Machine learning: lecture 13

Tommi S. Jaakkola
MIT AI Lab
tommi@ai.mit.edu

Topics

- A bit more general view of the EM algorithm
  - regularized mixtures
- Extensions of mixture models
  - hierarchical mixture models
  - conditional mixture models: mixtures of experts

Mixture models: review

- A two component Gaussian mixture model:

$$p(\mathbf{x}|\theta) \;=\; \sum_{j=1,2} p_j p(\mathbf{x}|\mu_j, \Sigma_j)$$

where $\theta = \{p_1, p_2, \mu_1, \mu_2, \Sigma_1, \Sigma_2\}$.

- Only iterative solutions are available for finding the parameters that maximize the log-likelihood

$$l(\theta; D) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\theta)$$

where $D = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$.

The estimation involves resolving which mixture component should be responsible for which data point

The EM algorithm

- The EM-algorithm finds a local maximum of $l(\theta; D)$

  E-step: evaluate the expected complete log-likelihood

$$
\begin{aligned}
J(\theta; \theta^{(t)}) &= \sum_{i=1}^{n} E_{j \sim P(j|\mathbf{x}_i, \theta^{(t)})} \log \left(p_j p(\mathbf{x}_i | \mu_j, \Sigma_j) \right) \\
&= \sum_{i=1}^{n} \sum_{j=1,2} P(j|\mathbf{x}_i, \theta^{(t)}) \log \left(p_j p(\mathbf{x}_i | \mu_j, \Sigma_j) \right)
\end{aligned}
$$

  M-step: find the new parameters by maximizing the expected complete log-likelihood

$$
\theta^{(t+1)} \leftarrow \arg\max_{\theta} J(\theta; \theta^{(t)})
$$

Regularized EM algorithm

- To maximize a penalized (regularized) log-likelihood

$$l'(\theta; D) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\theta) + \log p(\theta)$$

we only need to modify the M-step of the EM-algorithm.

Specifically, in the M-step, we find find θ that maximize a penalized expected complete log-likelihood:

$$\begin{aligned} J(\theta; \theta^{(t)}) &= \sum_{i=1}^{n} E_{j \sim P(j|\mathbf{x}_i, \theta^{(t)})} \log \Big(p_j p(\mathbf{x}_i|\mu_j, \Sigma_j) \Big) \\ &\quad + \log p(p_1, p_2) + \log p(\Sigma_1) + \log p(\Sigma_1) \end{aligned}$$

where, for example, $p(p_1, p_2)$ could be a *Dirichlet* and each $p(\Sigma_j)$ a *Wishart* prior.

Regularized EM: demo

Selecting the number of components

- As a simple strategy for selecting the appropriate number of mixture components, we can find k that minimize the following asymptotic approximation to the description length:

