Perceptron, neural network, and the back-propagation algorithm

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Machine learning

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Today

- Rosenblatt's perceptron
  - Biological analogy
  - Historical learning algorithm
  - Novikoff's convergence theorem
- Signal-flow notation and model of an artificial neuron
- Least-mean-squares
  - Minimization of the empirical risk
  - Method of gradient descent
  - The least-mean-square algorithm
- The back-propagation algorithm
  - Derivation for a single-layer network
  - Propagation for a multilayer network
  - An example of the activation function
- Additional information on learning networks
  - Regularization in neural networks
  - Some remarks on the back-propagation

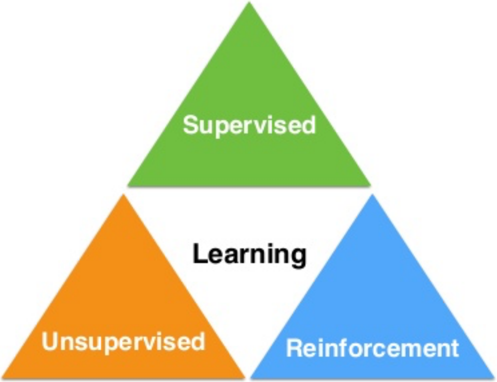
Literature

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

Supervised learning (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**:

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

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

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

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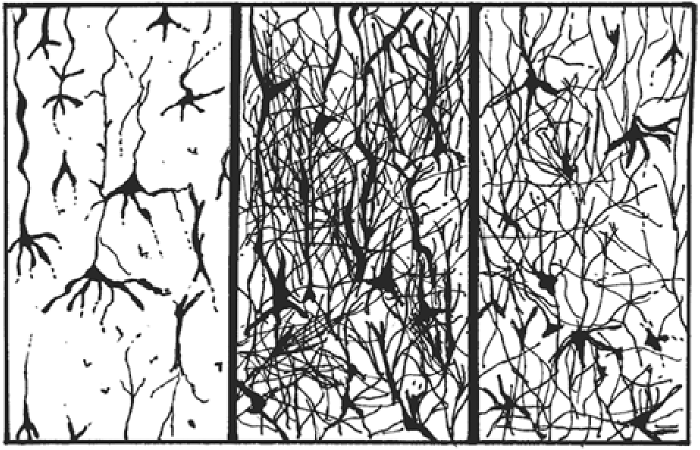
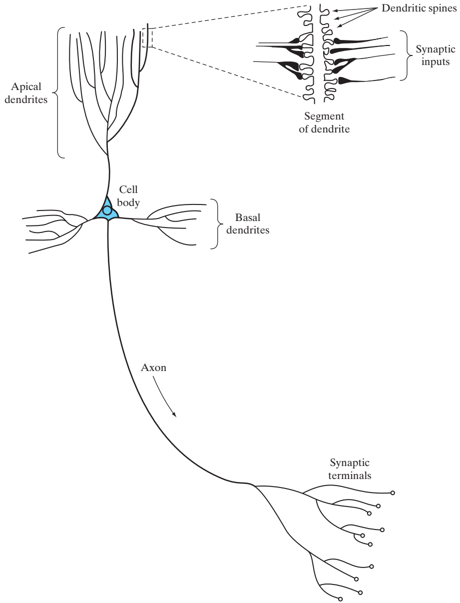
Neurons in the human body

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

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- Expert systems
- Knowledge engineering
- Recurrent architectures – Hopfield net
- Learning algorithm – back-propagation by Hinton and Rumelhart

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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

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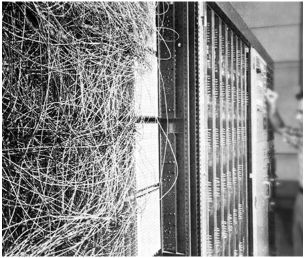

(Photo downloaded from http://www.usbdata.co/rosenblatt-perceptron.html)

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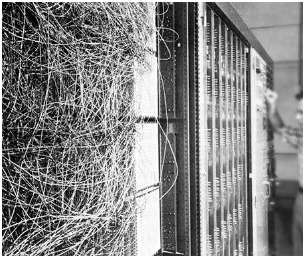

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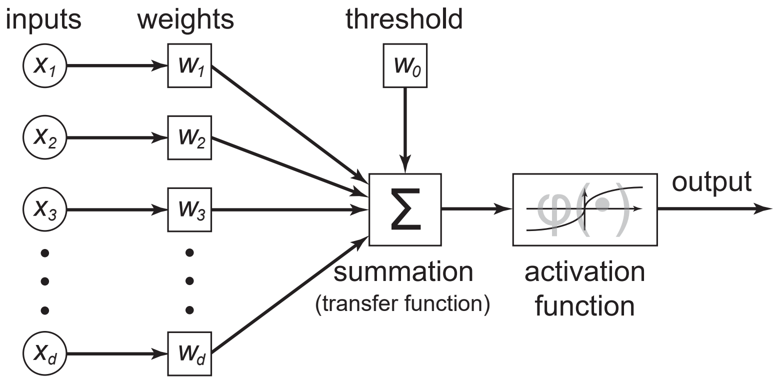
The **Mark I Perceptron** machine was the first implementation of the perceptron algorithm. The machine was connected to a **Camera** that used **20x20** cadmium sulfide **photocells** to produce a 400-pixel image. The main visible feature is a **Patchboard** that **allowed experimentation with** different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

Rosenblatt's perceptron



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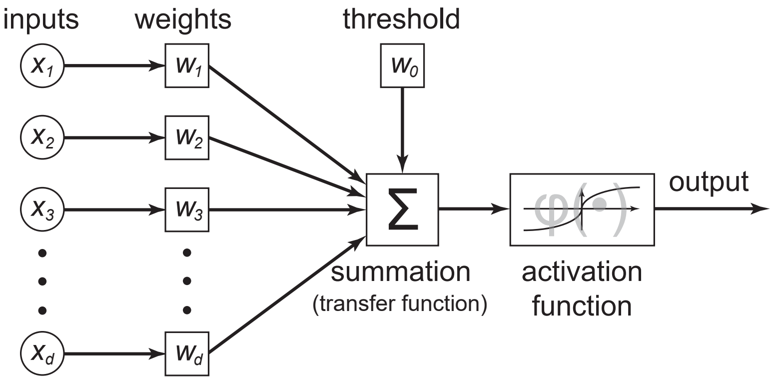

Let $\boldsymbol{w} = (w_1, w_2, ..., w_d)^T$ be the weight vector, then a new observation $\boldsymbol{x} = (x_1, x_2, ..., x_d)^T$ is classified as

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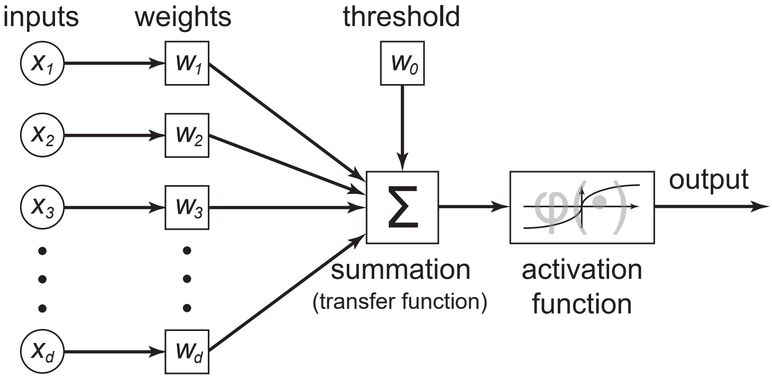

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$$g(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \phi\left(\sum_{k=1}^{d} w_k x_k + w_0\right) > 0\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

Rosenblatt's perceptron (training algorithm)

Initialize w_0 and $\boldsymbol{w}$ randomly or set $w_0 = 0$ and $\boldsymbol{w} = \mathbf{0}$.

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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:

Iris data

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

Iris data

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

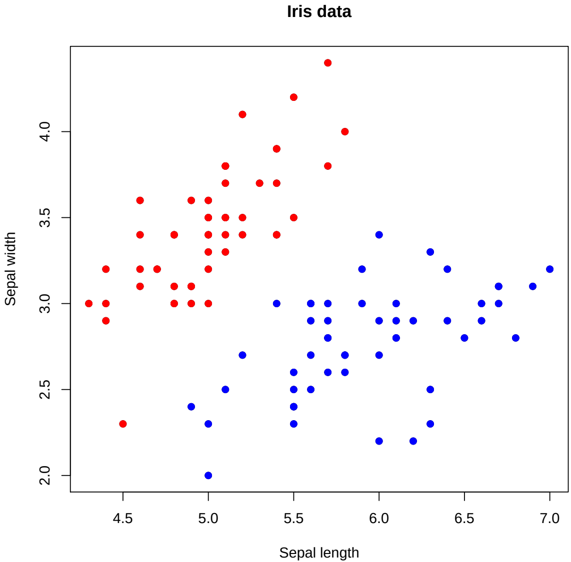
Iris **setosa**

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)



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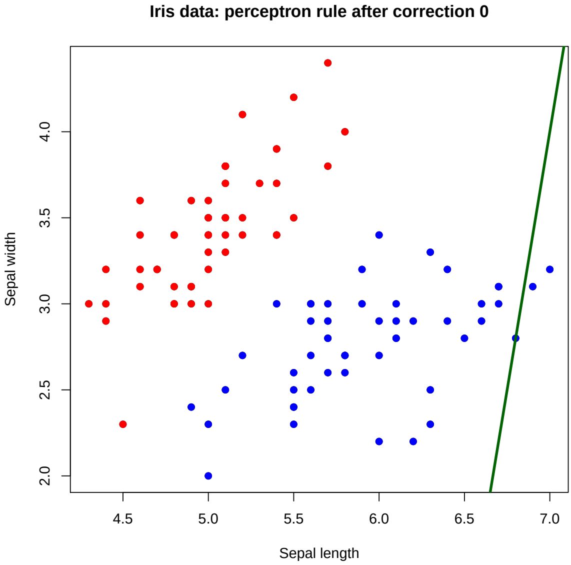

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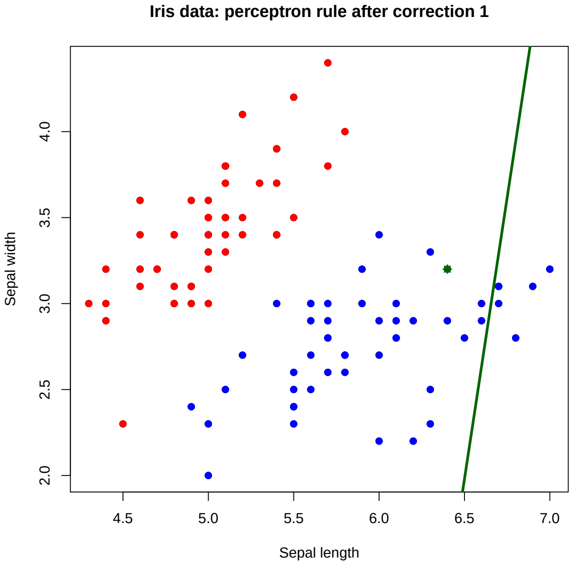

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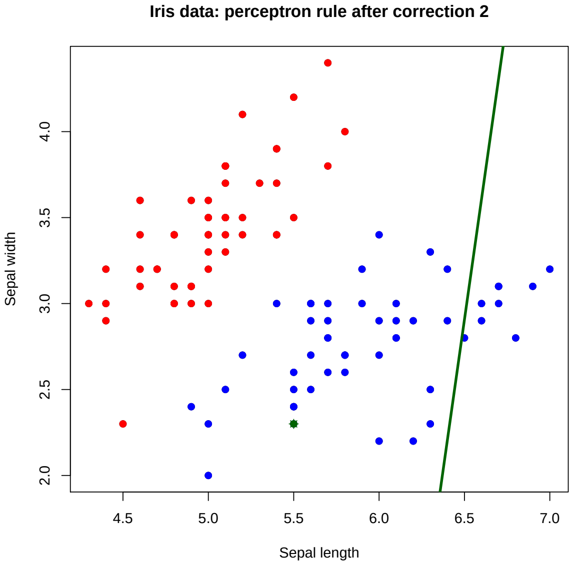

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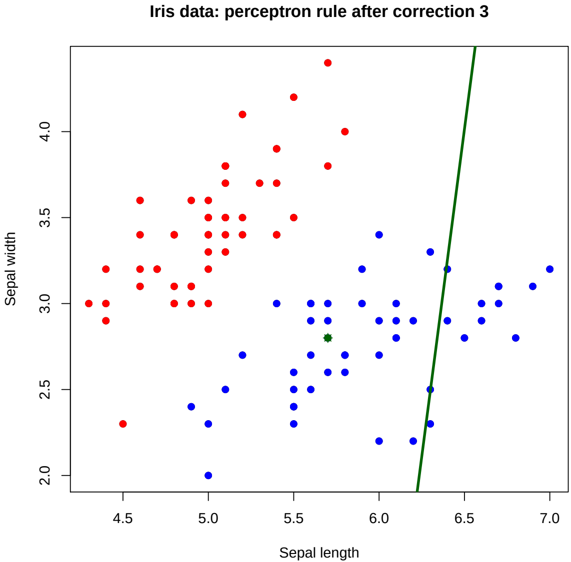

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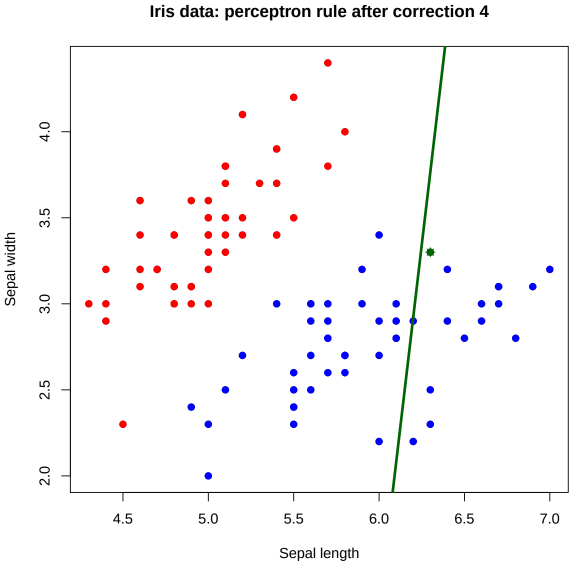

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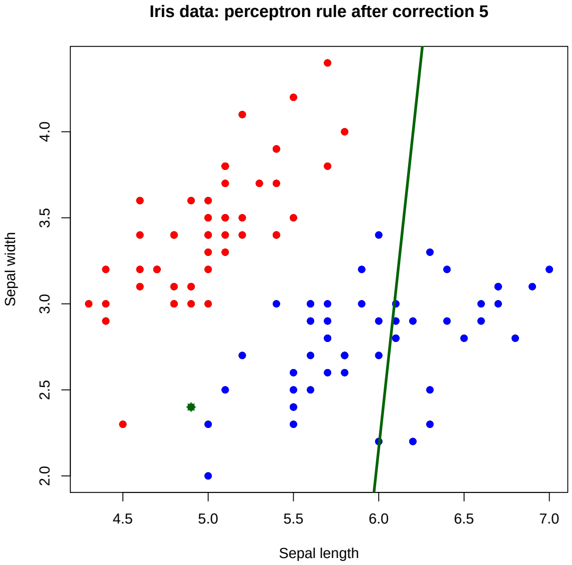

