

CS 2750 Machine Learning Lecture 4

Density estimation

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Parametric density estimation

Parametric density estimation:

- A set of random variables $\mathbf{X} = \{X_1, X_2, \dots, X_d\}$
- **A model of the distribution** over variables in X
with **parameters** Θ : $\hat{p}(\mathbf{X} | \Theta)$
- **Data** $D = \{D_1, D_2, \dots, D_n\}$

Objective: find parameters Θ such that $p(\mathbf{X} | \Theta)$ describes data D the best

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Parameter estimation (learning)

- Maximum likelihood (ML)
 $\Theta_{ML} = \arg \max_{\Theta} p(D | \Theta, \xi)$
- Maximum a posteriori probability (MAP)
 $\Theta_{MAP} = \arg \max_{\Theta} p(\Theta | D, \xi)$
- Bayesian parameter estimation
 - use the posterior density
 $p(\Theta | D, \xi)$
- Expected value

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

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Probability of a binary outcome

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 $(1-\theta)$

Assume: we know the probability θ

Probability of an outcome of a coin flip x_i

$$P(x_i | \theta) = \theta^{x_i} (1-\theta)^{(1-x_i)} \quad \text{Bernoulli distribution}$$

- Combines the probability of a head and a tail
- So that x_i is going to pick its correct probability
- Gives θ for $x_i = 1$
- Gives $(1-\theta)$ for $x_i = 0$

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The goodness of fit to the data

Learning: we do not know the value of the parameter θ

Our learning goal:

- Find the parameter θ that fits the data D the best?

One solution to the “best”: Maximize the likelihood

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

Intuition:

- more likely are the data given the model, the better is the fit

Assuming a sequence of n Bernoulli trials:

$$P(D | \theta) = \prod_{i=1}^n \theta^{x_i} (1-\theta)^{(1-x_i)}$$

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Maximum likelihood (ML) estimate.

Likelihood of data:

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

Maximum likelihood estimate

$$\theta_{ML} = \arg \max_{\theta} P(D | \theta, \xi)$$

Optimize log-likelihood (the same as maximizing likelihood)

$$\theta_{ML} = \arg \max_{\theta} \log P(D | \theta, \xi)$$

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

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

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Maximum a posteriori estimate

Maximum a posteriori estimate

- Selects the mode of the **posterior distribution**

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

Likelihood of data \downarrow **prior** \downarrow
$$p(\theta | D, \xi) = \frac{P(D | \theta, \xi) p(\theta | \xi)}{P(D | \xi)}$$
 (via Bayes rule)
$$P(D | \theta, \xi) = \prod_{i=1}^n \theta^{x_i} (1-\theta)^{(1-x_i)} = \theta^{N_1} (1-\theta)^{N_2}$$

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

How to choose the prior probability?

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Prior distribution

Choice of prior: Beta distribution

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

$\Gamma(x)$ - a Gamma function $\Gamma(x) = (x-1)\Gamma(x-1)$
For integer values of x $\Gamma(n) = (n-1)!$

Why to use Beta distribution?

Beta distribution “fits” Bernoulli trials - **conjugate choices**

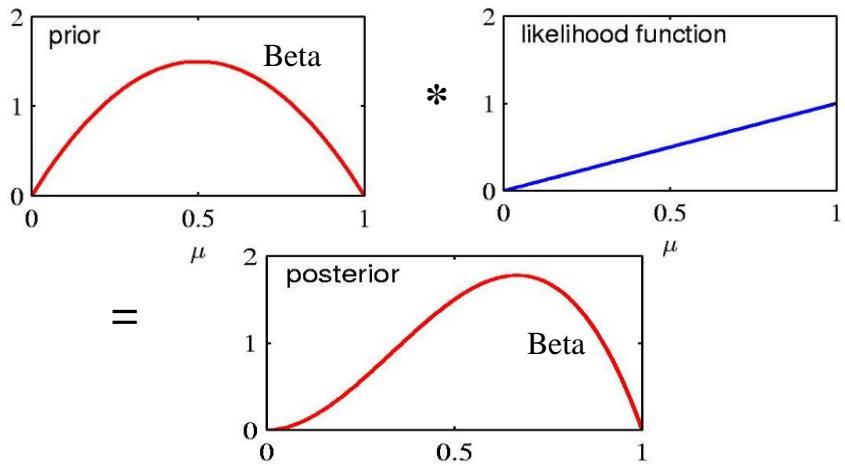
$$P(D | \theta, \xi) = \theta^{N_1} (1-\theta)^{N_2}$$

