CS 2750 Machine Learning
Lecture 4

Density estimation II.

Milos Hauskrecht
milos@cs.pitt.edu
5329 Sennott Square

Outline

Outline:

- **Density estimation:**
  - Maximum likelihood (ML)
  - Bayesian parameter estimates
  - MAP
- **Bernoulli distribution.**
- **Binomial distribution**
- **Multinomial distribution**
- **Normal distribution**
- **Exponential family**

Density estimation

Data: $D = \{D_1, D_2, .., D_n\}$

$D_i = \mathbf{x}_i$ a vector of attribute values

Objective: try to estimate the underlying 'true' probability distribution over variables $\mathbf{X}$, $p(\mathbf{X})$, using examples in D

true distribution $p(\mathbf{X})$ $\rightarrow$ n samples $D = \{D_1, D_2, .., D_n\}$ $\rightarrow$ estimate $\hat{p}(\mathbf{X})$

Standard (iid) assumptions: ?

Parameter estimation (learning)

- **Maximum likelihood (ML)**

$$\Theta_{ML} = \arg\max_{\Theta} p(D \mid \Theta, \xi)$$

- **Bayesian parameter estimation**

keep the posterior density $p(\Theta \mid D, \xi)$

- **Maximum a posteriori probability (MAP)**

$$\Theta_{MAP} = \arg\max_{\Theta} p(\Theta \mid D, \xi)$$

- **Expected value**

$$\Theta_{EXP} = \int_{\Theta} \Theta p(\Theta \mid D, \xi) d\Theta$$

Bernoulli trials

Data: D a sequence of outcomes x_i such that

- **head** $x_i = 1$
- **tail** $x_i = 0$

Model: probability of a head θ
probability of a tail $(1-\theta)$

Probability of an outcome of a coin flip

$$P(x_i \mid \theta) = \theta^{x_i}(1-\theta)^{(1-x_i)}$$ **Bernoulli distribution**

ML Solution: $$\theta_{ML} = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2}$$

N_1, N_2 - Number of heads and tails respectively

Posterior distribution

Posterior density

Likelihood of data **prior**

$$p(\theta \mid D, \xi) = \frac{P(D \mid \theta, \xi)\, p(\theta \mid \xi)}{P(D \mid \xi)}$$ **(via Bayes rule)**

Normalizing factor

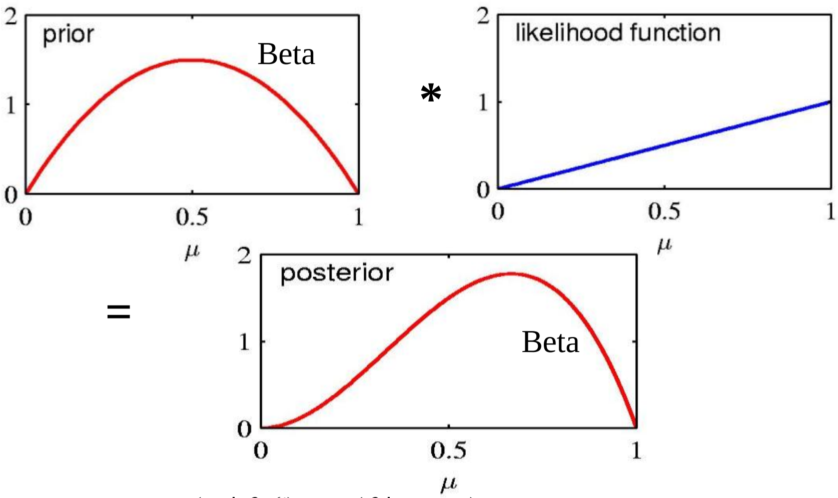
$$P(D \mid \theta, \xi) = \prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{(1-x_i)} = \theta^{N_1}(1-\theta)^{N_2}$$

$p(\theta \mid \xi)$ - is the prior probability on θ

Conjugate choice of prior: Beta

$$p(\theta \mid \xi) = Beta(\theta \mid \alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \theta^{\alpha_1 - 1}(1-\theta)^{\alpha_2 - 1}$$

