Machine Learning: Foundations

(NGCM Introductory Course)

Mahesan Niranjan

School of Electronics and Computer Science
University of Southampton

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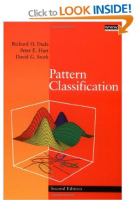
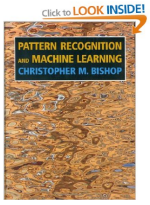
Good Books

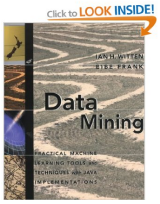
Well worth investing in books if you want to do more in this subject



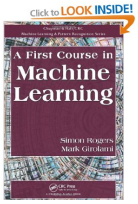
R.O.Duda, P.E.Hart & D.G.Stork
Pattern Classification



C.M. Bishop
Pattern Recognition and Machine Learning



I.H. Witten & E. Frank
Data Mining



S. Rogers & M. Girolami
A First Course in Machine Learning

"There is nothing to be learnt from a professor, which is not to be met with in books"
- David Hume (1711-1776)

(**WikiPedia:** "Hume had little respect for the professors of his time [...] He did not graduate")

Machine Learning as Data-driven Modelling

Data	$\{\boldsymbol{x}_n,\ \boldsymbol{y}_n\}_{n=1}^N \qquad \{\boldsymbol{x}_n\}_{n=1}^N$
Function Approximator	$\boldsymbol{y} = f(\boldsymbol{x}, \boldsymbol{\theta}) + v$
Parameter Estimation	$E_0 = \sum_{n=1}^N \{\|\| \boldsymbol{y}_n - f(\boldsymbol{x}_n; \boldsymbol{\theta}) \|\|\}^2$
Prediction	$\hat{\boldsymbol{y}}_{N+1} = f\left(\boldsymbol{x}_{N+1}, \hat{\boldsymbol{\theta}}\right)$
Regularization	$E_1 = \sum_{n=1}^N \{\|\| \boldsymbol{y}_n - f(\boldsymbol{x}_n) \|\|\}^2 + g(\|\|\boldsymbol{\theta}\|\|)$
Modelling Uncertainty	$p\left(\boldsymbol{\theta} \mid \{\boldsymbol{x}_n, \boldsymbol{y}_n\}_{n=1}^N\right)$
Probabilistic Inference	$\boldsymbol{E}[g(\boldsymbol{\theta})] = \int g(\boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta} = \frac{1}{N_s} \sum_{n=1}^{N_s} g\left(\boldsymbol{\theta}^{(n)}\right)$
Sequential Estimation	$\boldsymbol{\theta}(n-1\|n-1) \longrightarrow \boldsymbol{\theta}(n\|n-1) \longrightarrow \boldsymbol{\theta}(n\|n)$ Kalman & Particle Filters; Reinforcement Learning

Gaussian Densities: Univariate and Multivariate

- Univariate Gaussian

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2}\frac{(x-m)^2}{\sigma^2}\right\}$$

- Multivariate Gaussian

$$p(\boldsymbol{x}) = \frac{1}{(2\pi)^{p/2}(\det \boldsymbol{C})^{1/2}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{m})^t\, \boldsymbol{C}^{-1}\, (\boldsymbol{x}-\boldsymbol{m})\right\}$$

Mean $\boldsymbol{m}$ is a vector
Covariance, C, matrix: symmetric, positive definite!

$$\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{m}, \boldsymbol{C}),\ \boldsymbol{y} = \boldsymbol{A}\boldsymbol{x} \implies \boldsymbol{y} \sim \mathcal{N}(\boldsymbol{A}\boldsymbol{m}, \boldsymbol{A}\boldsymbol{C}\boldsymbol{A}^T)$$

Estimation

Univariate Mean	$\widehat{m} = \frac{1}{N}\sum_{n=1}^{N} x_n$
Univariate Covariance	$\widehat{\sigma} = \frac{1}{N}\sum_{n=1}^{N}(x_n - \widehat{m})^2$
Multivariate Mean	$\widehat{\boldsymbol{m}} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n$
Covariance Matrix	$\widehat{C} = \frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{x}_n - \boldsymbol{m})(\boldsymbol{x}_n - \boldsymbol{m})^T$

- These are known as maximum likelihood estimates (see later).

Bayesian Decision Theory

- Classes: $\omega_i,\ i = 1, ..., K$
- Prior Probabilities: $P[\omega_1], ..., P[\omega_K]$;
  $P[\omega_i] \geq 0, \quad \sum_{i=1}^{K} P[\omega_i] = 1$
- Likelihoods (class conditional probabilities): $p(\boldsymbol{x}|\omega_i),\ i = 1, .., K$
- Posterior Probability: $P[\omega_j \,|\, \boldsymbol{x}]$

$$P[\omega_j \,|\, \boldsymbol{x}] = \frac{p(\boldsymbol{x} \,|\, \omega_j)\ P[\omega_j]}{\sum_{i=1}^{K} p(\boldsymbol{x} \,|\, \omega_i)\ P[\omega_i]}$$

- From prior knowledge: $P[\omega_i]$; From traing data: $p(\boldsymbol{x}|\omega_i)$
- Decision rule: Assign $\boldsymbol{x}$ to the class that maximizes posterior probability.
- The denominator is a constant; *i.e.* does not depend on ω_j
- Hence the decision rule becomes:

$$\boldsymbol{x} \in \max_j p(\boldsymbol{x} \,|\, \omega_j)\ P[\omega_j]$$

Bayes' Classifier for Gaussian Densities

Make assumptions, cancel common terms when making comparisons...

- Decision rule from: $p(\boldsymbol{x} \mid \omega_j)\ P[\omega_j]$
- Assume the two classes are Gaussian distributed with distinct means and identical covariance matrices
  $p(\boldsymbol{x} \mid \omega_j) = \mathcal{N}(\boldsymbol{m}_j, \boldsymbol{C})$
- Substitute into Bayes' classifier decision rule

$$\begin{aligned} P[\omega_1|\boldsymbol{x}] &\lessgtr P[\omega_2|\boldsymbol{x}] \\ p(\boldsymbol{x}|\omega_1)\ P[\omega_1] &\lessgtr p(\boldsymbol{x}|\omega_2)\ P[\omega_2] \end{aligned}$$

$$\begin{aligned} &\frac{1}{(2\pi)^{p/2}(\det(C))^{1/2}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{m}_1)^t \boldsymbol{C}^{-1}(\boldsymbol{x}-\boldsymbol{m}_1)\right\} P[\omega_1] \lessgtr \\ &\frac{1}{(2\pi)^{p/2}(\det(C))^{1/2}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{m}_2)^t \boldsymbol{C}^{-1}(\boldsymbol{x}-\boldsymbol{m}_2)\right\} P[\omega_2] \end{aligned}$$

