

#### Parametric Distributions

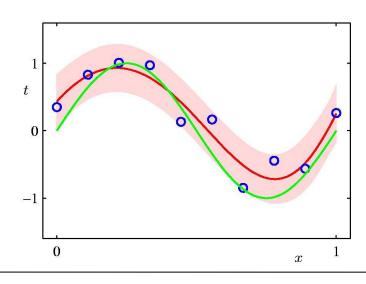
Basic building blocks:  $p(\mathbf{x}|\boldsymbol{\theta})$ 

Need to determine  $\boldsymbol{\theta}$  given  $\{\mathbf{x}_1,\dots,\mathbf{x}_N\}$ 

Representation:  $\theta^*$  or  $p(\theta)$ ?

### Recall Curve Fitting

$$p(t|x, \mathbf{x}, \mathbf{t}) = \int p(t|x, \mathbf{w}) p(\mathbf{w}|\mathbf{x}, \mathbf{t}) d\mathbf{w}$$



# Binary Variables (1)

Coin flipping: heads=1, tails=0

$$p(x=1|\mu) = \mu$$

#### Bernoulli Distribution

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

$$\mathbb{E}[x] = \mu$$

$$\operatorname{var}[x] = \mu(1-\mu)$$

# Binary Variables (2)

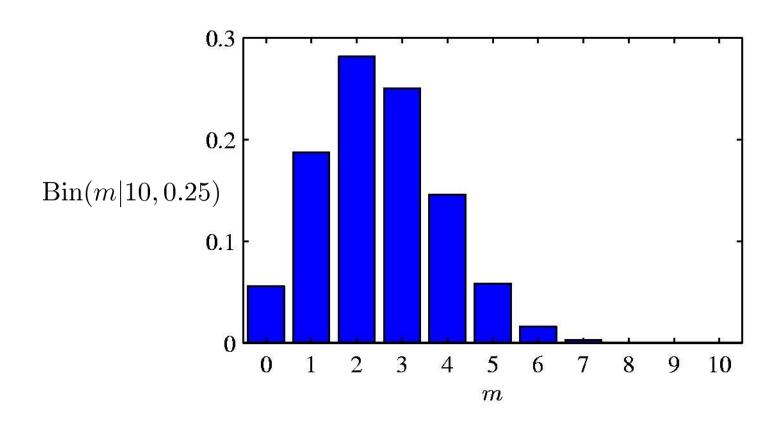
### N coin flips:

$$p(m \text{ heads}|N,\mu)$$

#### **Binomial Distribution**

$$\operatorname{Bin}(m|N,\mu) = \binom{N}{m} \mu^m (1-\mu)^{N-m}$$
 
$$\mathbb{E}[m] \equiv \sum_{m=0}^{N} m \operatorname{Bin}(m|N,\mu) = N\mu$$
 
$$\operatorname{var}[m] \equiv \sum_{m=0}^{N} (m - \mathbb{E}[m])^2 \operatorname{Bin}(m|N,\mu) = N\mu (1-\mu)$$

## **Binomial Distribution**



# Parameter Estimation (1)

#### ML for Bernoulli

Given:  $\mathcal{D} = \{x_1, \dots, x_N\}, m \text{ heads } (1), N-m \text{ tails } (0)$ 

$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \prod_{n=1}^{N} \mu^{x_n} (1-\mu)^{1-x_n}$$

$$\ln p(\mathcal{D}|\mu) = \sum_{n=1}^{N} \ln p(x_n|\mu) = \sum_{n=1}^{N} \{x_n \ln \mu + (1 - x_n) \ln(1 - \mu)\}$$

$$\mu_{\rm ML} = \frac{1}{N} \sum_{n=1}^{N} x_n = \frac{m}{N}$$

# Parameter Estimation (2)

**Example:** 
$$\mathcal{D} = \{1, 1, 1\} \rightarrow \mu_{\text{ML}} = \frac{3}{3} = 1$$

Prediction: all future tosses will land heads up

Overfitting to  $\mathcal{D}$ 

#### **Beta Distribution**

Distribution over  $\mu \in [0, 1]$ .

Beta
$$(\mu|a,b)$$
 =  $\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1}$   
 $\mathbb{E}[\mu]$  =  $\frac{a}{a+b}$   
 $\operatorname{var}[\mu]$  =  $\frac{ab}{(a+b)^2(a+b+1)}$ 

# Bayesian Bernoulli

$$p(\mu|a_0, b_0, \mathcal{D}) \propto p(\mathcal{D}|\mu)p(\mu|a_0, b_0)$$

$$= \left(\prod_{n=1}^N \mu^{x_n} (1-\mu)^{1-x_n}\right) \operatorname{Beta}(\mu|a_0, b_0)$$

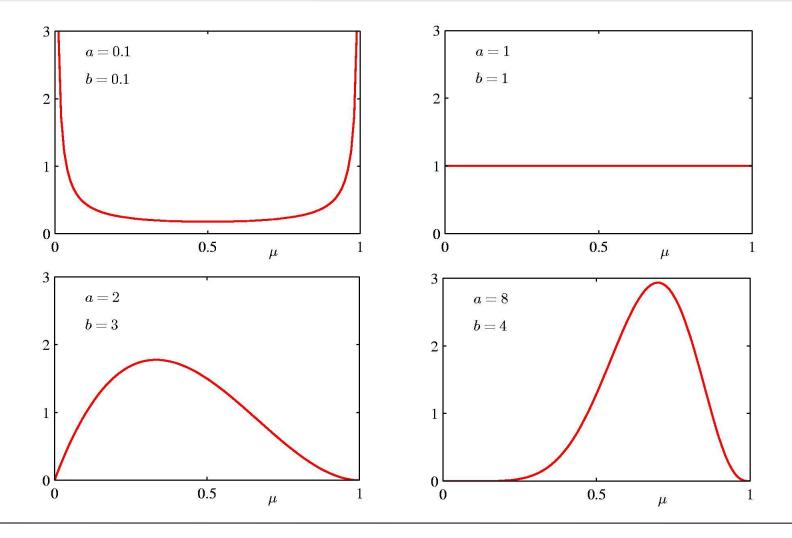
$$\propto \mu^{m+a_0-1} (1-\mu)^{(N-m)+b_0-1}$$

$$\propto \operatorname{Beta}(\mu|a_N, b_N)$$

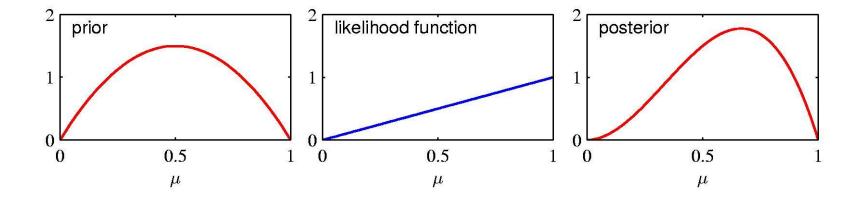
$$a_N = a_0 + m \qquad b_N = b_0 + (N-m)$$

The Beta distribution provides the *conjugate* prior for the Bernoulli distribution.

