Probability Distribution

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Outline

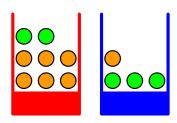
- Probability Theory
- Binary Variables
- Multinomial Variables
- The Gaussian Distribution
- Exponential Family

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Simple Example

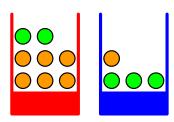
- Uncertainty is a key concept in the fields of pattern recognition and machine learning
- Probability theory provides a consistent framework for the quantification and manipulation of uncertainty and forms one of the central foundations for our study



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 - 2 apples and 6 oranges in the red box
 - 3 apples and 1 orange in the blue box
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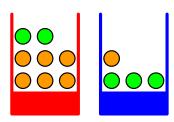
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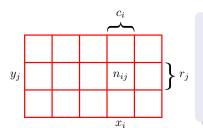
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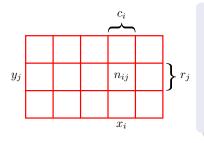
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A General Example

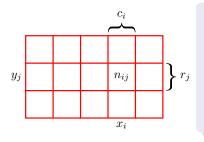


- two random variables X and Y
- suppose X can take any of the values $(x_i)_{i=1}^M$
- suppose that Y can take the values $(y_j)_{j=1}^L$
- consider a total of N trials in which we sample both of the variables X and Y
- let n_{ij} be the number of such trials in which $X = x_i$ and $Y = y_j$
- let r_j be the number of trials in which $Y = y_j$
- let c_i be the number of trials in which $X = x_i$





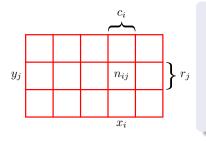
•
$$P(X = x_i) =$$



•
$$P(X = x_i) = c_i/N$$

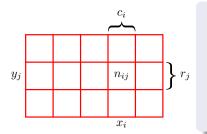
•
$$P(Y = y_i) = r_i/N$$

• joint probability
$$P(X = x_i, Y = y_i) =$$



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- $P(Y = y_i) = r_i/N$
- joint probability $P(X = x_i, Y = y_i) = n_{ii}/N$
- conditional probability $P(Y = y_i | X = x_i) =$



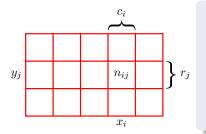
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The rules of probability

- **1** sum rule: $P(X = x_i) = \sum_{i=1}^{L} P(X = x_i, Y = y_i)^{a}$
- 2 product rule: $P(X = x_i, Y = y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N}$



•
$$P(X = x_i) = c_i/N$$

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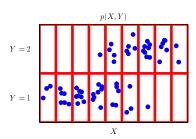
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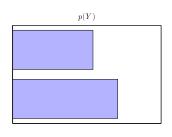
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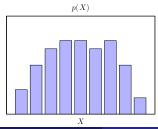
 $^{a}P(X=x_{i})$ is sometimes called the marginal probability

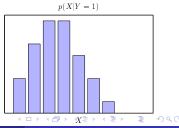
^bWe can derive the Bayes's Theorem.

An Illustration









Example: revisit

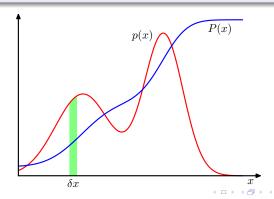
Assume:
$$p(B = r) = 4/10$$
, $p(B = b) = 6/10$
 $p(F = a|B = b) = ?$
 $p(F = a) = ?$
 $p(B = r|F = o) = ?$

Probability Density

Considering probabilities with respect to continuous variables

Informal definition

If the probability of a real-valued variable x falling in the interval $(x, x + \delta x)$ is given by $p(x)\delta x$ for $\delta x \to 0$, then p(x) is called the probability density over x



Probability Density (cont'd)

The probability that x will lie in an interval (a, b) is given by

$$P(x \in (a,b)) = \int_a^b p(x) dx$$

Cumulative distribution function

The probability that x lies in the interval $(-\infty, z)$ is given by

$$P(z) = \int_{-\infty}^{z} p(x) dx$$

Note that If x is a discrete variable, then p(x) is sometimes called a probability mass function



Expectations

The average value of some function f(x) under a probability distribution p(x) is called the expectation of f(x), denoted by $\mathcal{E}[f]$

Expectation

For a discrete distribution,

$$\mathcal{E}[f] = \sum_{x} p(x)f(x)$$

For a continuous distribution.

$$\mathcal{E}[f] = \int p(x)f(x)dx$$



Expectations (cont'd)

