2015-09-14

STA 414/2104: Machine Learning

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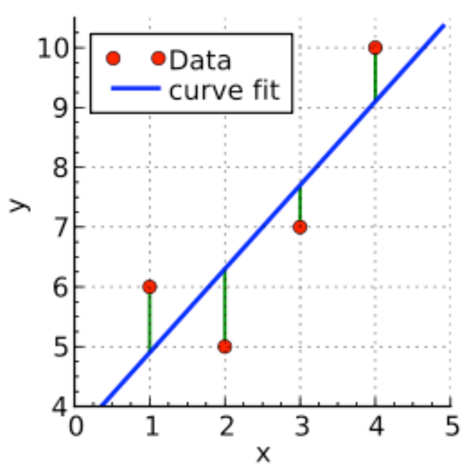
Lecture 2

Linear Least Squares

From last class: Minimize **the sum of the squares of the errors** between the predictions $y(\mathbf{x}_n, \mathbf{w})$ for each data point x_n and the corresponding real-valued targets t_n.



Source: Wikipedia

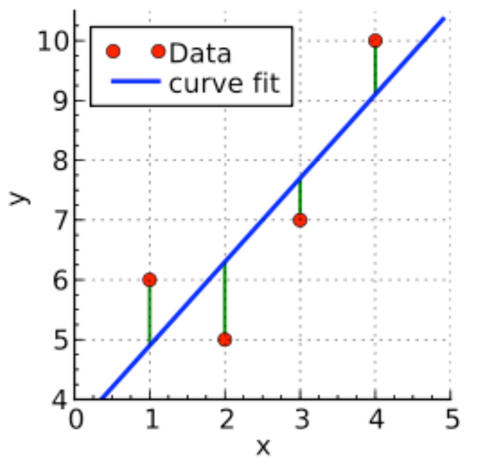
Loss function: sum-of-squared error function:

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}(\mathbf{x}_n^T\mathbf{w} - t_n)^2$$

$$= \frac{1}{2}(\mathbf{X}\mathbf{w} - \mathbf{t})^{\mathbf{T}}(\mathbf{X}\mathbf{w} - \mathbf{t}).$$

Linear Least Squares

If $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ is nonsingular, then the unique solution is given by:



Source: Wikipedia

optimal weights

vector of target values

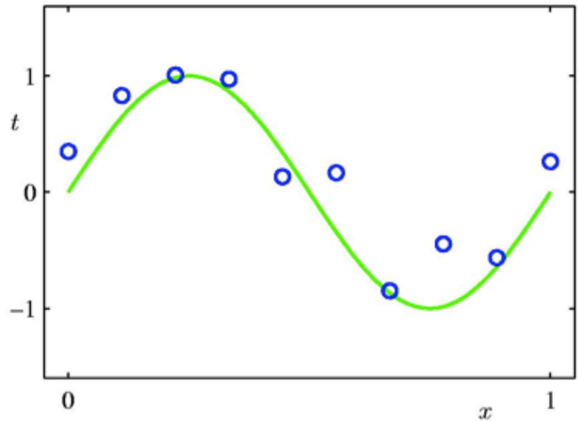
$$\mathbf{w}^* = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{t}$$

the design matrix has one input vector per row

- At an arbitrary input $\mathbf{x}_0$, the prediction is $y(\mathbf{x}_0, \mathbf{w}) = \mathbf{x}_0^T\mathbf{w}^*$.
- The entire model is characterized by d+1 parameters $\mathbf{w}^*$.

Example: Polynomial Curve Fitting

Consider observing a training set consisting of N 1-dimensional observations:
$\mathbf{x} = (x_1, x_2, ..., x_N)^T$, together with corresponding real-valued targets:
$\mathbf{t} = (t_1, t_2, ..., t_N)^T$.



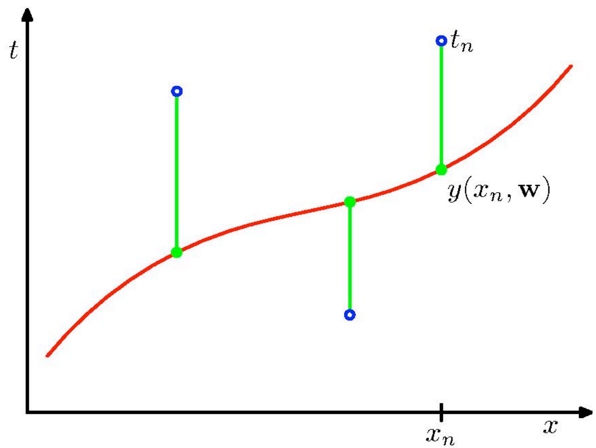
Goal: Fit the data using a polynomial function of the form:

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + ... + w_M x^M = \sum_{j=0}^{M} w_j x^j.$$

Note: the polynomial function is a nonlinear function of x, but it is a linear function of the coefficients **w** $\rightarrow$ **Linear Models**.

Example: Polynomial Curve Fitting

• As for the least squares example: we can minimize the sum of the squares of the errors between the predictions $y(x_n, \mathbf{w})$ for each data point x_n and the corresponding target values t_n.



Loss function: sum-of-squared error function:

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y(x_n, \mathbf{w}) - t_n)^2.$$

• Similar to the linear least squares: Minimizing sum-of-squared error function has a unique solution $\mathbf{w}^*$.

