Machine Learning/Advanced Machine Learning

Lecture 6.1: Multilayer Perceptrons

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Based on slides originally made by Jes Frellsen

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Learning Objectives for Week 6

- Reflect the structure of MLP networks
- Apply MLP networks and reflect their role in deep learning
- Use Tensorflow to build simple models and train them
- Explain backpropagation
- Use simple regularisation methods with neural networks
- Explain radial basis function networks
- Explain the principle of convolutional neural networks

Outline of lecture

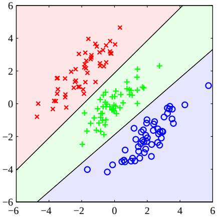
Feed-forward neural networks

Training neural networks

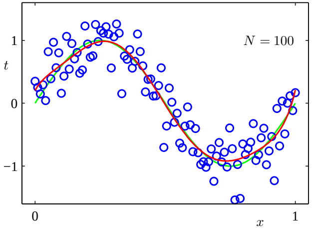
Re-cap: Categories of Machine Learning

Supervised learning: $\mathcal{D} = \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\}$

Classification

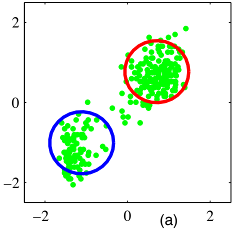


Regression

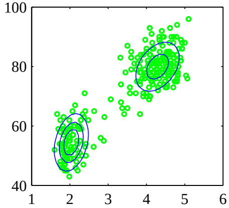


Unsupervised learning: $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$

Clustering

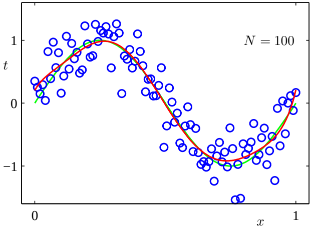


Density estimation



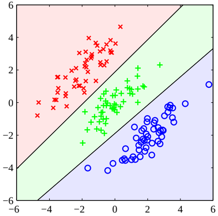
Linear models for regression and classification

Regression



$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=1}^{M} w_j \phi_i(\mathbf{x}) = \mathbf{w}^\mathsf{T} \boldsymbol{\phi}(\mathbf{x})$$

Classification



$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \phi_i(\mathbf{x})\right) = f(\mathbf{w}^\mathsf{T} \boldsymbol{\phi}(\mathbf{x}))$$

where f is an **activation function** such as the **sigmoid** or **softmax**.

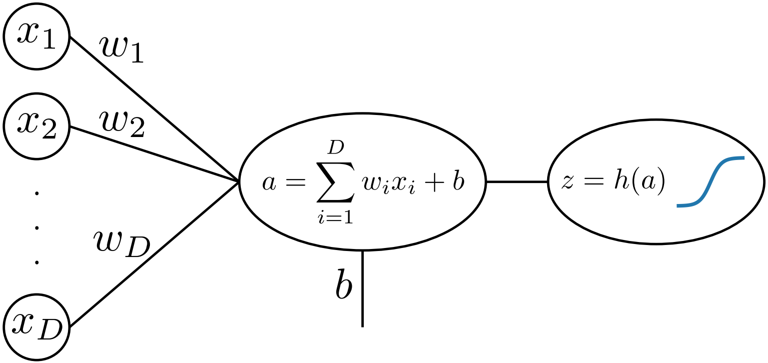
Advantages:

- Useful computational properties: have **closed form expressions**
- Can model “arbitrary” complicated functions.

Disadvantages:

- We have to **choose** the basis functions $\phi_i(\cdot)$, and these are **not adapted to data**.