## **Beta Distribution**



## Prior · Likelihood = Posterior



## Properties of the Posterior

As the size of the data set, N, increase

$$a_N \rightarrow m$$
 $b_N \rightarrow N-m$ 

$$\mathbb{E}[\mu] = \frac{a_N}{a_N + b_N} \rightarrow \frac{m}{N} = \mu_{\text{ML}}$$

$$\text{var}[\mu] = \frac{a_N b_N}{(a_N + b_N)^2 (a_N + b_N + 1)} \rightarrow 0$$

#### Prediction under the Posterior

What is the probability that the next coin toss will land heads up?

$$p(x = 1|a_0, b_0, \mathcal{D}) = \int_0^1 p(x = 1|\mu) p(\mu|a_0, b_0, \mathcal{D}) d\mu$$

$$= \int_0^1 \mu p(\mu|a_0, b_0, \mathcal{D}) d\mu$$

$$= \mathbb{E}[\mu|a_0, b_0, \mathcal{D}] = \frac{a_N}{b_N}$$

### Multinomial Variables

1-of-K coding scheme:  $\mathbf{x} = (0, 0, 1, 0, 0, 0)^{\mathrm{T}}$ 

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k}$$

$$\forall k: \mu_k \geqslant 0 \quad \text{and} \quad \sum_{k=1}^K \mu_k = 1$$

$$\mathbb{E}[\mathbf{x}|\boldsymbol{\mu}] = \sum_{\mathbf{x}} p(\mathbf{x}|\boldsymbol{\mu})\mathbf{x} = (\mu_1, \dots, \mu_K)^{\mathrm{T}} = \boldsymbol{\mu}$$

$$\sum_{\mathbf{x}} p(\mathbf{x}|\boldsymbol{\mu}) = \sum_{k=1}^{K} \mu_k = 1$$

#### ML Parameter estimation

Given:  $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ 

$$p(\mathcal{D}|\boldsymbol{\mu}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \mu_k^{x_{nk}} = \prod_{k=1}^{K} \mu_k^{(\sum_n x_{nk})} = \prod_{k=1}^{K} \mu_k^{m_k}$$

Ensure  $\sum_k \mu_k = 1$ , use a Lagrange multiplier,  $\lambda$ .

$$\sum_{k=1}^{K} m_k \ln \mu_k + \lambda \left( \sum_{k=1}^{K} \mu_k - 1 \right)$$

$$\mu_k = -m_k/\lambda \qquad \mu_k^{\rm ML} = \frac{m_k}{N}$$

### The Multinomial Distribution

$$\operatorname{Mult}(m_1, m_2, \dots, m_K | \boldsymbol{\mu}, N) = \begin{pmatrix} N \\ m_1 m_2 \dots m_K \end{pmatrix} \prod_{k=1}^{N} \mu_k^{m_k}$$

$$\mathbb{E}[m_k] = N \mu_k$$

$$\operatorname{var}[m_k] = N \mu_k (1 - \mu_k)$$

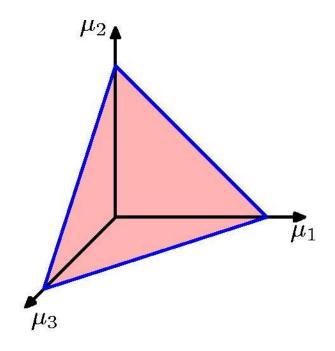
$$\operatorname{cov}[m_j m_k] = -N \mu_j \mu_k$$

### The Dirichlet Distribution

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

$$\alpha_0 = \sum_{k=1}^K \alpha_k$$

Conjugate prior for the multinomial distribution.



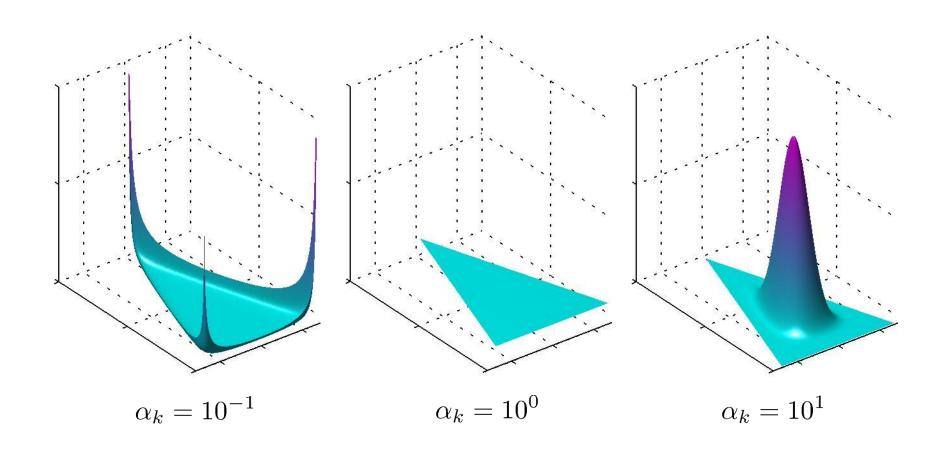
# Bayesian Multinomial (1)

$$p(\boldsymbol{\mu}|\mathcal{D}, \boldsymbol{\alpha}) \propto p(\mathcal{D}|\boldsymbol{\mu})p(\boldsymbol{\mu}|\boldsymbol{\alpha}) \propto \prod_{k=1}^{K} \mu_k^{\alpha_k + m_k - 1}$$

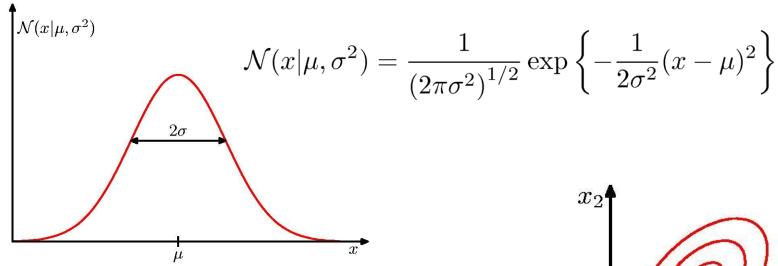
$$p(\boldsymbol{\mu}|\mathcal{D}, \boldsymbol{\alpha}) = \operatorname{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha} + \mathbf{m})$$

$$= \frac{\Gamma(\alpha_0 + N)}{\Gamma(\alpha_1 + m_1) \cdots \Gamma(\alpha_K + m_K)} \prod_{k=1}^K \mu_k^{\alpha_k + m_k - 1}$$

# Bayesian Multinomial (2)



### The Gaussian Distribution

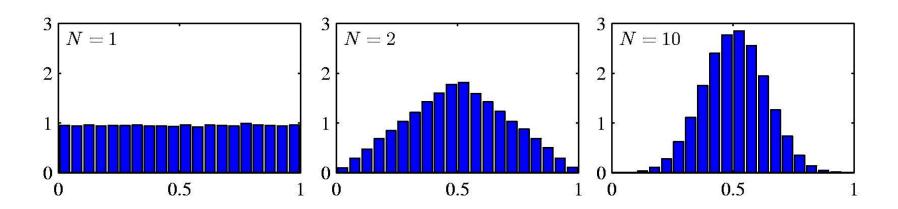


$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right\}$$

#### Central Limit Theorem

The distribution of the sum of N i.i.d. random variables becomes increasingly Gaussian as N grows.

Example: N uniform [0,1] random variables.



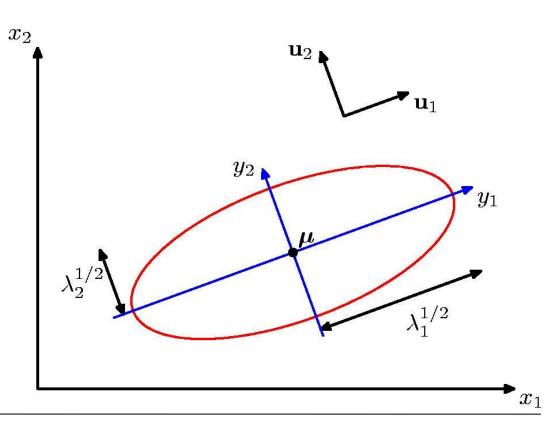
# Geometry of the Multivariate Gaussian

$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})$$

$$\mathbf{\Sigma}^{-1} = \sum_{i=1}^{D} \frac{1}{\lambda_i} \mathbf{u}_i \mathbf{u}_i^{\mathrm{T}}$$