Posterior distribution is again a Beta distribution

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

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Posterior distribution



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

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Maximum a posterior probability

Maximum a posteriori estimate

- Selects the mode of the **posterior distribution**

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

$$\begin{aligned} p(\theta | D, \xi) &= \frac{P(D | \theta, \xi) \text{Beta}(\theta | \alpha_1, \alpha_2)}{P(D | \xi)} = \text{Beta}(\theta | \alpha_1 + N_1, \alpha_2 + N_2) \\ &= \frac{\Gamma(\alpha_1 + \alpha_2 + N_1 + N_2)}{\Gamma(\alpha_1 + N_1)\Gamma(\alpha_2 + N_2)} \theta^{\alpha_1 - 1} (1 - \theta)^{\alpha_2 - 1} \end{aligned}$$

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

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

Both ML or MAP estimates pick one value of the parameter

- **Assume:** there are two different parameter settings that are close in terms of their probability values. Using only one of them may introduce a strong bias, if we use them, for example, for predictions.

Bayesian parameter estimate

- Remedies the limitation of one choice
- Keeps all possible parameter values
- Where $p(\theta | D, \xi) \approx Beta(\theta | \alpha_1 + N_1, \alpha_2 + N_2)$
- **The posterior can be used to define $p(A | D)$:**

$$p(A | D) = \int_{\Theta} p(A | \Theta) p(\Theta | D, \xi) d\Theta$$

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Binomial distribution

Example problem: a biased coin

Outcomes: two possible values -- head or tail

Data: a set of order-independent outcomes for N trials

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

can be calculated from the trial data !!!

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

Probability of an outcome

$$P(N_1 | N, \theta) = \binom{N}{N_1} \theta^{N_1} (1-\theta)^{N-N_1} \quad \text{Binomial distribution}$$

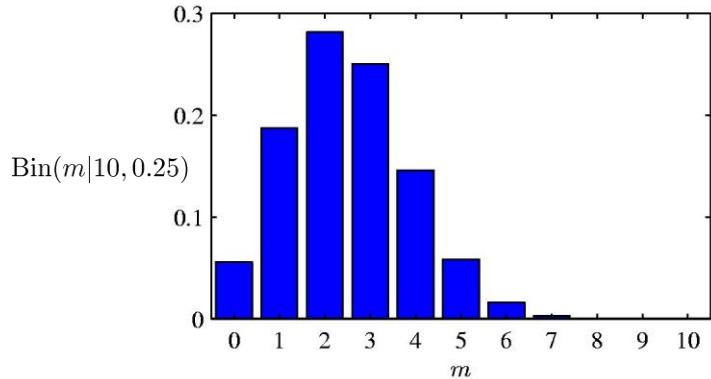
Objective:

We would like to estimate the probability of a **head** $\hat{\theta}$

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Binomial distribution

Binomial distribution:



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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

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

Constant from the point of optimization !!!

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

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

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Posterior density

Posterior density

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

Prior choice

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

Likelihood

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

Posterior

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

MAP estimate

$$\theta_{MAP} = \arg \max_{\theta} p(\theta | D, \xi)$$
$$\theta_{MAP} = \frac{\alpha_1 + N_1 - 1}{\alpha_1 + \alpha_2 + N_1 + N_2 - 2}$$

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Expected value of the parameter

The result is the same as for Bernoulli distribution

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

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

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

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

θ_i - probability of an outcome i

Probability of data (likelihood)

$$P(N_1, N_2, \dots, N_k | \boldsymbol{\theta}, \xi) = \frac{N!}{N_1! N_2! \dots N_k!} \theta_1^{N_1} \theta_2^{N_2} \dots \theta_k^{N_k} \quad \text{Multinomial distribution}$$

ML estimate:

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

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Posterior density and MAP estimate

Choice of the prior: Dirichlet distribution

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

Dirichlet is the **conjugate choice** for multinomial

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

Posterior density

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

MAP estimate:

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

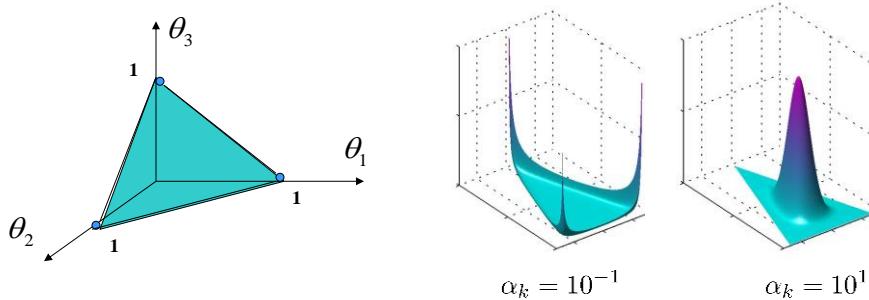
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Dirichlet distribution

Dirichlet distribution:

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

Assume: k=3



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Expected value

The result is analogous to the result for binomial

$$E(\boldsymbol{\theta}) = \int_{\boldsymbol{\theta} \leq 1, \sum \theta_i = 1} \boldsymbol{\theta} \cdot Dir(\boldsymbol{\theta} | \boldsymbol{\eta}) d\boldsymbol{\theta} = \left(\frac{\eta_1}{\eta_1 + \eta_2 + \eta_k}, \dots, \frac{\eta_i}{\eta_1 + \eta_2 + \eta_k}, \dots, \frac{\eta_k}{\eta_1 + \eta_2 + \eta_k} \right)$$

Expectation based parameter estimate

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

Represents the predictive probability of an event $x=i$

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

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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)**

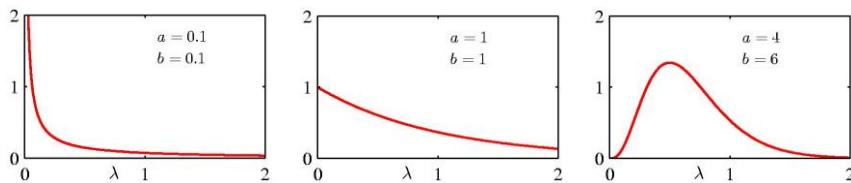
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Gamma distribution

- **Gamma distribution**

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

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



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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:

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

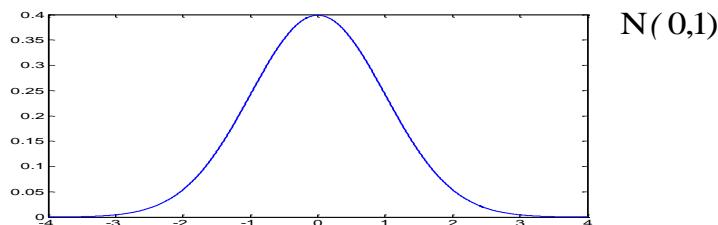
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Gaussian (normal) distribution

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

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

- **Example:**



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Parameter estimates

- **Loglikelihood**

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

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

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

- 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:**

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

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Multivariate normal distribution

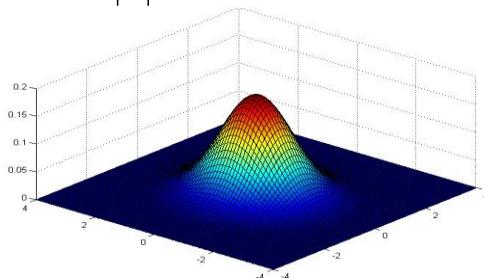
- **Multivariate normal:** $\mathbf{x} \sim N(\boldsymbol{\mu}, \Sigma)$

- **Parameters:** $\boldsymbol{\mu}$ - mean
 Σ - covariance matrix

- **Density function:**

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

- **Example:**



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Partitioned Gaussian Distributions

- Multivariate Gaussian:

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

– what are marginals and conditionals?