Posterior distribution



$$p(\theta \mid D, \xi) = \frac{P(D \mid \theta, \xi) Beta(\theta \mid \alpha_1, \alpha_2)}{P(D \mid \xi)} = Beta(\theta \mid \alpha_1 + N_1, \alpha_2 + N_2)$$

Maximum a posterior probability

Maximum a posteriori estimate

– Selects the mode of the **posterior distribution**

$$\theta_{MAP} = \arg\max_{\theta} p(\theta \mid D, \xi)$$

$$p(\theta \mid D, \xi) = \frac{P(D \mid \theta, \xi) Beta(\theta \mid \alpha_1, \alpha_2)}{P(D \mid \xi)} = Beta(\theta \mid \alpha_1 + N_1, \alpha_2 + N_2)$$

$$= \frac{\Gamma(\alpha_1 + \alpha_2 + N_1 + N_2)}{\Gamma(\alpha_1 + N_1)\Gamma(\alpha_2 + N_2)} \theta^{N_1 + \alpha_1 - 1} (1 - \theta)^{N_2 + \alpha_2 - 1}$$

Notice that parameters of the prior act like counts of heads and tails (sometimes they are also referred to as **prior counts**)

MAP Solution: $$\theta_{MAP} = \frac{\alpha_1 + N_1 - 1}{\alpha_1 + \alpha_2 + N_1 + N_2 - 2}$$

Bayesian framework

- **Predictive probability of an outcome $x=1$ in the next trial**

  $P(x=1|D,\xi)$

$$P(x=1|D,\xi)=\int_0^1 P(x=1|\theta,\xi)\overbrace{p(\theta|D,\xi)}^{\text{Posterior density}}d\theta$$

$$=\int_0^1 \theta p(\theta|D,\xi)d\theta = E(\theta)$$

- **Equivalent to the expected value of the parameter**
  - expectation is taken with respect to the posterior distribution

$$p(\theta|D,\xi)=Beta(\theta|\alpha_1+N_1,\alpha_2+N_2)$$

Expected value of the parameter

How to obtain the expected value?

$$E(\theta)=\int_0^1 \theta Beta(\theta|\eta_1,\eta_2)d\theta=\int_0^1 \theta\frac{\Gamma(\eta_1+\eta_2)}{\Gamma(\eta_1)\Gamma(\eta_2)}\theta^{\eta_1-1}(1-\theta)^{\eta_2-1}d\theta$$

$$=\frac{\Gamma(\eta_1+\eta_2)}{\Gamma(\eta_1)\Gamma(\eta_2)}\int_0^1 \theta^{\eta_1}(1-\theta)^{\eta_2-1}d\theta$$

$$=\frac{\Gamma(\eta_1+\eta_2)}{\Gamma(\eta_1)\Gamma(\eta_2)}\frac{\Gamma(\eta_1+1)\Gamma(\eta_2)}{\Gamma(\eta_1+\eta_2+1)}\underbrace{\int_0^1 Beta(\eta_1+1,\eta_2)d\theta}_{1}$$

$$=\frac{\eta_1}{\eta_1+\eta_2}$$

Note: $\Gamma(\alpha+1)=\alpha\Gamma(\alpha)$ for integer values of α

Expected value of the parameter

- **Substituting the results for the posterior:**

$$p(\theta \mid D, \xi) = Beta(\theta \mid \alpha_1 + N_1, \alpha_2 + N_2)$$

- **We get** $$E(\theta) = \frac{\alpha_1 + N_1}{\alpha_1 + N_1 + \alpha_2 + N_2}$$

- **Note that the mean of the posterior is yet** another "reasonable" parameter choice:

$$\hat{\theta} = E(\theta)$$

Binomial distribution

Example: a biased coin

Outcomes: two possible values -- head or tail

Data: D a set of order-independent outcomes

We treat *D* as a multi-set !!!

