder

- For:
  - a random pair (X, Y),
  - a loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$

  one seeks a classifier close to:

$$g^* = \arg\min_g \mathbb{E}[\ell(g(X), Y)] \, .$$

- **Strategy:** Given a *training sample* $(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), ..., (\boldsymbol{x}_n, y_n)$ of (X, Y), one minimizes the empirical version of $\mathbb{E}[\ell(g(X), Y)]$:

$$\frac{1}{n} \sum_{i=1}^{n} \ell\big(g(\boldsymbol{x}_i), y_i\big) \, .$$

- **Method:** Numerical optimization, *e.g.*, **gradient descent**.

- **Stochastic gradient descent:** Use a single (randomly drawn) observation to iteratively approximate g^*.

Contents

Method of gradient descent

- Consider a cost function $\mathcal{E}$ that is **continuously differentiable** function of some unknown weight (parameter) vector $\boldsymbol{w}$.
- In the **method of gradient descent**, the successive adjustments are applied to $\boldsymbol{w}$ in the direction of gradient descent, *i.e.* in the direction opposite to the gradient vector $\nabla\mathcal{E}$:

$$\boldsymbol{g} = \nabla\mathcal{E}(\boldsymbol{w}) = \left(\frac{\partial\mathcal{E}}{\partial w_1}\boldsymbol{e}_{w_1}, \frac{\partial\mathcal{E}}{\partial w_2}\boldsymbol{e}_{w_2}, ..., \frac{\partial\mathcal{E}}{\partial w_m}\boldsymbol{e}_{w_m}\right)^T .$$

- The step of the algorithm is then defined as

$$\boldsymbol{w}(n+1) = \boldsymbol{w}(n) - \gamma\boldsymbol{g}(n)\,,$$

  where γ is the **learning rate**.
- When going from iteration n to iteration $n+1$, the **correction** is applied to the weights:

$$\begin{aligned}\Delta\boldsymbol{w}(n) &= \boldsymbol{w}(n+1) - \boldsymbol{w}(n)\\ &= -\gamma\boldsymbol{g}(n)\,.\end{aligned}$$

Method of gradient descent

- Let us show that the constructed algorithm fulfills the idea of the **iterative descent**, *i.e.* that it satisfies

$$\mathcal{E}\big(\boldsymbol{w}(n+1)\big) < \mathcal{E}\big(\boldsymbol{w}(n)\big)\,.$$

- Using the first-order Taylor series expansion around $\boldsymbol{w}(n)$ to approximate $\mathcal{E}\big(\boldsymbol{w}(n+1)\big)$ as

$$\mathcal{E}\big(\boldsymbol{w}(n+1)\big) \approx \mathcal{E}\big(\boldsymbol{w}(n)\big) + \boldsymbol{g}^T(n)\Delta\boldsymbol{w}(n)$$

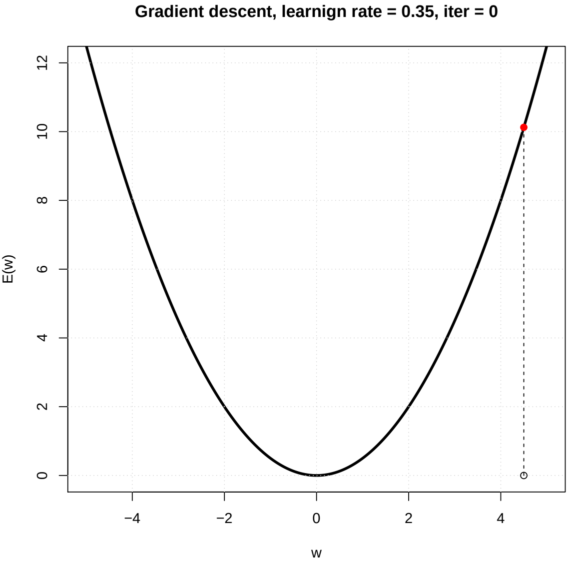
is justified for γ small enough.

- Substituting $\Delta\boldsymbol{w}(n)$ gives:

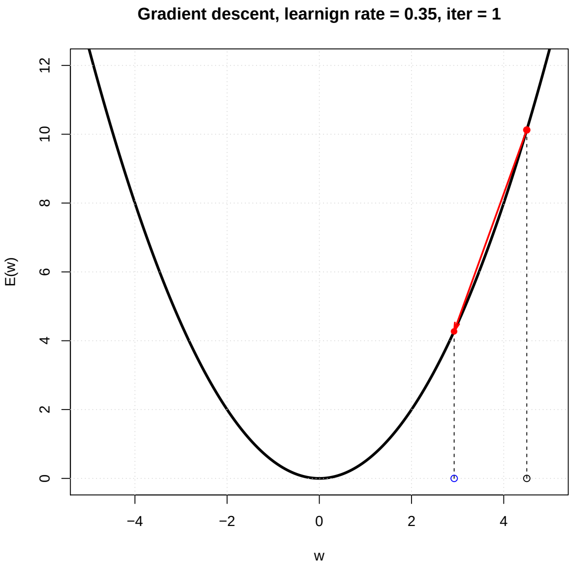
$$\begin{aligned}\mathcal{E}\big(\boldsymbol{w}(n+1)\big) &\approx \mathcal{E}\big(\boldsymbol{w}(n)\big) - \gamma\boldsymbol{g}^T(n)\boldsymbol{g}(n)\\ &= \mathcal{E}\big(\boldsymbol{w}(n)\big) - \gamma\|\boldsymbol{g}(n)\|^2\,,\end{aligned}$$

and thus for a positive learning rate the cost function decreases on each iteration.

Method of gradient descent: example (slow learning rate)



Method of gradient descent: example (slow learning rate)



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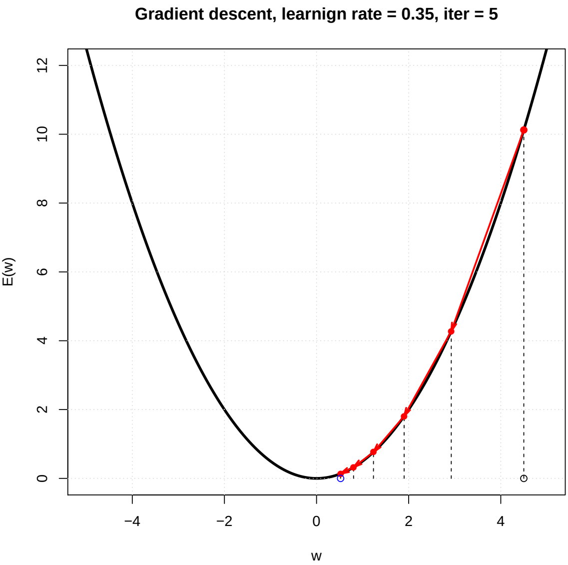
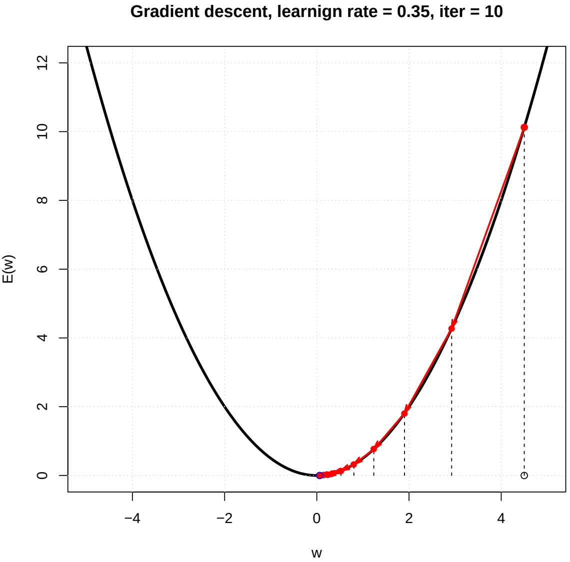
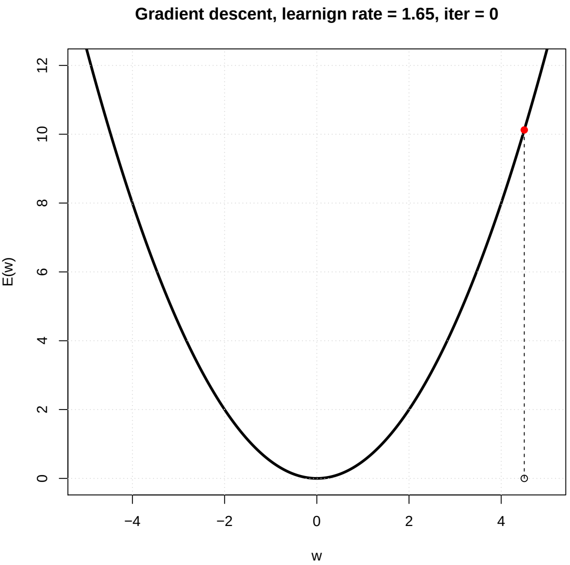


