STA 414/2104

Lecture 2, 15 January 2018

With thanks to Russ Salakhutdinov

The exponential family, maximum likelihood, and optimization

Outline

- Seven distributions and their ML estimates
  - Bernoulli, binomial, and multinomial discrete
  - Beta and Dirichlet multivariate extension of beta
  - Normal and Student's *t*
- Mixture of Gaussians
- The Exponential Family and its ML estimates
  maximum likelihood

The Bernoulli Distribution

- Consider a single binary random variable $x \in \{0, 1\}$. For example, *x* can describe the outcome of flipping a coin:

  Coin flipping: heads = 1, tails = 0.

- The probability of *x*=1 will be denoted by the parameter *μ*, not *p* as you may have encountered in earlier courses, so that:

$$p(x = 1|\mu) = \mu \qquad 0 \leq \mu \leq 1.$$

- The probability distribution, known as the **Bernoulli distribution**, can be written as:

$$\begin{aligned} \mathrm{Bern}(x|\mu) &= \mu^x (1-\mu)^{1-x} \\ \mathbb{E}[x] &= \mu \\ \mathrm{var}[x] &= \mu(1-\mu) \end{aligned}$$

Parameter Estimation

- Suppose we observed a dataset $\mathcal{D} = \{x_1, ..., x_N\}$

We can construct the likelihood function, which is a function of μ.

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

- Equivalently, we can consider the log of the likelihood function:

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

- Note that the likelihood function depends on the N observations x_n only through the sum $\sum_n x_n$

order is not relevant

Sufficient Statistic

Parameter Estimation

- Suppose we observed a dataset $\mathcal{D} = \{x_1, \ldots, x_N\}$

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

Let's find the μ which maximizes the likelihood function. Setting the derivative of the log-likelihood function w.r.t μ to zero, we obtain:

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

where m is the number of heads. If N is small, then problematic

This is a simplistic example of **parameter estimation**.

The Binomial Distribution

- We can work out the distribution of the number *m* of observations of *x*=1 (e.g. the number of heads).

The probability of observing *m* heads given *N* coin flips and a parameter μ is given by the **binomial distribution**:

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

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

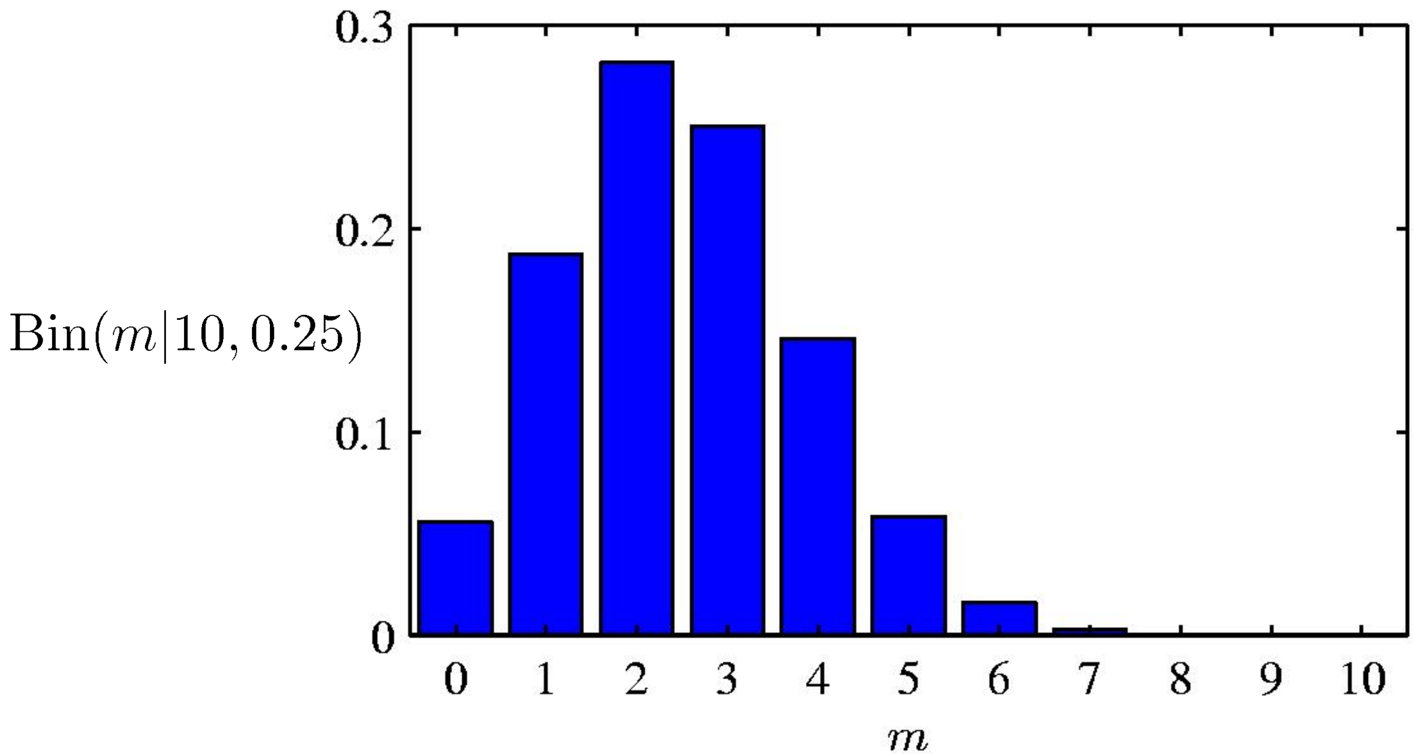
- Review exercise: show that the mean and variance are:

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

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

Example

Below is a histogram plot of the binomial distribution as a function of *m* for *N*=10 and μ = 0.25.



Beta Distribution

We can define a **distribution** over $\mu \in [0,1]$ (e.g. it can be used as a prior over the parameter μ of the Bernoulli distribution).