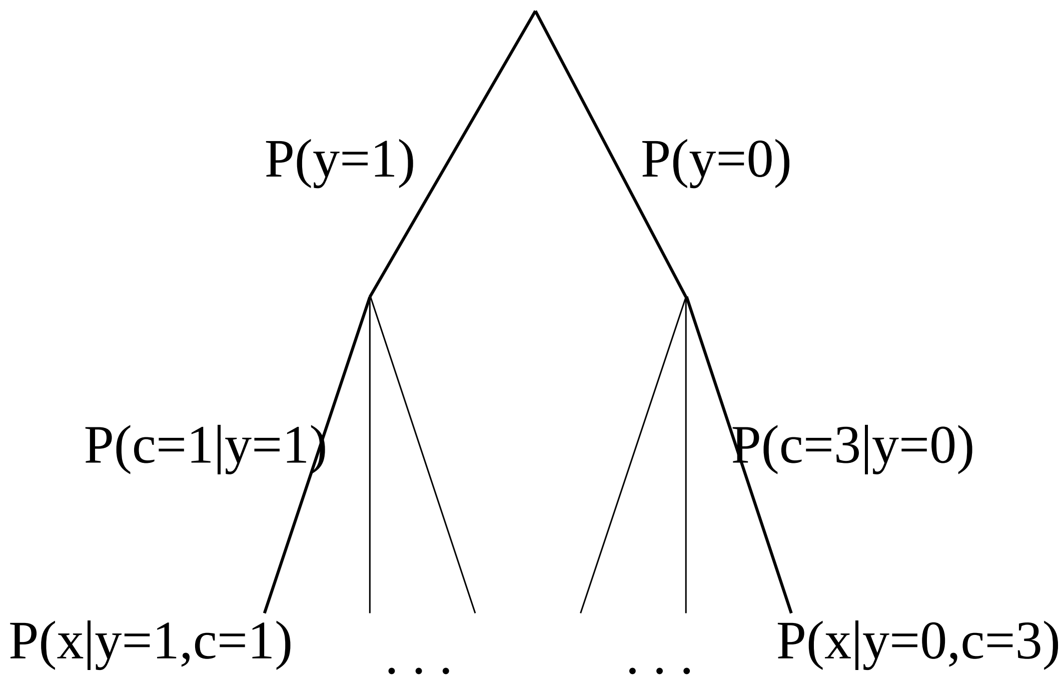
$$\mathsf{DL} \approx -\log p(\mathsf{data}|\hat{\theta}_k) + \frac{d_k}{2}\log(n)$$

where n is the number of training points, $\hat{\theta}_k$ is the maximum likelihood parameter estimate for the k-component mixture, and d_k is the (effective) number of parameters in the k-mixture.

Extensions: hierarchical mixture models

- We have already used hierarchical mixture models in the digit classification problem

  Data generation model:



  It is not necessary for the top level division to be "observable" as it is in this classification context.

Hierarchical mixture models cont'd

- To estimate such hierachical models from data, we have to resolve which leaf (path) in the tree is responsible for generating which data point

  Only the E-step needs to be revised: the expectation over assignments is now taken with respect to

$$P(y=j, c=k|\mathbf{x}) = \overbrace{P(y=j|\mathbf{x})}^{\text{First level}} \overbrace{P(c=k|y=j,\mathbf{x})}^{\text{Second level}},$$

  For example, for a hierarchical mixture of Gaussians, we evaluate

$$J(\theta;\theta^{(t)}) \;=\; \sum_{i=1}^{n} E_{(j,k)\sim P(j,k|\mathbf{x}_i,\theta^{(t)})} \log \Big(p_j\, p_{k|j}\, p(\mathbf{x}_i|\mu_{j,k},\Sigma_{j,k}) \Big)$$

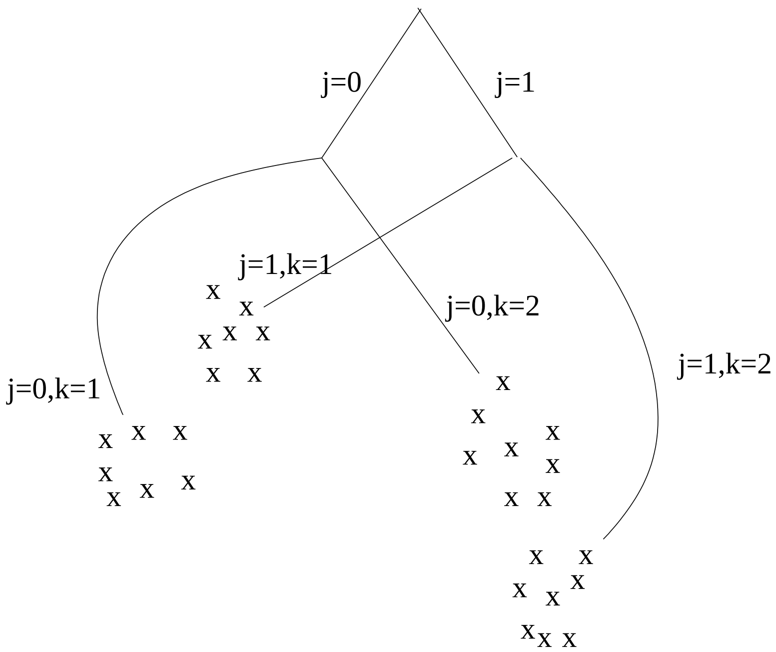
  where p_j and $p_{k|j}$ are the prior selection probabilities