In both the continuous and discrete cases, if given a finite number N of points drawn from the probability distribution or probability density, then we can approximate it as a finite sum over these points

$$\mathcal{E}[f] \cong \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

How about expectations of functions of several variables



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How about expectations of functions of several variables

 $\mathcal{E}_x[f(x,y)]$: the average of the function f(x,y) with respect to the distribution of x

Conditional expectation

$$\mathcal{E}_{x}[f|y] =$$

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$$\mathcal{E}_{x}[f|y] = \sum_{x} p(x|y)f(x)$$

Variance

The variance of f(x)

$$var[f] = \mathcal{E}\left[\left(f(x) - \mathcal{E}[f(x)]\right)^2\right] = \mathcal{E}[f(x)^2] - \mathcal{E}[f(x)]^2$$

Covariance



Variance

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Covariance

• For two random variables x, y

$$cov[x,y] = \mathcal{E}_{x,y}\left[\left\{x - \mathcal{E}[x]\right\}\right]\left[\left\{y - \mathcal{E}[y]\right\}\right] = \mathcal{E}_{x,y}[xy] - \mathcal{E}[x]\mathcal{E}[y]$$

For two vectors of random variables x and y,

$$\textit{cov}[\mathbf{x}, \mathbf{y}] = \mathcal{E}_{\mathbf{x}, \mathbf{y}}\left[\{\mathbf{x} - \mathcal{E}[\mathbf{x}]\}\right] \left[\{\mathbf{y}^\top - \mathcal{E}[\mathbf{y}^\top]\}\right] = \mathcal{E}_{\mathbf{x}, \mathbf{y}}[\mathbf{x}\mathbf{y}^\top] - \mathcal{E}[\mathbf{x}]\mathcal{E}[\mathbf{y}^\top]$$

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Bernoulli Distribution

Consider a single binary random variable $x \in \{0, 1\}$)

- The probability of x=1 will be denoted by the parameter μ so that $p(x=1|\mu)=\mu$, where $0\leq \mu \leq 1$
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- easily it follows that $p(x = 0|\mu) = 1 \mu$
- the probability distribution over x can be written in the form

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

 easily to verify that this distribution is normalized and that it has mean and variance given by

$$\mathcal{E}[\mathbf{x}] = \mu$$

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



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Likelihood function

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With
$$\frac{\partial \ln p(\mathcal{D}|\mu)}{\partial \mu} = 0 \rightarrow \mu_{ML} = \frac{1}{N} \sum_{n=1}^{N} x_n$$



Overfitting of ML

If we denote the number of observations of x = 1 (heads) within this data set by m, then

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

Example: Suppose now flip the coin 5 (N=5) times, and happen to observe 5 (m=5) heads. Then, $\mu_{ML} = 1$. What does it mean?

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The ML solution would predict that all future observations should give heads.



Binomial Distribution

Consider an extreme example of the over-fitting associated with maximum likelihood

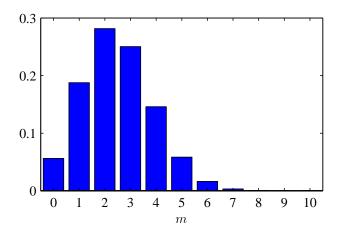
- binomial distribution: the distribution of the number m of observations of x = 1, given that the dataset has size N: $\mu^m (1 \mu)^{N-m}$
- If we work the distribution of the number m of observations of x = 1 given that the dataset has size N, we can obtain the binomial distribution

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

 $^{^{}a}$ The number of ways of choosing m objects out of a total of N identical objects.

Binomial Distribution (cont'd)

Histogram plot of the binomial distribution as a function of \emph{m} for $\emph{N}=$ 10 and $\mu=$ 0.25



The Beta Distribution

Problem by maximum likelihood estimation in the binomial distribution -

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Conjugate prior

- Remember the likelihood function takes the form $\mu^{x}(1-\mu)^{1-x}$
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We therefore choose a prior, called the beta distribution, given by

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



The Beta Distribution (cont'd)

The beta distribution is normalized,



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The beta distribution is normalized,

$$\int_0^1 \mathsf{Beta}(\mu|a,b) d\mu = 1$$

The mean and variance of the beta distribution are given by

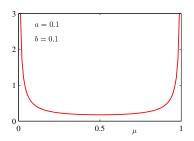
$$\mathcal{E}[\mu] = \frac{a}{a+b}$$

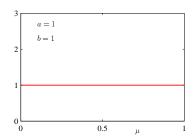
$$var[\mu] = \frac{ab}{(a+b)^2(a+b+1)}$$

