
PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 2: PROBABILITY DISTRIBUTIONS

Parametric Distributions

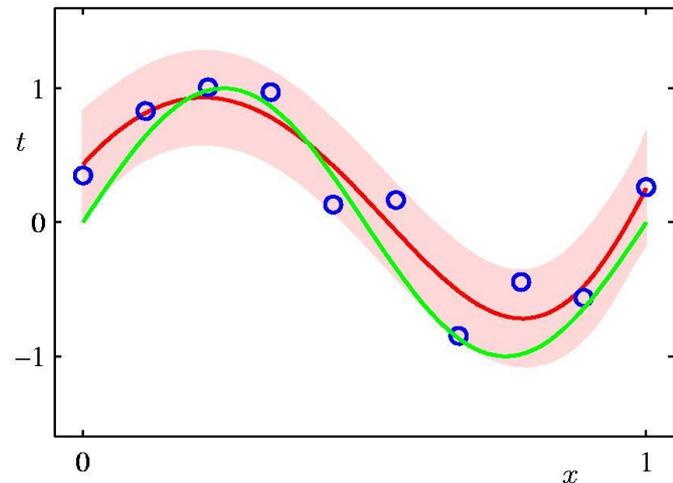
Basic building blocks: $p(\mathbf{x}|\boldsymbol{\theta})$

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

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

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

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

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

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

Binary Variables (2)

N coin flips:

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

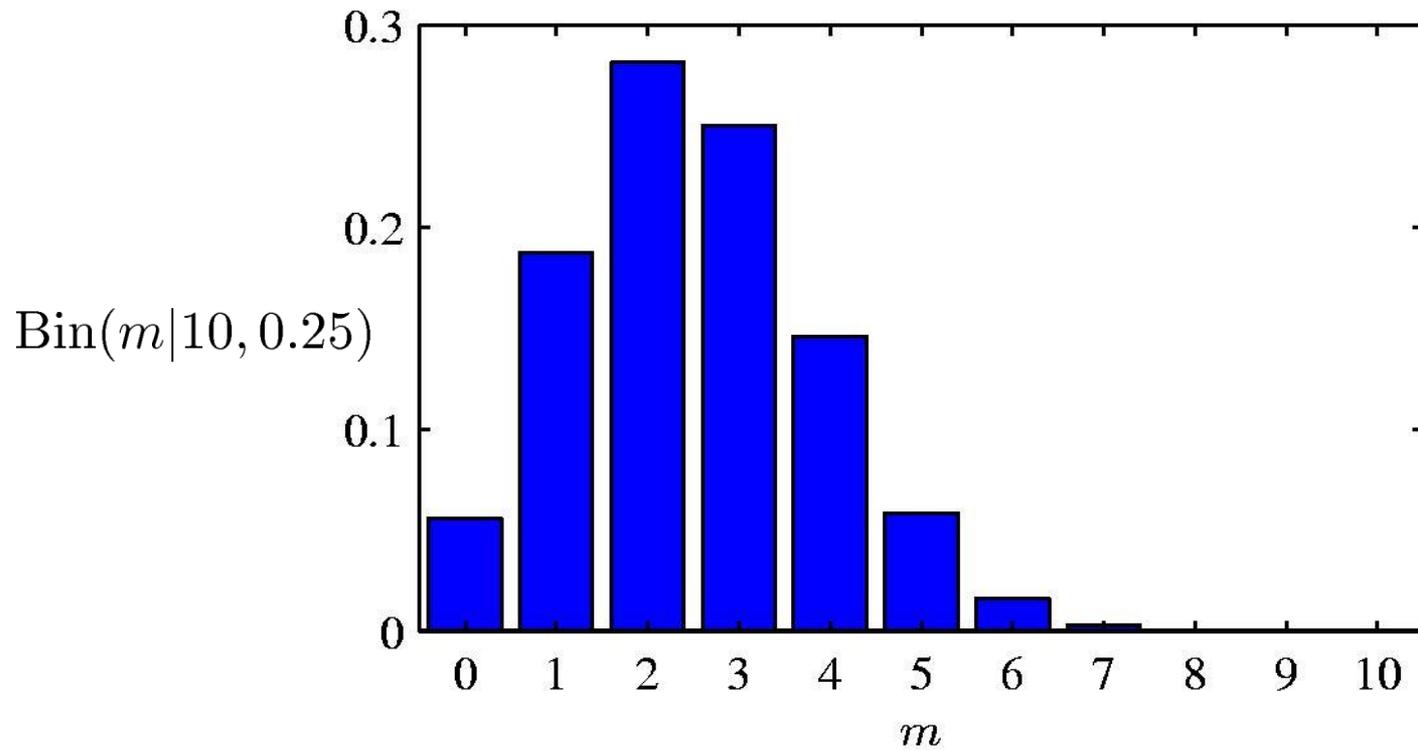
Binomial Distribution

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

$$\mathbb{E}[m] \equiv \sum_{m=0}^N m \text{Bin}(m | N, \mu) = N\mu$$

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

Binomial Distribution



Parameter Estimation (1)

ML for Bernoulli

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

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

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

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

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

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

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

$$\text{var}[\mu] = \frac{ab}{(a+b)^2(a+b+1)}$$



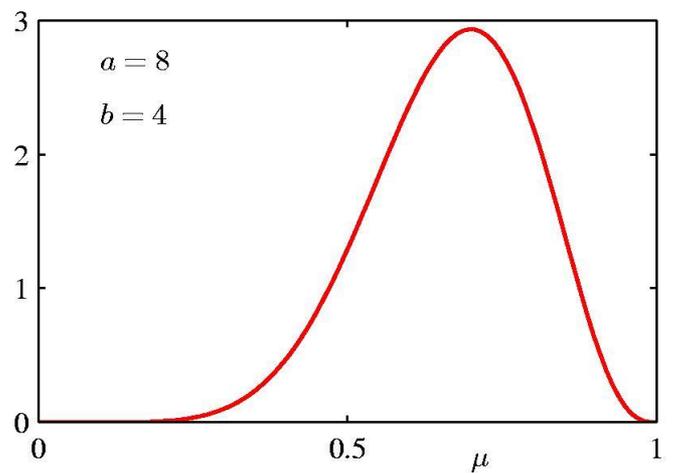
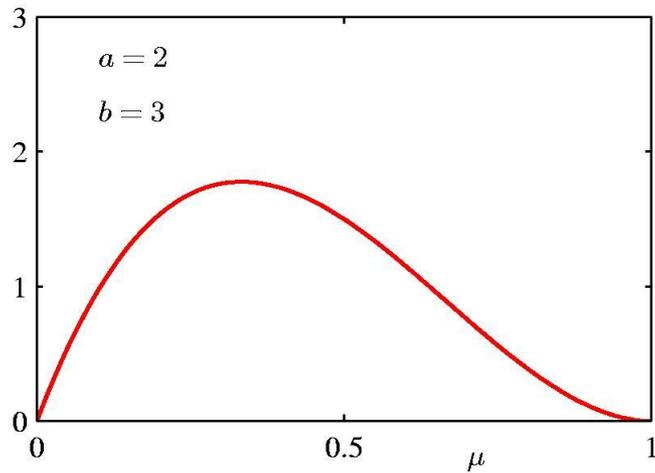
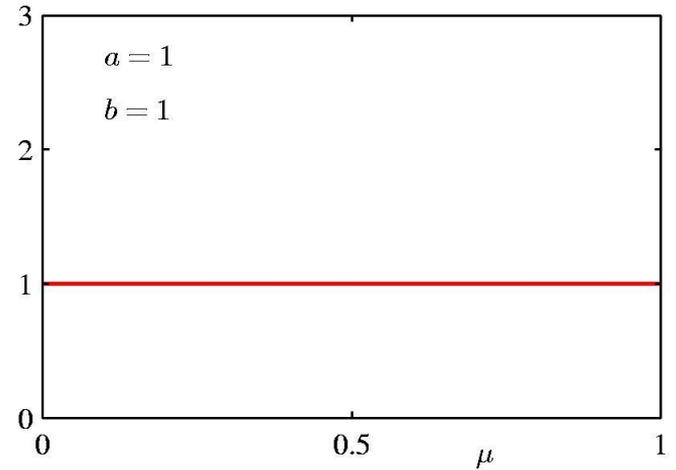
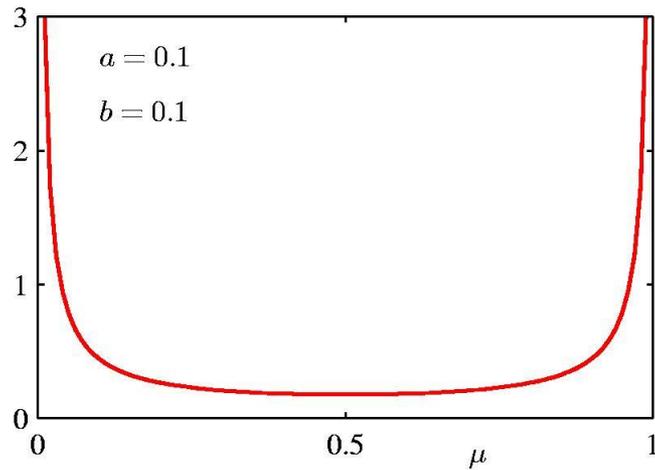
Bayesian Bernoulli

$$\begin{aligned} p(\mu|a_0, b_0, \mathcal{D}) &\propto p(\mathcal{D}|\mu)p(\mu|a_0, b_0) \\ &= \left(\prod_{n=1}^N \mu^{x_n} (1 - \mu)^{1-x_n} \right) \text{Beta}(\mu|a_0, b_0) \\ &\propto \mu^{m+a_0-1} (1 - \mu)^{(N-m)+b_0-1} \\ &\propto \text{Beta}(\mu|a_N, b_N) \end{aligned}$$

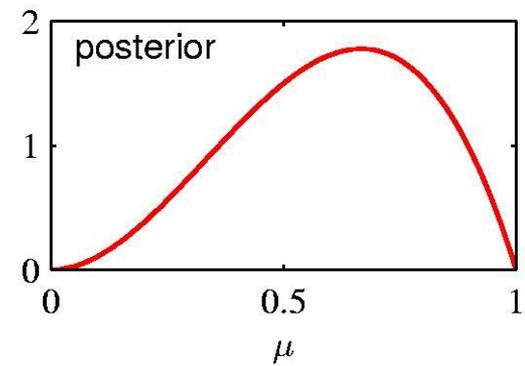
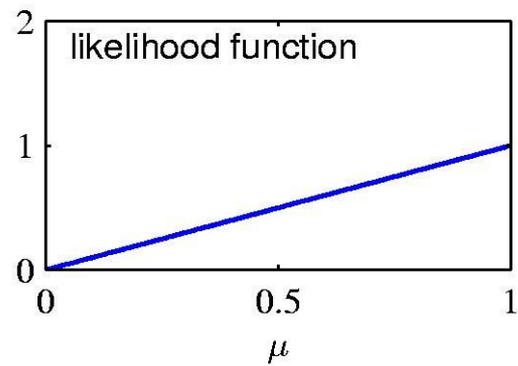
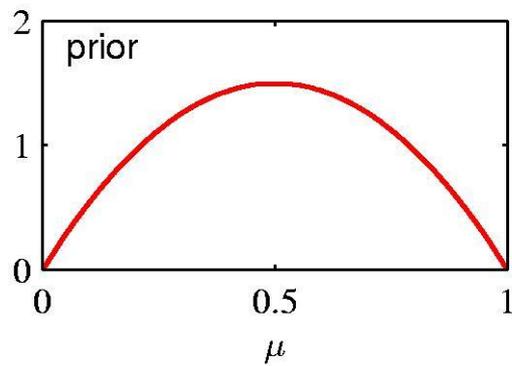
$$a_N = a_0 + m \quad b_N = b_0 + (N - m)$$

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?

$$\begin{aligned} p(x = 1|a_0, b_0, \mathcal{D}) &= \int_0^1 p(x = 1|\mu)p(\mu|a_0, b_0, \mathcal{D}) d\mu \\ &= \int_0^1 \mu p(\mu|a_0, b_0, \mathcal{D}) d\mu \\ &= \mathbb{E}[\mu|a_0, b_0, \mathcal{D}] = \frac{a_N}{b_N} \end{aligned}$$



Multinomial Variables

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

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

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

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

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

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, λ .