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

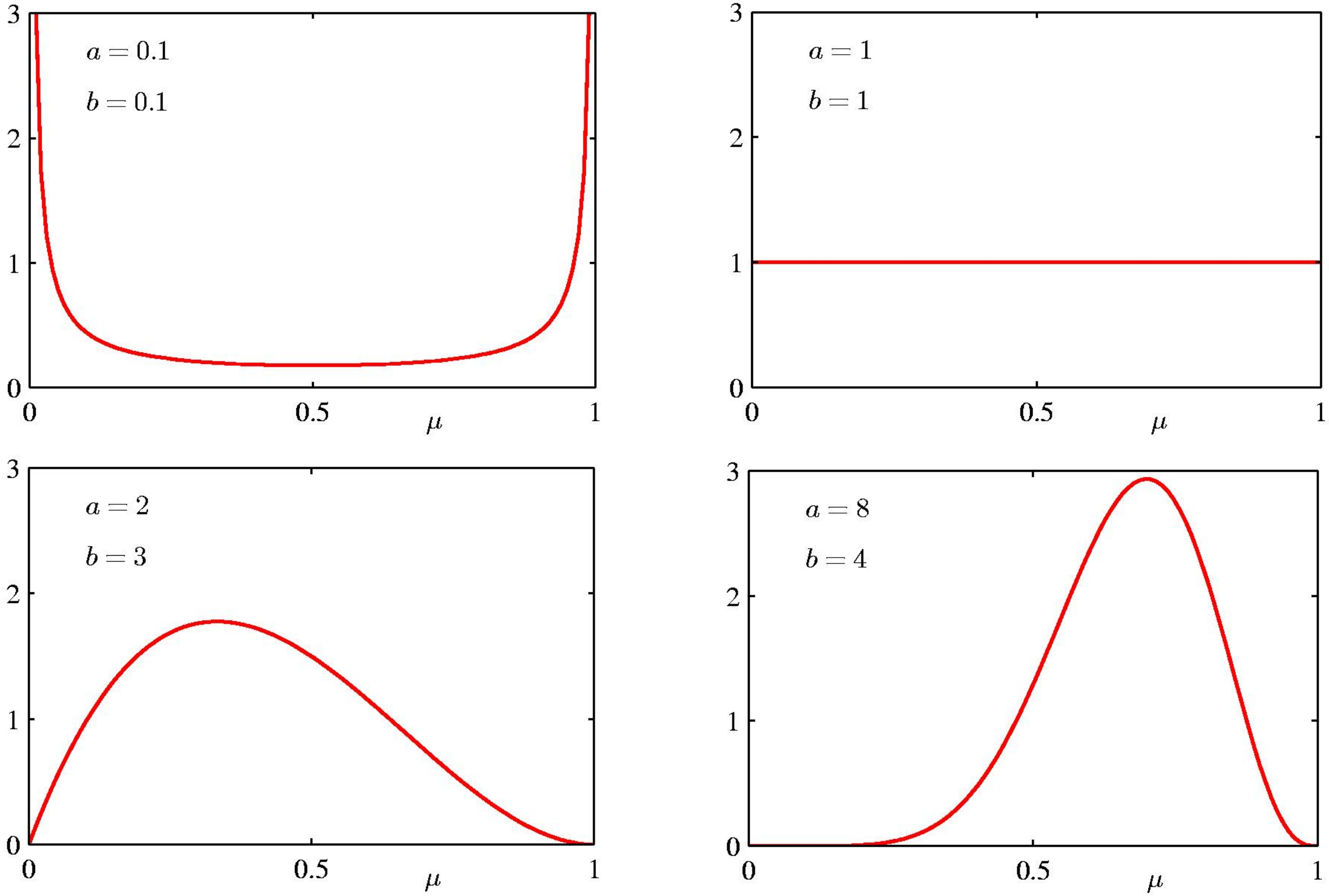
where the gamma function is defined as:

$$\Gamma(x) \equiv \int_0^\infty u^{x-1}e^{-u}du.$$

and ensures that the beta distribution is normalized.

Beta Distribution

if a = b, symmetry
a=1, b=1, uniform distribution
if a,b>0, hill shape



The beta distribution can be used to specify a posterior distribution over μ.
See for example John Rice's 3rd edition, Section 3.5 Example E; or Bishop 2.1.1

Multinomial Variables

- Consider a random variable that can take on one of *K* mutually exclusive states (e.g. rolling a die).

- We will use the so-called 1-of-*K* encoding scheme. For example, if a random variable can take on *K*=6 states, and a particular observation of the variable corresponds to the state x_3=1, then **x** will be represented as:

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

- If we denote the probability of x_k=1 by the parameter μ_k, then the distribution over **x** is defined as:

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{x_k} \qquad \forall k : \mu_k \geqslant 0 \quad \text{and} \quad \sum_{k=1}^{K} \mu_k = 1$$

Multinomial Variables

- A multinomial variable can be viewed as a generalization of the Bernoulli trial to more than two outcomes.

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

- It is easy to see that the above probabilities sum to 1:

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

and that

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

Maximum Likelihood Estimation

- Suppose we observed a dataset $\mathcal{D} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$

We can construct the likelihood function, which is a function of μ.

m_k : number of times side k is rolled

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

- Note that the likelihood function depends on the *N* data points only though the following *K* quantities:

$$m_k = \sum_n x_{nk}, \quad k = 1, ..., K.$$

where each represents the number of observations of x_k=1.

- These m_k are the sufficient statistics for this distribution.

Maximum Likelihood Estimation

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

To find a maximum likelihood estimate for μ, we maximize the log-likelihood taking into account the constraint that $\sum_k \mu_k = 1$

- Create a Lagrangian function:

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

which leads to:

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

and thus we estimate μ_k as the fraction of observations for which x_k=1.

Is this simplistic?

The Multinomial Distribution

We can construct the joint distribution of the quantities $\{m_1, m_2, \ldots, m_k\}$ given the parameters $\boldsymbol{\mu}$ and the total number N of observations:

N! / (m1! m2! … mK!)

$$
\begin{aligned}
\mathrm{Mult}(m_1, m_2, \ldots, m_K|\boldsymbol{\mu}, N) &= \binom{N}{m_1 m_2 \ldots m_K} \prod_{k=1}^{K} \mu_k^{m_k} \\
\mathbb{E}[m_k] &= N\mu_k \\
\mathrm{var}[m_k] &= N\mu_k(1-\mu_k) \\
\mathrm{cov}[m_j m_k] &= -N\mu_j\mu_k
\end{aligned}
$$

- The normalization coefficient is the number of ways of partitioning N objects into K groups with m_k objects in the kth group

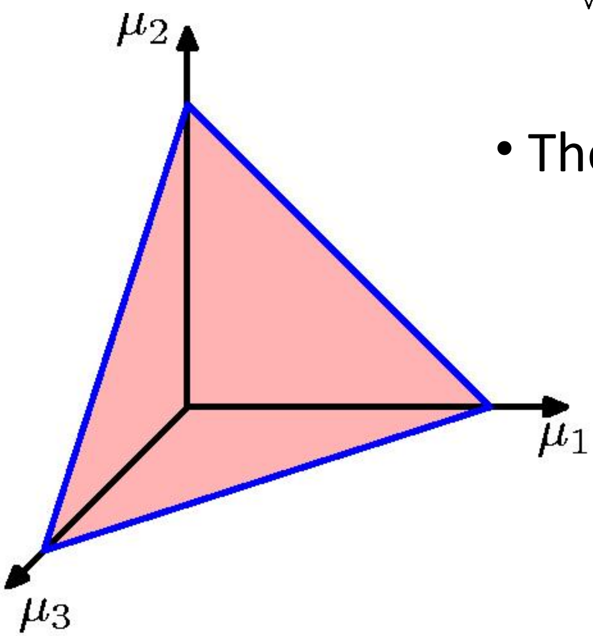
- This is known as the **multinomial distribution**. Note that

$$\sum_k m_k = N.$$

example: rolling a die multiple times without knowing probability of a side turning up…

The Dirichlet Distribution

Consider a distribution over μ_k – subject to constraints:



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

- The **Dirichlet distribution** is defined as:

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

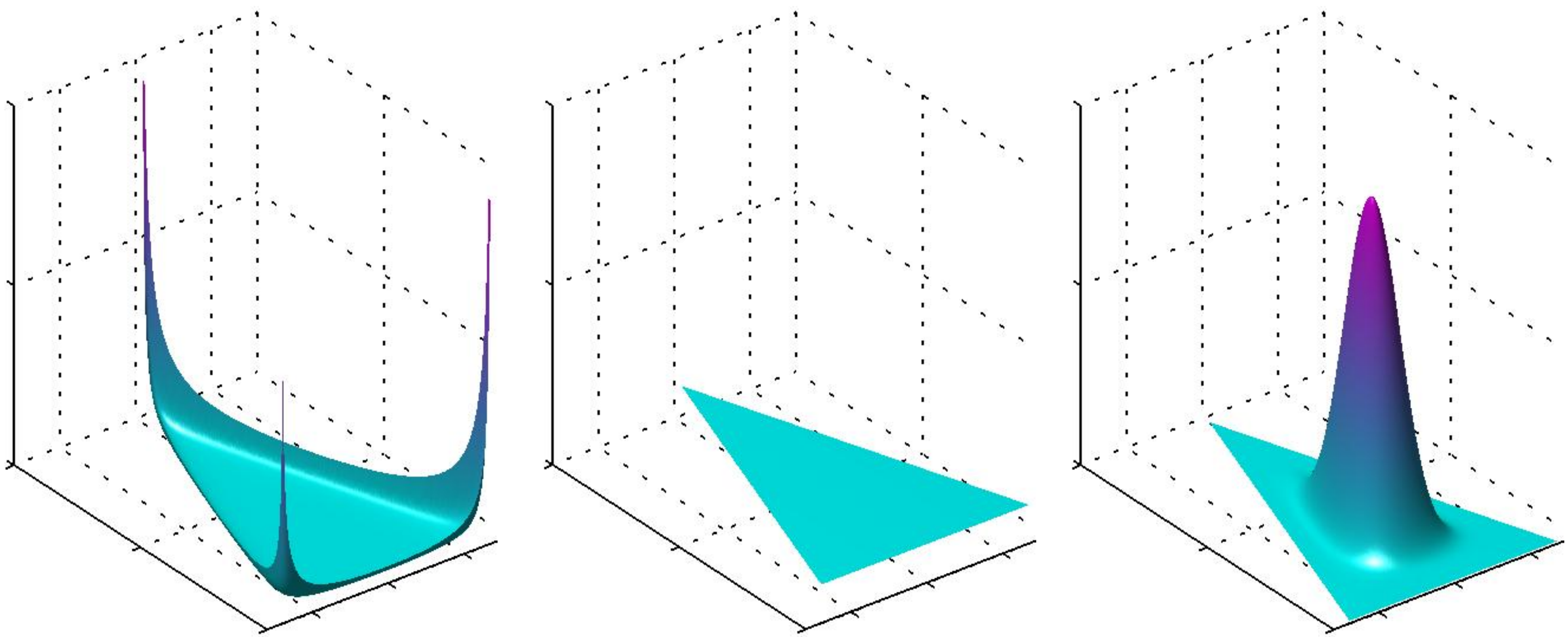
$$\alpha_0 = \sum_{k=1}^{K} \alpha_k$$

where $\alpha_1, \ldots, \alpha_k$ are the parameters of the distribution, and $\Gamma(\cdot)$ is the gamma function.

- The Dirichlet distribution is confined to a *simplex* (the generalization of a triangle to arbitrary dimension) as a consequence of the constraints.

The Dirichlet Distribution

- Plots of the Dirichlet distribution over three variables.



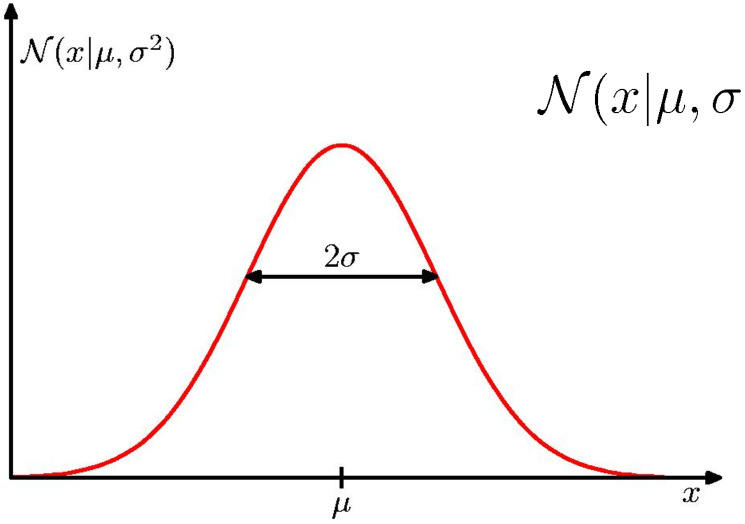
$\alpha_k = 10^{-1}$ $\alpha_k = 10^{0}$ $\alpha_k = 10^{1}$

similar to beta distribution plot

uniform distribution

Gaussian Univariate Distribution

- In the case of a single variable *x*, the Gaussian distribution takes the form



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

which is governed by two parameters:

- μ (mean)
- σ^2 (variance)

- The Gaussian distribution satisfies:

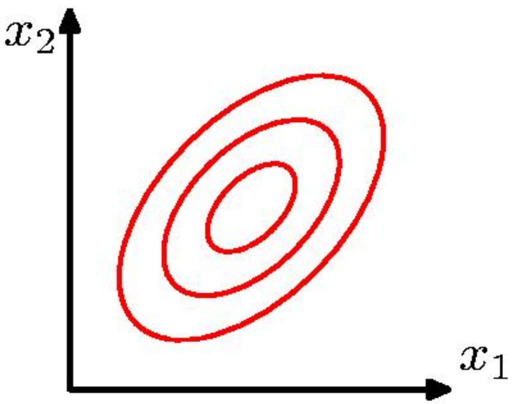
$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu,\sigma^2\right)\,\mathrm{d}x = 1$$

Multivariate Gaussian Distribution

- For a *D*-dimensional vector **x**, the Gaussian distribution takes the form

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



which is governed by two parameters:

- $\boldsymbol{\mu}$ is a *D*-dimensional mean vector
- $\boldsymbol{\Sigma}$ is a *D*-by-*D* covariance matrix

and $|\boldsymbol{\Sigma}|$ denotes the determinant of $\boldsymbol{\Sigma}$.

Z^T \Sigma Z > 0 for Z \neq 0

- The covariance matrix is a positive definite matrix. (Appendix C of Christopher Bishop's book gives a review of matrices.)

Central Limit Theorem

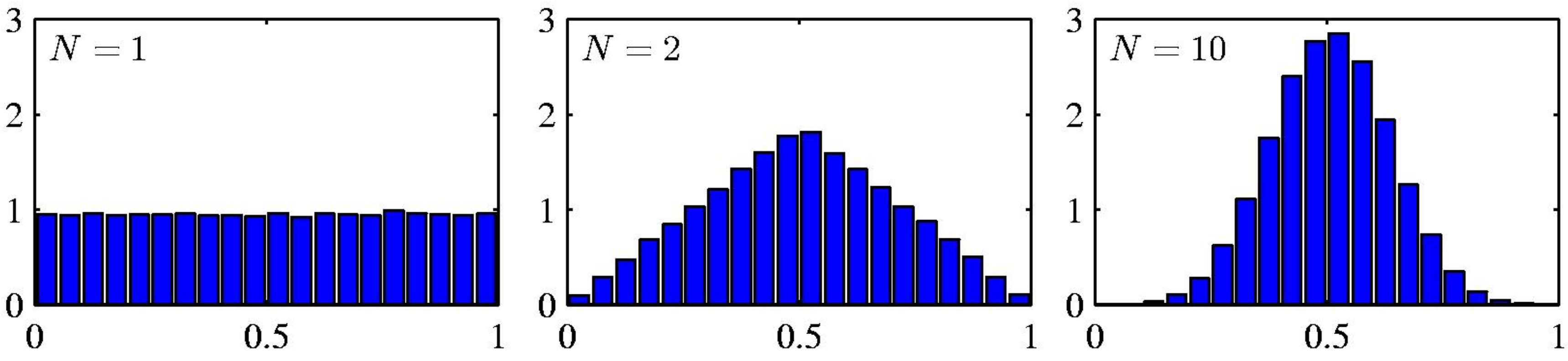
- The distribution of the sum of *N* i.i.d. random variables becomes increasingly Gaussian as *N* grows.

- Consider *N* variables, each of which has a uniform distribution over the interval [0,1].

- Let us look at the distribution over the mean:

$$\frac{x_1 + x_2 + ... + x_N}{N}.$$

- As *N* increases, the distribution tends towards a Gaussian distribution.



