高级机器学习

PRML基础知识回顾

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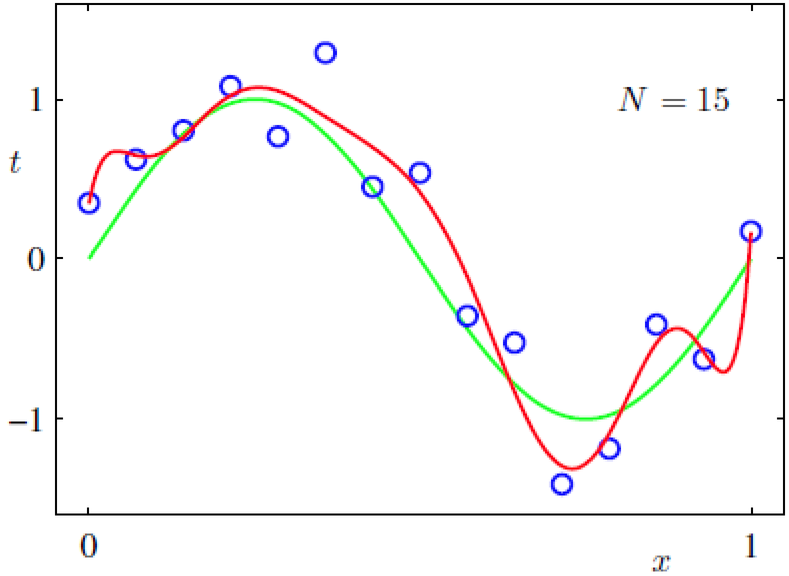
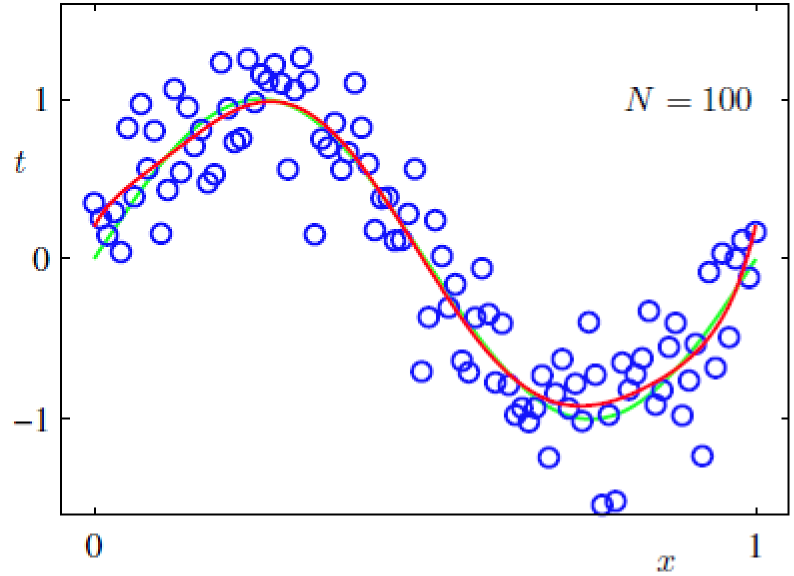
Review – curve fitting

- Polynomial curve fitting
  - Curve $$y(x,\mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$
  - Loss $$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2$$





  - Regularized $$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n,\mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

Review – Bayes related

- Bayes' theorem
  - $$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$ posterior $\propto$ likelihood $\times$ prior
- Maximize likelihood
  - $$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n|y(x_n, \mathbf{w}), \beta^{-1}\right).$$
  - $$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi).$$

Equivalent to minimizing the *sum-of-squares error function*

- Maximize a posteriori
  - $$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}\right\}$$
  - $$p(\mathbf{w}|\mathbf{x}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$
  - $$\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}.$$

equivalent to minimizing the regularized sum-of-squares error

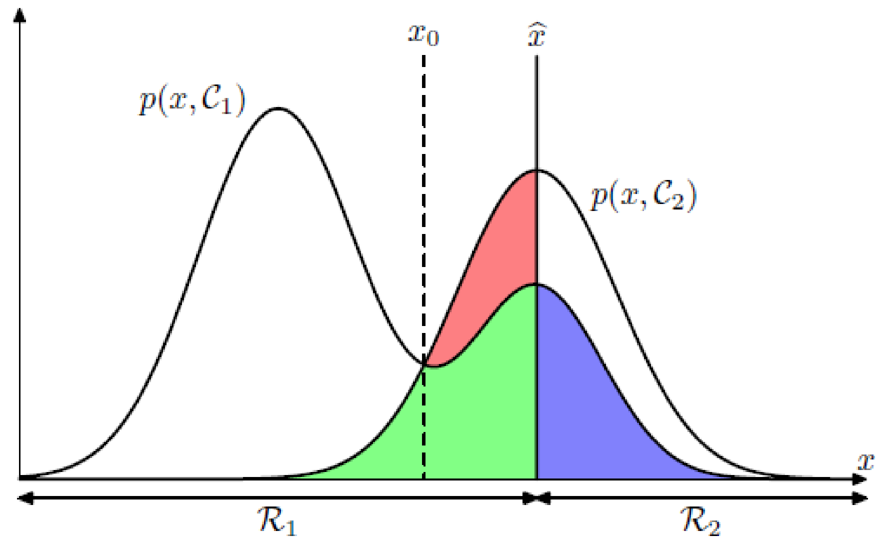
- Bayesian curve fitting
  - Not MAP but integrate over all values like w.

Review – decision theory

- Model selection
  - Cross-validation
  - Add a plenty term to likelihood e.g., AIC or BIC
- Decision theory
  - Misclassification rate

$$p(\text{mistake}) = \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2)\,\mathrm{d}\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1)\,\mathrm{d}\mathbf{x}$$

class=argmax $_{Ck}$ p(C_k|x)



  - Expected loss

$$\mathbb{E}[L] = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj}\, p(\mathbf{x}, \mathcal{C}_k)\,\mathrm{d}\mathbf{x}$$

class=argmin $_j$ $\sum_k L_{kj}\, p(\mathcal{C}_k|\mathbf{x})$

$$\mathbb{E}[L] = \iint L(t, y(\mathbf{x}))\, p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t \quad L(t, y(\mathbf{x})) = \{y(\mathbf{x}) - t\}^2 \quad \mathbf{y}(\mathbf{x}) = \mathbb{E}_t[\mathbf{t}|\mathbf{x}]$$

Review – inference and decision

- Inference and decision
  - Generative model
    - $p(\mathcal{C}_k|\mathbf{x}) = \dfrac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})}$ $p(\mathbf{x}) = \sum_k p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k).$
    - model the joint distribution
  - Discriminative model
    - model the conditional probabilities $p(\mathcal{C}_k|\mathbf{x})$ directly
  - Discriminant function
    - a discriminant function $f(\mathbf{x})$ which maps each input x directly onto a class label

Review – information theory

- Information theory
  - Entropy $\mathrm{H}[x] = -\sum_{x} p(x) \log_2 p(x)$ $\mathrm{H}[\mathbf{x}] = -\int p(\mathbf{x}) \ln p(\mathbf{x}) \,\mathrm{d}\mathbf{x}.$
  - Conditional entropy $\mathrm{H}[\mathbf{y}|\mathbf{x}] = -\iint p(\mathbf{y}, \mathbf{x}) \ln p(\mathbf{y}|\mathbf{x}) \,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{x}$
  - Relative entropy

$$\begin{aligned} \mathrm{KL}(p\|q) &= -\int p(\mathbf{x}) \ln q(\mathbf{x}) \,\mathrm{d}\mathbf{x} - \left(-\int p(\mathbf{x}) \ln p(\mathbf{x}) \,\mathrm{d}\mathbf{x}\right) \\ &= -\int p(\mathbf{x}) \ln \left\{\frac{q(\mathbf{x})}{p(\mathbf{x})}\right\} \mathrm{d}\mathbf{x}. \end{aligned}$$

  - Mutual information

$$\begin{aligned} \mathrm{I}[\mathbf{x}, \mathbf{y}] &\equiv \mathrm{KL}(p(\mathbf{x}, \mathbf{y}) \| p(\mathbf{x}) p(\mathbf{y})) \\ &= -\iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x}) p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})}\right) \mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y} \end{aligned}$$

$$\mathrm{I}[\mathbf{x}, \mathbf{y}] = \mathrm{H}[\mathbf{x}] - \mathrm{H}[\mathbf{x}|\mathbf{y}] = \mathrm{H}[\mathbf{y}] - \mathrm{H}[\mathbf{y}|\mathbf{x}].$$