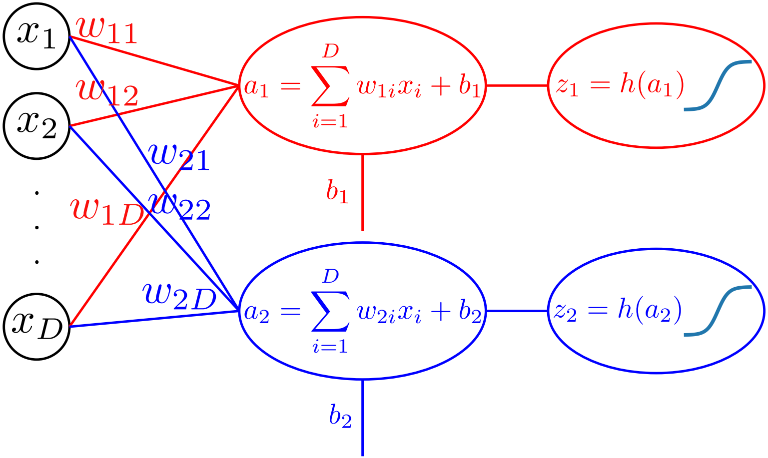
Artificial neuron



Input: $\mathbf{x} = (x_1, \ldots, x_D)^\intercal$
Weights: $\mathbf{w} = (w_1, \ldots, w_D)^\intercal$
Bias: b

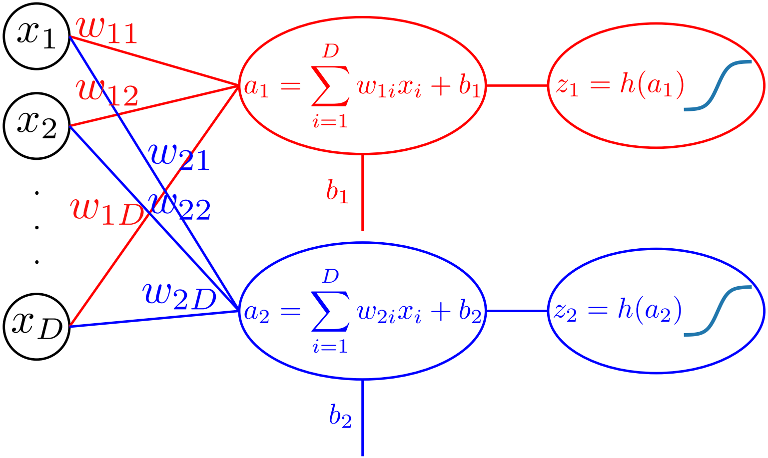
Activation: $a = \sum_{i=1}^{D} w_i x_i + b = \mathbf{w}^\intercal \mathbf{x} + b$
Output: $z = h(a)$
Where $h(\cdot)$ is a **nonlinear activation function**.

Combining artificial neurons



$\mathbf{x}$ $\quad \mathbf{a} = W\mathbf{x} + \mathbf{b} \quad \mathbf{z} = h(\mathbf{a})$

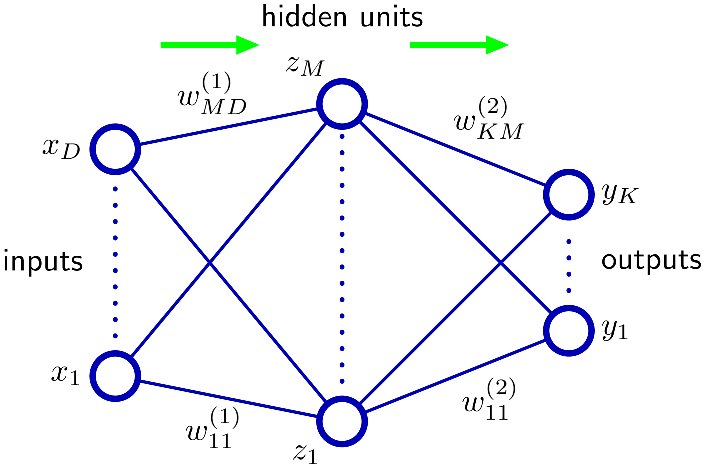
Combining artificial neurons



$\mathbf{x}$ $\quad$ $\mathbf{a} = W\mathbf{x} + \mathbf{b}$ $\quad$ $\mathbf{z} = h(\mathbf{a})$