$$\Delta^2 = \sum_{i=1}^D \frac{y_i^2}{\lambda_i}$$

$$y_i = \mathbf{u}_i^{\mathrm{T}}(\mathbf{x} - \boldsymbol{\mu})$$



## Moments of the Multivariate Gaussian (1)

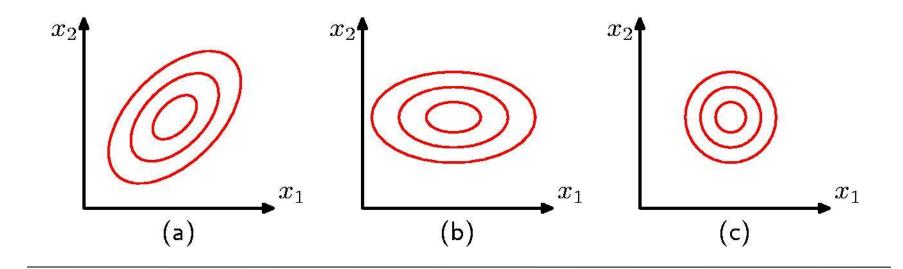
$$\mathbb{E}[\mathbf{x}] = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\mathbf{\Sigma}|^{1/2}} \int \exp\left\{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right\} \mathbf{x} \, d\mathbf{x}$$
$$= \frac{1}{(2\pi)^{D/2}} \frac{1}{|\mathbf{\Sigma}|^{1/2}} \int \exp\left\{-\frac{1}{2} \mathbf{z}^{\mathrm{T}} \mathbf{\Sigma}^{-1} \mathbf{z}\right\} (\mathbf{z} + \boldsymbol{\mu}) \, d\mathbf{z}$$

thanks to anti-symmetry of z

$$\mathbb{E}[\mathbf{x}] = oldsymbol{\mu}$$

## Moments of the Multivariate Gaussian (2)

$$\mathbb{E}[\mathbf{x}\mathbf{x}^{\mathrm{T}}] = \boldsymbol{\mu}\boldsymbol{\mu}^{\mathrm{T}} + \boldsymbol{\Sigma}$$
  $\operatorname{cov}[\mathbf{x}] = \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^{\mathrm{T}}\right] = \boldsymbol{\Sigma}$ 



#### Partitioned Gaussian Distributions

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$\mathbf{x} = egin{pmatrix} \mathbf{x}_a \ \mathbf{x}_b \end{pmatrix} \qquad \qquad oldsymbol{\mu} = egin{pmatrix} oldsymbol{\mu}_a \ oldsymbol{\mu}_b \end{pmatrix} \qquad \qquad oldsymbol{\Sigma} = egin{pmatrix} oldsymbol{\Sigma}_{aa} & oldsymbol{\Sigma}_{ab} \ oldsymbol{\Sigma}_{ba} & oldsymbol{\Sigma}_{bb} \end{pmatrix} .$$

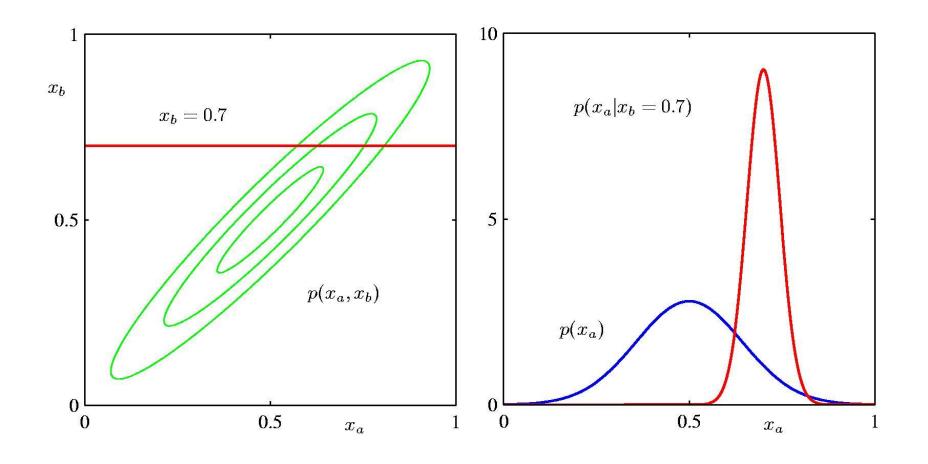
$$oldsymbol{\Lambda} \equiv oldsymbol{\Sigma}^{-1} \qquad \qquad oldsymbol{\Lambda} = egin{pmatrix} oldsymbol{\Lambda}_{aa} & oldsymbol{\Lambda}_{ab} \ oldsymbol{\Lambda}_{ba} & oldsymbol{\Lambda}_{bb} \end{pmatrix}$$

## Partitioned Conditionals and Marginals

$$egin{aligned} p(\mathbf{x}_a|\mathbf{x}_b) &= \mathcal{N}(\mathbf{x}_a|oldsymbol{\mu}_{a|b},oldsymbol{\Sigma}_{a|b}) \ oldsymbol{\Sigma}_{a|b} &= & oldsymbol{\Lambda}_{aa}^{-1} = oldsymbol{\Sigma}_{aa} - oldsymbol{\Sigma}_{ab}oldsymbol{\Sigma}_{bb}^{-1}oldsymbol{\Sigma}_{ba} \ oldsymbol{\mu}_{a|b} &= & oldsymbol{\Sigma}_{a|b}\left\{oldsymbol{\Lambda}_{aa}oldsymbol{\mu}_{a} - oldsymbol{\Lambda}_{ab}(\mathbf{x}_b - oldsymbol{\mu}_{b})
ight\} \ &= & oldsymbol{\mu}_{a} - oldsymbol{\Lambda}_{aa}^{-1}oldsymbol{\Lambda}_{ab}(\mathbf{x}_b - oldsymbol{\mu}_{b}) \ &= & oldsymbol{\mu}_{a} + oldsymbol{\Sigma}_{ab}oldsymbol{\Sigma}_{bb}^{-1}(\mathbf{x}_b - oldsymbol{\mu}_{b}) \end{aligned}$$

$$p(\mathbf{x}_a) = \int p(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_b$$
$$= \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$$

# Partitioned Conditionals and Marginals



# Bayes' Theorem for Gaussian Variables

#### Given

$$p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$$
  
 $p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\mathbf{x} + \mathbf{b}, \mathbf{L}^{-1})$ 

we have

$$p(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\mathrm{T}})$$
$$p(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{x}|\mathbf{\Sigma}\{\mathbf{A}^{\mathrm{T}}\mathbf{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\}, \boldsymbol{\Sigma})$$

where

$$\mathbf{\Sigma} = (\mathbf{\Lambda} + \mathbf{A}^{\mathrm{T}} \mathbf{L} \mathbf{A})^{-1}$$

## Maximum Likelihood for the Gaussian (1)

Given i.i.d. data  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)^T$ , the log likelihood function is given by

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{ND}{2} \ln(2\pi) - \frac{N}{2} \ln|\boldsymbol{\Sigma}| - \frac{1}{2} \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu})$$

#### Sufficient statistics

$$\sum_{n=1}^{N} \mathbf{x}_n \qquad \qquad \sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^{\mathrm{T}}$$

## Maximum Likelihood for the Gaussian (2)

Set the derivative of the log likelihood function to zero,

$$\frac{\partial}{\partial \boldsymbol{\mu}} \ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}) = 0$$

and solve to obtain

$$\mu_{\mathrm{ML}} = rac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n.$$

Similarly

$$\mathbf{\Sigma}_{\mathrm{ML}} = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}}) (\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^{\mathrm{T}}.$$

## Maximum Likelihood for the Gaussian (3)

#### Under the true distribution

$$egin{array}{lll} \mathbb{E}[oldsymbol{\mu}_{ ext{ML}}] &=& oldsymbol{\mu} \ \mathbb{E}[oldsymbol{\Sigma}_{ ext{ML}}] &=& rac{N-1}{N}oldsymbol{\Sigma}. \end{array}$$

#### Hence define

$$\widetilde{\Sigma} = \frac{1}{N-1} \sum_{n=1}^{N} (\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}}) (\mathbf{x}_n - \boldsymbol{\mu}_{\mathrm{ML}})^{\mathrm{T}}.$$

## Sequential Estimation

### Contribution of the $N^{ m th}$ data point, ${f x}_N$

$$\begin{array}{lll} \boldsymbol{\mu}_{\mathrm{ML}}^{(N)} & = & \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_{n} \\ & = & \frac{1}{N} \mathbf{x}_{N} + \frac{1}{N} \sum_{n=1}^{N-1} \mathbf{x}_{n} \\ & = & \frac{1}{N} \mathbf{x}_{N} + \frac{N-1}{N} \boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)} \\ & = & \boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)} + \frac{1}{N} (\mathbf{x}_{N} - \boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)}) \\ & & \stackrel{>}{\longrightarrow} \text{correction given } \mathbf{x}_{N} \\ & & \stackrel{>}{\longrightarrow} \text{old estimate} \end{array}$$

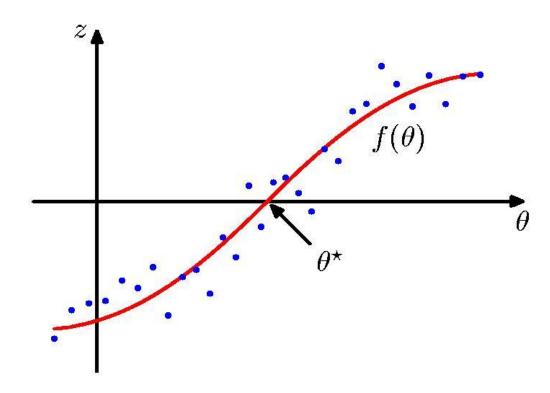
# The Robbins-Monro Algorithm (1)

Consider  $\theta$  and z governed by  $p(z,\theta)$  and define the *regression function* 

$$f(\theta) \equiv \mathbb{E}[z|\theta] = \int zp(z|\theta) dz$$

Seek  $\theta^*$  such that  $f(\theta^*) = 0$ .