Review – probability distribution

- Bernoulli

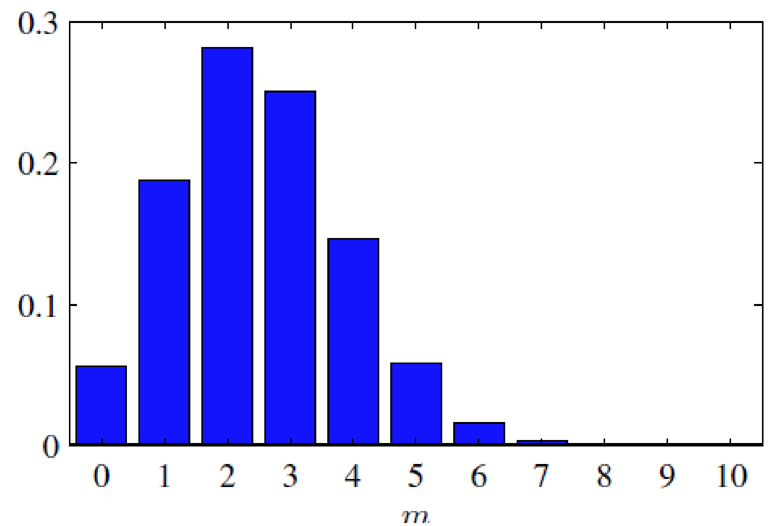
$$\mathrm{Bern}(x|\mu) = \mu^x(1-\mu)^{1-x}$$

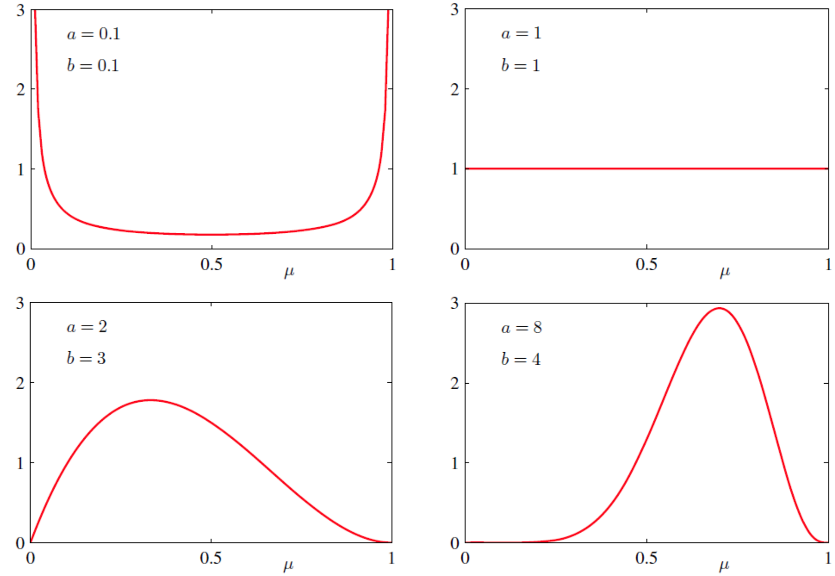
- Binomial

$$\mathrm{Bin}(m|N,\mu) = \binom{N}{m}\mu^m(1-\mu)^{N-m}$$

- Beta

$$\mathrm{Beta}(\mu|a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}$$





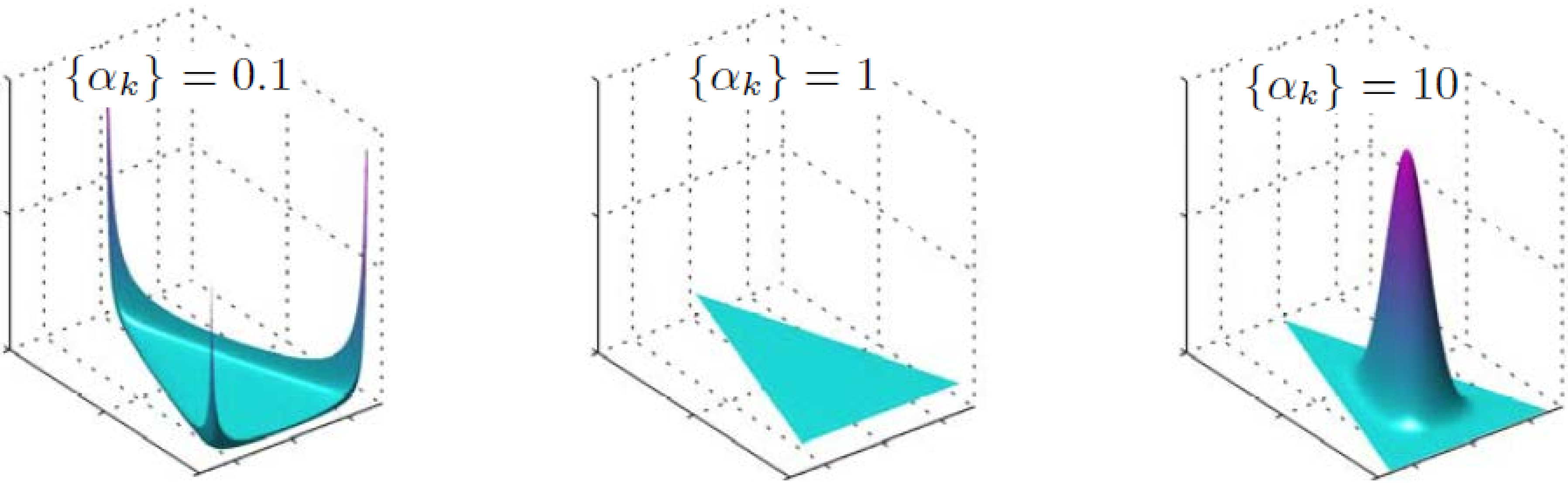
Review – probability distribution

- Generalization of the Bernoulli $p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k}$
- Multinomial

$$\mathrm{Mult}(m_1, m_2, \ldots, m_K|\boldsymbol{\mu}, N) = \binom{N}{m_1 m_2 \ldots m_K} \prod_{k=1}^{K} \mu_k^{m_k}$$

- Dirichelet

$$\mathrm{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_K)} \prod_{k=1}^{K} \mu_k^{\alpha_k - 1}$$