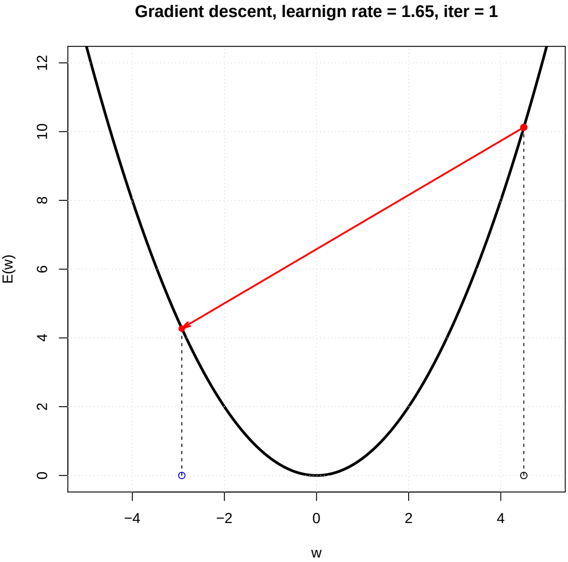
Method of gradient descent: example (slow learning rate)



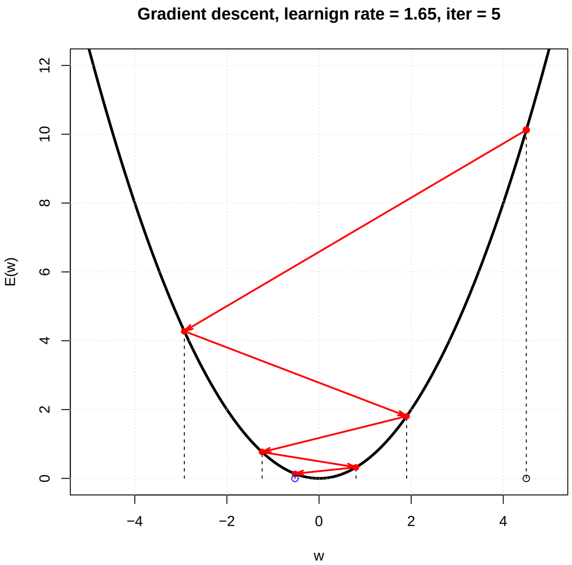
Method of gradient descent: example (fast learning rate)



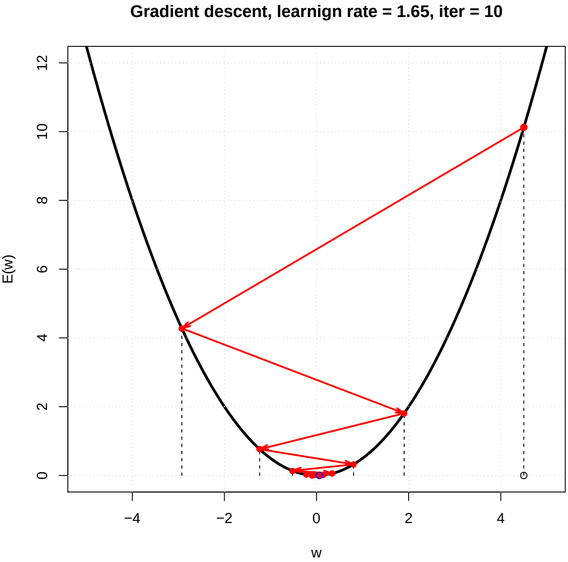
Method of gradient descent: example (fast learning rate)



Method of gradient descent: example (fast learning rate)



Method of gradient descent: example (fast learning rate)

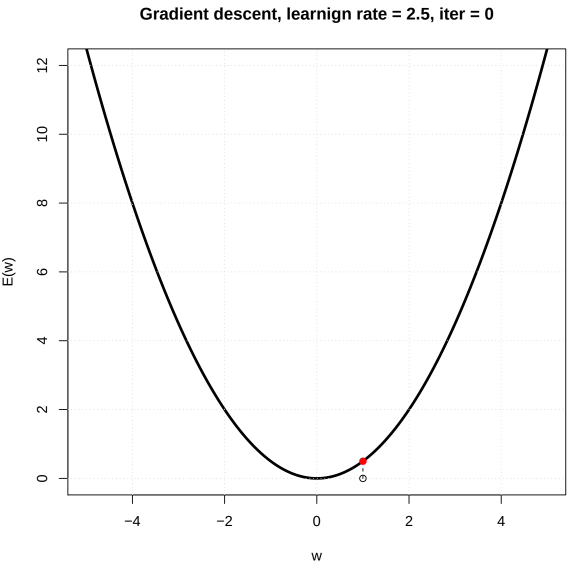


Method of gradient descent, choice of learning rate

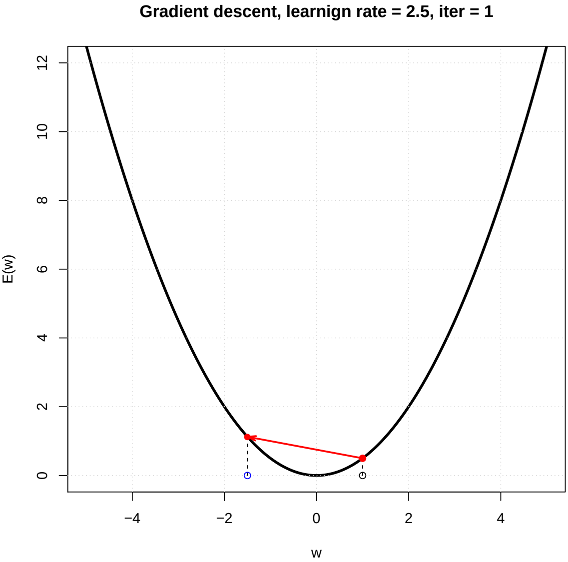
The method **converges** to the optimal solution **slowly**.
Moreover, the **learning rate** γ has a profound influence on its convergence behavior:

- When γ is small, the transient response of the algorithm is **overdamped**, and the trajectory of $\boldsymbol{w}(n)$ follows a smooth path in the parameter space.
- When γ is large, the transient response is **underdamped**, and the trajectory of $\boldsymbol{w}(n)$ follows a zigzagging (oscillatory) path.
- When γ exceeds a certain critical value, the algorithm becomes unstable and may diverge.