# The Robbins-Monro Algorithm (2)



Assume we are given samples from  $p(z,\theta)$ , one at the time.

# The Robbins-Monro Algorithm (3)

Successive estimates of  $\theta^*$  are then given by

$$\theta^{(N)} = \theta^{(N-1)} - a_{N-1} z(\theta^{(N-1)}).$$

Conditions on  $a_N$  for convergence :

$$\lim_{N \to \infty} a_N = 0 \qquad \sum_{N=1}^{\infty} a_N = \infty \qquad \sum_{N=1}^{\infty} a_N^2 < \infty$$

## Robbins-Monro for Maximum Likelihood (1)

#### Regarding

$$-\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \frac{\partial}{\partial \theta} \ln p(x_n|\theta) = \mathbb{E}_x \left[ -\frac{\partial}{\partial \theta} \ln p(x|\theta) \right]$$

as a regression function, finding its root is equivalent to finding the maximum likelihood solution  $\theta_{\rm ML}$ . Thus

$$\theta^{(N)} = \theta^{(N-1)} - a_{N-1} \frac{\partial}{\partial \theta^{(N-1)}} \left[ -\ln p(x_N | \theta^{(N-1)}) \right].$$

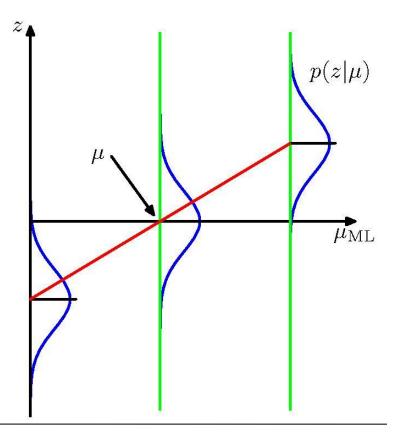
#### Robbins-Monro for Maximum Likelihood (2)

Example: estimate the mean of a Gaussian.

$$z = \frac{\partial}{\partial \mu_{\rm ML}} \left[ -\ln p(x|\mu_{\rm ML}, \sigma^2) \right]$$
$$= -\frac{1}{\sigma^2} (x - \mu_{\rm ML})$$

The distribution of z is Gaussian with mean  $\mu-\mu_{\rm ML}$ .

For the Robbins-Monro update equation,  $a_N=\sigma^2/N$ .



## Bayesian Inference for the Gaussian (1)

Assume  $\sigma^2$  is known. Given i.i.d. data  $\mathbf{x} = \{x_1, \dots, x_N\}$  , the likelihood function for  $\mu$  is given by

$$p(\mathbf{x}|\mu) = \prod_{n=1}^{N} p(x_n|\mu) = \frac{1}{(2\pi\sigma^2)^{N/2}} \exp\left\{-\frac{1}{2\sigma^2} \sum_{n=1}^{N} (x_n - \mu)^2\right\}.$$

This has a Gaussian shape as a function of  $\mu$  (but it is *not* a distribution over  $\mu$ ).

# Bayesian Inference for the Gaussian (2)

Combined with a Gaussian prior over  $\mu$ ,

$$p(\mu) = \mathcal{N}\left(\mu|\mu_0, \sigma_0^2\right).$$

this gives the posterior

$$p(\mu|\mathbf{x}) \propto p(\mathbf{x}|\mu)p(\mu).$$

Completing the square over  $\mu$ , we see that

$$p(\mu|\mathbf{x}) = \mathcal{N}\left(\mu|\mu_N, \sigma_N^2\right)$$

# Bayesian Inference for the Gaussian (3)

#### ... where

$$\mu_{N} = \frac{\sigma^{2}}{N\sigma_{0}^{2} + \sigma^{2}}\mu_{0} + \frac{N\sigma_{0}^{2}}{N\sigma_{0}^{2} + \sigma^{2}}\mu_{ML}, \qquad \mu_{ML} = \frac{1}{N}\sum_{n=1}^{N}x_{n}$$

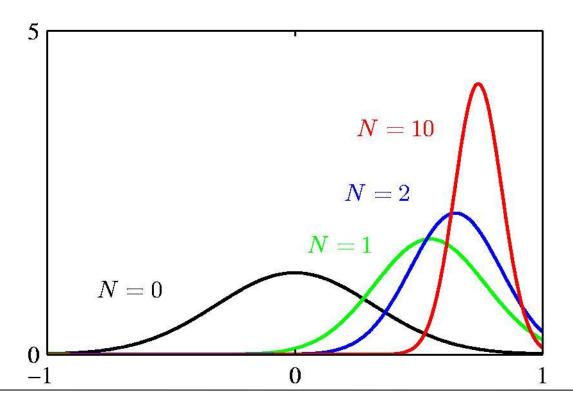
$$\frac{1}{\sigma_{N}^{2}} = \frac{1}{\sigma_{0}^{2}} + \frac{N}{\sigma^{2}}.$$

#### Note:

$$egin{array}{|c|c|c|c|c|} \hline N=0 & N 
ightarrow \infty \\ \hline \mu_N & \mu_0 & \mu_{
m ML} \\ \sigma_N^2 & \sigma_0^2 & 0 \\ \hline \end{array}$$

## Bayesian Inference for the Gaussian (4)

Example:  $p(\mu|\mathbf{x}) = \mathcal{N}\left(\mu|\mu_N, \sigma_N^2\right)$  for  $N=0,\ 1,\ 2$  and 10.



## Bayesian Inference for the Gaussian (5)

#### Sequential Estimation

$$p(\mu|\mathbf{x}) \propto p(\mu)p(\mathbf{x}|\mu)$$

$$= \left[p(\mu)\prod_{n=1}^{N-1}p(x_n|\mu)\right]p(x_N|\mu)$$

$$\propto \mathcal{N}\left(\mu|\mu_{N-1},\sigma_{N-1}^2\right)p(x_N|\mu)$$

The posterior obtained after observing N-1 data points becomes the prior when we observe the  $N^{\rm th}$  data point.

# Bayesian Inference for the Gaussian (6)

Now assume  $\mu$  is known. The likelihood function for  $\lambda=1/\sigma^2$  is given by

$$p(\mathbf{x}|\lambda) = \prod_{n=1}^{N} \mathcal{N}(x_n|\mu, \lambda^{-1}) \propto \lambda^{N/2} \exp\left\{-\frac{\lambda}{2} \sum_{n=1}^{N} (x_n - \mu)^2\right\}.$$

This has a Gamma shape as a function of  $\lambda$ .