N_1 - number of heads seen N_2 - number of tails seen

Model: probability of a head θ

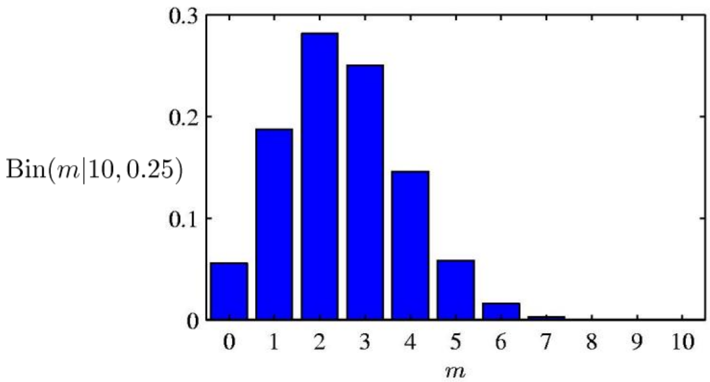
probability of a tail $(1-\theta)$

Probability of an outcome

$$P(D \mid \theta) = \binom{N}{N_1} \theta^{N_1} (1-\theta)^{N_2}$$ **Binomial distribution**

Binomial distribution

Binomial distribution:



Maximum likelihood (ML) estimate.

Likelihood of data:

$$P(D \mid \theta) = \binom{N}{N_1} \theta^{N_1} (1-\theta)^{N_2} = \frac{N!}{N_1! N_2!} \theta^{N_1} (1-\theta)^{N_2}$$

Log-likelihood

$$l(D, \theta) = \log \binom{N}{N_1} \theta^{N_1} (1-\theta)^{N_2} = \underline{\log \frac{N!}{N_1! N_2!}} + N_1 \log \theta + N_2 \log(1-\theta)$$

Constant from the point of optimization !!!

ML Solution: $\theta_{ML} = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2}$

The same as for Bernoulli and D with an iid sequence of examples

Posterior density

Posterior density

$$p(\theta \mid D, \xi) = \frac{P(D \mid \theta, \xi)\, p(\theta \mid \xi)}{P(D \mid \xi)}$$ **(via Bayes rule)**

Prior choice

$$p(\theta \mid \xi) = Beta(\theta \mid \alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \theta^{\alpha_1 - 1}(1-\theta)^{\alpha_2 - 1}$$

Likelihood

$$P(D \mid \theta) = \frac{\Gamma(N_1 + N_2)}{\Gamma(N_1)\Gamma(N_2)} \theta^{N_1}(1-\theta)^{N_2}$$

Posterior $p(\theta \mid D, \xi) = Beta(\alpha_1 + N_1, \alpha_2 + N_2)$

MAP estimate $\theta_{MAP} = \arg\max_{\theta} p(\theta \mid D, \xi)$

$$\theta_{MAP} = \frac{\alpha_1 + N_1 - 1}{\alpha_1 + \alpha_2 + N_1 + N_2 - 2}$$

Expected value of the parameter

The result is the same as for Bernoulli distribution

$$E(\theta) = \int_0^1 \theta Beta(\theta \mid \eta_1, \eta_2) d\theta = \frac{\eta_1}{\eta_1 + \eta_2}$$

Expected value of the parameter

$$E(\theta) = \frac{\alpha_1 + N_1}{\alpha_1 + N_1 + \alpha_2 + N_2}$$

Predictive probability of event x=1

$$P(x = 1 \mid \theta, \xi) = E(\theta) = \frac{\alpha_1 + N_1}{\alpha_1 + N_1 + \alpha_2 + N_2}$$

Binomial distribution

Example: a biased coin

Outcomes: two possible values -- head or tail

Data: D a set of order-independent outcomes

We treat *D* as a multi-set !!!

N_1 - number of heads seen N_2 - number of tails seen

Model: probability of a head θ

probability of a tail $(1-\theta)$

Probability of an outcome

$$P(D|\theta) = \binom{N}{N_1}\theta^{N_1}(1-\theta)^{N_2}$$ **Binomial distribution**

Maximum likelihood (ML) estimate.

Likelihood of data:

$$P(D|\theta) = \binom{N}{N_1}\theta^{N_1}(1-\theta)^{N_2} = \frac{N!}{N_1!N_2!}\theta^{N_1}(1-\theta)^{N_2}$$

Log-likelihood

$$l(D,\theta) = \log\binom{N}{N_1}\theta^{N_1}(1-\theta)^{N_2} = \underline{\log\frac{N!}{N_1!N_2!}} + N_1\log\theta + N_2\log(1-\theta)$$

Constant from the point of optimization !!!

