Machine Learning

Weeks 7 & 8: Artificial Neural Networks

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Autumn Semester 2016/17

Overview of Lecture

- Rapid summary of work so far...
- Non-linear class boundaries (fixed non-linear parts)
  - Quadratic discriminant function
  - Radial basis functions
- Multi-layer perceptron
  - Error back-propagation algorithm
  - Speed-up tricks
  - Over-fitting and regularization

Summary $W1 \rightarrow W6$

- Mult-variate Gaussian: $p(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{m}, \boldsymbol{C})$ $\leftarrow$ Lab 1
- Bayesian decision theory: $P[\omega_j]$, $p(\boldsymbol{x}|\omega_j)$, $P[\omega_j|\boldsymbol{x}]$
- Optimal classifiers and posterior probabilities under specific assumtions
  - Linear and quadratic $\leftarrow$ Lab 3
  - Distance to means (Euclidean $|\boldsymbol{x} - \boldsymbol{m}_1|$ and Mahalanobis $(\boldsymbol{x} - \boldsymbol{m}_1)^t \boldsymbol{C}^{-1}(\boldsymbol{x} - \boldsymbol{m}_1)$)
- Linear discriminant functions
  - Perceptron algorithm and convergence analysis $\leftarrow$ Lab 2
  - Fisher linear discriminant $\leftarrow$ Lab 3
- Implementing Classifiers
  - Nearest Neighbour, Quantifying performance of classifiers (ROC) $\leftarrow$ Lab 3
  - Cross validation and uncertainty in results. $\leftarrow$ Lab 4
- Linear Regression: $\min |\boldsymbol{Ya} - \boldsymbol{f}|^2$
  - Pseudo-inverse: $\boldsymbol{a} = (\boldsymbol{Y}^t\boldsymbol{Y})^{-1}\boldsymbol{Y}^t\boldsymbol{f}$; Gradient search: $\boldsymbol{a}^{(k+1)} \leftarrow \boldsymbol{a}^{(k)} - \eta \nabla_a E$
  - Regularization $\leftarrow$ Lab 4
- Estimation: Maximum likelihood and Bayesian estimation
- Unsupervised learning
  - PCA, Derivation of PCA using Lagrange multipliers $\leftarrow$ Lab 1
  - Mixture Gaussian: $p(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, EM and K-Means clustering

Radial Basis Functions

- We fix nonlinear part in a data-dependent way
- Estimate only a linear part (by linear regression)

The Model:

$$g(\mathbf{x}) = \sum_{j=1}^{M} \lambda_j \, \phi\left(|\boldsymbol{x} - \boldsymbol{m}_j| \,/\, \sigma\right)$$

- We think of *centers* $\boldsymbol{m}_j$ in the input space
- *'Radial'* comes from distances to these centers (scaled by σ)
- We refer to $\phi(.)$ as basis functions
- Note similarity to Fourier transform – signal expressed as sum of sine waves (basis functions)
- $\boldsymbol{m}_j$, $j = 1, .., M$, σ and the functional form of $\phi(.)$ are fixed by some sensible (*ad hoc*) way
- λ_j, $j = 1, .., M$ are the unknowns

Radial Basis Functions (cont'd)

- Data is $\{\boldsymbol{x}_n,\ f_n\}_{n=1}^{N}$
- Similar to linear regression, we will hope to achieve

$$\begin{aligned} f_n &= g\left(\boldsymbol{x}_n\right) \\ &= \sum_{j=1}^{M} \lambda_j\, \phi\left(|\, \boldsymbol{x}_n - \boldsymbol{m}_j\, |\, /\, \sigma\right) \end{aligned}$$

- *i.e.* at each input $\boldsymbol{x}_n$, the function should output our target f_n
- Usually, $M < N$ *i.e.* we have fewer basis functions than there are items of data

Radial basis functions (cont'd)

What basis functions?