Method of gradient descent: example (divergent case)



Method of gradient descent: example (divergent case)



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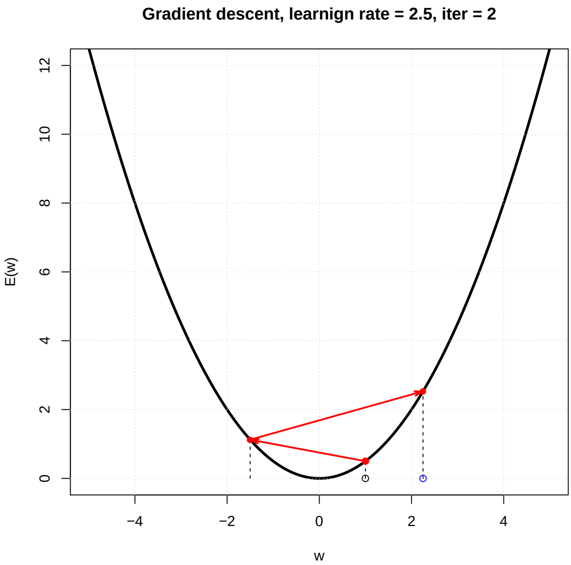
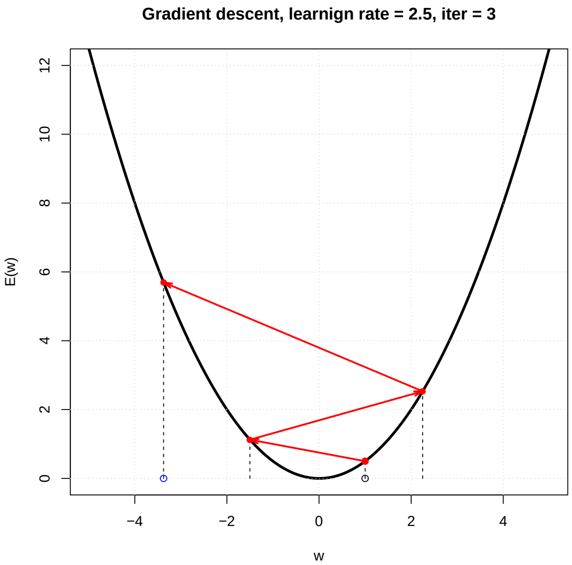
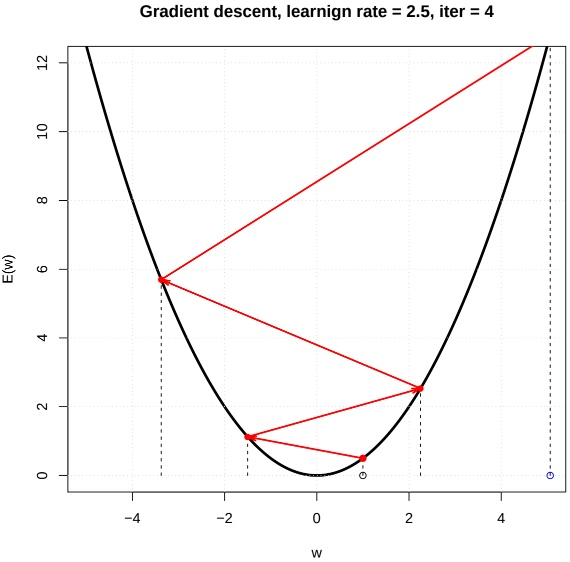


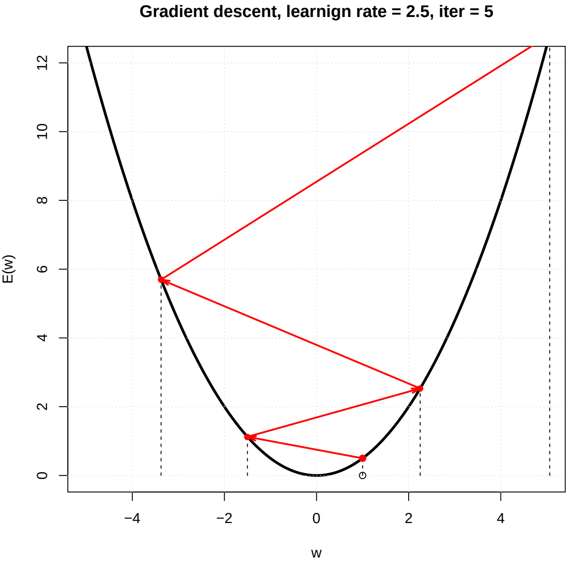
Method of gradient descent: example (divergent case)



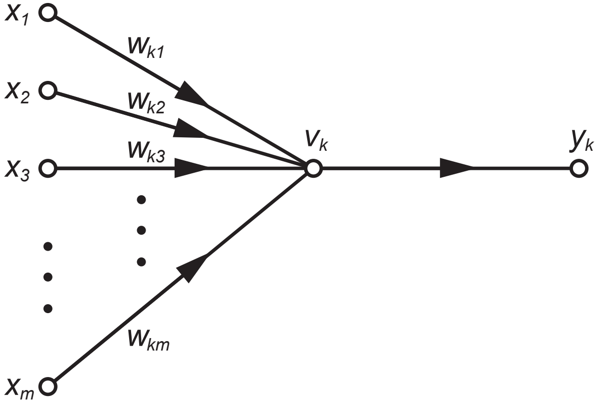
Method of gradient descent: example (divergent case)



Method of gradient descent: example (divergent case)



A signal-flow graph of a simplified neuron



Method of gradient descent: iris data

- A simplified neuron has the following prediction function:

$$p_{\boldsymbol{w}}(\boldsymbol{x}) = \sum_{q=1}^{m} w_q x_q \,.$$

- For a data sample $(\boldsymbol{x}_1, y_1)$, $(\boldsymbol{x}_2, y_2)$ ..., $(\boldsymbol{x}_n, y_n)$, let us measure its empirical error by a convex function, *e.g.* using the quadratic loss:

$$\mathcal{E}(\boldsymbol{w}) = \frac{1}{2} \times \frac{1}{n} \sum_{j=1}^{n} e_j(\boldsymbol{w})^2 = \frac{1}{2} \times \frac{1}{n} \sum_{j=1}^{n} \big(y_j - p_{\boldsymbol{w}}(\boldsymbol{x}_j)\big)^2 \,.$$

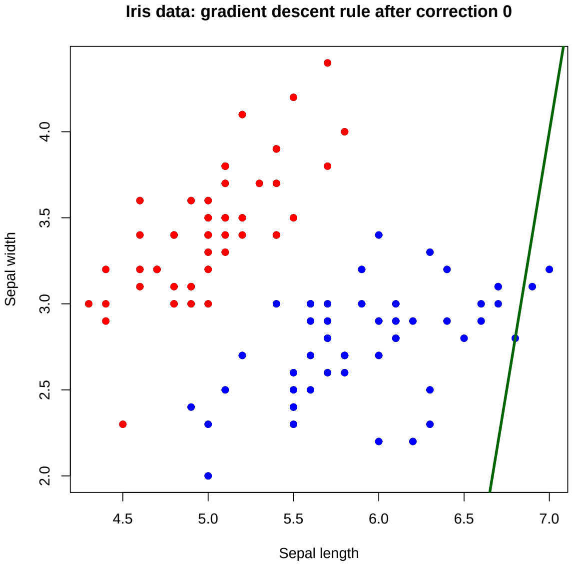
- The gradient equals:

$$\boldsymbol{g} = \nabla \mathcal{E}(\boldsymbol{w}) = -\frac{1}{n} \sum_{j=1}^{n} \big(y_j - p_{\boldsymbol{w}}(\boldsymbol{x}_j)\big) \boldsymbol{x}_j \,.$$

