Inf2b - Learning

Lecture 15: Multi-layer neural networks (2)

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http://www.inf.ed.ac.uk/teaching/courses/inf2b/
https://piazza.com/ed.ac.uk/spring2020/infr08028
Office hours: Wednesdays at 14:00-15:00 in IF-3.04

Jan-Mar 2020

Today's Schedule

1. Training of neural networks (recap)
2. Activation functions
3. Experimental comparison of different classifiers
4. Overfitting and generalisation
5. Deep Neural Networks

Training of neural networks (recap)

- Optimisation problem (training):

$$\min_{\boldsymbol{w}} E(\boldsymbol{w}) = \min_{\boldsymbol{w}} \frac{1}{2}\sum_{n=1}^{N}(y_n - t_n)^2$$

- No analytic solution (no closed form)
- Employ an iterative method (requires initial values) e.g. Gradient descent (steepest descent), Newton's method, Conjugate gradient methods
- Gradient descent

$$w_i^{(\text{new})} \leftarrow w_i - \eta \frac{\partial}{\partial w_i} E(\boldsymbol{w}), \qquad (\eta > 0)$$

Training of the single-layer neural network (recap)

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}(\,y_n - t_n\,)^2 \;=\; \frac{1}{2}\sum_{n=1}^{N}(\,g(a_n) - t_n\,)^2$$

$$\text{where} \quad y_n = g(a_n), \quad a_n = \sum_{i=0}^{D} w_i x_{ni}, \quad \frac{\partial\, a_n}{\partial\, w_i} = x_{ni}$$

$$\begin{aligned}
\frac{\partial E(\boldsymbol{w})}{\partial w_i} &= \frac{\partial E(\boldsymbol{w})}{\partial y_n}\,\frac{\partial y_n}{\partial a_n}\,\frac{\partial a_n}{\partial w_i} \\
&= \sum_{n=1}^{N}(y_n - t_n)\,\frac{\partial\, g(a_n)}{\partial a_n}\,\frac{\partial\, a_n}{\partial w_i} \\
&= \sum_{n=1}^{N}(y_n) - t_n)\, g'(a_n)\, x_{ni}
\end{aligned}$$

Multi-layer neural networks (recap)

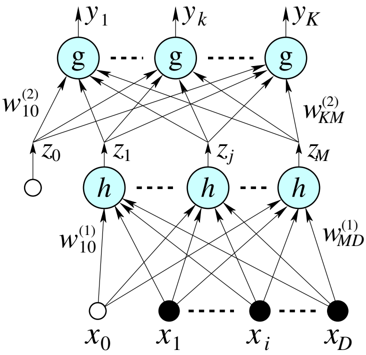
Multi-layer perceptron (MLP)

- Hidden-to-output weights:

$$w_{kj}^{(2)} \leftarrow w_{kj}^{(2)} - \eta \frac{\partial E}{\partial w_{kj}^{(2)}}$$

- Input-to-hidden weights:

$$w_{ji}^{(1)} \leftarrow w_{ji}^{(1)} - \eta \frac{\partial E}{\partial w_{ji}^{(1)}}$$



The derivatives of the error function (two-layers) (recap)

$$E_n = \frac{1}{2}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

$$y_{nk} = g(a_{nk}), \quad a_{nk} = \sum_{j=1}^{M} w_{kj}^{(2)} z_{nj}$$

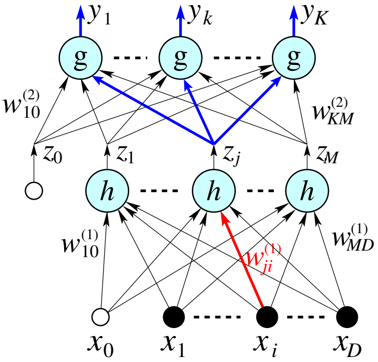
$$z_{nj} = h(b_{nj}), \quad b_{nj} = \sum_{i=0}^{D} w_{ji}^{(1)} x_{ni}$$

$$\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \frac{\partial E_n}{\partial y_{nk}} \frac{\partial y_{nk}}{\partial a_{nk}} \frac{\partial a_{nk}}{\partial w_{kj}^{(2)}}$$

