1. Feedforward neural networks

1.1. The perceptron

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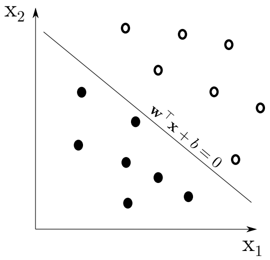
The perceptron

- A simplification of the perceptron is a binary classifier.
- Assume a set of observations in a column vector $\mathbf{x} = \{x_1 \cdots x_D\}^\top$, that can be arbitrarily labelled as "black" (-1) and "white" (+1) classes.



A classification function can be constructed from a *separating hyperplane* between both classes:

$$\mathbf{w}^\top \mathbf{x} + b = 0 \qquad (1)$$

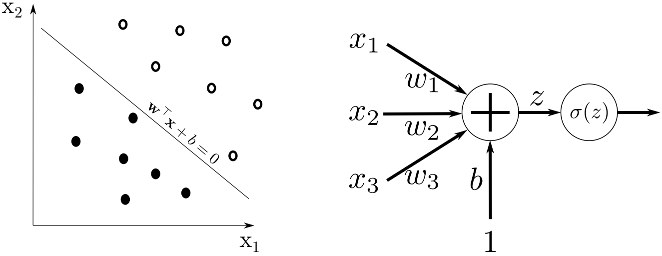
The classifier is defined as

$$f(\mathbf{x}) = \mathrm{sign}\left(\mathbf{w}^\top \mathbf{x} + b\right) \qquad (2)$$

Ìč

The classifier is a function with weights **w** and a bias b, and a generic *activation function* σ:

$$f(\mathbf{x}) = \sigma\left(\mathbf{w}^\top \mathbf{x} + b\right) = \sigma\left(\sum_d w_d x_d + b\right)$$



The separating hyperplane in an example of 2 dimensions (left), and a representation of the classification function for the case of 3 dimensions.

The Minimum Mean Square Error criterion

- In order to illustrate the idea of MMSE we can take the simplest actication, which is the linear one:

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$$

- The training criterion is then (MMSE)

$$\min_{\mathbf{w},b} \mathbb{E}\left[e_i^2\right] = \min \mathbb{E}\left[\left(y_i - \mathbf{w}^\top \mathbf{x}_i - b\right)^2\right] \tag{3}$$

  Of course, the actual expectation cannot be computed, because the probability density functions of the random variables are not available, so the expectation will be approximated by a sample average.

The Minimum Mean Square Error criterion

- Assuming that N labelled samples $\mathbf{x}_i, y_i$ are available, we introduce here matrix $\mathbf{X} = [\mathbf{x}_1, \cdots, \mathbf{x}_N]$ and vector $\mathbf{y} = [y_1, \cdots, y_N]$ containing all training samples and labels.
- We extend both the input data and the weight vector to obtain a compact solution as follows:

$$\mathbf{x} \rightarrow \begin{bmatrix} \mathbf{x} \\ 1 \end{bmatrix}, \qquad \mathbf{w} \rightarrow \begin{bmatrix} \mathbf{w} \\ b \end{bmatrix}$$

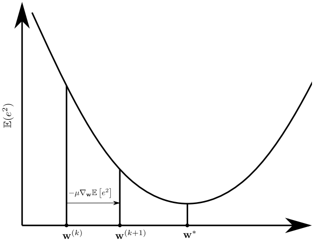
- In this case, nulling the gradient gives

$$\mathbf{w} = \left(\mathbf{X}\mathbf{X}^\top\right)^{-1}\mathbf{X}\mathbf{y} \tag{4}$$

(derivation as an exercise) which is a compact solution, i.e. no iterations needed.

The Least Mean Square solution

Here we derive a recursive solution. The method is based on a *gradient descent* approach: compute the gradient of the error wrt $\mathbf{w}$ and move the weights in its opposite direction.