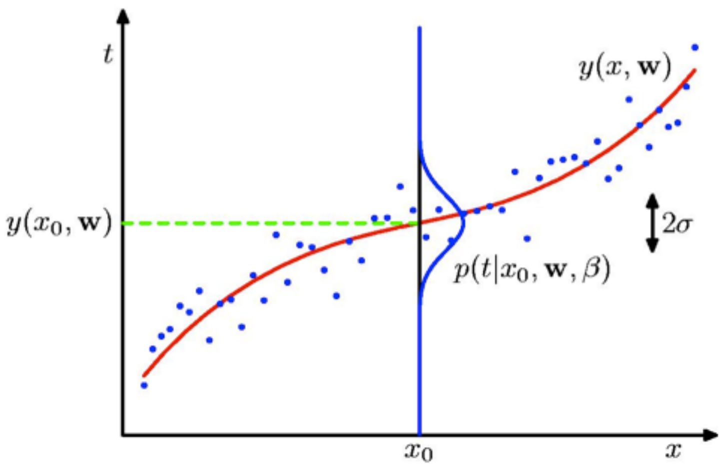
Probabilistic Perspective

• So far we saw that polynomial curve fitting can be expressed in terms of error minimization. We now view it from probabilistic perspective.

• Suppose that our model arose from a statistical model:

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon,$$

where ϵ is a random error having Gaussian distribution with zero mean, and is independent of **x**.



Thus we have:

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}),$$

where β is a precision parameter, corresponding to the inverse variance.

I will use probability distribution and probability density interchangeably. It should be obvious from the context.

Maximum Likelihood

If the data are assumed to be independently and identically distributed (*i.i.d assumption*), the likelihood function takes form:

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{i=1}^{N} \mathcal{N}(t_n | y(\mathbf{x}_n, \mathbf{w}), \beta^{-1}).$$

It is often convenient to maximize the log of the likelihood function:

$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \underbrace{-\frac{\beta}{2} \sum_{n=1}^{N} (y(\mathbf{x}_n, \mathbf{w}) - t_n)^2}_{\beta E(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi).$$

- Maximizing log-likelihood with respect to **w** (under the assumption of a Gaussian noise) is equivalent to minimizing the *sum-of-squared error* function.

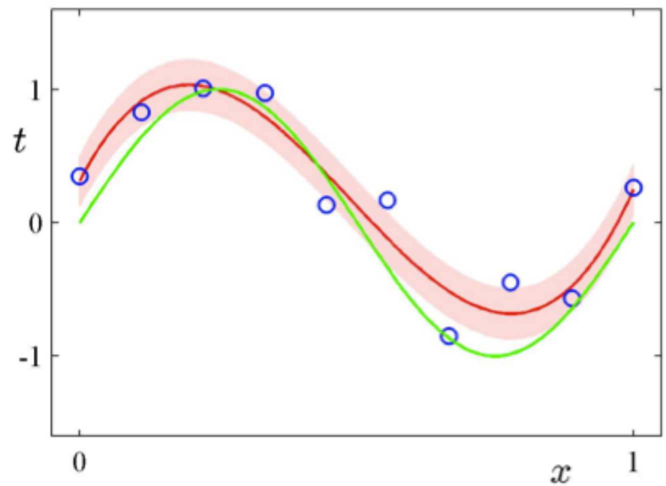
- Determine $\mathbf{w}_{ML}$ by maximizing log-likelihood. Then maximizing w.r.t. β:

$$\frac{1}{\beta_{ML}} = \frac{1}{N} \sum_{n} (y(\mathbf{x}_n, \mathbf{w}_{ML}) - t_n)^2.$$

Predictive Distribution

Once we determined the parameters **w** and β, we can make prediction for new values of **x**:

$$p(t|\mathbf{x}, \mathbf{w}_{ML}, \beta_{ML}) = \mathcal{N}(t|y(\mathbf{x}, \mathbf{w}_{ML}), \beta_{ML}^{-1}).$$



Later we will consider Bayesian linear regression.

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, so that:

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

- The probability distribution, known as 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 maximize 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 $\sum_n x_n$

Sufficient Statistic

Parameter Estimation

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

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

- 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.

Binomial Distribution

- We can also 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:

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

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

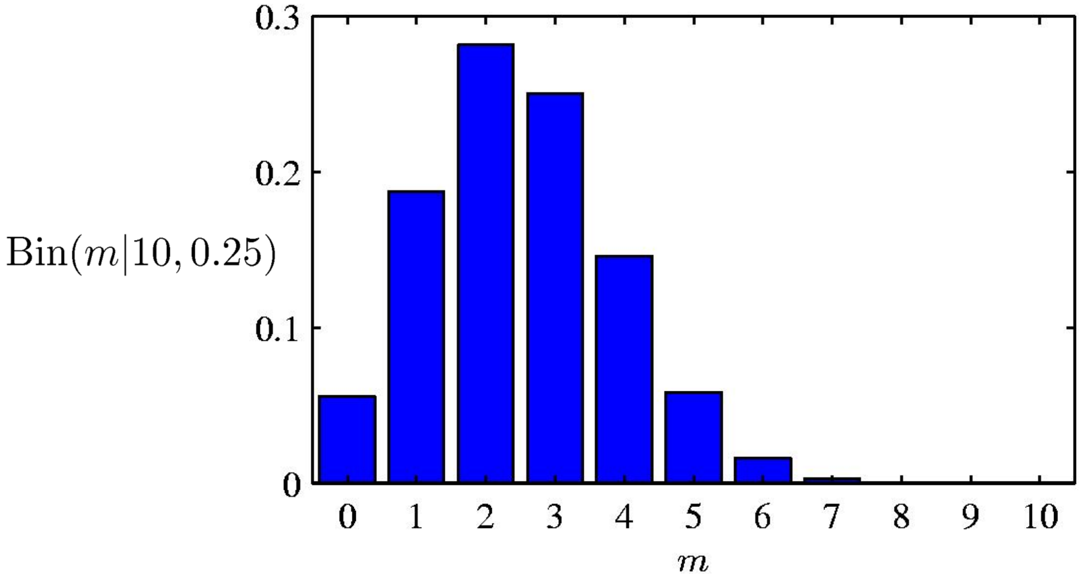
- The mean and variance can be easily derived as:

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

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

Example

• 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 a prior over the parameter μ of the Bernoulli distribution).

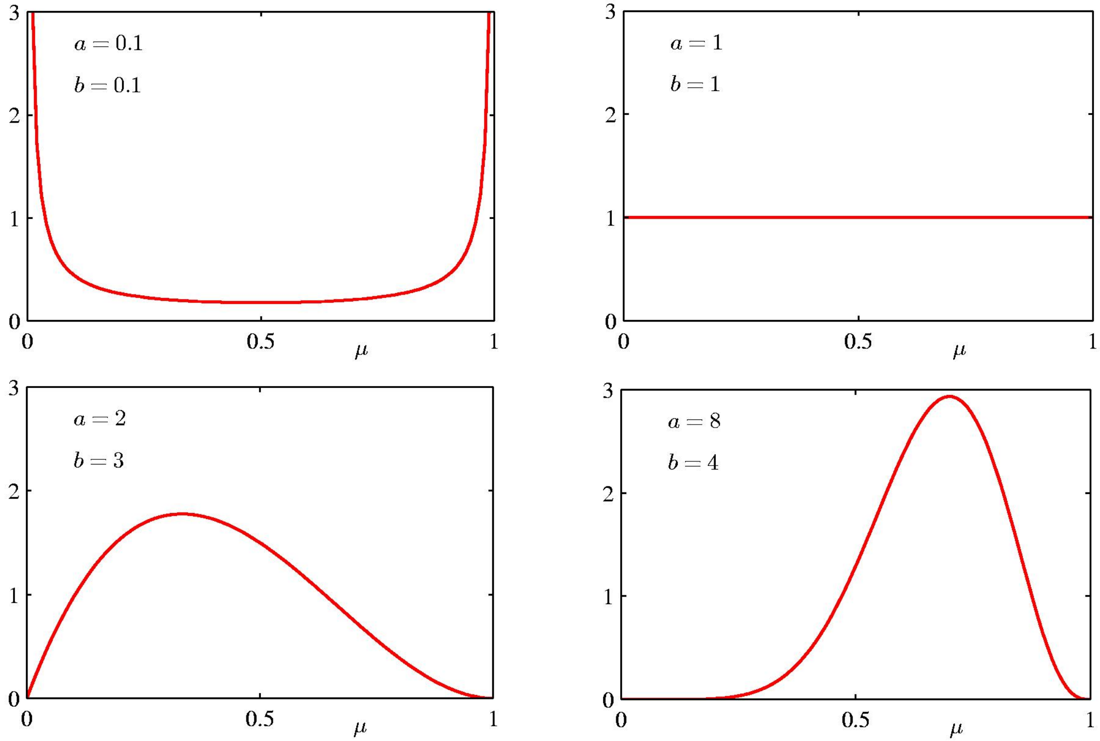
$$
\begin{aligned}
\mathrm{Beta}(\mu|a,b) &= \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\mu^{a-1}(1-\mu)^{b-1} \\
\mathbb{E}[\mu] &= \frac{a}{a+b} \\
\mathrm{var}[\mu] &= \frac{ab}{(a+b)^2(a+b+1)}
\end{aligned}
$$

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



Multinomial Variables

• Consider a random variable that can take on one of K possible mutually exclusive states (e.g. roll of a dice).

• We will use so-called 1-of-K encoding scheme.

• 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 resented 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

- Multinomial distribution can be viewed as a generalization of Bernoulli distribution 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 distribution is normalized:

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

and

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

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.

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

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

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

which represents the number of observations of $x_k=1$.

- These are called 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 solution for μ, we need to maximize the log-likelihood taking into account the constraint that $\sum_k \mu_k = 1$

- Forming the Lagrangian:

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

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

which is the fraction of observations for which x_k=1.