ML Solution: $\theta_{ML} = \frac{N_1}{N} = \frac{N_1}{N_1+N_2}$

The same as for Bernoulli and D with iid sequence of examples

Posterior density

Posterior density

$$p(\theta \mid D, \xi) = \frac{P(D \mid \theta, \xi)\, p(\theta \mid \xi)}{P(D \mid \xi)} \quad \textbf{(via Bayes rule)}$$

Prior choice

$$p(\theta \mid \xi) = Beta(\theta \mid \alpha_1, \alpha_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \theta^{\alpha_1 - 1}(1-\theta)^{\alpha_2 - 1}$$

Likelihood

$$P(D \mid \theta) = \frac{\Gamma(N_1 + N_2)}{\Gamma(N_1)\Gamma(N_2)} \theta^{N_1}(1-\theta)^{N_2}$$

Posterior $p(\theta \mid D, \xi) = Beta(\alpha_1 + N_1, \alpha_2 + N_2)$

MAP estimate $\theta_{MAP} = \arg\max_{\theta} p(\theta \mid D, \xi)$

$$\theta_{MAP} = \frac{\alpha_1 + N_1 - 1}{\alpha_1 + \alpha_2 + N_1 + N_2 - 2}$$

Multinomial distribution

Example: Multi-way coin toss, roll of dice

- **Data:** a set of N outcomes (multi-set)

  N_i - a number of times an outcome i has been seen

Model parameters: $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots \theta_k)$ **s.t.** $\sum_{i=1}^{k} \theta_i = 1$

θ_i - probability of an outcome i

Probability of data (likelihood)

$$P(N_1, N_2, \ldots N_k \mid \boldsymbol{\theta}, \xi) = \frac{N!}{N_1! N_2! \ldots N_k!} \theta_1^{N_1} \theta_2^{N_2} \ldots \theta_k^{N_k}$$

Multinomial distribution

ML estimate:

$$\theta_{i,ML} = \frac{N_i}{N}$$

Posterior density and MAP estimate

Choice of the prior: Dirichlet distribution

$$Dir(\boldsymbol{\theta} \mid \alpha_1,..,\alpha_k) = \frac{\Gamma(\sum_{i=1}^{k} \alpha_i)}{\prod_{i=1}^{k} \Gamma(\alpha_i)} \theta_1^{\alpha_1 - 1} \theta_2^{\alpha_2 - 1} \ldots \theta_k^{\alpha_k - 1}$$

Dirichlet is the conjugate choice for multinomial

$$P(D \mid \boldsymbol{\theta}, \xi) = P(N_1, N_2, \ldots N_k \mid \boldsymbol{\theta}, \xi) = \frac{N!}{N_1! N_2! \ldots N_k!} \theta_1^{N_1} \theta_2^{N_2} \ldots \theta_k^{N_k}$$

Posterior density

$$p(\boldsymbol{\theta} \mid D, \xi) = \frac{P(D \mid \boldsymbol{\theta}, \xi) Dir(\boldsymbol{\theta} \mid \alpha_1, \alpha_2,..\alpha_k)}{P(D \mid \xi)} = Dir(\boldsymbol{\theta} \mid \alpha_1 + N_1,.., \alpha_k + N_k)$$

MAP estimate:

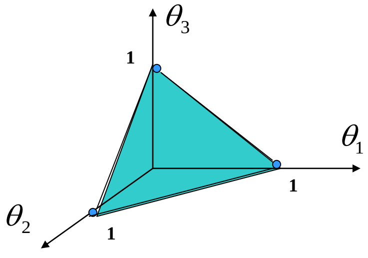
$$\theta_{i,MAP} = \frac{\alpha_i + N_i - 1}{\sum_{i=1,..k} (\alpha_i + N_i) - k}$$