- Linear: $\phi(\alpha) = \alpha$
- Gaussian: $\phi(\alpha) = \exp(-\alpha^2/\sigma^2)$
- Multi-quadric: $\phi(\alpha) = \sqrt{1+\alpha^2}$
- Thin plate splines: $\phi(\alpha) = \alpha^2 \log(\alpha)$

- Gaussian very popular in practice
  - Local basis functions
  - $\boldsymbol{m}_j$ obtained by clustering

Radial basis functions (cont'd): Estimating λ_j

- $N \times M$ matrix Y

$$\begin{bmatrix} \phi(|\boldsymbol{x}_1 - \boldsymbol{m}_1|/\sigma) & \phi(|\boldsymbol{x}_1 - \boldsymbol{m}_2|/\sigma) & \dots & \phi(|\boldsymbol{x}_1 - \boldsymbol{m}_M|/\sigma) \\ \phi(|\boldsymbol{x}_2 - \boldsymbol{m}_1|/\sigma) & \phi(|\boldsymbol{x}_2 - \boldsymbol{m}_2|/\sigma) & \dots & \phi(|\boldsymbol{x}_2 - \boldsymbol{m}_M|/\sigma) \\ \vdots & \vdots & \dots & \vdots \\ \phi(|\boldsymbol{x}_N - \boldsymbol{m}_1|/\sigma) & \phi(|\boldsymbol{x}_N - \boldsymbol{m}_2|/\sigma) & \dots & \phi(|\boldsymbol{x}_N - \boldsymbol{m}_M|/\sigma) \end{bmatrix}$$

- Targets $N \times 1$ vector

$$\begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{bmatrix}$$

- Minimize error

$$\widehat{\boldsymbol{\lambda}} = \min_{\lambda} |Y \boldsymbol{\lambda} - \boldsymbol{f}|^2$$

- Solution similar to linear regression; e.g. pseudo inverse

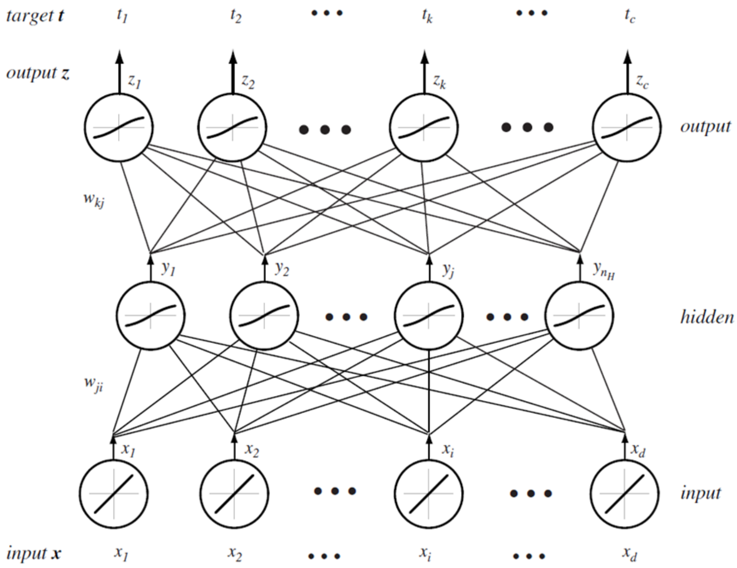
$$\widehat{\boldsymbol{\lambda}} = (Y^T Y)^{-1} Y^T \boldsymbol{f}$$

- Clustering and other rules to set $\boldsymbol{m}_j$ and σ

Lab Five: from 12 November

- Implement your own RBF
- Boston housing problem and a problem of your choice
- Compare with linear regression
- Cross validation to evaluate uncertainty
- Comparisons on out-of-sample data

Multi-layer perceptron



$$g_k(\boldsymbol{x}) = f\left(\sum_{j=1}^{n_H} w_{jk}\, f\left(\sum_{i=1}^{d} w_{ji}\, x_i + w_{j0}\right) + w_{k0}\right)$$

Each unit is a logistic

- Weighted sum of inputs – net activation

$$\mathrm{net}_j = \sum_{i=1}^{d} x_i\, w_{ji} + w_{j0}$$

- Squashed by a nonlinearity

$$y_j = f\left(\mathrm{net}_j\right)$$

- Simple threshold

$$f(\mathrm{net}) = \begin{cases} 1 & \text{if net} \geq 0 \\ -1 & \text{if net} < 0 \end{cases}$$