Multinomial Distribution

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

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

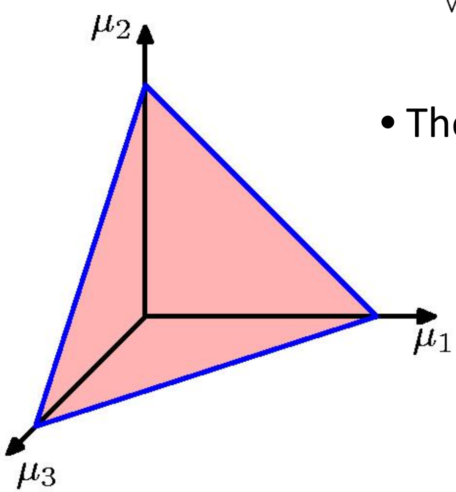
- The normalization coefficient is the number of ways of partitioning N objects into K groups of size $m_1,m_2,\ldots,m_K$.

- Note that

$$\sum_k m_k = N.$$

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:

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

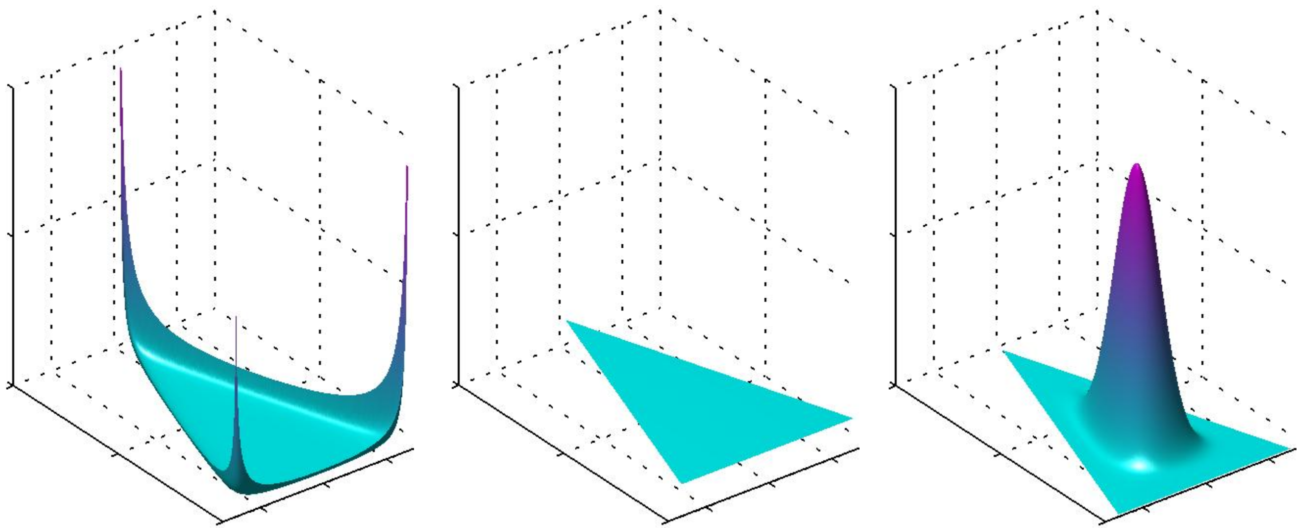
$$\alpha_0 = \sum_{k=1}^{K} \alpha_k$$

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

- The Dirichlet distribution is confined to a simplex as a consequence of the constraints.

Dirichlet Distribution

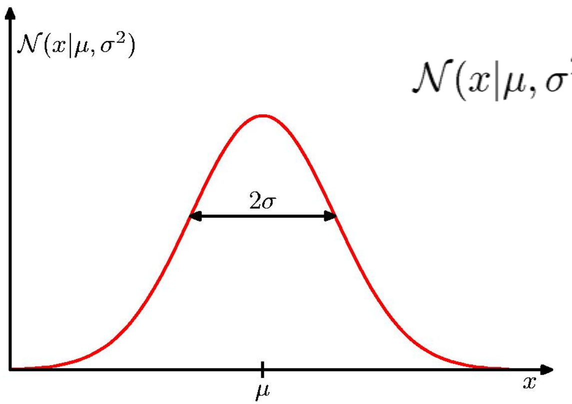
- Plots of the Dirichlet distribution over three variables.



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

Gaussian Univariate Distribution

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

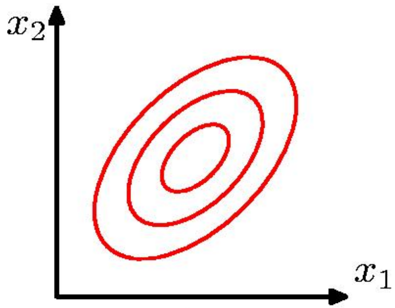
$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

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

Multivariate Gaussian Distribution

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

- μ is a D-dimensional mean vector.
- Σ is a D by D covariance matrix.

and $|\Sigma|$ denotes the determinant of Σ.

- Note that the covariance matrix is a symmetric positive definite matrix.