Geometry of the Gaussian Distribution

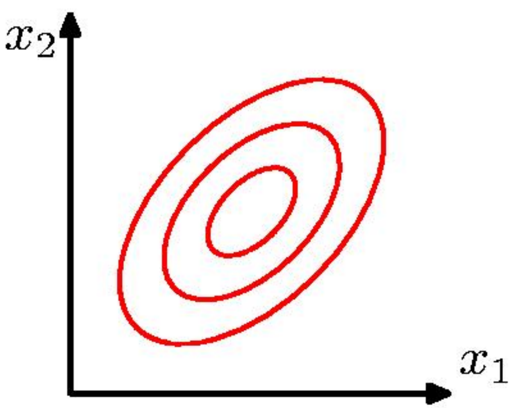
- For a D-dimensional vector **x**, the Gaussian distribution takes the form

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

Let us analyse the functional dependence of the Gaussian on **x** through the quadratic form:

$$\underbrace{\Delta^2}_{\text{a scalar}} = (\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})$$

- Here Δ is known as the Mahalanobis distance. generalization of standard deviation



The Gaussian distribution will be constant on surfaces in **x**-space for which Δ is constant.

Geometry of the Gaussian Distribution

- For a D-dimensional vector **x**, the Gaussian distribution takes the form

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

- Consider the eigenvalue equation for the covariance matrix:

$$\boldsymbol{\Sigma}\mathbf{u}_i = \lambda_i \mathbf{u}_i, \quad \text{where} \quad i = 1, ..., D.$$

- You should be able to show that the covariance can be expressed in terms of its eigenvectors:

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

- The inverse of the covariance is:

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

Geometry of the Gaussian Distribution

- For a *D*-dimensional vector **x**, the Gaussian distribution takes the form

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

- Remember:

$$\Delta^2 = (\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu}) \qquad \boldsymbol{\Sigma}^{-1} = \sum_{i=1}^{D} \frac{1}{\lambda_i} \mathbf{u}_i \mathbf{u}_i^{\mathrm{T}}$$

- Hence:

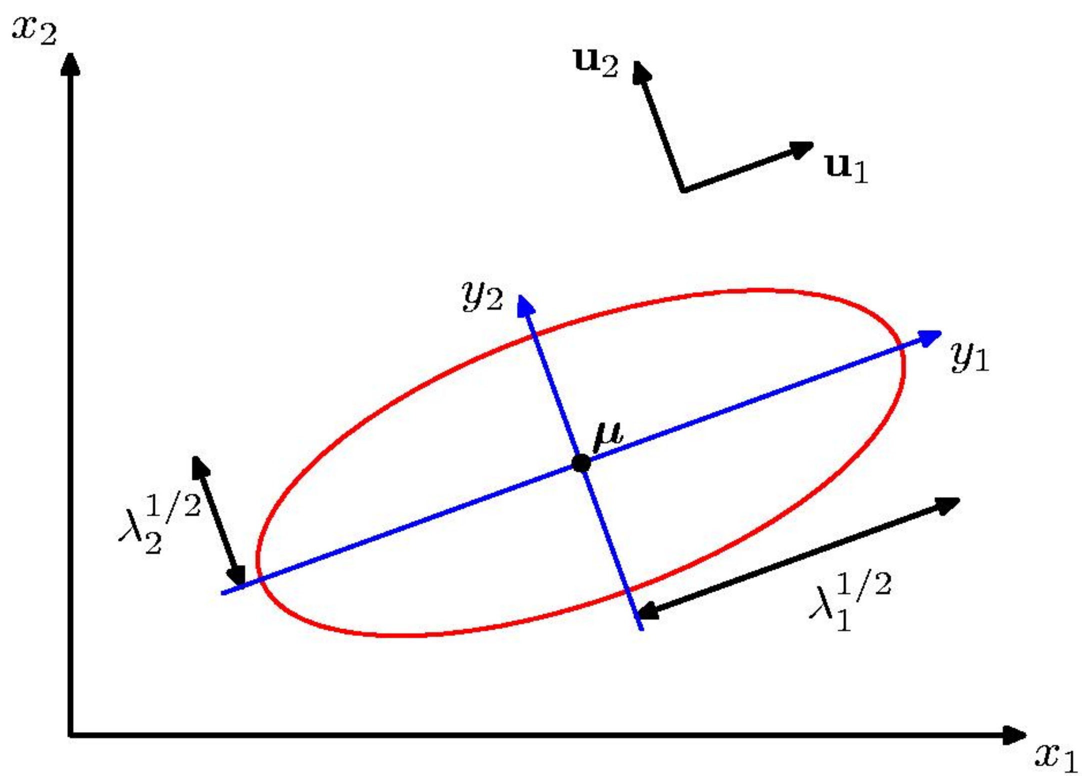
$$\Delta^2 = \sum_{i=1}^{D} \frac{y_i^2}{\lambda_i} \qquad y_i = \mathbf{u}_i^{\mathrm{T}} (\mathbf{x}-\boldsymbol{\mu})$$

- We can interpret $\{y_i\}$ as a new coordinate system defined by the orthonormal vectors $\mathbf{u}_i$ that are shifted and rotated.

Geometry of the Gaussian Distribution

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

$$\Delta^2 = \sum_{i=1}^{D} \frac{y_i^2}{\lambda_i} \qquad y_i = \mathbf{u}_i^{\mathrm{T}}(\mathbf{x}-\boldsymbol{\mu})$$



- Red curve: surface of constant probability density
- The axes are defined by the eigenvectors $\mathbf{u}_i$ of the covariance matrix with corresponding eigenvalues

Moments of the Gaussian Distribution

- The expectation of **x** under the Gaussian distribution is:

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

cancels z out since oddxeven function

This is an even function of **z**, so this multiplied by **z** will vanish by symmetry.

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

Moments of the Gaussian Distribution

- Additional algebra leads to the second-order raw moments of the Gaussian distribution:

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

- The second-order central moments are given by the covariance matrix:

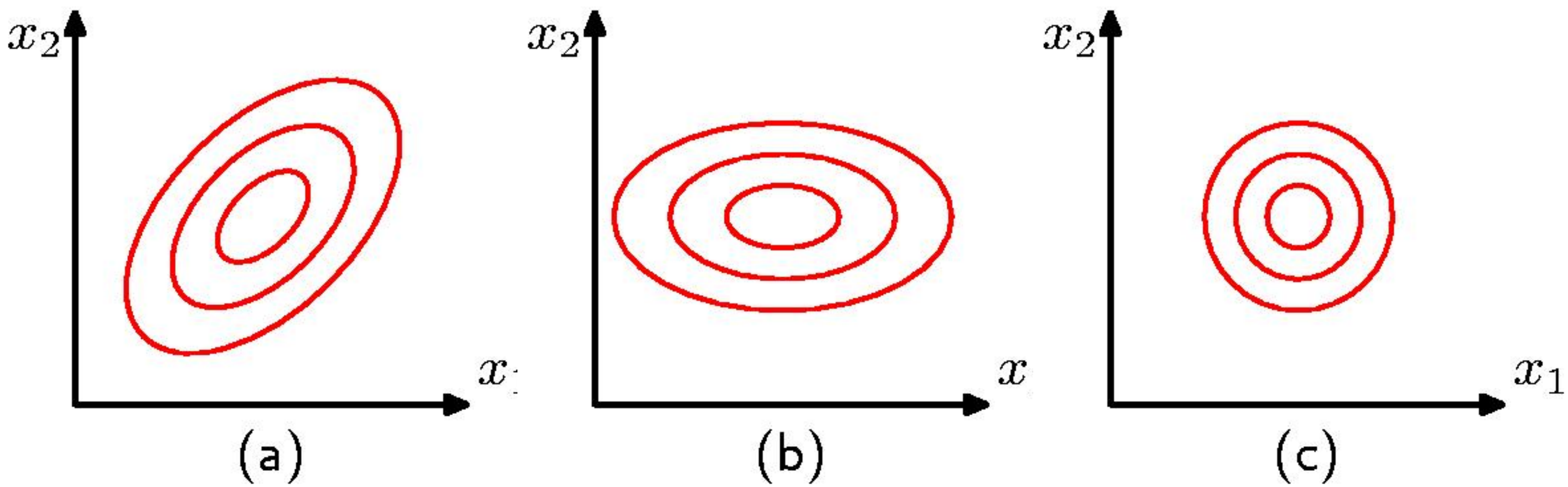
$$\mathrm{cov}[\mathbf{x}] = \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^{\mathrm{T}}\right] = \boldsymbol{\Sigma}$$