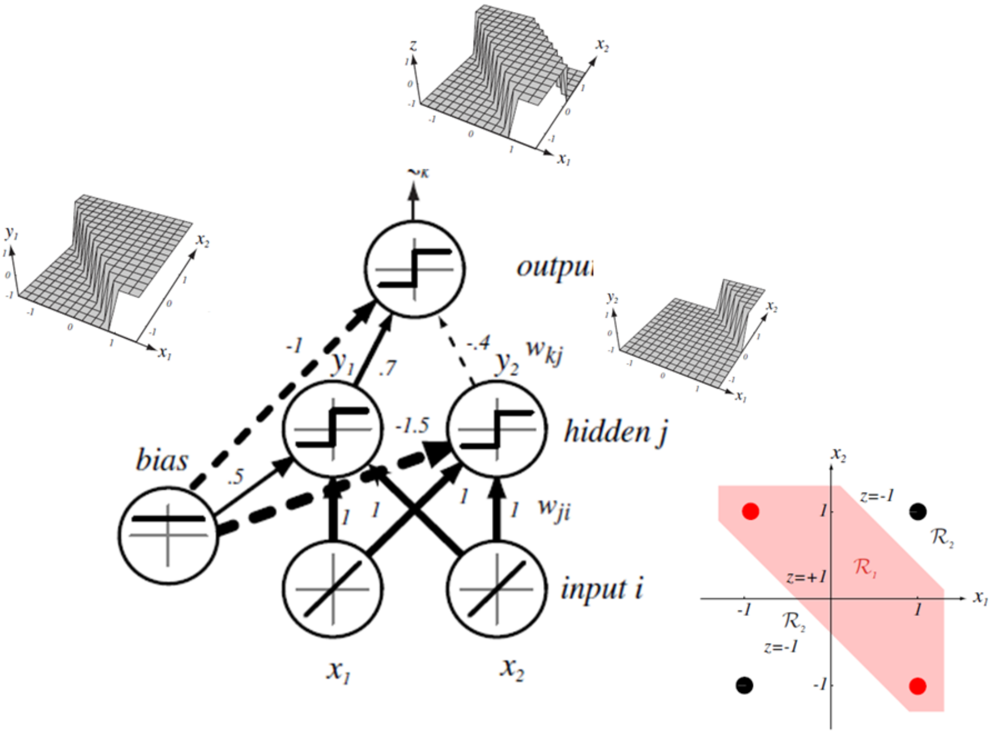
- Sigmoid (logistic)

$$f(\mathrm{net}) = \frac{1}{1 + \exp(-\mathrm{net})}$$

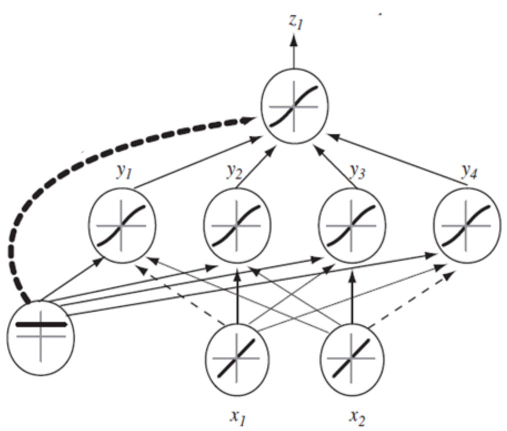
- Hyperbolic tangent

$$\begin{aligned} f(\mathrm{net}) &= \tanh(b\,\mathrm{net}) \\ &= \left[\frac{\exp(b\,\mathrm{net}) - \exp(-b\,\mathrm{net})}{\exp(b\,\mathrm{net}) + \exp(-b\,\mathrm{net})}\right] \end{aligned}$$

XOR Using a MLP



MLP Constructing Complex Functions



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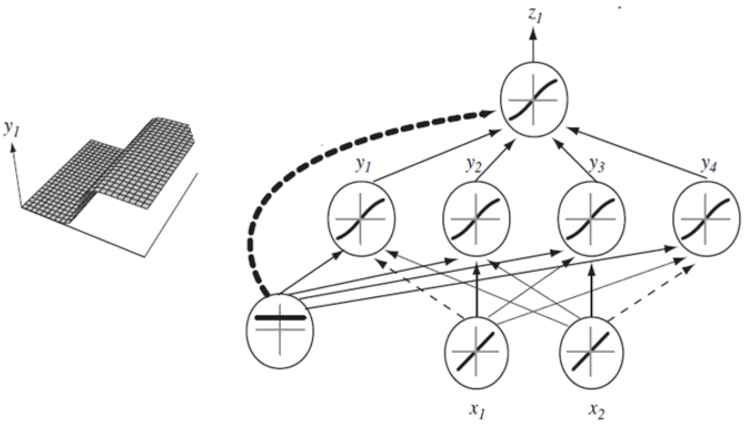