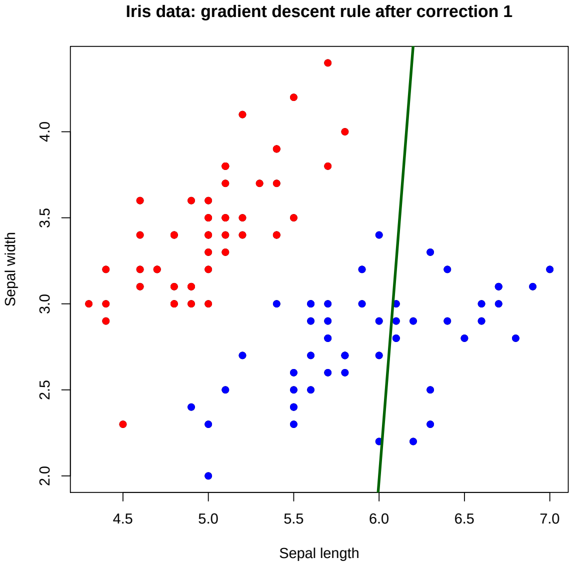
- The step of the algorithm is then:

$$\boldsymbol{w}(i+1) = \boldsymbol{w}(i) - \gamma \boldsymbol{g}(i) = \boldsymbol{w}(i) + \frac{\gamma}{n} \sum_{j=1}^{n} \big(y_j - \boldsymbol{w}(i)^T \boldsymbol{x}_j\big) \boldsymbol{x}_j \,.$$

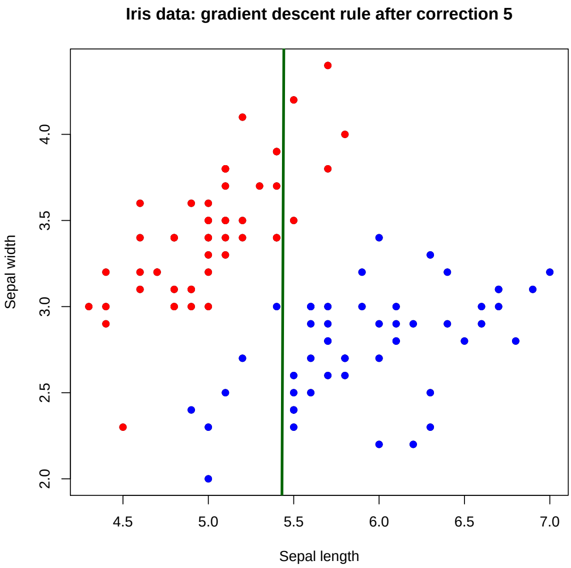
Method of gradient descent: iris data



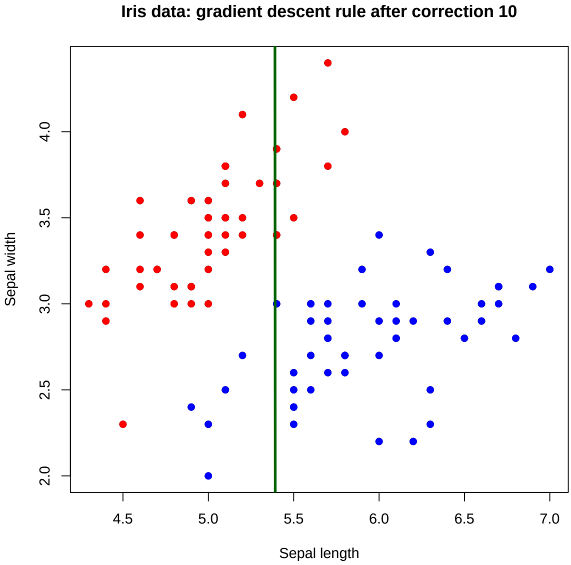
Method of gradient descent: iris data



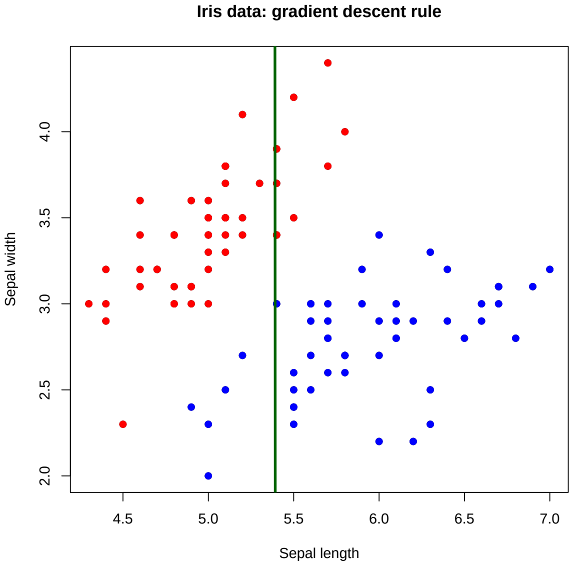
Method of gradient descent: iris data



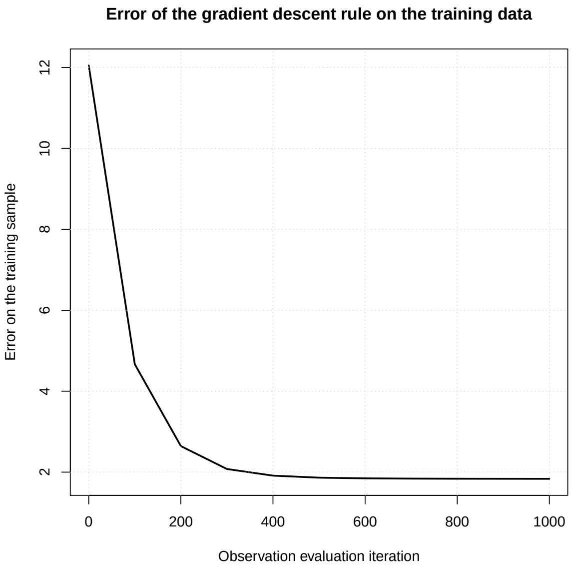
Method of gradient descent: iris data



Method of gradient descent: iris data



Method of gradient descent: iris data



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The least-mean-square algorithm

- The **least-mean-square (LMS) algorithm** attempts to minimize the **instantaneous value** of the cost function

$$\mathcal{E}(\hat{\boldsymbol{w}}) = \frac{1}{2}e^2(n)\,,$$

where $e(n)$ is the error measured at time n.
- Differentiating $\mathcal{E}(\hat{\boldsymbol{w}})$ w.r.t. $\hat{\boldsymbol{w}}$ gives:

$$\frac{\partial \mathcal{E}(\hat{\boldsymbol{w}})}{\partial \hat{\boldsymbol{w}}} = e(n)\frac{\partial e(n)}{\partial \hat{\boldsymbol{w}}}\,.$$

- When operating on the linear neuron, the error can be expressed as:

$$e(n) = d(n) - \boldsymbol{x}^T(n)\hat{\boldsymbol{w}}(n)\,.$$

- Thus

$$\frac{\partial e(n)}{\partial \hat{\boldsymbol{w}}} = -\boldsymbol{x}(n) \quad \text{and} \quad \frac{\partial \mathcal{E}(\hat{\boldsymbol{w}})}{\partial \hat{\boldsymbol{w}}(n)} = -\boldsymbol{x}(n)e(n) = \hat{\boldsymbol{g}}(n)\,.$$

- Now, LMS can be formulated as follows:

$$\hat{\boldsymbol{w}}(n+1) = \hat{\boldsymbol{w}}(n) + \gamma\boldsymbol{x}(n)e(n)\,.$$

The least-mean-square algorithm

Input:

- Input signals $\boldsymbol{x}(n)$ with correct outputs $d(n)$ for n=1,2,...
- Learning rate γ.

Initialization:

- Set $\hat{\boldsymbol{w}}(1) = \mathbf{0}$.