Bayes' classifier for simple densities (cont'd)

Distinct Means; Equal, isotropic covariance matrix

- Suppose the densities are isotropic and priors are equal
  i.e. $\boldsymbol{C} = \sigma^2 \boldsymbol{I}$ and $P[\omega_1] = P[\omega_2]$
- The comparison simplifies to (see algebra on board):

$$\begin{aligned} (\boldsymbol{x}-\boldsymbol{m}_1)^t(\boldsymbol{x}-\boldsymbol{m}_1) &\lessgtr (\boldsymbol{x}-\boldsymbol{m}_2)^t(\boldsymbol{x}-\boldsymbol{m}_2) \\ |\boldsymbol{x}-\boldsymbol{m}_1| &\lessgtr |\boldsymbol{x}-\boldsymbol{m}_2| \end{aligned}$$

- The above is a simple *distance to mean* classifier
- Under the above simplistic assumptions, we only need to store one template per class (the means)!

Bayes' classifier for simple densities (cont'd)

Distinct Means; Common covariance matrix (but not isotropic)

- Cancel common terms and take log

$$(\boldsymbol{x}-\boldsymbol{m}_1)^t\,\boldsymbol{C}^{-1}\,(\boldsymbol{x}-\boldsymbol{m}_1) \lessgtr (\boldsymbol{x}-\boldsymbol{m}_2)^t\,\boldsymbol{C}^{-1}\,(\boldsymbol{x}-\boldsymbol{m}_2) - \log\left\{\frac{P[\omega_1]}{P[\omega_2}\right\}$$

- Also simplifies to a linear classifier!

$$\boldsymbol{w}^t\,\boldsymbol{x} + b \lessgtr 0$$

$$\begin{aligned}\boldsymbol{w} &= 2\boldsymbol{C}^{-1}(\boldsymbol{m}_2-\boldsymbol{m}_1)\\ b &= \left(\boldsymbol{m}_1^t\boldsymbol{C}^{-1}\boldsymbol{m}_1 - \boldsymbol{m}_2^t\boldsymbol{C}^{-1}\boldsymbol{m}_2\right) - \log\left\{\frac{P[\omega_1]}{P[\omega_2]}\right\}\end{aligned}$$

- Also a distance to template classifier, where the distance is

$$(\boldsymbol{x}-\boldsymbol{m}_1)^t\,\boldsymbol{C}^{-1}\,(\boldsymbol{x}-\boldsymbol{m}_1)$$

  Known as Mahalanobis distance

Posterior probabilities for simple Gaussian cases

- Bayes classifier:

$$P[\omega_1|\boldsymbol{x}] = \frac{p(\boldsymbol{x}|\omega_1)\,P[\omega_1]}{p(\boldsymbol{x}|\omega_1)\,P[\omega_1] + p(\boldsymbol{x}|\omega_2)\,P[\omega_2]}$$

- Restrictive assumptions:
  - Gaussian $p(\boldsymbol{x}|\omega_j) = \mathcal{N}(\boldsymbol{m}_j, \boldsymbol{C}_j)$
  - Equal covariance matrices: $\boldsymbol{C}_1 = \boldsymbol{C}_2 = C$
- Substitute, divide through by numerator term and cancel common terms to get

$$P[\omega_1|\boldsymbol{x}] = \frac{1}{1+\exp\{-(\boldsymbol{w}^t\boldsymbol{x}+w_0)\}}$$

- The functional form $1/(1+\exp(-\alpha))$ is known as sigmoid / logistic.

Summary:

Bayesian decision theory is fundamental to machine learning; we started from a probabilistic setting in which we described the posterior probability of membership and derived several results starting from this premise:

- Under certain assumptions...
  - The class boundary is linear
  - The posterior probability has a sigmoidal shapedefault
  - The optimal classifier reduces to a distance to template classifier
- ...and under certain other assumptions...
  - The best classifier is still a distance to template classifier, but instead of Euclidean distance we need to use Mahalanobis distance.
- ...and under certain other assumptions...
  - The optimal classifier is a quadratic classifier

Fisher Linear Discriminant Analysis

- In the $p-$ dimensional ($\mathcal{R}^p$) input space, find a direction on which projected data is maximally separable:
  - Projected means should be far apart
  - Projected scatter of each class should be small
- Projection of $\boldsymbol{x}_n$ onto direction $\boldsymbol{w}$ is $\boldsymbol{w}^t\boldsymbol{x}_n$;
  - Projected mean for class j will be at $\boldsymbol{w}^t\boldsymbol{m}_j$
  - Variance of projections is $\boldsymbol{w}^t\boldsymbol{C}_j\boldsymbol{w}$, where $\boldsymbol{C}_j$ is the covariance matrix of data in class j.
- Fisher Ratio:

$$J_F = \frac{(\boldsymbol{w}^t\boldsymbol{m}_1 - \boldsymbol{w}^t\boldsymbol{m}_2)^2}{\boldsymbol{w}^t\boldsymbol{C}_1\boldsymbol{w} + \boldsymbol{w}^t\boldsymbol{C}_2\boldsymbol{w}}$$

- We can write the numerator as $\boldsymbol{w}^t\boldsymbol{C}_B\boldsymbol{w}$, where $\boldsymbol{C}_B = (\boldsymbol{m}_1 - \boldsymbol{m}_2)(\boldsymbol{m}_1 - \boldsymbol{m}_2)^t$, the between-class scatter matrix.
- $\boldsymbol{C}_W = \boldsymbol{C}_1 + \boldsymbol{C}_2$, the within class scatter matrix.

