Inf2b - Learning

Lecture 15: Multi-layer neural networks (2)

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(Credit: Iain Murray and Steve Renals)

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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

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Today's Schedule

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)

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

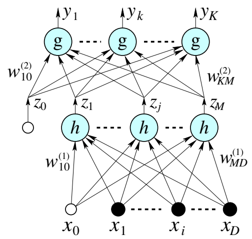
where $y_n = g(a_n), \quad a_n = \sum_{i=0}^{D} w_i x_{ni}, \quad \frac{\partial\, a_n}{\partial\, w_i} = x_{ni}$

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

Multi-layer neural networks (recap)

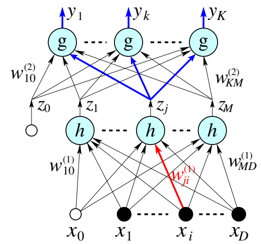
Multi-layer perceptron (MLP)

- Hidden-to-output weights:
$$w_{kj}^{(2)} \leftarrow w_{kj}^{(2)} - \eta\frac{\partial E}{\partial w_{kj}^{(2)}}$$
- Input-to-hidden weights:
$$w_{ji}^{(1)} \leftarrow w_{ji}^{(1)} - \eta\frac{\partial E}{\partial w_{ji}^{(1)}}$$



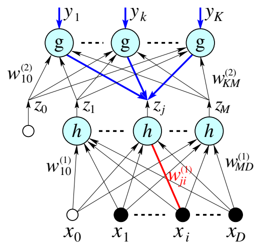
The derivatives of the error function (two-layers) (recap)

$$E_n = \frac{1}{2}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$
$$y_{nk} = g(a_{nk}), \quad a_{nk} = \sum_{j=1}^{M} w_{kj}^{(2)} z_{nj}$$
$$z_{nj} = h(b_{nj}), \quad b_{nj} = \sum_{i=0}^{D} w_{ji}^{(1)} x_{ni}$$
$$\frac{\partial E_n}{\partial w_{kj}^{(2)}} = \frac{\partial E_n}{\partial y_{nk}}\frac{\partial y_{nk}}{\partial a_{nk}}\frac{\partial a_{nk}}{\partial w_{kj}^{(2)}} = (y_{nk} - t_{nk})\, g'(a_{nk})\, z_{nj}$$
$$\frac{\partial E_n}{\partial w_{ji}^{(1)}} = \frac{\partial E_n}{\partial z_{nj}}\frac{\partial z_{nj}}{\partial b_{nj}}\frac{\partial b_{nj}}{\partial w_{ji}^{(1)}} = \left(\sum_{k=1}^{K}(y_{nk} - t_{nk})\frac{\partial y_{nk}}{\partial z_{nj}}\right)h'(b_{nj})\, x_{ni}$$
$$= \left(\sum_{k=1}^{K}(y_{nk} - t_{nk})g'(a_{nk})w_{kj}^{(2)}\right)h'(b_{nj})\, x_{ni}$$



Error back propagation (recap)

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



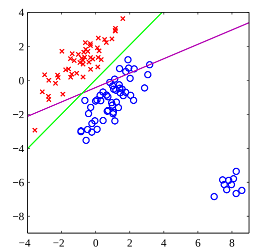
Some questions on activation functions

- 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

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

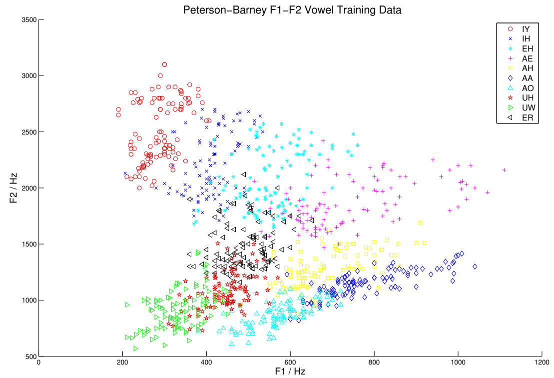
$$= \sum_{n=1}^{N} E_n, \quad \text{where} \quad E_n = \frac{1}{2}\sum_{k=1}^{K}(y_{nk} - t_{nk})^2$$

- 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 $\boldsymbol{x}$.