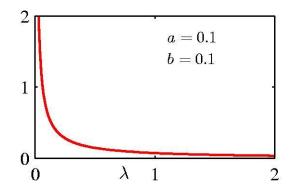
# Bayesian Inference for the Gaussian (7)

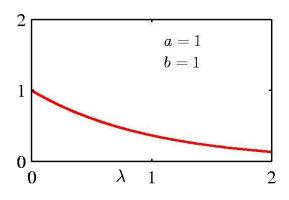
#### The Gamma distribution

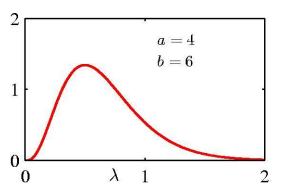
$$Gam(\lambda|a,b) = \frac{1}{\Gamma(a)}b^a\lambda^{a-1}\exp(-b\lambda)$$

$$\mathbb{E}[\lambda] = \frac{a}{b}$$

$$\operatorname{var}[\lambda] = \frac{a}{b^2}$$







# Bayesian Inference for the Gaussian (8)

Now we combine a Gamma prior,  $Gam(\lambda|a_0,b_0)$ , with the likelihood function for  $\lambda$  to obtain

$$p(\lambda|\mathbf{x}) \propto \lambda^{a_0-1} \lambda^{N/2} \exp\left\{-b_0 \lambda - \frac{\lambda}{2} \sum_{n=1}^{N} (x_n - \mu)^2\right\}$$

which we recognize as  $Gam(\lambda|a_N,b_N)$  with

$$a_N = a_0 + \frac{N}{2}$$

$$b_N = b_0 + \frac{1}{2} \sum_{n=1}^{N} (x_n - \mu)^2 = b_0 + \frac{N}{2} \sigma_{\text{ML}}^2.$$

### Bayesian Inference for the Gaussian (9)

If both  $\mu$  and  $\lambda$  are unknown, the joint likelihood function is given by

$$p(\mathbf{x}|\mu,\lambda) = \prod_{n=1}^{N} \left(\frac{\lambda}{2\pi}\right)^{1/2} \exp\left\{-\frac{\lambda}{2}(x_n - \mu)^2\right\}$$

$$\propto \left[\lambda^{1/2} \exp\left(-\frac{\lambda\mu^2}{2}\right)\right]^N \exp\left\{\lambda\mu \sum_{n=1}^{N} x_n - \frac{\lambda}{2} \sum_{n=1}^{N} x_n^2\right\}.$$

We need a prior with the same functional dependence on  $\mu$  and  $\lambda$ .

#### Bayesian Inference for the Gaussian (10)

#### The Gaussian-gamma distribution

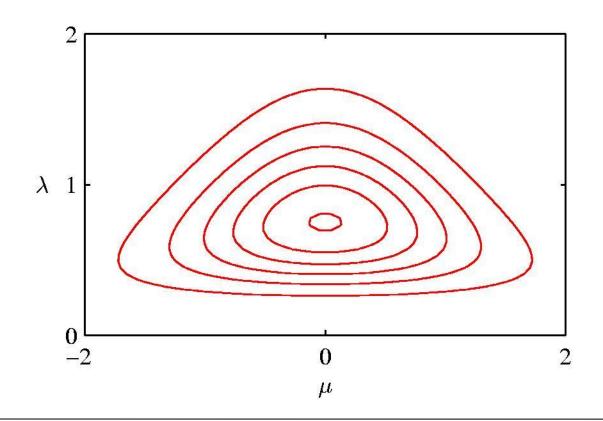
$$p(\mu, \lambda) = \mathcal{N}(\mu | \mu_0, (\beta \lambda)^{-1}) \operatorname{Gam}(\lambda | a, b)$$

$$\propto \exp\left\{-\frac{\beta \lambda}{2} (\mu - \mu_0)^2\right\} \lambda^{a-1} \exp\left\{-b\lambda\right\}$$

- Linear in  $\lambda$ .
- Quadratic in  $\mu$ . Gamma distribution over  $\lambda$ .
  - Independent of  $\mu$ .

#### Bayesian Inference for the Gaussian (11)

#### The Gaussian-gamma distribution



#### Bayesian Inference for the Gaussian (12)

#### Multivariate conjugate priors

- $\mu$  unknown,  $\Lambda$  known:  $p(\mu)$  Gaussian.
- $\Lambda$  unknown,  $\mu$  known:  $p(\Lambda)$  Wishart,

$$W(\mathbf{\Lambda}|\mathbf{W}, \nu) = B|\mathbf{\Lambda}|^{(\nu-D-1)/2} \exp\left(-\frac{1}{2}\text{Tr}(\mathbf{W}^{-1}\mathbf{\Lambda})\right).$$

•  $\Lambda$  and  $\mu$  unknown:  $p(\mu, \Lambda)$  Gaussian-Wishart,  $p(\mu, \Lambda | \mu_0, \beta, \mathbf{W}, \nu) = \mathcal{N}(\mu | \mu_0, (\beta \Lambda)^{-1}) \, \mathcal{W}(\Lambda | \mathbf{W}, \nu)$ 

$$p(x|\mu, a, b) = \int_0^\infty \mathcal{N}(x|\mu, \tau^{-1}) \operatorname{Gam}(\tau|a, b) d\tau$$

$$= \int_0^\infty \mathcal{N}(x|\mu, (\eta\lambda)^{-1}) \operatorname{Gam}(\eta|\nu/2, \nu/2) d\eta$$

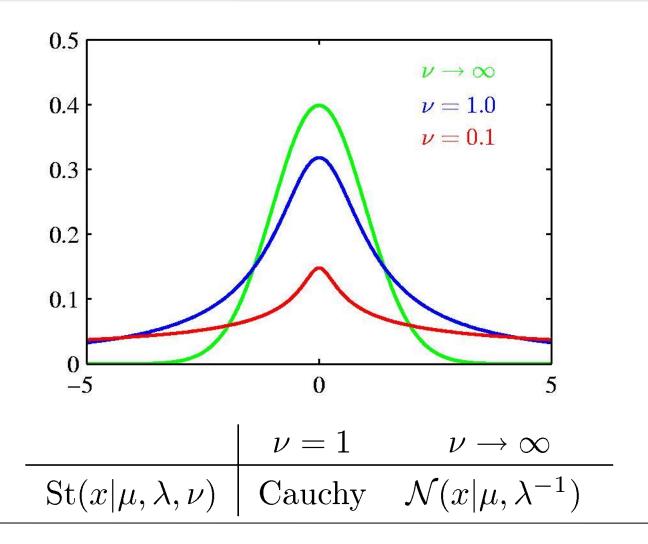
$$= \frac{\Gamma(\nu/2 + 1/2)}{\Gamma(\nu/2)} \left(\frac{\lambda}{\pi\nu}\right)^{1/2} \left[1 + \frac{\lambda(x - \mu)^2}{\nu}\right]^{-\nu/2 - 1/2}$$

$$= \operatorname{St}(x|\mu, \lambda, \nu)$$

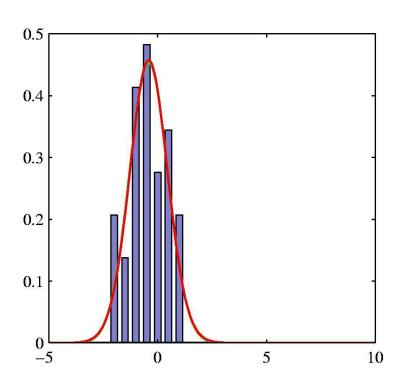
#### where

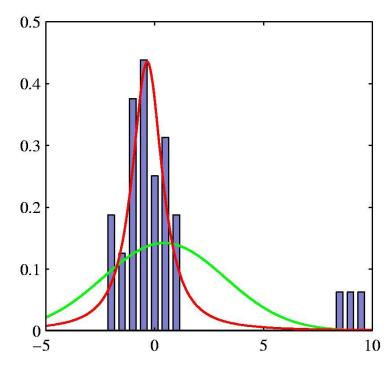
$$\lambda = a/b$$
  $\eta = \tau b/a$   $\nu = 2a$ .

Infinite mixture of Gaussians. -----



Robustness to outliers: Gaussian vs t-distribution.





#### The D-variate case:

$$\operatorname{St}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda},\nu) = \int_0^\infty \mathcal{N}(\mathbf{x}|\boldsymbol{\mu},(\eta\boldsymbol{\Lambda})^{-1})\operatorname{Gam}(\eta|\nu/2,\nu/2)\,\mathrm{d}\eta$$
$$= \frac{\Gamma(D/2+\nu/2)}{\Gamma(\nu/2)} \frac{|\boldsymbol{\Lambda}|^{1/2}}{(\pi\nu)^{D/2}} \left[1 + \frac{\Delta^2}{\nu}\right]^{-D/2-\nu/2}$$

where  $\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})$ .