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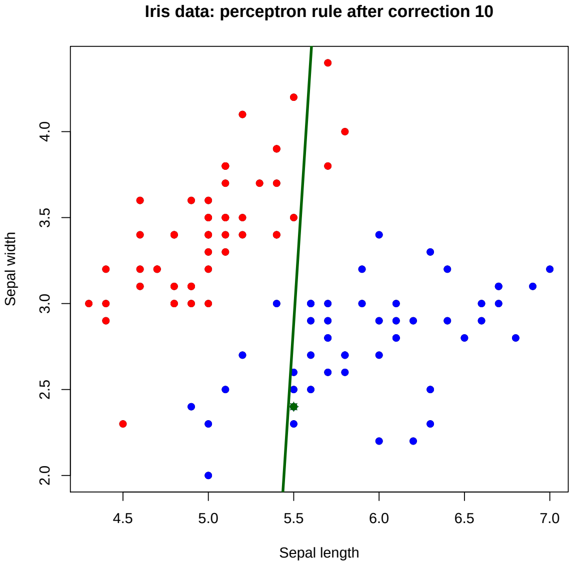

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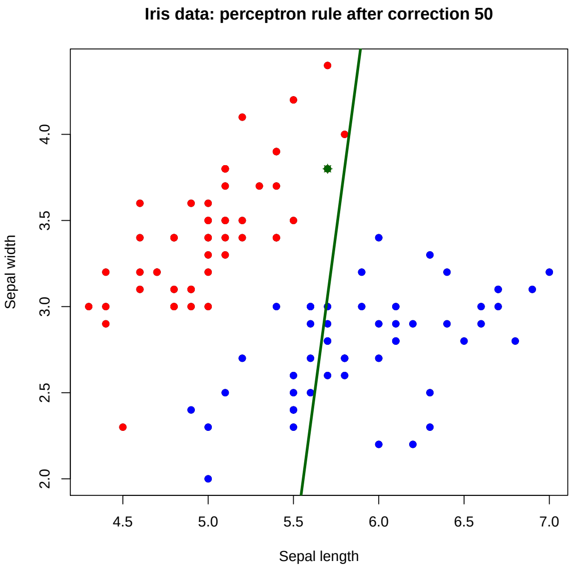

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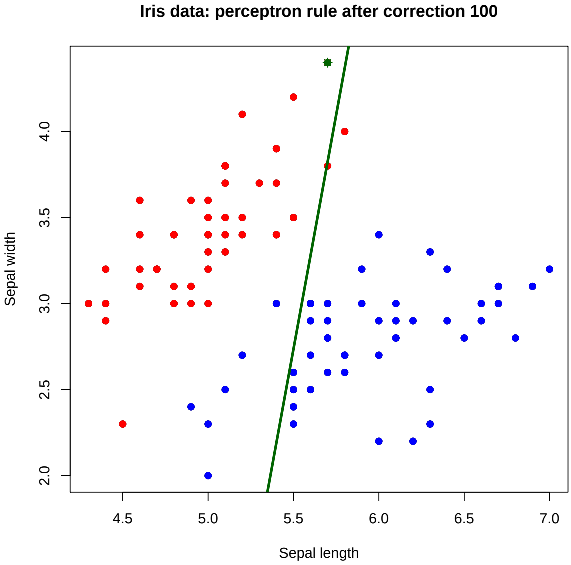

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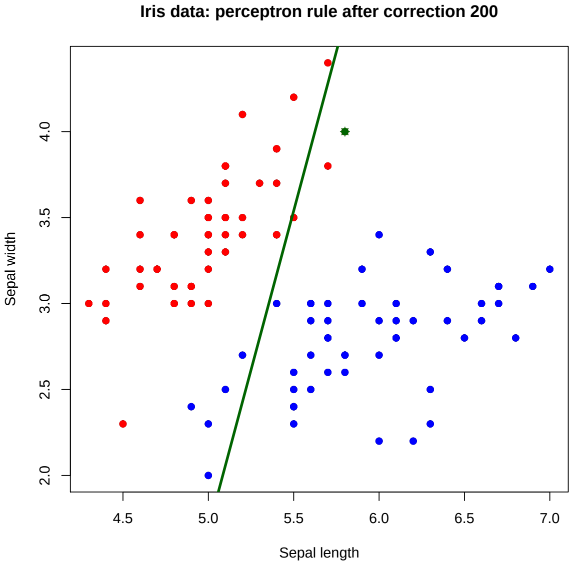

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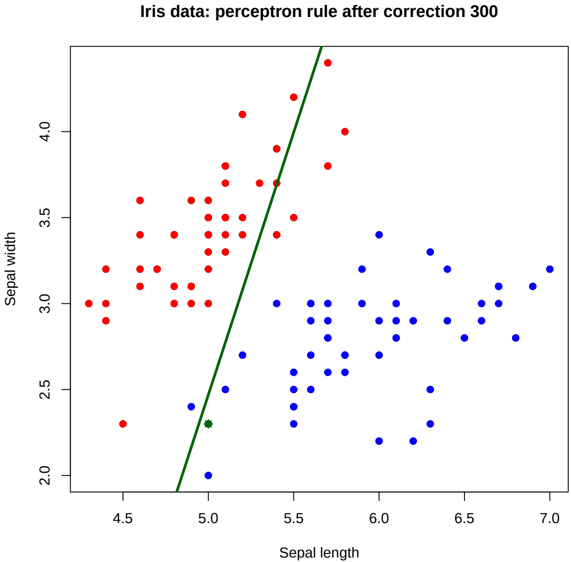

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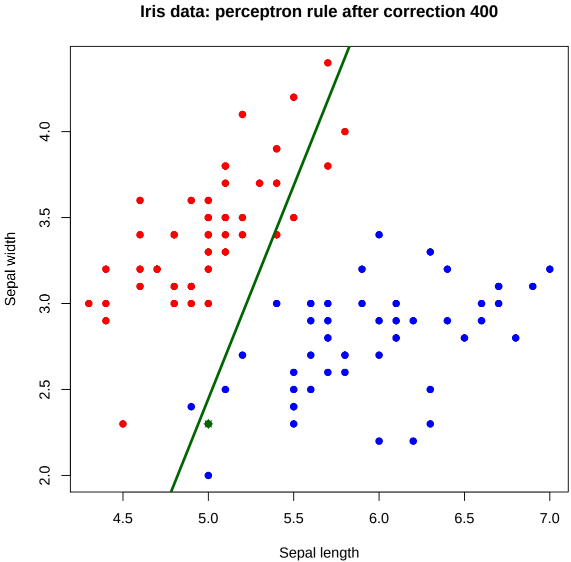

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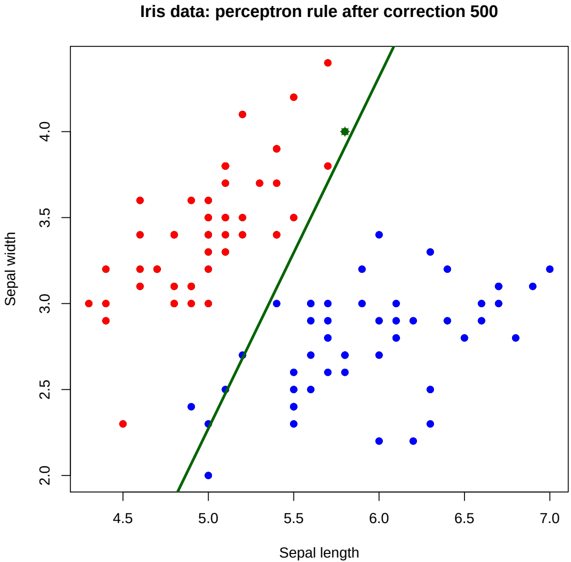

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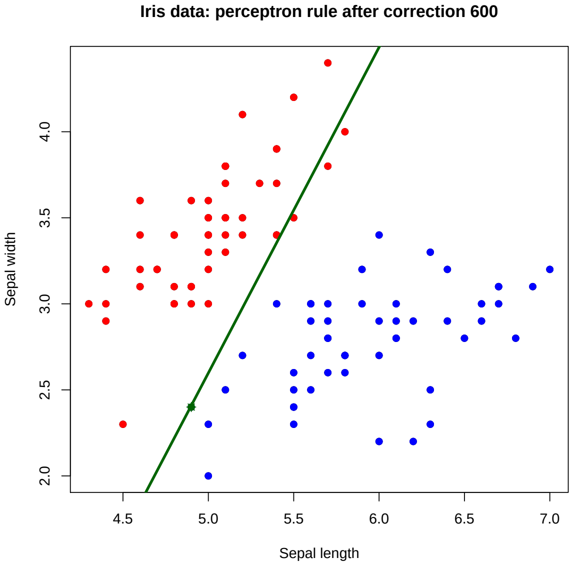

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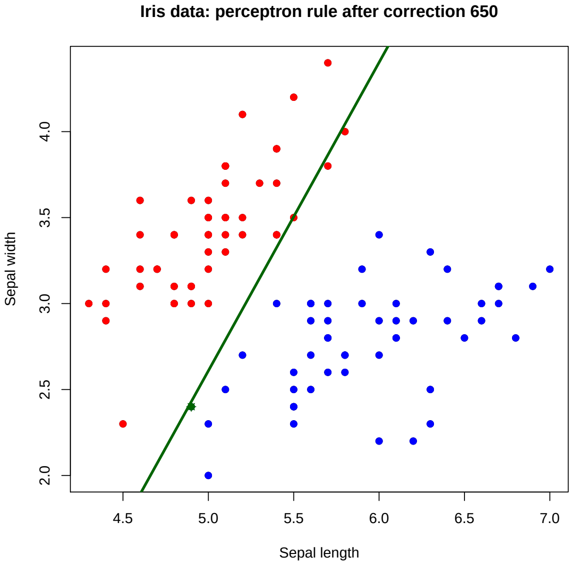

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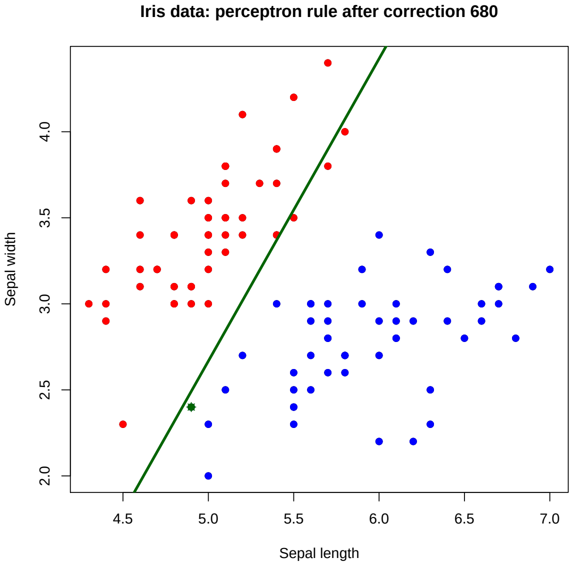

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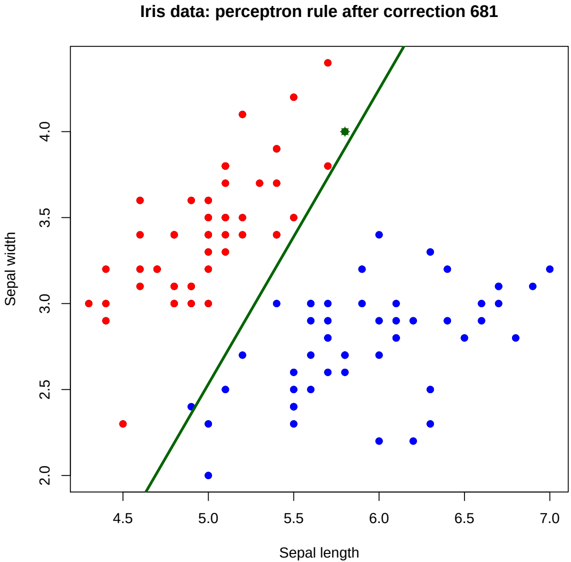

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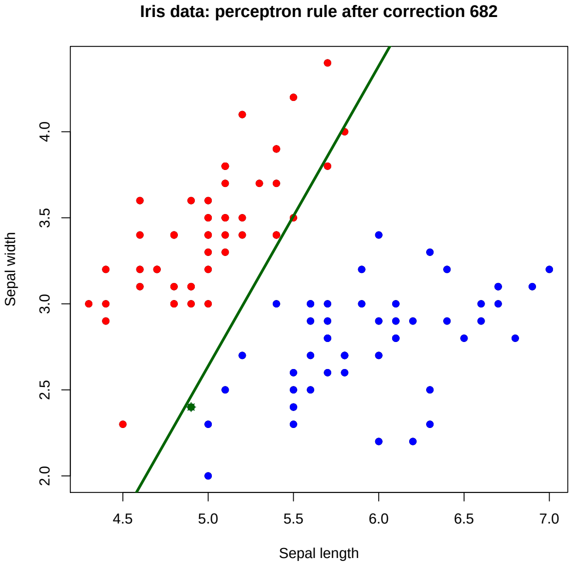

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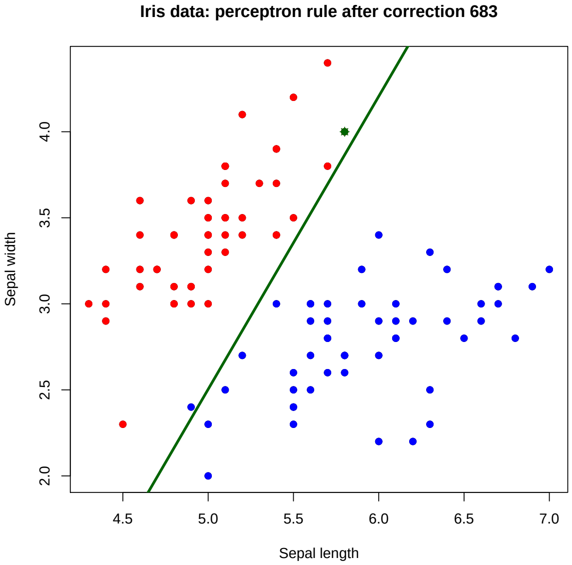