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

$$\mu_k = -m_k / \lambda \quad \mu_k^{\text{ML}} = \frac{m_k}{N}$$

The Multinomial Distribution

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

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

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

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

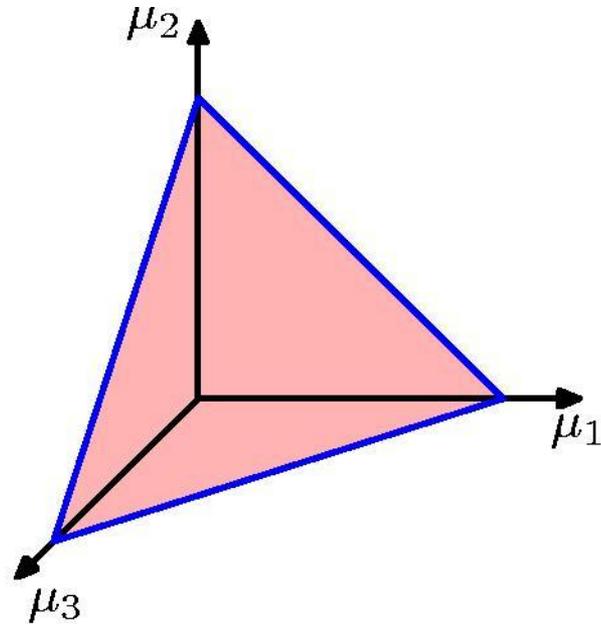


The Dirichlet Distribution

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

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

Conjugate prior for the multinomial distribution.

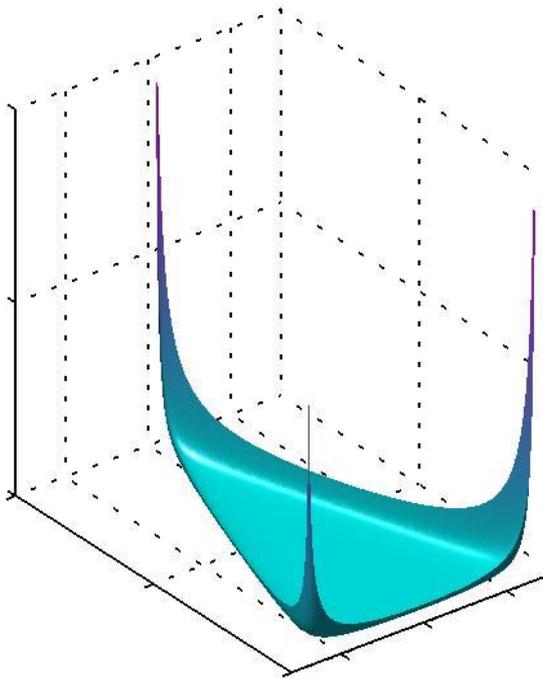


Bayesian Multinomial (1)

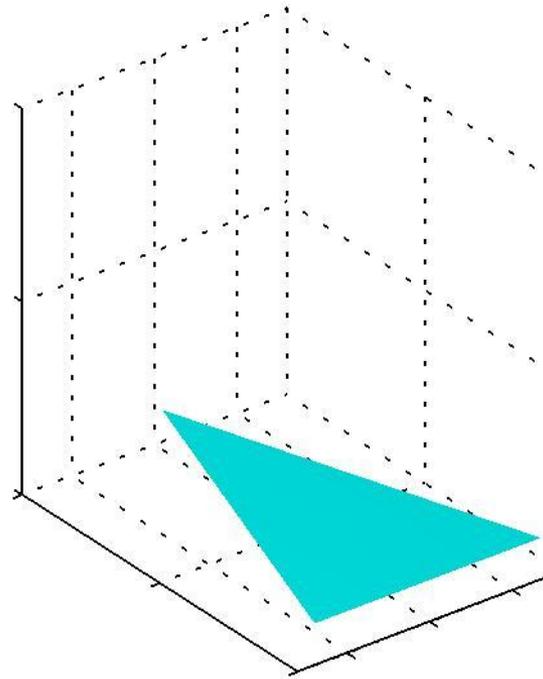
$$p(\boldsymbol{\mu}|\mathcal{D}, \boldsymbol{\alpha}) \propto p(\mathcal{D}|\boldsymbol{\mu})p(\boldsymbol{\mu}|\boldsymbol{\alpha}) \propto \prod_{k=1}^K \mu_k^{\alpha_k + m_k - 1}$$

$$\begin{aligned} p(\boldsymbol{\mu}|\mathcal{D}, \boldsymbol{\alpha}) &= \text{Dir}(\boldsymbol{\mu}|\boldsymbol{\alpha} + \mathbf{m}) \\ &= \frac{\Gamma(\alpha_0 + N)}{\Gamma(\alpha_1 + m_1) \cdots \Gamma(\alpha_K + m_K)} \prod_{k=1}^K \mu_k^{\alpha_k + m_k - 1} \end{aligned}$$

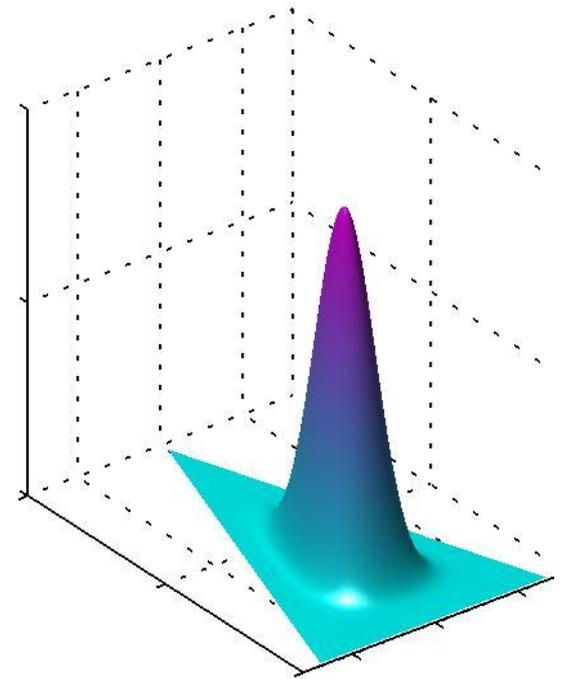
Bayesian Multinomial (2)



$$\alpha_k = 10^{-1}$$

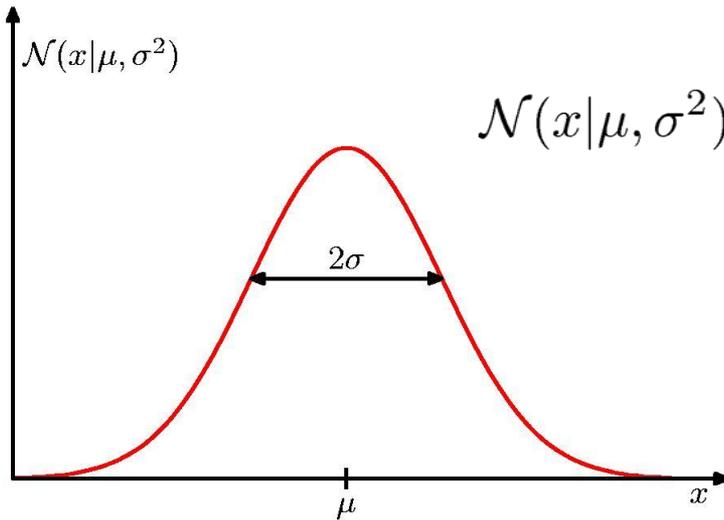


$$\alpha_k = 10^0$$

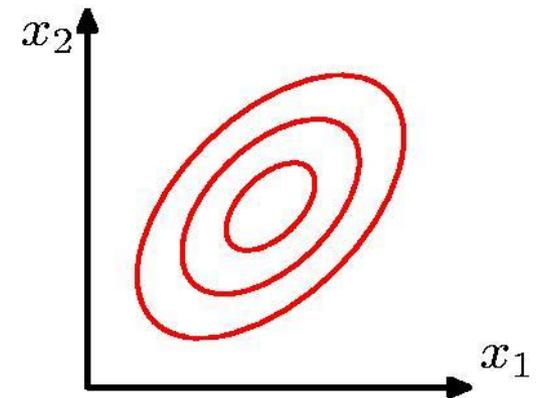


$$\alpha_k = 10^1$$

The Gaussian Distribution



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

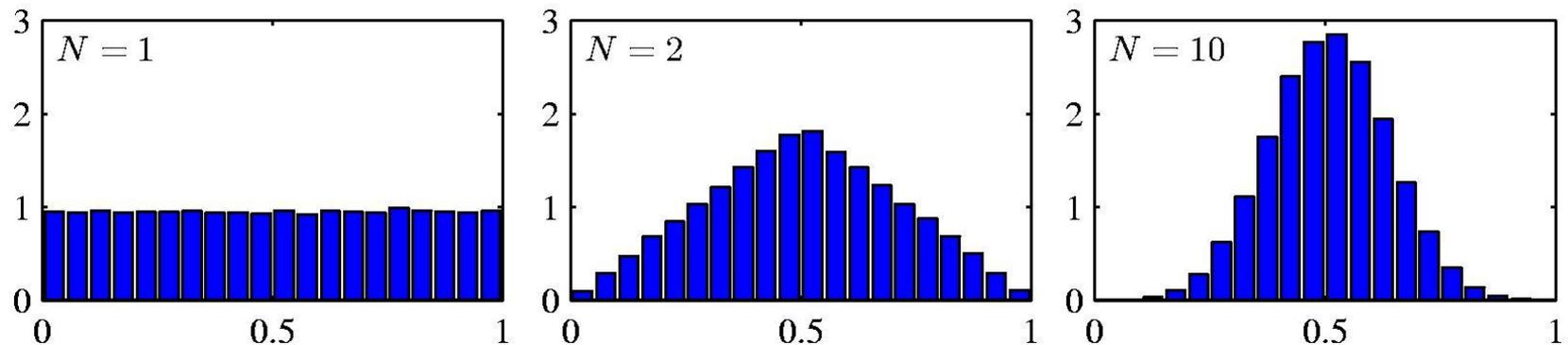


$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

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.