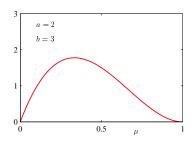
The parameters a and b are often called hyperparameters

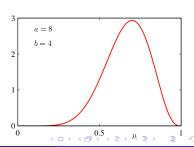


The Beta Distribution (cont'd)









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$$p(\mu|m, l, a, b) \propto \mu^{m+a-1} (1-\mu)^{l+b-1}$$

where I = N - m

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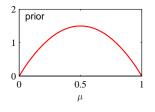
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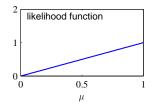
$$p(\mu|m, l, a, b) = \frac{\Gamma(m+a+l+b)}{\Gamma(m+a)\Gamma(l+b)} \mu^{m+a-1} (1-\mu)^{l+b-1}$$

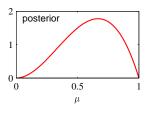


Illustration

The prior is given by a beta distribution with parameters a = 2, b = 2, and the likelihood function, given by binomial distribution with N = m = 1, corresponds to a single observation of x = 1







We can see that the posterior is given by a beta distribution with parameters a = 3, b = 2

We can interpret a, b in the prior as an effective number of observations of x = 1 and x = 0, respectively

The Beta Distribution - Prediction

Prediction, given the prior and observations \mathcal{D} ,



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

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$$P(x = 1|\mathcal{D}) = \int_0^1 p(x = 1|\mu)p(\mu|\mathcal{D})d\mu$$
$$= \int_0^1 \mu p(\mu|\mathcal{D})d\mu$$
$$= \mathcal{E}[\mu|\mathcal{D}]$$
$$= \frac{m+a}{m+a+l+b}$$

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Introduction

- Consider a discrete variable that can take one of possible K values
- Convenient representation with a vector where one element equals 1, others 0, e.g., $\mathbf{x} = (0, 0, 1, 0, 0, 0)^{\top}$
- If denoting the probability of $x_k = 1$ by the parameter μ_k , then the distribution of **x** is given

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

where $\boldsymbol{\mu} = (\mu_1, \cdots, \mu_K)^{\top}$, s.t., $\mu_k \geq 0$ and $\sum_k \mu_k = 1$

Generalization of the Bernoulli Distribution

• the distribution is normalized

Generalization of the Bernoulli Distribution

the distribution is normalized

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

and that

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

the likelihood function

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

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the likelihood function

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

^aThe number of observations of $x_k = 1$, and $m_k = \sum_n x_{nk}$

Maximum Likelihood Estimator

By a Lagrange multiplier λ and maximizing

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

$$\Rightarrow \mu_k^{\text{ML}} = \frac{m_k}{N}$$

Multinomial Distribution

Consider the joint distribution of the quantities m_1, \dots, m_K , the multinomial distribution takes the form

$$\mathsf{Mult}(m_1,\cdots,m_K|\mu,N) = \underbrace{\begin{pmatrix} N \\ m_1m_2\cdots m_K \end{pmatrix}}_{\substack{N:\\ m_1!m_2!\cdots m_K!}} \prod_{k=1}^K \mu^{m_k}$$

The variables m_k are subject to the constraint $\sum_{k=1}^{K} m_k = N$

Dirichlet Distribution

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$$p(\mu|\alpha) \propto \prod_{k=1}^K \mu_k^{\alpha_k - 1}, \text{ s.t. } \left\{ \begin{array}{l} 0 \leq \mu_k \leq 1 \\ \sum_k \mu_k = 1 \end{array} \right.$$

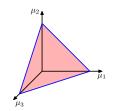
• The normalized form the distribution by

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

This is called the Dirichlet distribution.

$$^{a}\alpha_{0}=\sum_{k=1}^{K}\alpha_{k}$$

Dirichlet Distribution (cont'd)

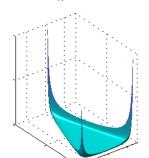


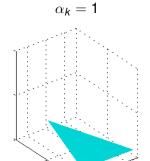
The domain of the \leftarrow Dirichlet distribution with K = 3

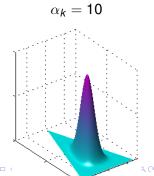
Plots of the Dirichlet distribution (K = 3)











- Probability Theory
- 2 Binary Variables
- Multinomial Variables
- 4 The Gaussian Distribution
- Exponential Family



Single Variable Gaussian

For a single variable x

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

where μ is the mean and σ^2 is the variance

Multivariable Gaussian

For a d-dimensional vector **x**

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

where μ is a d-dimensional mean vector and Σ is a $d \times d$ covariance matrix, and $|\Sigma|$ denotes the determinant of Σ