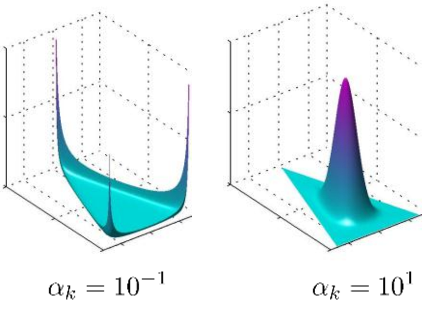
Dirichlet distribution

Dirichlet distribution:

$$Dir(\boldsymbol{\theta} \mid \alpha_1,..,\alpha_k) = \frac{\Gamma(\sum_{i=1}^{k} \alpha_i)}{\prod_{i=1}^{k} \Gamma(\alpha_i)} \theta_1^{\alpha_1 - 1} \theta_2^{\alpha_2 - 1} \ldots \theta_k^{\alpha_k - 1}$$

Assume: k=3





Expected value

The result is analogous to the result for binomial

$$E(\boldsymbol{\theta}) = \int_{0 \le \theta_i \le 1, \sum \theta_i = 1} \boldsymbol{\theta} \; Dir(\boldsymbol{\theta} \mid \boldsymbol{\eta}) d\boldsymbol{\theta} = \left(\frac{\eta_1}{\eta_1 + \eta_2 + \eta_k}, \ldots \frac{\eta_i}{\eta_1 + \eta_2 + \eta_k}, \ldots \frac{\eta_k}{\eta_1 + \eta_2 + \eta_k} \right)$$

Expectation based parameter estimate

$$E(\boldsymbol{\theta}) = \left(\frac{\alpha_1 + N_1}{\alpha_1 + N_1 + \ldots + \alpha_k + N_k} \ldots \frac{\alpha_i + N_i}{\alpha_1 + N_1 + \ldots + \alpha_k + N_k} \ldots \frac{\alpha_k + N_k}{\alpha_1 + N_1 + \ldots + \alpha_k + N_k} \right)$$

Represents the predictive probability of an event x=i

$$P(x = i \mid \boldsymbol{\theta}, \xi) = \frac{\alpha_i + N_i}{\alpha_1 + N_1 + \ldots + \alpha_k + N_k}$$

Other distributions

The same ideas can be applied to other distributions

- Typically we choose distributions that behave well so that computations lead to a nice solutions

- **Exponential family of distributions**

Conjugate choices for some of the distributions from the exponential family:

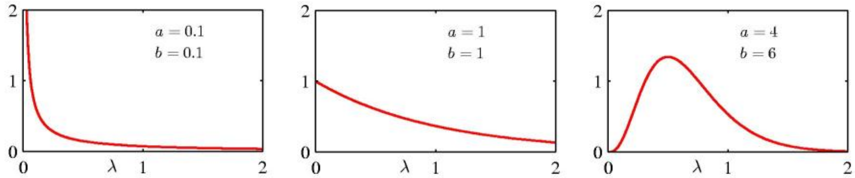
- **Binomial – Beta**
- **Multinomial - Dirichlet**
- **Exponential – Gamma**
- **Poisson – Inverse Gamma**
- **Gaussian - Gaussian (mean) and Wishart (covariance)**

Gamma distribution

- **Gamma distribution**

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

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



Other distributions

Exponential distribution:

- A special case of Gamma for a=1

$$p(x|b) = \left(\frac{1}{b}\right) e^{-\frac{x}{b}}$$

Poisson distribution:

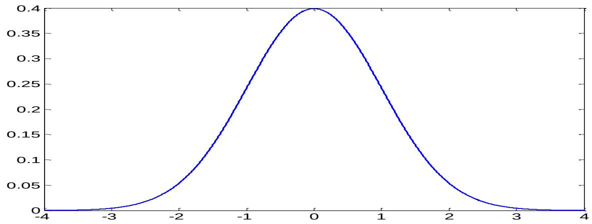
$$p(x|\lambda) = \frac{e^{-\lambda}\lambda^x}{x!} \qquad \text{for} \quad x \in \{0,1,2,\ldots\}$$

Gaussian (normal) distribution

- **Gaussian:** $x \sim N(\mu, \sigma)$
- **Parameters:** μ - mean
  σ - standard deviation
- **Density function:**

$$p(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2\sigma^2}(x-\mu)^2\right]$$