$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \mu\nabla_{\mathbf{w}}\mathbb{E}\left[e^2\right] \quad (5)$$

where

$$\nabla_{\mathbf{w}}\mathbb{E}\left[e^2\right] = \mathbf{X}\mathbf{X}^\top\mathbf{w} - \mathbf{X}\mathbf{y} \quad (6)$$

The Least Mean Square solution

Now we approximate Eq. (6) by using a single sample:

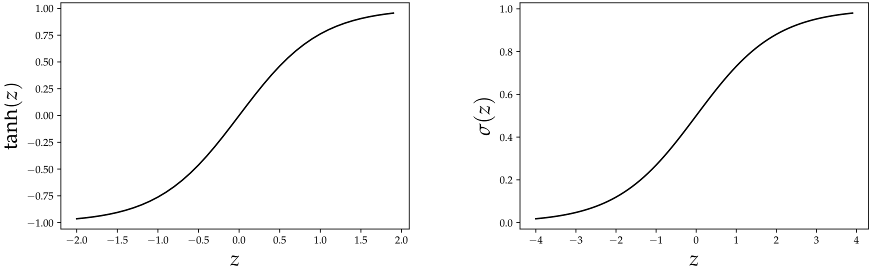
$$\begin{aligned}\nabla_{\mathbf{w}}\mathbb{E}\left[e^2\right] &= \mathbf{X}\mathbf{X}^\top\mathbf{w} - \mathbf{X}\mathbf{y} \\ &\approx \mathbf{x}_k\mathbf{x}_k^\top\mathbf{w} - \mathbf{x}_k y_k \\ &= \mathbf{x}_k\left(\mathbf{x}_k^\top\mathbf{w} - y_k\right) \\ &= -e_k\mathbf{x}_k\end{aligned} \tag{7}$$

Where $e_k = y_k - \mathbf{x}_k^\top\mathbf{w}$. This leads to the following update rule

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} + \mu e_k\mathbf{x}_k \tag{8}$$

Soft activations

- In neural networks the neuron includes an activation $\sigma(\cdot)$.
- It can be a *sigmoid* function that produces an output that can be interpreted as a soft state or a probability of a state.



Hyperbolic tangent function (left) and logistic function.

Soft activations

- The logistic function or the hyperbolic tangent are classic neural network activations, but nowadays, the logistic is used in combination with other functions that will be studied further.
- The hyperbolic tangent, the logistic function and their derivatives are:

$$
\begin{aligned}
\tanh(z) &= \tfrac{e^z - e^{-z}}{e^z + e^{-z}}, & \tfrac{d}{dz}\tanh(z) &= 1 - \tanh^2(z) \\
\sigma(z) &= \tfrac{1}{1+e^{-z}}, & \tfrac{d}{dz}\sigma(z) &= \sigma(z)\left(1 - \sigma(z)\right)
\end{aligned}
\tag{9}
$$

Soft activations

Now, if the output of the classifier is

$$f(\mathbf{x}) = \tanh\left(\mathbf{w}^\top \mathbf{x}_i + b\right) \tag{10}$$

then the criterion to optimize the parameters will be

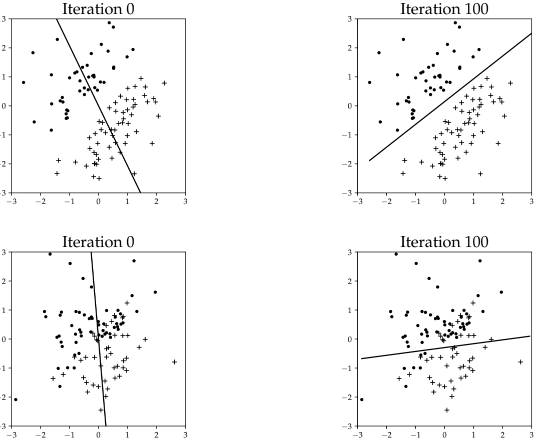
$$\min_{\mathbf{w},b} \mathbb{E}\left[e_i^2\right] \approx \min_{\mathbf{w},b} \sum_{i=1}^{N} \left(y_i - \tanh\left(\mathbf{w}^\top \mathbf{x}_i + b\right)\right)^2 \tag{11}$$

which leads to the update rule

$$\begin{aligned} \mathbf{w}^{(k+1)} &= \mathbf{w}^{(k)} + \mu \sum_{i=1}^{N} e_i \left(1 - f^2(\mathbf{x}_i)\right) \mathbf{x}_i \\ b^{(k+1)} &= b^{(k)} + \mu \sum_{i=1}^{N} e_i \left(1 - f^2(\mathbf{x}_i)\right) \end{aligned} \tag{12}$$

The proof is left as an exercise.

Example of the MMSE applied to a perceptron



Example of the application of the MMSE criterion to a perceptron with hyperbolic tangent activation. The first row corresponds to a separable case and the second one to a non separable one. In both cases the algorithm converges to a solution.