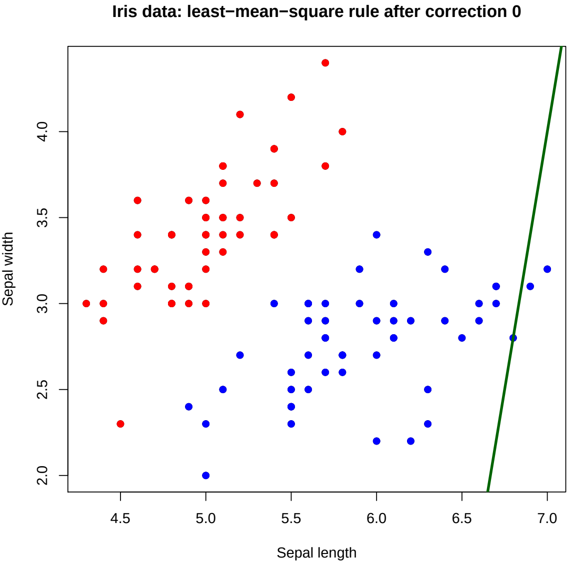
Iterations:

- For $n = 1, 2, \dots$, compute
  - $e(n) = d(n) - \hat{\boldsymbol{w}}^T(n)\boldsymbol{x}(n)$,
  - $\hat{\boldsymbol{w}}(n+1) = \hat{\boldsymbol{w}}(n) + \gamma \boldsymbol{x}(n) e(n)$.

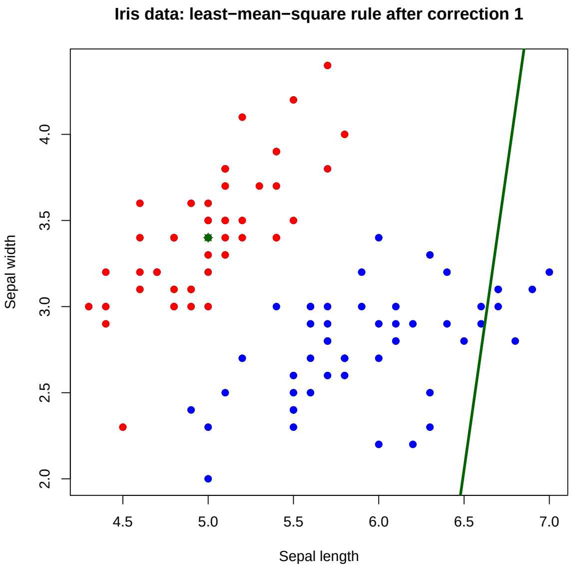
Remarks:

- The inverse of the learning rate acts as a **measure of the memory** of the LMS algorithm: the smaller γ is set, the longer the memory span over which the LMS remembers the past data will be.
- Having $\hat{\boldsymbol{w}}(n)$ in place of $\boldsymbol{w}(n)$ emphasizes that the LMS algorithm produces the **instantaneous estimate** of the weights, which would result from the gradient descent.
- For this last reason, the LMS-updated weights $\hat{\boldsymbol{w}}(n)$ trace a random trajectory in the parameter space: **stochastic gradient descent**.

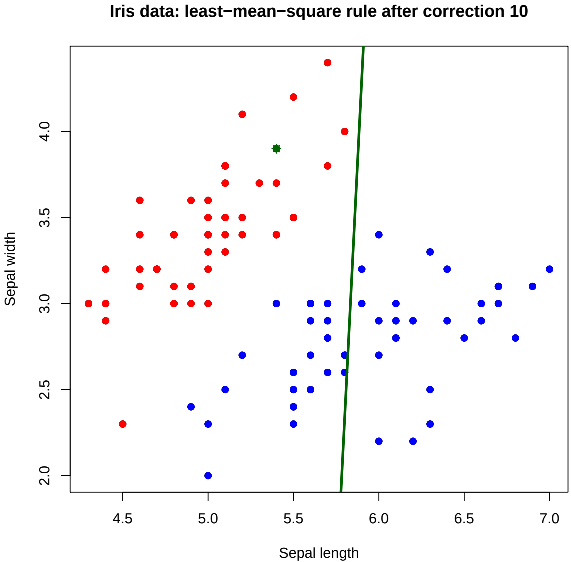
The least-mean-square algorithm: iris data



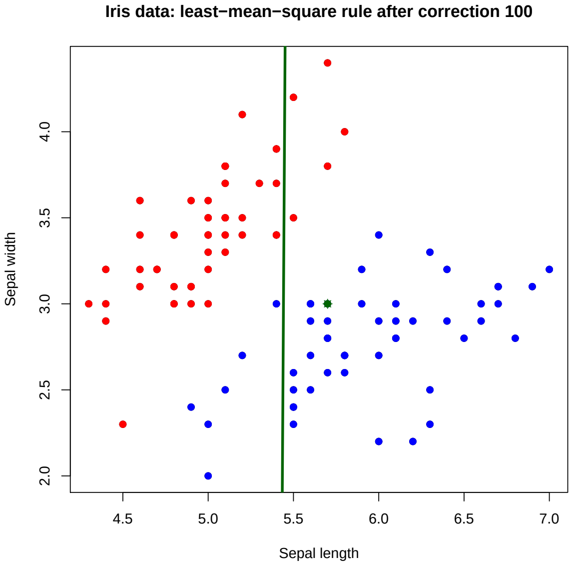
The least-mean-square algorithm: iris data



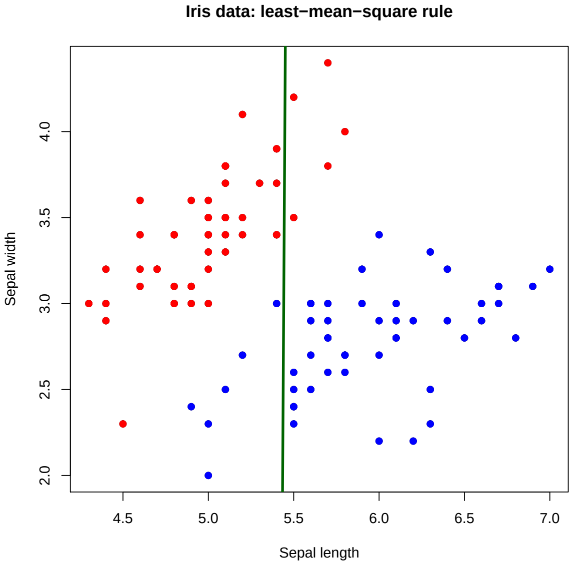
The least-mean-square algorithm: iris data



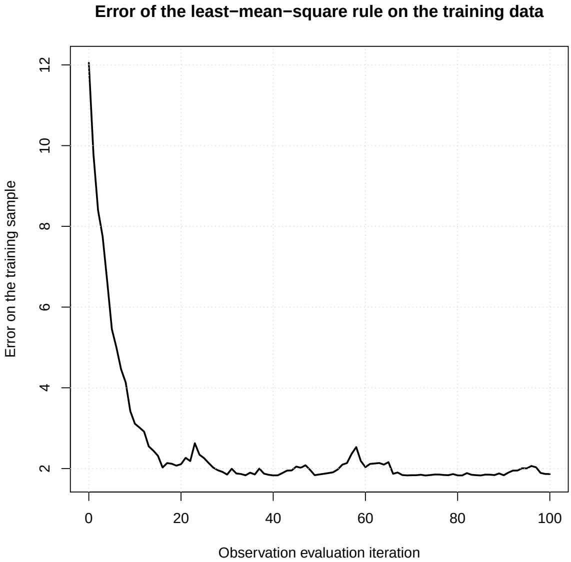
The least-mean-square algorithm: iris data



The least-mean-square algorithm: iris data



The least-mean-square algorithm: iris data



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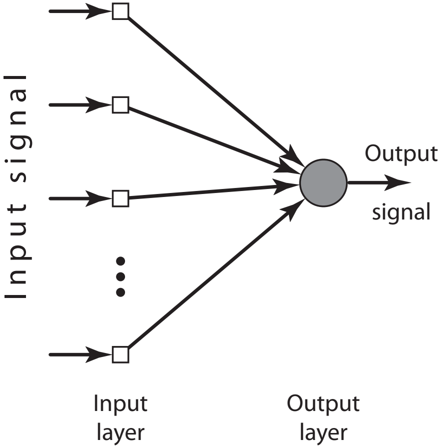
Single layer perceptron



Preliminaries

- **Error signal** produced at the output of neuron j is defined by

$$e_j(n) = d_j(n) - y_j(n)\,,$$

where $d_j(n)$ is the correct output.