Hierarchical mixture models cont'd

- Arranging the mixture components into a hierarchy is useful only with additional "topological" constraints. The hierarchical mixture (as stated previously) is otherwise equivalent to a flat mixture.

  To adequately reveal any hierarchical organization in the data, we have to prime the model to find such structure.

  - initialize parameters similarly within branches
  - tying parameters, etc.



Conditional mixtures: mixtures of experts

- Many regression or classification problems can be decomposed into smaller (easier) sub problems
- Examples:
  1. Dealing with style in handwritten character recognition
  2. Dealing with dialect/accent in speech recognition

     etc.
- Each sub-problem could be solved by a specific "expert"
- Unlike in ordinary mixtures, the selection of which expert to rely on must depend on the context (i.e., the input $\mathbf{x}$)

Experts

- Suppose we have several "experts" or component regression models generating conditional Gaussian outputs

$$P(y|\mathbf{x}, \theta_i) = N(y;\, \mathbf{w}_i^T \mathbf{x} + w_{i0},\, \sigma_i^2)$$

where

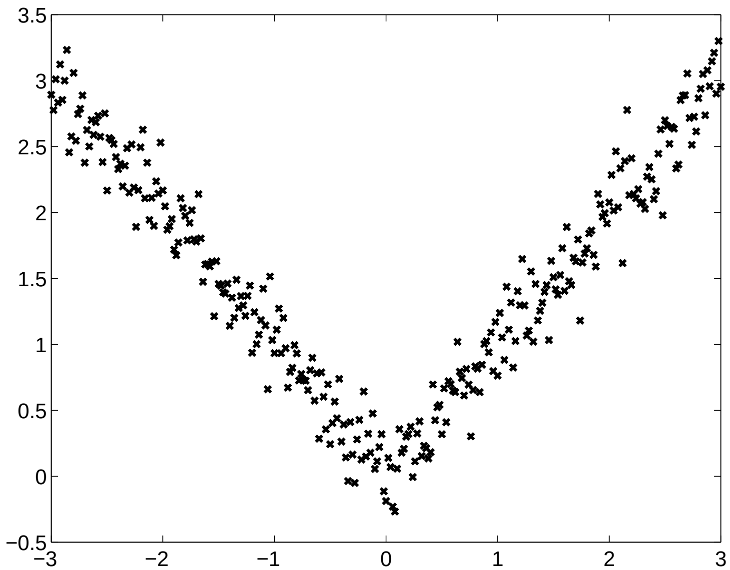
$$\begin{aligned} \text{mean of } y \text{ given } \mathbf{x} &= \mathbf{w}_i^T \mathbf{x} + w_{i0} \\ \text{variance of } y \text{ given } \mathbf{x} &= \sigma_i^2 \end{aligned}$$

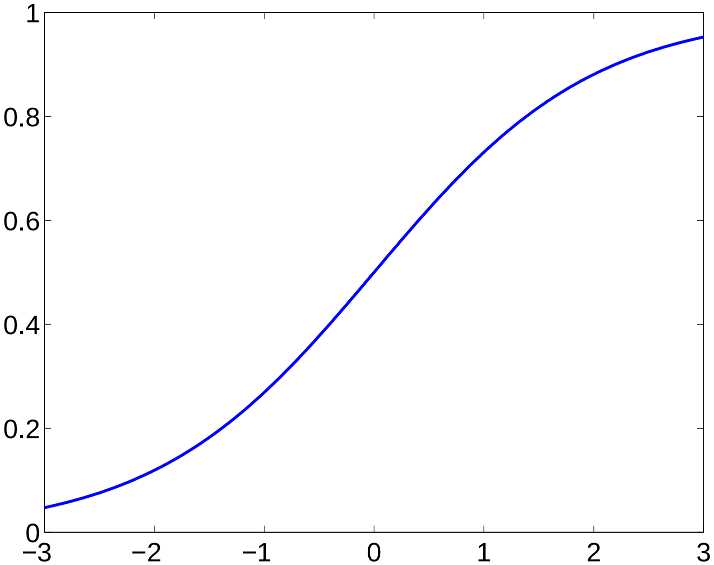
$\theta_i = \{\mathbf{w}_i, w_{i0}, \sigma_i^2\}$ denotes the parameters of the i^{th} expert.