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

Because the parameter matrix **Σ** governs the covariance of **x** under the Gaussian distribution, it is called the covariance matrix.

Moments of the Gaussian Distribution

- Contours of constant probability density:



Covariance matrix is of general form.

Diagonal, axis-aligned covariance matrix

Spherical covariance matrix (proportional to identity matrix)

Partitioned Gaussian Distribution

- Consider a *D*-dimensional Gaussian distribution: $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- Let us partition a datum **x** into two disjoint subsets $\mathbf{x}_a$ and $\mathbf{x}_b$:

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

- In many situations, it will be more convenient to work with the precision matrix (inverse of the covariance matrix):

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

- Note that $\boldsymbol{\Lambda}_{aa}$ is not given by the inverse of $\boldsymbol{\Sigma}_{aa}$. doesnt correspond

Conditional Distribution

- It turns out that the conditional distribution is also a Gaussian distribution:

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

Covariance does not depend on $\mathbf{x}_b$

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

linear gaussian

Linear function of $\mathbf{x}_b$

Marginal Distribution

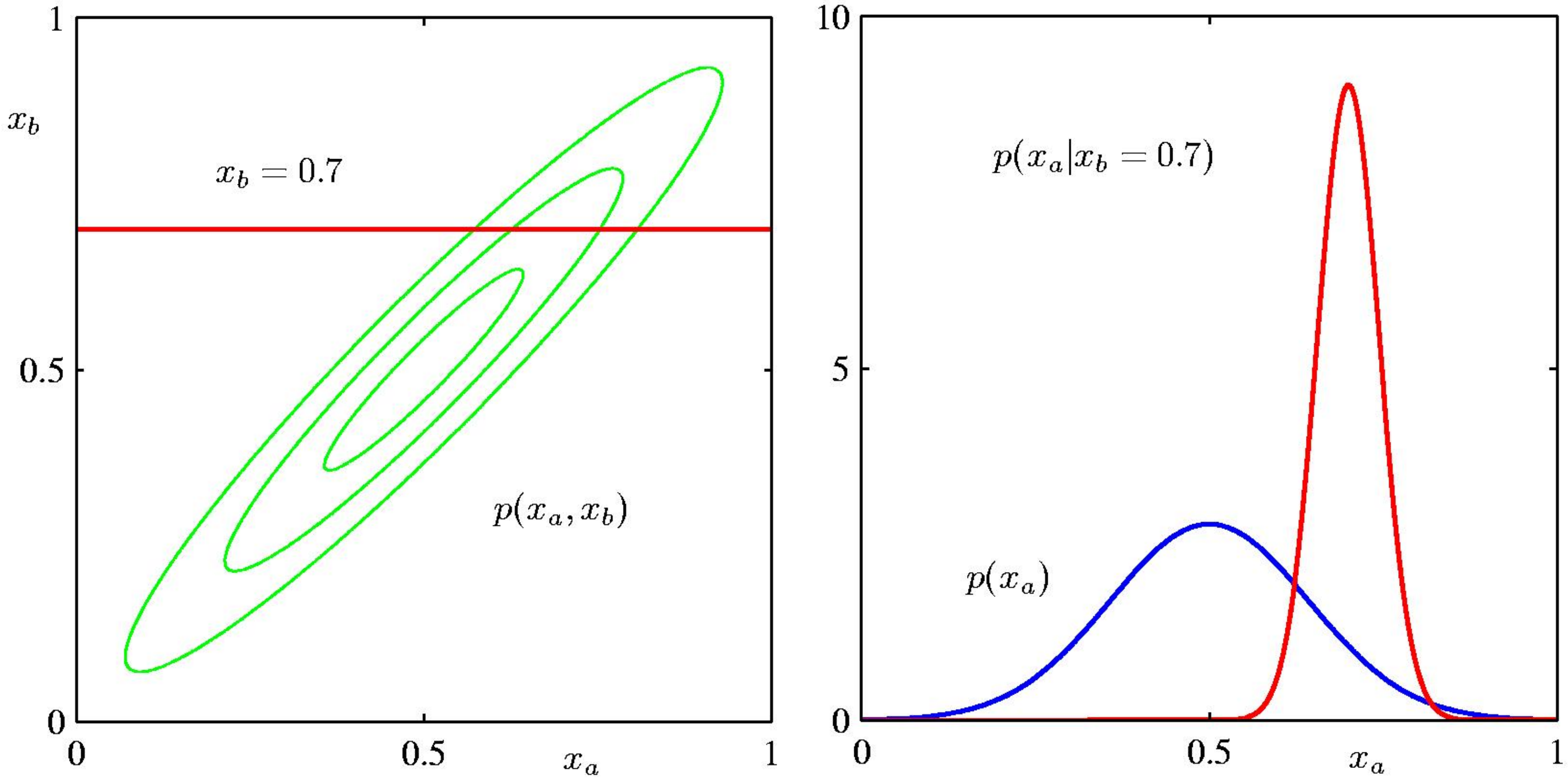
- It turns out that the marginal distribution is also a Gaussian distribution:

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

- For a marginal distribution, the mean and covariance are most simply expressed in terms of partitioned covariance matrix.

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

Conditional and Marginal Distributions



Maximum Likelihood Estimation

- Suppose we observed i.i.d data $\mathbf{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$.

We can construct the log-likelihood function, which is a function of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$:

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

- Note that the likelihood function depends on the *N* data points only through the following sums:

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

Sufficient Statistics

Maximum Likelihood Estimation

- To find a maximum likelihood (ML) estimate of the mean, we 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:

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

More difficult to find is the ML estimate of **Σ** which is:

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

Maximum Likelihood Estimation

- Evaluating the expectation of the ML estimates under the true distribution, we obtain:

Unbiased estimate

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

Biased estimate

- Note that the maximum likelihood estimate of **Σ** is biased.