Properties: 
$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}$$
, if  $\nu > 1$   $\operatorname{cov}[\mathbf{x}] = \frac{\nu}{(\nu - 2)} \boldsymbol{\Lambda}^{-1}$ , if  $\nu > 2$   $\operatorname{mode}[\mathbf{x}] = \boldsymbol{\mu}$ 

#### Periodic variables

- Examples: calendar time, direction, ...
- We require

$$p(\theta) \geqslant 0$$

$$\int_0^{2\pi} p(\theta) d\theta = 1$$

$$p(\theta + 2\pi) = p(\theta).$$

### von Mises Distribution (1)

This requirement is satisfied by

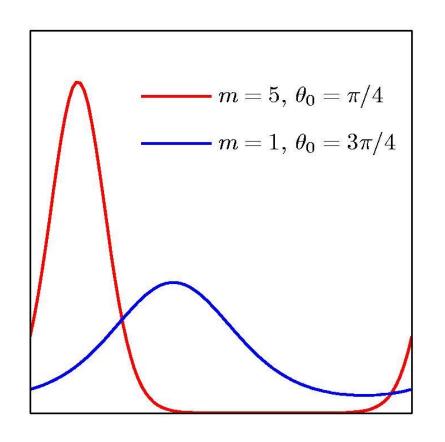
$$p(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp\{m\cos(\theta - \theta_0)\}\$$

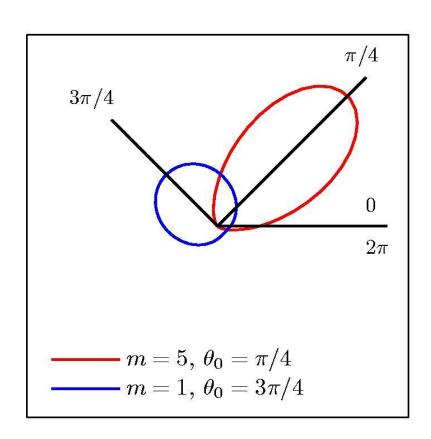
where

$$I_0(m) = \frac{1}{2\pi} \int_0^{2\pi} \exp\{m\cos\theta\} d\theta$$

is the 0<sup>th</sup> order modified Bessel function of the 1<sup>st</sup> kind.

### von Mises Distribution (4)





#### Maximum Likelihood for von Mises

Given a data set,  $\mathcal{D} = \{\theta_1, \dots, \theta_N\}$ , the log likelihood function is given by

$$\ln p(\mathcal{D}|\theta_0, m) = -N \ln(2\pi) - N \ln I_0(m) + m \sum_{n=1}^{N} \cos(\theta_n - \theta_0).$$

Maximizing with respect to  $\theta_0$  we directly obtain

$$\theta_0^{\mathrm{ML}} = \tan^{-1} \left\{ \frac{\sum_n \sin \theta_n}{\sum_n \cos \theta_n} \right\}.$$

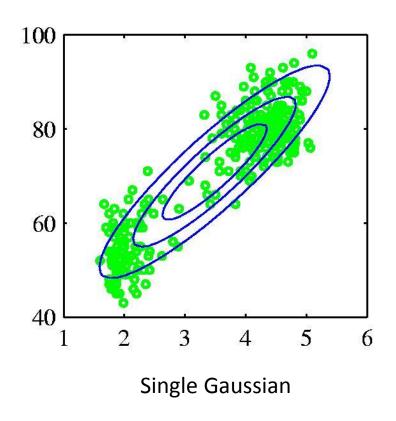
Similarly, maximizing with respect to m we get

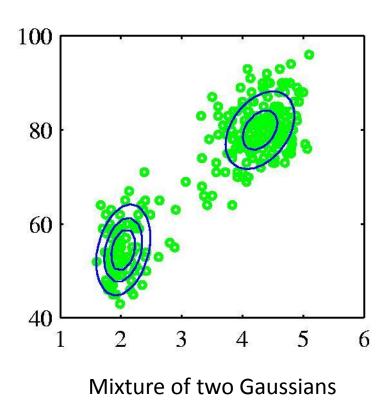
$$\frac{I_1(m_{\rm ML})}{I_0(m_{\rm ML})} = \frac{1}{N} \sum_{n=1}^{N} \cos(\theta_n - \theta_0^{\rm ML})$$

which can be solved numerically for  $m_{
m ML}$ .

### Mixtures of Gaussians (1)

#### Old Faithful data set



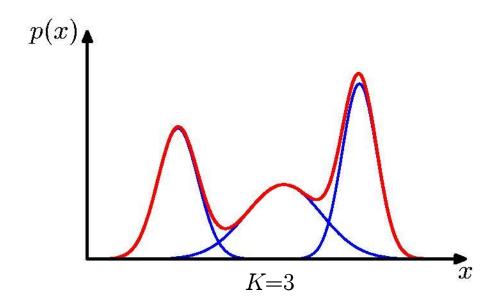


### Mixtures of Gaussians (2)

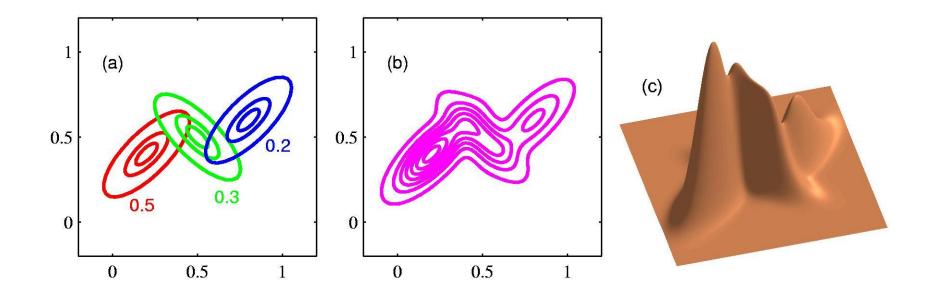
Combine simple models into a complex model:

$$p(\mathbf{x}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x}|oldsymbol{\mu}_k, oldsymbol{\Sigma}_k)$$
 Component Mixing coefficient

$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^K \pi_k = 1$$



# Mixtures of Gaussians (3)



## Mixtures of Gaussians (4)

Determining parameters  $\mu$ ,  $\Sigma$ , and  $\pi$  using maximum log likelihood

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

Log of a sum; no closed form maximum.

Solution: use standard, iterative, numeric optimization methods or the *expectation* maximization algorithm (Chapter 9).

# The Exponential Family (1)

$$p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp \{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\}$$

where  $\eta$  is the *natural parameter* and

$$g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp \left\{ \boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x}) \right\} d\mathbf{x} = 1$$

so  $g(\eta)$  can be interpreted as a normalization coefficient.

### The Exponential Family (2.1)

#### The Bernoulli Distribution

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

$$= \exp \{x \ln \mu + (1 - x) \ln(1 - \mu)\}$$

$$= (1 - \mu) \exp \left\{ \ln \left(\frac{\mu}{1 - \mu}\right) x \right\}$$

#### Comparing with the general form we see that

$$\eta = \ln\left(rac{\mu}{1-\mu}
ight) \quad ext{and so} \quad \mu = \sigma(\eta) = rac{1}{1+\exp(-\eta)}.$$
 Logistic sigmoid

# The Exponential Family (2.2)

# The Bernoulli distribution can hence be written as

$$p(x|\eta) = \sigma(-\eta) \exp(\eta x)$$

#### where

$$u(x) = x$$
 $h(x) = 1$ 
 $g(\eta) = 1 - \sigma(\eta) = \sigma(-\eta).$ 

## The Exponential Family (3.1)

#### The Multinomial Distribution

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{M} \mu_k^{x_k} = \exp\left\{\sum_{k=1}^{M} x_k \ln \mu_k\right\} = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right)$$

where, 
$$\mathbf{x}=(x_1,\ldots,x_M)^{\mathrm{T}}$$
,  $\boldsymbol{\eta}=(\eta_1,\ldots,\eta_M)^{\mathrm{T}}$  and

$$\eta_k = \ln \mu_k$$
 $\mathbf{u}(\mathbf{x}) = \mathbf{x}$ 
 $h(\mathbf{x}) = 1$ 
 $g(\boldsymbol{\eta}) = 1$ .