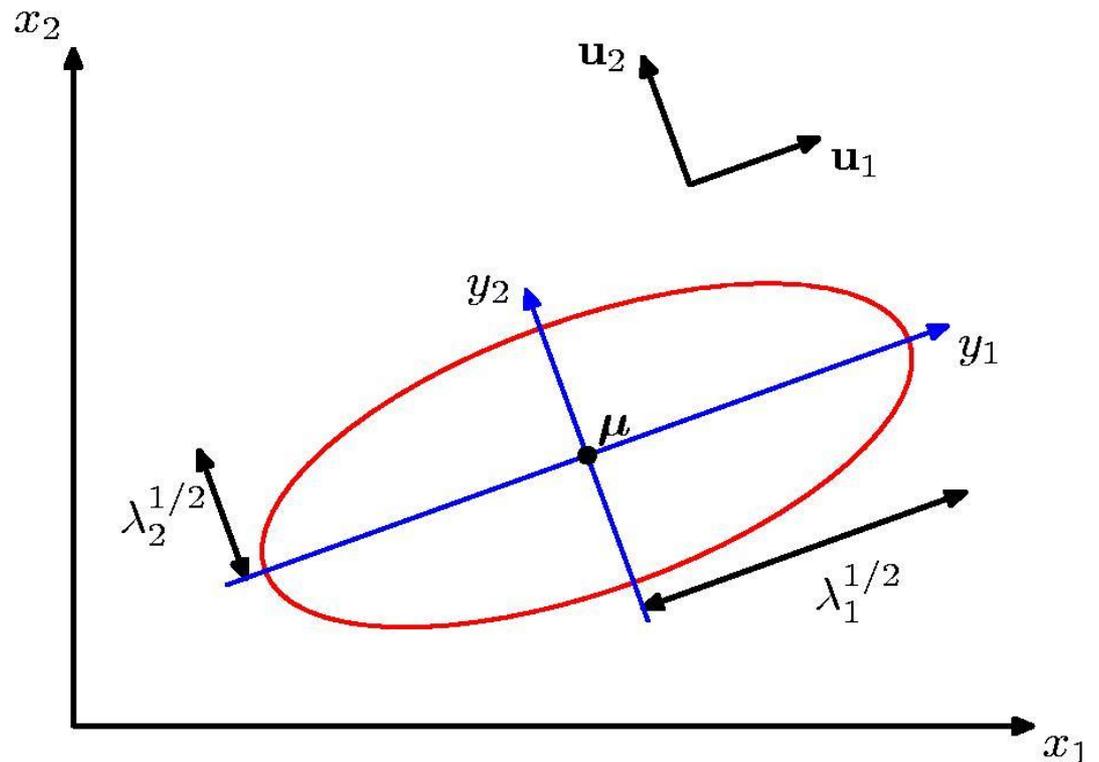
Geometry of the Multivariate Gaussian

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

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

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

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



Moments of the Multivariate Gaussian (1)

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

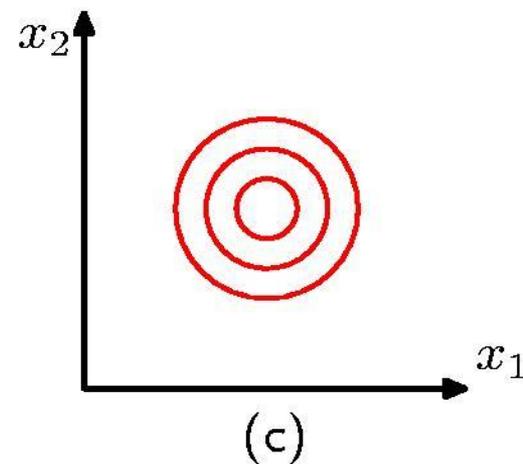
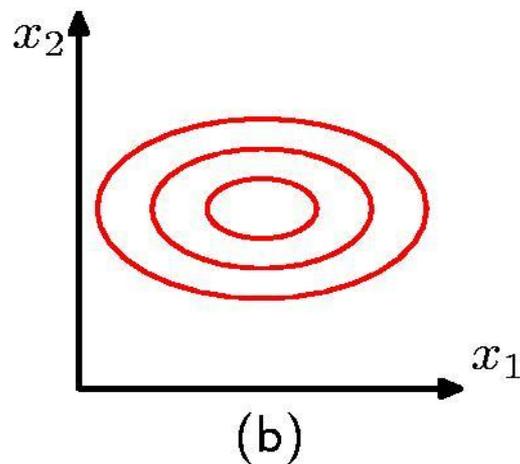
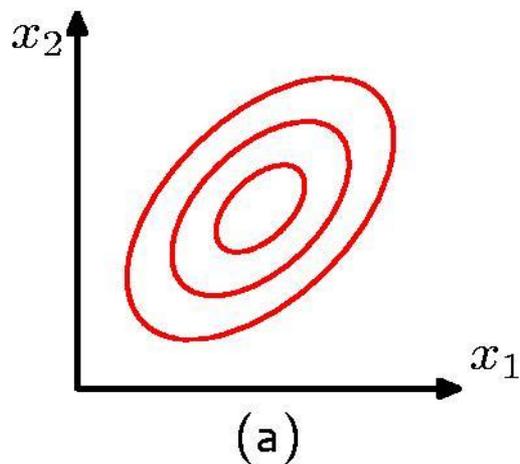
thanks to anti-symmetry of \mathbf{z}

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

Moments of the Multivariate Gaussian (2)

$$\mathbb{E}[\mathbf{x}\mathbf{x}^T] = \boldsymbol{\mu}\boldsymbol{\mu}^T + \boldsymbol{\Sigma}$$

$$\text{cov}[\mathbf{x}] = \mathbb{E} [(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^T] = \boldsymbol{\Sigma}$$



Partitioned Gaussian Distributions

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

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{pmatrix}$$

$$\boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{pmatrix}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{pmatrix}$$

$$\boldsymbol{\Lambda} \equiv \boldsymbol{\Sigma}^{-1}$$

$$\boldsymbol{\Lambda} = \begin{pmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{pmatrix}$$

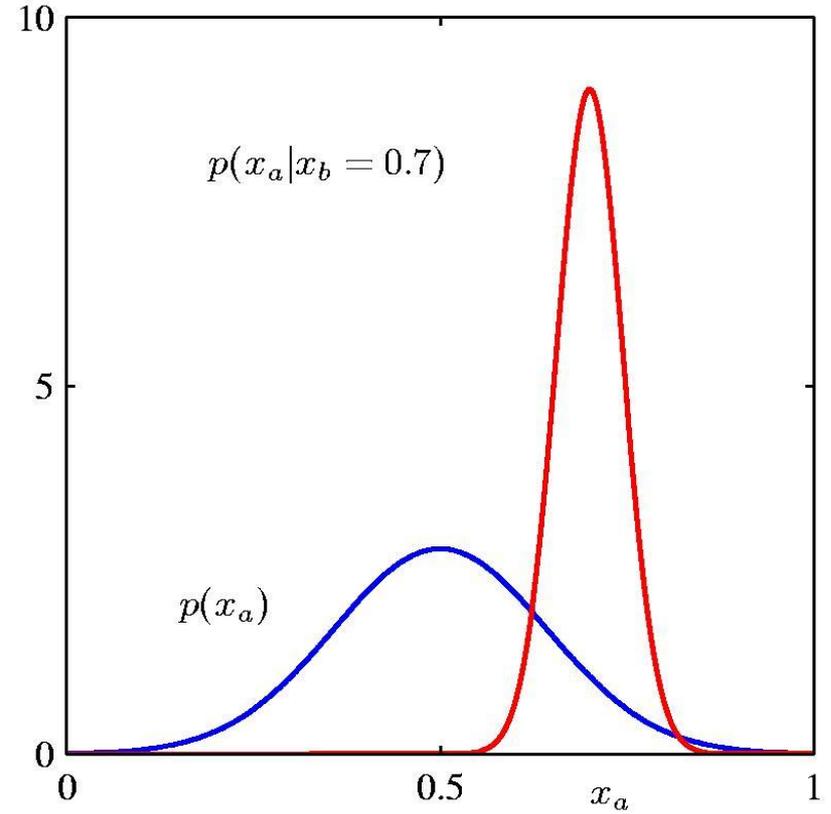
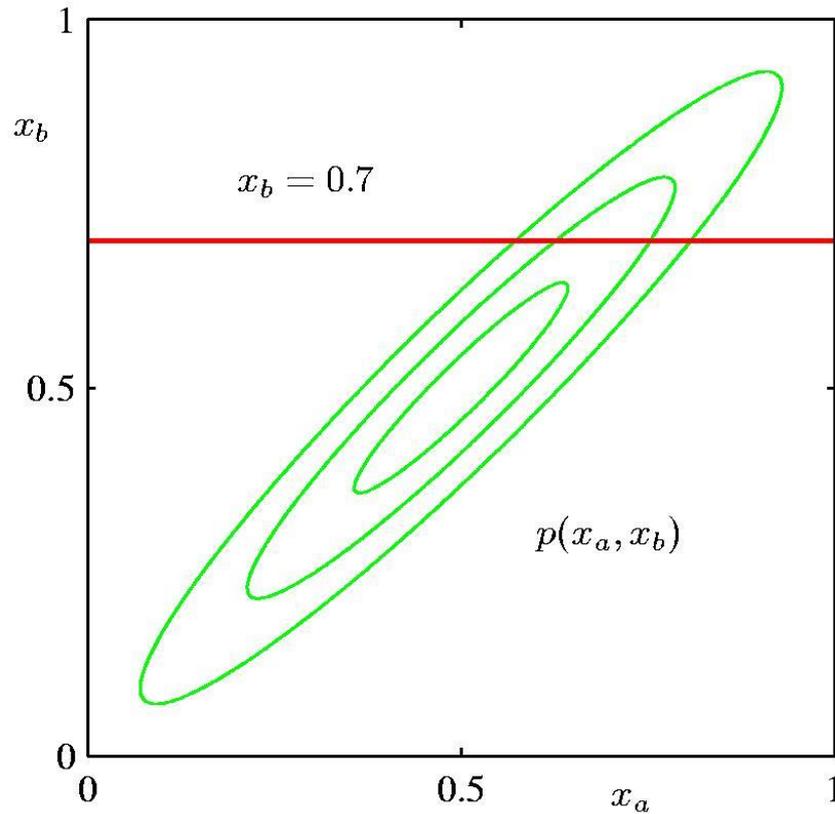
Partitioned Conditionals and Marginals