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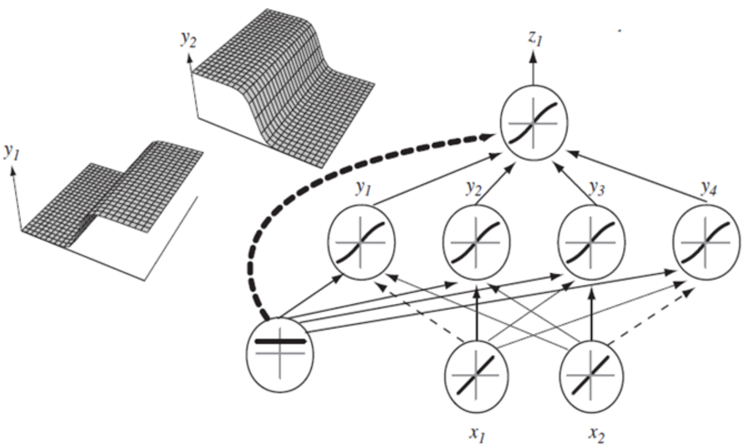

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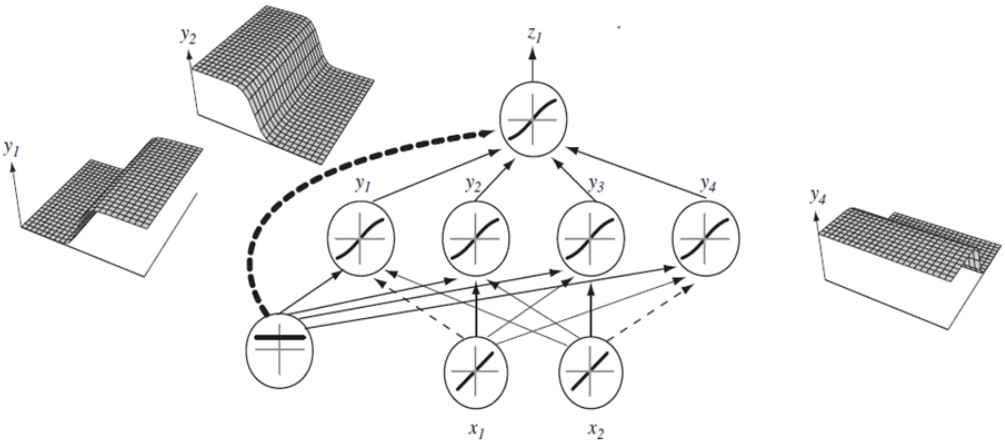

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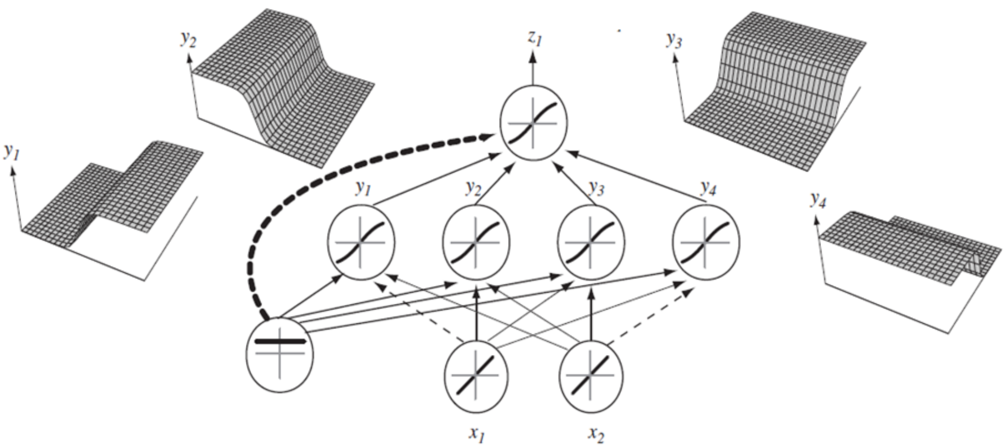