NOTE: The  ${'}_k$  parameters are not independent since the corresponding  $\mu_k$  must satisfy  ${}_M$ 

$$\sum_{k=1}^{M} \mu_k = 1.$$

# The Exponential Family (3.2)

Let 
$$\mu_M = 1 - \sum_{k=1}^{M-1} \mu_k$$
. This leads to

$$\eta_k = \ln\left(rac{\mu_k}{1-\sum_{j=1}^{M-1}\mu_j}
ight) ext{ and } \mu_k = rac{\exp(\eta_k)}{1+\sum_{j=1}^{M-1}\exp(\eta_j)}.$$

Here the  $\eta_k$  parameters are independent. Note that

$$0\leqslant \mu_k\leqslant 1$$
 and  $\sum_{k=1}^{M-1}\mu_k\leqslant 1.$ 

# The Exponential Family (3.3)

# The Multinomial distribution can then be written as

$$p(\mathbf{x}|\boldsymbol{\mu}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left(\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right)$$

where

$$\boldsymbol{\eta} = (\eta_1, \dots, \eta_{M-1}, 0)^{\mathrm{T}}$$
 $\mathbf{u}(\mathbf{x}) = \mathbf{x}$ 
 $h(\mathbf{x}) = 1$ 

$$g(\boldsymbol{\eta}) = \left(1 + \sum_{k=1}^{M-1} \exp(\eta_k)\right)^{-1}.$$

# The Exponential Family (4)

#### The Gaussian Distribution

$$p(x|\mu, \sigma^{2}) = \frac{1}{(2\pi\sigma^{2})^{1/2}} \exp\left\{-\frac{1}{2\sigma^{2}}(x-\mu)^{2}\right\}$$

$$= \frac{1}{(2\pi\sigma^{2})^{1/2}} \exp\left\{-\frac{1}{2\sigma^{2}}x^{2} + \frac{\mu}{\sigma^{2}}x - \frac{1}{2\sigma^{2}}\mu^{2}\right\}$$

$$= h(x)g(\eta) \exp\left\{\eta^{T}\mathbf{u}(x)\right\}$$

#### where

$$\boldsymbol{\eta} = \begin{pmatrix} \mu/\sigma^2 \\ -1/2\sigma^2 \end{pmatrix} \qquad h(\mathbf{x}) = (2\pi)^{-1/2}$$
$$\mathbf{u}(x) = \begin{pmatrix} x \\ x^2 \end{pmatrix} \qquad g(\boldsymbol{\eta}) = (-2\eta_2)^{1/2} \exp\left(\frac{\eta_1^2}{4\eta_2}\right).$$

### ML for the Exponential Family (1)

#### From the definition of $g(\eta)$ we get

$$\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp\left\{\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right\} d\mathbf{x} + g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp\left\{\boldsymbol{\eta}^{\mathrm{T}} \mathbf{u}(\mathbf{x})\right\} \mathbf{u}(\mathbf{x}) d\mathbf{x} = 0$$

$$1/g(\boldsymbol{\eta})$$

$$\mathbb{E}[\mathbf{u}(\mathbf{x})]$$

Thus

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

## ML for the Exponential Family (2)

Give a data set,  $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ , the likelihood function is given by

$$p(\mathbf{X}|\boldsymbol{\eta}) = \left(\prod_{n=1}^{N} h(\mathbf{x}_n)\right) g(\boldsymbol{\eta})^N \exp\left\{\boldsymbol{\eta}^T \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)\right\}.$$

Thus we have

$$-\nabla \ln g(oldsymbol{\eta}_{\mathrm{ML}}) = rac{1}{N} \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)$$

#### Conjugate priors

For any member of the exponential family, there exists a prior

$$p(\boldsymbol{\eta}|\boldsymbol{\chi}, \nu) = f(\boldsymbol{\chi}, \nu)g(\boldsymbol{\eta})^{\nu} \exp\left\{\nu \boldsymbol{\eta}^{\mathrm{T}} \boldsymbol{\chi}\right\}.$$

Combining with the likelihood function, we get

$$p(\boldsymbol{\eta}|\mathbf{X}, \boldsymbol{\chi}, \nu) \propto g(\boldsymbol{\eta})^{\nu+N} \exp \left\{ \boldsymbol{\eta}^{\mathrm{T}} \left( \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n) + \nu \boldsymbol{\chi} \right) \right\}.$$

Prior corresponds to  $\nu$  pseudo-observations with value  $\chi$ .

## Noninformative Priors (1)

With little or no information available a-priori, we might choose a non-informative prior.

- $\lambda$  discrete, K-nomial :  $p(\lambda) = 1/K$ .
- $\lambda \in [a,b]$  real and bounded:  $p(\lambda) = 1/b a$ .
- $\lambda$  real and unbounded: improper!

A constant prior may no longer be constant after a change of variable; consider  $p(\lambda)$  constant and  $\lambda = \eta^2$ :

$$p_{\eta}(\eta) = p_{\lambda}(\lambda) \left| \frac{\mathrm{d}\lambda}{\mathrm{d}\eta} \right| = p_{\lambda}(\eta^2) 2\eta \propto \eta$$

# Noninformative Priors (2)

#### Translation invariant priors. Consider

$$p(x|\mu) = f(x - \mu) = f((x + c) - (\mu + c)) = f(\widehat{x} - \widehat{\mu}) = p(\widehat{x}|\widehat{\mu}).$$

For a corresponding prior over  $\mu$ , we have

$$\int_{A}^{B} p(\mu) d\mu = \int_{A-c}^{B-c} p(\mu) d\mu = \int_{A}^{B} p(\mu - c) d\mu$$

for any A and B. Thus  $p(\mu) = p(\mu - c)$  and  $p(\mu)$  must be constant.

# Noninformative Priors (3)

Example: The mean of a Gaussian,  $\mu$ ; the conjugate prior is also a Gaussian,

$$p(\mu|\mu_0, \sigma_0^2) = \mathcal{N}(\mu|\mu_0, \sigma_0^2)$$

As  $\sigma_0^2 \to \infty$ , this will become constant over  $\mu$ .

# Noninformative Priors (4)

Scale invariant priors. Consider  $p(x|\sigma) = (1/\sigma)f(x/\sigma)$  and make the change of variable  $\widehat{x} = cx$ 

$$p_{\widehat{x}}(\widehat{x}) = p_x(x) \left| \frac{\mathrm{d}x}{\mathrm{d}\widehat{x}} \right| = p_x \left( \frac{\widehat{x}}{c} \right) \frac{1}{c} = \frac{1}{c\sigma} f\left( \frac{\widehat{x}}{c\sigma} \right) = p_x(\widehat{x}|\widehat{\sigma}).$$

For a corresponding prior over  $\sigma$ , we have

$$\int_{A}^{B} p(\sigma) d\sigma = \int_{A/c}^{B/c} p(\sigma) d\sigma = \int_{A}^{B} p\left(\frac{1}{c}\sigma\right) \frac{1}{c} d\sigma$$

for any A and B. Thus  $p(\sigma) \propto 1/\sigma$  and so this prior is improper too. Note that this corresponds to  $p(\ln \sigma)$  being constant.

# Noninformative Priors (5)

Example: For the variance of a Gaussian,  $\sigma^2$ , we have

$$\mathcal{N}(x|\mu,\sigma^2) \propto \sigma^{-1} \exp\left\{-((x-\mu)/\sigma)^2\right\}.$$

If  $\lambda=1/\sigma^2$  and  $p(\sigma)\propto 1/\sigma$ , then  $p(\lambda)\propto 1/\lambda$ .

We know that the conjugate distribution for  $\lambda$  is the Gamma distribution,

$$\operatorname{Gam}(\lambda|a_0,b_0) \propto \lambda^{a_0-1} \exp(-b_0\lambda).$$

A noninformative prior is obtained when  $a_0=0$  and  $b_0=0$ .

# Nonparametric Methods (1)

Parametric distribution models are restricted to specific forms, which may not always be suitable; for example, consider modelling a multimodal distribution with a single, unimodal model.