- As before, we define the **cost function** penalizing neuron j as

$$\mathcal{E}_j(n) = \frac{1}{2} e_j^2(n)\,.$$

- The **induced local field** $v_j(n)$ produced at the input of the activation function associated with neuron j is therefore

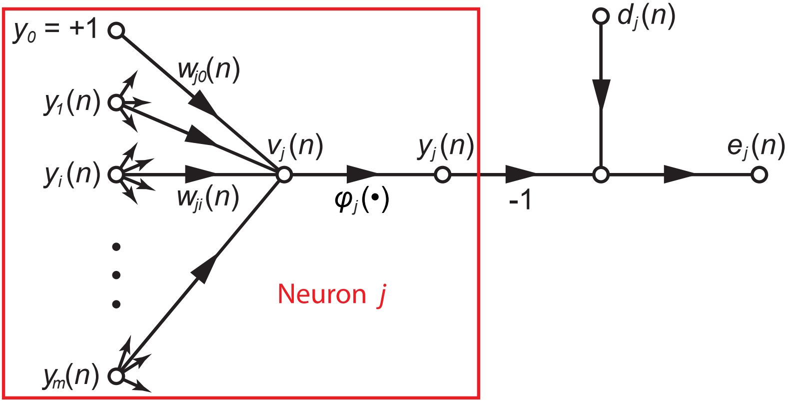
$$v_j(n) = \sum_{i=0}^{m} w_{ji}(n) y_i(n)\,,$$

where m is the number of inputs excluding bias applied to neuron j.

- The **output signal** $y_j(n)$ appearing at the output of neuron j at iteration n equals:

$$y_j(n) = \phi\big(v_j(n)\big)\,.$$

A signal-flow graph of a neuron and its output



Derivation for a single (output-layer) neuron

- In a manner similar to the LMS algorithm, the back-propagation algorithm applies a correction $\Delta w_{ji}(n)$ to the synaptic weight w_{ji}, which is proportional to the partial derivative $\frac{\partial \mathcal{E}(n)}{\partial w_{ji}(n)}$. Applying of the **chain rule** of the calculus, this gradient can be expressed as:

$$\frac{\partial \mathcal{E}(n)}{\partial w_{ji}(n)} = \frac{\partial \mathcal{E}(n)}{\partial e_j(n)} \times \frac{\partial e_j(n)}{\partial y_j(n)} \times \frac{\partial y_j(n)}{\partial v_j(n)} \times \frac{\partial v_j(n)}{\partial w_{ji}(n)} \,.$$

- Partial derivatives equal:

$$\begin{aligned}
\frac{\partial \mathcal{E}(n)}{\partial e_j(n)} &= e_j(n)\,, \\
\frac{\partial e_j(n)}{\partial y_j(n)} &= -1\,, \\
\frac{\partial y_j(n)}{\partial v_j(n)} &= \phi_j'(v_j(n))\,, \\
\frac{\partial v_j(n)}{\partial w_{ji}(n)} &= y_i(n)\,.
\end{aligned}$$

Derivation for a single (output-layer) neuron

- From these, the partial derivative can be composed as:

$$\frac{\partial \mathcal{E}(n)}{\partial w_{ji}(n)} = -e_j(n)\phi_j'\big(v_j(n)\big)y_i(n)\,.$$

- This partial derivative represents a **sensitivity factor**, which determines the direction of search in the parameter space for synaptic weight w_{ji}.
- The correction $\Delta w_{ji}(n)$ applied to $w_{ji}(n)$ is defined as:

$$\Delta w_{ji}(n) = -\gamma \frac{\partial \mathcal{E}(n)}{\partial w_{ji}(n)}\,,$$

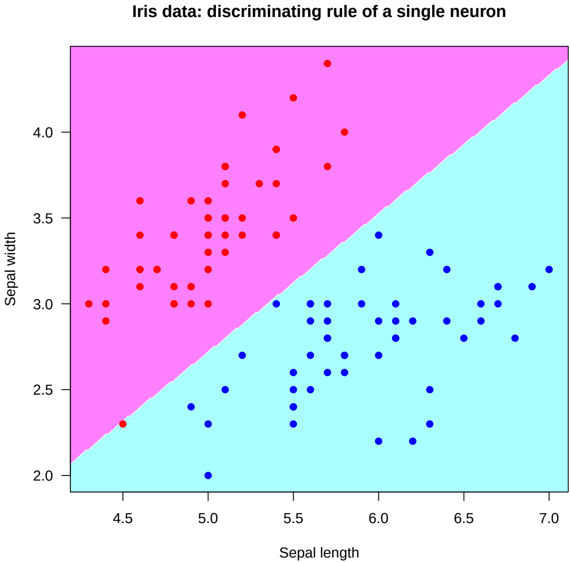
  with γ being the **learning parameter** of the back-propagation algorithm.
- Accordingly, one can generalize

$$\Delta w_{ji}(n) = \gamma \delta_j(n) y_i(n)$$

  where the **local gradient** $\delta_j(n)$ is defined by

$$\delta_j(n) = -\frac{\partial \mathcal{E}(n)}{\partial v_j(n)} = -\frac{\partial \mathcal{E}(n)}{\partial e_j(n)}\frac{\partial e_j(n)}{\partial y_j(n)}\frac{\partial y_j(n)}{\partial v_j(n)} = e_j(n)\phi_j'\big(v_j(n)\big)\,.$$

Single neuron: iris data



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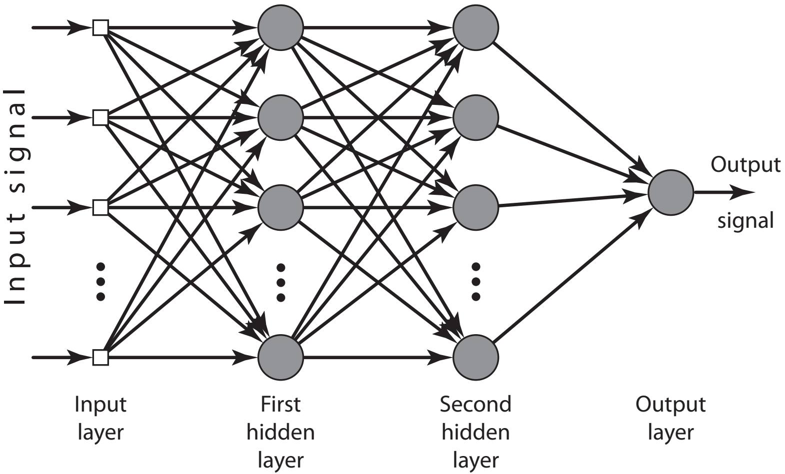
Multilayer neural network (example)



