CS 2750 Machine Learning
Lecture 5

Density estimation II.

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Outline

Outline:

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

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

Standard (iid) assumptions: Samples

- **are independent of each other**
- **come from the same (identical) distribution (fixed $p(\mathbf{X})$)**

Parametric density estimation

Parametric density estimation:

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

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

Parameter estimation (learning)

- **Maximum likelihood (ML)**

  maximize $p(D \mid \Theta, \xi)$

  – yields: one set of parameters Θ_{ML}

  – the target distribution is approximated as:

  $$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \mathbf{\Theta}_{ML})$$

- **Bayesian parameter estimation**

  – uses the posterior distribution over possible parameters

  $$p(\Theta \mid D, \xi) = \frac{p(D \mid \Theta, \xi)\, p(\Theta \mid \xi)}{p(D \mid \xi)}$$

  – Yields: all possible settings of Θ (and their "weights")

  – The target distribution is approximated as:

  $$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid D) = \int_{\mathbf{\Theta}} p(X \mid \mathbf{\Theta})\, p(\mathbf{\Theta} \mid D, \xi)\, d\mathbf{\Theta}$$

Parameter estimation.

Other possible criteria:

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

  maximize $p(\mathbf{\Theta} \mid D, \xi)$ (mode of the posterior)

  – Yields: one set of parameters $\mathbf{\Theta}_{MAP}$

  – Approximation:

  $$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \mathbf{\Theta}_{MAP})$$

- **Expected value of the parameter**

  $\hat{\mathbf{\Theta}} = E(\mathbf{\Theta})$ (mean of the posterior)

  – Expectation taken with regard to posterior $p(\mathbf{\Theta} \mid D, \xi)$

  – Yields: one set of parameters

  – Approximation:

  $$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \hat{\mathbf{\Theta}})$$

Parameter estimation. Coin example.

Coin example: we have a coin that can be biased

Outcomes: two possible values -- head or tail

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 $(1-\theta)$

Objective:

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

Probability of an 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 $(1-\theta)$

Probability of an outcome of a coin flip

$$P(x_i \mid \theta) = \theta^{x_i}(1-\theta)^{(1-x_i)}$$ ⟵ **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 $x_i = 0$

Probability of a sequence of outcomes.

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: a sequence of coin flips D = H H T H T H
encoded as D= 110101

What is the probability of observing a data sequence **D:**

$$P(D \mid \theta) = \theta\theta(1-\theta)\theta(1-\theta)\theta$$

$$P(D \mid \theta) = \prod_{i=1}^{6} \theta^{x_i}(1-\theta)^{(1-x_i)}$$

Assumption of sample independence

Maximum likelihood (ML) estimate.

Likelihood of data:

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

Maximum likelihood estimate

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

Optimize log-likelihood (the same as maximizing likelihood)

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

$$\sum_{i=1}^{n} x_i \log\theta + (1-x_i)\log(1-\theta) = \log\theta \underbrace{\sum_{i=1}^{n} x_i}_{N_1} + \log(1-\theta) \underbrace{\sum_{i=1}^{n} (1-x_i)}_{N_2}$$

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

Maximum likelihood (ML) estimate.

Optimize log-likelihood

$$l(D,\theta) = N_1 \log\theta + N_2 \log(1-\theta)$$

Set derivative to zero

$$\frac{\partial l(D,\theta)}{\partial\theta} = \frac{N_1}{\theta} - \frac{N_2}{(1-\theta)} = 0$$

Solving $$\theta = \frac{N_1}{N_1 + N_2}$$

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

Maximum likelihood (ML) estimate.

Optimize log-likelihood

$$l(D,\theta) = N_1 \log\theta + N_2 \log(1-\theta)$$

Set derivative to zero

$$\frac{\partial l(D,\theta)}{\partial\theta} = \frac{N_1}{\theta} - \frac{N_2}{(1-\theta)} = 0$$

Solving $$\theta = \frac{N_1}{N_1 + N_2}$$

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

Maximum likelihood estimate. Example

- **Assume** the unknown and possibly biased coin
- Probability of the head is θ
- **Data:**

  H H T T H H T H T H T T T H T H H H H T H H H H T
  - **Heads:** 15
  - **Tails:** 10

What is the ML estimate of the probability of a head and a tail?

Maximum likelihood estimate. Example

- Assume the unknown and possibly biased coin
- Probability of the head is θ
- **Data:**

  H H T T H H T H T H T T T H T H H H H T H H H H T
  - **Heads:** 15
  - **Tails:** 10

What is the ML estimate of the probability of head and tail ?

Head: $$\theta_{ML} = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2} = \frac{15}{25} = 0.6$$

Tail: $$(1 - \theta_{ML}) = \frac{N_2}{N} = \frac{N_2}{N_1 + N_2} = \frac{10}{25} = 0.4$$

Posterior distribution

Bayesian and MAP approaches rely on the posterior density

$$p(\theta \mid D, \xi)$$

Can be calculated as:

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

How to choose the prior probability?