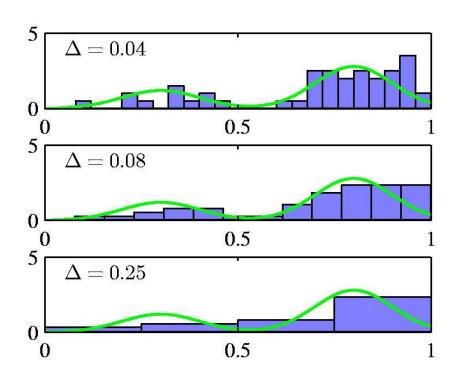
Nonparametric approaches make few assumptions about the overall shape of the distribution being modelled.

# Nonparametric Methods (2)

Histogram methods partition the data space into distinct bins with widths  $\Delta_i$  and count the number of observations,  $n_i$ , in each bin.

$$p_i = \frac{n_i}{N\Delta_i}$$

- •Often, the same width is used for all bins,  $\Delta_i = \Delta$ .
- $ullet\Delta$  acts as a smoothing parameter.



•In a D-dimensional space, using M bins in each dimension will require  $M^D$  bins!

# Nonparametric Methods (3)

Assume observations drawn from a density  $p(\mathbf{x})$  and consider a small region  $\mathcal{R}$  containing  $\mathbf{x}$  such that

$$P = \int_{\mathcal{R}} p(\mathbf{x}) \, \mathrm{d}\mathbf{x}.$$

The probability that K out of N observations lie inside  $\mathcal{R}$  is  $\mathrm{Bin}(K|N,P)$  and if N is large

If the volume of  $\mathcal{R}$ , V, is sufficiently small,  $p(\mathbf{x})$  is approximately constant over  $\mathcal{R}$  and

$$P \simeq p(\mathbf{x})V$$

Thus

$$p(\mathbf{x}) = \frac{K}{NV}.$$

V small, yet K>0, therefore N large?

# Nonparametric Methods (4)

**Kernel Density Estimation:** fix V, estimate K from the data. Let  $\mathcal{R}$  be a hypercube centred on  $\mathbf{x}$  and define the kernel function (Parzen window)

$$k((\mathbf{x} - \mathbf{x}_n)/h) = \begin{cases} 1, & |(x_i - x_{ni})/h| \leq 1/2, & i = 1, \dots, D, \\ 0, & \text{otherwise.} \end{cases}$$

It follows that

$$K = \sum_{n=1}^{N} k\left(\frac{\mathbf{x} - \mathbf{x}_n}{h}\right) \text{ and hence } p(\mathbf{x}) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{h^D} k\left(\frac{\mathbf{x} - \mathbf{x}_n}{h}\right).$$

# Nonparametric Methods (5)

To avoid discontinuities in p(x), use a smooth kernel, e.g. a Gaussian

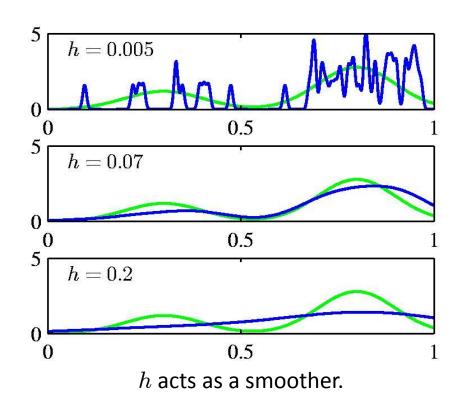
$$p(\mathbf{x}) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi h^2)^{D/2}}$$
$$\exp\left\{-\frac{\|\mathbf{x} - \mathbf{x}_n\|^2}{2h^2}\right\}$$

Any kernel such that

$$k(\mathbf{u}) \geqslant 0,$$

$$\int k(\mathbf{u}) \, d\mathbf{u} = 1$$

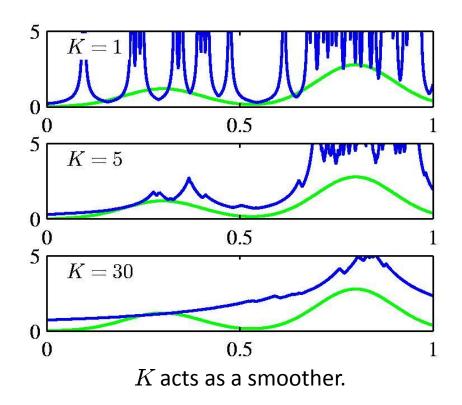
will work.



### Nonparametric Methods (6)

Nearest Neighbour Density Estimation: fix K, estimate V from the data. Consider a hypersphere centred on  $\mathbf{x}$  and let it grow to a volume,  $V^*$ , that includes K of the given N data points. Then

$$p(\mathbf{x}) \simeq \frac{K}{NV^{\star}}.$$



# Nonparametric Methods (7)

Nonparametric models (not histograms) requires storing and computing with the entire data set.

Parametric models, once fitted, are much more efficient in terms of storage and computation.

#### K-Nearest-Neighbours for Classification (1)

Given a data set with  $N_k$  data points from class  $\mathcal{C}_k$  and  $\sum_k N_k = N$ , we have

$$p(\mathbf{x}) = \frac{K}{NV}$$

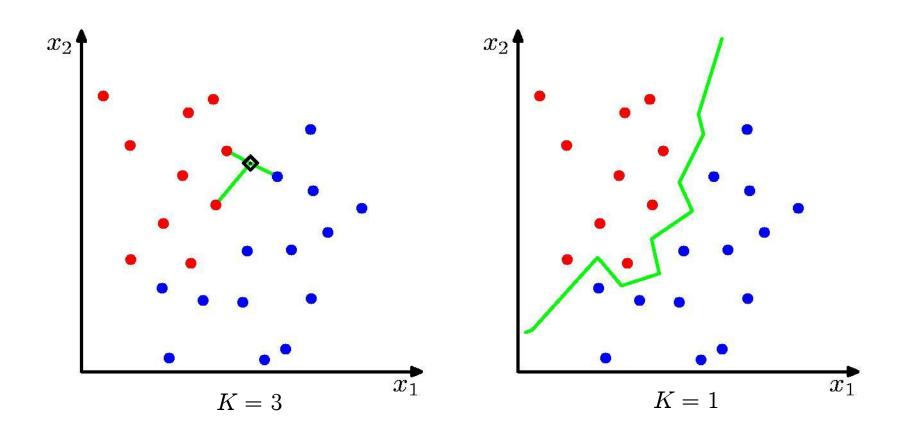
and correspondingly

$$p(\mathbf{x}|\mathcal{C}_k) = \frac{K_k}{N_k V}.$$

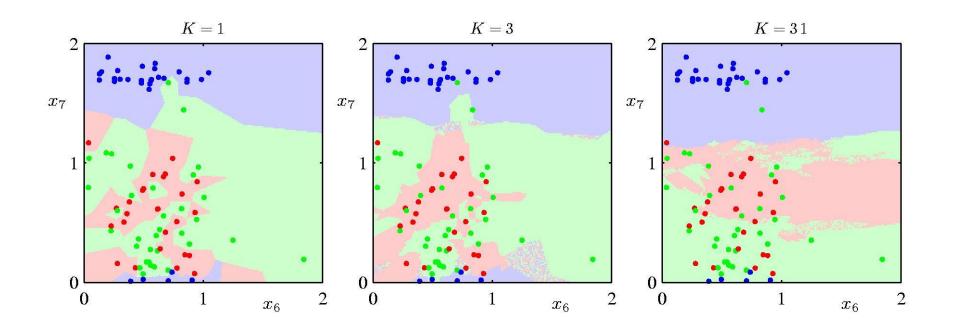
Since  $p(C_k) = N_k/N$ , Bayes' theorem gives

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{p(\mathbf{x})} = \frac{K_k}{K}.$$

#### K-Nearest-Neighbours for Classification (2)



#### K-Nearest-Neighbours for Classification (3)



- K acts as a smother
- For  $N \to \infty$ , the error rate of the 1-nearest-neighbour classifier is never more than twice the optimal error (obtained from the true conditional class distributions).