10417/10617 Intermediate Deep Learning: Fall2020

Russ Salakhutdinov

Machine Learning Department rsalakhu@cs.cmu.edu

Lecture 3

Bernoulli Distribution

ullet 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:

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

• The probability distribution, known as Bernoulli distribution, can be written as:

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

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

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

Parameter Estimation

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

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

Statistic

• Note that the likelihood function depends on the N observations $\mathbf{x_n}$ only through the sum $\sum x_n$

Parameter Estimation

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

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

ullet Setting the derivative of the log-likelihood function w.r.t μ to zero, we obtain:

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

where m is the number of heads.

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:

$$p(\mathbf{x}|oldsymbol{\mu}) = \prod_{k=1}^K \mu_k^{x_k} ~~ orall k: \mu_k \geqslant 0 ~~ ext{and} ~~ \sum_{k=1}^K \mu_k = 1$$

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

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

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

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

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

These are called the sufficient statistics for this distribution.

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

- 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:

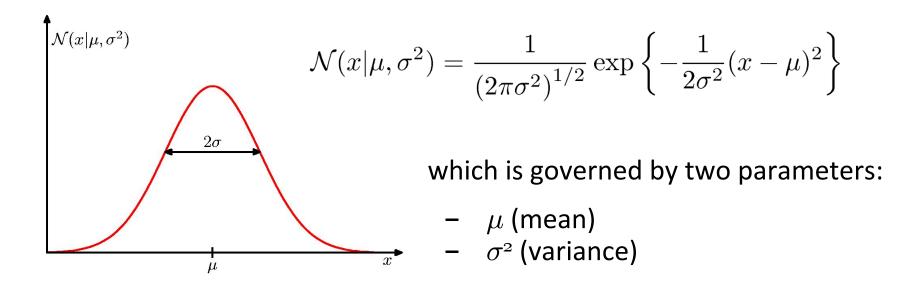
$$\sum_{k=1}^{K} m_k \ln \mu_k + \lambda \left(\sum_{k=1}^{K} \mu_k - 1 \right)$$

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

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

Gaussian Univariate Distribution

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



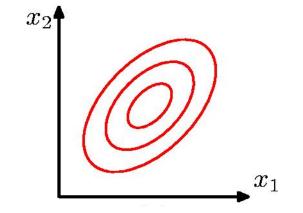
The Gaussian distribution satisfies:

$$\mathcal{N}(x|\mu, \sigma^2) > 0$$
$$\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) dx = 1$$

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 .

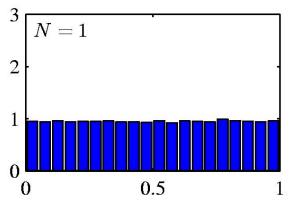
 Note that the covariance matrix is a symmetric positive definite matrix.

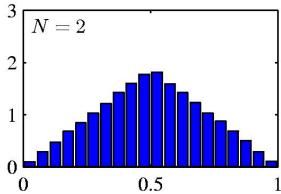
Central Limit Theorem

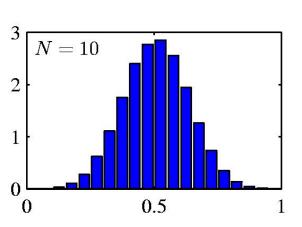
- The distribution of the sum of N i.i.d. random variables becomes increasingly Gaussian as N grows.
- Consider N variables, each of which has a uniform distribution over the interval [0,1].
- Let us look at the distribution over the mean:

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

• As N increases, the distribution tends towards a Gaussian distribution.







Moments of the Gaussian Distribution

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

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

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

The term in z in the factor $(z+\mu)$ will vanish by symmetry.