- We need to find an appropriate way of allocating tasks to these experts (linear regression models)

Mixtures of experts

Example:





- Here we need a switch or a gating network that selects the appropriate expert (linear regression model) as a function of the input $\mathbf{x}$

Gating network

- A simple gating network is a probability distribution over the choice of the experts conditional on the input $\mathbf{x}$
- Example: in case of two experts (0 and 1), the gating network can be a logistic regression model

$$P(\text{expert} = 1|\mathbf{x}, \mathbf{v}, v_0) = g(\,\mathbf{v}^T\mathbf{x} + v_0\,)$$

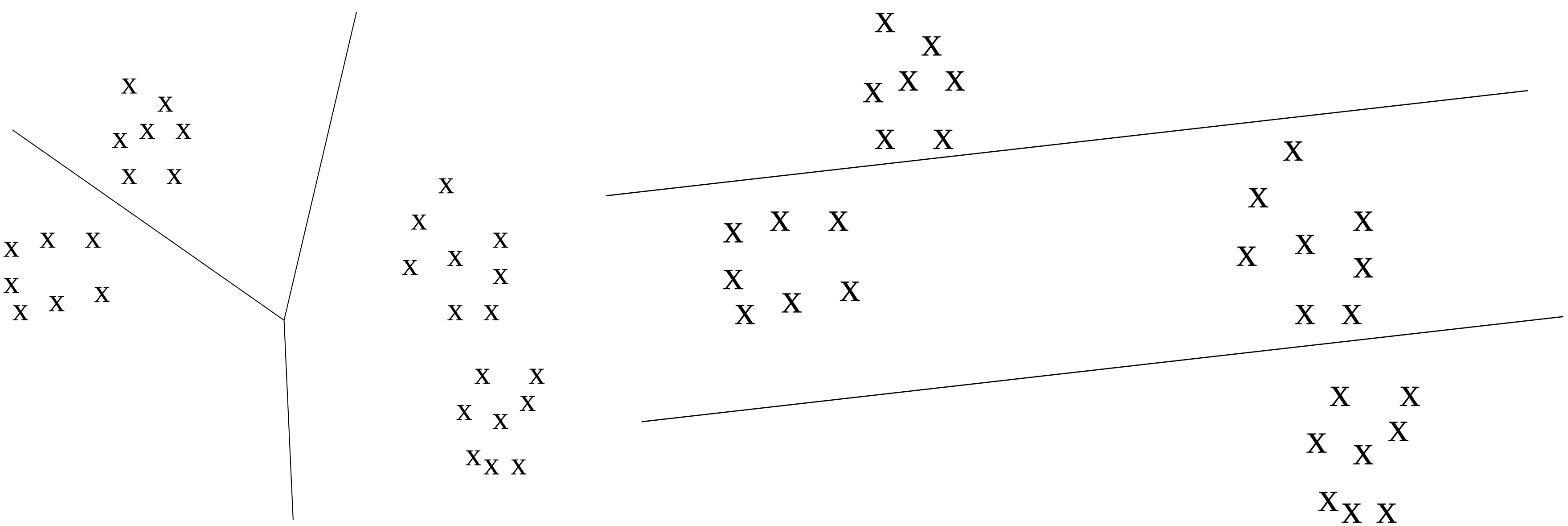
  where $g(z) = (1 + e^{-z})^{-1}$ is the logistic function.
- In case of $m > 2$ experts, the gating network can be a softmax model