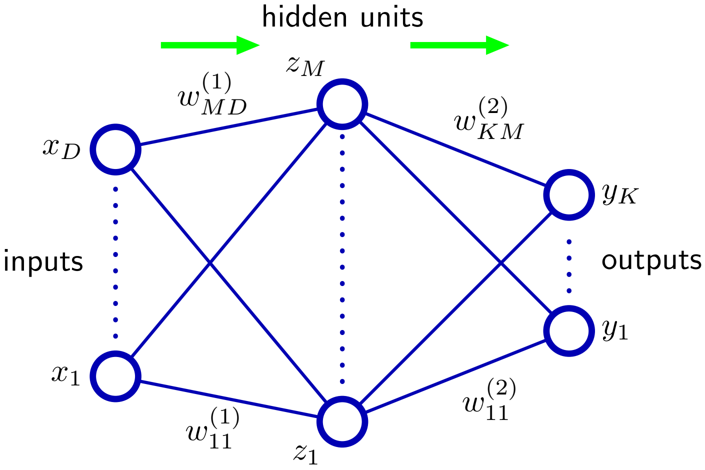
Where $W = \begin{bmatrix} w_{11} & w_{12} & \dots & w_{1D} \\ w_{21} & w_{22} & \dots & w_{2D} \end{bmatrix}$ and h is applied element wise.

A two-layer neural network



$\mathbf{x}$ $\quad$ $\mathbf{z} = h(W^{(1)}\mathbf{x} + \mathbf{b}^{(1)})$ $\quad$ $\mathbf{y} = \sigma(W^{(2)}\mathbf{z} + \mathbf{b}^{(2)})$

A two-layer neural network

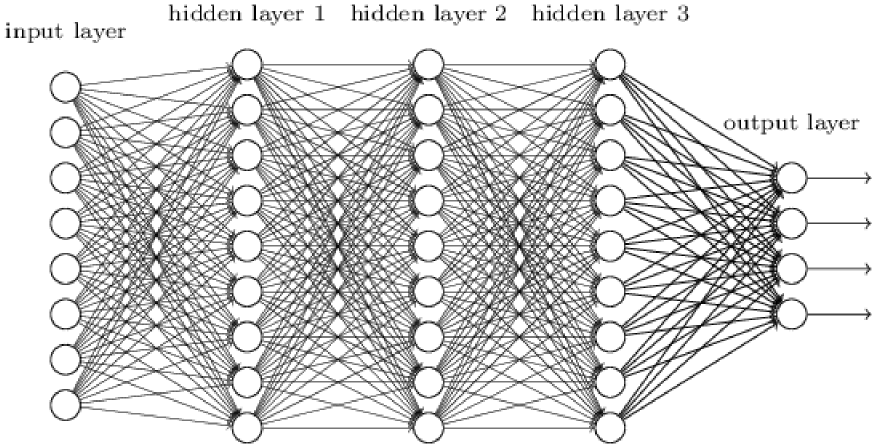


$\mathbf{x}$ $\quad$ $\mathbf{z} = h(W^{(1)}\mathbf{x} + \mathbf{b}^{(1)})$ $\quad$ $\mathbf{y} = \sigma(W^{(2)}\mathbf{z} + \mathbf{b}^{(2)})$

$$\mathbf{y}(\mathbf{x}, \mathbf{W}, \mathbf{b}) = \sigma(W^{(2)}h(W^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) + \mathbf{b}^{(2)})$$

Figure(s) from Bishop.

A deep neural network



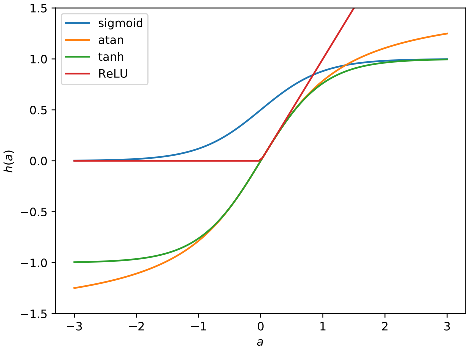
$$\mathbf{y}(\mathbf{x}, \mathbf{W}, \mathbf{b}) = f^{(4)}(f^{(3)}(f^{(2)}(f^{(1)}(\mathbf{x}))))$$

where

$$f^{(\ell)}(\mathbf{z}) = h^{(\ell)}(W^{(\ell)}\mathbf{z} + b^{(\ell)})$$

Figure from neuralnetworksanddeeplearning.com/chap6.html

Activations functions



For hidden layers:

- Sigmoid: $h(a) = \frac{1}{1+\exp(-a)}$
- Arctangent[1]: $h(a) = \operatorname{atan}(a)$
- Hyperbolic tangent: $h(a) = \tanh(a)$
- **Rectified linear**[2]: $h(a) = \max(0, a)$

For output layer:

- Regression: identity, $h(a) = a$
- Binary classification: sigmoid, $h(a) = \frac{1}{1+\exp(-a)}$
- Multiclass classification: softmax, $h(a_k) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$

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[2] The inverse of $\tan$.