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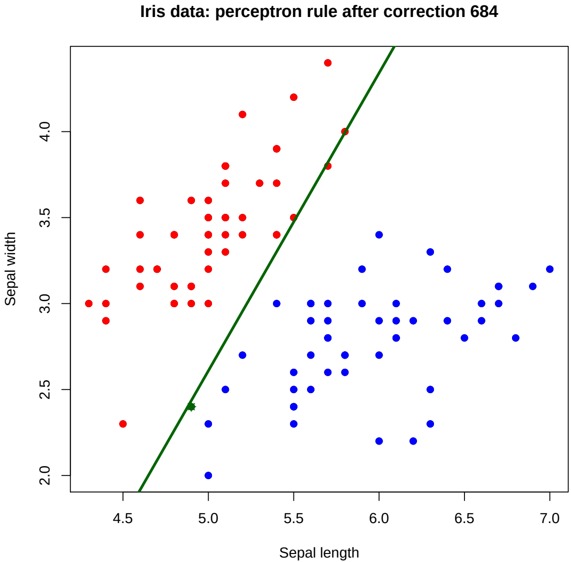

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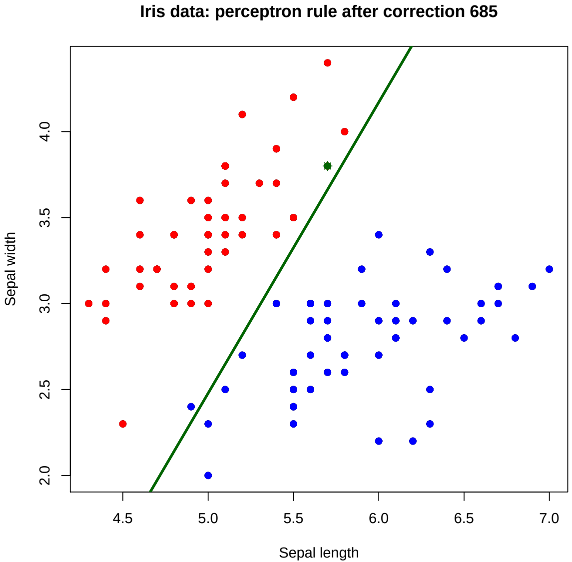

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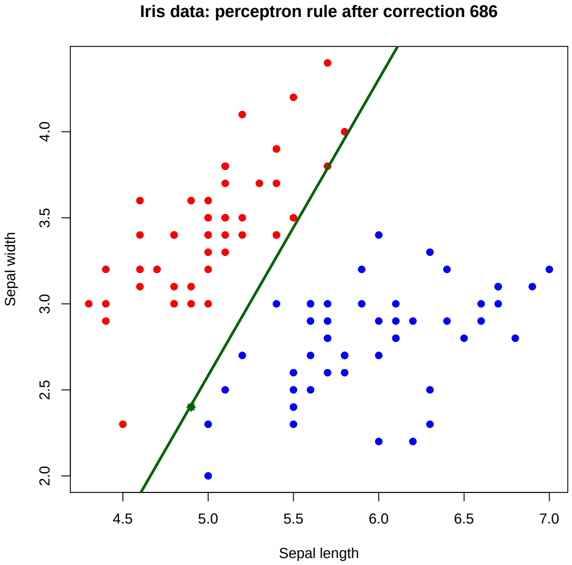

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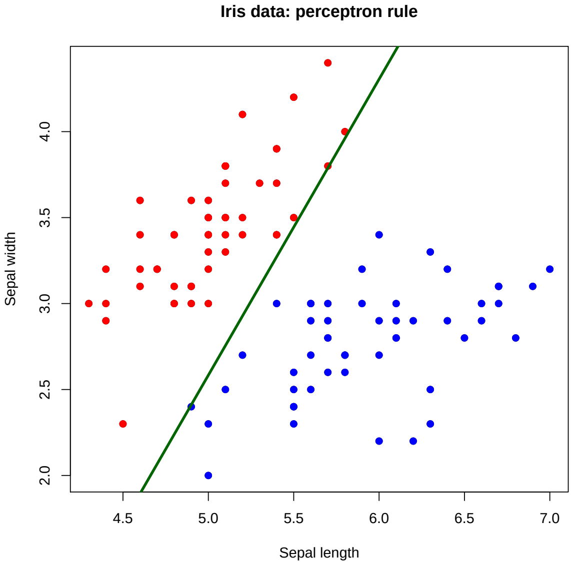

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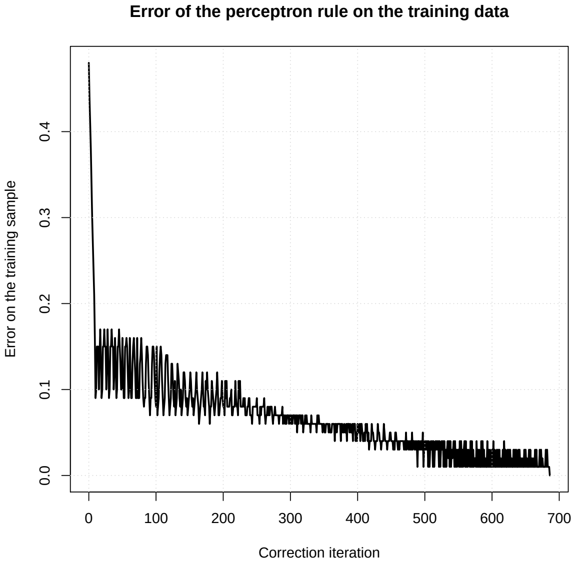

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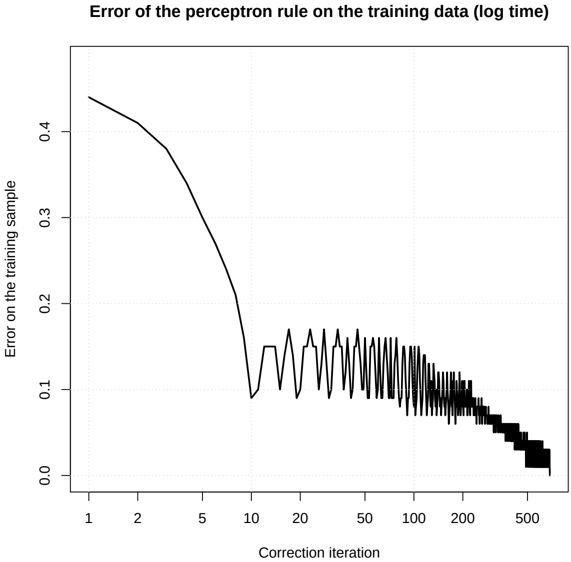

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  $\tilde{\mathcal{X}} = \{\boldsymbol{x} \,|\, (\boldsymbol{x}, y) \in (\mathcal{X}, \mathcal{Y}),\ y = 1\} \cup \{-\boldsymbol{x} \,|\, (\boldsymbol{x}, y) \in (\mathcal{X}, \mathcal{Y}),\ y = 0\}$.

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- 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.

Novikoff's convergence theorem

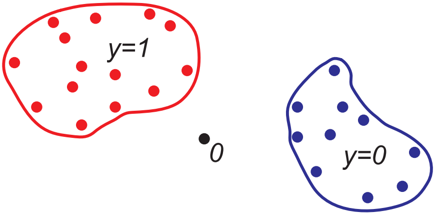
- Let $w_0 = 0$ and set $\gamma = 1$.
- Let $(\mathcal{X}, \mathcal{Y}) = (\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_i, y_i), \ldots$ be an infinite training sequence.
- In addition, let (construct)
  $\tilde{\mathcal{X}} = \{\boldsymbol{x} \,|\, (\boldsymbol{x}, y) \in (\mathcal{X}, \mathcal{Y}),\ y = 1\} \cup \{-\boldsymbol{x} \,|\, (\boldsymbol{x}, y) \in (\mathcal{X}, \mathcal{Y}),\ y = 0\}$.
- 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*

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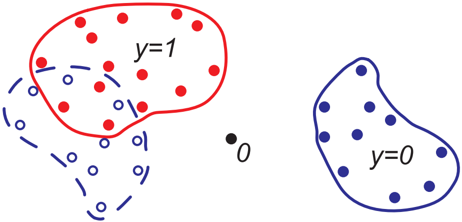

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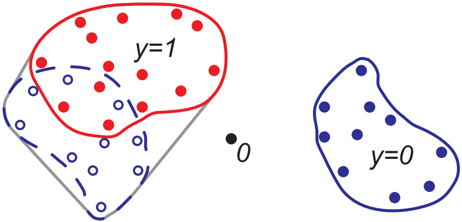

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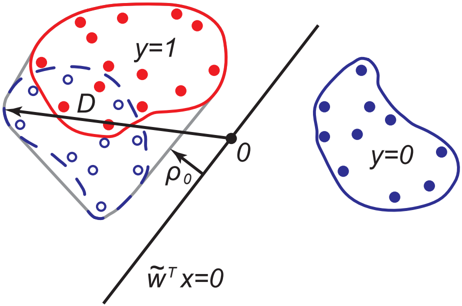

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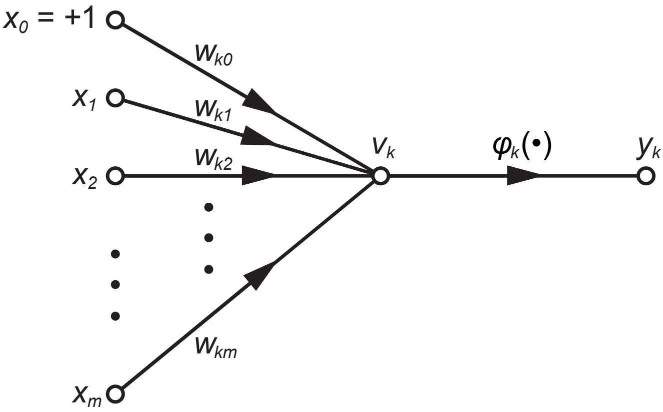
3. The signal at node is transmitted to each outgoing link originating from that node, with the transmission entirely independent of the transfer functions of the outgoing links: **synaptic divergence** or **fan-out**.

A signal-flow graph of a neuron



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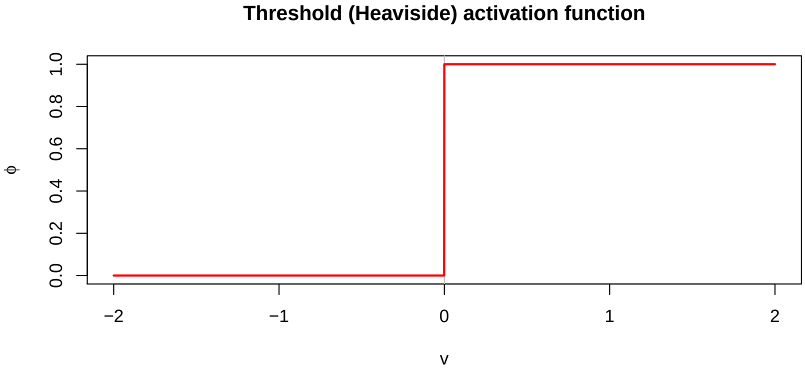
3. The weighted sum of the input signals defines the **induced local field** of the neuron in question.
4. The **activation link** squashes the induced local field of the neuron to produce **output**.

Activation function $\phi(v)$

- **Threshold (Heaviside) function:**

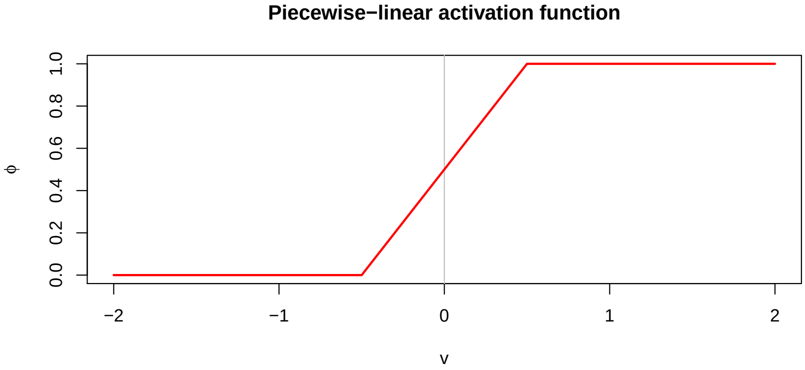
$$\phi(v) = \begin{cases} 1 & \text{if } v \geq 0\,, \\ 0 & \text{if } v < 0\,. \end{cases}$$



Activation function $\phi(v)$

- **Piecewise-linear function:**

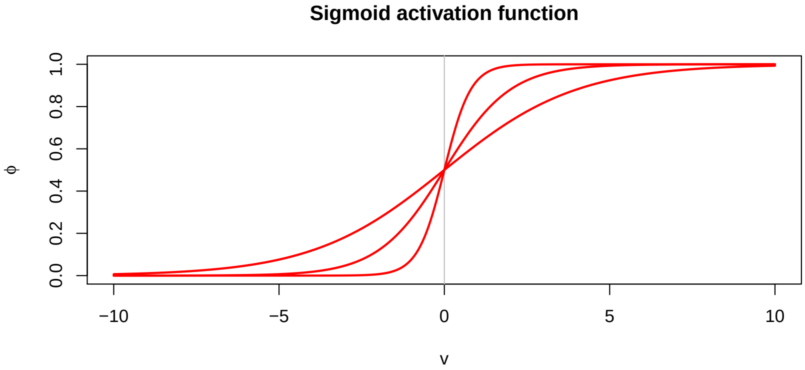
$$\phi(v) = \begin{cases} 1 & \text{if } v \geq \frac{1}{2}\,, \\ v + \frac{1}{2} & \text{if } -\frac{1}{2} < v < \frac{1}{2}\,, \\ 0 & \text{if } v \leq -\frac{1}{2}\,. \end{cases}$$



Activation function $\phi(v)$

- **Sigmoid function:**

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



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Minimization of the empirical risk (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* $(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_n, y_n)$ 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^*.