$$P(\text{expert} = j|\mathbf{x}, \eta) = \frac{\exp(\,\mathbf{v}_j^T\mathbf{x} + v_{j0}\,)}{\sum_{j'=1}^{m} \exp(\,\mathbf{v}_{j'}^T\mathbf{x} + v_{j'0}\,)}$$

  where $\eta = \{\mathbf{v}_1, \ldots, \mathbf{v}_m, v_{10}, \ldots, v_{m0}\}$ are the parameters in the gating network

Gating network cont'd

$$P(\text{expert} = j|\mathbf{x}, \eta) = \frac{\exp(\,\mathbf{v}_j^T\mathbf{x} + v_{j0}\,)}{\sum_{j'=1}^{m} \exp(\,\mathbf{v}_{j'}^T\mathbf{x} + v_{j'0}\,)}$$

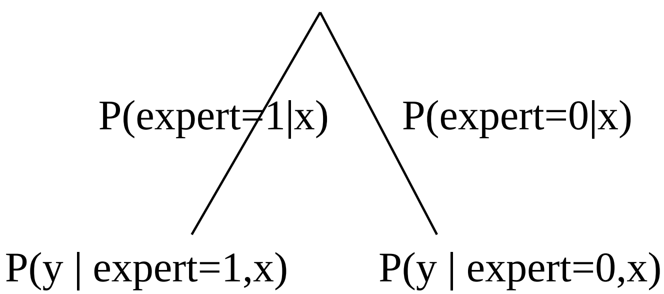


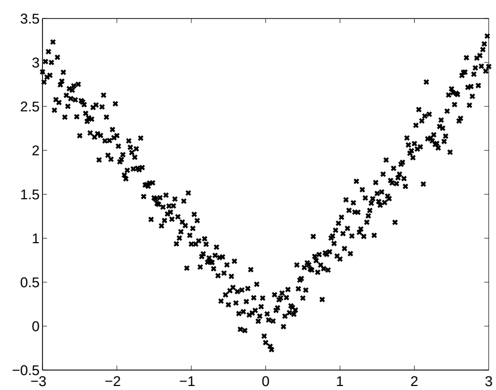
Mixtures of experts model

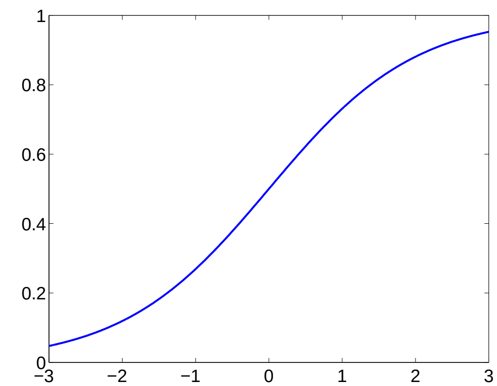
- The probability distribution over the (regression) output y given the input $\mathbf{x}$ is a conditional mixture model

$$P(y|\mathbf{x}, \theta, \eta) = \sum_{j=1}^{m} P(\text{expert} = j|\mathbf{x}, \eta)\, P(y|\mathbf{x}, \theta_j)$$

where η defines the parameters of the gating network (e.g., logistic) and θ_j are the parameters of each expert (e.g., linear regression model).