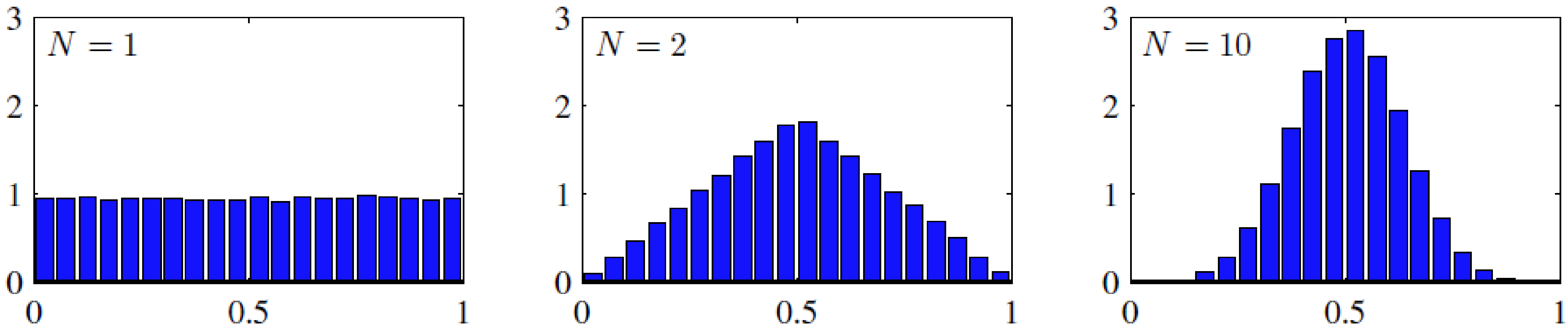
Review – probability distribution

- Gaussian

$X_n \sim [0,1]$

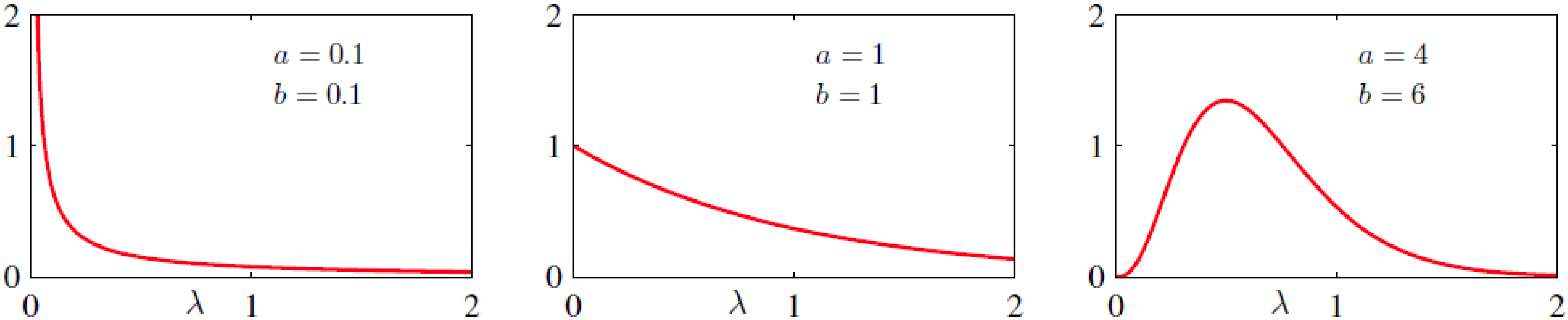
$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

$$(x_1 + \cdots + x_N)/N.$$



- Gamma

$$\mathrm{Gam}(\lambda|a,b) = \frac{1}{\Gamma(a)} b^a \lambda^{a-1} \exp(-b\lambda)$$

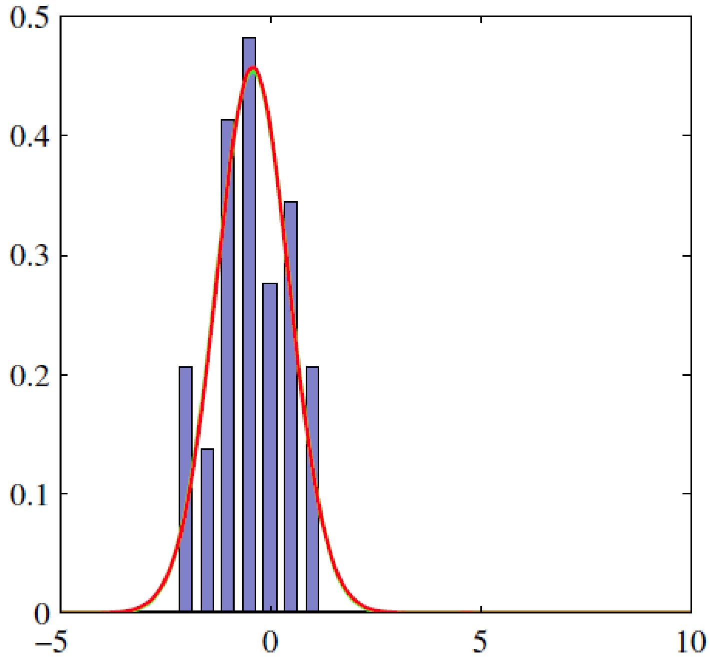


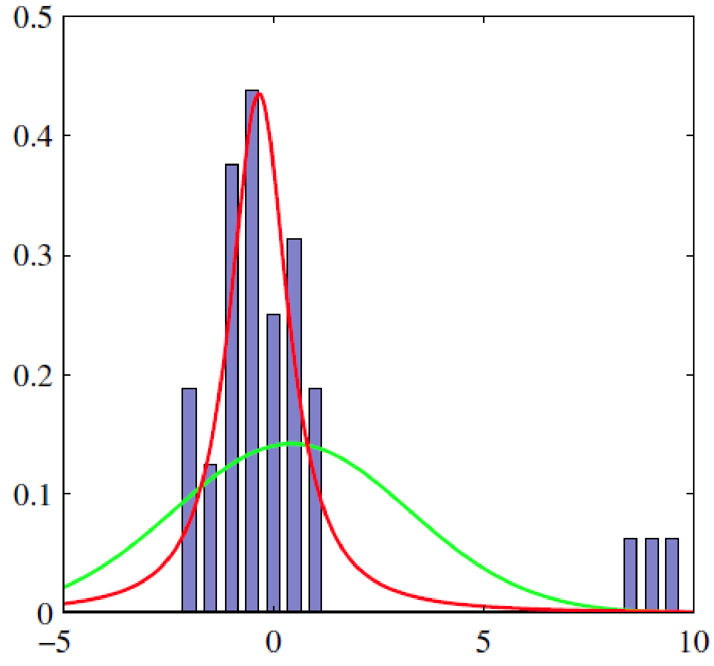
Review – probability distribution

- Student T

$$\mathrm{St}(x|\mu,\lambda,\nu) = \frac{\Gamma(\nu/2+1/2)}{\Gamma(\nu/2)}\left(\frac{\lambda}{\pi\nu}\right)^{1/2}\left[1+\frac{\lambda(x-\mu)^2}{\nu}\right]^{-\nu/2-1/2}$$

$$\mathcal{N}(x|\mu,\tau^{-1}) \qquad \mathrm{Gam}(\tau|a,b)$$





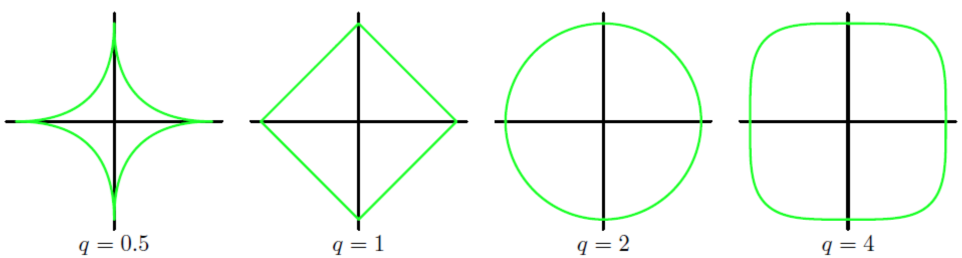
Review – linear regression model

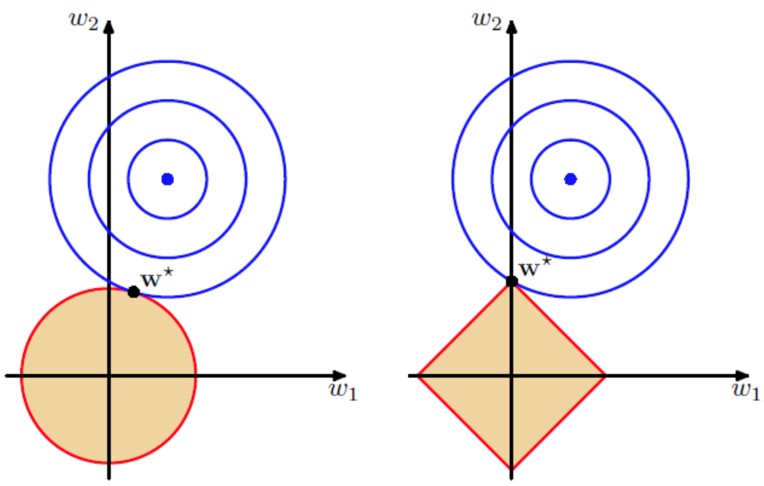
- Maximum likelihood and least squares

$$p(\mathbf{t}|\mathbf{x}, \mathrm{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n | y(x_n, \mathrm{w}), \beta^{-1}\right) \qquad \ln p(\mathbf{t}|\mathbf{x}, \mathrm{w}, \beta) = -\frac{\beta}{2}\sum_{n=1}^{N}\{y(x_n, \mathrm{w}) - t_n\}^2 + \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi)$$

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j \qquad E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