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

$$\begin{aligned}\boldsymbol{\Sigma}_{a|b} &= \boldsymbol{\Lambda}_{aa}^{-1} = \boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab} \boldsymbol{\Sigma}_{bb}^{-1} \boldsymbol{\Sigma}_{ba} \\ \boldsymbol{\mu}_{a|b} &= \boldsymbol{\Sigma}_{a|b} \{ \boldsymbol{\Lambda}_{aa} \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) \} \\ &= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) \\ &= \boldsymbol{\mu}_a + \boldsymbol{\Sigma}_{ab} \boldsymbol{\Sigma}_{bb}^{-1} (\mathbf{x}_b - \boldsymbol{\mu}_b)\end{aligned}$$

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

Partitioned Conditionals and Marginals



Bayes' Theorem for Gaussian Variables

Given

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

we have

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

where

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

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

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

Sufficient statistics

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

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

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

$$\boldsymbol{\mu}_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n.$$

Similarly

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

Maximum Likelihood for the Gaussian (3)

Under the true distribution

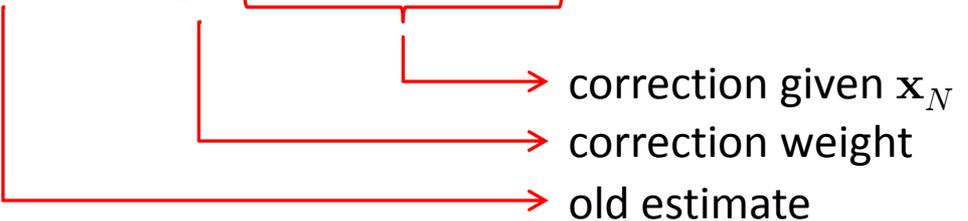
$$\begin{aligned}\mathbb{E}[\boldsymbol{\mu}_{\text{ML}}] &= \boldsymbol{\mu} \\ \mathbb{E}[\boldsymbol{\Sigma}_{\text{ML}}] &= \frac{N-1}{N} \boldsymbol{\Sigma}.\end{aligned}$$

Hence define

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

Sequential Estimation

Contribution of the N^{th} data point, \mathbf{x}_N

$$\begin{aligned}\boldsymbol{\mu}_{\text{ML}}^{(N)} &= \frac{1}{N} \sum_{n=1}^N \mathbf{x}_n \\ &= \frac{1}{N} \mathbf{x}_N + \frac{1}{N} \sum_{n=1}^{N-1} \mathbf{x}_n \\ &= \frac{1}{N} \mathbf{x}_N + \frac{N-1}{N} \boldsymbol{\mu}_{\text{ML}}^{(N-1)} \\ &= \boldsymbol{\mu}_{\text{ML}}^{(N-1)} + \frac{1}{N} (\mathbf{x}_N - \boldsymbol{\mu}_{\text{ML}}^{(N-1)})\end{aligned}$$


correction given \mathbf{x}_N
correction weight
old estimate

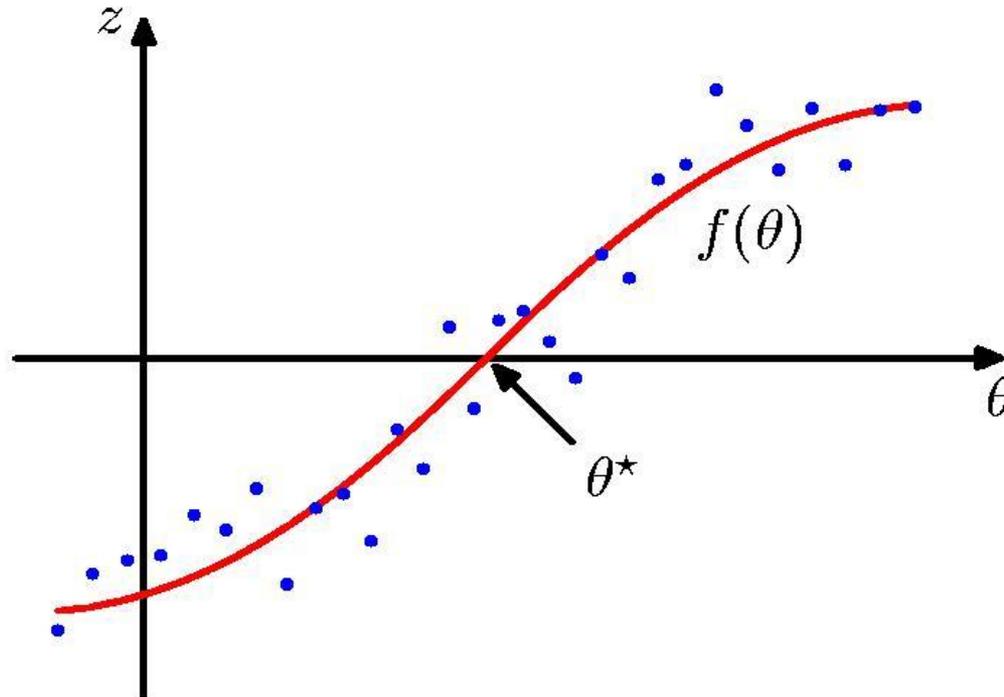
The Robbins-Monro Algorithm (1)

Consider θ 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 θ^* 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 θ^* are then given by

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

Conditions on a_N for convergence :

$$\lim_{N \rightarrow \infty} a_N = 0 \quad \sum_{N=1}^{\infty} a_N = \infty \quad \sum_{N=1}^{\infty} a_N^2 < \infty$$



Robbins-Monro for Maximum Likelihood (1)

Regarding

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

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

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

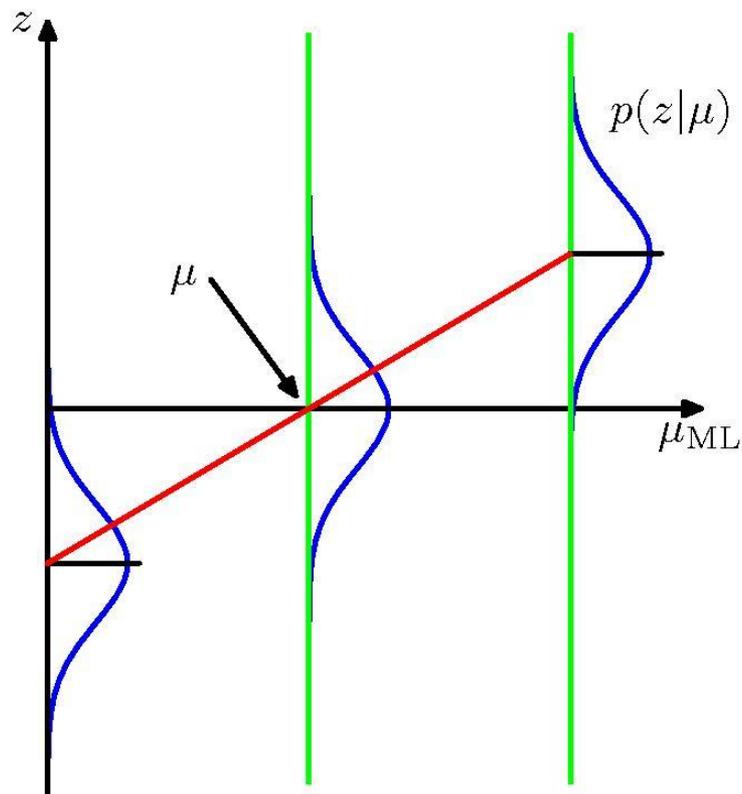
Robbins-Monro for Maximum Likelihood (2)

Example: estimate the mean of a Gaussian.

$$\begin{aligned} z &= \frac{\partial}{\partial \mu_{\text{ML}}} [-\ln p(x|\mu_{\text{ML}}, \sigma^2)] \\ &= -\frac{1}{\sigma^2}(x - \mu_{\text{ML}}) \end{aligned}$$

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

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



Bayesian Inference for the Gaussian (1)

Assume σ^2 is known. Given i.i.d. data

$\mathbf{x} = \{x_1, \dots, x_N\}$, the likelihood function for μ 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 μ (but it is *not* a distribution over μ).

Bayesian Inference for the Gaussian (2)

Combined with a Gaussian prior over μ ,

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

this gives the posterior

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

Completing the square over μ , we see that

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

Bayesian Inference for the Gaussian (3)

... where

$$\mu_N = \frac{\sigma^2}{N\sigma_0^2 + \sigma^2}\mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2}\mu_{\text{ML}}, \quad \mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^N x_n$$

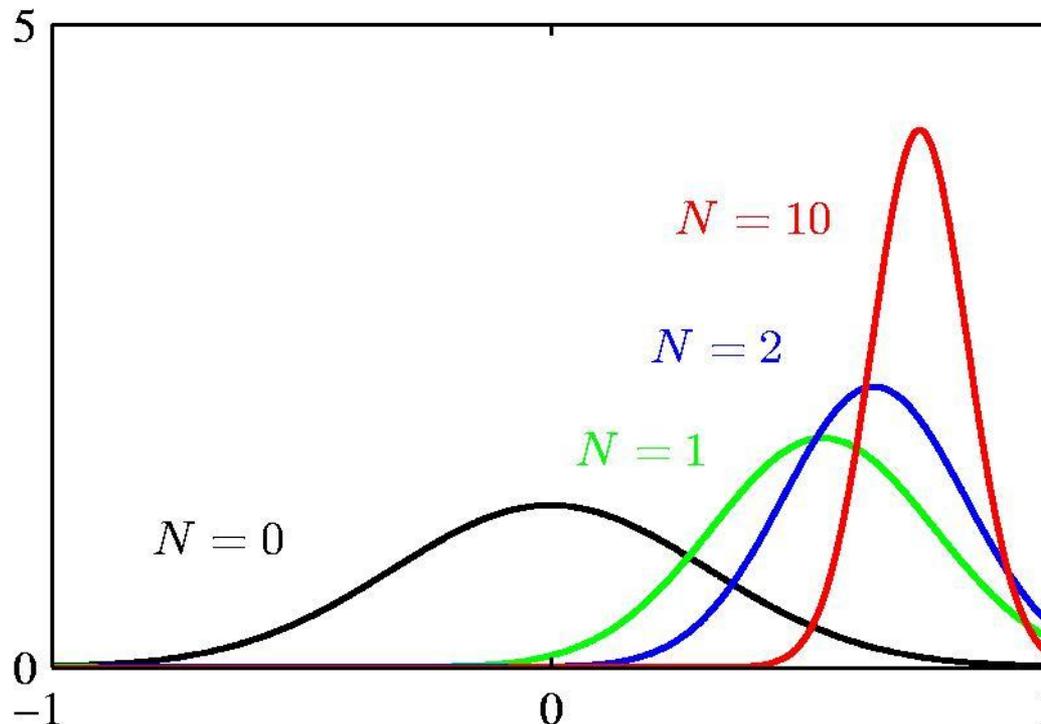
$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}.$$

Note:

	$N = 0$	$N \rightarrow \infty$
μ_N	μ_0	μ_{ML}
σ_N^2	σ_0^2	0

Bayesian Inference for the Gaussian (4)

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



Bayesian Inference for the Gaussian (5)