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- 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 $\nabla\mathcal{E}$:

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

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

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- 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

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

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

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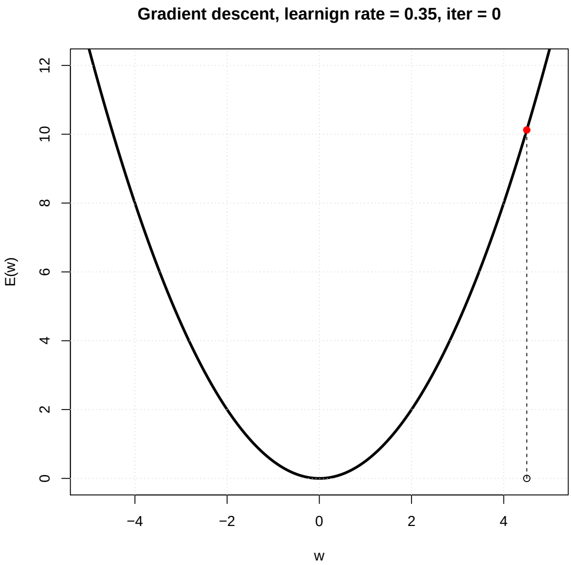
  is justified for γ small enough.
- Substituting $\Delta\boldsymbol{w}(n)$ gives:

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

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

Method of gradient descent: example (slow learning rate)



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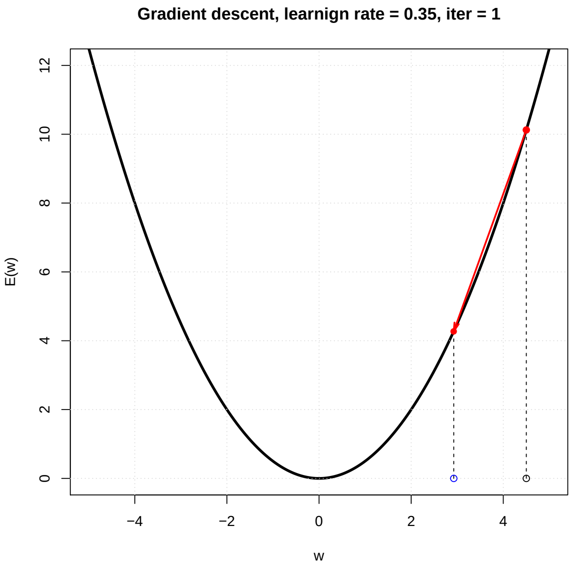

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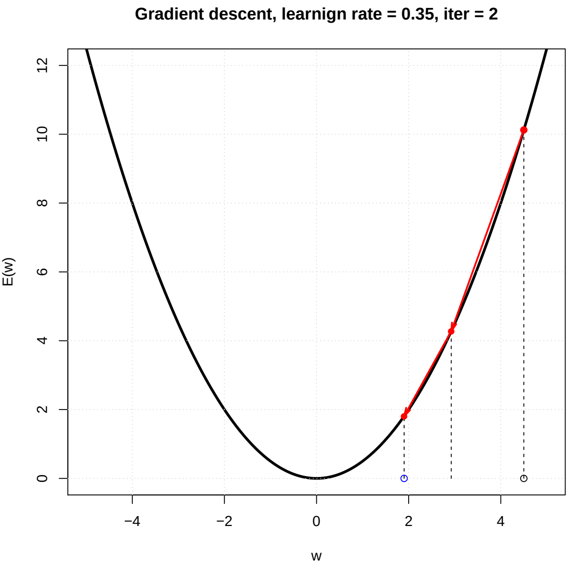

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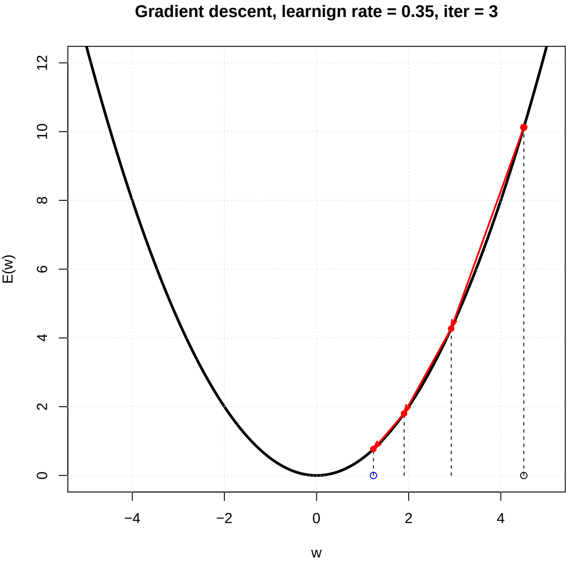

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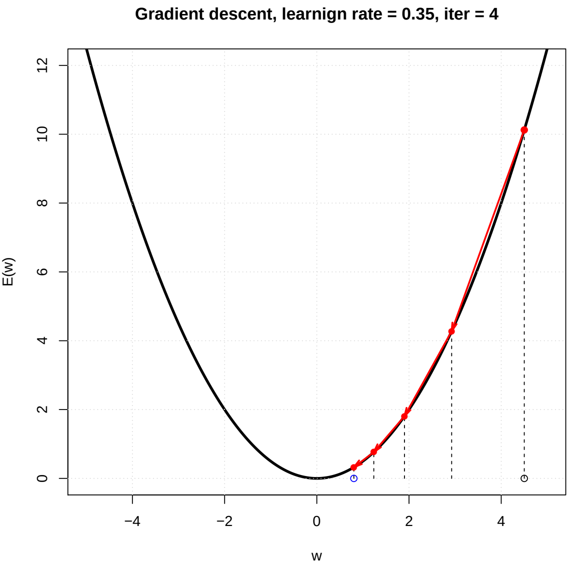

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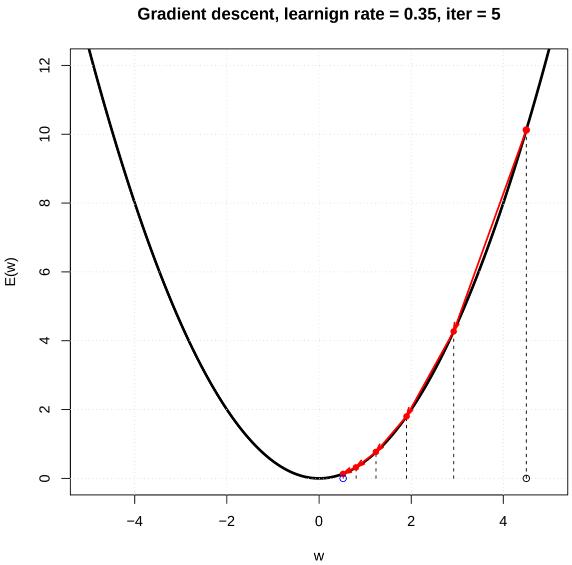

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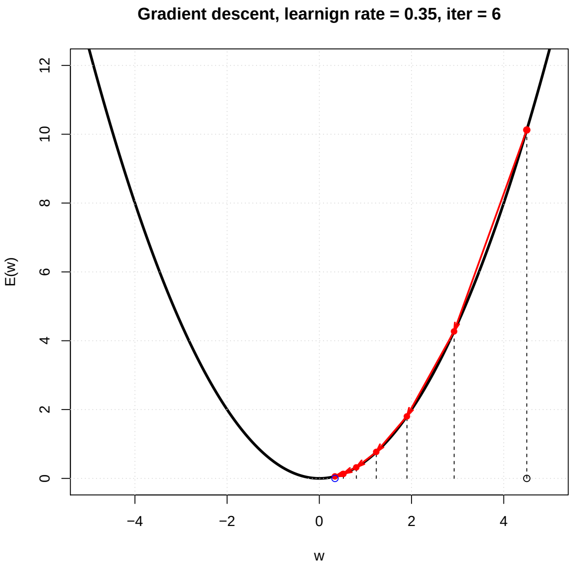

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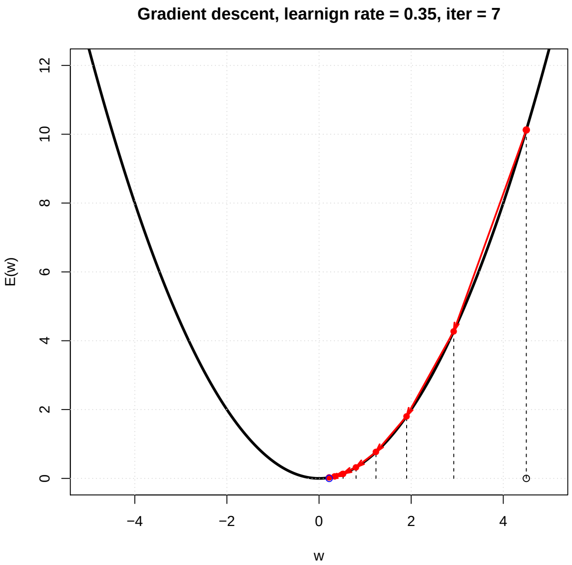

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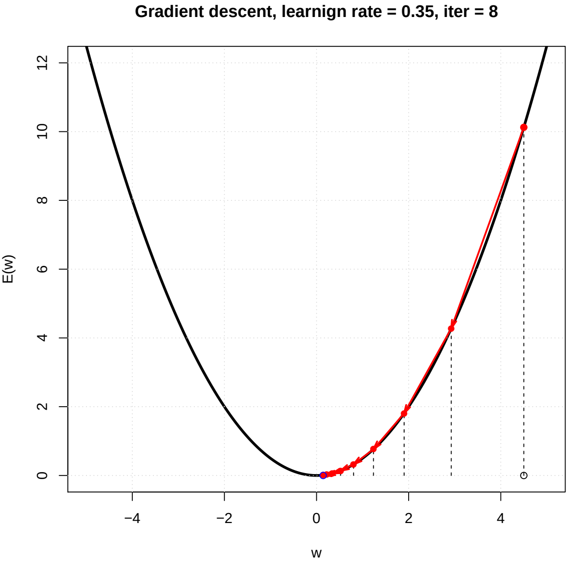

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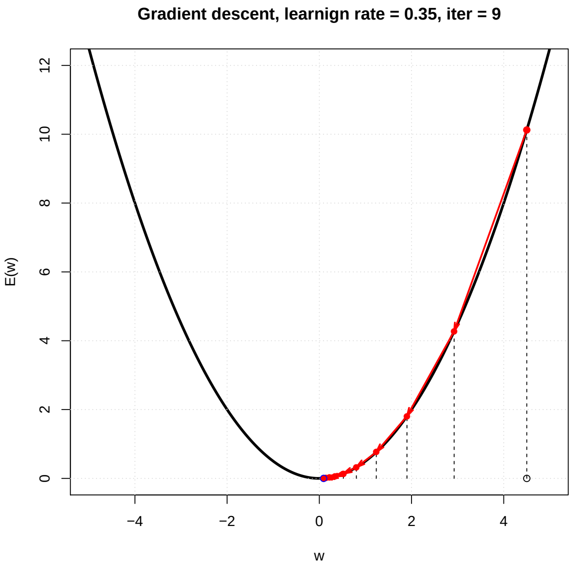

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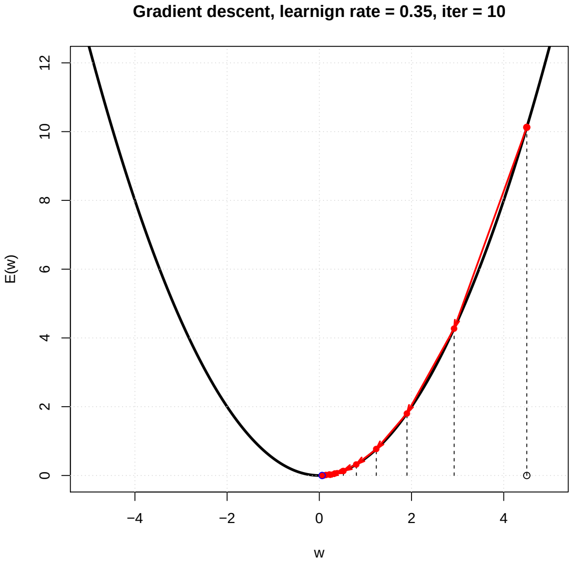

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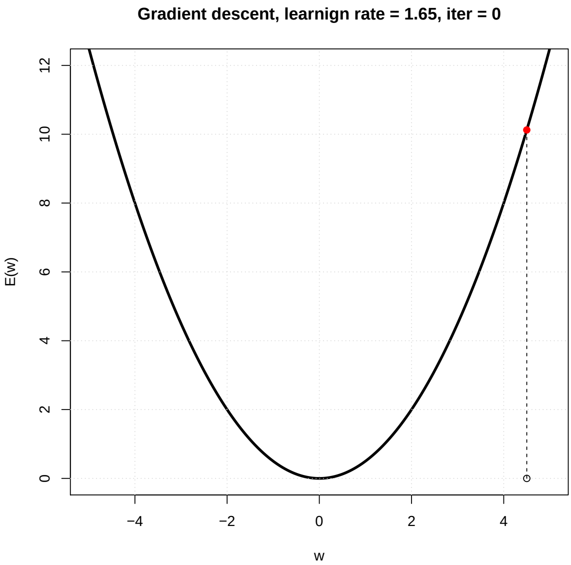

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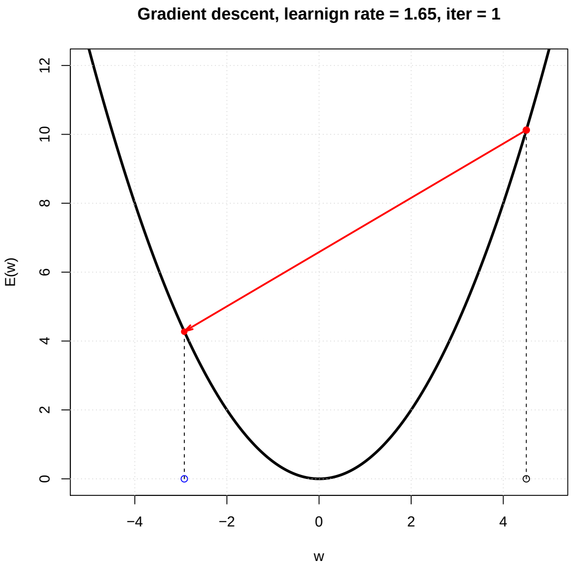

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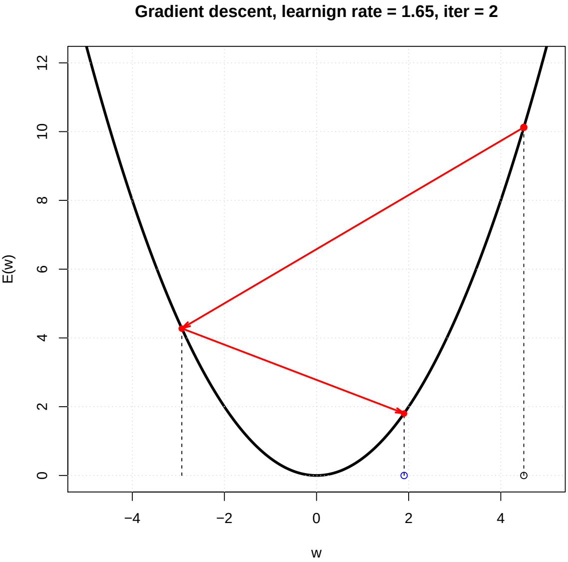

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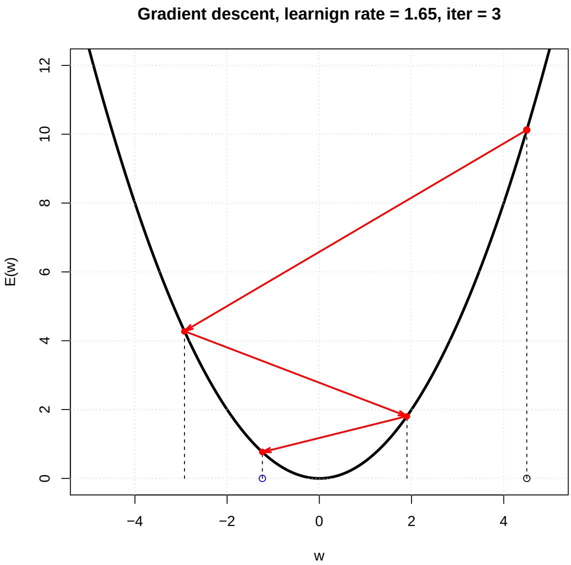