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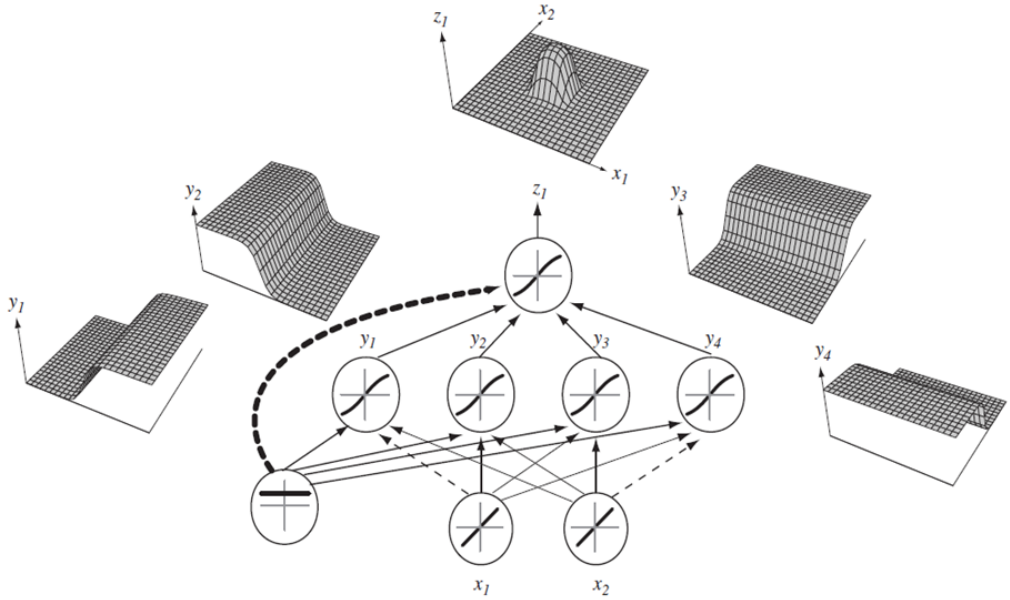
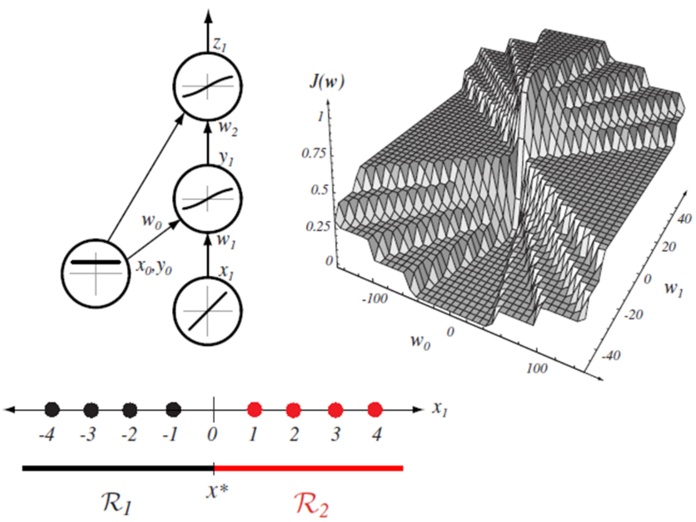


Error Function for MLP



- Not smooth and quadratic like for the linear model
- Large variation in gradient
- Local minima
- Gradient descent training with clever tricks

Training Multi-Layer Neural Networks

Error Back-propagation algorithm

- Error

$$J(\mathbf{w}) = \frac{1}{2}\sum_{k=1}^{c}(t_k - z_k)^2 = \frac{1}{2}||\mathbf{t} - \mathbf{z}||^2$$

- Change in weight for gradient descent

$$\Delta\mathbf{w} = -\eta\frac{\partial J}{\partial \mathbf{w}}$$

Or in component form

$$\Delta w_{pq} = -\eta\frac{\partial J}{\partial w_{pq}}$$

- Gradient descent update

$$\mathbf{w}(m+1) = \mathbf{w}(m) + \Delta\mathbf{w}(m)$$

Error Back Propagation Algorithm

- Hidden to output layer weights

$$\frac{\partial J}{\partial w_{kj}} = \frac{\partial J}{\partial \mathrm{net}_k}\frac{\partial \mathrm{net}_k}{\partial w_{kj}} = -\delta_k\frac{\partial \mathrm{net}_k}{\partial w_{kj}}$$

where, change in error with respect to the activation of the unit,

$$\delta_k = -\frac{\partial J}{\partial \mathrm{net}_k}$$

  - Easy form for δ_k

$$\delta_k = -\frac{\partial J}{\partial \mathrm{net}_k} = -\frac{\partial J}{\partial z_k}\frac{\partial z_k}{\partial \mathrm{net}_k} = (t_k - z_k)\, f'(\mathrm{net}_k)$$

