Statistical Data Mining and Machine Learning
Hilary Term 2016

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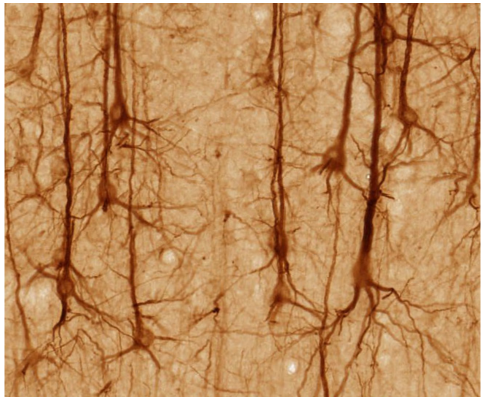
Slides and other materials available at:
http://www.stats.ox.ac.uk/~sejdinov/sdmml

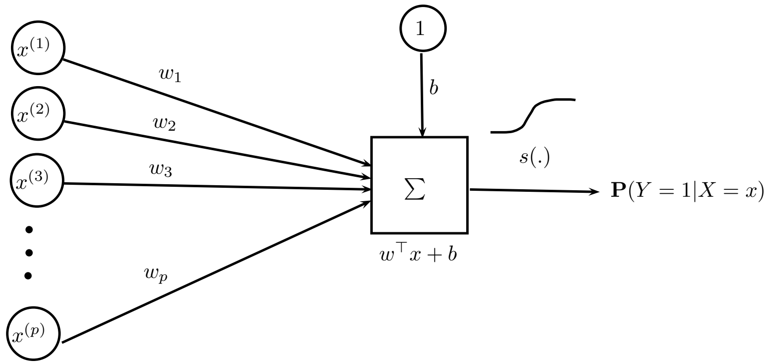
Neural Networks

Biological inspiration

- Basic computational elements: neurons.
- Receives signals from other neurons via dendrites.
- Sends processed signals via axons.
- Axon-dendrite interactions at synapses.
- $10^{10} - 10^{11}$ neurons.
- $10^{14} - 10^{15}$ synapses.

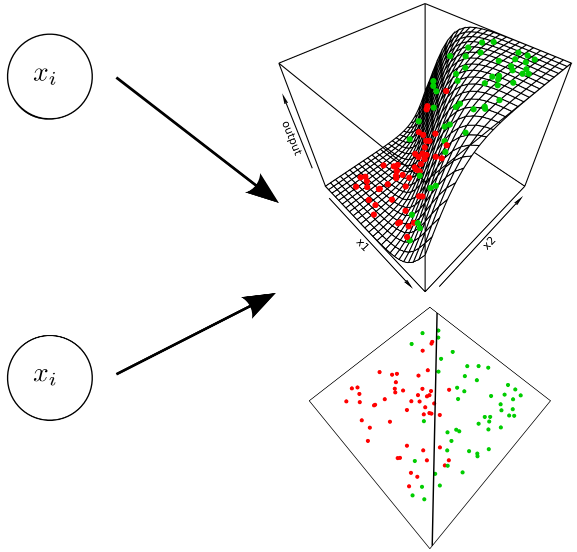


Single Neuron Classifier

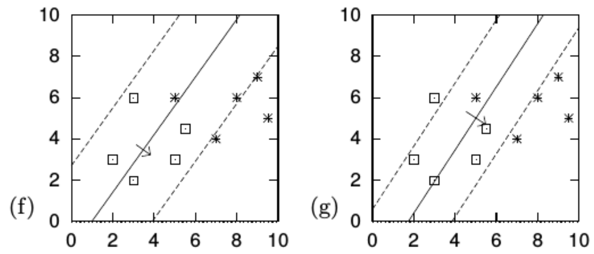


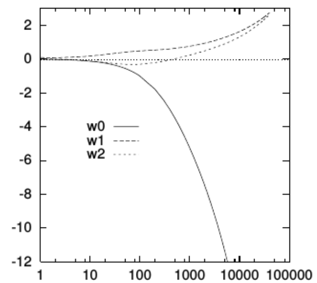
- **activation** $w^\top x + b$ (linear in **inputs** x)
- **activation/transfer function** s gives the **output/activity** (potentially nonlinear in x)
- common nonlinear activation function $s(a) = \frac{1}{1+e^{-a}}$: **logistic regression**
- learn w and b via gradient descent