Central Limit Theorem

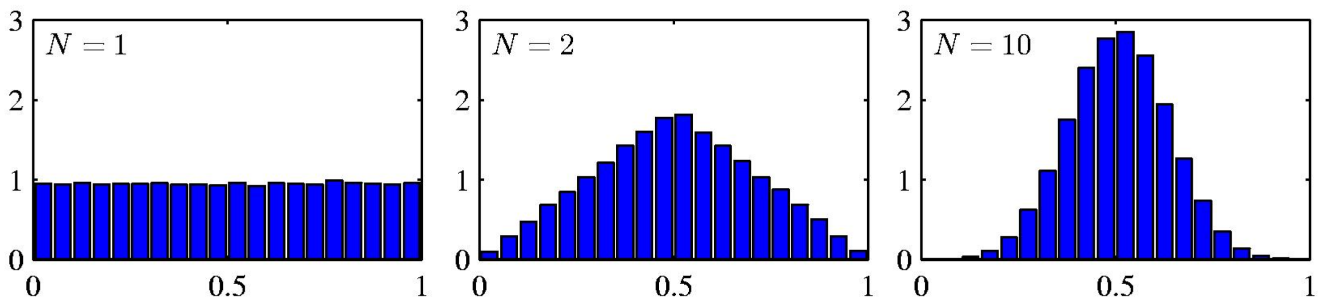
• The distribution of the sum of N i.i.d. random variables becomes increasingly Gaussian as N grows.

• 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

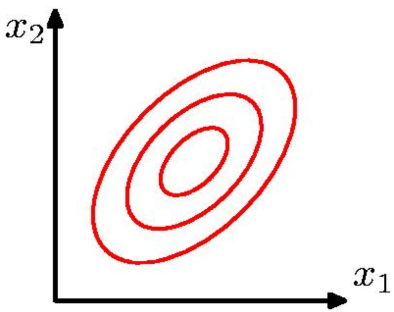
- For a D-dimensional vector **x**, the Gaussian distribution takes form:

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

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

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

- Here Δ is known as Mahalanobis distance.



- 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 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:

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

- 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:

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

Geometry of the Gaussian Distribution

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

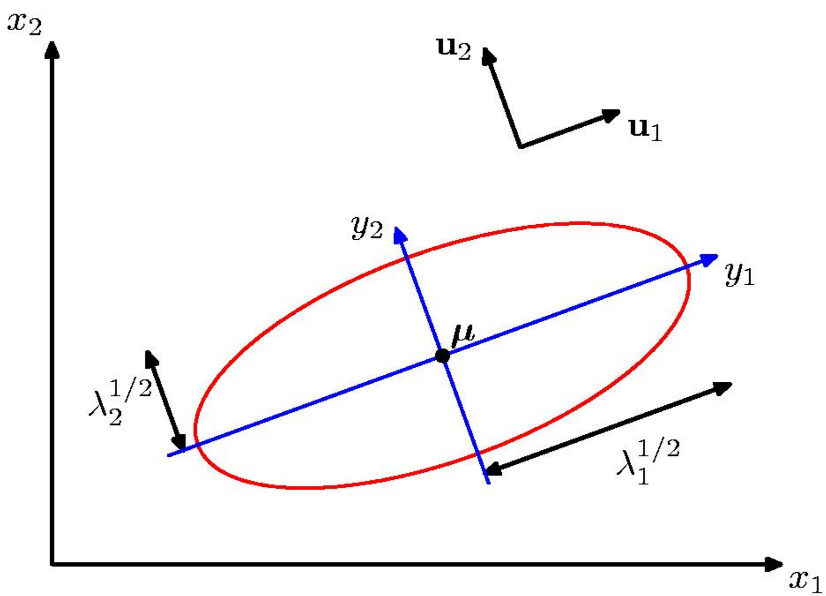
$$\Delta^2 = \sum_{i=1}^{D} \frac{y_i^2}{\lambda_i} \qquad y_i = \mathbf{u}_i^{\mathrm{T}} (\mathbf{x}-\boldsymbol{\mu})$$

- We can interpret $\{y_i\}$ as a new coordinate system defined by the orthonormal vectors 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 axis are defined by the eigenvectors u_i of the covariance matrix with corresponding eigenvalues.

Moments of the Gaussian Distribution

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

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

The term in z in the factor (z+μ) will vanish by symmetry.

0 by symmetry

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

Moments of the Gaussian Distribution

- The second order moments of the Gaussian distribution:

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

- The covariance is given by:

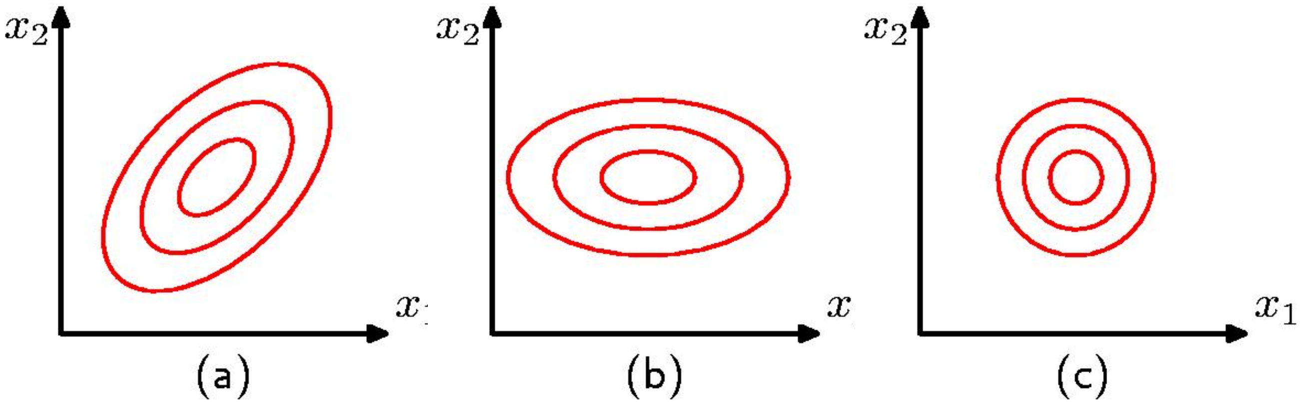
$$\operatorname{cov}[\mathbf{x}] = \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^{\mathrm{T}}\right] = \boldsymbol{\Sigma}$$

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

- 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 (proportional to identity) covariance matrix.