Fisher Linear Discriminant Analysis

- Fisher criterion to maximize

$$J(\boldsymbol{w}) = \frac{\boldsymbol{w}^t \boldsymbol{C}_B \boldsymbol{w}}{\boldsymbol{w}^t \boldsymbol{C}_W \boldsymbol{w}}$$

- Set gradient to zero

$$\nabla_{\boldsymbol{w}} = \frac{2\boldsymbol{C}_B\boldsymbol{w} \times (\boldsymbol{w}^t \boldsymbol{C}_W \boldsymbol{w}) - 2\boldsymbol{C}_W\boldsymbol{w} \times (\boldsymbol{w}^t \boldsymbol{C}_B \boldsymbol{w})}{(\boldsymbol{w}^t \boldsymbol{C}_W \boldsymbol{w})^2}$$

- Equate this to zero and observe
  - $\boldsymbol{w}^t\boldsymbol{C}_W\boldsymbol{w}$ and $\boldsymbol{w}^t\boldsymbol{C}_B\boldsymbol{w}$ are scalars
  - $\boldsymbol{C}_B\boldsymbol{w}$ points in the same direction as $\boldsymbol{m}_1 - \boldsymbol{m}_2$
  - We are only interested in the direction of $\boldsymbol{w}$

$$\boldsymbol{w}_F = \alpha\boldsymbol{C}_w^{-1}(\boldsymbol{m}_1 - \boldsymbol{m}_2)$$

Linear Regression & Perceptron

Formulation → derivation → solution

- Data: $\{\boldsymbol{x}_n,\ f_n\}_{n=1}^N$
  Input: $\boldsymbol{x}_n \in \mathcal{R}^p$; target / output f_n real valued
- Model: $f = \boldsymbol{w}^t\boldsymbol{x} + w_0$
  Output linear function of input (including a constant w_0)
- Work in $(p+1)$ dimensional space to avoid treating w_0 separately

$$\boldsymbol{y} = \begin{pmatrix} \boldsymbol{x} \\ 1 \end{pmatrix} \quad \boldsymbol{a} = \begin{pmatrix} \boldsymbol{w} \\ w_0 \end{pmatrix}$$

- Data: $\{\boldsymbol{y}_n,\ f_n\}_{n=1}^N$
- Model: $f = \boldsymbol{y}^t\boldsymbol{a}$
- $p+1$ unknowns held in vector $\boldsymbol{a}$

Error and Minimization

- $E = \sum_{n=1}^{N} \{\boldsymbol{y}_n^t \boldsymbol{a} - f_n\}^2$
- $E = \sum_{n=1}^{N} \left\{ \left(\sum_{j=1}^{(p+1)} a_j \, y_{nj} \right) - f_n \right\}^2$
- To find the best $\boldsymbol{a}$ we minimize E – differentiate with respect to each of the unknowns in $\boldsymbol{a}$ and set to zero.
- $$\frac{\partial E}{\partial a_i} = 2 \sum_{n=1}^{N} \left\{ \left(\sum_{j=1}^{(p+1)} a_j \, y_{nj} \right) - f_n \right\} (y_{ni})$$
- There are $(p+1)$ derivatives (with respect to each a_i)
- Equating them to zero gives $(p+1)$ equations in $(p+1)$ unknowns

Solution to Regression

- $(p+1)$ simultaneous equations to solve:
  i^{th} row, j^{th} column shown

$$\begin{pmatrix} & \cdots & \\ \cdots & \cdots & \cdots \\ \vdots & \sum_{n=1}^{N} y_{ni} y_{nj} & \cdots \\ \vdots & \cdots & \vdots \\ \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_{(p+1)} \end{pmatrix} = \begin{pmatrix} \vdots \\ \sum_{n=1}^{N} f_n y_{ni} \\ \vdots \end{pmatrix}$$

Derivation in vector/matrix form

- $\boldsymbol{Y}$: $N \times (p+1)$ matrix n^{th} row is $\boldsymbol{y}_n^t$
- $\boldsymbol{f}$: $N \times 1$ vector of outputs
- Error $E = ||\boldsymbol{Y}\,\boldsymbol{a} - \boldsymbol{f}||^2$
- Gradient

$$\nabla_{\boldsymbol{a}} E = 2\boldsymbol{Y}^t(\boldsymbol{Y}\boldsymbol{a} - \boldsymbol{f})$$

- Equating the gradient to zero gives

$$\begin{aligned} \boldsymbol{Y}^t\boldsymbol{Y}\boldsymbol{a} &= \boldsymbol{Y}^t\boldsymbol{f} \\ \boldsymbol{a} &= (\boldsymbol{Y}^t\boldsymbol{Y})^{-1}\,\boldsymbol{Y}^t\,\boldsymbol{f} \end{aligned}$$

Solution by Gradient Descent

- Gradient vector: $\nabla_{\boldsymbol{a}} E = 2\boldsymbol{Y}^t(\boldsymbol{Y}\boldsymbol{a} - \boldsymbol{f})$
- Steepest descent algorithm:

```
Initialize a at random
Update a^(k+1) = a^(k) − η ∇_a E
Until Convergence
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- Second order (Newton's) method