Geometrical Form

Mahalanobis distance

The functional dependence of the Gaussian on ${\bf x}$ is through the quadratic form

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

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The quantity Δ is called the Mahalanobis distance from μ to \mathbf{x} and reduces to the Euclidean distance when Σ is the identity matrix

Consider the eigenvector equation for the covariance matrix

$$\Sigma \mu_i = \lambda_i \mu_i$$

Since Σ is a real, symmetric matrix, its eigenvalues will be real, and its eigenvectors can be chosen to form an orthonormal set, so that,

$$\boldsymbol{\mu}_i^{\top} \boldsymbol{\mu}_j = \mathrm{I}_{ij}$$



The covariance matrix can be expressed as an expansion in terms of its eigenvectors in the form

$$\Sigma = \sum_{i=1}^d \lambda_i \boldsymbol{\mu}_i \boldsymbol{\mu}_j^\top$$

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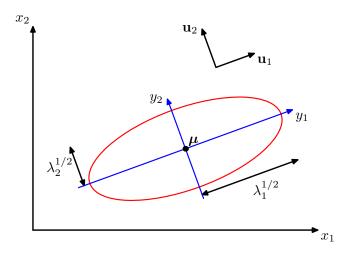
$$\Sigma^{-1} = \sum_{i=1}^d rac{1}{\lambda_i} \mu_i \mu_j^{ op} ext{ and } \Delta^2 = (\mathbf{x} - \mu)^{ op} \Sigma^{-1} (\mathbf{x} - \mu),$$

therefore we have,

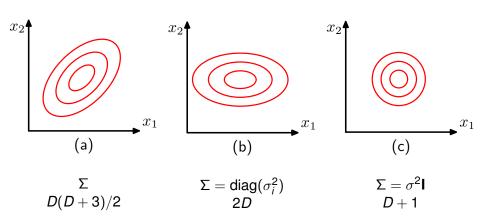
$$\Delta^2 = \sum_{i=1}^d rac{y_i^2}{\lambda_i}, \ y_i = oldsymbol{\mu}_i^ op(\mathbf{x} - oldsymbol{\mu})$$

- We can interpret $\{y_i\}$ as a new coordinate system defined by the orthonormal vectors μ_i that are shifted and rotated with respect to the original x_i coordinates
- Forming the vector $\mathbf{y} = (y_1, \dots, y_d)^{\top}$, we have

$$y = U(x - \mu)$$

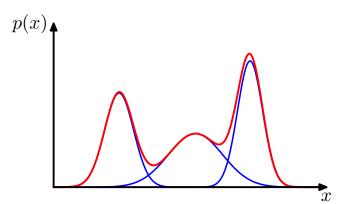


One of Limitations of Gaussian Distribution



Mixture of Gaussians

Another limitations of Gaussian distribution is that it is uni-modal The superpositions, formed by taking linear combinations of more basic distributions, can be formulated as probabilistic models known as mixture distribution

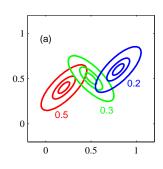


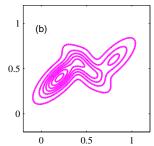
Mixture of Gaussians (cont'd)

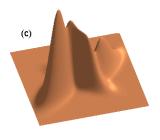
Consider a superposition of K Gaussian densities of the form

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

which is called a mixture of Gaussians







- Probability Theory
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General Form

The exponential family of distributions over \mathbf{x} , given parameters η , is defined to be the set of distributions of the form

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

- η are called the natural parameters of the distribution, and $\mathbf{u}(\mathbf{x})$ is some function of \mathbf{x}
- the function $g(\eta)$ can be interpreted as the coefficient that the distribution is normalized and therefore satisfies

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



Bernoulli Distribution

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

Expressing the right-hand side as the exponential of the logarithm, we have

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



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$$\begin{cases} \eta = \ln\left(\frac{\mu}{1-\mu}\right) \\ \sigma(\eta) = \frac{1}{1+\exp(-\eta)} \end{cases}$$



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Bernoulli Distribution (cont'd)

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

Bernoulli Distribution (cont'd)

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

$$u(x) = x$$

$$h(x) = 1$$

$$g(\eta) = \sigma(-\eta)$$



Multinomial Distribution

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

where $\mathbf{x} = (x_1, \cdots, x_N)^{\top}$

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 $h(\mathbf{x}) = 1$
 $g(\eta) = 1$