[2] Often called ReLU, but this is a misnomer as it means *rectified linear unit*

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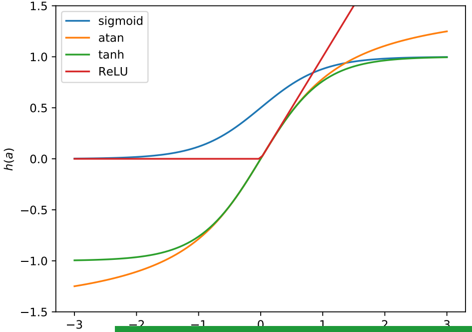

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Exercise

Why do we need activation functions in the **hidden layers**?

Why do we need activation functions in the **output layer for classification**?

[2] The inverse of $\tan$.
[2] Often called ReLU, but this is a misnomer as it means *rectified linear unit*

Universal approximation theorem

Neural networks are universal approximators (Bishop):

"A two-layer network with linear outputs can uniformly **approximate any continuous function** on a compact input domain (compact subset of $\mathbb{R}^N$) to **arbitrary accuracy** provided the network has **sufficiently large number of hidden units**"

How do we program neural networks?

We could in principle program them directly in Python / NumPy

However, we need **derivatives / gradients** for training (later)

We will use **TensorFlow**, which has automatic differentiations.

TensorFlow works in a **declarative** style:

- First you declare/define a **dataflow graph**.
- Then you use a session to run/evaluate operations in the graph.

Example: Notebook 1

TensorFlow

PyTorch

Outline of lecture

Feed-forward neural networks

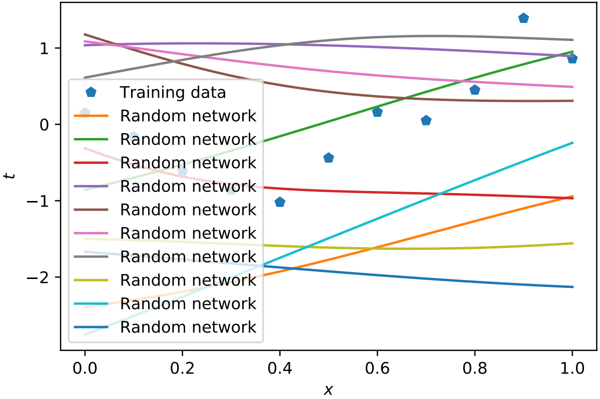
Training neural networks

Training neural networks

We looked a the definition of a neural network, or a **neural network function** $\mathbf{y}(\mathbf{x}, \mathbf{W}, \mathbf{b})$.

If we are given some data as **input vectors X** $= \{\mathbf{x}_n\}_{n=1}^N$ **and target vectors t** $= \{\mathbf{t}_n\}_{n=1}^N$:

- How can we find $\mathbf{W}$ and $\mathbf{b}$?



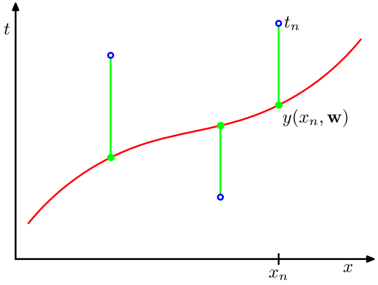
Example: Notebook 2

Regression with neural networks

We find $\mathbf{W}$ and $\mathbf{b}$ by minimizing an **error function** that **measures the misfit** between $\mathbf{y}(\mathbf{x}, \mathbf{W}, \mathbf{b})$ and $\mathbf{t} = \{\mathbf{t}_n\}_{n=1}^N$.