```
Initialize a at random
Update a^(k+1) = a^(k) − η H^{-1} ∇_a E
Until Convergence
```

- Rapid convergence with second order method, but cost of computing and inverting $\boldsymbol{H}$ can be high (more on this under Neural Networks)

Gradient and Stochastic Gradient Descent

- Error $E = \sum_{n=1}^{N} e_n^2$
- True gradient:

$$\nabla_{\boldsymbol{a}} E = 2 \sum_{n=1}^{N} \left\{ \mathbf{y_n^t a} - \mathbf{f_n} \right\} (\mathbf{y_n})$$

- Gradient computed on n^{th} data:

$$\nabla_{\boldsymbol{a}} e_n = 2 \left\{ \mathbf{y_n^t a} - \mathbf{f_n} \right\} (\mathbf{y_n})$$

Regularization

- Pseudo inverse solution: $\boldsymbol{a} = (\boldsymbol{Y}^t \boldsymbol{Y})^{-1} \boldsymbol{Y}^t \boldsymbol{f}$
- This can be ill conditioned, so we could *regularize* by

$$\boldsymbol{a} = \left(\boldsymbol{Y}^t \boldsymbol{Y} + \gamma \boldsymbol{I} \right)^{-1} \boldsymbol{Y}^t \boldsymbol{f}$$

  where γ is a small constant.
- We achieve precisely this by minimizing an error of the form

$$||\boldsymbol{Ya} - \boldsymbol{f}||^2 + \gamma ||\boldsymbol{a}||^2$$

  Here a quadratic penalty term has been included
- Homework: Differentiate this error and derive the regularized solution
- Sparse solutions are obtained by regularizing with an l_1 norm (sum of absolute values of $\boldsymbol{a}$, i.e. $\sum_{j=1}^{p} |a_j|$): Known as *Lasso*

Perceptron

- Number of misclassified examples as measure of error
  Piecewise constant (cannot differentiate)
- Suitable error measure:

$$E_P = -\sum \boldsymbol{y}_n^t \boldsymbol{a}$$

  - Summation taken over misclassified examples
  - We started with $\boldsymbol{y}_n^t \boldsymbol{a} > 0$ for positive class and $\boldsymbol{y}_n^t \boldsymbol{a} < 0$ for the negative class; we then switch the signs of negative class examples and required $\boldsymbol{y}_n^t \boldsymbol{a} > 0$ for all the training data; so for the misclassified examples $-\sum \boldsymbol{y}_n^t \boldsymbol{a}$ should be as small as possible.

Perceptron

Learning rule

- Gradient:

$$\frac{\partial E}{\partial \boldsymbol{a}} = -\sum \boldsymbol{y}_n$$

- Gradient algorithm: $\boldsymbol{a}^{(k+1)} = a^{(k)} + \sum \boldsymbol{y}_n$
- Stochastic gradient algorithm:

$$\boldsymbol{a}^{(k+1)} = a^{(k)} + \boldsymbol{y}_n$$

- Note what $\boldsymbol{y}_n$ is. It is an item of data that is taken at random and happens to be misclassified by the current value of $\boldsymbol{a}$ at iteration k.

Perceptron

Convergence of the learning rule

- Learning Rule: $\boldsymbol{a}^{(k+1)} = \boldsymbol{a}^{(k)} + \boldsymbol{y}(k)$
  where $\boldsymbol{y}(k)$ is a misclassified input.
- Training criterion
  - We start with requiring $\boldsymbol{a}^t\,\boldsymbol{y}(k) \leqslant 0$, depending on the example belonging to class 1 or class 2.
  - If we switch the signs of examples of class 2, we require $\boldsymbol{a}^t\,\boldsymbol{y}(k) > 0$ for all k.
- On misclassified data $\boldsymbol{a}^t\,\boldsymbol{y}(k) < 0$
- If $\widehat{\boldsymbol{a}}$ is a solution (separable data), for all k, $\widehat{\boldsymbol{a}}\,\boldsymbol{y}(k) > 0$
- We prove convergence by showing:
  $||\boldsymbol{a}^{(k+1)} - \widehat{\boldsymbol{a}}||^2 < ||\boldsymbol{a}^{(k)} - \widehat{\boldsymbol{a}}||^2$ for this update rule. *i.e.* the learning rule brings the guess closer to a valid solution.

Perceptron

Convergence of the learning rule (cont'd)

- For perceptron criterion, the magnitude of $\boldsymbol{a}$ is not relevant (only the direction is). Hence for some scalar α, we wish to show

$$||\boldsymbol{a}^{(k+1)} - \alpha\,\widehat{\boldsymbol{a}}||^2 < ||\boldsymbol{a}^{(k)} - \alpha\,\widehat{\boldsymbol{a}}||^2$$

- From the update formula

$$\boldsymbol{a}^{(k+1)} - \alpha\,\widehat{\boldsymbol{a}} = \boldsymbol{a}^{(k)} - \alpha\,\widehat{\boldsymbol{a}} + \boldsymbol{y}(k)$$

- Taking magnitudes

$$||\boldsymbol{a}^{(k+1)} - \alpha\widehat{\boldsymbol{a}}||^2 = ||\boldsymbol{a}^{(k)} - \alpha\widehat{\boldsymbol{a}}||^2 + 2(\boldsymbol{a}^{(k)} - \alpha\widehat{\boldsymbol{a}})^t\boldsymbol{y}(k) + ||\boldsymbol{y}(k)||^2$$