- Example:

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

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

Precision matrix

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Partitioned Conditionals and Marginals

- Conditional density:

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

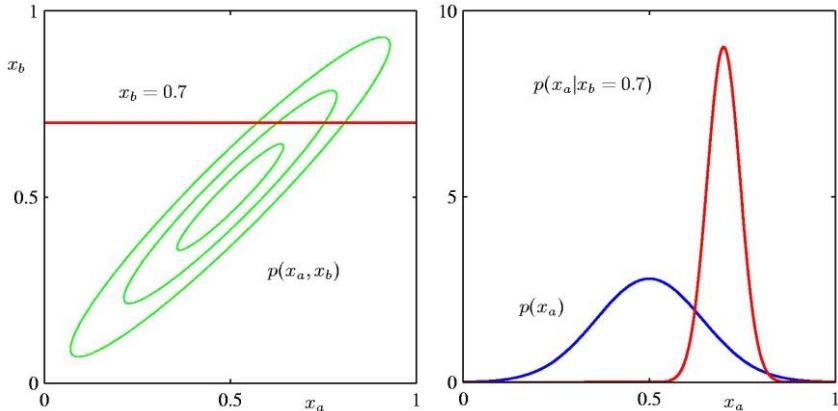
$$\begin{aligned} \boldsymbol{\Sigma}_{a|b} &= \boldsymbol{\Lambda}_{aa}^{-1} = \boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab}\boldsymbol{\Sigma}_{bb}^{-1}\boldsymbol{\Sigma}_{ba} \\ \boldsymbol{\mu}_{a|b} &= \boldsymbol{\Sigma}_{a|b} \{ \boldsymbol{\Lambda}_{aa}\boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{ab}(\mathbf{x}_b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

- Marginal Density:

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

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Partitioned Conditionals and Marginals



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Parameter estimates

- **Loglikelihood**
$$l(D, \mu, \Sigma) = \log \prod_{i=1}^n p(\mathbf{x}_i | \mu, \Sigma)$$
- **ML estimates of the mean and covariances:**

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

- Covariance estimate is biased

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

- **Unbiased estimate:**

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

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Posterior of a multivariate normal

- Assume a prior on the mean μ that is normally distributed:

$$p(\mu) \approx N(\mu_p, \Sigma_p)$$

- Then the posterior of μ is normally distributed

$$\begin{aligned} p(\mu | D) &\approx \left(\prod_{i=1}^n \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp \left[-\frac{1}{2} (\mathbf{x}_i - \mu)^T \Sigma^{-1} (\mathbf{x}_i - \mu) \right] \right) \\ &\quad * \frac{1}{(2\pi)^{d/2} |\Sigma_p|^{1/2}} \exp \left[-\frac{1}{2} (\mu - \mu_p)^T \Sigma_p^{-1} (\mu - \mu_p) \right] \\ &= \frac{1}{(2\pi)^{d/2} |\Sigma_n|^{1/2}} \exp \left[-\frac{1}{2} (\mu - \mu_n)^T \Sigma_n^{-1} (\mu - \mu_n) \right] \end{aligned}$$

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Posterior of a multivariate normal

- Then the posterior of μ is normally distributed

$$p(\mu | D) = \frac{1}{(2\pi)^{d/2} |\Sigma_n|^{1/2}} \exp \left[-\frac{1}{2} (\mu - \mu_n)^T \Sigma_n^{-1} (\mu - \mu_n) \right]$$

$$\Sigma_n^{-1} = n\Sigma^{-1} + \Sigma_p^{-1}$$

$$\mu_n = \Sigma_p \left(\Sigma_p + \frac{1}{n} \Sigma \right)^{-1} \left(\frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \right) + \frac{1}{n} \Sigma \left(\Sigma_p + \frac{1}{n} \Sigma \right)^{-1} \mu_p$$

$$\Sigma_n = \Sigma_p \left(\Sigma_p + \frac{1}{n} \Sigma \right)^{-1} \frac{1}{n} \Sigma$$

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Sequential Bayesian parameter estimation

- Sequential Bayesian approach

- Under the iid the estimates of the posterior can be computed incrementally for a sequence of data points

$$p(\Theta | D, \xi) = \frac{p(D | \Theta, \xi) p(\Theta | \xi)}{\int_{\Theta} p(D | \Theta, \xi) p(\Theta | \xi) d\Theta}$$

- If we use a conjugate prior we get back the same posterior
- Assume we split the data D in the last element \mathbf{x} and the rest

$$p(D | \Theta) = P(x | \Theta) P(D_{n-1} | \Theta)$$

- Then:

$$p(\Theta | D, \xi) = \frac{P(x | \Theta) \overbrace{P(D_{n-1} | \Theta) p(\Theta | \xi)}^{\text{A "new" prior}}}{\int_{\Theta} P(x | \Theta) P(D_{n-1} | \Theta) p(\Theta | \xi) d\Theta}$$

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