- We can correct the bias by defining a different estimator:

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

Sequential Estimation

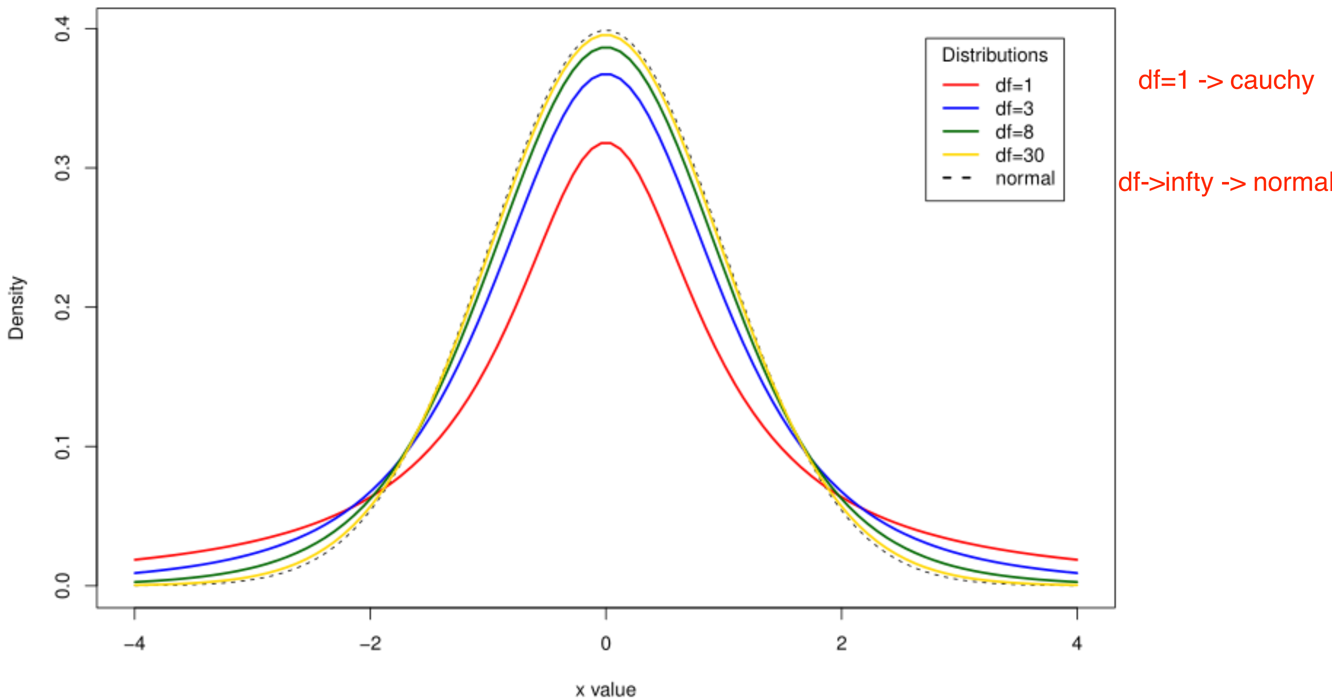
- Sequential estimation allows data points to be processed one at a time and then discarded. This is important for *online algorithms*.

- Let's consider the contribution of the N^{th} data point $\mathbf{x}_n$:

$$
\begin{aligned}
\boldsymbol{\mu}_{\mathrm{ML}}^{(N)} &= \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n \\
&= \frac{1}{N}\mathbf{x}_N + \frac{1}{N}\sum_{n=1}^{N-1}\mathbf{x}_n \\
&= \frac{1}{N}\mathbf{x}_N + \frac{N-1}{N}\boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)} \\
&= \underbrace{\boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)}}_{\text{old estimate}} + \underbrace{\frac{1}{N}}_{\text{correction weight}}\underbrace{\left(\mathbf{x}_N - \boldsymbol{\mu}_{\mathrm{ML}}^{(N-1)}\right)}_{\text{correction given } \mathbf{x}_N}
\end{aligned}
$$

Student’s *t*-distribution

• You’re familiar with the *t*-distribution (aka Students’ *t*-distribution) as the quotient of a standard normal and a χ^2 distribution



• In Bayesian machine learning, we often generalize the *t*-distribution. A common parameterization is to consider a Gaussian distribution with known mean (not necessarily zero!) and unknown variance such that the variance has a Gamma prior distribution