- Regularized least squares





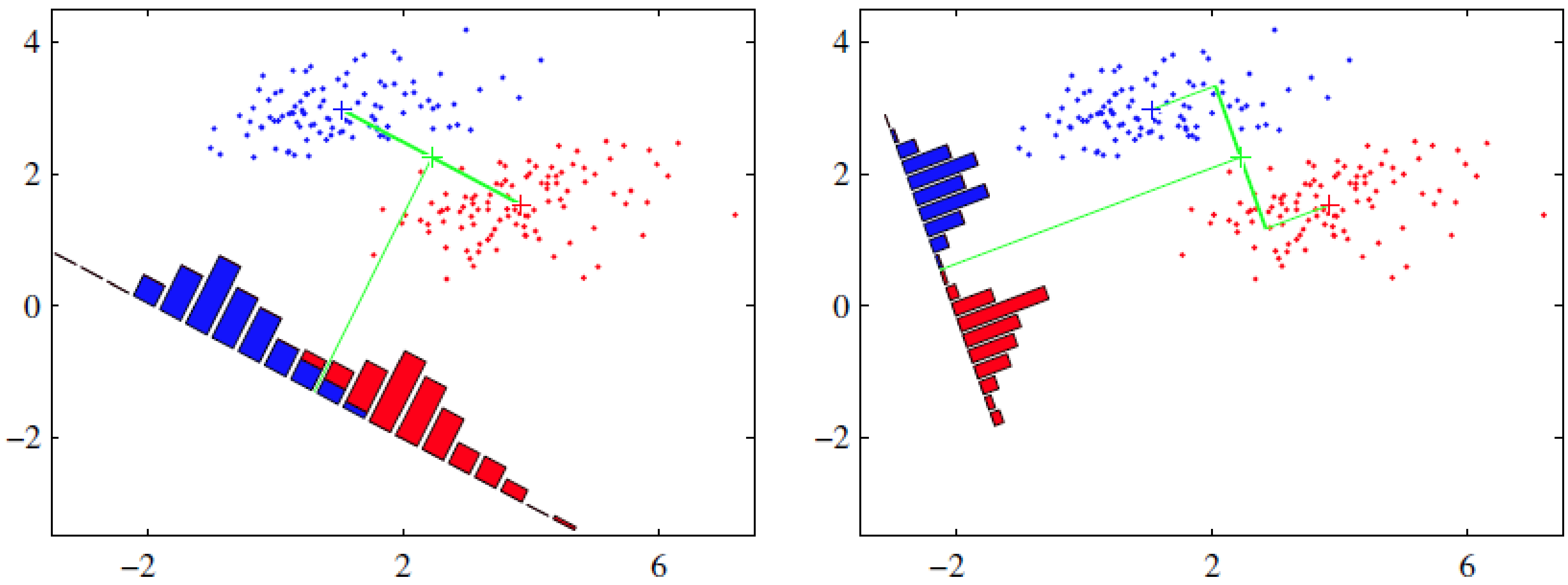
- Bayesian Linear Regression

Review – linear classification model

- Fisher linear discriminant

$$\mathbf{m}_1 = \frac{1}{N_1}\sum_{n \in \mathcal{C}_1} \mathbf{x}_n, \qquad \mathbf{m}_2 = \frac{1}{N_2}\sum_{n \in \mathcal{C}_2} \mathbf{x}_n. \qquad m_2 - m_1 = \mathbf{w}^{\mathrm{T}}(\mathbf{m}_2 - \mathbf{m}_1)$$

$$s_k^2 = \sum_{n \in \mathcal{C}_k} (y_n - m_k)^2 \qquad J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2} \qquad J(\mathbf{w}) = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}}$$



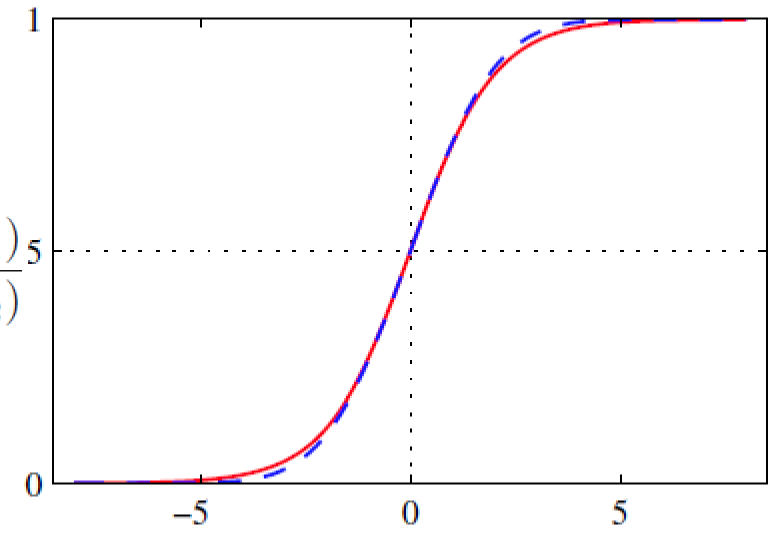
Review – linear classification model

- Naive Bayes

$$p(\mathcal{C}_1|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

$$= \frac{1}{1+\exp(-a)} = \sigma(a) \quad a = \ln\frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

$$p(\mathbf{x}|\mathcal{C}_k) = \prod_{i=1}^{D} \mu_{ki}^{x_i}(1-\mu_{ki})^{1-x_i} \qquad x_i \in \{0,1\}$$



- Logistic regression

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right) \qquad \frac{d\sigma}{da} = \sigma(1-\sigma)$$

Cross-entropy loss

$$p(\mathbf{t}|\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n}\{1-y_n\}^{1-t_n} \qquad E(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{w}) = -\sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$

- Bayesian logistic regression
  - Laplace approximation $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_0, \mathbf{S}_0)$ $\quad p(\mathbf{w}|\mathbf{t}) \propto p(\mathbf{w})p(\mathbf{t}|\mathbf{w})$

$$q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_{\mathrm{MAP}}, \mathbf{S}_N)$$

Review – neural network

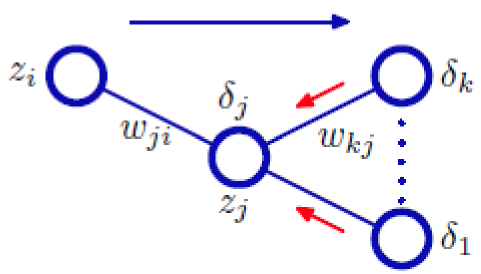
- Feed-forward Network Functions

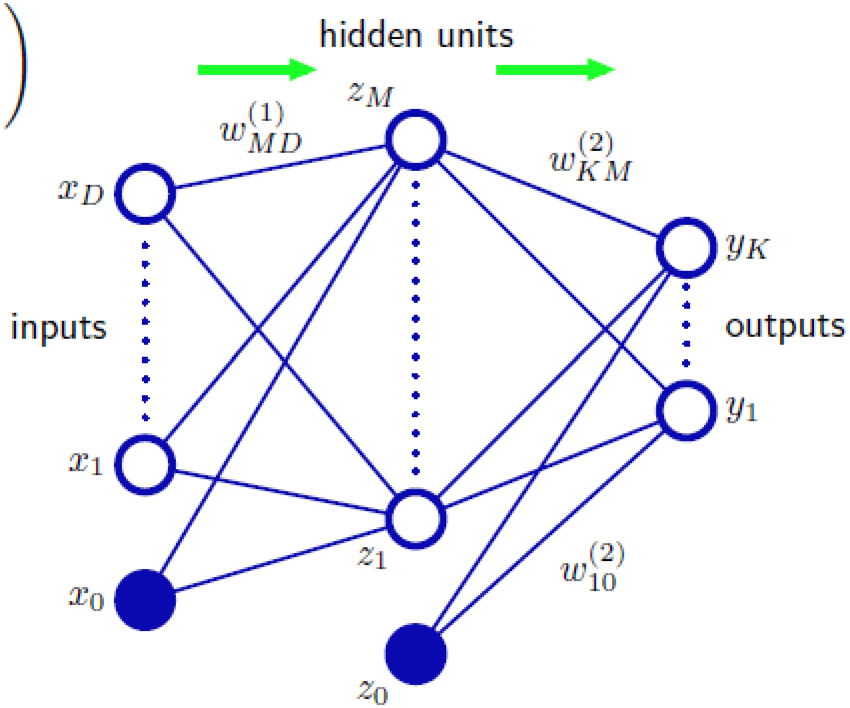
$$y_k(\mathbf{x},\mathbf{w}) = \sigma\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}\right) + w_{k0}^{(2)}\right)$$

- loss function

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N} \|\mathbf{y}(\mathbf{x}_n,\mathbf{w}) - \mathbf{t}_n\|^2.$$