$$= (y_{nk} - t_{nk})\, g'(a_{nk})\, z_{nj}$$

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \frac{\partial E_n}{\partial z_{nj}} \frac{\partial z_{nj}}{\partial b_{nj}} \frac{\partial b_{nj}}{\partial w_{ji}^{(1)}} = \left(\sum_{k=1}^{K}(y_{nk} - t_{nk})\frac{\partial y_{nk}}{\partial z_{nj}}\right) h'(b_{nj})\, x_{ni}$$

$$= \left(\sum_{k=1}^{K}(y_{nk} - t_{nk}) g'(a_{nk}) w_{kj}^{(2)}\right) h'(b_{nj})\, x_{ni}$$



Error back propagation (recap)

$$\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \frac{\partial E_n}{\partial y_{nk}} \frac{\partial y_{nk}}{\partial a_{nk}} \frac{\partial a_{nk}}{\partial w_{kj}^{(2)}}$$

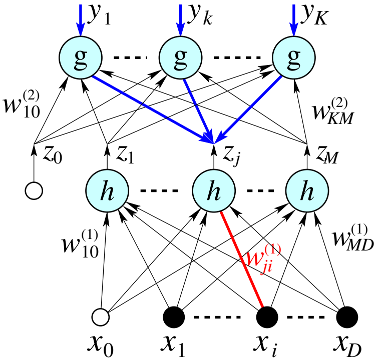
$$= (y_{nk} - t_{nk})\, g'(a_{nk})\, z_{nj}$$

$$= \delta_{nk}^{(2)}\, z_{nj}, \qquad \delta_{nk}^{(2)} = \frac{\partial E_n}{\partial a_{nk}}$$

$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \frac{\partial E_n}{\partial z_{nj}} \frac{\partial z_{nj}}{\partial b_{nj}} \frac{\partial b_{nj}}{\partial w_{ji}^{(1)}}$$

$$= \left(\sum_{k=1}^{K} (y_{nk} - t_{nk}) g'(a_{nk}) w_{kj}^{(2)} \right) h'(b_{nj})\, x_{ni}$$

$$= \left(\sum_{k=1}^{K} \delta_{nk}^{(2)} w_{kj}^{(2)} \right) h'(b_{nj})\, x_{ni}$$



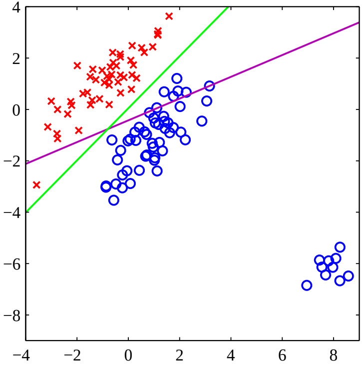
Some questions on activation functions

- Is the logistic sigmoid function necessary for single-layer single-output-node network?
  - No, in terms of classification.
    We can replace it with $g(a) = a$. However, decision boundaries can be different. (NB: A linear decision boundary ($a = 0.5$) is formed in either case.)
- What benefits are there in using the logistic sigmoid function in the case above?
  - The output can be regarded as a posterior probability.
  - Compared with a linear output node ($g(a) = a$), 'logistic regression' normally forms a more robust decision boundary against noise.

Logistic sigmoid vs a linear output node

Binary classification problem with the least squares error (LSE):

$$g(a) = \frac{1}{1 + \exp(-a)} \quad \text{vs} \quad g(a) = a$$



(after Fig 4.4b in PRML C. M. Bishop (2006))

Implementations of gradient descent

$$E(w) = \frac{1}{2}\sum_{n=1}^{N} \| \mathbf{y}_n - \mathbf{t}_n \|^2 \; = \; \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

$$= \sum_{n=1}^{N} E_n, \quad \text{where} \;\; E_n = \frac{1}{2}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

- Batch gradient descent:

$$w_{ki} \;\leftarrow\; w_{ki} - \eta \frac{\partial E}{\partial w_{ki}}$$

- Incremental (online) gradient descent:
  Update weights for each $\mathbf{x}_n$