- If we drop the negative term ${\boldsymbol{a}^{(k)}}^t\boldsymbol{y}(k)$ from RHS, the equality becomes an inequality

$$||\boldsymbol{a}^{(k+1)} - \alpha\widehat{\boldsymbol{a}}||^2 < ||\boldsymbol{a}^{(k)} - \alpha\widehat{\boldsymbol{a}}||^2 - 2\alpha\widehat{\boldsymbol{a}}^t\boldsymbol{y}(k) + ||\boldsymbol{y}(k)||^2$$

Perceptron

Convergence of the learning rule (cont'd)

- Of the three terms on the right hand side, we know $\widehat{\boldsymbol{a}}^t \boldsymbol{y}(k) > 0$, because $\widehat{\boldsymbol{a}}$ is assumed to be a solution.
- If we select

$$\beta^2 = \max_i ||\boldsymbol{y}_i||^2 \quad \gamma = \min_i \widehat{\boldsymbol{a}}^t \boldsymbol{y}_i$$

i.e. largest of the positive term and smallest of the negative term, then for $\alpha = \beta^2/\gamma$,

$$||\boldsymbol{a}^{(k+1)} - \alpha\widehat{\boldsymbol{a}}||^2 < ||\boldsymbol{a}^{(k)} - \alpha\widehat{\boldsymbol{a}}||^2 - \beta^2$$

- (Note the inequality remains true when the right hand side is replaced by a quantity larger than what it previously was.)
- Every correction takes the guess closer to a true solution.
- From an initialization $\boldsymbol{a}^{(1)}$, we will find a solution in *at most* $k_0 = \frac{||\boldsymbol{a}(1) - \alpha\widehat{\boldsymbol{a}}||^2}{\beta^2}$ updates.

Estimation

Maximum likelihood on simple examples

- We have data $\boldsymbol{x}_k$
- We have a model: *e.g.* the data came from a Gaussian density
- We have parameters relating to the model: *e.g.* mean of the Gaussian
- Our task is to estimate the parameters given the data
- Frequentist thought
  - The given data is a particular realization of the underlying system
  - Repeated experiments will give different estimates
  - If each experiment uses a lot of data, the variation may be small
  - We define a probabilistic model and maximize likelihood
  - Bias and Variance in estimation
- Bayesian thought
  - We are interested in the uncertainty in parameters
  - We have a prior uncertainty
  - There is some information in the data
  - We combine these to get a posterior uncertainty

Likelihood & Log likelihood

- $p(\boldsymbol{x} \mid \omega_j)$
- Parametric form $p(\boldsymbol{x} \mid \omega_j, \boldsymbol{\theta}_j)$
  For example
$$p(\boldsymbol{x} \mid \omega_j, \boldsymbol{\theta}_j) = \mathcal{N}(\boldsymbol{m}_j, \boldsymbol{C}_j)$$

- Dataset $\mathcal{D} = \boldsymbol{x}_1, \boldsymbol{x}_2, ..., \boldsymbol{x}_n$ of identical and independently distributed samples (iid)
  - All samples were drawn from this distribution
  - Independent draws (previous value does not affect the next draw)
- Likelihood of an item of data (function of the parameter!)
$$p(\boldsymbol{x}_k|\boldsymbol{\theta})$$
- Likelihood of the set of data
$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{i=1}^{n} p(\boldsymbol{x}_k|\boldsymbol{\theta})$$
- Log likelihood
$$l(\boldsymbol{\theta}) = \ln p(\mathcal{D}|\boldsymbol{\theta})$$

Maximum Likelihood

- Maximum likelihood
$$\widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} l(\boldsymbol{\theta})$$
- Maximize by taking derivative
$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} = \begin{bmatrix} \frac{\partial}{\partial \theta_1} \\ \vdots \\ \frac{\partial}{\partial \theta_n} \end{bmatrix}$$
$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} l = \sum_{k=1}^{n} \boldsymbol{\nabla}_{\boldsymbol{\theta}} p(\mathcal{D}|\boldsymbol{\theta})$$

... and equating to zero
$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} l = \mathbf{0}.$$

... and solve for the unknown parameter values.

Example: Multivariate Gaussian $\mathcal{N}(\boldsymbol{m}, C)$

Mean unknown, (Covariance known)

- ... product of Gaussians; taking log removes exp and turns $\prod$ into $\sum$
- ... write it out for a single data point

$$\ln\, p\left(\boldsymbol{x}_k|\boldsymbol{m}\right) \;=\; \frac{1}{2}\ln(2\pi)^d \det C \;-\; \frac{1}{2}\left(\boldsymbol{x}_k-\boldsymbol{m}\right)^T\; C^{-1}\; \left(\boldsymbol{x}_k-\boldsymbol{m}\right)$$

- ... the derivative