Sequential Estimation

$$\begin{aligned} p(\mu|\mathbf{x}) &\propto p(\mu)p(\mathbf{x}|\mu) \\ &= \left[p(\mu) \prod_{n=1}^{N-1} p(x_n|\mu) \right] p(x_N|\mu) \\ &\propto \mathcal{N}(\mu|\mu_{N-1}, \sigma_{N-1}^2) p(x_N|\mu) \end{aligned}$$

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

Bayesian Inference for the Gaussian (6)

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

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

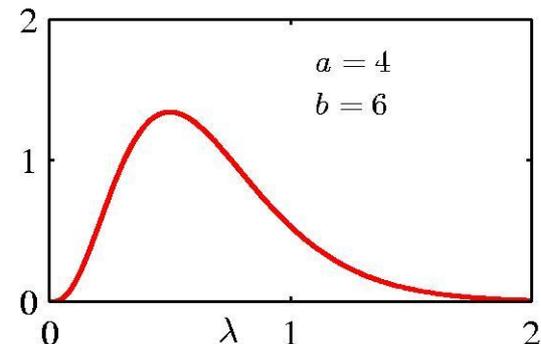
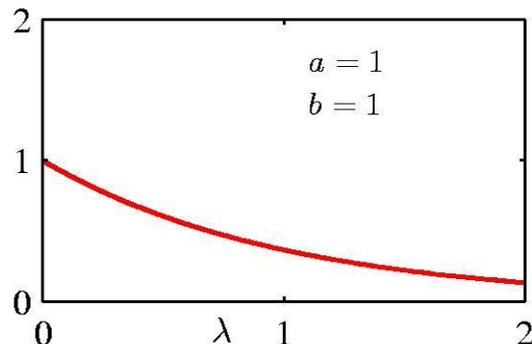
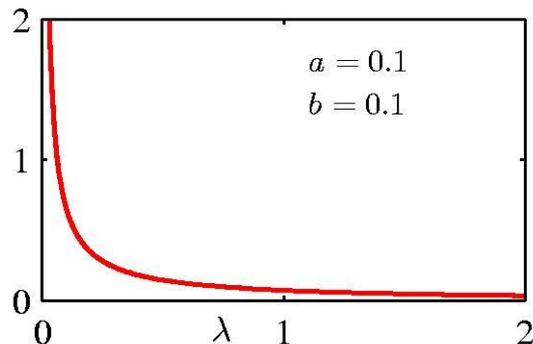
This has a Gamma shape as a function of λ .

Bayesian Inference for the Gaussian (7)

The Gamma distribution

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

$$\mathbb{E}[\lambda] = \frac{a}{b} \qquad \text{var}[\lambda] = \frac{a}{b^2}$$



Bayesian Inference for the Gaussian (8)

Now we combine a Gamma prior, $\text{Gam}(\lambda|a_0, b_0)$, with the likelihood function for λ 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 $\text{Gam}(\lambda|a_N, b_N)$ with

$$\begin{aligned} a_N &= a_0 + \frac{N}{2} \\ b_N &= b_0 + \frac{1}{2} \sum_{n=1}^N (x_n - \mu)^2 = b_0 + \frac{N}{2} \sigma_{\text{ML}}^2. \end{aligned}$$

Bayesian Inference for the Gaussian (9)

If both μ and λ 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 μ and λ .

Bayesian Inference for the Gaussian (10)

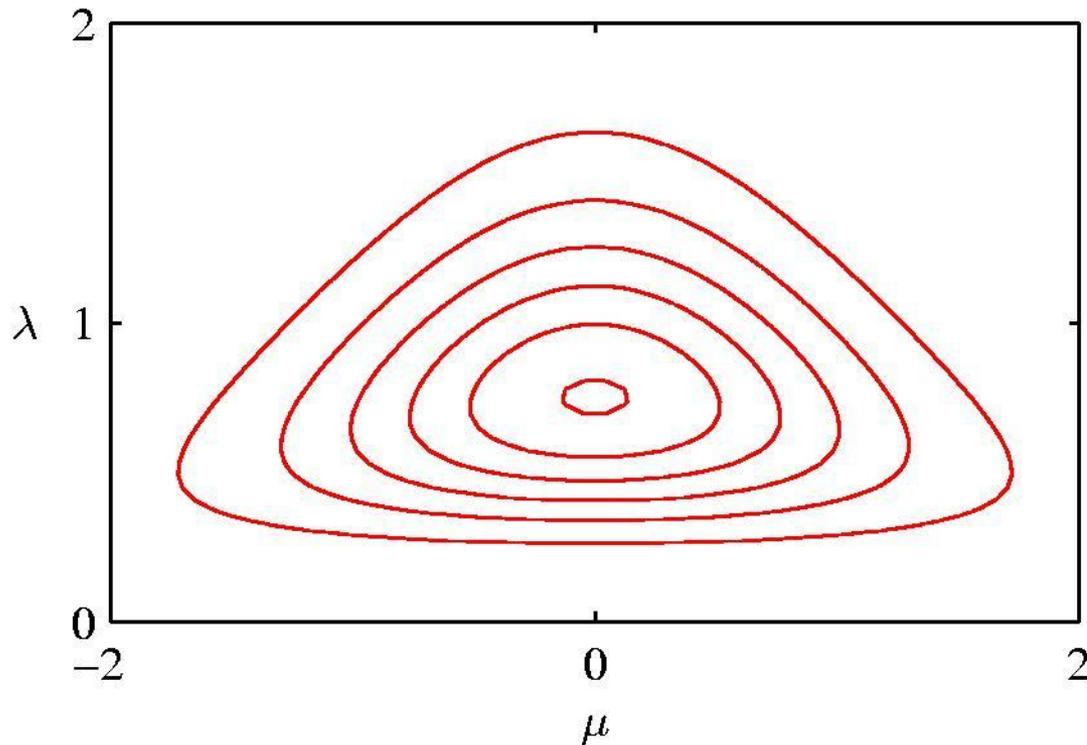
The Gaussian-gamma distribution

$$p(\mu, \lambda) = \mathcal{N}(\mu | \mu_0, (\beta\lambda)^{-1}) \text{Gam}(\lambda | a, b)$$
$$\propto \underbrace{\exp\left\{-\frac{\beta\lambda}{2}(\mu - \mu_0)^2\right\}}_{\text{Quadratic in } \mu} \underbrace{\lambda^{a-1} \exp\{-b\lambda\}}_{\text{Gamma distribution over } \lambda}$$

- Quadratic in μ .
 - Linear in λ .
 - Gamma distribution over λ .
 - Independent of μ .
-

Bayesian Inference for the Gaussian (11)

The Gaussian-gamma distribution



Bayesian Inference for the Gaussian (12)

Multivariate conjugate priors

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

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

- $\boldsymbol{\Lambda}$ and $\boldsymbol{\mu}$ unknown: $p(\boldsymbol{\mu}, \boldsymbol{\Lambda})$ Gaussian-Wishart, $p(\boldsymbol{\mu}, \boldsymbol{\Lambda}|\boldsymbol{\mu}_0, \beta, \mathbf{W}, \nu) =$

$$\mathcal{N}(\boldsymbol{\mu}|\boldsymbol{\mu}_0, (\beta\boldsymbol{\Lambda})^{-1}) \mathcal{W}(\boldsymbol{\Lambda}|\mathbf{W}, \nu)$$

Student's t-Distribution

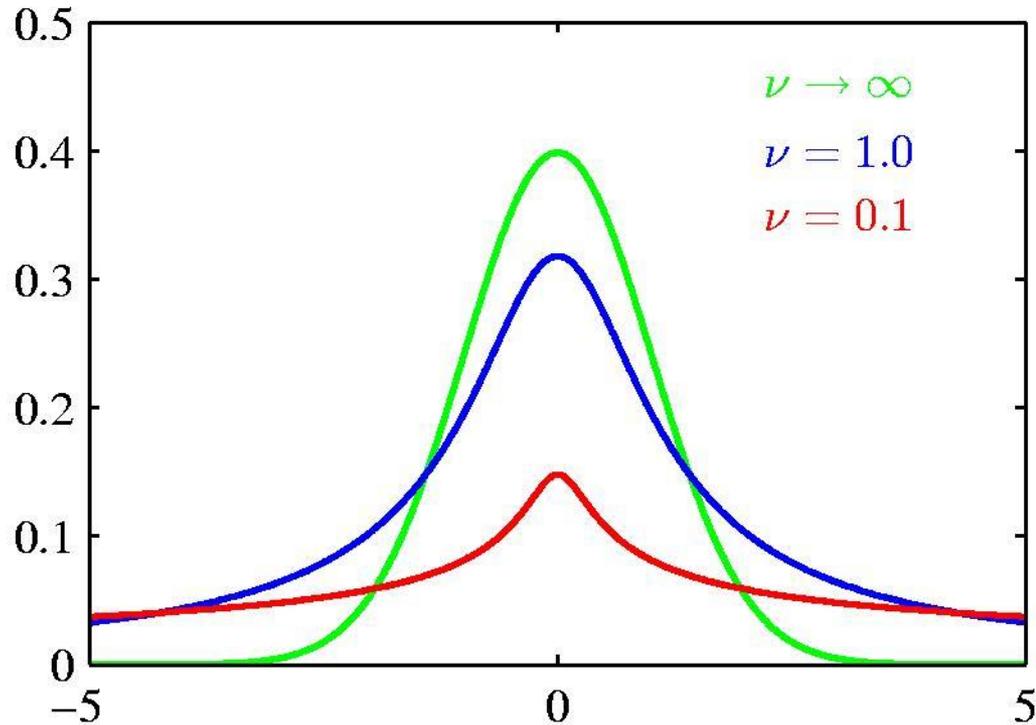
$$\begin{aligned} p(x|\mu, a, b) &= \int_0^\infty \mathcal{N}(x|\mu, \tau^{-1}) \text{Gam}(\tau|a, b) d\tau \\ &= \int_0^\infty \mathcal{N}(x|\mu, (\eta\lambda)^{-1}) \text{Gam}(\eta|\nu/2, \nu/2) d\eta \quad \leftarrow \\ &= \frac{\Gamma(\nu/2 + 1/2)}{\Gamma(\nu/2)} \left(\frac{\lambda}{\pi\nu} \right)^{1/2} \left[1 + \frac{\lambda(x - \mu)^2}{\nu} \right]^{-\nu/2 - 1/2} \\ &= \text{St}(x|\mu, \lambda, \nu) \end{aligned}$$

where

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

Infinite mixture of Gaussians.