- The allocation of experts is made conditionally on the input

Estimation of mixtures of experts

- The estimation would be again easy if we had the assignment of which expert should account for which training example
- In other words, if we had $\{(\mathbf{x}_1, k_1, y_1), \ldots, (\mathbf{x}_n, k_n, y_n)\}$, where k_i indicates the expert assigned to the i^{th} example

1. Separately for each expert j

$$\text{Find } \theta_j \text{ that maximize} \quad \sum_{i=1:\, k_i=j}^{n} \log P(y_i|\mathbf{x}_i, \theta_j)$$

   (linear regression based on points "labeled" j)

2. For the gating network

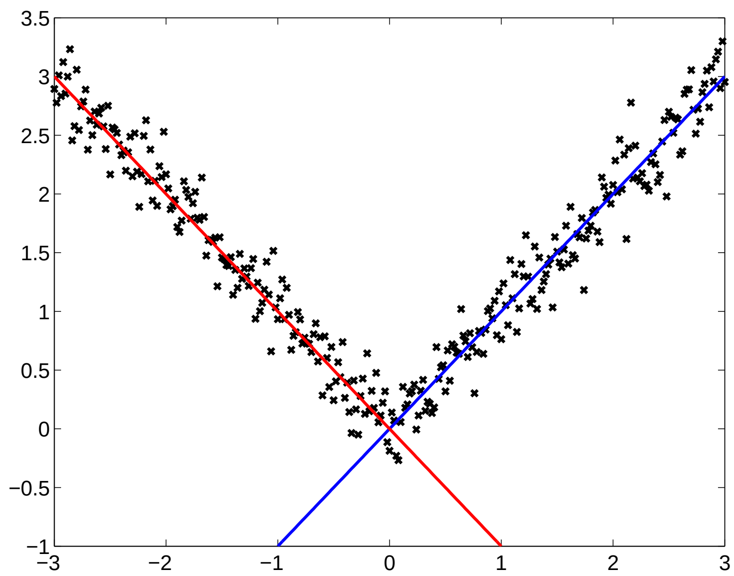
$$\text{Find } \eta \text{ that maximize} \quad \sum_{i=1}^{n} \log P(\text{expert} = k_i|\mathbf{x}_i, \eta)$$

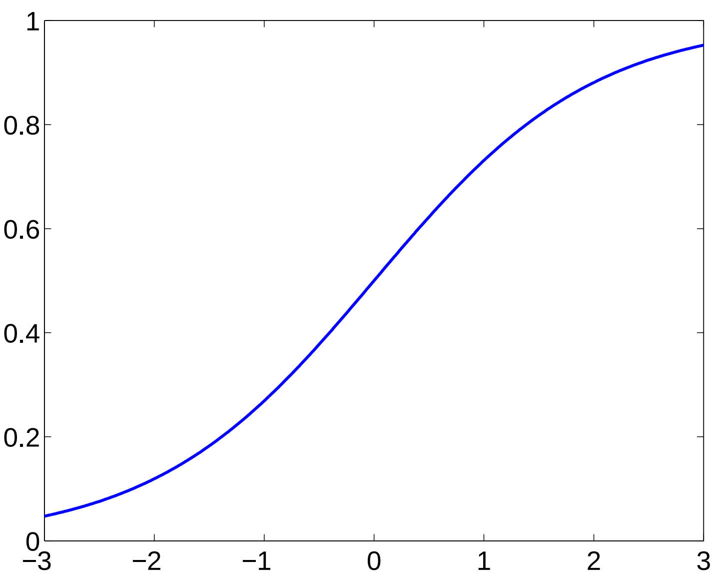
   (softmax regression problem to predict the assignments)

Estimation of mixtures of experts

- Similarly to mixture models, we now have to evaluate the posterior probability (here given both $\mathbf{x}_i$ AND y_i) that the output came from a particular expert:

$$
\begin{aligned}
\hat{p}(j|i) \quad &\leftarrow \quad P(\text{expert} = j|\mathbf{x}_i, y_i, \eta, \theta) \\
&= \frac{P(\text{expert} = j|\mathbf{x}_i, \eta)\, P(y_i|\mathbf{x}_i, \theta_j)}{\sum_{j'=1}^{m} P(\text{expert} = j'|\mathbf{x}_i, \eta)\, P(y_i|\mathbf{x}_i, \theta_{j'})}
\end{aligned}
$$