- Error Backpropagation

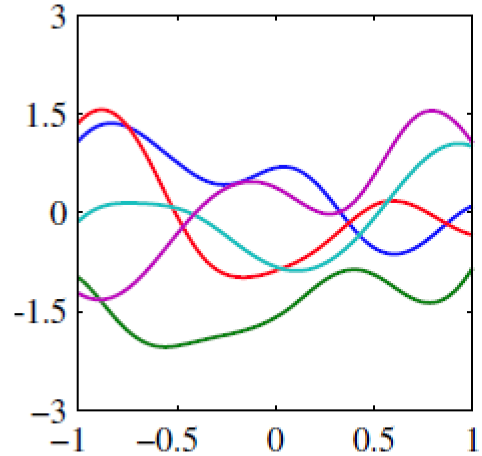


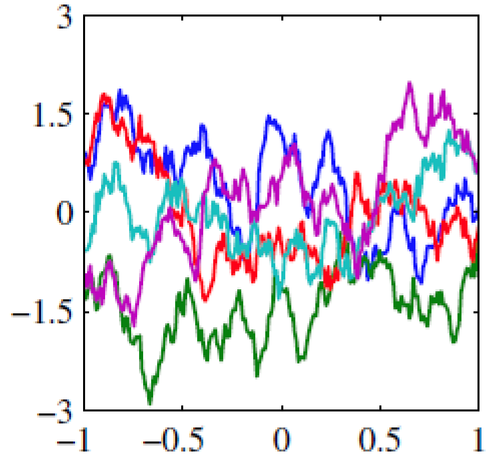


- Regularization
  - *weight decay*
  - *Early stopping*

Review – kernel methods

- $k(x, x') = \phi(x)^{\mathrm{T}}\phi(x') = \sum_{i=1}^{M} \phi_i(x)\phi_i(x')$
- Gaussian Processes
  - Linear regression + prior + kernel trick

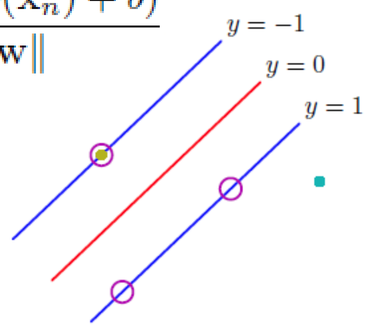




- Kernel SVM
  - SVM + kernel trick

Review – support vector machine

- Maximum Margin Classifiers
  - Distance from point to surface $\frac{t_n y(\mathbf{x}_n)}{\|\mathbf{w}\|} = \frac{t_n(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b)}{\|\mathbf{w}\|}$
  - Maximize the closest distance



$$\arg\max_{\mathbf{w},b} \left\{ \frac{1}{\|\mathbf{w}\|} \min_n \left[t_n \left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b \right) \right] \right\}$$

  - distances not vary with the scales of w and b
  - Closest point $t_n \left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b \right) = 1$ $\min_n \left[t_n \left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b \right) \right] = 1$
  - Others statisfy $t_n \left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b \right) \geqslant 1$
  - Objective $\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$ $t_n \left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b \right) \geqslant 1$

Review – support vector machine

- Maximum Margin Classifiers
  - Objective $\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 \qquad t_n\left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)+b\right) \geqslant 1$
  - Lagrangian function $L(\mathbf{w},b,\mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n\left\{t_n(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)+b)-1\right\}$
  - KKT condition + kernel trick

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n,\mathbf{x}_m)$$

$$a_n \geqslant 0, \qquad n=1,\ldots,N,$$

$$\sum_{n=1}^{N} a_n t_n = 0. \qquad a_n\left\{t_n y(\mathbf{x}_n)-1\right\} = 0.$$

  - Predict $y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x},\mathbf{x}_n) + b.$
  - Dual and KKT

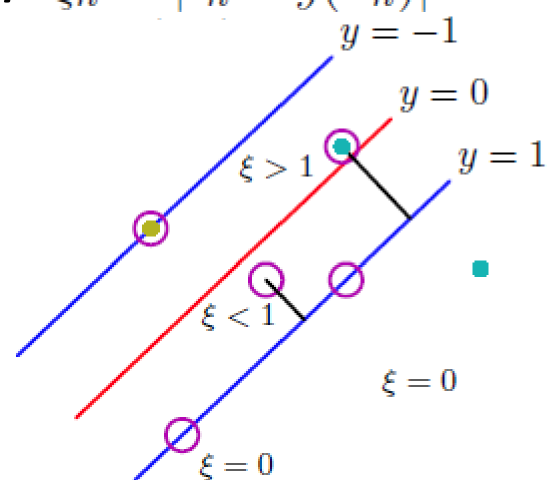
$$\begin{aligned} min \quad & f(x) \\ s.t. \quad & h(x)=0 \\ & g(x)\le 0 \end{aligned}$$

$$\begin{aligned} \nabla(x)+\lambda\nabla h(x)+\mu\nabla g(x)&=0 \\ \mu g(x)&=0 \\ \mu&\ge 0 \\ h(x)&=0 \\ g(x)&\le 0 \end{aligned}$$

Review – support vector machine

- Soft margin SVMs
  - Allow some be misclassified and make penalty
  - introduce *slack variables* $\xi_n = 0$ *or* $\xi_n = |t_n - y(\mathbf{x}_n)|$

$$C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2 \quad t_n y(\mathbf{x}_n) \geqslant 1 - \xi_n$$

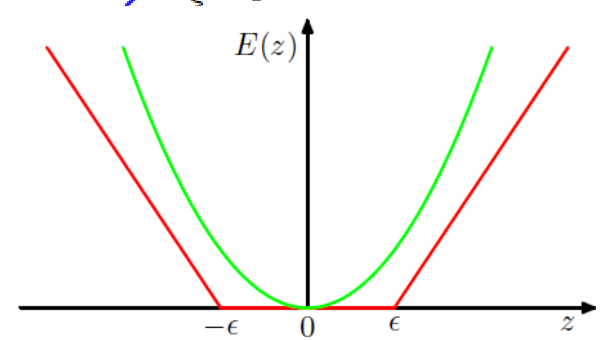


- SVM for regression

$$C\sum_{n=1}^{N}E_\epsilon(y(\mathbf{x}_n) - t_n) + \frac{1}{2}\|\mathbf{w}\|^2$$

$$E_\epsilon(y(\mathbf{x}) - t) = \begin{cases} 0, & \text{if } |y(\mathbf{x}) - t| < \epsilon; \\ |y(\mathbf{x}) - t| - \epsilon, & \text{otherwise} \end{cases}$$

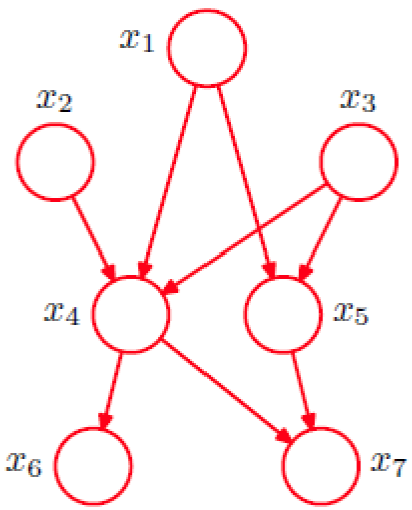
a sparse solution, and the only terms that have to be evaluated in the predictive model