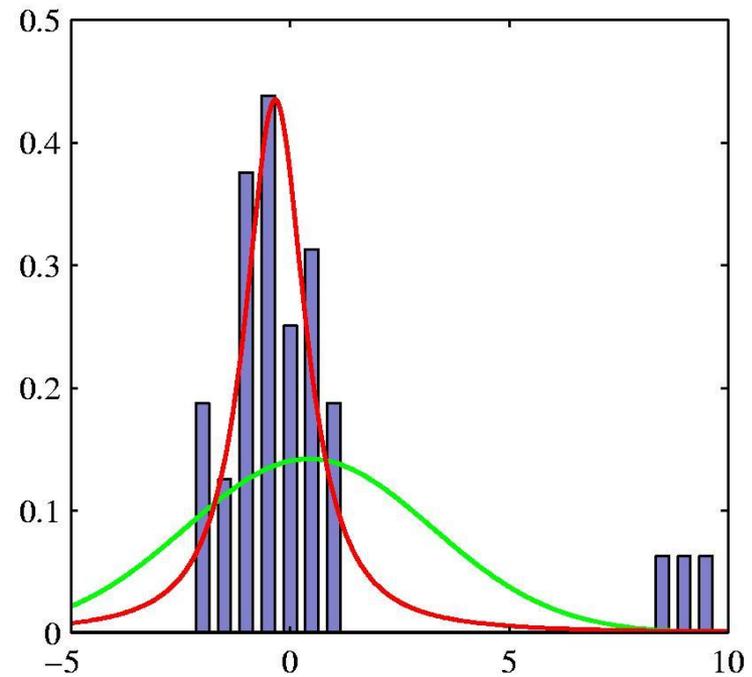
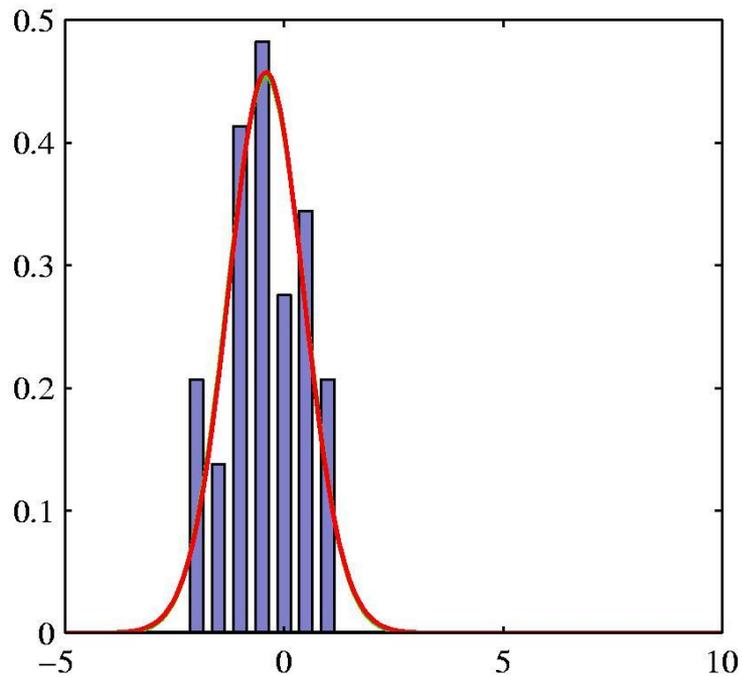
Student's t-Distribution



	$\nu = 1$	$\nu \rightarrow \infty$
$\text{St}(x \mu, \lambda, \nu)$	Cauchy	$\mathcal{N}(x \mu, \lambda^{-1})$

Student's t-Distribution

Robustness to outliers: **Gaussian** vs **t-distribution**.



Student's t-Distribution

The D -variate case:

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

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

Properties:

$$\begin{aligned}\mathbb{E}[\mathbf{x}] &= \boldsymbol{\mu}, & \text{if } \nu > 1 \\ \text{cov}[\mathbf{x}] &= \frac{\nu}{(\nu - 2)} \boldsymbol{\Lambda}^{-1}, & \text{if } \nu > 2 \\ \text{mode}[\mathbf{x}] &= \boldsymbol{\mu}\end{aligned}$$

Periodic variables

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

$$\begin{aligned} p(\theta) &\geq 0 \\ \int_0^{2\pi} p(\theta) \, d\theta &= 1 \\ p(\theta + 2\pi) &= p(\theta). \end{aligned}$$

von Mises Distribution (1)

This requirement is satisfied by

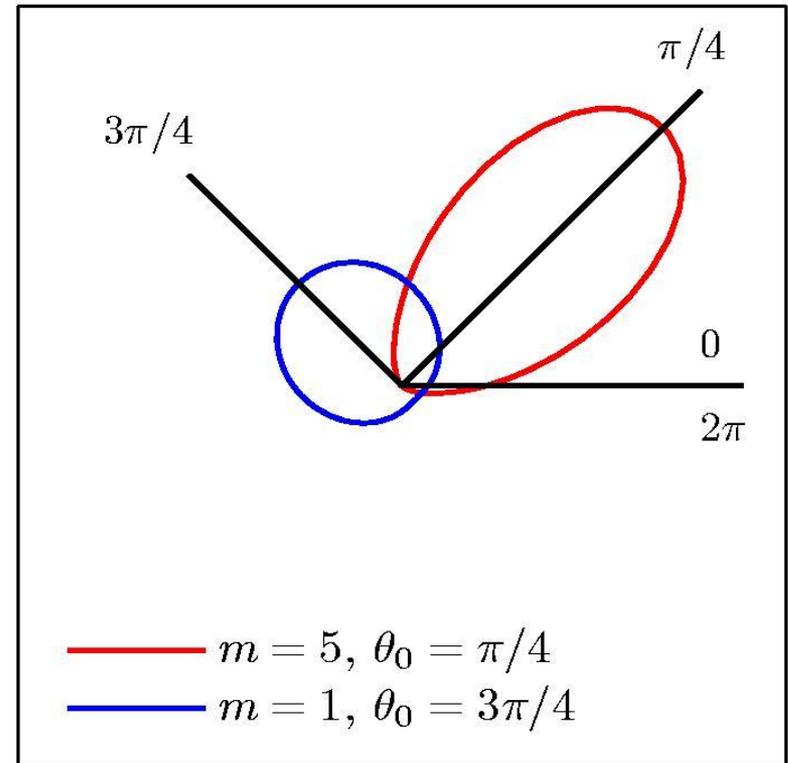
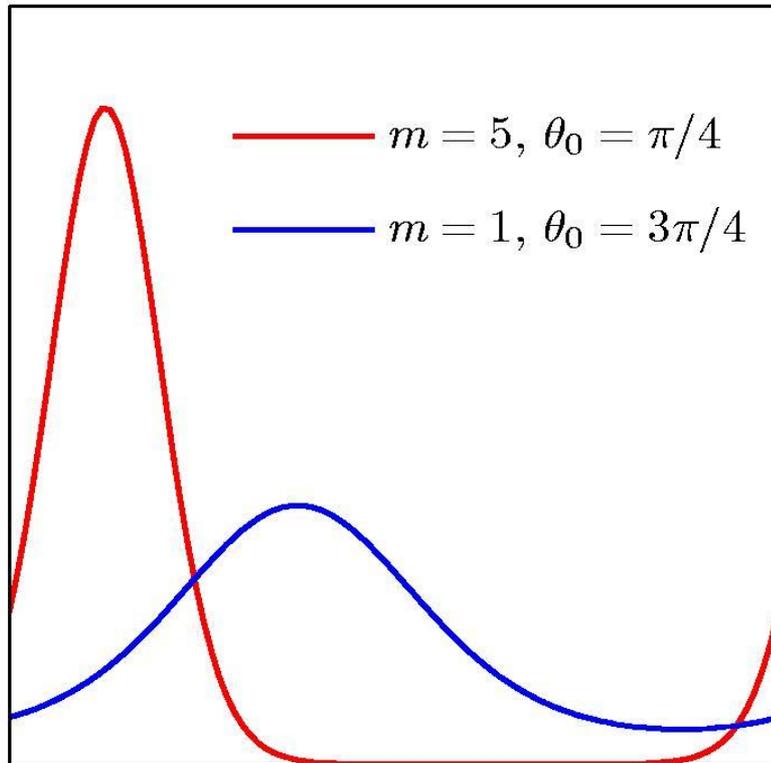
$$p(\theta|\theta_0, m) = \frac{1}{2\pi I_0(m)} \exp \{m \cos(\theta - \theta_0)\}$$

where

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

is the 0th order modified Bessel function of the 1st 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 θ_0 we directly obtain

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

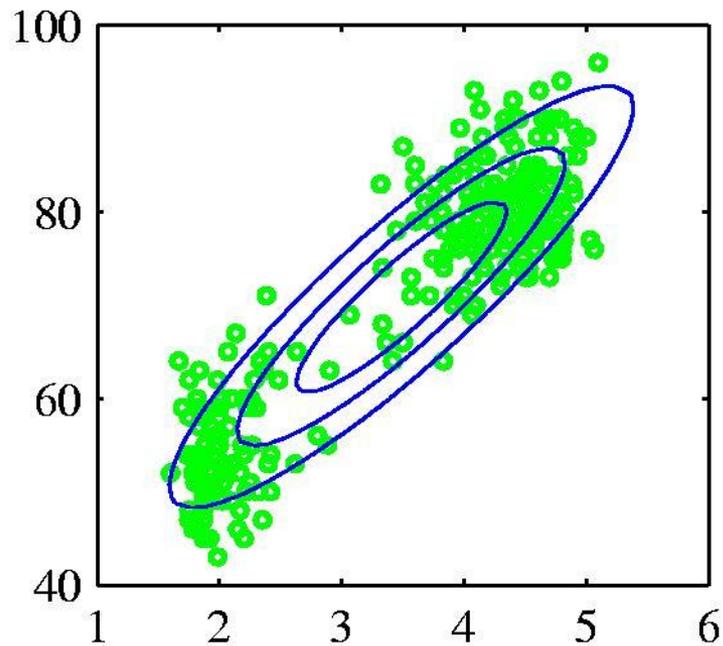
Similarly, maximizing with respect to m we get

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

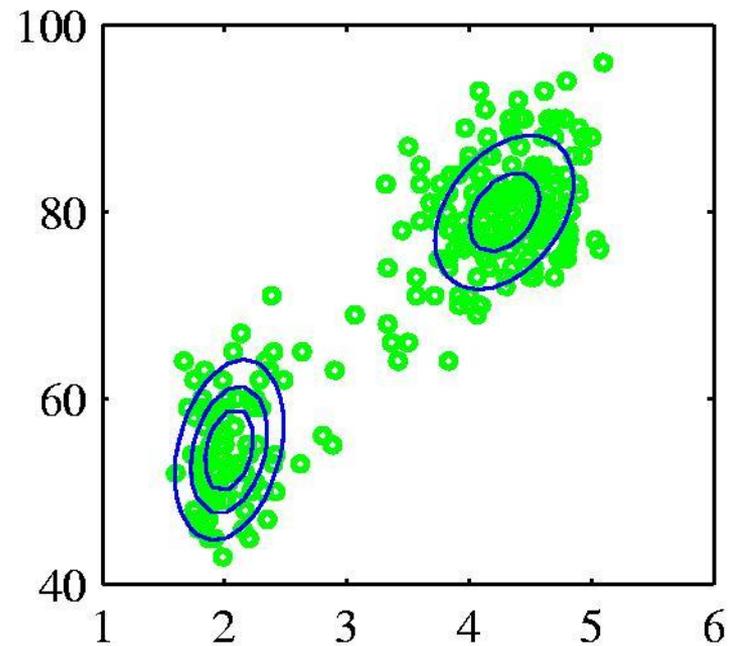
which can be solved numerically for m_{ML} .