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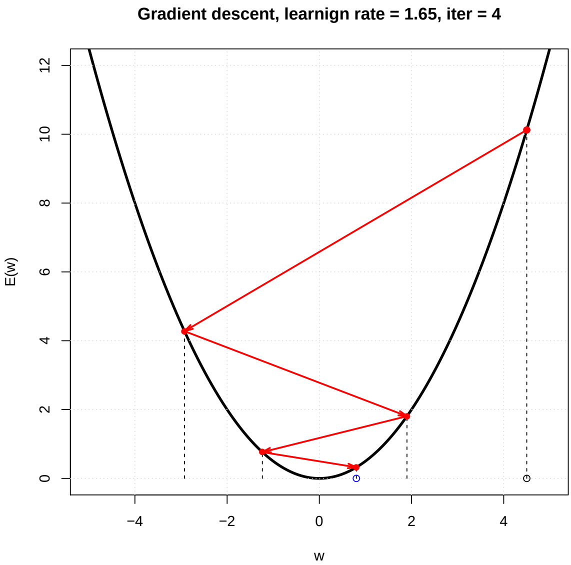

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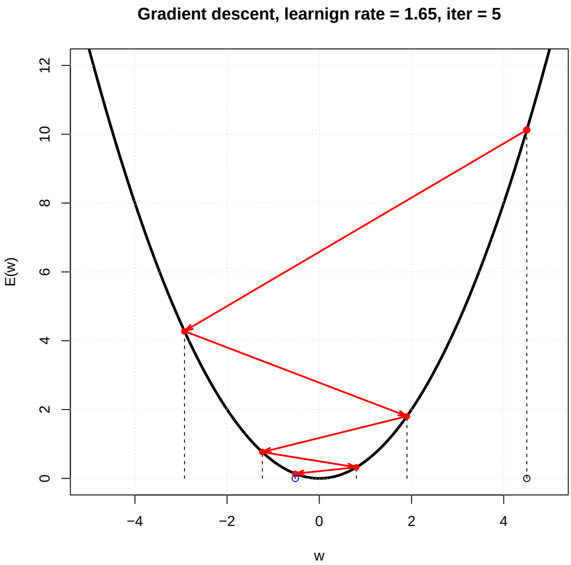

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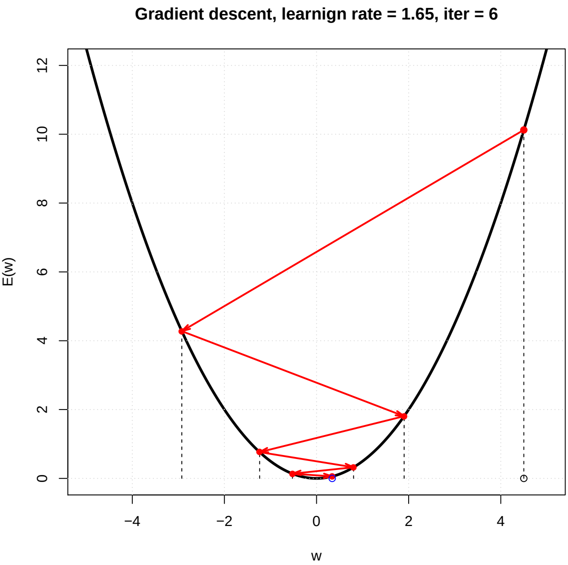

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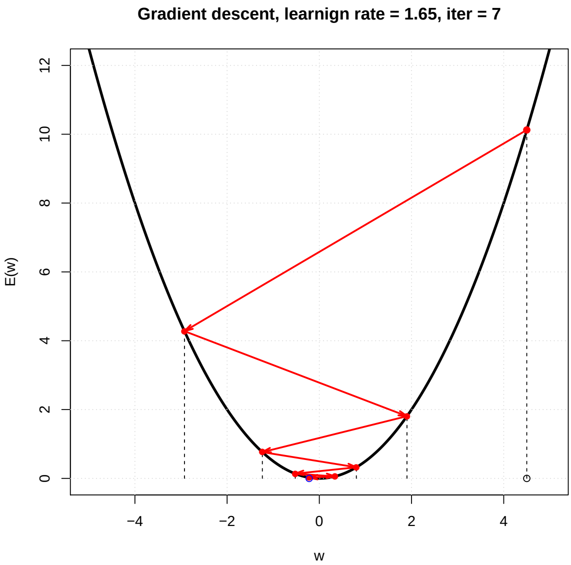

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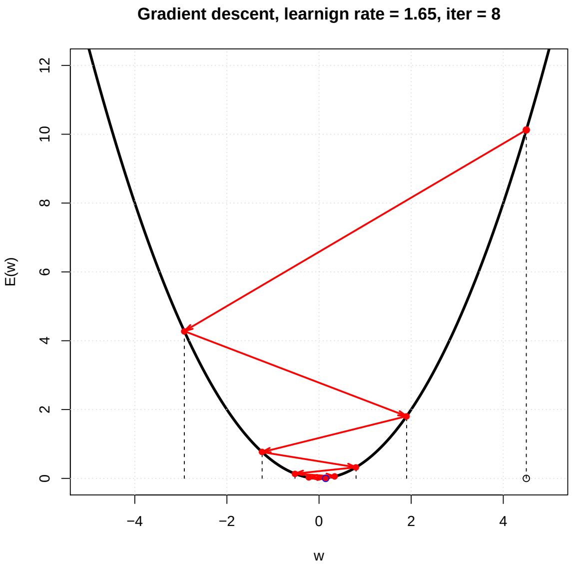

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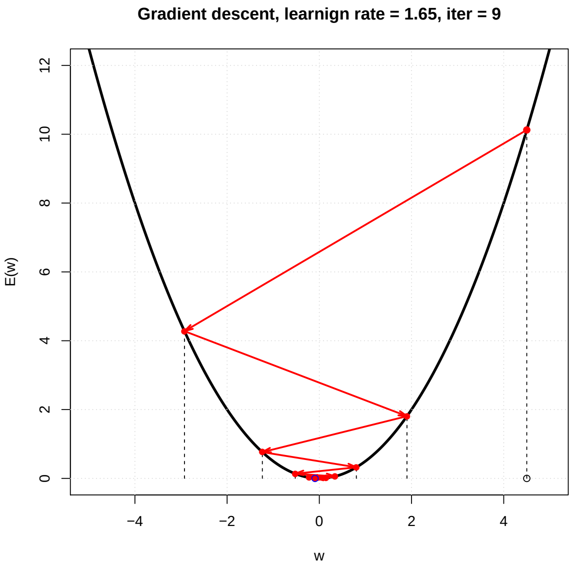

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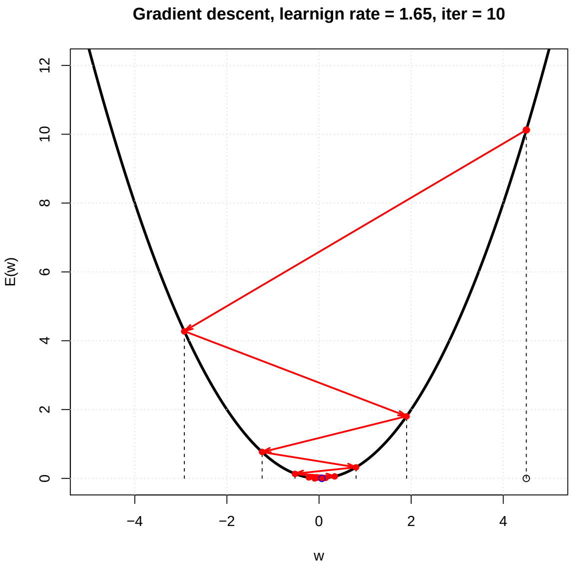

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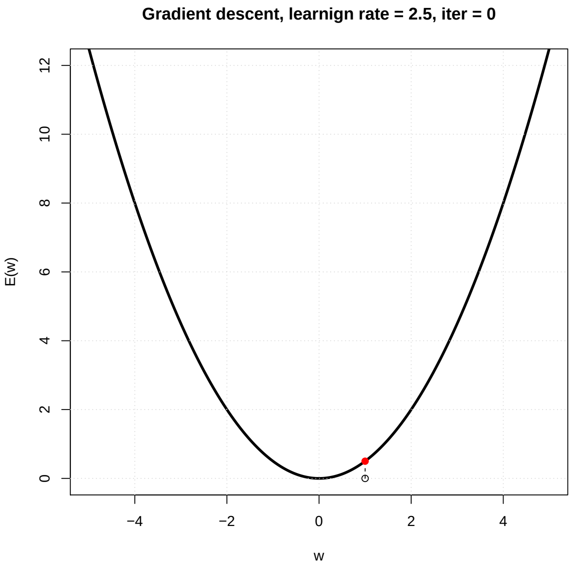
- When γ exceeds a certain critical value, the algorithm becomes unstable and may diverge.

Method of gradient descent: example (divergent case)



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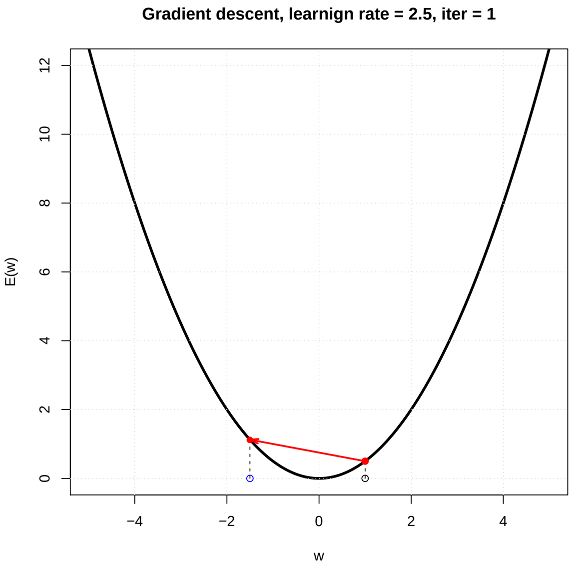

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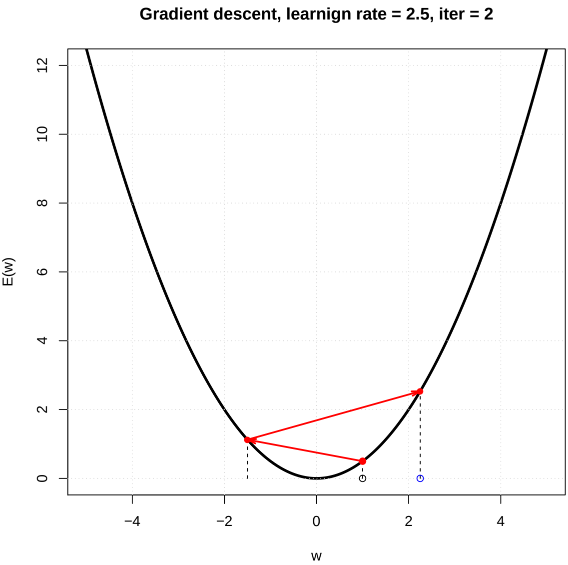

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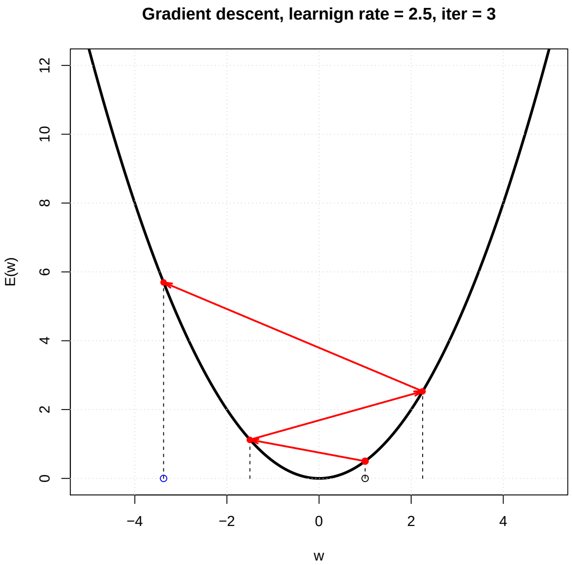

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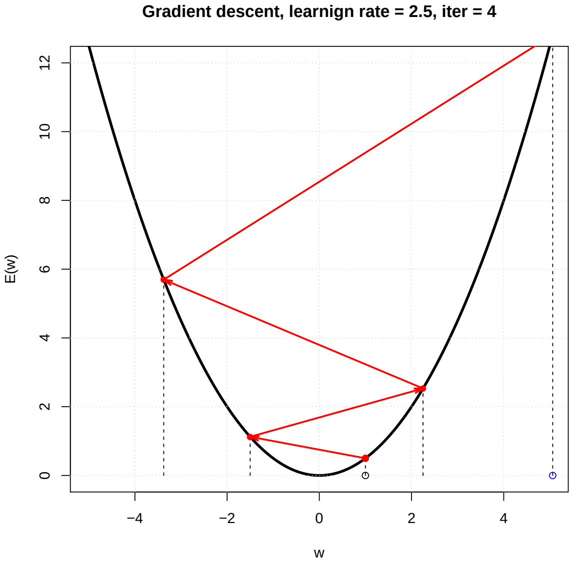

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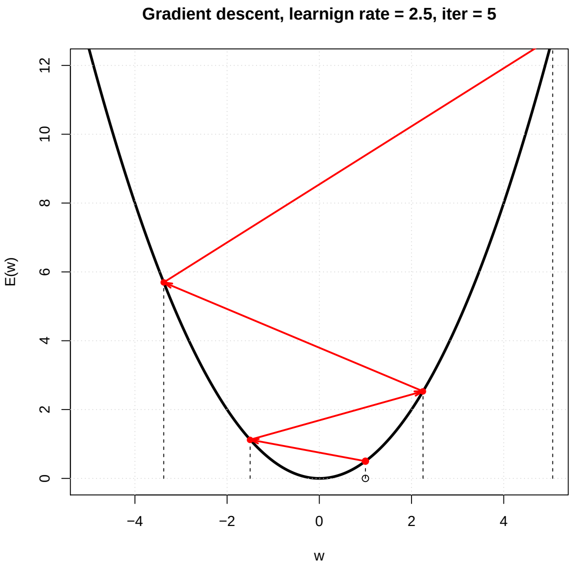
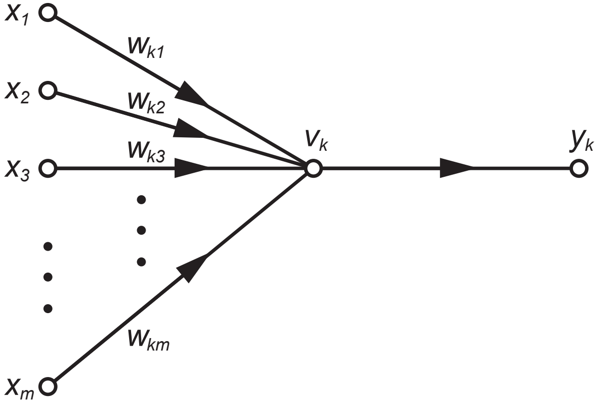