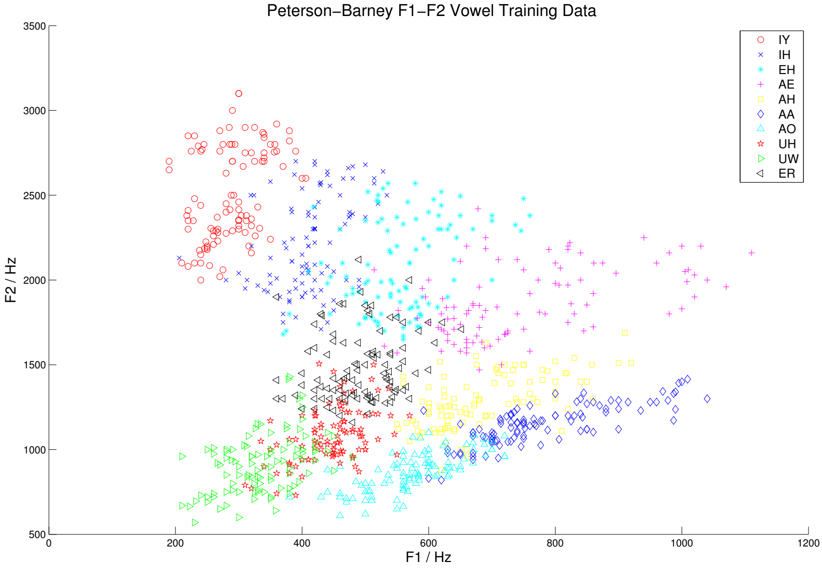
$$w_{ki} \;\leftarrow\; w_{ki} - \eta \frac{\partial E_n}{\partial w_{ki}}$$

- Stochastic gradient descent: c.f. Batch/Mini-batch training
  Update weights for randomly chosen $\boldsymbol{x}$.

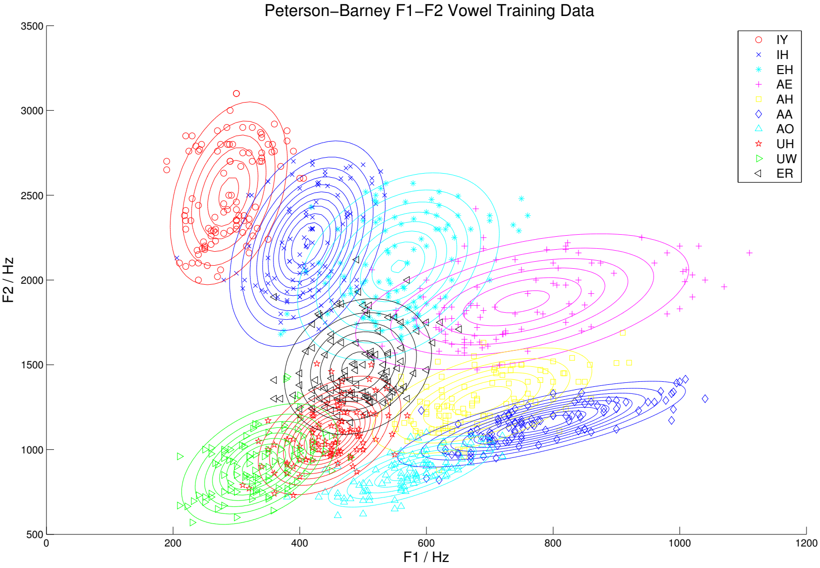
Experimental comparison

- Task: spoken vowel classification
- Classifiers:
  - Gaussian classifier
  - Single layer network (SLN)
  - Multi-layer perceptron (MLP)

Classifying spoken vowels (lecture 09) — Training data



Gaussian for each class



Details of the classifiers

- **Gaussian classifier**: (2-dimensional) Gaussian for each class. Training involves estimating mean vector and covariance matrix for each class, assume equal priors. (50 parameters)
- **Single layer network**: 2 inputs, 10 outputs. Iterative training of weight matrix. (30 parameters)
- **MLP**: two inputs, 25 hidden units, 10 outputs. Trained by gradient descent (backprop). (335 parameters)
- For SLN and MLP normalise feature vectors to mean=0 and sd=1:

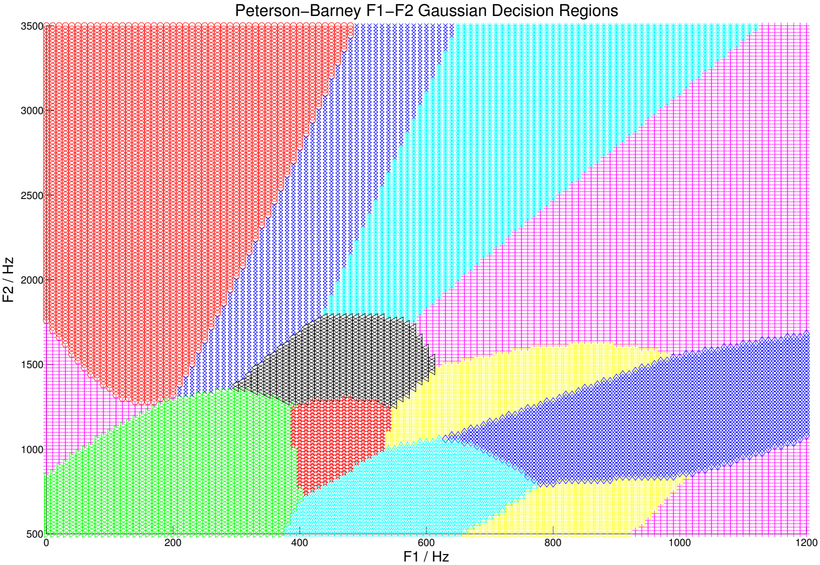
  $$z_{ni} = \frac{x_i^n - mi}{s_i}$$

  m_i is sample mean of feature i computed from the training set, s_i is standard deviation.

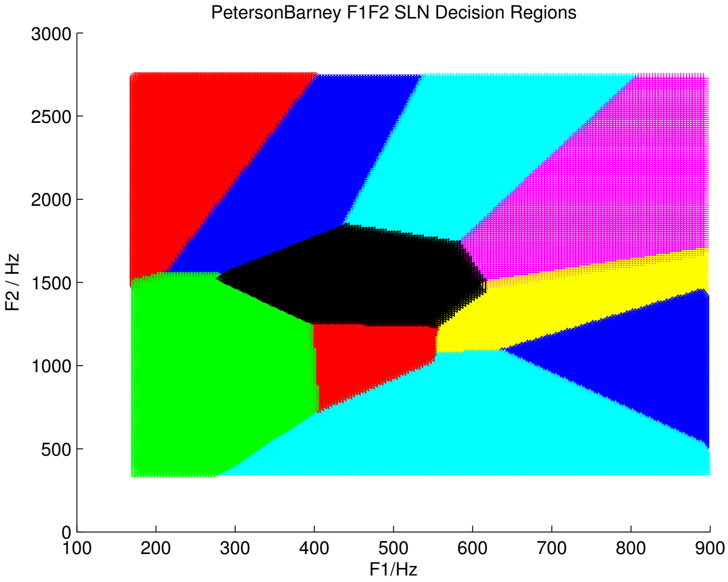
Results

Gaussian classifier:	86.5% correct
Single layer network:	85.5% correct
MLP:	86.5% correct