Single Neuron Classifier



Overfitting

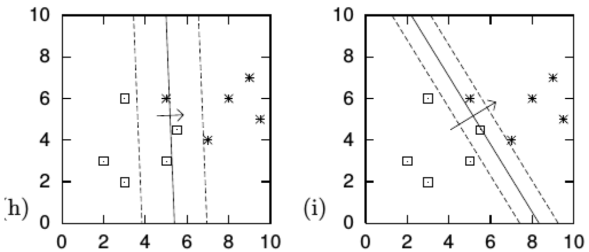


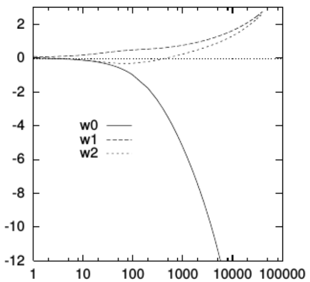


iterations 30,80

Figures from D. MacKay, **Information Theory, Inference and Learning Algorithms**

Overfitting

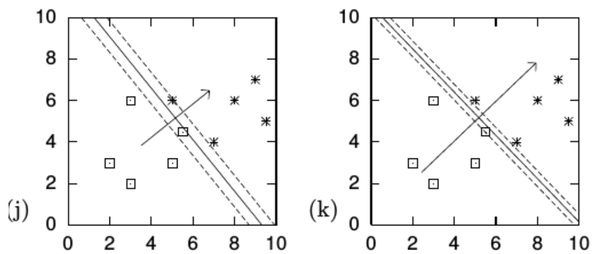


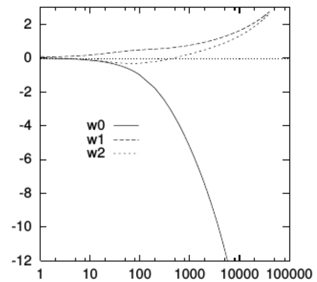


iterations 500,3000

Figures from D. MacKay, **Information Theory, Inference and Learning Algorithms**

Overfitting





iterations 10000,40000

prevent overfitting by:

- **early stopping**: just halt the gradient descent
- regularization: L_2-regularization called **weight decay** in neural networks literature.

Figures from D. MacKay, **Information Theory, Inference and Learning Algorithms**

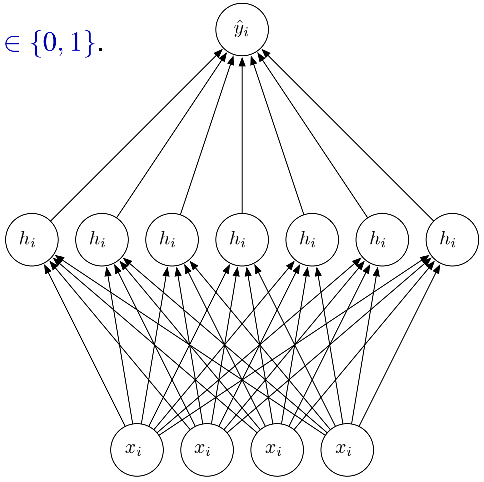
Multilayer Networks

- Data vectors $x_i \in \mathbb{R}^p$, binary labels $y_i \in \{0, 1\}$.
- **inputs** $x_{i1}, \dots, x_{ip}$
- **output** $\hat{y}_i = \mathbb{P}(Y = 1|X = x_i)$
- **hidden unit activities** $h_{i1}, \dots, h_{im}$
  - Compute **hidden unit activities**:

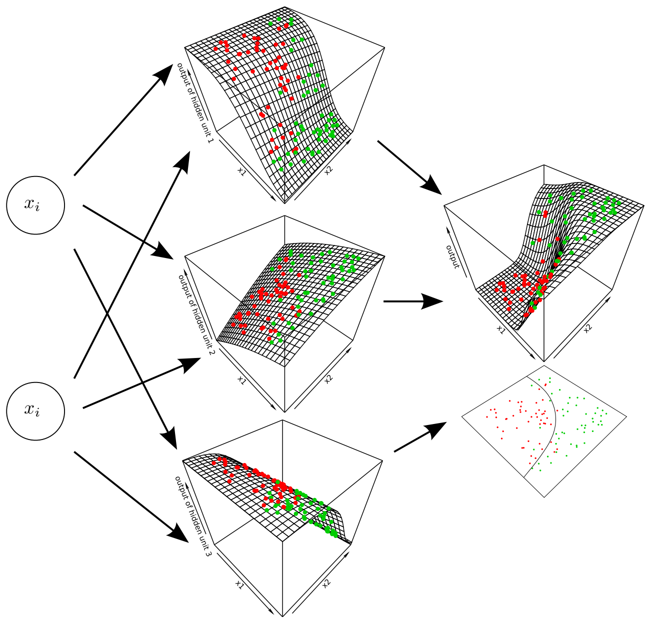
$$h_{il} = s\left(b_l^h + \sum_{j=1}^{p} w_{jl}^h x_{ij}\right)$$

  - Compute **output probability**:

$$\hat{y}_i = s\left(b^o + \sum_{l=1}^{m} w_k^o h_{il}\right)$$



Multilayer Networks



Training a Neural Network

- Objective function: L_2-regularized log-loss

$$J = -\sum_{i=1}^{n} y_i \log \hat{y}_i + (1 - y_i)\log(1 - \hat{y}_i) + \frac{\lambda}{2}\left(\sum_{jl}(w_{jl}^h)^2 + \sum_{l}(w_l^o)^2\right)$$

where

$$\hat{y}_i = s\left(b^o + \sum_{l=1}^{m} w_l^o h_{il}\right) \qquad h_{il} = s\left(b_l^h + \sum_{j=1}^{p} w_{jl}^h x_{ij}\right)$$

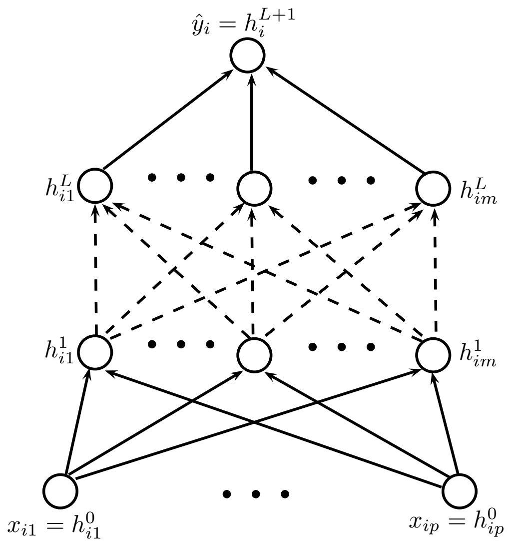
- Optimize parameters $\theta = \left\{b^h, w^h, b^o, w^o\right\}$, where $b^h \in \mathbb{R}^m$, $w^h \in \mathbb{R}^{p \times m}$, $b^o \in \mathbb{R}$, $w^o \in \mathbb{R}^m$ with gradient descent.

$$\frac{\partial J}{\partial w_l^o} = \lambda w_l^o + \sum_{i=1}^{n} \frac{\partial J}{\partial \hat{y}_i}\frac{\partial \hat{y}_i}{\partial w_l^o} = \lambda w_l^o + \sum_{i=1}^{n}(\hat{y}_i - y_i)h_{il},$$

$$\frac{\partial J}{\partial w_{jl}^h} = \lambda w_{jl}^h + \sum_{i=1}^{n} \frac{\partial J}{\partial \hat{y}_i}\frac{\partial \hat{y}_i}{\partial h_{il}}\frac{\partial h_{il}}{\partial w_{jl}^h} = \lambda w_{jl}^h + \sum_{i=1}^{n}(\hat{y}_i - y_i)w_l^o h_{il}(1 - h_{il})x_{ij}.$$