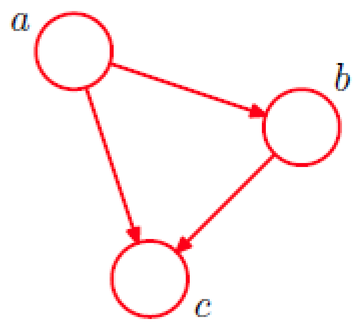


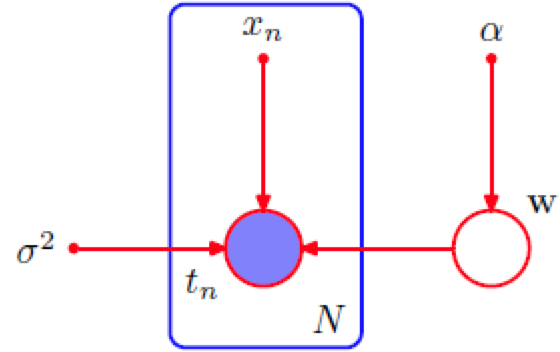
Review – graphical models

- Bayesian networks

$$p(a,b,c) = p(c|a,b)p(b|a)p(a)$$



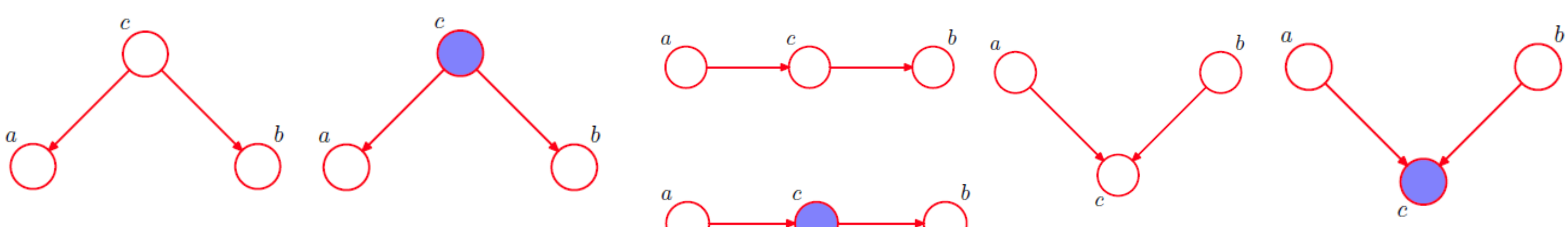




$$p(\mathbf{t}, \mathrm{w}|\mathbf{x}, \alpha, \sigma^2) = p(\mathrm{w}|\alpha) \prod_{n=1}^{N} p(t_n|\mathrm{w}, x_n, \sigma^2)$$

$$p(x_1)p(x_2)p(x_3)p(x_4|x_1,x_2,x_3)p(x_5|x_1,x_3)p(x_6|x_4)p(x_7|x_4,x_5)$$

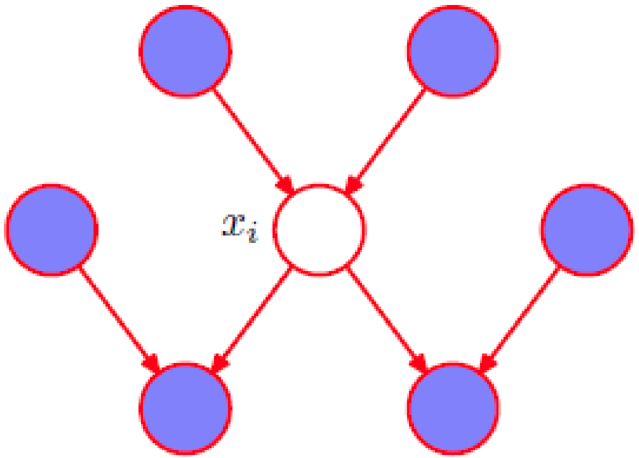
- Conditional independence



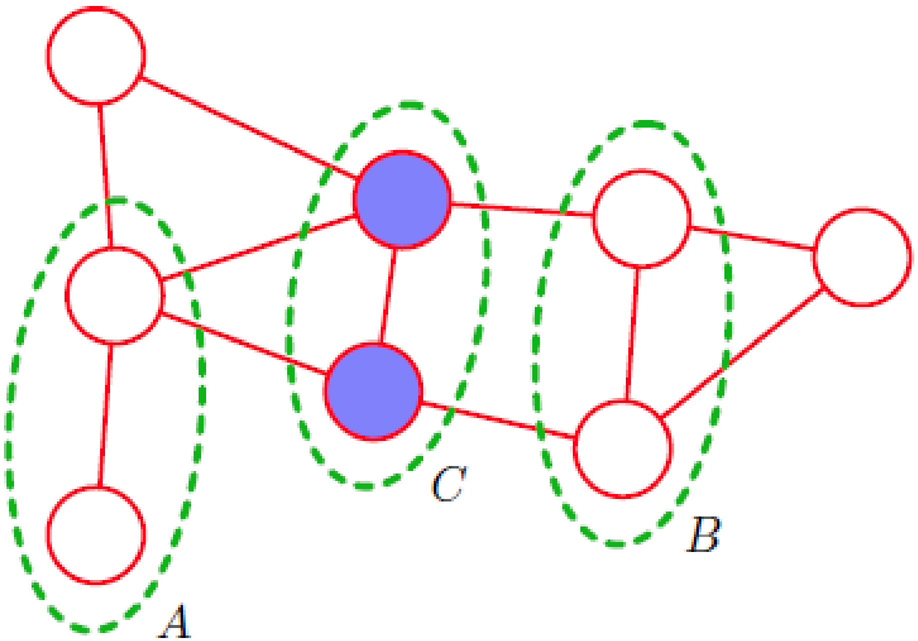
Review – graphical models

The Markov blanket of a node $\mathbf{x}_i$ comprises the set of parents, children and co-parents of the node. It has the property that the conditional distribution of $\mathbf{x}_i$, conditioned on all the remaining variables in the graph, is dependent only on the variables in the Markov blanket.

$$X \perp \{U - MB - \{X\}\} \mid MB$$



An example of an undirected graph in which every path from any node in set A to any node in set B passes through at least one node in set C. Consequently the conditional independence property $A \perp\!\!\!\perp B \mid C$ holds for any probability distribution described by this graph.



Review – EM

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q\|p)$$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} \right\}$$

$$\mathrm{KL}(q\|p) = -\sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})}{q(\mathbf{Z})} \right\}$$

E step Evaluate $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$.

M step Evaluate $\boldsymbol{\theta}^{\text{new}}$ given by

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) \tag{9.32}$$

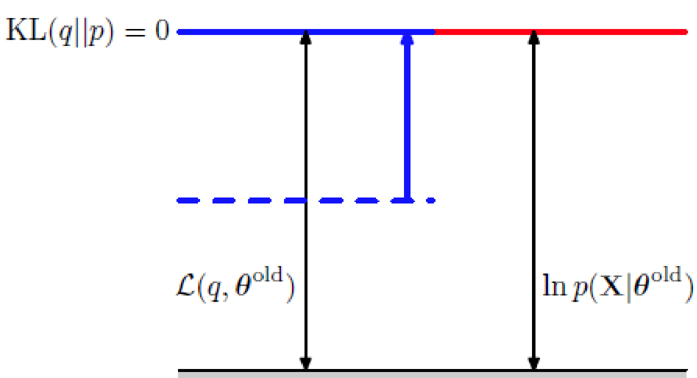
where

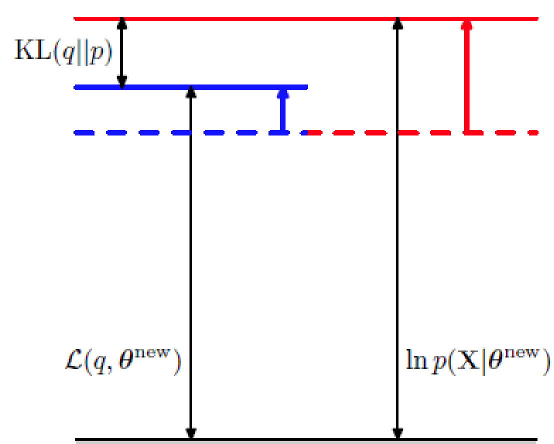
$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}). \tag{9.33}$$

Check for convergence of either the log likelihood or the parameter values. If the convergence criterion is not satisfied, then let

$$\boldsymbol{\theta}^{\text{old}} \leftarrow \boldsymbol{\theta}^{\text{new}} \tag{9.34}$$

and return to step 2.