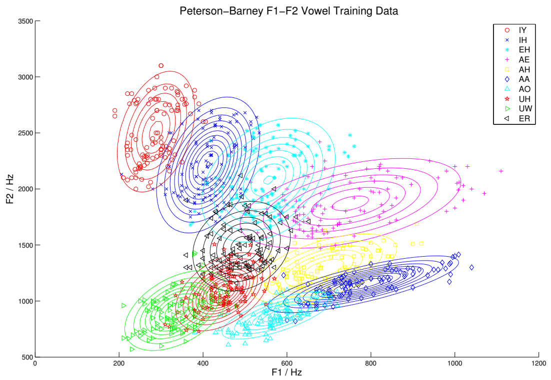
Experimental comparison

- 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



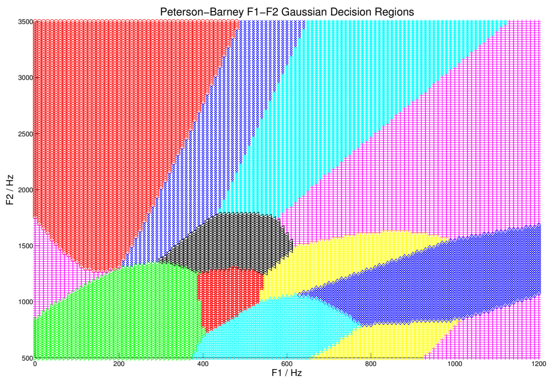
Details of the classifiers

- **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.

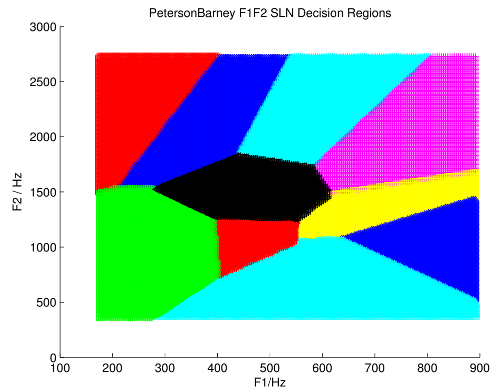
Results

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

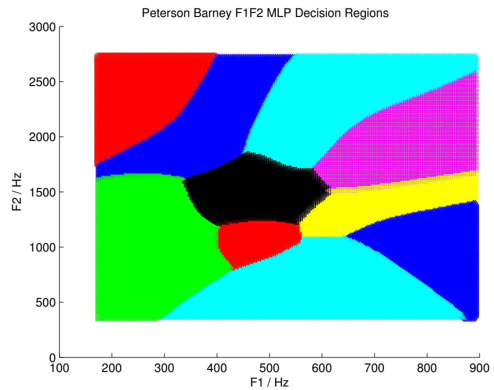
Decision Regions: Gaussian classifier



Decision Regions: Single-layer perceptron



Decision Regions: Multi-layer perceptron



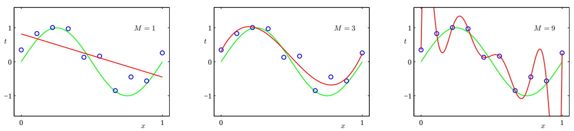
Problems with multi-layer neural networks

- 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?

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

  - Cross-validation error?

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

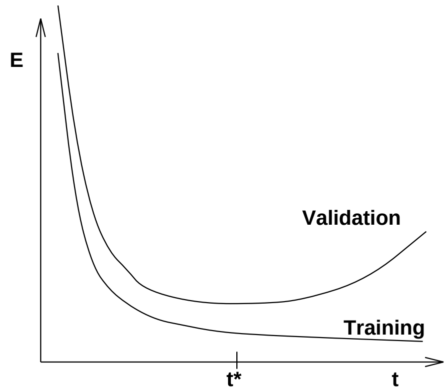
Overtraining in neural networks (†)

- 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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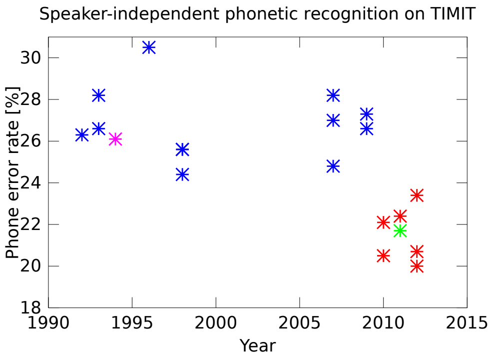
  - Slow convergence ('vanishing gradients')
  - Difficult to find the optimal network topology
- Poor generalisation (under some conditions)
  - Very good performance on the training set
  - Poor performance on the test set

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 → 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/`