    Error at output $\times$ slope of nonlinearity
  - Also with respect to weights net is differentiated easily

$$\frac{\partial \mathrm{net}_k}{\partial w_{kj}} = y_j$$

Error back propagation (cont'd)

- Units internal to the network have no explicit error signal
- Chain rule of differentiation helps!

$$\frac{\partial J}{\partial w_{ji}} = \frac{\partial J}{\partial y_j}\,\frac{\partial y_j}{\partial \mathrm{net}_j}\,\frac{\partial \mathrm{net}_j}{\partial w_{ji}}$$

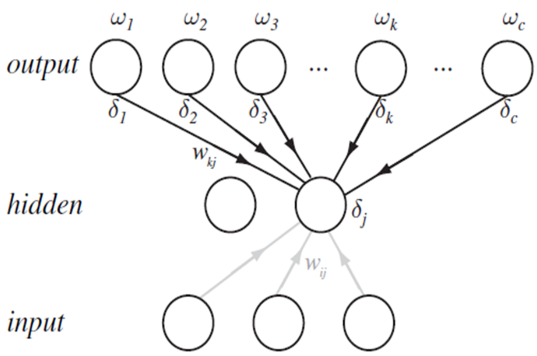
$$\begin{aligned}
\frac{\partial J}{\partial y_j} &= \frac{\partial}{\partial y_j}\left[\frac{1}{2}\sum_{k=1}^{c}(t_k - z_k)^2\right] \\
&= -\sum_{k=1}^{c}(t_k - z_k)\,\frac{\partial z_k}{\partial y_j} \\
&= -\sum_{k=1}^{c}(t_k - z_k)\,\frac{\partial z_k}{\partial \mathrm{net}_k}\,\frac{\partial \mathrm{net}_k}{\partial y_j} \\
&= -\sum_{k=1}^{c}(t_k - z_k)\,f'(\mathrm{net}_k)\,w_{kj}
\end{aligned}$$

Error propagation (cont'd)

$$\delta_j = f'(\mathrm{net}_j)\sum_{k=1}^{c} w_{kj}\,\delta_k$$

and the update rule

$$\delta w_{ji} = \eta\, x_i\, \delta_j = \eta\left[\sum_{k=1}^{c} w_{kj}\delta_k\right] f'(\mathrm{net}_j)\, x_i$$



- Signal y_j propagates forward
- δ_j's propagate backwards

- Having gradient enables us to update weights
- Can sum over all data and update with true gradient
- Or use sample-by-sample stochastic update
- Gradient descent can be slow (large flat regions)
- Can get stuck in local minima

Speeding-up Training: Newton's Method

Taylor expansion

$$J(\boldsymbol{w} + \Delta \boldsymbol{w}) = J(\boldsymbol{w}) + \left(\frac{\partial J(\boldsymbol{w})}{\partial \boldsymbol{w}}\right)^T \Delta \boldsymbol{w} + \frac{1}{2} \Delta \boldsymbol{w}^T H \Delta w + \ldots$$

- We can consider the change in objective function

  $$\Delta J(\boldsymbol{w}) = J(\boldsymbol{w} + \Delta \boldsymbol{w}) - J(\boldsymbol{w})$$

  and ask for what $\Delta \boldsymbol{w}$ is this minimized?

  $$\left(\frac{\partial J(\boldsymbol{w})}{\partial \boldsymbol{w}}\right) + H \Delta \boldsymbol{w} = 0$$

  $$\Delta \boldsymbol{w} = - H^{-1} \left(\frac{\partial J(\boldsymbol{w})}{\partial \boldsymbol{w}}\right)$$