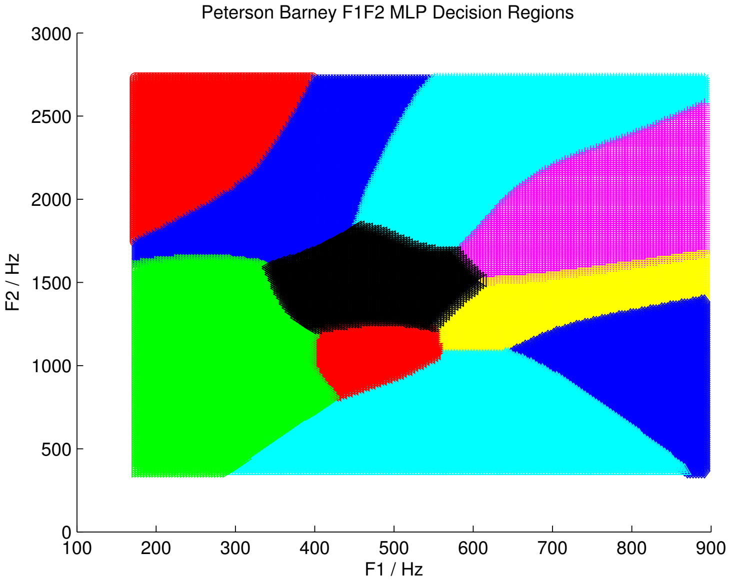
Decision Regions: Gaussian classifier



Decision Regions: Single-layer perceptron



Decision Regions: Multi-layer perceptron



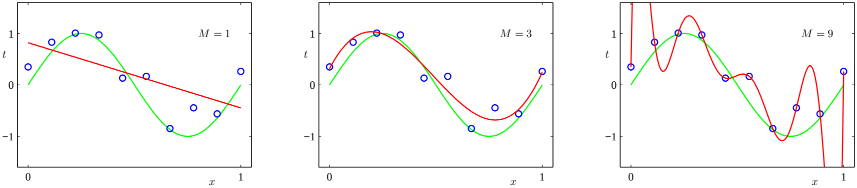
Problems with multi-layer neural networks

- Still difficult to train
  - Computationally very expensive (e.g. weeks of training)
  - Slow convergence ('vanishing gradients')
  - Difficult to find the optimal network topology
- Poor generalisation (under some conditions)
  - Very good performance on the training set
  - Poor performance on the test set

Overfitting and generalisation

Example of curve fitting by a polynomial function:

$$y(x, \boldsymbol{w}) = w_0 + w_1\, x + w_2\, x^2 + \ldots + w_M\, x^M = \sum_{k=0}^{M} w_k\, x^k$$



(after Fig 1.4 in PRML C. M. Bishop (2006))

- cf. memorising the training data

Generalisation in neural networks

- How many hidden units (or, how many weights) do we need?
- Optimising training set performance does not necessarily optimise test set performance
  - Network too "flexible": Too many weights compared with the number of training examples
  - Network not flexible enough: Not enough weights (hidden units) to represent the desired mapping
- **Generalisation Error**: The predicted error on unseen data. How can the generalisation error be estimated?
  - Training error?

$$E_{\mathrm{train}} = \frac{1}{2} \sum_{\mathrm{trainingset}} \sum_{k=1}^{K} (y_k - t_k)^2$$

  - Cross-validation error?

$$E_{\mathrm{xval}} = \frac{1}{2} \sum_{\mathrm{validationset}} \sum_{k=1}^{K} (y_k - t_k)^2$$

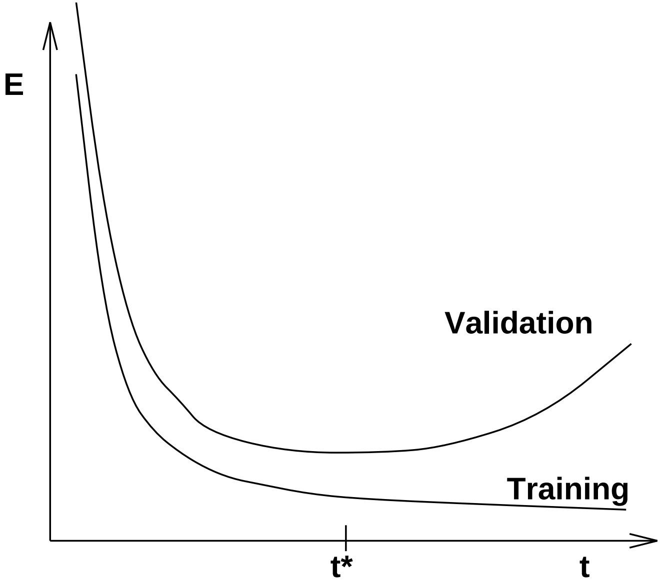
Overtraining in neural networks (†)