The **sum-of-squares** error function is given by

$$E(\mathbf{W}, \mathbf{b}) = \frac{1}{2} \sum_{n=1}^{N} ||\mathbf{y}(x_n, \mathbf{W}, \mathbf{b}) - \mathbf{t}_n||^2.$$

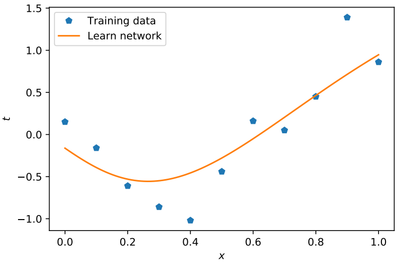


Recall, this corresponds to **finding the MLE** of $\mathbf{W}$ and $\mathbf{b}$ with the likelihood function

$$p(\mathbf{t}|\mathbf{X}, \mathbf{W}, \mathbf{b}, \beta) = \prod_{n=1}^{N} p(\mathbf{t}_n|\mathbf{x}_n, \mathbf{W}, \mathbf{b}, \beta)$$

where

$$p(\mathbf{t}_n|\mathbf{x}_n, \mathbf{W}, \mathbf{b}, \beta) = \mathcal{N}(\mathbf{t}_n|\mathbf{y}(x_n, \mathbf{W}, \mathbf{b}), \beta^{-1}I)$$

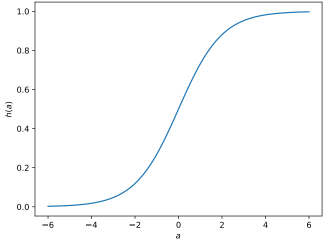


Binary classification with neural networks

Now consider a classification problem, where $t_n \in \{0, 1\}$.

In this cases we use the **sigmoid activation** function

$$y(\mathbf{x}, \mathbf{W}, \mathbf{b}) = \sigma(a^{(L)}) = \frac{1}{1 + \exp(-a^{(L)})}$$

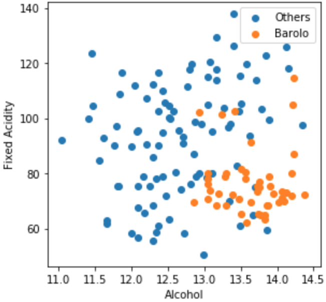


We then use the binomial distribution

$$p(t|\mathbf{x}, \mathbf{W}, \mathbf{b}) = y(\mathbf{x}, \mathbf{W}, \mathbf{b})^t (1 - y(\mathbf{x}, \mathbf{W}, \mathbf{b}))^{1-t} \quad (1)$$

Assuming i.i.d. training data we get the likelihood function

$$p(\mathbf{t}|\mathbf{X}, \mathbf{W}, \mathbf{b}, \beta) = \prod_{n=1}^{N} p(t_n|\mathbf{x}_n, \mathbf{W}, \mathbf{b}) \quad (2)$$



We then set the error function to the negative log-likelihood

$$E(\mathbf{W}, \mathbf{b}) = -\sum_{n=1}^{N} t_n \ln y(\mathbf{x}_n, \mathbf{W}, \mathbf{b}) + (1 - t_n) \ln(1 - y(\mathbf{x}_n, \mathbf{W}, \mathbf{b})) \quad (3)$$

Which is also called the **cross-entropy error function**

Binary classification with neural networks

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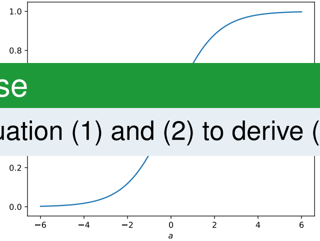

Exercise

Use equation (1) and (2) to derive (3).

We then use the binomial distribution

$$p(t|\mathbf{x}, \mathbf{W}, \mathbf{b}) = y(\mathbf{x}, \mathbf{W}, \mathbf{b})^t (1 - y(\mathbf{x}, \mathbf{W}, \mathbf{b}))^{1-t} \qquad (1)$$

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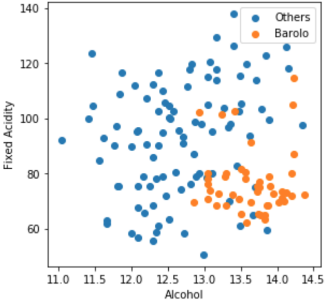
$$p(\mathbf{t}|\mathbf{X}, \mathbf{W}, \mathbf{b}, \beta) = \prod_{n=1}^{N} p(t_n|\mathbf{x}_n, \mathbf{W}, \mathbf{b}) \qquad (2)$$



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Which is also called the **cross-entropy error function**

Multi-class classification with neural networks

Now consider a classification problem, where $t_n \in \{0, 1\}^K$.