Partitioned Gaussian Distribution

- Consider a D-dimensional Gaussian distribution: $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- Let us partition **x** into two disjoint subsets x_a and 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 Λ_{aa} is not given by the inverse of Σ_{aa}.

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 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 function of x_b.

Marginal Distribution

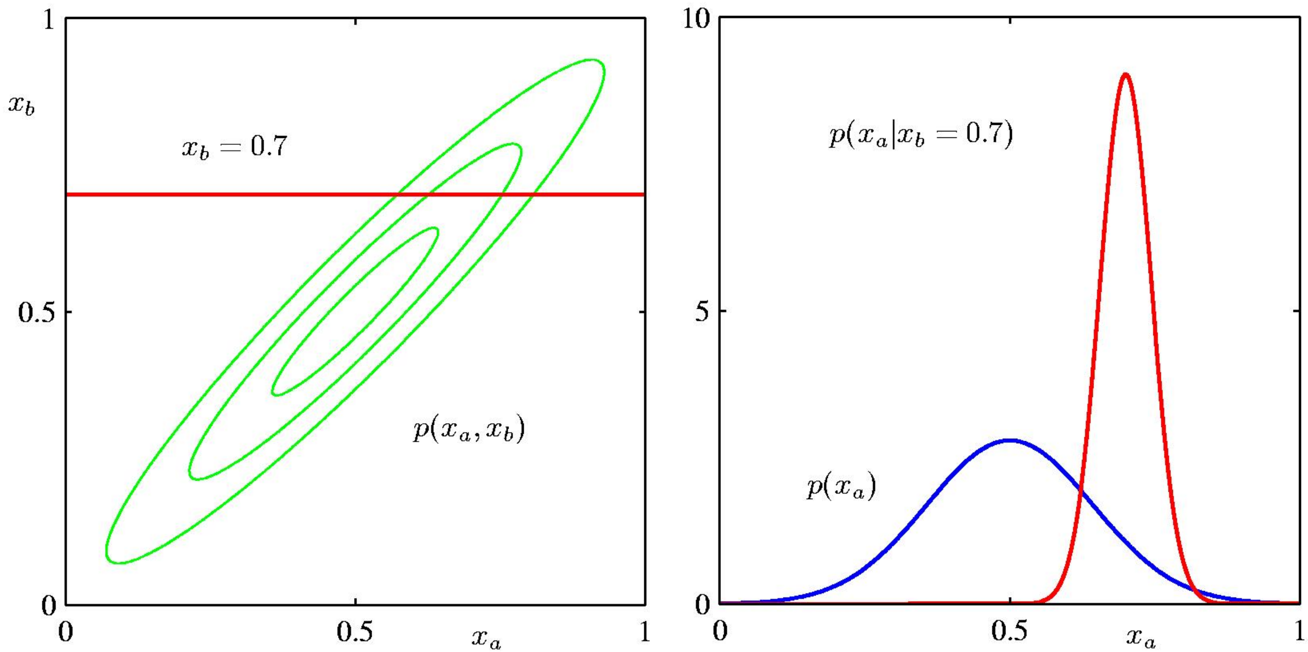
- It turns out that the marginal distribution is also a Gaussian distribution:

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

- 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 μ and Σ:

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

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

Sufficient Statistics

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

Maximum Likelihood Estimation

- To find a maximum likelihood 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:

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

- Similarly, we can find the ML estimate of Σ:

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

Maximum Likelihood Estimation

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

Unbiased estimate

$$\mathbb{E}[\boldsymbol{\mu}_{\mathrm{ML}}] = \boldsymbol{\mu}$$

$$\mathbb{E}[\boldsymbol{\Sigma}_{\mathrm{ML}}] = \frac{N-1}{N}\boldsymbol{\Sigma}.$$

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. Important for on-line applications.

- Let us consider the contribution of the N^{th} data point x_n:

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

the only reason we do this is to release memories

Student's t-Distribution

- Consider Student's t-Distribution

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

Infinite mixture of Gaussians

where

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

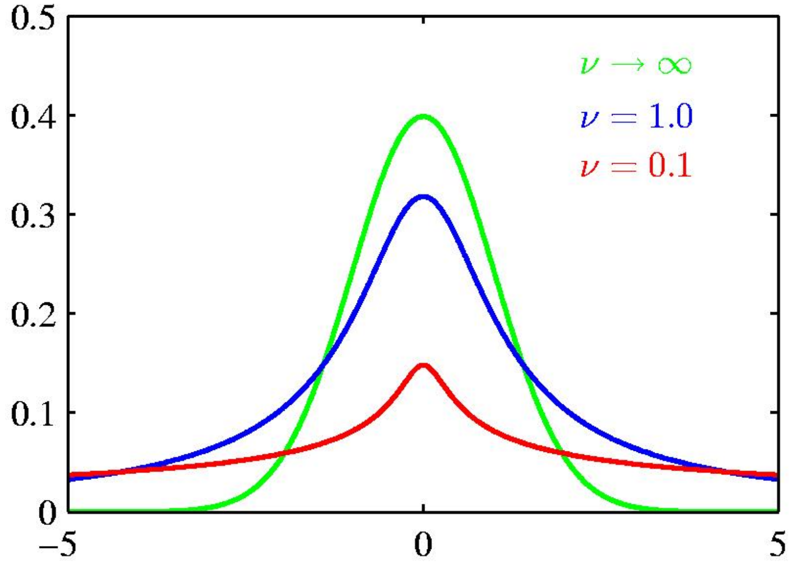
Sometimes called the precision parameter.

Degrees of freedom

Student's t-Distribution

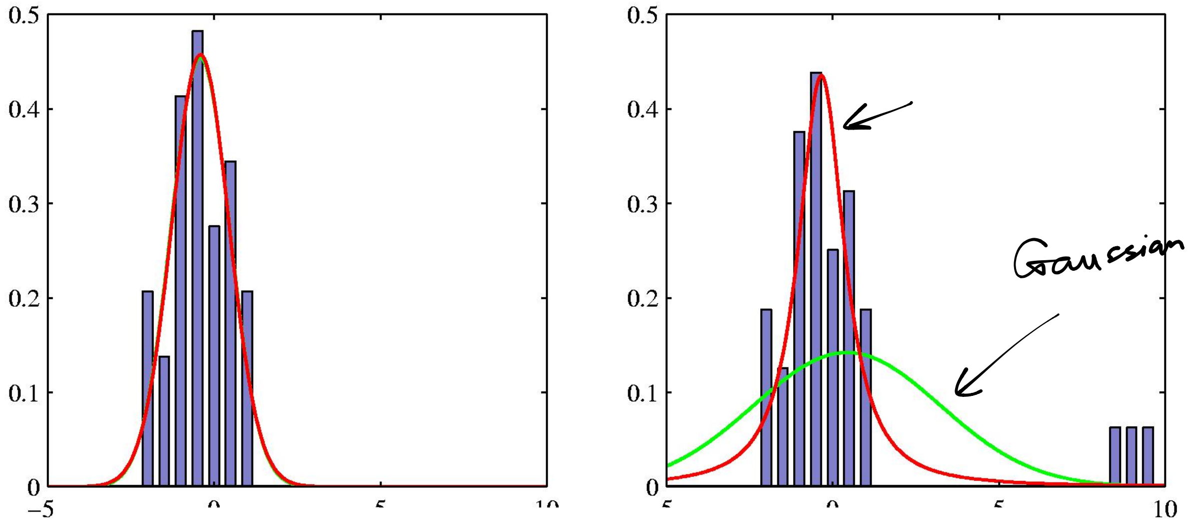
- Setting $\nu = 1$ recovers Cauchy distribution
- The limit $\nu \to \infty$ corresponds to a Gaussian distribution.

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



Student’s t-Distribution

- Robustness to outliners: Gaussian vs. t-Distribution.



Student's t-Distribution

- The multivariate extension of the t-Distribution:

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

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

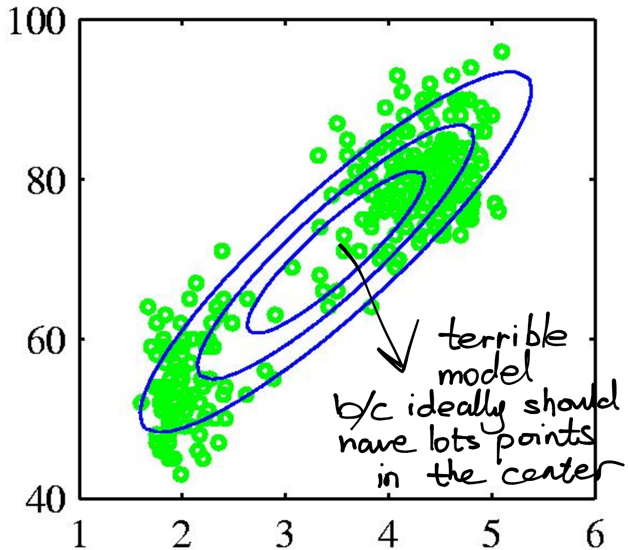
- Properties:

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

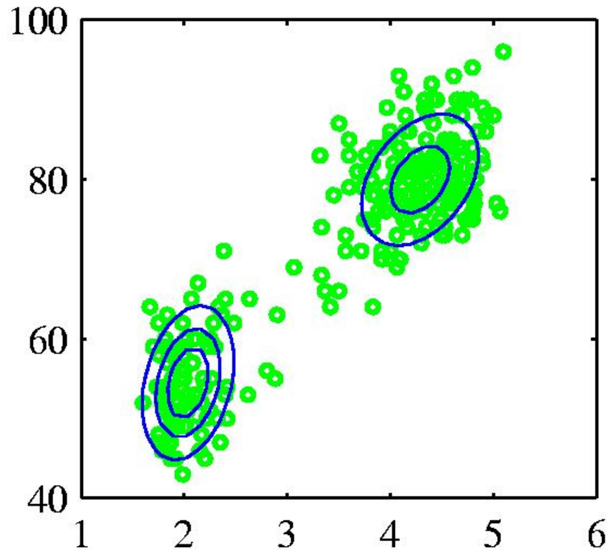
Mixture of Gaussians

- When modeling real-world data, Gaussian assumption may not be appropriate.