Student's *t*-distribution

- Therefore, Student's *t*-distribution is

assume tau's distribution is gamma

tau^-1 is called precision

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

Infinite mixture of Gaussians

where

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

Sometimes called the precision parameter

Degrees of freedom

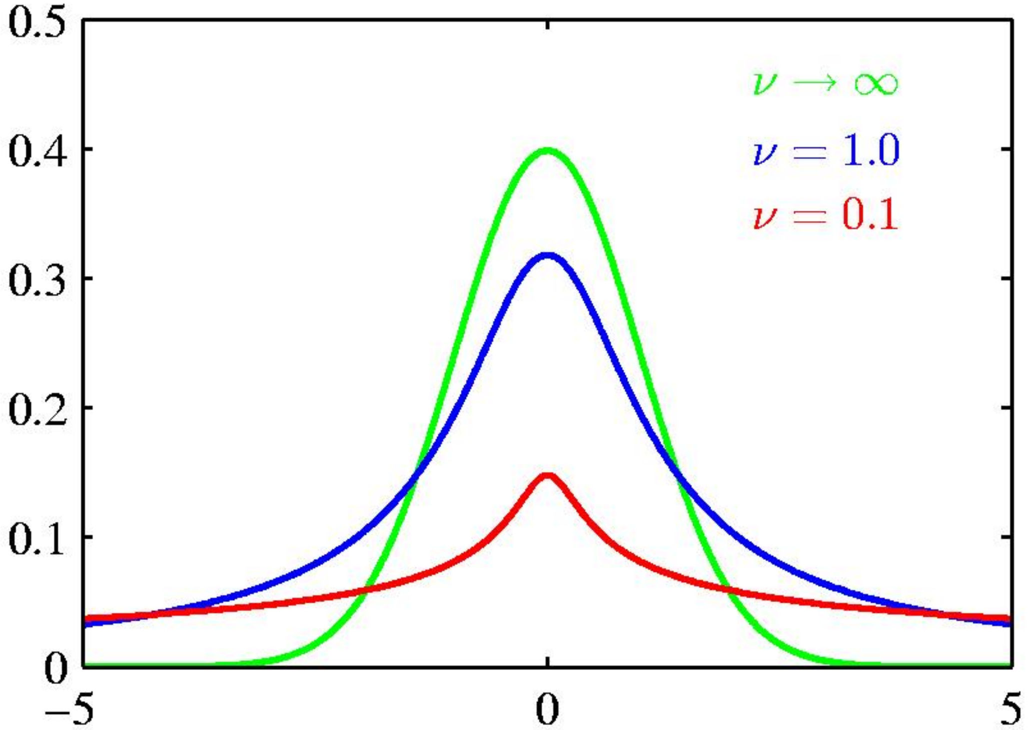
Student's *t*-distribution

- Setting ν = 1 recovers the Cauchy distribution

The limit $\nu \rightarrow \infty$ corresponds to a Gaussian distribution

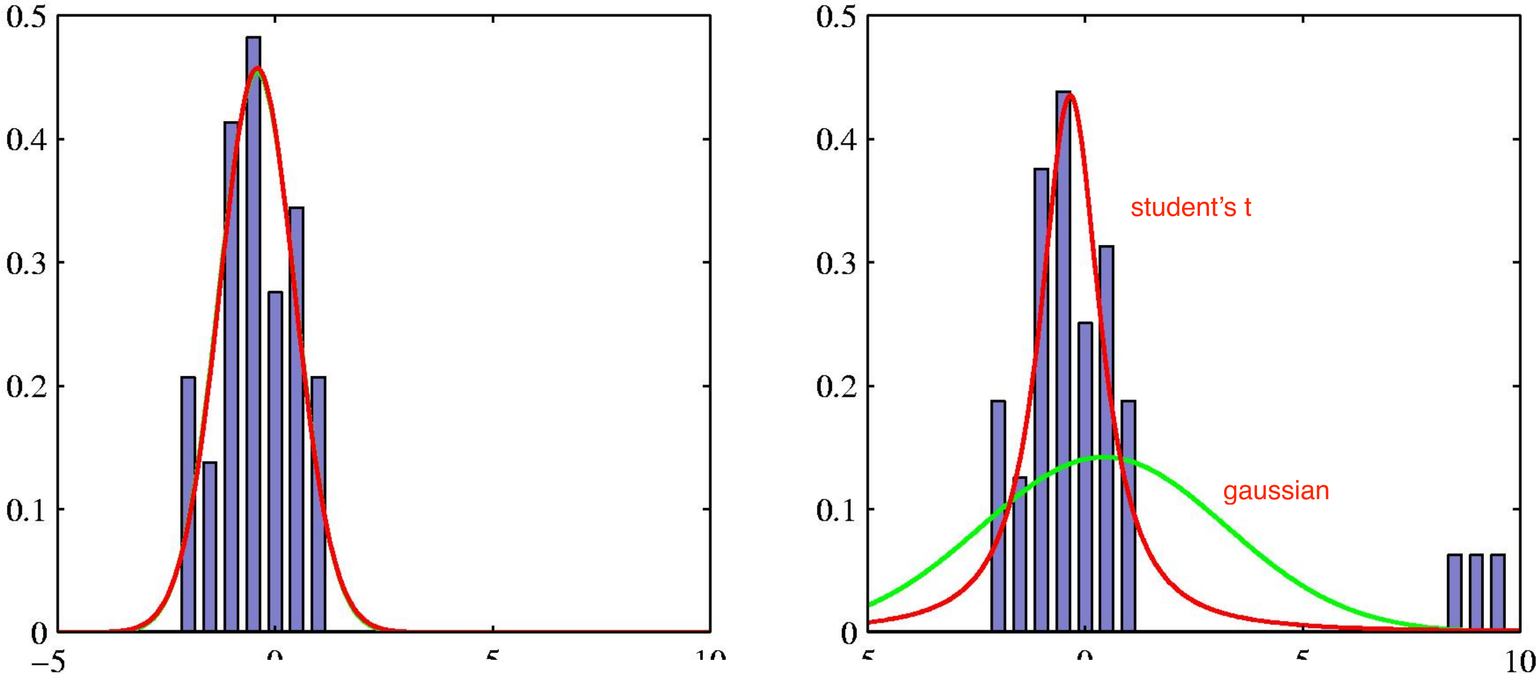
	$\nu = 1$	$\nu \rightarrow \infty$
$\mathrm{St}(x\|\mu, \lambda, \nu)$	Cauchy	$\mathcal{N}(x\|\mu, \lambda^{-1})$

cauchy: more relaxted about the outliers



Student’s *t*-distribution

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



Student's *t*-distribution

- The multivariate extension of the *t*-distribution:

integrating out the precision

$$\mathrm{St}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Lambda},\nu) = \int_0^{\infty} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu},(\eta\boldsymbol{\Lambda})^{-1})\mathrm{Gam}(\eta|\nu/2,\nu/2)\,\mathrm{d}\eta$$

$$= \frac{\Gamma(D/2+\nu/2)}{\Gamma(\nu/2)}\frac{|\boldsymbol{\Lambda}|^{1/2}}{(\pi\nu)^{D/2}}\left[1+\frac{\Delta^2}{\nu}\right]^{-D/2-\nu/2}$$

v is degree of freedom

lambda is precision

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

- Properties:

$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}, \qquad \text{if } \nu > 1$$

$$\mathrm{cov}[\mathbf{x}] = \frac{\nu}{(\nu-2)}\boldsymbol{\Lambda}^{-1}, \qquad \text{if } \nu > 2$$

$$\mathrm{mode}[\mathbf{x}] = \boldsymbol{\mu}$$

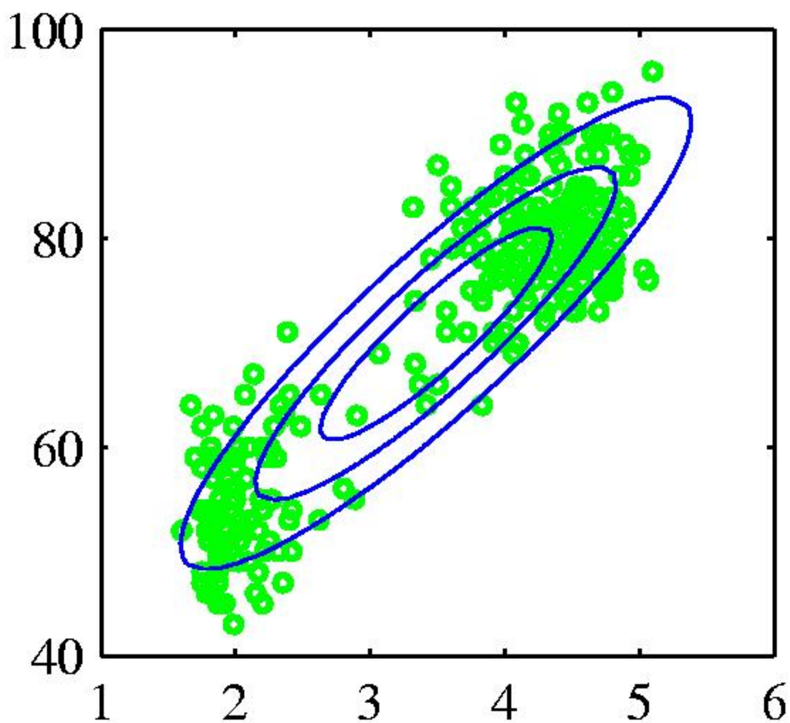
Outline

- Seven distributions and their ML estimates
  - Bernoulli, binomial, and multinomial
  - Beta and Dirichlet
  - Normal and Student's *t*
- **Mixture of Gaussians**
- The Exponential Family and its ML estimates

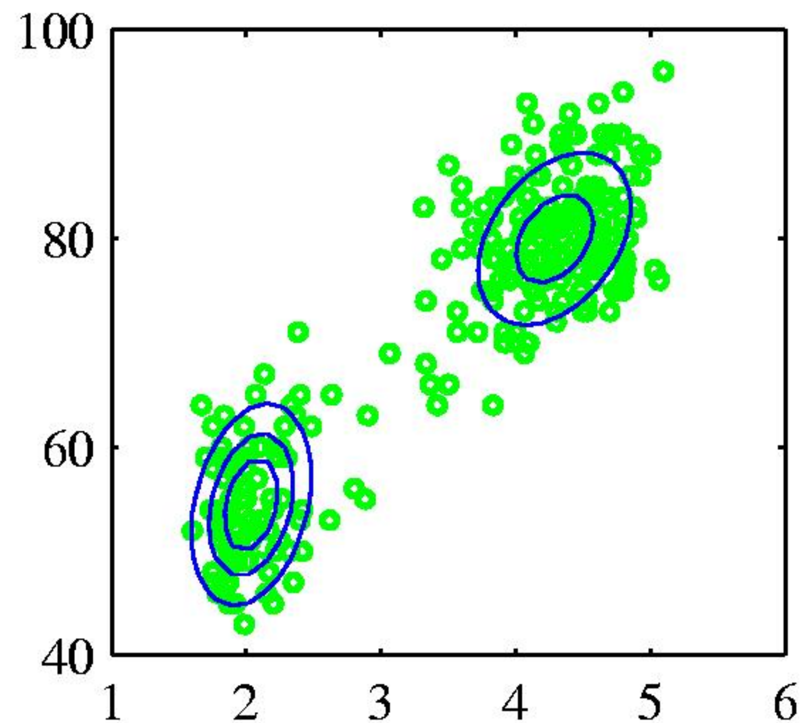
Mixture of Gaussians

- When modelling real-world data, assuming a normal distribution may not be appropriate