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

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:

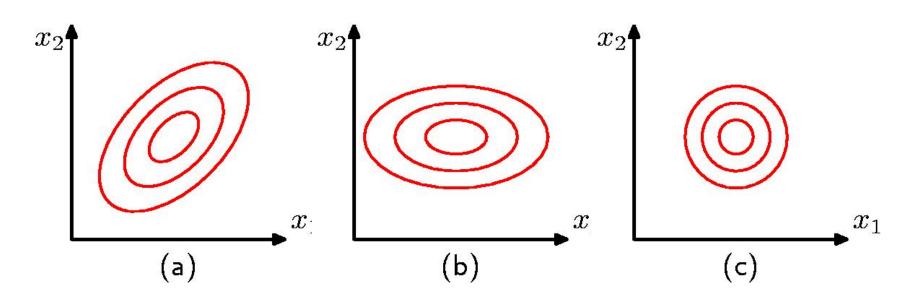
$$ext{cov}[\mathbf{x}] = \mathbb{E}\left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^{\mathrm{T}} \right] = \mathbf{\Sigma}$$

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

ullet 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, axisaligned 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 \mathbf{x} into two disjoint subsets \mathbf{x}_a and \mathbf{x}_b :

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

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

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

 \bullet Note that \varLambda_{aa} is not given by the inverse of $\varSigma_{aa}.$

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 notdepend on x_b.

$$egin{array}{lcl} oldsymbol{\Sigma}_{a|b} &=& oldsymbol{\Lambda}_{aa}^{-1} = oldsymbol{\Sigma}_{aa} - oldsymbol{\Sigma}_{ab} oldsymbol{\Sigma}_{bb}^{-1} oldsymbol{\Sigma}_{ba} \ oldsymbol{\mu}_{a|b} &=& oldsymbol{\Sigma}_{a|b} \left\{ oldsymbol{\Lambda}_{aa} oldsymbol{\mu}_{a} - oldsymbol{\Lambda}_{ab} (\mathbf{x}_{b} - oldsymbol{\mu}_{b})
ight\} \ &=& oldsymbol{\mu}_{a} - oldsymbol{\Lambda}_{aa}^{-1} oldsymbol{\Lambda}_{ab} (\mathbf{x}_{b} - oldsymbol{\mu}_{b}) \ &=& oldsymbol{\mu}_{a} + oldsymbol{\Sigma}_{ab} oldsymbol{\Sigma}_{bb}^{-1} (\mathbf{x}_{b} - oldsymbol{\mu}_{b}) \end{array}$$

Linear function of x_h .

Marginal Distribution

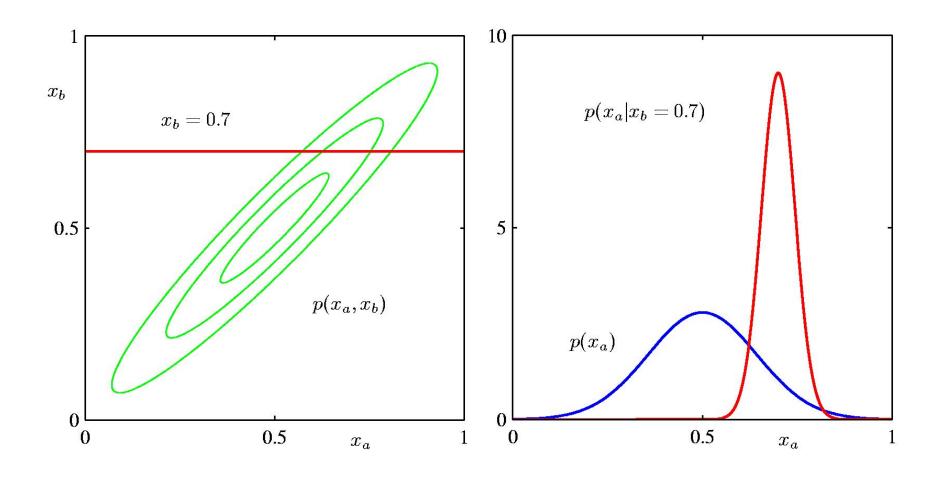
• It turns out that the marginal distribution is also a Gaussian distribution:

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

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

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

Conditional and Marginal Distributions



- ullet 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

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

• 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:

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

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

$$oldsymbol{\Sigma}_{ ext{ML}} = rac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - oldsymbol{\mu}_{ ext{ML}}) (\mathbf{x}_n - oldsymbol{\mu}_{ ext{ML}})^{ ext{T}}.$$

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

Unbiased estimate

$$\mathbb{E}[m{\mu}_{ ext{ML}}] = m{\mu}$$
 $\mathbb{E}[m{\Sigma}_{ ext{ML}}] = rac{N-1}{N}m{\Sigma}.$ Biased estimate

- ullet Note that the maximum likelihood estimate of Σ is biased.
- We can correct the bias by defining a different estimator:

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

Consider Student's t-Distribution

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

where

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



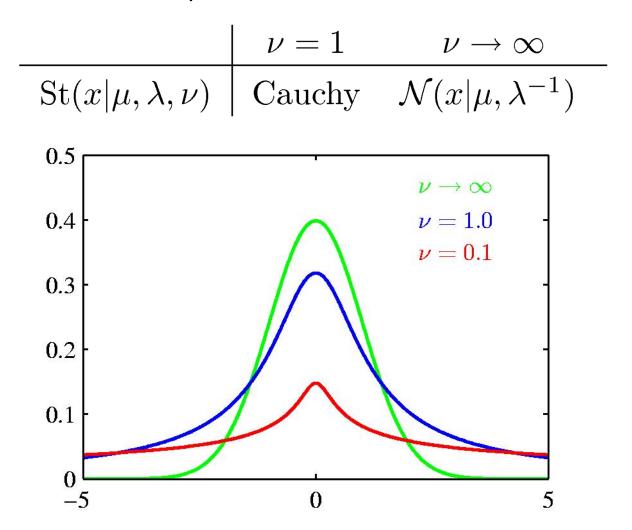
Sometimes called the precision

parameter.

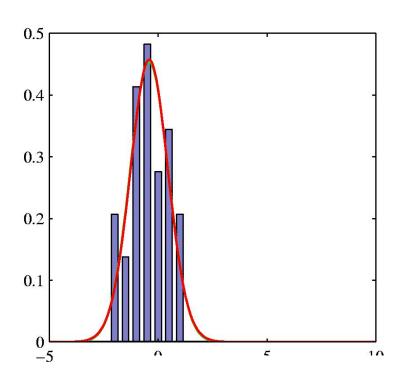


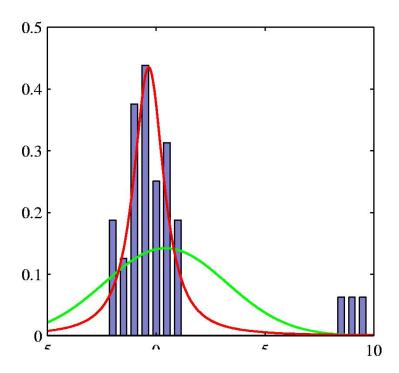
Degrees of freedom

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



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





• The multivariate extension of the t-Distribution:

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

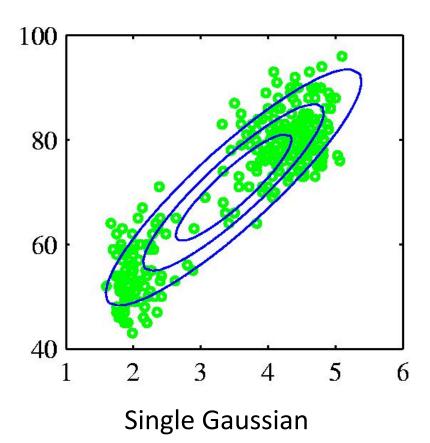
where
$$\Delta^2 = (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Lambda} (\mathbf{x} - \boldsymbol{\mu})$$