- L_2-regularization often called **weight decay**.
- Multiple hidden layers: **Backpropagation** algorithm

Multiple hidden layers



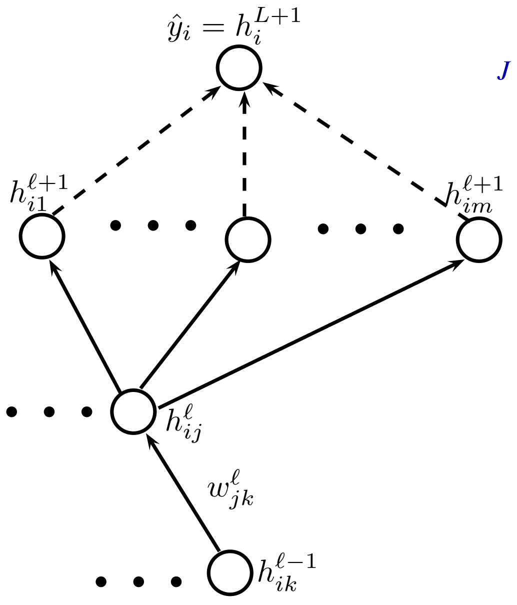
$$h_i^{\ell+1} = \underline{s}\left(W^{\ell+1} h_i^{\ell}\right)$$

- $W^{\ell+1} = \left(w_{jk}^{\ell}\right)_{jk}$: weight matrix at the $(\ell + 1)$-th layer, weight w_{jk}^{ℓ} on the edge between $h_{ik}^{\ell-1}$ and h_{ij}^{ℓ}
- $\underline{s}$: entrywise (logistic) transfer function

$$\hat{y}_i = \underline{s}\left(W^{L+1}\underline{s}\left(W^L\left(\cdots \underline{s}\left(W^1 x_i\right)\right)\right)\right)$$

- **Many** hidden layers can be used: they are usually thought of as forming a hierarchy from low-level to high-level features.

Backpropagation



$$J = -\sum_{i=1}^{n} y_i \log h_i^{L+1} + (1-y_i)\log(1-h_i^{L+1})$$

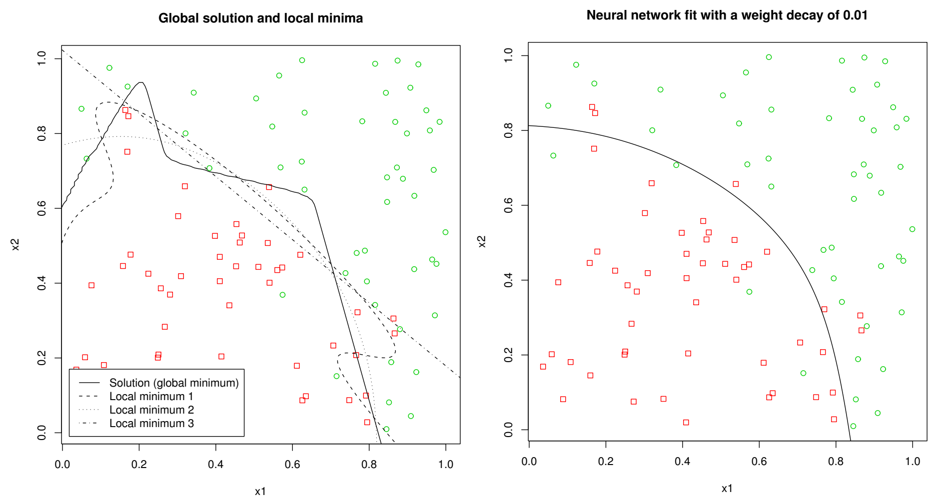
- Gradients wrt h_{ij}^{ℓ} computed by recursive applications of chain rule, and propagated through the network backwards.