Derivation for a hidden neuron

- **Problem:** When neuron j is located in a hidden layer, there is **no specified desired response** for it.
- For a **hidden neuron** j, one may define the local gradient $\delta_j(n)$ as:

$$\begin{aligned} \delta_j(n) &= -\frac{\partial \mathcal{E}(n)}{\partial y_j(n)} \frac{\partial y_j(n)}{\partial v_j(n)} \\ &= -\frac{\partial \mathcal{E}(n)}{\partial y_j(n)} \phi_j'(v_j(n)) \,, \quad \text{neuron } j \text{ is hidden} \,. \end{aligned}$$

- To **calculate the partial derivative** $\frac{\partial \mathcal{E}(n)}{\partial y_j(n)}$, one may proceed as follows (denoting C the set of all output neurons for generality):

$$\mathcal{E}(n) = \frac{1}{2} \sum_{k \in C} e_k^2(n) \,, \quad \text{neuron } k \text{ is an output node} \,.$$

- Differentiating this w.r.t. the output of neuron j $y_j(n)$, one gets

$$\frac{\partial \mathcal{E}(n)}{\partial y_j(n)} = \sum_{k \in C} e_k \frac{\partial e_k(n)}{\partial y_j(n)} \,.$$

Derivation for a hidden neuron

- Application of the chain rule to the partial derivative $\frac{\partial e_k(n)}{\partial y_j(n)}$ gives:

$$\frac{\partial \mathcal{E}(n)}{\partial y_j(n)} = \sum_{k \in C} e_k(n) \frac{\partial e_k(n)}{\partial v_k(n)} \frac{\partial v_k(n)}{\partial y_j(n)} \, .$$

- Using

$$\begin{aligned} e_k(n) &= d_k(n) - y_k(n) \\ &= d_k(n) - \phi_k\big(v_k(n)\big) \, , \quad \text{neuron } k \text{ is an output node} \, , \end{aligned}$$

  one gets

$$\frac{\partial e_k(n)}{\partial v_k(n)} = -\phi_k'\big(v_k(n)\big) \, .$$

- Taking into account that the induced local field for neuron k is

$$v_k(n) = \sum_{j=0}^{m} w_{kj}(n) y_j(n) \, ,$$

  (with m being the number of inputs) one obtains

$$\frac{\partial v_k(n)}{\partial y_j(n)} = w_{kj}(n) \, .$$

Derivation for a hidden neuron

- The desired partial derivative equals

$$\begin{aligned}\frac{\partial \mathcal{E}(n)}{\partial y_j(n)} &= -\sum_{k \in C} e_k(n)\phi_k'\big(v_k(n)\big)w_{kj}(n) \\ &= -\sum_{k \in C} \delta_k(n) w_{kj}(n)\,,\end{aligned}$$

  with $\delta_k(n) = e_k(n)\phi_k'\big(v_k(n)\big)$ as before.
- Finally, the **back-propagation formula** for the local gradient $\delta_j(n)$ can be written as:

$$\delta_j(n) = \phi_j'\big(v_j(n)\big)\sum_{k \in C} \delta_k(n) w_{kj}(n)\,, \quad \text{neuron } j \text{ is hidden}\,.$$

Summarizing:

1. If neuron j is an **output neuron**, the local gradient equals

$$\delta_j(n) = \phi_j'(n) e_j(n)\,.$$

2. If neuron j is a **hidden neuron**, the local gradient equals

$$\delta_j(n) = \phi_j'(n)\sum_{k} \delta_k(n) w_{kj}(n)\,, \quad k \text{ indexes next layer neurons}\,.$$

Summary of the back-propagation algorithm

- The back-propagation algorithm applies correction $\Delta w_{ji}(n)$ to the synaptic weight connecting neuron i to neuron j, defined by the delta rule:

$$\begin{pmatrix} \textit{Weight} \\ \textit{correction} \\ \Delta w_{ji}(n) \end{pmatrix} = \begin{pmatrix} \textit{learning} \\ \textit{rate} \\ \gamma \end{pmatrix} \times \begin{pmatrix} \textit{local} \\ \textit{gradient} \\ \delta_j(n) \end{pmatrix} \times \begin{pmatrix} \textit{input signal} \\ \textit{of neuron } j\,, \\ y_i(n) \end{pmatrix}$$

- To increase the rate of learning while avoiding the danger of instability one may include a momentum term:

$$\Delta w_{ji}(n) = \alpha \Delta w_{ji}(n-1) + \gamma \delta_j(n) y_j(n)\,,$$

  where α is usually a positive number called **momentum constant**. This rule is also called the generalized delta rule (delta rule is its special case with $\alpha = 0$).
- **Criterion of convergence**:
  The back-propagation algorithm is considered to have converged when the absolute rate of change in the average square error per epoch is sufficiently small.

Summary of the back-propagation algorithm

1. **Initialization:** Pick the synaptic weights and thresholds from a uniform distribution with mean 0 and variance chosen due to the shape of the sigmoid function.
2. **Presentation of training examples:** Present the network an epoch of training examples, repeating for each example steps 3. and 4.
3. **Forward computation (classification):** Passing layers $l = 1, ..., L$, compute outputs and errors:

$$y^{(0)}(n) = x_j(n);\ y_j^{(l)}(n) = \phi_j\Big(\sum_i w_{ji}^{(l)}(n) y_i^{(l-1)}(n)\Big);\ e_j(n) = d_j(n) - y_j^{(L)}(n)$$

4. **Backward computation:** Passing layers $l = 1, ..., L$, compute local gradients:

$$\delta_j^{(l)}(n) = \begin{cases} \phi_j'\big(\sum_i w_{ji}^{(L)}(n) y_i^{(L-1)}(n)\big)\, e_j^{(L)}(n) & \text{if output}\,, \\ \phi_j'\big(\sum_i w_{ji}^{(l)}(n) y_i^{(l-1)}(n)\big)\, \sum_k \delta_k^{(l+1)}(n) w_{kj}^{(l+1)}(n) & \text{if hidden}\,. \end{cases}$$

   Adjust synaptic weights:

$$w_{ji}^{(l)}(n+1) = w_{ji}^{(l)}(n) + \alpha w_{ji}^{(l)}(n-1) + \gamma \delta_j^{(l)}(n) y_i^{(l-1)}(n)\,.$$

5. **Iteration:** Feed randomly permuted epochs till convergence.

Contents

An example of $\phi(\cdot)$: logistic function

- In its general form logistic function is defined by:

$$\phi_j\big(v_j(n)\big) = \frac{1}{1+\exp\big(-av_j(n)\big)}\,, \quad a>0\,,$$

  where $v_j(n)$ is the induced local field of neuron j.

- Differentiating w.r.t. $v_j(n)$ one gets:

$$\phi_j'\big(v_j(n)\big) = \frac{a\exp\big(-av_j(n)\big)}{\Big(1+\exp\big(-av_j(n)\big)\Big)^2} = ay_j(n)\big(1-y_j(n)\big)\,.$$

- Denoting network output $o_j(n) = y_j(n)$, the local gradient equals

$$\begin{aligned}\delta_j(n) &= \phi_j'\big(v_j(n)\big)\,e_j(n)\\ &= a\big(d_j(n)-o_j(n)\big)o_j(n)\big(1-o_j(n)\big)\,, \quad j \text{ is an output neuron}\,,\end{aligned}$$

- and respectively

$$\begin{aligned}\delta_j(n) &= \phi_j'\big(v_j(n)\big)\,\sum_k \delta_k(n)w_{kj}(n)\\ &= ay_j(n)\big(1-y_j(n)\big)\sum_k \delta_k(n)w_{kj}(n)\,, \quad j \text{ is a hidden neuron}\,.\end{aligned}$$

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Complexity regularization

- In designing a multilayer perceptron by whatever method, we are in effect building **a non-linear model** of the physical phenomenon responsible for the generation of the input-output examples used to train the network.
- Insofar as the network design is statistical in nature, we need an appropriate **tradeoff** between **reliability** of the training data and **goodness** of the model.
- In the context of back-propagation learning, or any other supervised learning procedure for that matter, we may realize this tradeoff by minimizing the **total risk**, expressed as a function of the parameter vector $\boldsymbol{w}$, as follows:

$$R(\boldsymbol{w}) = \mathcal{E}_{av}(\boldsymbol{w}) + \lambda \mathcal{E}_c(\boldsymbol{w}) \,.$$

- $\mathcal{E}_{av}(\boldsymbol{w})$ is the standard **performance metric**, which depends on both the network (model) and the input data, and in back-propagation learning is typically defined as a mean-square error.
- $\mathcal{E}_c(\boldsymbol{w})$ is the **complexity penalty**, where the notion of complexity is measured in terms of the network (weights) alone.
- λ is a **regularization parameter**.