  ... giving us the update

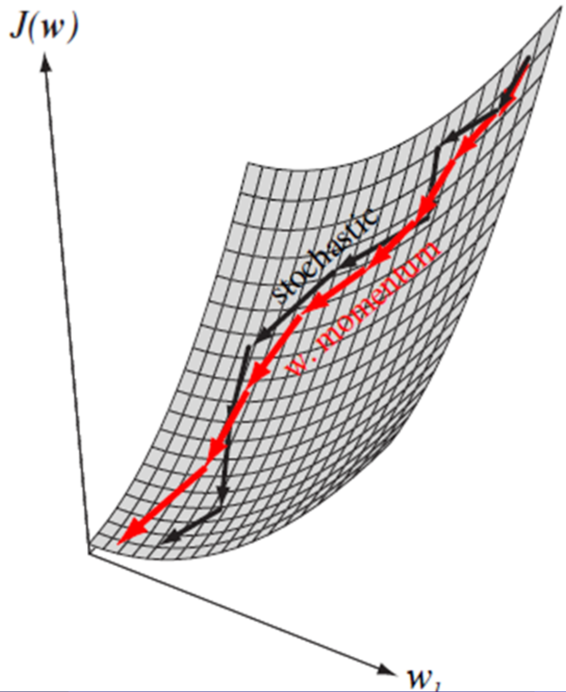
  $$\begin{aligned} \boldsymbol{w}(m+1) &= \boldsymbol{w}(m) + \Delta \boldsymbol{w} \\ &= \boldsymbol{w}(m) - H^{-1}(m) \left(\frac{\partial J(\boldsymbol{w}(m))}{\partial \boldsymbol{w}}\right) \end{aligned}$$

- However
  - N weights $\rightarrow$ N^2 storage for Hessian
  - Matrix inversion $\mathcal{O}(N^3)$ complexity

Momentum

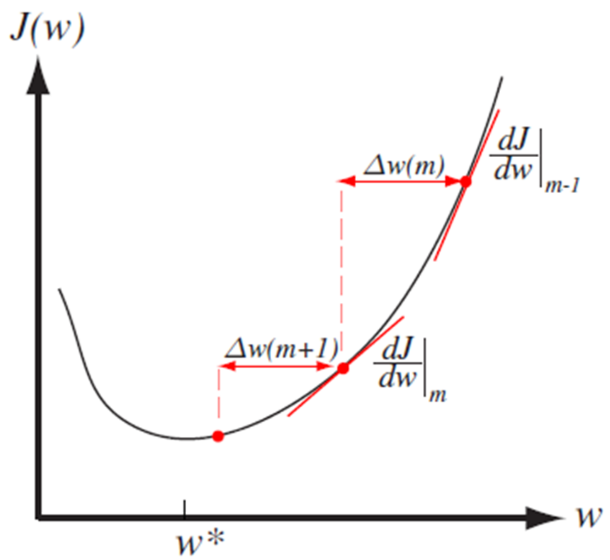
- Slow learning in regions in which gradient is small

$$\boldsymbol{w}(m+1) = \boldsymbol{w}(m) + (1-\alpha)\,\Delta \boldsymbol{w}_{\mathrm{BP}}(m) + \alpha\,\Delta \boldsymbol{w}(m-1)$$



QuickProp

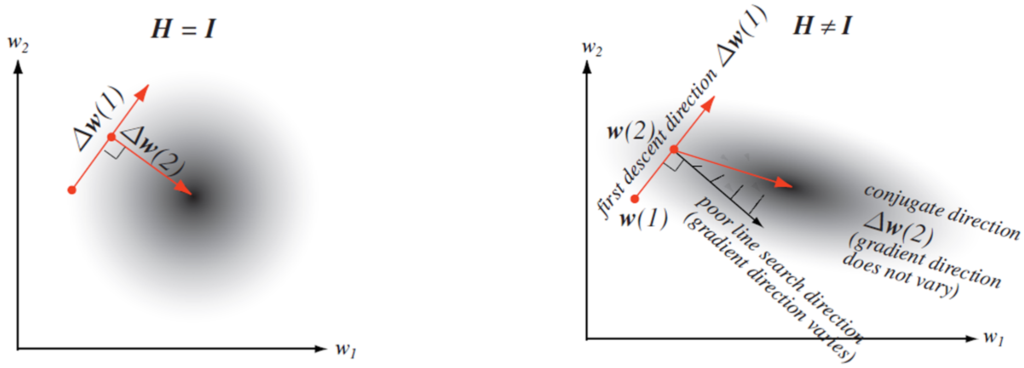
Two successive evaluations to approximate local curvature



$$\Delta w(m+1) = \frac{\partial J \,/\, \partial w\,|_m}{\partial J \,/\, \partial w\,|_{m-1} \;-\; \partial J \,/\, \partial w\,|_m}\,\Delta w(m)$$