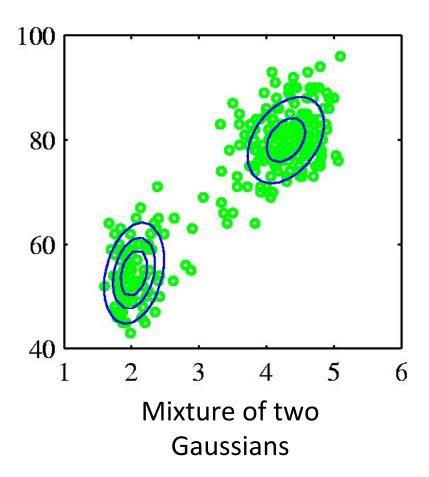
• Properties:

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

Mixture of Gaussians

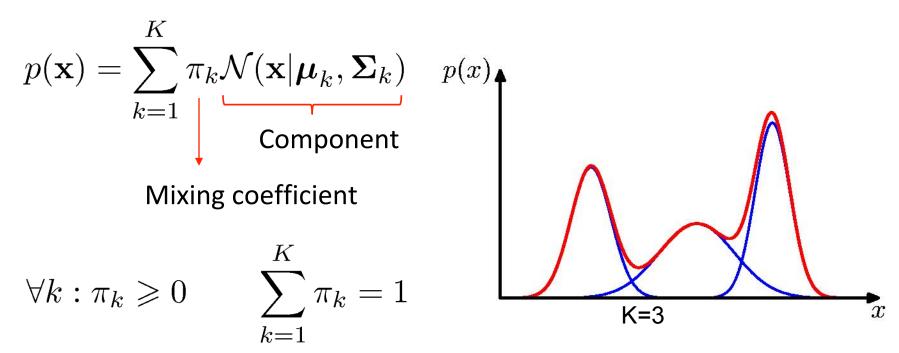
- When modeling real-world data, Gaussian assumption may not be appropriate.
- Consider the following example: Old Faithful Dataset





Mixture of Gaussians

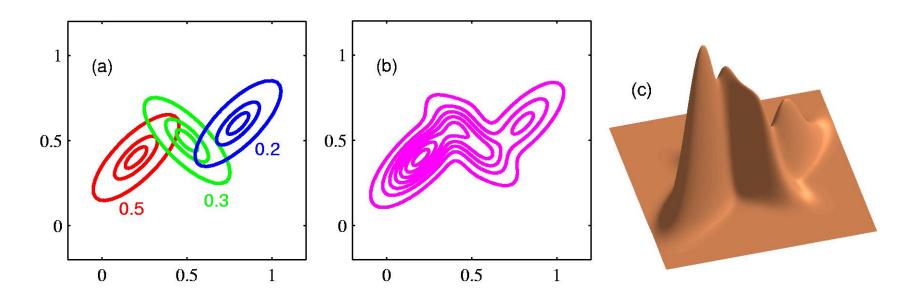
 We can combine simple models into a complex model by defining a superposition of K Gaussian densities of the form:



- 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 ν
- (b) Contours of marginal probability density $p(\mathbf{x}) = \sum_{k=1}^{n} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
- (c) A surface plot of the distribution p(x).

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

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

Log of a sum: no closed form 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 distributions of the form:

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

where

- η is the vector of natural parameters
- u(x) is the vector of sufficient statistics
- The function $g(\eta)$ can be interpreted as the coefficient that ensures that the distribution $p(\mathbf{x} \mid \eta)$ is normalized:

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

ML for the Exponential Family

• Remember the Exponential Family:

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

• From the definition of the normalizer $g(\eta)$:

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

• We can take a derivative w.r.t η :

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

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

Thus

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

ML for the Exponential Family

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 :

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

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

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

• Thus

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

• Note that the covariance of $\mathbf{u}(\mathbf{x})$ can be expressed in terms of the second derivative of $\mathbf{g}(\eta)$, and similarly for the higher moments.

ML for the Exponential Family

- ullet 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 .

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

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

Therefore we have

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

Sufficient Statistic