Mixtures of Gaussians (1)

Old Faithful data set



Single Gaussian



Mixture of two Gaussians

Mixtures of Gaussians (2)

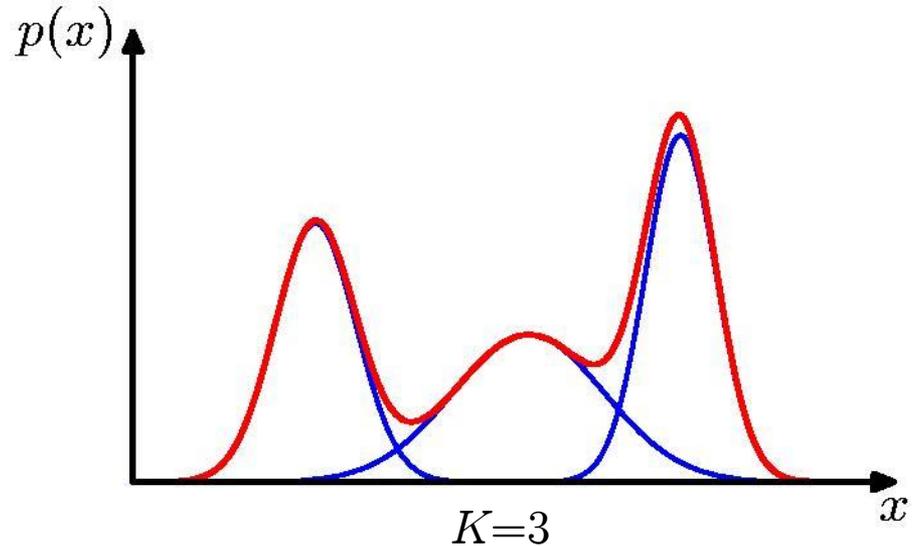
Combine simple models
into a complex model:

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

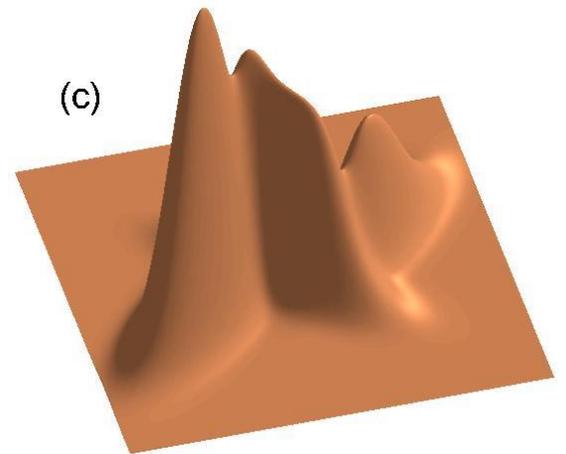
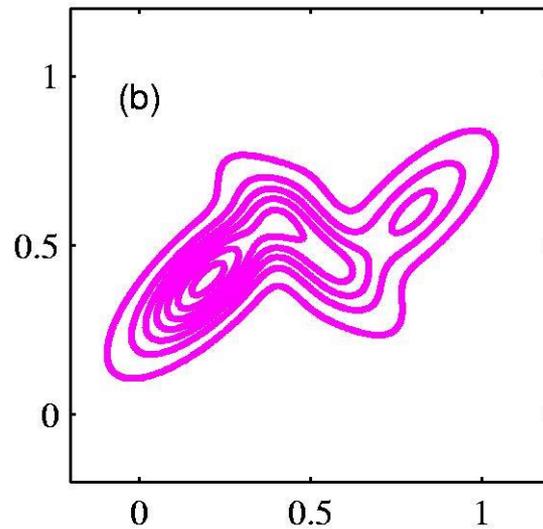
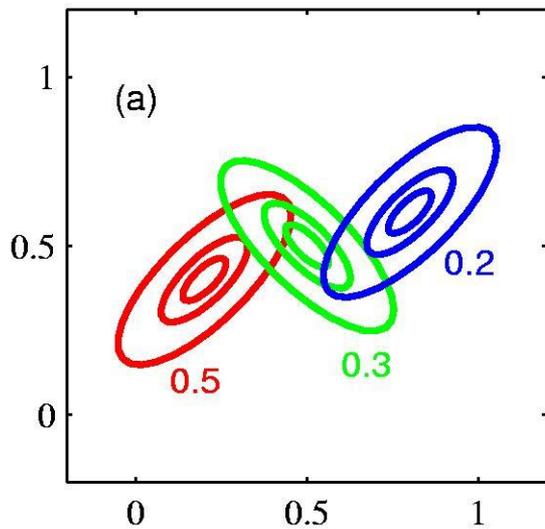
↑
Mixing coefficient

Component

$$\forall k : \pi_k \geq 0 \quad \sum_{k=1}^K \pi_k = 1$$



Mixtures of Gaussians (3)



Mixtures of Gaussians (4)

Determining parameters μ , Σ , and π using maximum log likelihood

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

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)

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

where $\boldsymbol{\eta}$ is the *natural parameter* and

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

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

The Exponential Family (2.1)

The Bernoulli Distribution

$$\begin{aligned} p(x|\mu) &= \text{Bern}(x|\mu) = \mu^x (1 - \mu)^{1-x} \\ &= \exp \{x \ln \mu + (1 - x) \ln(1 - \mu)\} \\ &= (1 - \mu) \exp \left\{ \ln \left(\frac{\mu}{1 - \mu} \right) x \right\} \end{aligned}$$

Comparing with the general form we see that

$$\eta = \ln \left(\frac{\mu}{1 - \mu} \right) \quad \text{and so} \quad \mu = \underbrace{\sigma(\eta)}_{\text{Logistic sigmoid}} = \frac{1}{1 + \exp(-\eta)}.$$

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

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

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

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

NOTE: The η_k parameters are not independent since the corresponding μ_k must satisfy

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

The Exponential Family (3.2)

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

$$\eta_k = \ln \left(\frac{\mu_k}{1 - \sum_{j=1}^{M-1} \mu_j} \right) \quad \text{and} \quad \mu_k = \frac{\exp(\eta_k)}{\underbrace{1 + \sum_{j=1}^{M-1} \exp(\eta_j)}_{\text{Softmax}}}.$$

Here the η_k parameters are independent. Note that

$$0 \leq \mu_k \leq 1 \quad \text{and} \quad \sum_{k=1}^{M-1} \mu_k \leq 1.$$

The Exponential Family (3.3)

The Multinomial distribution can then be written as

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

where

$$\begin{aligned}\boldsymbol{\eta} &= (\eta_1, \dots, \eta_{M-1}, 0)^T \\ \mathbf{u}(\mathbf{x}) &= \mathbf{x} \\ h(\mathbf{x}) &= 1 \\ g(\boldsymbol{\eta}) &= \left(1 + \sum_{k=1}^{M-1} \exp(\eta_k) \right)^{-1}.\end{aligned}$$

The Exponential Family (4)

The Gaussian Distribution

$$\begin{aligned} p(x|\mu, \sigma^2) &= \frac{1}{(2\pi\sigma^2)^{1/2}} \exp \left\{ -\frac{1}{2\sigma^2} (x - \mu)^2 \right\} \\ &= \frac{1}{(2\pi\sigma^2)^{1/2}} \exp \left\{ -\frac{1}{2\sigma^2} x^2 + \frac{\mu}{\sigma^2} x - \frac{1}{2\sigma^2} \mu^2 \right\} \\ &= h(x)g(\boldsymbol{\eta}) \exp \{ \boldsymbol{\eta}^T \mathbf{u}(x) \} \end{aligned}$$

where

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

ML for the Exponential Family (1)

From the definition of $g(\boldsymbol{\eta})$ we get

$$\nabla g(\boldsymbol{\eta}) \underbrace{\int h(\mathbf{x}) \exp \{ \boldsymbol{\eta}^T \mathbf{u}(\mathbf{x}) \} d\mathbf{x}}_{1/g(\boldsymbol{\eta})} + g(\boldsymbol{\eta}) \underbrace{\int h(\mathbf{x}) \exp \{ \boldsymbol{\eta}^T \mathbf{u}(\mathbf{x}) \} \mathbf{u}(\mathbf{x}) d\mathbf{x}}_{\mathbb{E}[\mathbf{u}(\mathbf{x})]} = 0$$

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

$$-\nabla \ln g(\boldsymbol{\eta}_{\text{ML}}) = \frac{1}{N} \underbrace{\sum_{n=1}^N \mathbf{u}(\mathbf{x}_n)}_{\text{Sufficient statistic}}$$

Sufficient statistic

Conjugate priors

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

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

Combining with the likelihood function, we get

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

Prior corresponds to ν pseudo-observations with value $\boldsymbol{\chi}$.

Noninformative Priors (1)

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

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

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

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

Noninformative Priors (2)

Translation invariant priors. Consider

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

For a corresponding prior over μ , 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, μ ; the conjugate prior is also a Gaussian,

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

As $\sigma_0^2 \rightarrow \infty$, this will become constant over μ .

Noninformative Priors (4)

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

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

For a corresponding prior over σ , 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, σ^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 λ is the Gamma distribution,

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

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.

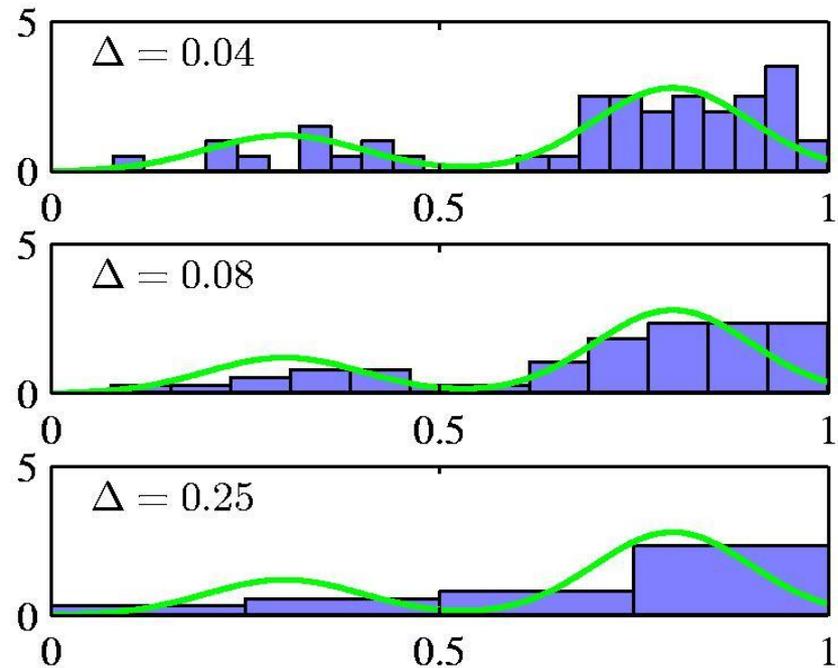
Nonparametric approaches make few assumptions about the overall shape of the distribution being modelled.