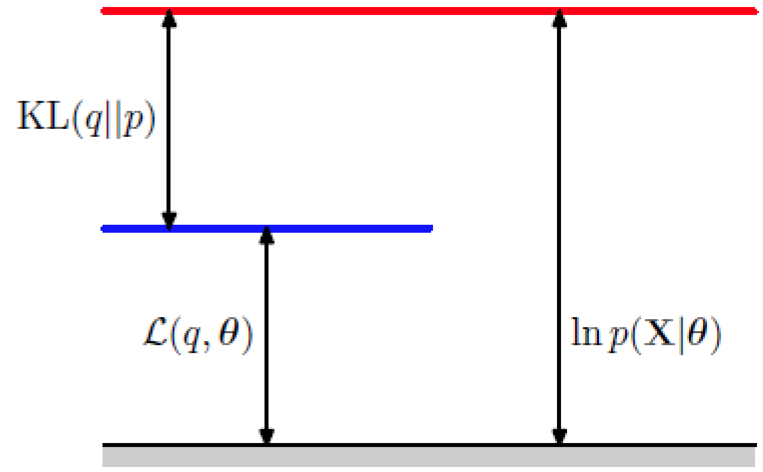
Review – approximate inference

- Variational Inference

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q\|p)$$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} \right\}$$

$$\mathrm{KL}(q\|p) = -\sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})}{q(\mathbf{Z})} \right\}$$



- Mean field

$$\begin{aligned} \mathcal{L}(q) &= \int \prod_i q_i \left\{ \ln p(\mathbf{X}, \mathbf{Z}) - \sum_i \ln q_i \right\} \mathrm{d}\mathbf{Z} \\ &= \int q_j \left\{ \int \ln p(\mathbf{X}, \mathbf{Z}) \prod_{i \neq j} q_i \, \mathrm{d}\mathbf{Z}_i \right\} \mathrm{d}\mathbf{Z}_j - \int q_j \ln q_j \, \mathrm{d}\mathbf{Z}_j + \mathrm{c} \\ &= \int q_j \ln \widetilde{p}(\mathbf{X}, \mathbf{Z}_j) \, \mathrm{d}\mathbf{Z}_j - \int q_j \ln q_j \, \mathrm{d}\mathbf{Z}_j + \mathrm{const} \end{aligned}$$

$$\ln q_j^\star(\mathbf{Z}_j) = \mathbb{E}_{i \neq j}[\ln p(\mathbf{X}, \mathbf{Z})] + \mathrm{c}$$

Review – approximate inference

- exponential family

$$q(\mathbf{z}) = h(\mathbf{z})g(\boldsymbol{\eta}) \exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{z})\right\}$$

$$\mathrm{KL}(p\|q) = -\ln g(\boldsymbol{\eta}) - \boldsymbol{\eta}^{\mathrm{T}}\mathbb{E}_{p(\mathbf{z})}[\mathbf{u}(\mathbf{z})] + \mathrm{const}$$

- With property

$$-\nabla \ln g(\boldsymbol{\eta}) = \mathbb{E}_{p(\mathbf{z})}[\mathbf{u}(\mathbf{z})]$$

$$\mathbb{E}_{q(\mathbf{z})}[\mathbf{u}(\mathbf{z})] = \mathbb{E}_{p(\mathbf{z})}[\mathbf{u}(\mathbf{z})].$$

- Objective

$$\mathrm{KL}\,(p\|q) = \mathrm{KL}\left(\frac{1}{p(\mathcal{D})}\prod_i f_i(\boldsymbol{\theta}) \middle\| \frac{1}{Z}\prod_i \widetilde{f}_i(\boldsymbol{\theta})\right)$$

$$\mathrm{KL}\left(\frac{f_j(\boldsymbol{\theta})q^{\backslash j}(\boldsymbol{\theta})}{Z_j} \middle\| q^{\mathrm{new}}(\boldsymbol{\theta})\right)$$

1. Initialize all of the approximating factors $\widetilde{f}_i(\boldsymbol{\theta})$.
2. Initialize the posterior approximation by setting

$$q(\boldsymbol{\theta}) \propto \prod_i \widetilde{f}_i(\boldsymbol{\theta}).$$

3. Until convergence:
   (a) Choose a factor $\widetilde{f}_j(\boldsymbol{\theta})$ to refine.
   (b) Remove $\widetilde{f}_j(\boldsymbol{\theta})$ from the posterior by division

$$q^{\backslash j}(\boldsymbol{\theta}) = \frac{q(\boldsymbol{\theta})}{\widetilde{f}_j(\boldsymbol{\theta})}.$$

   (c) Evaluate the new posterior by setting the sufficient statistics (moments) of $q^{\mathrm{new}}(\boldsymbol{\theta})$ equal to those of $q^{\backslash j}(\boldsymbol{\theta})f_j(\boldsymbol{\theta})$, including evaluation of the normalization constant

$$Z_j = \int q^{\backslash j}(\boldsymbol{\theta})f_j(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}. \quad (10.206)$$

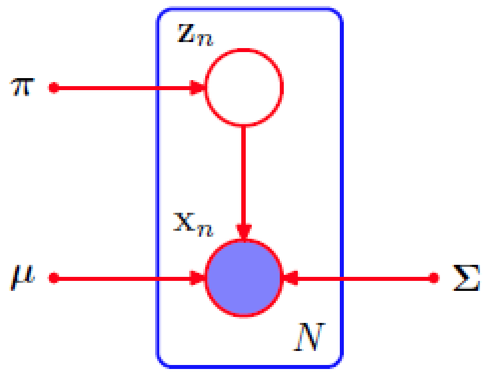
   (d) Evaluate and store the new factor

$$\widetilde{f}_j(\boldsymbol{\theta}) = Z_j\frac{q^{\mathrm{new}}(\boldsymbol{\theta})}{q^{\backslash j}(\boldsymbol{\theta})}. \quad (10.207)$$

Review – mixture model and EM

- K-means
- GMM

$$p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}. \qquad \sum_{k=1}^{K} \pi_k = 1$$



$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}$$

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

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

$$\begin{aligned} \gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) &= \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}. \end{aligned}$$

Review – GMM and EM

- Objective

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \ln\left\{\sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\boldsymbol{\theta})\right\}$$

- EM

$$\mathcal{Q}(\boldsymbol{\theta},\boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\theta})$$

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta},\boldsymbol{\theta}^{\text{old}})$$

$$\ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\left\{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}$$

$$p(\mathbf{Z}|\mathbf{X},\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}) \propto \prod_{n=1}^{N}\prod_{k=1}^{K}\left[\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right]^{z_{nk}}$$

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi})] = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\left\{\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}$$

$$\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K}\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)} = \gamma(z_{nk})$$ =p(z_nk=1|X)

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\left(\mathbf{x}_n-\boldsymbol{\mu}_k^{\text{new}}\right)\left(\mathbf{x}_n-\boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}}$$

$$\pi_k^{\text{new}} = \frac{N_k}{N}$$

Review – sampling methods

- Objective e.g., Monte Carlo EM

$$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})\,\mathrm{d}\mathbf{z}$$