A signal-flow graph of a simplified neuron



Method of gradient descent: iris data

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

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

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- The step of the algorithm is then:

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

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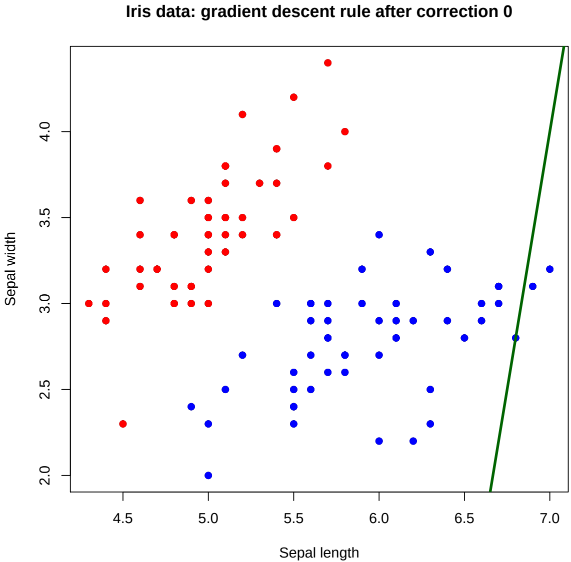

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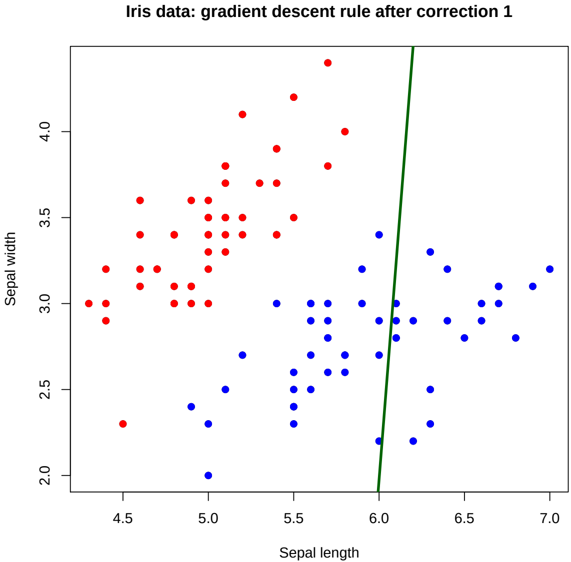

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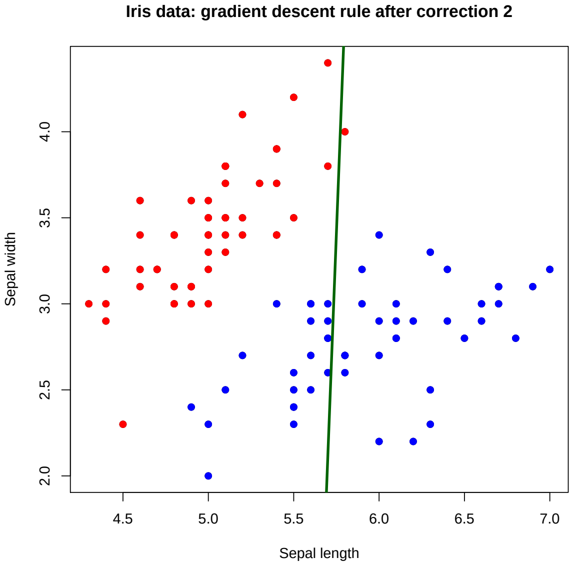

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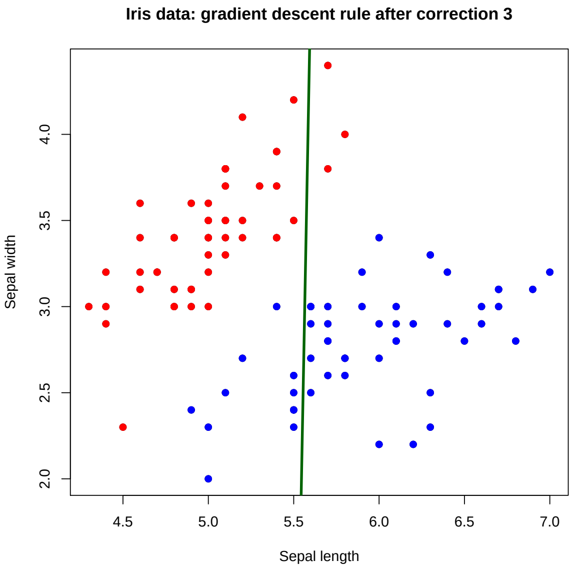

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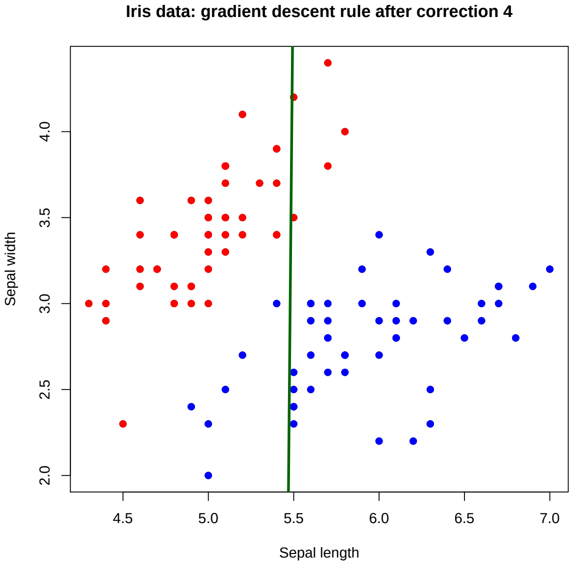

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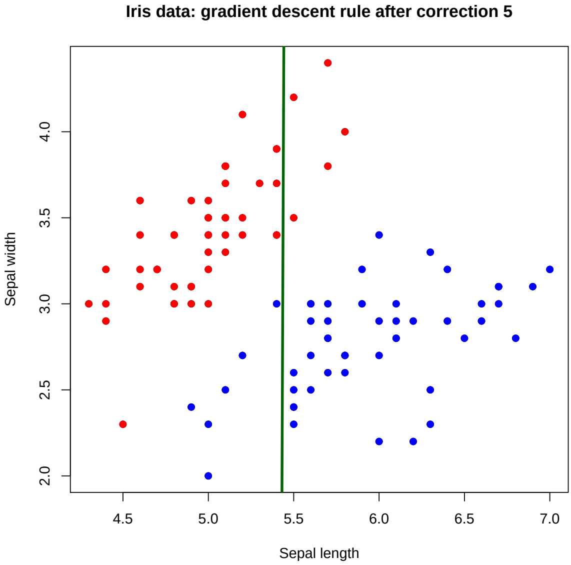

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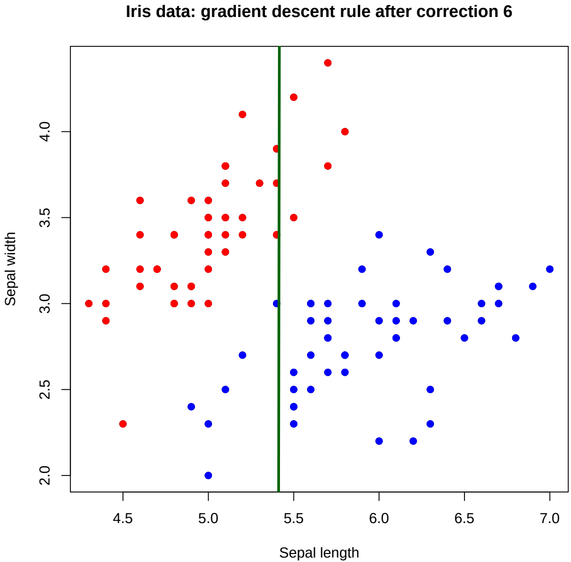

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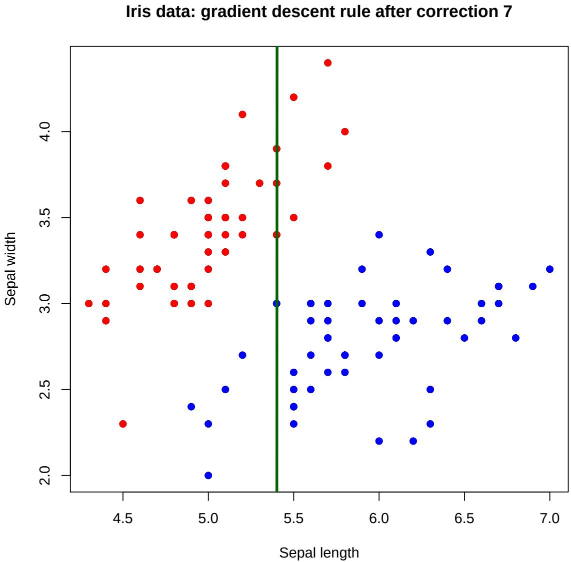

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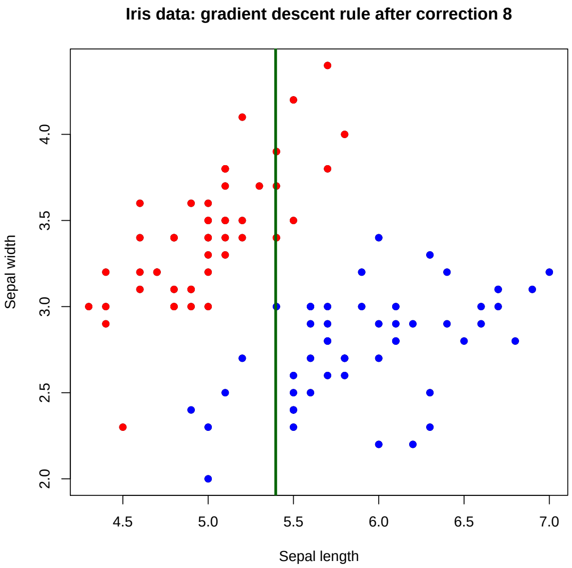

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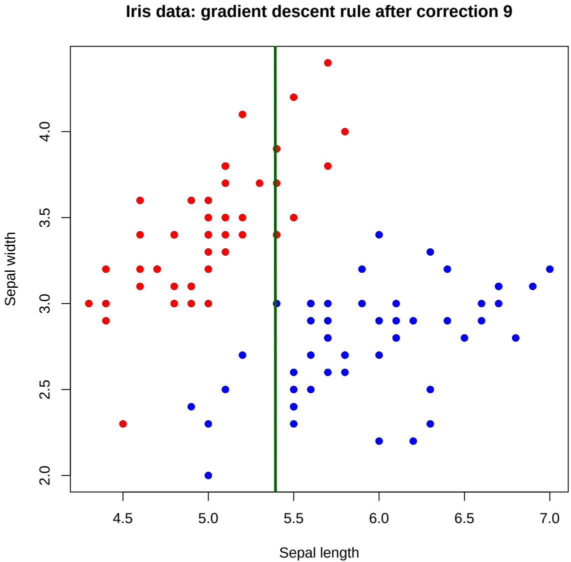

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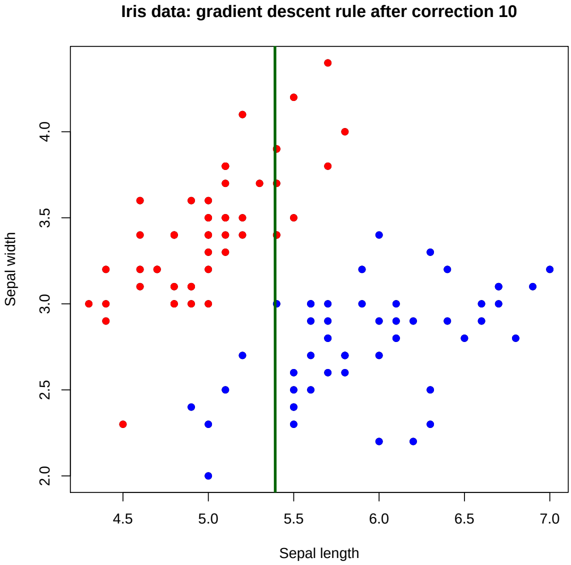

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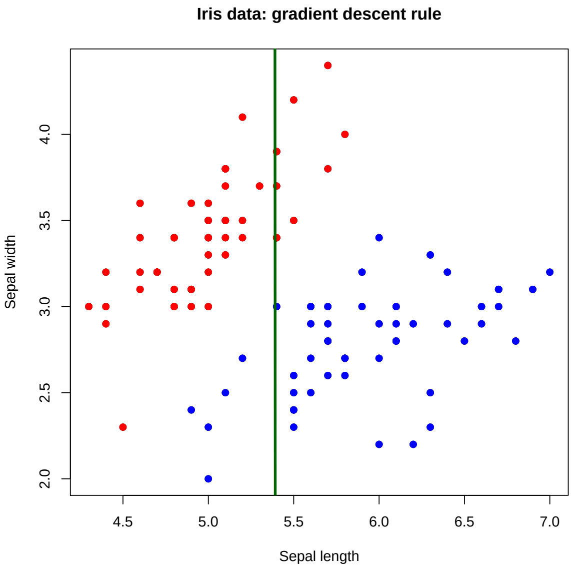

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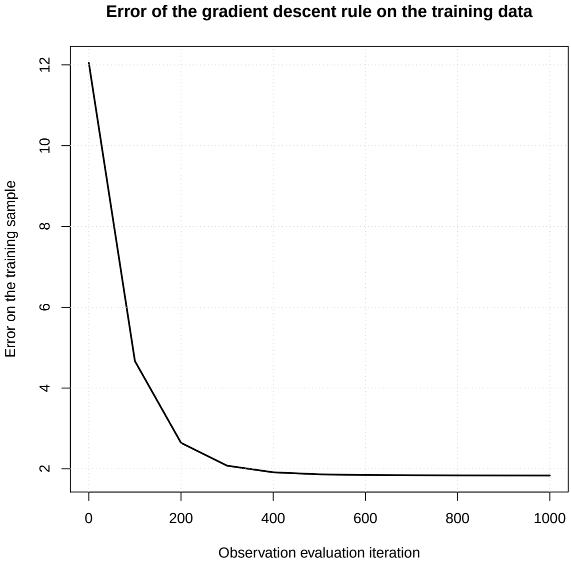

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- The **least-mean-square (LMS) algorithm** attempts to minimize the **instantaneous value** of the cost function

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

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- Now, LMS can be formulated as follows:

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

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Input:

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

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

Iterations:

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- For this last reason, the LMS-updated weights $\hat{\boldsymbol{w}}(n)$ trace a random trajectory in the parameter space: **stochastic gradient descent**.