- **Example:**



$N(0,1)$

Parameter estimates

- **Loglikelihood**

$$l(D, \mu, \sigma) = \log \prod_{i=1}^{n} p(x_i \mid \mu, \sigma)$$

- **ML estimates of the mean and variance:**

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})^2$$

  – ML variance estimate is biased

$$E_n(\sigma^2) = E_n\left(\frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})^2\right) = \frac{n-1}{n}\sigma^2 \neq \sigma^2$$

- **Unbiased estimate:**

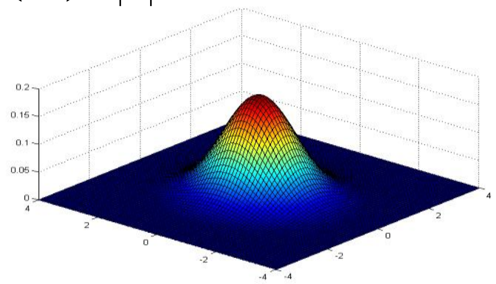
$$\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \hat{\mu})^2$$

Multivariate normal distribution

- **Multivariate normal:** $\mathbf{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- **Parameters:** $\boldsymbol{\mu}$ - mean
  $\boldsymbol{\Sigma}$ - covariance matrix
- **Density function:**

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

- **Example:**



Partitioned Gaussian Distributions

- **Multivariate Gaussian:**

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

  – **what are marginals and conditionals?**

- **Example:**

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

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

Precision matrix

Partitioned Conditionals and Marginals

- **Conditional density:**

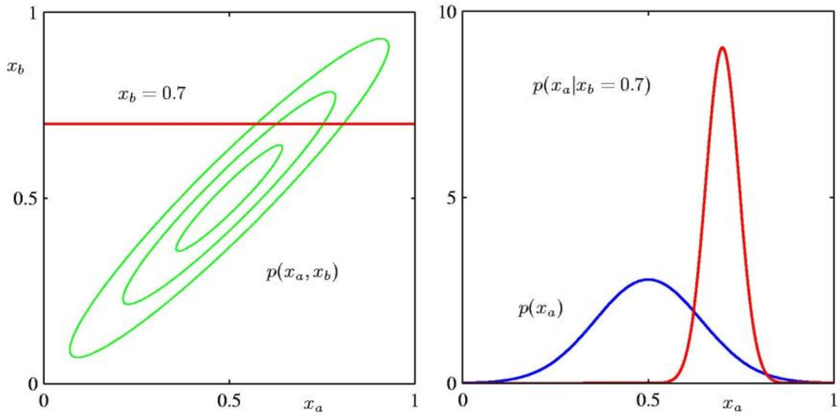
$$p(\mathbf{x}_a|\mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a|\boldsymbol{\mu}_{a|b}, \boldsymbol{\Sigma}_{a|b})$$

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

- **Marginal Density:**

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

Partitioned Conditionals and Marginals



Parameter estimates

- **Loglikelihood**

$$l(D, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \log \prod_{i=1}^{n} p(\mathbf{x}_i \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- **ML estimates of the mean and covariances:**

$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i \qquad \hat{\boldsymbol{\Sigma}} = \frac{1}{n}\sum_{i=1}^{n} (\mathbf{x}_i - \hat{\boldsymbol{\mu}})(\mathbf{x}_i - \hat{\boldsymbol{\mu}})^T$$

  – Covariance estimate is biased

$$E_n(\hat{\boldsymbol{\Sigma}}) = E_n\left(\frac{1}{n}\sum_{i=1}^{n} (\mathbf{x}_i - \hat{\boldsymbol{\mu}})(\mathbf{x}_i - \hat{\boldsymbol{\mu}})^T\right) = \frac{n-1}{n}\boldsymbol{\Sigma} \neq \boldsymbol{\Sigma}$$

- **Unbiased estimate:**

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n-1}\sum_{i=1}^{n} (\mathbf{x}_i - \hat{\boldsymbol{\mu}})(\mathbf{x}_i - \hat{\boldsymbol{\mu}})^T$$