- Overtraining (overfitting) corresponds to a network function too closely fit to the training set (too much flexibility)
- Undertraining corresponds to a network function not well fit to the training set (too little flexibility)
- Solutions
  - If possible increasing both network complexity in line with the training set size
  - Use prior information to constrain the network function
    Control the flexibility: **Structural Stabilisation**
  - Control the effective flexibility: **early stopping** and **regularisation**

Early stopping (†)

- Use validation set to decide when to stop training
- Training-set error monotonically decreases as training progresses
- Validation-set error will reach a minimum then start to increase
- "Effective Flexibility" increases as training progresses
- Network has an increasing number of "effective degrees of freedom" as training progresses
- Network weights become more tuned to training data
- Very effective — used in many practical applications such as speech recognition and optical character recognition

Early stopping



Regularisation — Penalising complexity (†)

- Original error function

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}||\mathbf{y}_n - \mathbf{t}_n||^2$$

- Regularised error function

$$\tilde{E}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}||\mathbf{y}_n - \mathbf{t}_n||^2 \; + \; \frac{\beta}{2}\sum_{\ell}||\boldsymbol{w}||^2$$

Ability of neural networks (†)

- Universal approximation thorem
  - "Univariate function and a set of affine functionals can uniformly approximate any continuous function of n real variables with support in the unit hypercube; only mild conditions are imposed on the univariate function. "
    (G. Cybenko (1989)

    $\longrightarrow$

    A single-output node nerural network with a single hidden layer with a finite neurons can approximate continuous functions.
  - K. Hornik (1990) doi:10.1016/0893-6080(91)90009-T
  - N. Guliyev, V. Ismailov (2018) 10.31219/osf.io/xgnw8

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Breakthrough (†)

1957 Frank Rosenblatt : 'Perceptron'

1986 D. Rumelhart, G. Hinton, and R. Williams: 'Backpropagation'

2006 G. Hinton etal (U. Toronto)

"Reducing the dimensionality of data with neural networks", Science.

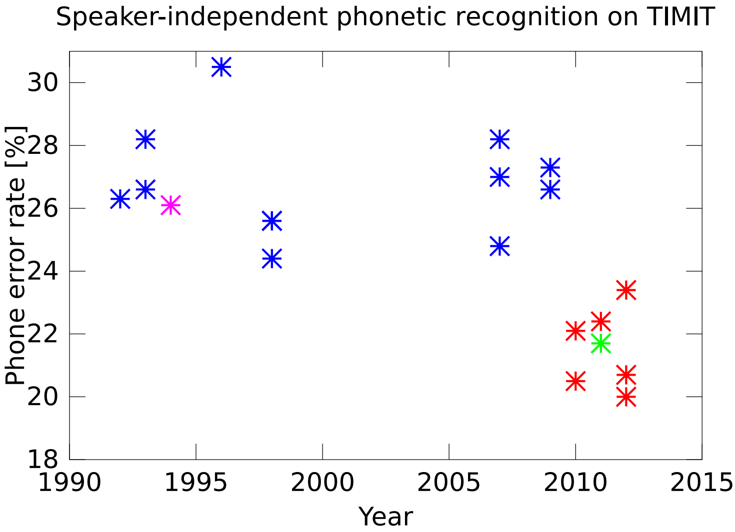
2009 J. Schmidhuber (Swiss AI Lab IDSIA)

Winner at ICDAR2009 handwriting recognition competition

2011- many papers from U.Toronto, Microsoft, IBM, Google, ...

- What's the ideas?
  - Pretraining
    - A single layer of feature detectors $\rightarrow$ Stack it to form several hidden layers
  - Fine-tuning, dropout
  - GPU
  - Convolutional network (CNN), Long short-term memory (LSTM)
  - Rectified linear unit (ReLU)

Breakthrough (†)



Summary

- Error back propagation training
- Logistic sigmoid vs linear node
- Decision boundaries
- Overfitting vs generalisation
- (Feed-forward network vs RNN)

- A very good reference:
  http://neuralnetworksanddeeplearning.com/