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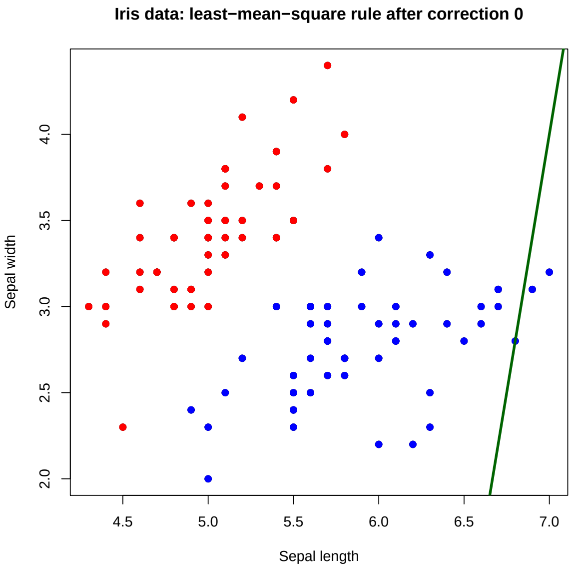

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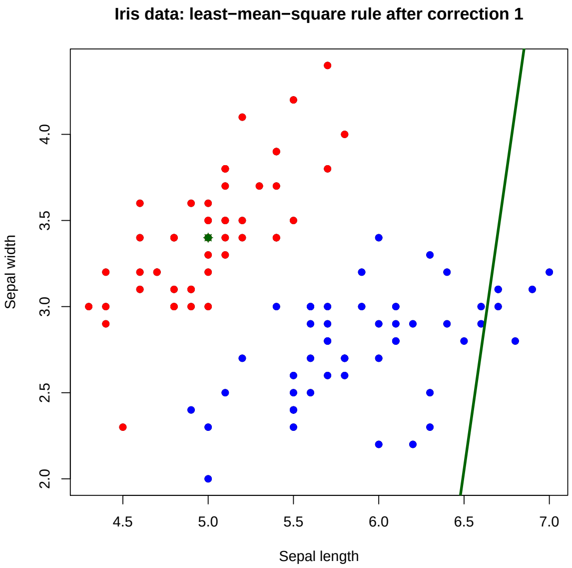

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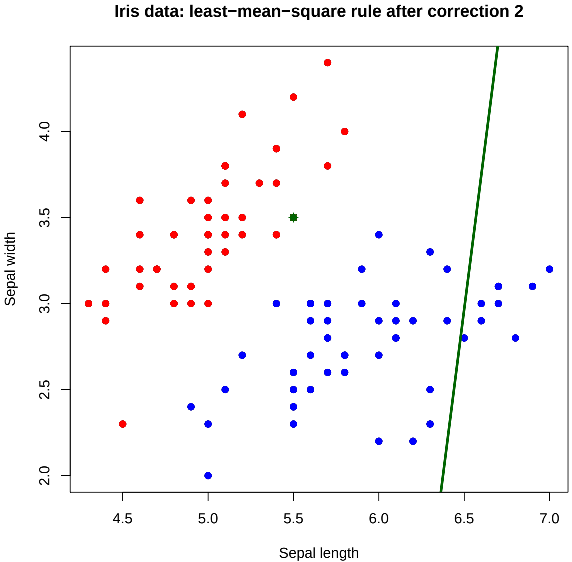

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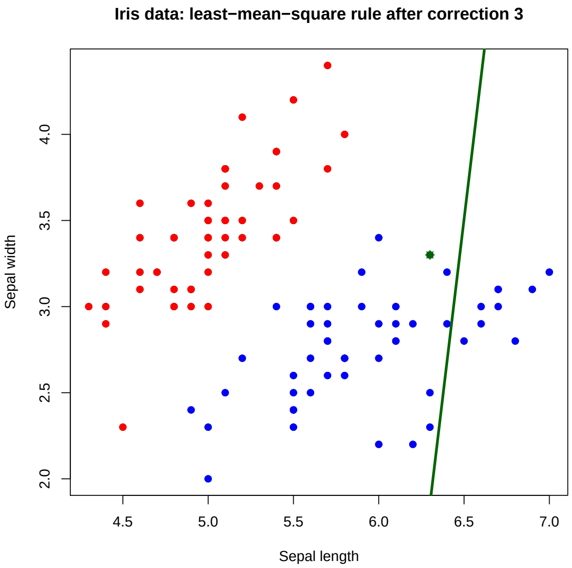

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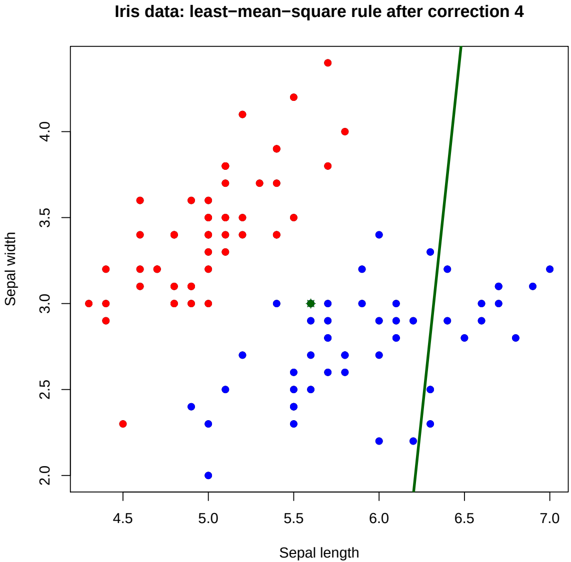

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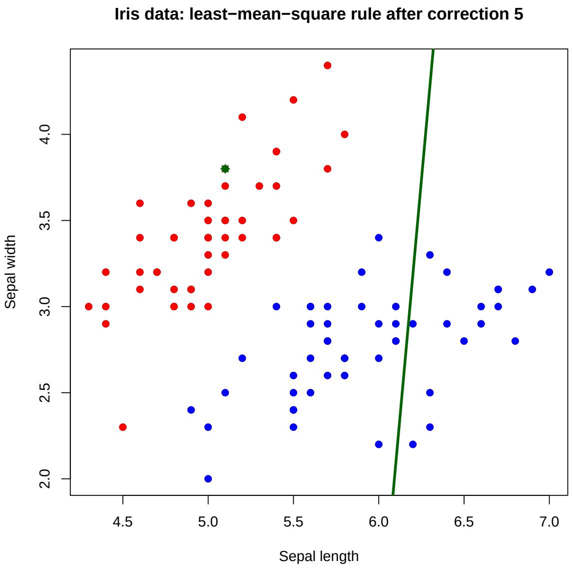

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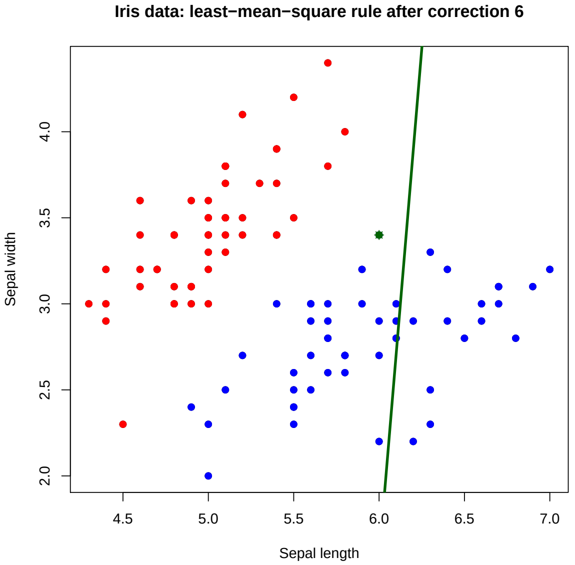

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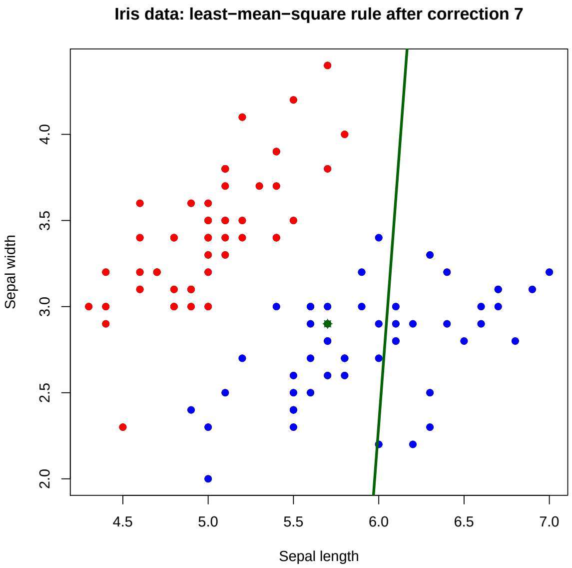

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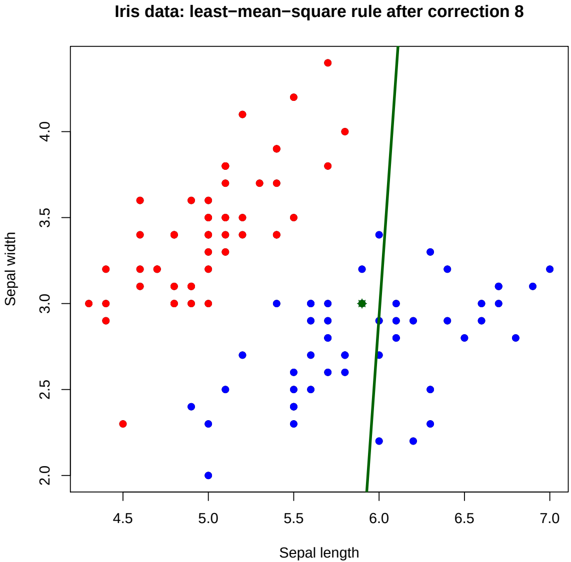

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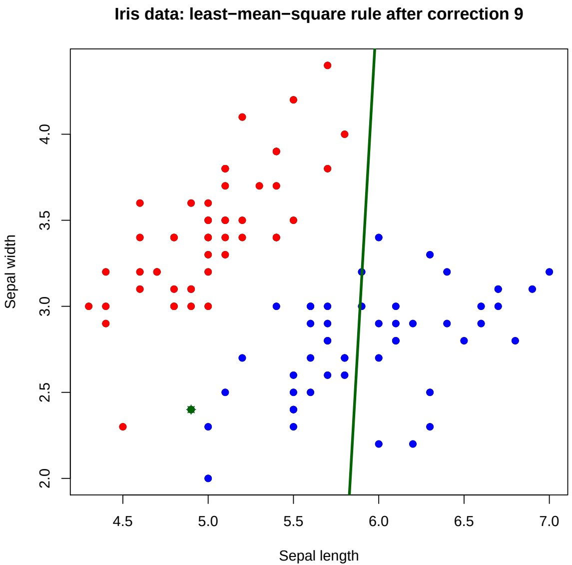

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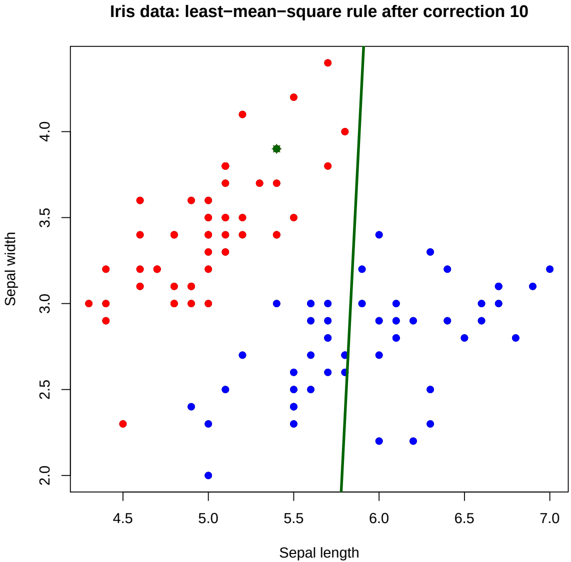

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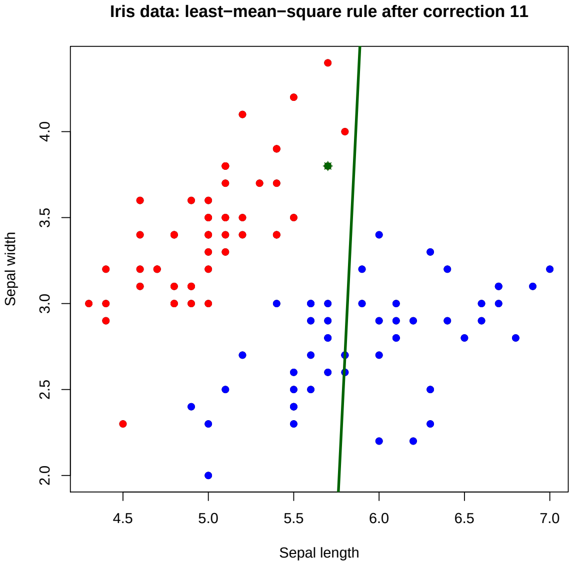

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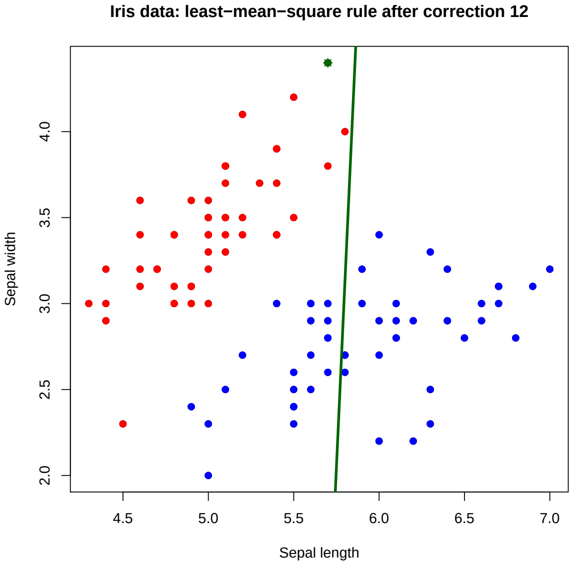

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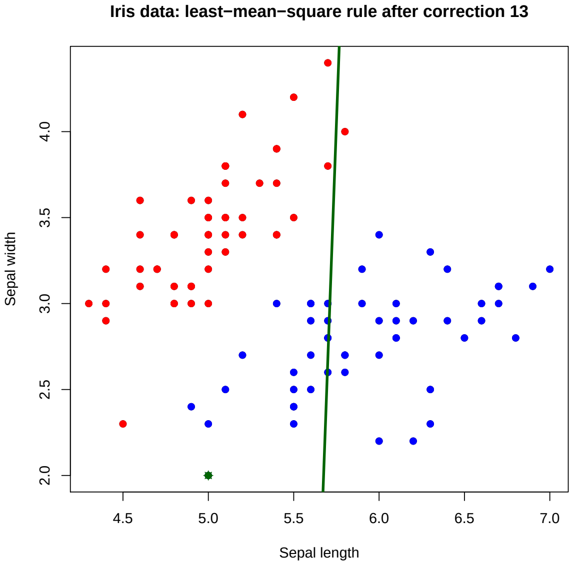