L^2 parameter regularization

- A simple and most common parameter norm penalty is the L^2 parameter norm penalty commonly known as **weight decay**:

$$\mathcal{E}_c(\boldsymbol{w}) \; = \frac{1}{2}\|\boldsymbol{w}\|_2^2 = \frac{1}{2}\sum_{k\in\mathcal{C}_{total}} w_k^2 \,.$$

- It is also called *ridge regression* of *Tikhonov regularization*.
- Such a model has the following **total risk**:

$$R(\boldsymbol{w}) = \frac{\lambda}{2}\boldsymbol{w}^\top\boldsymbol{w} + \mathcal{E}_{av}(\boldsymbol{w})\,,$$

- and the corresponding parameter **gradient**:

$$\boldsymbol{g} = \lambda\boldsymbol{w} + \nabla\mathcal{E}_{av}(\boldsymbol{w})\,.$$

- The **weight update** is:

$$\boldsymbol{w}(n+1) = (1-\gamma\lambda)\boldsymbol{w}(n) - \gamma\nabla\mathcal{E}_{av}\big(\boldsymbol{w}(n)\big)\,.$$

- The weight decay term now **multiplicatively shrinks the weight vector** by a constant factor, just **before** performing the usual **gradient update**.

L^1 parameter regularization

- While L^2 weight decay is the most common form of weight decay, another option is to use L^1 regularization.
- L^1 regularization on the model parameter $\boldsymbol{w}$ is defined as:

$$\mathcal{E}_c(\boldsymbol{w}) \;= \|\boldsymbol{w}\|_1 = \sum_{k \in \mathcal{C}_{total}} |w_k| \,.$$

- The **total risk** is given by:

$$R(\boldsymbol{w}) = \lambda \|\boldsymbol{w}\|_1 + \mathcal{E}_{av}(\boldsymbol{w}) \,,$$

- and the corresponding **gradient**:

$$\boldsymbol{g} = \lambda \text{sign}(\boldsymbol{w}) + \nabla \mathcal{E}_{av}(\boldsymbol{w}) \,.$$

- The **weight update** is then:

$$\boldsymbol{w}(n+1) = \boldsymbol{w}(n) - \gamma\lambda \text{sign}(\boldsymbol{w}) - \gamma \nabla \mathcal{E}_{av}\big(\boldsymbol{w}(n)\big) \,.$$

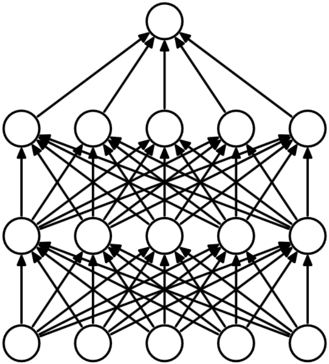
- The regularization **contribution** to the gradient is a **constant factor** with a sign equal (component-wise) to $\text{sign}(w_k)$.
- L^1 regularization introduces **sparsity** (some w_k have optimal value $= 0$). This is used for *feature selection*, see also *LASSO*.

The dropout strategy

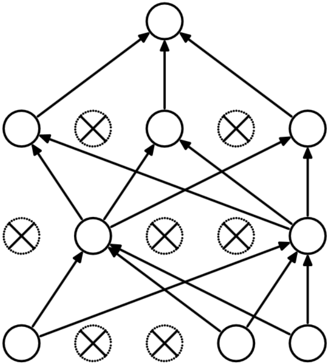
- **Dropout** provides a computationally inexpensive but powerful method of regularizing a broad family of models.
- To a first approximation, dropout can be thought of as a method of making **bagging** practical **for ensembles of** very many large **neural networks**.
- Bagging involves **training multiple models**, and evaluating multiple models on each test example. This **seems impractical** when each model is a large neural network, since training and evaluating such networks is costly in terms of computation time and memory.
- It is common to use ensembles of five to ten neural networks, but more than this rapidly becomes unwieldy.
- Dropout provides an **inexpensive approximation to** training and evaluating a **bagged** ensemble of exponentially many **neural networks**.
- Specifically, **dropout trains the ensemble consisting of all sub-networks** that can be formed by removing non-output neurons from an underlying base network.

The dropout strategy

- An example of applying the dropout strategy:



Standard neural network



After applying dropout

The dropout strategy

- In most modern neural networks, based on a series of affine transformations and nonlinearities, we can effectively **remove a neuron** from a network **by multiplying its output value by zero**.
- To **train with dropout**, we **use** a **minibatch-based learning** algorithm that makes small steps, such as *stochastic gradient descent*.
- Each time we **randomly sample a** different **binary mask** to apply to all of the input and hidden neurons in the network.
- Typically, an input neuron is included with probability 0.8 and a hidden neuron is included with probability 0.5. These probabilities constitute a **hyperparameter** to be fixed in advance.
- The forward propagation, back-propagation, and the learning update are run as usual.
- To **predict** an unknown observation, we **average the output from many masks**. Even 10–20 masks are often sufficient to obtain good performance.

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Stopping criteria

- In general, back-propagation algorithm *cannot be shown to converge*, and there are no well-defined criteria for stopping its operation.
- A necessary condition for $\boldsymbol{w}^*$ to be a (*local*!) minimum is that the gradient vector $\boldsymbol{g}(\boldsymbol{w})$ of the error surface w.r.t. the weight vector $\boldsymbol{w}$ must be zero at $\boldsymbol{w} = \boldsymbol{w}^*$.
- **The back-propagation algorithm is considered to have converged when the Euclidean norm of the gradient vector reaches a sufficiently small gradient threshold.**
- But with this criterion learning time may be long.
- **The back-propagation algorithm is considered to have converged when the absolute rate of change in the average squared error per epoch is sufficiently small.**
- The rate of convergence in the average squared error is typically considered to be small enough if it lies in the range of 0.1 t 1 percent per epoch (0.01 percent per epoch is used as well).

Remarks on the back-propagation algorithm

Heuristics for making the back-propagation algorithm perform better:

- **Stochastic learning** is preferable to the *large batch/entire training sample*, updates especially when the training data sample is large and highly redundant.
- **Maximizing information content**, *e.g. shuffling* observations to ensure that successive examples rarely belong to the same class.
- Correct choice of the **activation function**, *e.g.* a sigmoid one which is *odd in its argument*.
- Choosing **target values** properly w.r.t. the activation function.
- **Normalizing the inputs**: *mean removal*, *decorrelation*, *covariance equalization*.
- **Initialization**: not large (*saturation*!) and not small (*slowing down*!) initial values; *e.g. uniform distribution* with zero mean and variance equal to the reciprocal of the number of synaptic connections of a neuron.
- **Learning from hints**: include *prior information* about your task, *e.g.* sparsity (weight sharing) in the convolutional neural networks.
- **Learning rates**: learning rate can be *smaller in the last layers* than in the front layers.

Thank you for your attention!

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