$$\boldsymbol{\nabla}_{\boldsymbol{m}} \ln p\left(\boldsymbol{x}_k|\boldsymbol{m}\right) \;=\; C^{-1}\left(\boldsymbol{x}_k-\boldsymbol{m}\right)$$

- Given n data $\boldsymbol{x}_1, ..., \boldsymbol{x}_n$

$$\sum_{k=1}^{n} C^{-1}\left(\boldsymbol{x}_k-\widehat{\boldsymbol{m}}\right) \;=\; \mathbf{0}$$

- and the solution is...

$$\widehat{\boldsymbol{m}} \;=\; \frac{1}{n}\sum_{k=1}^{n} \boldsymbol{x}_k$$

Example: Univariate Gaussian $\mathcal{N}(m, \sigma^2)$

(Mean and variance unknown)

- Two parameters: $\theta_1 = m$ and $\theta_2 = \sigma^2$
- Log likelihood of a single data:

$$\ln p\left(x_k|\boldsymbol{\theta}\right) \;=\; \frac{1}{2}\ln 2\pi\theta_2 \;-\; \frac{1}{2\theta_2}(x_k-\theta_1)^2$$

- Derivative of the log likelihood

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} p\left(x_k|\boldsymbol{\theta}\right) \;=\; \begin{bmatrix} \frac{1}{\theta_2}\left(x_k-\theta_1\right)^2 \\ -\frac{1}{2\theta_2} \;+\; \frac{(x_k-\theta_1)^2}{2\theta_2^2} \end{bmatrix}$$

- Given n data $x_1, x_2, ..., x_n$, and considering the full log likelihood

$$\begin{aligned} \sum_{k=1}^{n} \frac{1}{\widehat{\theta}_2}\left(x_k-\widehat{\theta}_1\right) \;&=\; 0 \\ -\sum_{k=1}^{n} \frac{1}{\widehat{\theta}_2} + \sum_{k=1}^{n} \frac{1}{\widehat{\theta}_2^2}\left(x_k-\widehat{\theta}_1^2\right)^2 \;&=\; 0 \end{aligned}$$

Example

Univariate Gaussian, unknown mean and variance (cont'd)

- ... after some algebra

$$\widehat{m} = \frac{1}{n}\sum_{k=1}^{n} x_k$$

$$\widehat{\sigma}^2 = \frac{1}{n}\sum_{k=1}^{n}(x_k - \widehat{m})^2$$

- If we did this estimation from several datasets...

$$E\left[\frac{1}{n}\sum_{k=1}^{n}(x_k - \bar{x})^2\right] = \frac{n-1}{n}\sigma^2 \neq \sigma^2$$

  expected value of estimate is not the same as the true value!

For the multivariate Gaussian, we have seen the results:

$$\widehat{\boldsymbol{m}} =$$

$$\widehat{C} =$$

Bayesian Estimation

- Data: $\mathcal{D}$: $x_1, ...x_n$
- Likelihood (as seen before) $p(x|m) \sim \mathcal{N}(m, \sigma^2)$
- Prior uncertainty over parameters: $p(m) \sim \mathcal{N}(m_0, \sigma_0^2)$
  m_0 and σ_0^2 are known.
- Posterior via Bayes' formula

$$p(m|\mathcal{D}) = \frac{p(\mathcal{D}|m)p(m)}{\int p(\mathcal{D}|m)\, p(m)\, dm}$$

  Denominator is a constant, so we deal with

$$p(m|\mathcal{D}) = \alpha \prod_{k=1}^{n} p(x_k|m)\, p(m)$$

- Two ways forward from here
  - Maximum *a posteriori* estimation
  - Inference by integrating out parameters

Bayesian Estimation: Univariate Gaussian

(Only the mean is unknown)

- Data: $\mathcal{D}$: $x_1, ...x_n$
- Likelihood (as seen before) $p(x|m) \sim \mathcal{N}(m, \sigma^2)$
- Prior uncertainty over parameters: $p(m) \sim \mathcal{N}(m_0, \sigma_0^2)$
  m_0 and σ_0^2 are known.
- Substituting gives the posterior as a product of Gaussians

$$p(m|\mathcal{D}) = \alpha \prod_{k=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x_k - m}{\sigma}\right)^2\right] \times \frac{1}{\sigma_0\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{m - m_0}{\sigma_0}\right)^2\right]$$

- Which can be reduced to...

$$p(m|\mathcal{D}) = \alpha_2 \exp\left\{-\frac{1}{2}\left\{\left(\frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}\right) m^2 - 2\left(\frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{m_0}{\sigma_0^2}\right) m\right\}\right\}$$

- But then...

$$p(m|\mathcal{D}) = \frac{1}{\sigma_n} \exp\left\{-\frac{1}{2}\left(\frac{m - m_n}{\sigma_n}\right)^2\right\}$$

- Matching terms...

$$\frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}$$

$$\frac{m_n}{\sigma_n^2} = \frac{n}{\sigma^2} \quad \frac{m_0}{\sigma_0^2} \quad \frac{1}{n}\sum_{k=1}^{n}$$

Bayesian Estimation: Univariate Gaussian (cont'd)

- Finally...

$$m_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2}\right) \widehat{m}_n + \left(\frac{\sigma^2}{n\sigma_0^2 + \sigma^2}\right) m_0$$

$$\sigma_n^2 = \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2}$$

- We now have an estimate that combines *prior* information about the parameter ($p(m) = m_0$) with data ($x_1, ..., x_k$) to quantify uncertainty about the parameter:
  - Before seeing any data, we have a belief
  - As we see more and more data, our belief is taken over by what the data tells us.

Unsupervised Learning

- Given: $\{\boldsymbol{x}_n\}_{n=1}^N$ (as opposed to $\{\boldsymbol{x}_n, f_n\}_{n=1}^N$)
- We might extract cluster structures
  - Notion of distance between points of data
  - Criterion to determine how many clusters (often from prior knowledge)
  - Underlying probabilistic model
- We might project data onto a subspace $\boldsymbol{x}_n \in \mathcal{R}^d \longrightarrow \boldsymbol{y}_n \in \mathcal{R}^q$
  - $q = 2$ helps visualization
  - Subspace representation useful for
    - Data compression
    - Sometimes used to reduce features

Semi Supervised Learning:

$$\{\boldsymbol{x}_n, f_n\}_{n=1}^{N_1} \text{ and } \{\boldsymbol{x}_n\}_{n=N_1+1}^{N_2}$$

Principal Component Analysis:

- N data $\boldsymbol{x}_n \in \mathcal{R}^d$ distributed with mean $\boldsymbol{m}$ and covariance matrix $\boldsymbol{C}$.
- Project onto direction $\boldsymbol{u}$; find the direction that maximizes projected variance.
- Projected variance is $\boldsymbol{u}^t \boldsymbol{C} \boldsymbol{u}$
- We are only interested in the direction; not in increasing the projected variance by choosing $\boldsymbol{u}$ with large magnitude.
- Set up a constrained optimization problem

$$\max_{\boldsymbol{u}} \boldsymbol{u}^t \boldsymbol{C} \boldsymbol{u} \quad \text{subject to } \boldsymbol{u}^t \boldsymbol{u} = 1$$

- Lagrangian

$$\mathcal{L} = \boldsymbol{u}^t \boldsymbol{C} \boldsymbol{u} - \lambda \left[\boldsymbol{u}^t \boldsymbol{u} - 1 \right]$$

- $\frac{\partial \mathcal{L}}{\partial \boldsymbol{u}} = 0 \implies \boldsymbol{C}\boldsymbol{u} = \lambda \boldsymbol{u}$; *i.e.* principal directions are eigenvectors of covariance

Mixture Model

We write a mixture of Gaussian densities:

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- If the mixing proportions π_k satisfy
  - $\pi_k \geq 0$
  - $\sum_{k=1}^{K} \pi_k = 1$

  $p(\boldsymbol{x})$ is a proper probability density.

- More powerful model – useful when data is multi-modal
- Parameters are: proportions, means and covariance matrices
- Parameter estimation $(\boldsymbol{\pi}_k, \boldsymbol{\mu}_k \boldsymbol{\Sigma}_k)$ is not easy.
- z_{nk}: association of n^{th} data to k^{th} mode unknown (latent)

Algorithm:

$$\begin{aligned}
\pi_k &= \frac{1}{N} \sum_{n=1}^{N} q_{nk} \\
\boldsymbol{\mu}_k &= \frac{\sum_{n=1}^{N} q_{nk} \boldsymbol{x}_n}{\sum_{n=1}^{N} q_{nk}} \\
\boldsymbol{\Sigma}_k &= \frac{\sum_{n=1}^{N} q_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^t}{\sum_{n=1}^{N} q_{nk}}
\end{aligned}$$

$$q_{nk} = \frac{\pi_k p(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j p(\boldsymbol{x}_n | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

Expectation Maximization

Auxilliary Variable as Posteriors

Interpret:

- Mixture model as a Gaussian classifier with K classes
- π_k as prior probabilities
- Each of the $\mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ as class conditional densities / likelihoods.

$$\begin{aligned} p(z_{nk} = 1 | \boldsymbol{x}_n, \boldsymbol{\pi}, \Delta) &= \frac{p(z_{nk} = 1|\pi_k) p(\boldsymbol{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} p(z_{nk} = 1|\pi_k) p(\boldsymbol{x}_n | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \\ &= q_{nk} \end{aligned}$$

- Each data item has a weighted contribution to the estimation of parameters.
- Unknown assignment z_{nk}; **E**xpected value of this unknown assignment is q_{nk}, the posterior probability
- **M**aximize (the lower bound) to re-estimate parameters.

K-Means Clustering Algorithm

Input: $\boldsymbol{X} = \{\boldsymbol{x}_n^t\}_{n=1}^N$, K
Output: $\boldsymbol{C}$, `Idx`

`initialize:` $\boldsymbol{C} = \left\{\boldsymbol{c}_j^t\right\}_{j=1}^K$

`repeat`

. assign n^{th} sample to nearest $\boldsymbol{c}_j$
. `Idx(n)` $= \min_j \; ||\boldsymbol{x}_n - \boldsymbol{c}_j||^2$

. recompute $\boldsymbol{c}_j = \frac{1}{N_j} \sum_{n=j} \boldsymbol{x}_n$