In this cases we use the **softmax activation** function

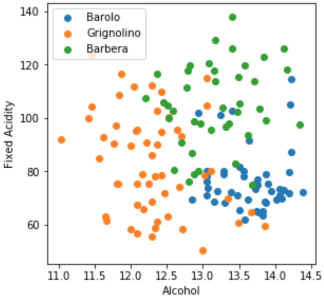
$$y_k(\mathbf{x}, \mathbf{W}, \mathbf{b}) = \sigma(\mathbf{a}^{(L)}) = \frac{\exp(a_k)}{\sum_{j=1}^{K} \exp(a_j)}$$

In this case we obtain the error function

$$E(\mathbf{W}, \mathbf{b}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{nk} \ln y_k(\mathbf{x}_n, \mathbf{W}, \mathbf{b}). \qquad (4)$$

from the log-likelihood function.

This is also called the **cross-entropy error function**



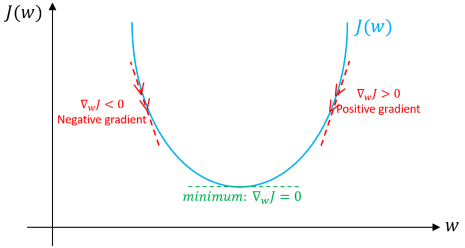
Parameter optimization and gradient descent

We want to find $\mathbf{W} = (\mathbf{W}, \mathbf{b})$ that **minimizes** $E(\mathbf{W})$, i.e. find $\mathbf{W}$ such that $\nabla E(\mathbf{W}) = 0$.

Gradient descent starts with an initial random point $\mathbf{W}^{(0)}$, and iteratively refines it by following the steepest descent direction:

$$\mathbf{W}^{(\tau+1)} = \mathbf{W}^{(\tau)} - \eta \nabla E(\mathbf{W}^{(\tau)})$$

where η is the called the **learning rate**.



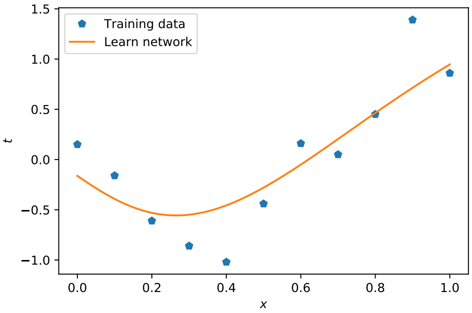
Normally the gradient is calculated on the full dataset (*batch* optimization).

To avoid getting stuck in local minima, we can calculate the gradient on **mini-batches**:

$$\mathbf{W}^{(\tau+1)} = \mathbf{W}^{(\tau)} - \eta \nabla E_s(\mathbf{W}^{(\tau)})$$

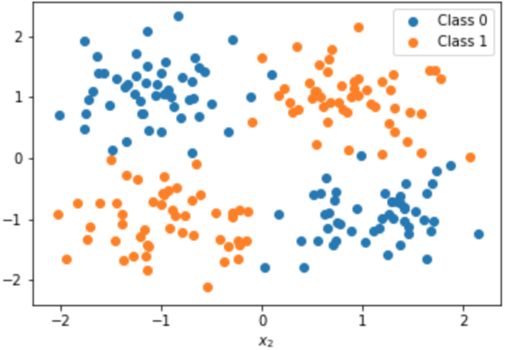
where E_s is the error on a subset of the data.

Examples: regression



Example: Notebook 3

Examples: binary classification



Example: Notebook 4

Next lecture

- Backpropagation
- Regularisation of neural networks
- Radial basis functions
- Brief introduction to CNNs

References I

Bishop, C. M. (2006). *Pattern Recognition and Machine Learning*. Springer.