Estimation of mixtures of experts

E-step: evaluate the posterior probabilities $\hat{p}(j|i)$ that partially assign experts to training examples

M-step(s):

1. Separately for each expert j

   Find θ_j that maximize $$\sum_{i=1}^{n} \hat{p}(j|i) \log P(y_i|\mathbf{x}_i, \theta_j)$$

   (weighted linear regression)

2. For the gating network

   Find η that maximize $$\sum_{i=1}^{n} \sum_{j=1}^{m} \hat{p}(j|i) \log P(\text{expert} = j|\mathbf{x}_i, \eta)$$

   (weighted softmax regression)

Mixtures of experts: demo

Mixtures of experts: additional considerations

- Softmax gating network

$$P(\text{expert} = j|\mathbf{x}, \eta) = \frac{\exp(\,\mathbf{v}_j^T\mathbf{x} + v_{j0}\,)}{\sum_{j'=1}^m \exp(\,\mathbf{v}_{j'}^T\mathbf{x} + v_{j'0}\,)}$$

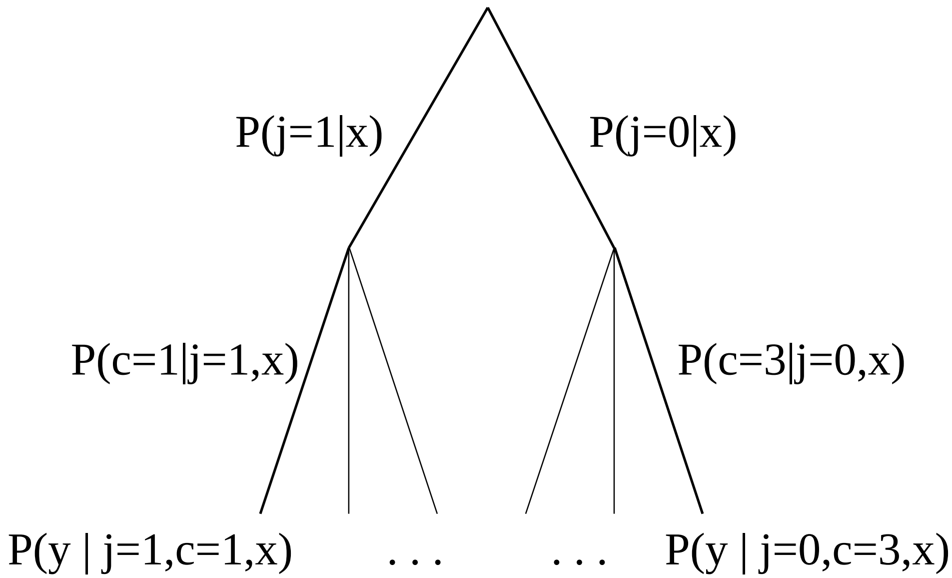
- Gaussian gating network

$$P(\text{expert} = j|\mathbf{x}, \eta) = \frac{\exp(\,-\frac{1}{2}(\mathbf{x}-\mathbf{v}_j)^T\Sigma_j^{-1}(\mathbf{x}-\mathbf{v}_j)\,)}{\sum_{j'=1}^m \exp(\,-\frac{1}{2}(\mathbf{x}-\mathbf{v}_{j'})^T\Sigma_{j'}^{-1}(\mathbf{x}-\mathbf{v}_{j'})\,)}$$

What if $\Sigma_1 = \ldots = \Sigma_m$? Are these still different?

Hierarchical mixtures of experts

- The "gates" can be arranged hierarchically:



where for example:

$$P(c = k|j = 1, \mathbf{x}, \eta_j) = \frac{\exp(\,\mathbf{v}_{1k}^T\mathbf{x} + v_{1k0}\,)}{\sum_{k'=1}^{3}\exp(\,\mathbf{v}_{1k'}^T\mathbf{x} + v_{1k'0}\,)}$$

- We can estimate these with the EM-algorithm similarly to hierarchical mixture models