`until` no change in $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots \boldsymbol{c}_k$

K-Means as Mixture Gaussian

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \pi_j \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- Set $\boldsymbol{\Sigma}_k = \sigma_k^2 \boldsymbol{I}$
- At every iteration, set largest q_{nk} (largest over k) to one and others to zero. Winner take all at each datapoint.
- Computation of q_{nk} is expectation of latent variable z_{nk} – **E** step
- Re-estimation of $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$ become maximum likelihood estimates from data assigned to each cluster (because q_{nk} is either one or zero) – **M** step

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

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

- *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

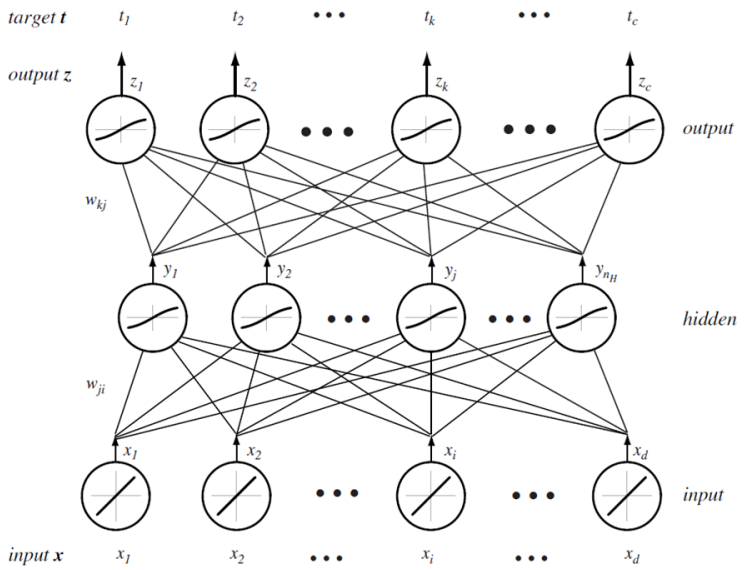
$$\widehat{\boldsymbol{\lambda}} = \min_{\lambda} |Y\,\boldsymbol{\lambda} - \boldsymbol{f}|^2$$

- 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

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

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

- Squashed by a nonlinearity

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

- Simple threshold

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

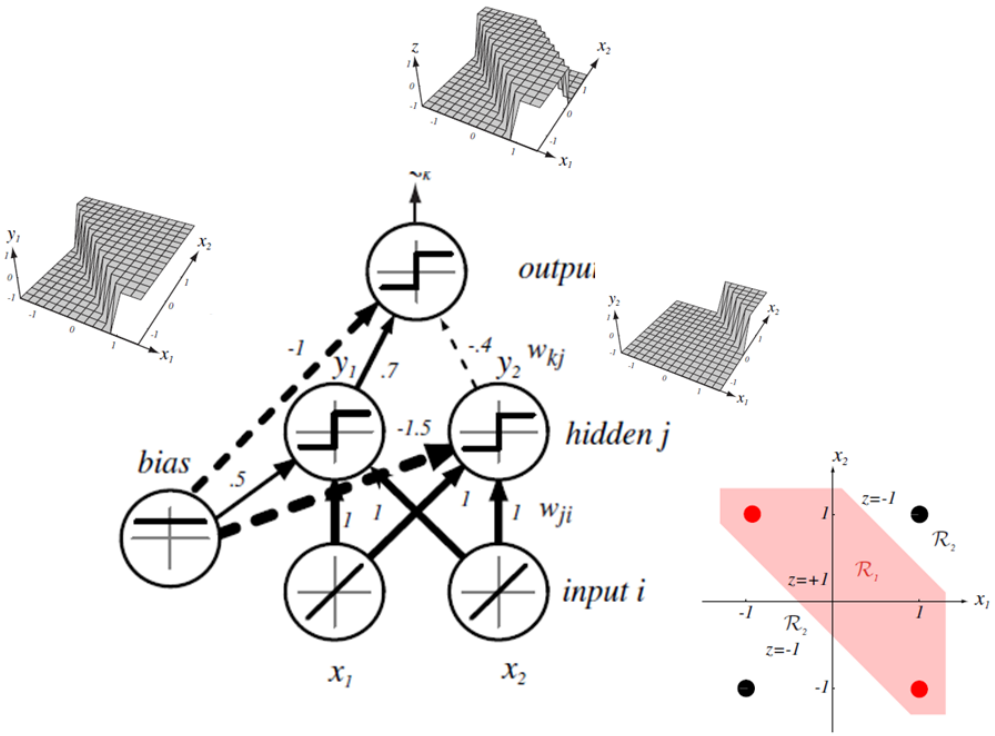
- Sigmoid (logistic)

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

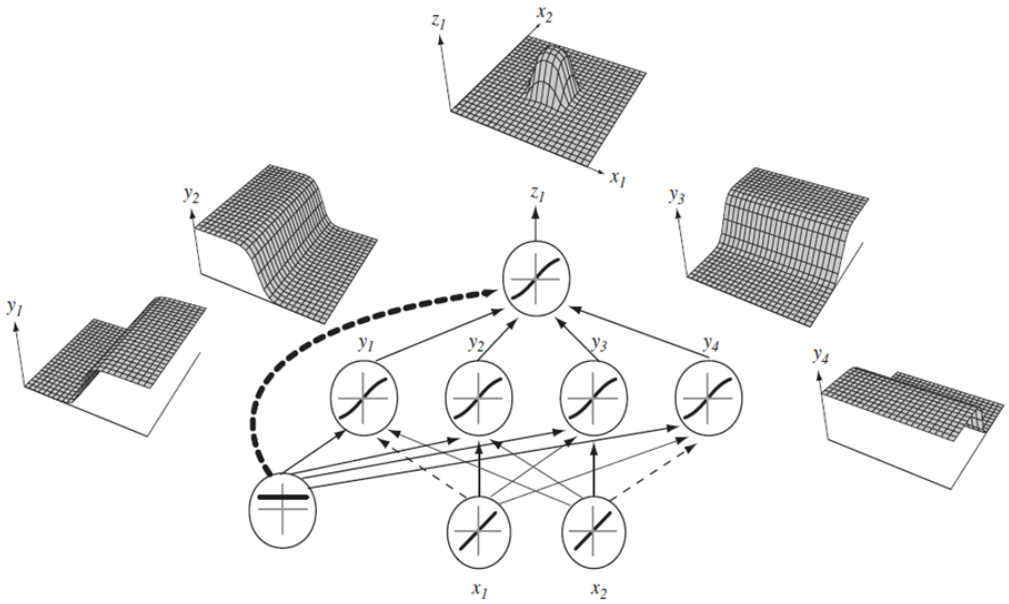
- Hyperbolic tangent

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

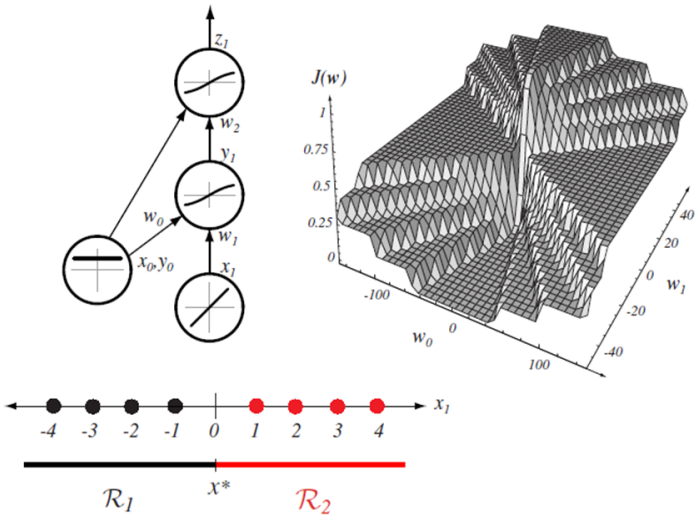
XOR Using a MLP



MLP Constructing Complex Functions



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

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

- Change in weight for gradient descent

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

  Or in component form

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

- Gradient descent update

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

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!

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

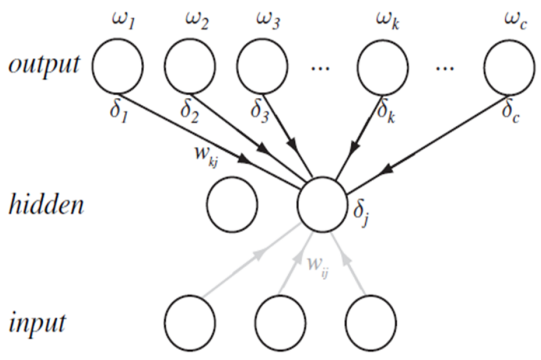
$$\begin{aligned}
\frac{\partial J}{\partial y_j} &= \frac{\partial}{\partial y_j}\left[\frac{1}{2}\sum_{k=1}^{c}(t_k - z_k)^2\right] \\
&= -\sum_{k=1}^{c}(t_k - z_k)\frac{\partial z_k}{\partial y_j} \\
&= -\sum_{k=1}^{c}(t_k - z_k)\frac{\partial z_k}{\partial \text{net}_k}\frac{\partial \text{net}_k}{\partial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

Error propagation (cont'd)

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

and the update rule

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



- 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

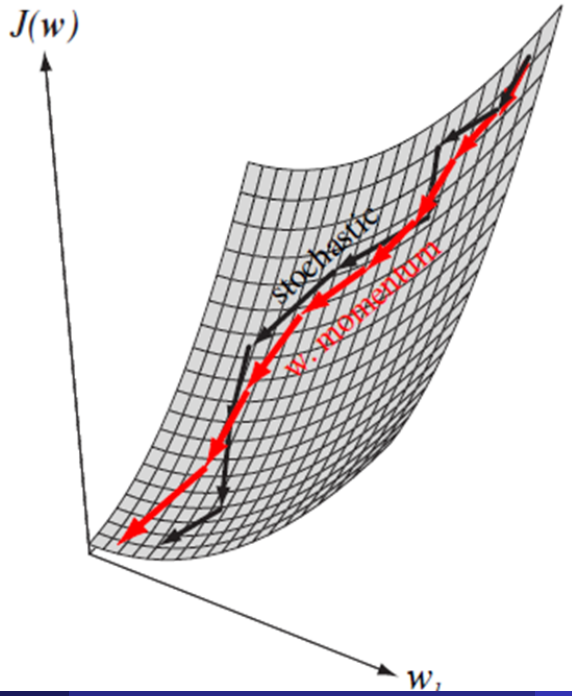
$$\begin{aligned}\boldsymbol{w}(m+1) &= \boldsymbol{w}(m) + \Delta\boldsymbol{w} \\ &= \boldsymbol{w}(m) - H^{-1}(m)\left(\frac{\partial J(\boldsymbol{w}(m))}{\partial \boldsymbol{w}}\right)\end{aligned}$$

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

Momentum

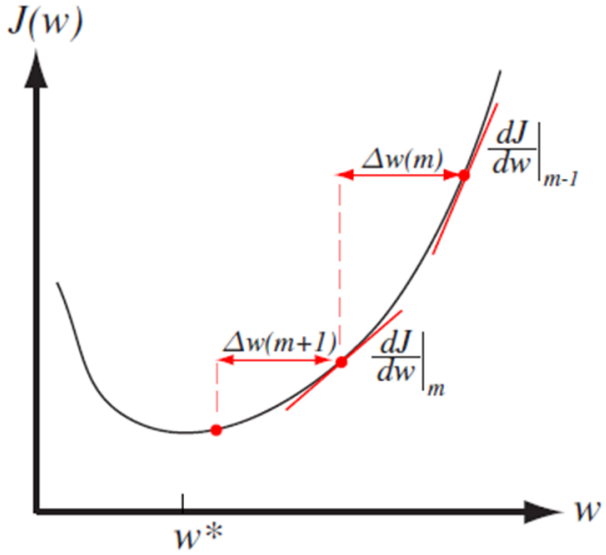
- Slow learning in regions in which gradient is small

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



QuickProp

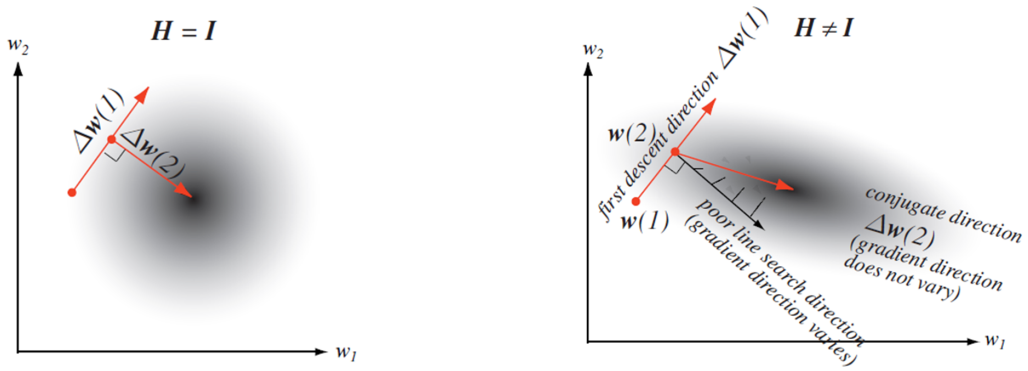
Two successive evaluations to approximate local curvature



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

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 $\Delta \boldsymbol{w}$

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

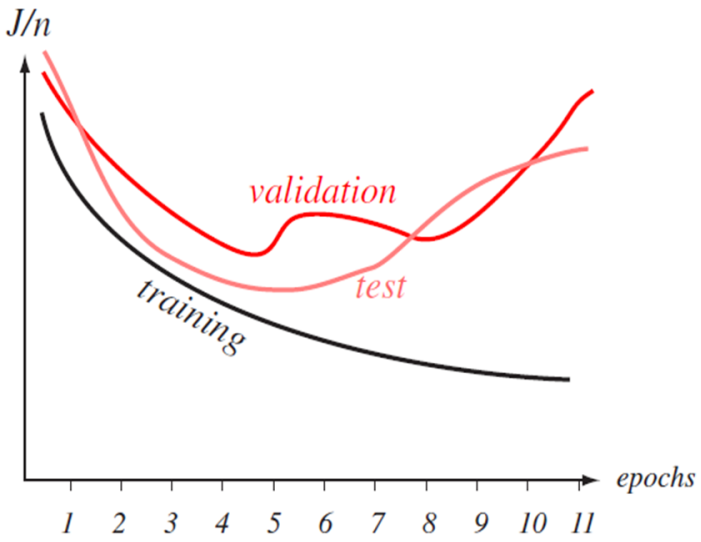
- Can be expressed as the gradient plus a component of previous search direction

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

- 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

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

- Suppose we train a neural net with c outputs

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

- Mininimising the error

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

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

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