Prior distribution

Choice of prior: Beta distribution

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

$\Gamma(x)$ - A Gamma function

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

Why to use Beta distribution?

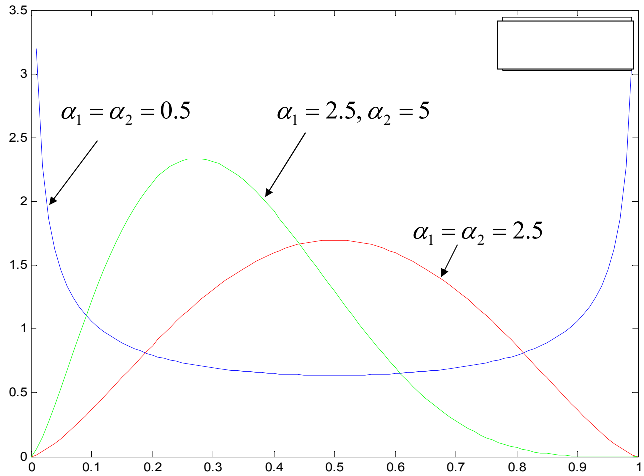
Beta distribution "**fits**" Bernoulli trials - **conjugate choice**

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

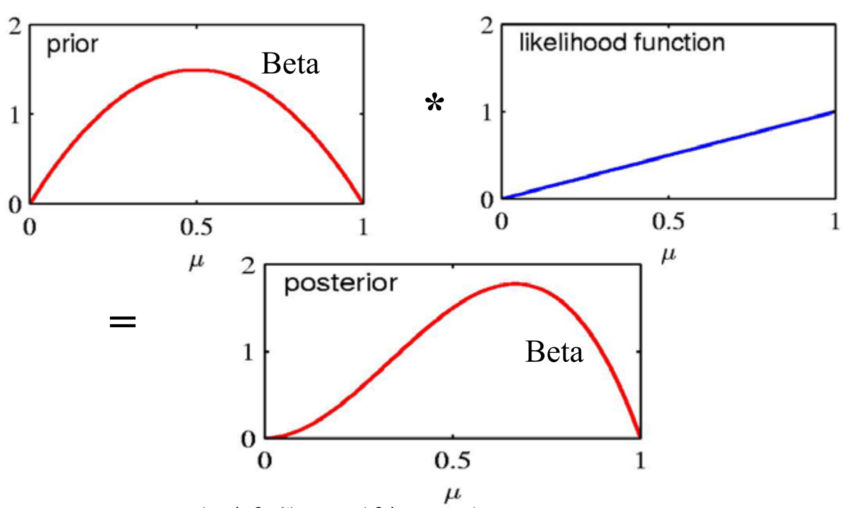
Posterior distribution is again a Beta distribution

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

Beta distribution



Posterior distribution



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

Bayesian framework

The ML estimate picks 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 $p(\theta \mid D, \xi) \approx Beta(\theta \mid \alpha_1 + N_1, \alpha_2 + N_2)$

- **The posterior can be used to define** $p(A \mid D)$**:**

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

Bayesian framework

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

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

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

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

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

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

Expected value of the parameter

How to obtain the expected value?

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

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

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

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

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:

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

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

MAP estimate example

- Assume the unknown and possibly biased coin
- Probability of the head is θ
- **Data:**

  H H T T H H T H T H T T T H T H H H H T H H H H T
  - **Heads:** 15
  - **Tails:** 10
- Assume $p(\theta \mid \xi) = Beta(\theta \mid 5,5)$

What is the MAP estimate?

MAP estimate example

- Assume the unknown and possibly biased coin
- Probability of the head is θ
- **Data:**

  H H T T H H T H T H T T T H T H H H H T H H H H T
  - **Heads:** 15
  - **Tails:** 10
- Assume $p(\theta \mid \xi) = Beta(\theta \mid 5,5)$

What is the MAP estimate ?

$$\theta_{MAP} = \frac{N_1 + \alpha_1 - 1}{N - 2} = \frac{N_1 + \alpha_1 - 1}{N_1 + N_2 + \alpha_1 + \alpha_2 - 2} = \frac{19}{33}$$

MAP estimate example

- Note that the prior and data fit (data likelihood) are combined
- **The MAP can be biased with large prior counts**
- **It is hard to overturn it with a smaller sample size**
- **Data:**

  H H T T H H T H T H T T T H T H H H H T H H H H T
  - **Heads:** 15
  - **Tails:** 10
- Assume

$$p(\theta \mid \xi) = Beta(\theta \mid 5,5) \qquad \theta_{MAP} = \frac{19}{33}$$

$$p(\theta \mid \xi) = Beta(\theta \mid 5,20) \qquad \theta_{MAP} = \frac{19}{48}$$