Conjugate Gradients

- Sequence of line searches (not just gradient update)



Conjugate Gradients (cont'd)

- One dimensional line searches in multiple dimensions
- Careful choice of successive directions to search, informed by local curvature
- $\Delta \boldsymbol{w}(m-1)$ direction of line search at step $m-1$
- For new direction to search, find $\Delta \boldsymbol{w}$

$$\Delta \boldsymbol{w}^T(m-1)\, H\, \Delta \boldsymbol{w} \;=\; 0$$

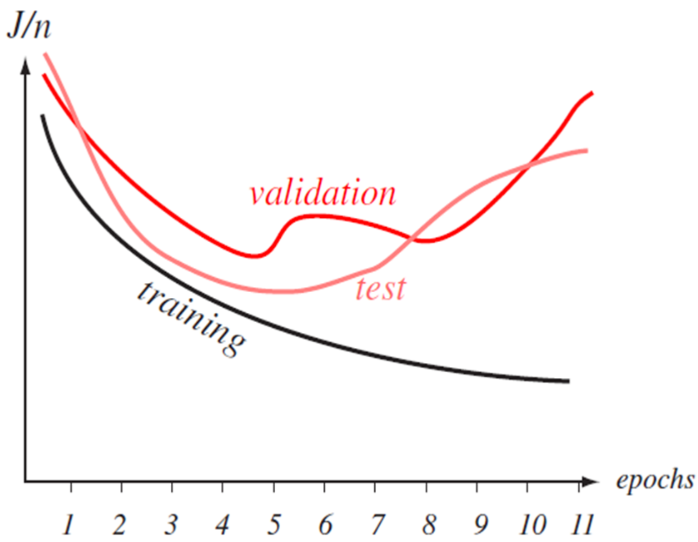
- Can be expressed as the gradient plus a component of previous search direction

$$\Delta \boldsymbol{w}(m) \;=\; \frac{\partial J(\boldsymbol{w}(m))}{\partial \boldsymbol{w}} + \beta_m\, \Delta \boldsymbol{w}(m-1)$$

- Need clever (approximate) way to set β_m: Fletcher-Reeves method

$$\beta_m \;=\; \frac{\nabla J^T(\boldsymbol{w}(m))\, \nabla J(\boldsymbol{w}(m))}{\nabla J^T(\boldsymbol{w}(m-1))\, \nabla J(\boldsymbol{w}(m-1))}$$

Performance on Out-of-Sample data



- Validation set to monitor error
- Stop (early) when validation error begins to increase

MLP As Posterior Probability Estimator

- Recall Bayes' decision

$$P[\omega_k|\mathbf{x}] = \frac{p(\mathbf{x}|\omega_k)\, p[\omega_k]}{\sum_{i=1}^{c} p(\mathbf{x}|\omega_i)\, p[\omega_i]}$$

- Suppose we train a neural net with c outputs

$$t_k(\mathbf{x}) = \begin{cases} 1 \text{ if } \mathbf{x} \in \omega_k \\ 0 \text{ otherwise} \end{cases}$$

- Mininimising the error

$$\sum_{\mathbf{x}} [g_k(\mathbf{x}, \mathbf{w} - t_k]^2$$

when we have infinite data, can be shown to be the same as minimizing

$$\sum_{k=1}^{c} \int [g_k(\mathbf{x}, \mathbf{w}) - P(\omega_k|\mathbf{x})]\; p(\mathbf{x})\, d\mathbf{x}$$

Summary

- Linear discriminant functions / regression (limited scope)
- Nonlinear models
  - More powerful
  - Difficult to train
- Some clever tricks
  - Variants of gradient descent
  - Fixed non-linear, variable linear models
- Estimators of $P[\omega_j \mid \boldsymbol{x}]$

What next:

- Coursework on MLP
  - How well does it approximate posterir probabilities?
  - How do we model time series?
- Guest lecture: Deep Neural Networks