Nonparametric Methods (2)

Histogram methods partition the data space into distinct bins with widths Δ_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, $\Delta_i = \Delta$.
- Δ 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

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

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

$$K \simeq NP.$$

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)

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

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)

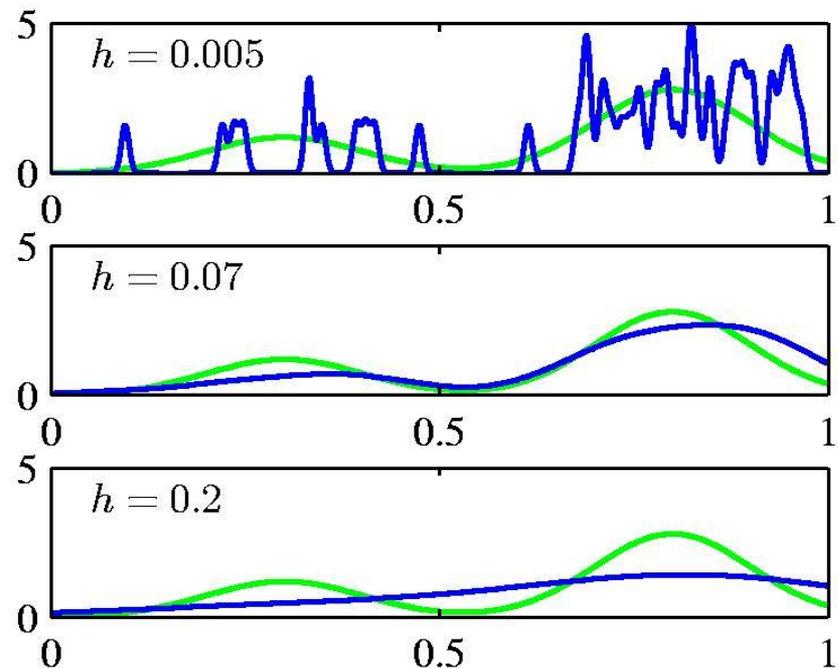
To avoid discontinuities in $p(\mathbf{x})$,
use a smooth kernel, e.g. a
Gaussian

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

Any kernel such that

$$\begin{aligned} k(\mathbf{u}) &\geq 0, \\ \int k(\mathbf{u}) \, d\mathbf{u} &= 1 \end{aligned}$$

will work.



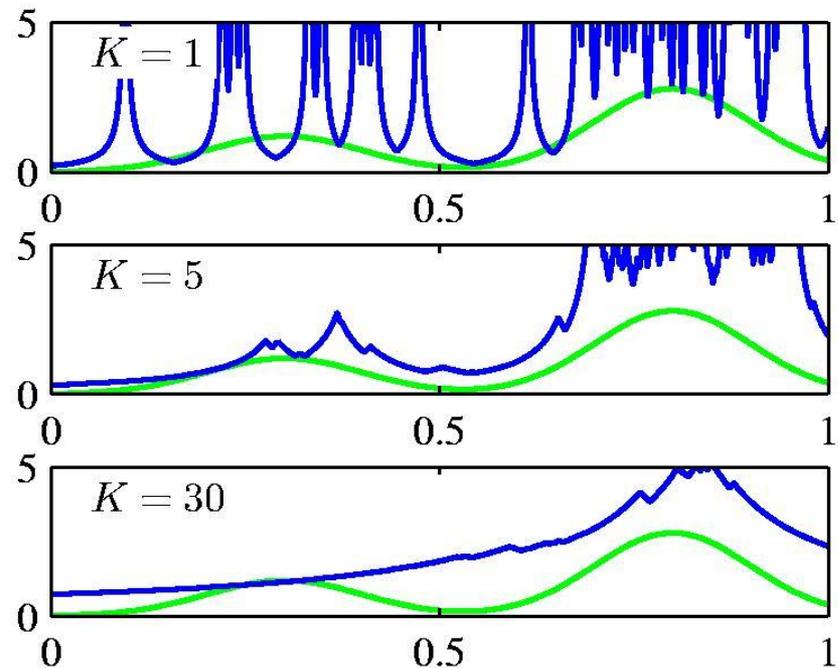
h acts as a smoother.

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

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



K acts as a smoother.

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

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

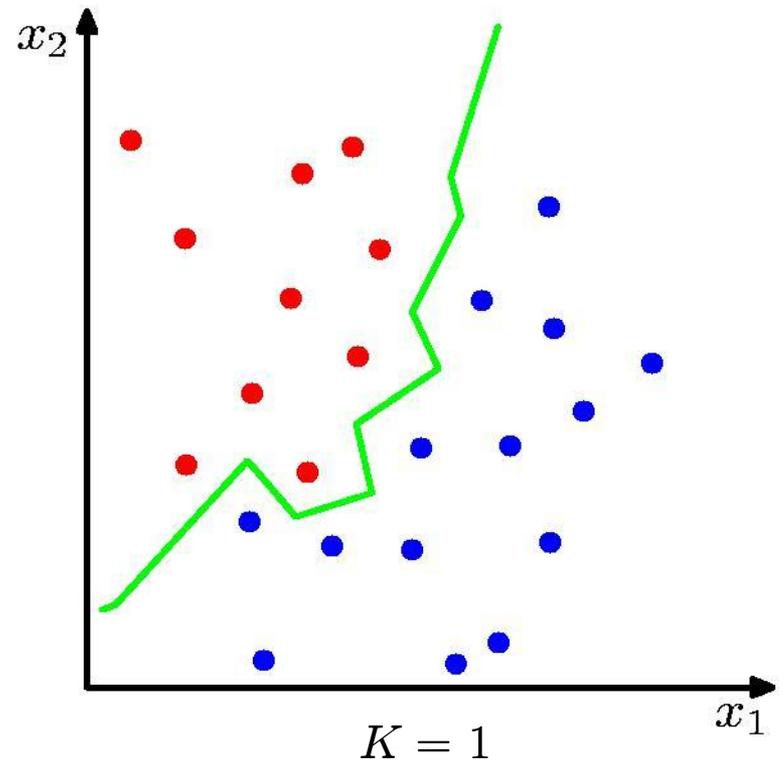
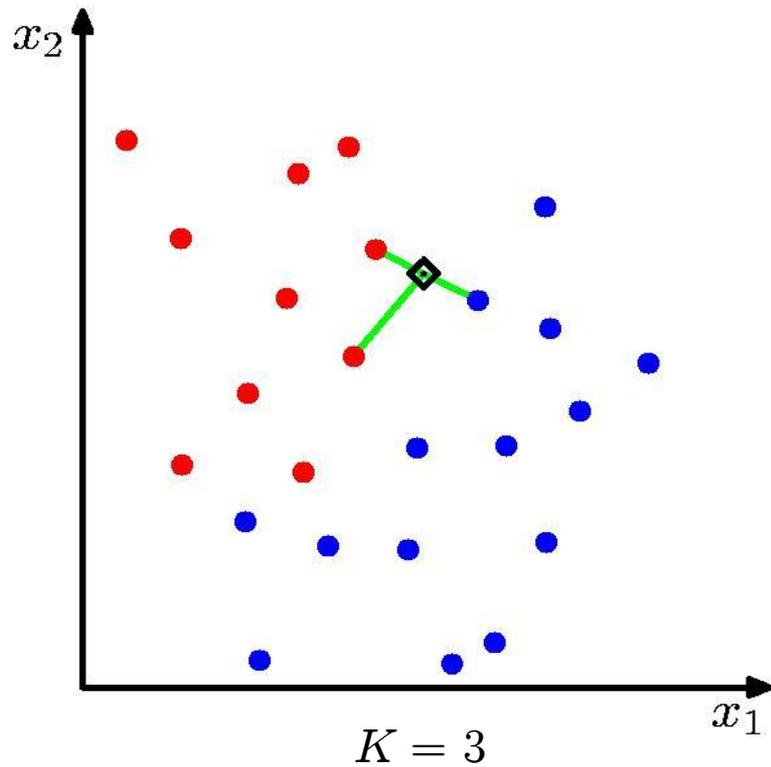
and correspondingly

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

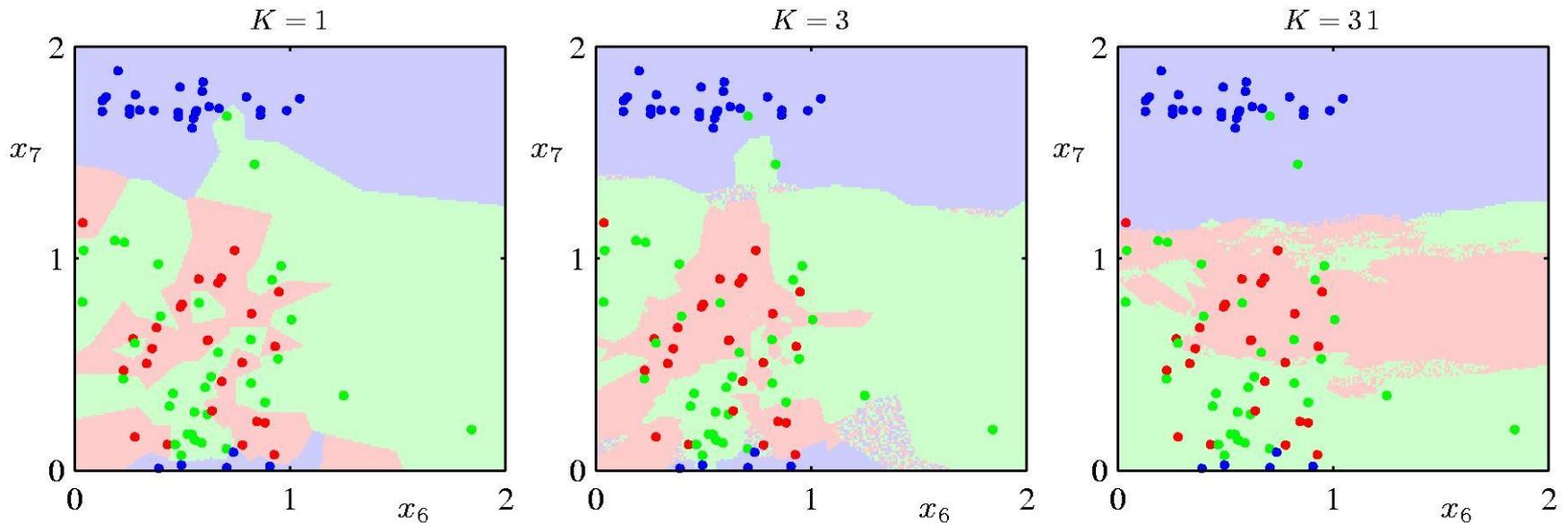
Since $p(\mathcal{C}_k) = N_k/N$, Bayes' theorem gives

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

K -Nearest-Neighbours for Classification (2)



K -Nearest-Neighbours for Classification (3)



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