$$\widehat{f} = \frac{1}{L}\sum_{l=1}^{L} f(\mathbf{z}^{(l)}).$$

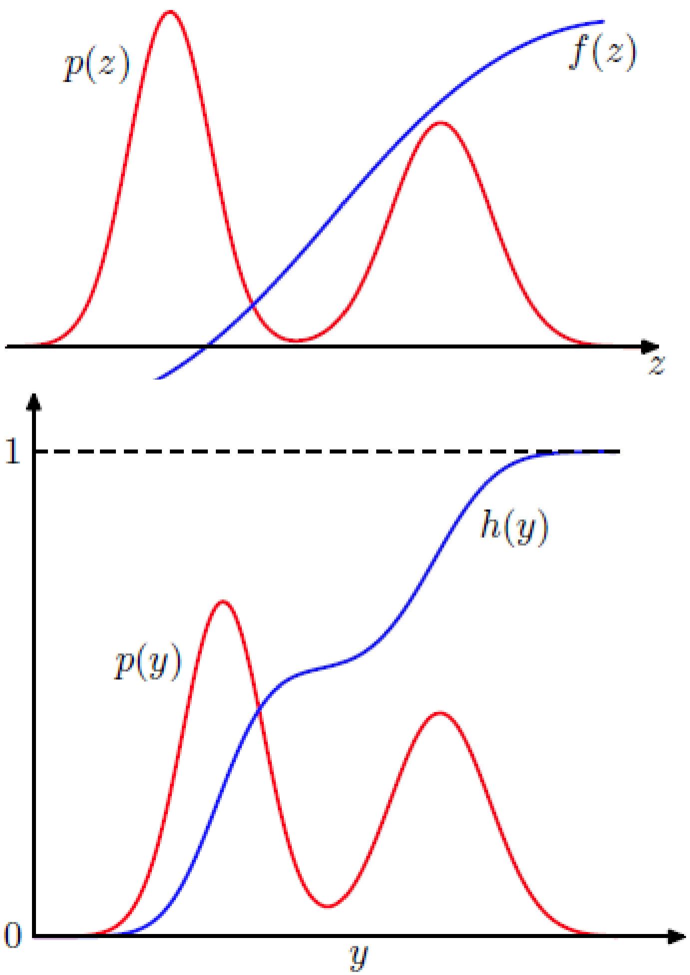
- Standard distributions

$$y = f(z)$$

$$p(y) = p(z)\left|\frac{dz}{dy}\right|$$

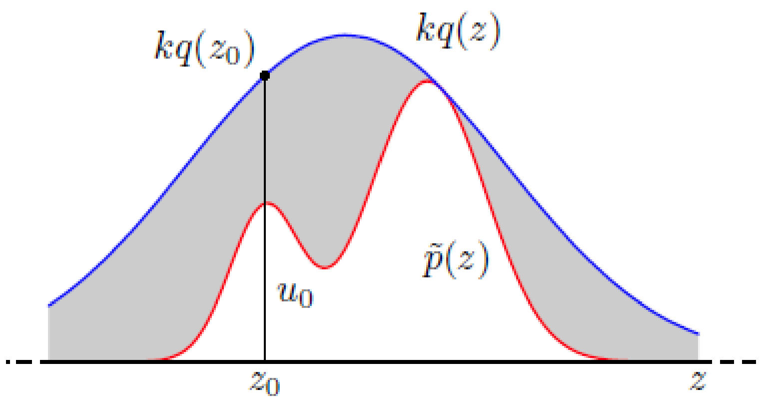
$$z = h(y) \equiv \int_{-\infty}^{y} p(\widehat{y})\,\mathrm{d}\widehat{y}$$

$$y = h^{-1}(z).$$



Review – sampling methods

- Rejection sampling
- Importance sampling
- Markov Chain Monte Carlo
  - Metropolis-Hastings
  - Gibbs Sampling
  - Slice Sampling
  - Hamiltonian Monte Carlo

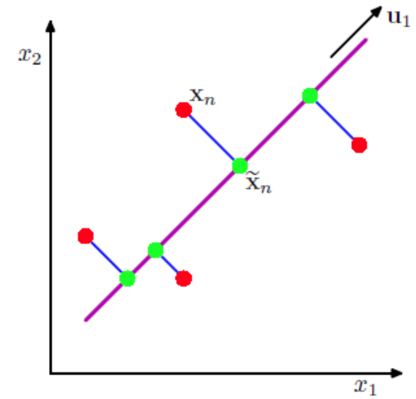


Review – Continuous latent variable

- PCA: maximize the projected variance

$$\overline{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n \qquad \frac{1}{N}\sum_{n=1}^{N}\left\{\mathbf{u}_1^{\mathrm{T}}\mathbf{x}_n - \mathbf{u}_1^{\mathrm{T}}\overline{\mathbf{x}}\right\}^2 = \mathbf{u}_1^{\mathrm{T}}\mathbf{S}\mathbf{u}_1$$

$$\mathbf{S} = \frac{1}{N}\sum_{n=1}(\mathbf{x}_n - \overline{\mathbf{x}})(\mathbf{x}_n - \overline{\mathbf{x}})^{\mathrm{T}}. \qquad \mathbf{u}_1^{\mathrm{T}}\mathbf{S}\mathbf{u}_1 + \lambda_1\left(1 - \mathbf{u}_1^{\mathrm{T}}\mathbf{u}_1\right)$$



- Probabilistic PCA

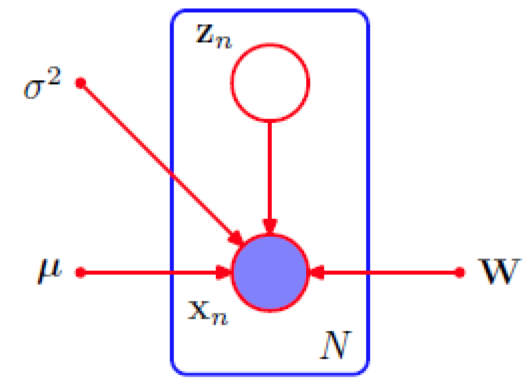
$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}). \qquad p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$$

$$p(\mathbf{z}|\mathbf{x}) = \mathcal{N}\left(\mathbf{z}|\mathbf{M}^{-1}\mathbf{W}^{\mathrm{T}}(\mathbf{x} - \boldsymbol{\mu}), \sigma^{-2}\mathbf{M}\right)$$

  - Maximum likelihood PCA

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \mathbf{W}, \sigma^2) = \sum_{n=1}^{N}\ln p(\mathbf{x}_n|\mathbf{W}, \boldsymbol{\mu}, \sigma^2)$$

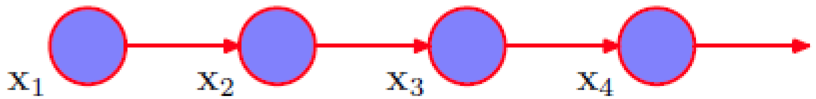
$$\mathbf{W}_{\mathrm{ML}} = \mathbf{U}_M(\mathbf{L}_M - \sigma^2\mathbf{I})^{1/2}\mathbf{R} \qquad \sigma^2_{\mathrm{ML}} = \frac{1}{D-M}\sum_{i=M+1}^{D}\lambda_i$$



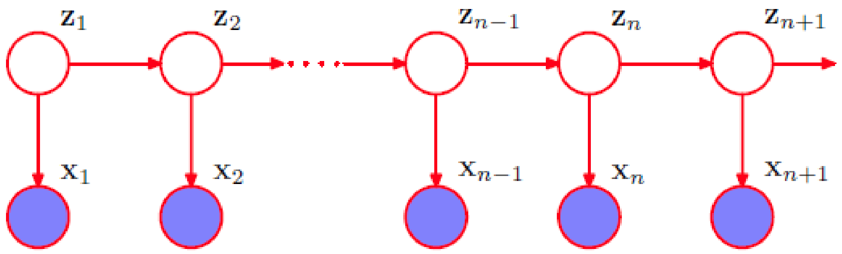
- Factor analysis
  - Ψ is a $D \times D$ diagonal matrix with different elements $\quad p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \boldsymbol{\Psi})$

Review – sequential data

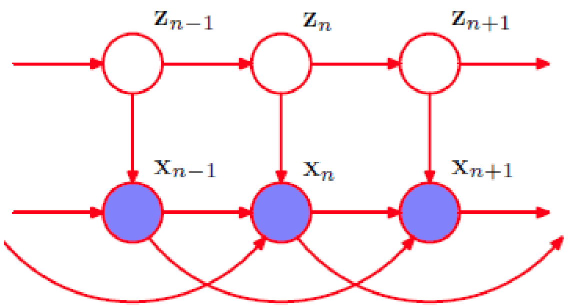
- Markov models



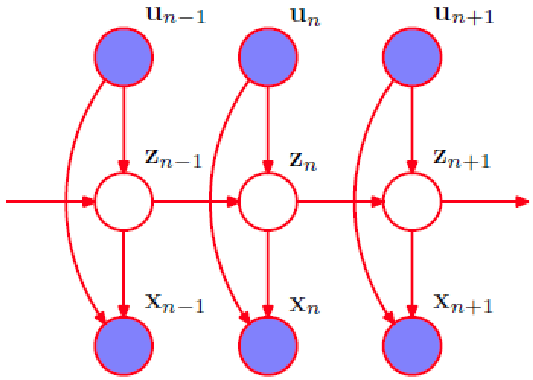
- Hidden Markov models



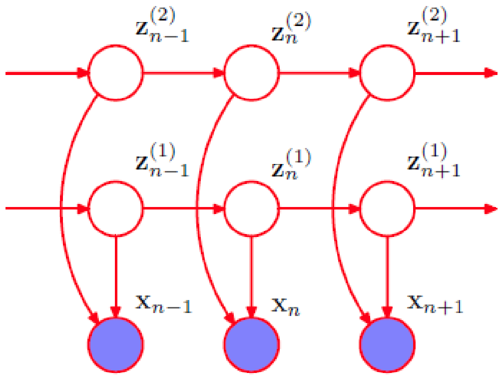
- autoregressive HMM



- input-output HMM



- Factorial HMM



- Linear Dynamical System

参考资料

- Christopher M. Bishop. Pattern Recognition and Machine Learning, Springer, 2006.