- Consider the following example: the Old Faithful dataset



Single Gaussian



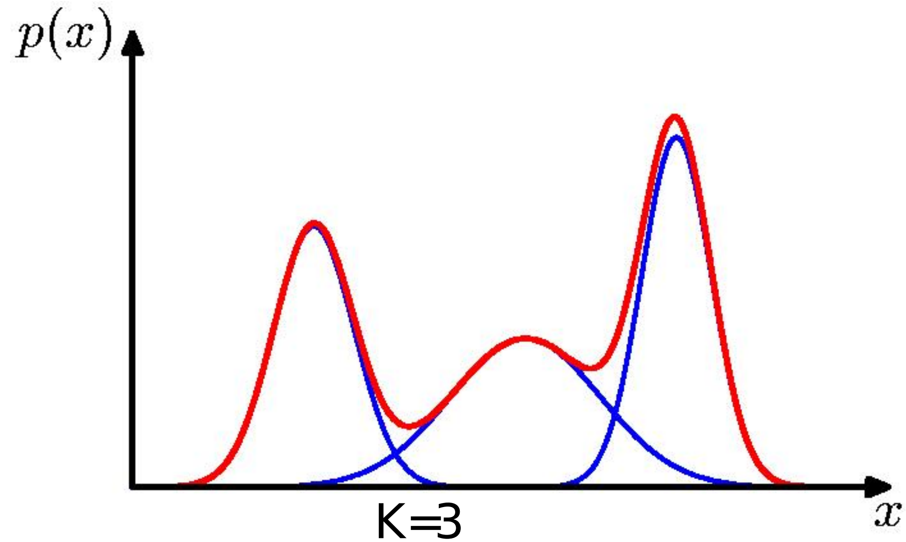
Mixture of two Gaussians

Mixture of Gaussians

- We can combine simple models into a complex model by defining a superposition of *K* Gaussian densities of the form:

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

Mixing coefficient



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

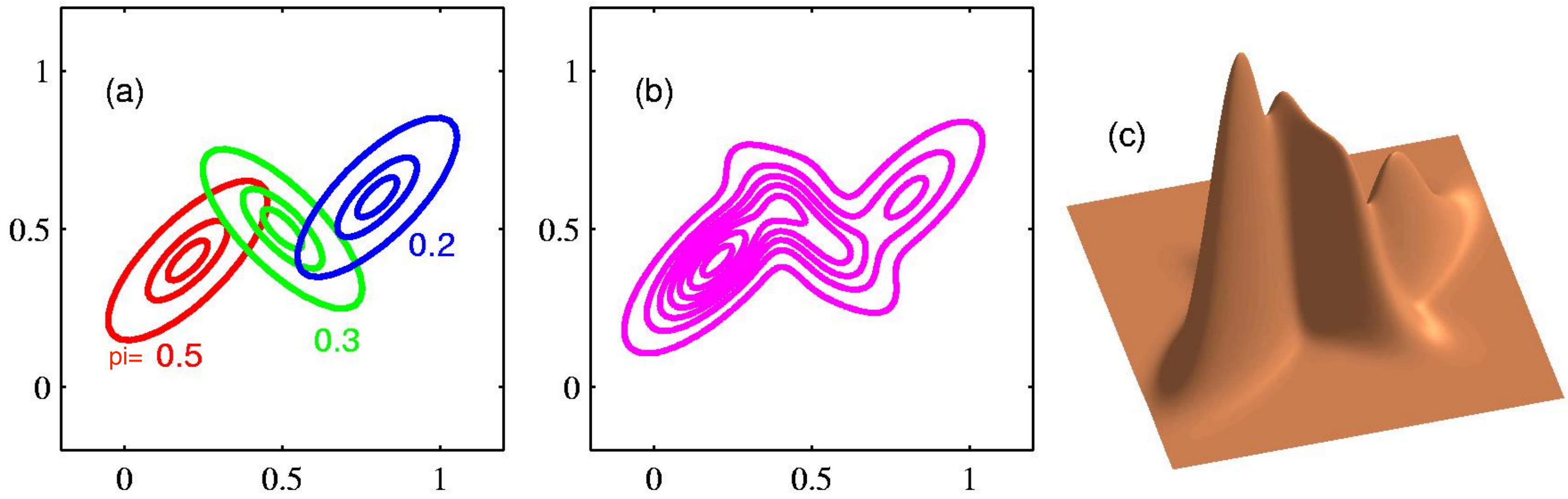
condition s.t. integration of pdf = 1

Note that each Gaussian component has its own mean $\boldsymbol{\mu}_k$ and covariance $\boldsymbol{\Sigma}_k$. The parameters π_k are called mixing coefficients.

- More generally, **mixture models** can comprise linear combinations of other distributions.

Mixture of Gaussians

- Illustration of a mixture of three Gaussians in a 2-dimensional space:



(a) Contours of constant density of each of the mixture components, along with the mixing coefficients

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

(c) A surface plot of the distribution $p(\mathbf{x})$.

Maximum Likelihood Estimation

Given a dataset $\mathbf{X}$, we can determine model parameters $\boldsymbol{\mu}_k$. $\boldsymbol{\Sigma}_k$, π_k by maximizing the log-likelihood function:

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \underbrace{\ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}}_{\text{Log of a sum: no closed-form solution}}$$

Solutions:

- Use standard, iterative, numerical optimization methods (e.g. conjugate gradients), or
- Use the Expectation Maximization algorithm (to come around March)

Outline

- Seven distributions and their ML estimates
  - Bernoulli, binomial, and multinomial
  - Beta and Dirichlet
  - Normal and Student's *t*
- Mixture of Gaussians
- **The Exponential Family and its ML estimates**

The Exponential Family

- The exponential family of distributions over **x** is defined to be a set of distributions of the form:

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

can separate x and mu

where

- $\boldsymbol{\eta}$ is the vector of natural parameters
- ***u(x)*** is the vector of sufficient statistics

The function $g(\boldsymbol{\eta})$ can be interpreted as the coefficient that ensures that the distribution $p(\mathbf{x}|\boldsymbol{\eta})$ is normalized:

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

Bernoulli Distribution

- The Bernoulli distribution is a member of the exponential family:

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

x is sufficient statistics

- Comparing with the general form of the exponential family:

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

we see that

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

Bernoulli Distribution

- The Bernoulli distribution is a member of the exponential family:

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

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

- The Bernoulli distribution can therefore be written as:

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

where

$$\begin{aligned} u(x) &= x \\ h(x) &= 1 \\ g(\eta) &= 1 - \sigma(\eta) = \sigma(-\eta). \end{aligned}$$

Multinomial Distribution

- The multinomial distribution is a member of the exponential family:

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

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

and

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

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

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

- Sometimes it's convenient to remove the constraint by expressing the distribution over the $M - 1$ parameters; Bishop makes a start in this direction

Gaussian Distribution

- The Gaussian distribution is a member of the exponential family:

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

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

Remember the exponential family: $p(\mathbf{x}|\boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta}) \exp\left\{\boldsymbol{\eta}^{\mathrm{T}}\mathbf{u}(\mathbf{x})\right\}$

From the definition of the normalizer *g*(***η***):

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

We can take a derivative w.r.t ***η***:

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

- Thus

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

The covariance of ***u(x)*** can be expressed in terms of the second derivative of *g*(***η***), and similarly for the higher moments.

ML for the Exponential Family

- Suppose we observed i.i.d data $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$.

We can construct the log-likelihood function, which is a function of the natural parameter $\boldsymbol{\eta}$.

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

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

- Exercise: differentiate the log w.r.t. $\boldsymbol{\eta}$ to find:

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