- Consider the following example: Old Faithful Dataset



Single Gaussian



Mixture of two Gaussians

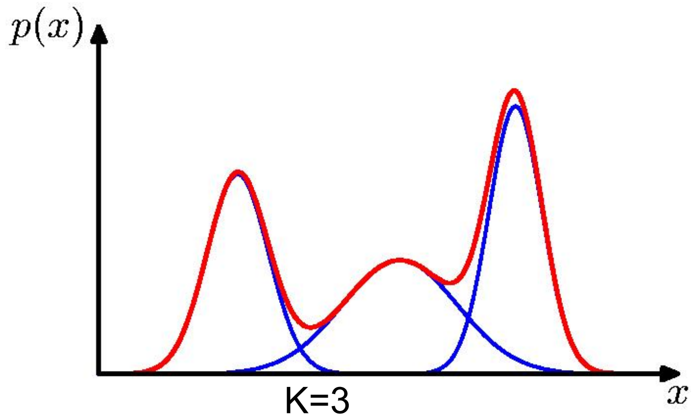
Mixture of Gaussians

• 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

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

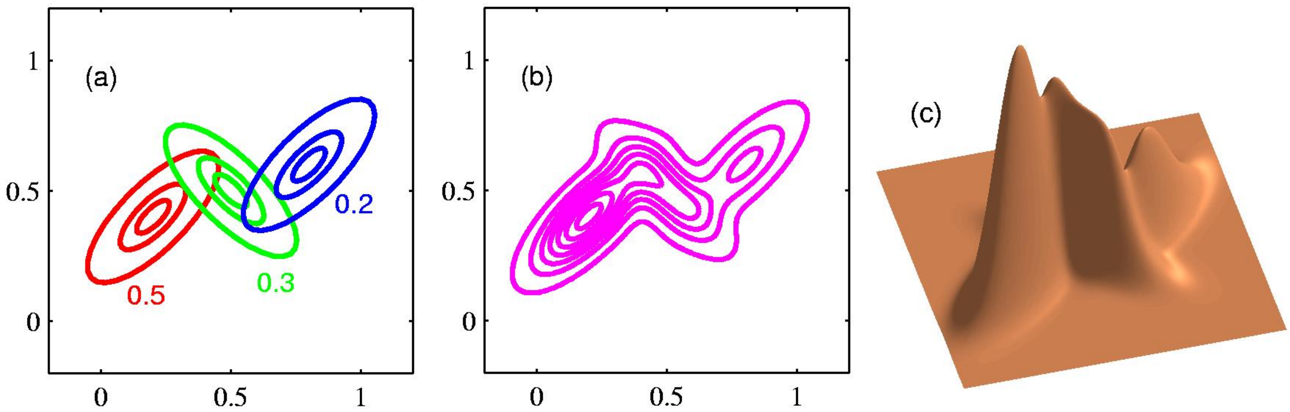


• Note that each Gaussian component has its own mean μ_k and covariance Σ_k. The parameters π_k are called mixing coefficients.

• Mote generally, mixture models can comprise linear combinations of other distributions.

Mixture of Gaussians

- Illustration of a mixture of 3 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(x).

Maximum Likelihood Estimation

• Given a dataset D, we can determine model parameters μ_k. Σ_k, π_k by maximizing the log-likelihood function:

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

• **Solution**: use standard, iterative, numeric optimization methods or the Expectation Maximization algorithm.

The Exponential Family

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

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

where

- η is the vector of natural parameters
- **u**(**x**) is the vector of sufficient statistics

• The function g(η) can be interpreted the coefficient that ensures that the distribution p(**x**|η) 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:

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

rewrite
in such form

- 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

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

generalization of Bern (2-value)

Multinomial Distribution (k-value)

- 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 μ_k must satisfy

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

- In some cases it will be convenient to remove the constraint by expressing the distribution over the M-1 parameters.

Multinomial Distribution

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

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

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

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

- Here the parameters η_k are independent.
- Note that:

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

Multinomial Distribution

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

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

- The Multinomial distribution can therefore 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

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

Gaussian Distribution (not surprisingly)

- The Gaussian distribution can be written as:

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

where

$$
\boldsymbol{\eta} = \begin{pmatrix} \mu/\sigma^2 \\ -1/2\sigma^2 \end{pmatrix} \qquad h(\mathbf{x}) = (2\pi)^{-1/2}
$$

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

sufficient statistics

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

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

ML for the Exponential Family

- Remember the Exponential Family:

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

- We can take a derivative w.r.t η:

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

- Thus

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

- Note that 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 $\mathbf{X} = \{\mathbf{x}_1, ..., \mathbf{x}_N\}$.

- We can construct the log-likelihood function, which is a function of the natural parameter η.

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

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

- Therefore we have

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