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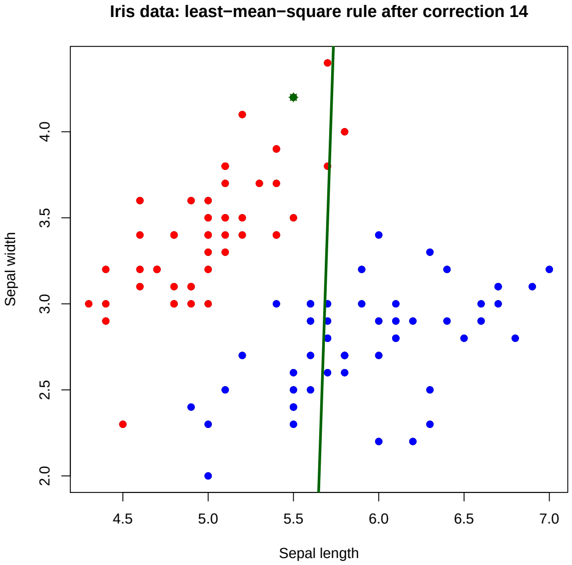

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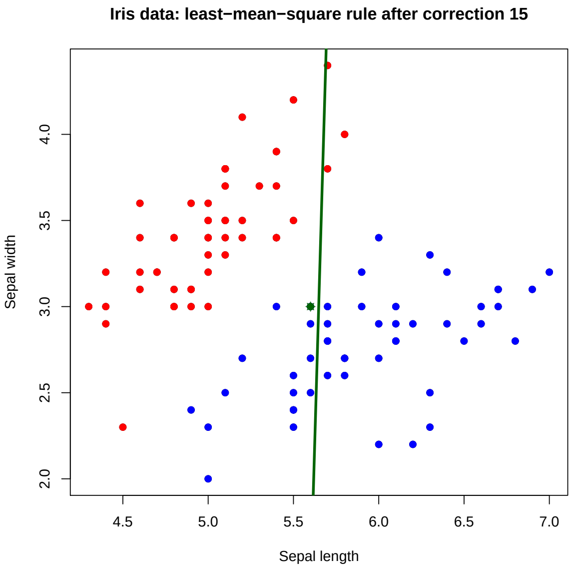

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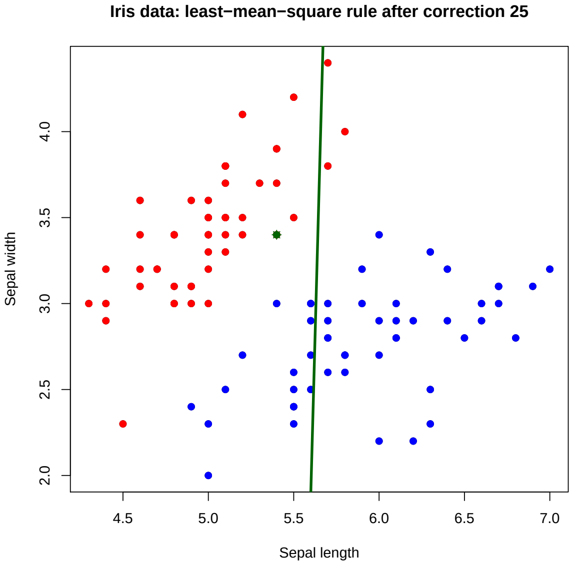

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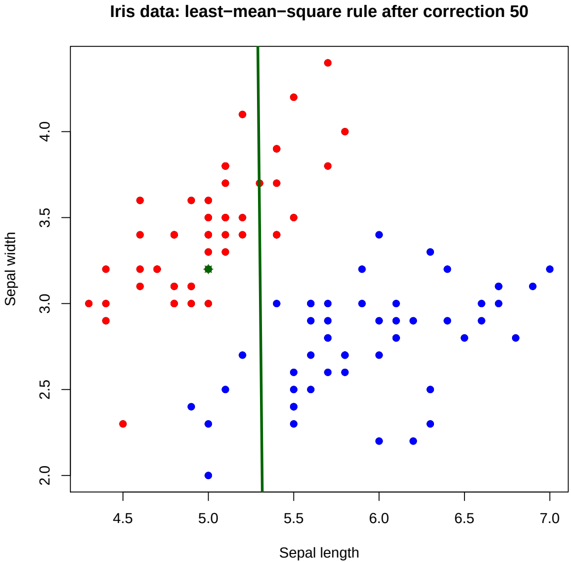

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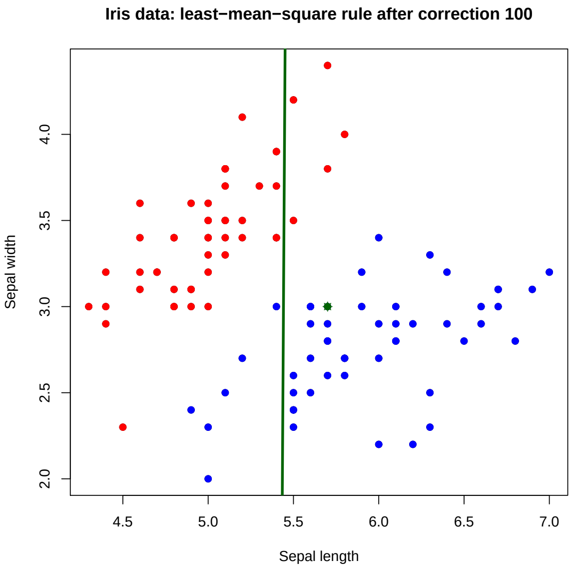

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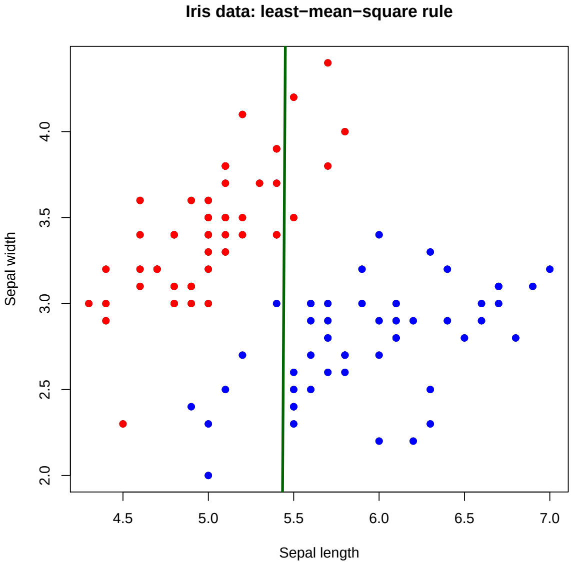

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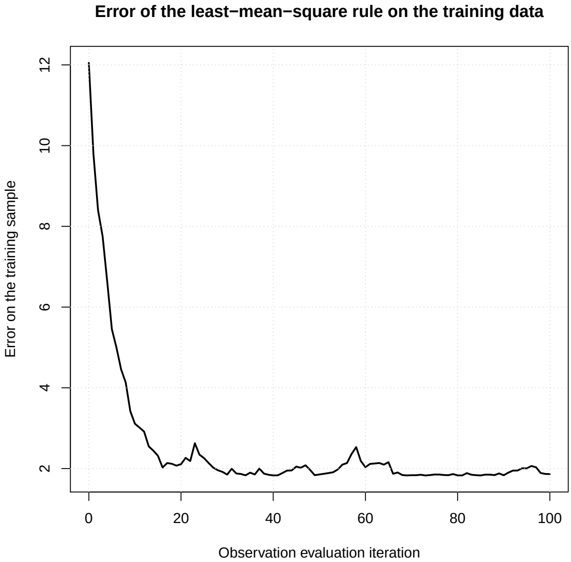

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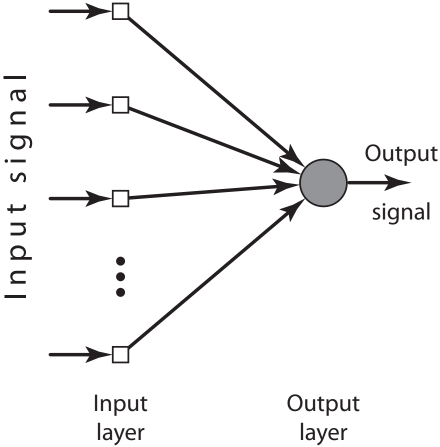
Single layer perceptron



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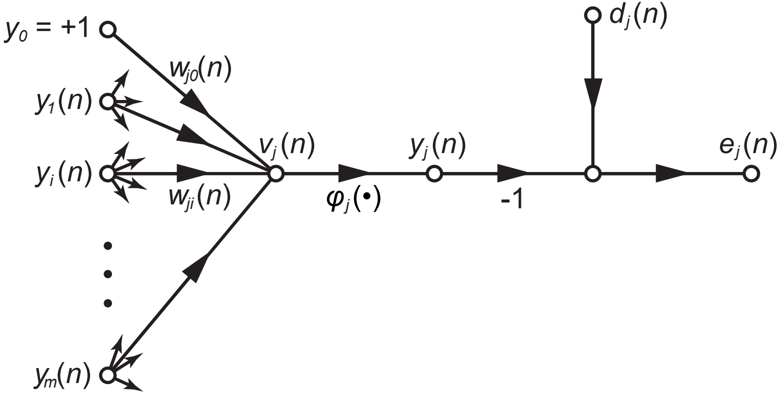
$$y_j(n) = \phi\big(v_j(n)\big)\,.$$

A signal-flow graph of a neuron and its output



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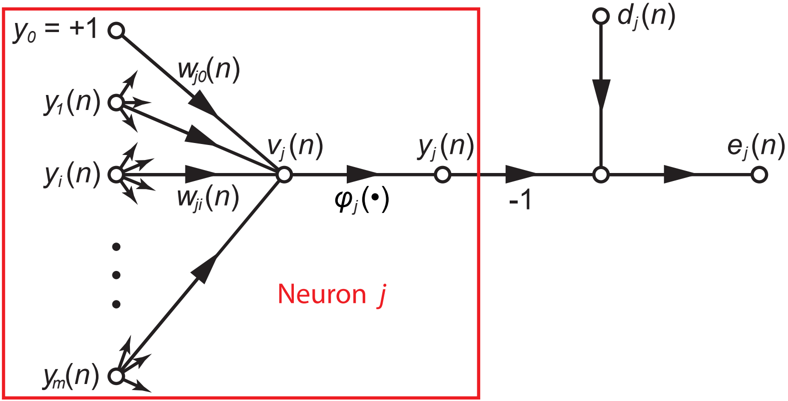

Derivation for a single (output-layer) neuron

- 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:

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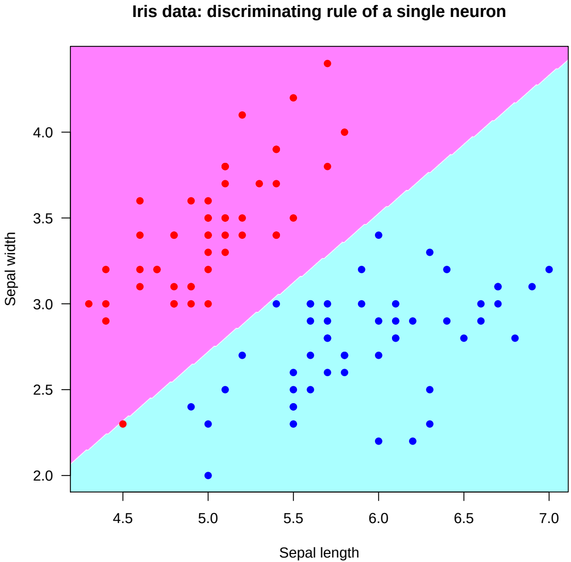
Single neuron: iris data



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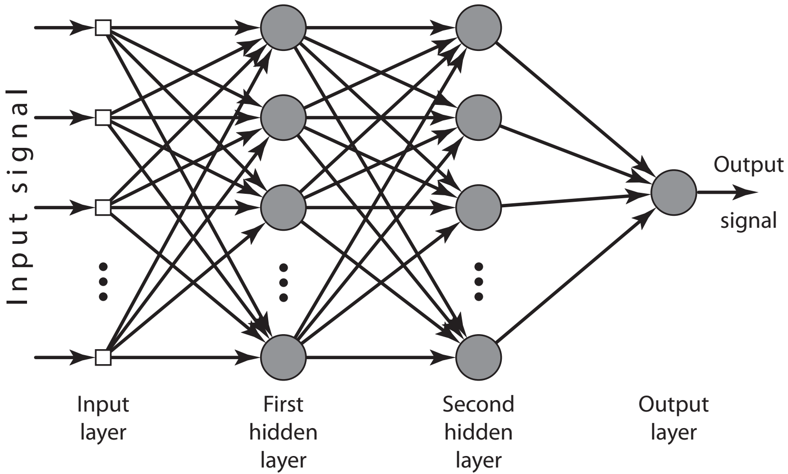
Multilayer neural network (example)



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

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

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

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

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Summarizing:

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

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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:

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

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

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- **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.

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

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

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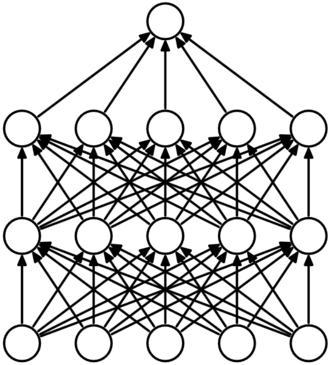
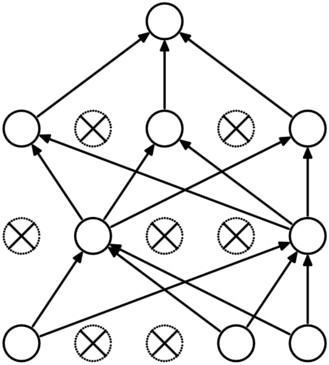
- Dropout provides an **inexpensive approximation to** training and evaluating a **bagged** ensemble of exponentially many **neural networks**.
- Specifically, **dropout trains the ensemble consisting of all sub-networks** that can be formed by removing non-output neurons from an underlying base network.

The dropout strategy

- An example of applying the dropout strategy:



Standard neural network



After applying dropout

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- To **predict** an unknown observation, we **average the output from many masks**. Even 10–20 masks are often sufficient to obtain good performance.

Contents

Rosenblatt's perceptron
- Biological analogy
- Historical learning algorithm
- Novikoff's convergence theorem

Signal-flow notation and model of an artificial neuron

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- Minimization of the empirical risk
- Method of gradient descent
- The least-mean-square algorithm

The back-propagation algorithm
- Derivation for a single-layer network
- Propagation for a multilayer network
- An example of the activation function

Additional information on learning networks
- Regularization in neural networks
- Some remarks on the back-propagation

Stopping criteria

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- 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).

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- **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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And some references

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