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$$\exp\left\{\sum_{k=1}^M x_k \ln \mu_k\right\}$$



$$\begin{split} & \exp\left\{\sum_{k=1}^{M} x_{k} \ln \mu_{k}\right\} \\ & = \exp\left\{\sum_{k=1}^{M-1} x_{k} \ln \mu_{k} + \left(1 - \sum_{k=1}^{M-1} x_{k}\right) \ln \left(1 - \sum_{k=1}^{M-1} \mu_{k}\right)\right\} \\ & = \exp\left\{\sum_{k=1}^{M-1} x_{k} \ln \left(\frac{\mu_{k}}{1 - \sum_{j=1}^{M-1} \mu_{j}}\right) + \ln \left(1 - \sum_{k=1}^{M-1} \mu_{k}\right)\right\} \end{split}$$

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$$\ln\left(\frac{\mu_k}{1 - \sum_{j=1}^{M-1} \mu_j}\right) = \eta_k \Rightarrow \mu_k = \frac{\exp(\eta_k)}{1 - \sum_j \exp(\eta_j)}^2$$

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$$egin{aligned} \mathbf{u}(\mathbf{x}) &= \mathbf{x} \\ h(\mathbf{x}) &= 1 \\ g(\eta) &= \left(1 + \sum_{k=1}^{M-1} \exp(\eta_k)
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$$p(x|\mu, \sigma^2)$$
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$$\begin{split} & \boldsymbol{\eta} = \left(\begin{array}{c} \mu/\sigma^2 \\ -1/2\sigma^2 \end{array} \right) \\ & \mathbf{u}(\mathbf{x}) = \left(\begin{array}{c} x \\ x^2 \end{array} \right) \\ & h(\mathbf{x}) = (2\pi)^{-1/2} \\ & g(\boldsymbol{\eta}) = (-2\eta_2)^{1/2} \exp\left(\frac{\eta_1^2}{4\eta_2} \right) \end{split}$$

Maximum Likelihood

- ullet estimating the parameter vector η in the general exponential family distribution
- if using the ML technique, we can take the gradient of $g(\eta) \int h(\mathbf{x}) \exp \left\{ \eta^\top \mathbf{u}(\mathbf{x}) \right\} d\mathbf{x} = 1$,

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Sufficient Statistics

Considering a set of i.i.d. data denoted by $\mathbf{X} = (\mathbf{x}_n)_{n=1}^N$, for which the likelihood function is given by

$$p(\mathbf{X}|\boldsymbol{\eta}) = \left(\prod_{n=1}^{N} h(\mathbf{x}_n)\right) g(\boldsymbol{\eta})^N \exp\left\{\boldsymbol{\eta}^\top \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)\right\}$$
$$\Rightarrow - \nabla \ln g(\boldsymbol{\eta}_{\mathsf{ML}}) = \frac{1}{N} \sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n)$$

- The solution for the MLE dependends on the data only through $\sum_{n} \mathbf{u}(\mathbf{x}_n)$
- this is called the sufficient statistic of the distribution $h(\mathbf{x})g(\eta) \exp \left\{ \eta^{\top} \mathbf{u}(\mathbf{x}) \right\}$
- we donot need to store the entire dataset itself but the value of the sufficient statistic

Sufficient Statistics (cont'd)

- for Bernoulli, Multinomial distribution, $\mathbf{u}(\mathbf{x}) = \mathbf{x}$, and so we only keep $\sum_{n} \mathbf{x}_{n}$
- for Gaussian, $\mathbf{u}(\mathbf{x}) = (\mathbf{x}, \mathbf{x}^2)^{\top}$, we should keep only $\sum_n \mathbf{x}_n$ and $\sum_n \mathbf{x}_n^2$

3

³Common distributions and the corresponding sufficient statistics are listed in PP. 108-109 of Pattern Classification

Conjugate Priors

- In general, for a given probability distribution $p(\mathbf{x}|\eta)$, we can seek a prior $p(\eta)$ that is conjugate to the likelihood function
- so the posterior distribution has the same functional form as the prior
- for any member of the exponential family, there exists a conjugate prior in the form

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

where $f(\chi, \nu)$ is a normalization coefficient, and $g(\eta)$ is the same function in the exponential family

$$p(oldsymbol{\eta} | \mathbf{X}, oldsymbol{\chi},
u) \propto g(oldsymbol{\eta})^{
u+N} \exp \left\{ oldsymbol{\eta}^{ op} \left(\sum_{n=1}^{N} \mathbf{u}(\mathbf{x}_n) +
u oldsymbol{\chi}
ight)
ight\}$$