$$\frac{\partial J}{\partial h_i^{L+1}} = -\frac{y_i}{h_i^{L+1}} + \frac{1-y_i}{1-h_i^{L+1}}$$

$$\frac{\partial J}{\partial h_{ij}^{\ell}} = \sum_{r=1}^{m} \frac{\partial J}{\partial h_{ir}^{\ell+1}} \frac{\partial h_{ir}^{\ell+1}}{\partial h_{ij}^{\ell}}$$

$$\frac{\partial J}{\partial w_{jk}^{\ell}} = \sum_{i=1}^{n} \frac{\partial J}{\partial h_{ij}^{\ell}} \frac{\partial h_{ij}^{\ell}}{\partial w_{jk}^{\ell}}$$

Neural Networks



R package implementing neural networks with a single hidden layer: `nnet`.

Neural Networks – Variations

- Other loss functions can be used, e.g. for regression:

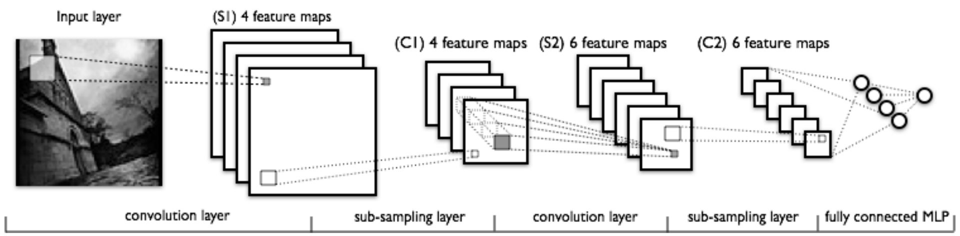
$$\sum_{i=1}^{n} |y_i - \hat{y}_i|^2$$

For multiclass classification, use **softmax** outputs:

$$\hat{y}_{ik} = \frac{\exp(b_k^o + \sum_\ell w_{\ell k}^o h_{i\ell})}{\sum_{k'} \exp(b_{k'}^o + \sum_\ell w_{\ell k'}^o h_{i\ell})} \qquad L(y_i, \hat{y}_i) = \sum_{k=1}^{K} \mathbb{1}(y_i = k) \log \hat{y}_{ik}$$

- Other activation functions can be used:
  - **rectified linear unit (ReLU)**: $s(z) = \max(0, z)$
  - **softplus**: $s(z) = \log(1 + \exp(z))$
  - **tanh**: $s(z) = \tanh(z)$

Deep Convolutional Neural Networks



- Input is a 2D image, $X \in \mathbb{R}^{p \times q}$.
- **Convolution**: detects simple object parts or features

$$A^m = s(X * W^m) \qquad A_{jk}^m = s\left(b^m + \sum_{fg} X_{j-f,k-g} W_{fg}^m\right)$$

Weights W^m now correspond to a **filter** to be learned - typically much smaller than the input thus encouraging sparse connectivity.

- **Pooling and Sub-sampling**: replace the output with a summary statistic of the nearby outputs, e.g. max-pooling (allows invariance to small translations in the input).

$$B_{jk}^m = \max\{A_{fg}^m : |f - j| \le w, |g - k| \le h\}$$

LeCun et al, Krizhevsky et al.

Dropout Training of Neural Networks

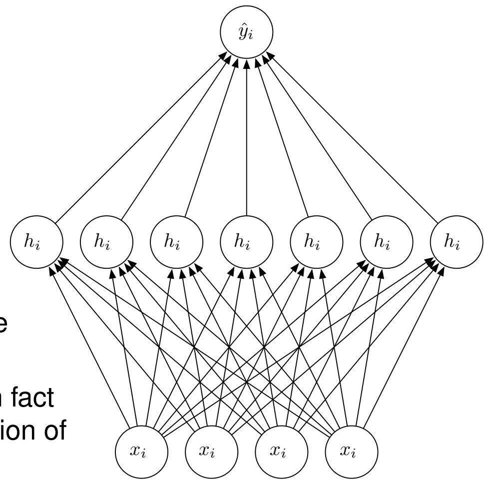
- Neural network with single layer of hidden units:
  - **Hidden unit activations**:

$$h_{ik} = s\left(b_k^h + \sum_{j=1}^{p} W_{jk}^h x_{ij}\right)$$

  - **Output probability**:

$$\hat{y}_i = s\left(b^o + \sum_{k=1}^{m} W_k^o h_{ik}\right)$$

- Large, overfitted networks often have co-adapted hidden units.
- What each hidden unit learns may in fact be useless, e.g. predicting the negation of predictions from other units.
- Can prevent co-adaptation by randomly **dropping out** units from network.

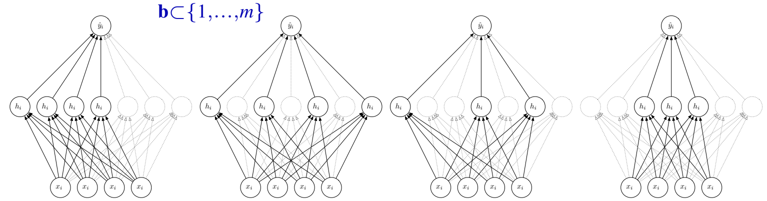


Hinton et al (2012).

Dropout Training of Neural Networks

- Model as an ensemble of networks:

$$p(y_i = 1|x_i, \theta) = \sum_{\mathbf{b} \subset \{1,\ldots,m\}} q^{|\mathbf{b}|}(1-q)^{m-|\mathbf{b}|} p(y_i = 1|x_i, \theta, \text{drop out units } \mathbf{b})$$



- **Weight-sharing** among all networks: each network uses a subset of the parameters of the full network (corresponding to the retained units).
- Training by stochastic gradient descent: at each iteration a network is sampled from ensemble, and its subset of parameters are updated.
- Biological inspiration: 10^{14} weights to be fitted in a lifetime of 10^9 seconds
  - Poisson spikes as a regularization mechanism which prevents co-adaptation: Geoff Hinton on Brains, Sex and Machine Learning

Dropout Training of Neural Networks

Classification of phonemes in speech.

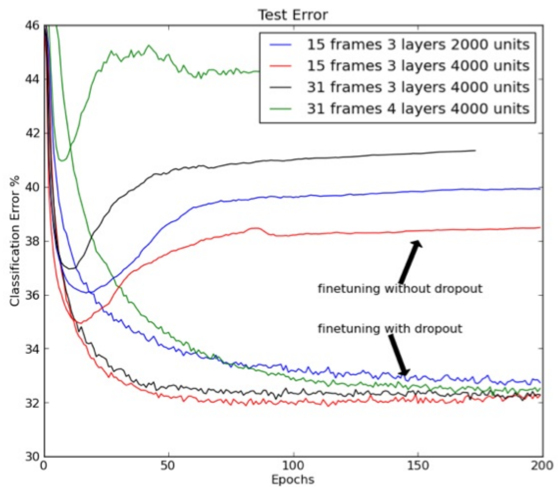


Figure from Hinton et al.

Neural Networks – Discussion

- Nonlinear hidden units introduce modelling flexibility.
- In contrast to user-introduced nonlinearities, features are global, and can be learned to maximize predictive performance.
- Neural networks with a single hidden layer and sufficiently many hidden units can model arbitrarily complex functions.
- Highly flexible framework, with many variations to solve different learning problems and introduce domain knowledge.
- Optimization problem is **not convex**, and objective function can have many local optima, plateaus and ridges.
- On large scale problems, often use **stochastic gradient descent**, along with a whole host of techniques for optimization, regularization, and initialization.
- Explosion of interest in the field recently and **many new developments** not covered here, especially by Geoffrey Hinton, Yann LeCun, Yoshua Bengio, Andrew Ng and others. See also `http://deeplearning.net/`.