CS 1675 Introduction to Machine Learning
Lecture 6

Density estimation I

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Homework assignments

Homework assignment 1 was due today

Homework assignment 2:

- **Due next week on Thursday**
- Two parts: **Report + Programs**

Submission:

- via Courseweb
- Report (submit in pdf)
- Programs (submit using the zip or tar archive)
- Deadline 9:30am (prior to the lecture)

Rules:

- Strict deadline
- No collaboration on the programming and the report part

Density estimation

Density estimation: is an unsupervised learning problem

- **Goal:** Learn a model that represent the relations among attributes in the data

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

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

Attributes:

- modeled by random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ with
  - **Continuous or discrete valued variables**

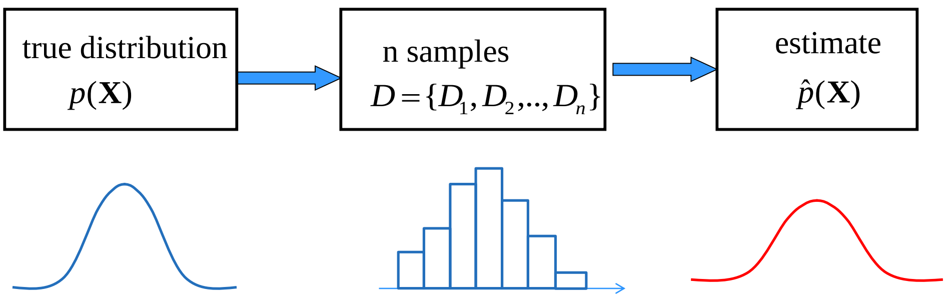
Density estimation: learn an underlying probability distribution model : $p(\mathbf{X}) = p(X_1, X_2, \ldots, X_d)$ **from D**

Density estimation

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

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

Objective: estimate the model of the underlying probability distribution over variables $\mathbf{X}$, $p(\mathbf{X})$, using examples in D

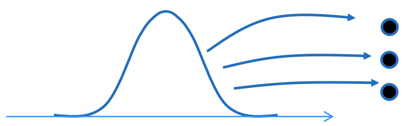


Density estimation: iid assumptions

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 $p(\mathbf{X})$)**



Independently drawn instances from the same fixed distribution

Density estimation

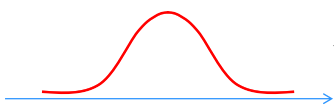
Types of density estimation:

(1) Parametric

- the distribution is modeled using a set of parameters Θ

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

- **Estimation:** find parameters Θ fitting the data D
- **Example:** estimate the mean and covariance of a normal distribution



$$\hat{p}(x) = N(x \mid \mu, \sigma)$$

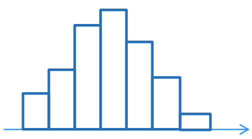
Density estimation

Types of density estimation:

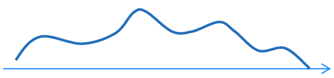
(2) Non-parametric

- The model of the distribution utilizes all examples in *D*
- As if all examples were parameters of the distribution
- $\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid D)$
- **Examples:**

histogram



Kernel density estimation



Learning via parameter estimation

In this lecture we consider **parametric density estimation**

Basic settings:

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

Question:

- How to measure the **goodness of fit** or alternatively **the error**?

ML Parameter estimation

Model $\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \mathbf{\Theta})$ **Data** $D = \{D_1, D_2, .., D_n\}$

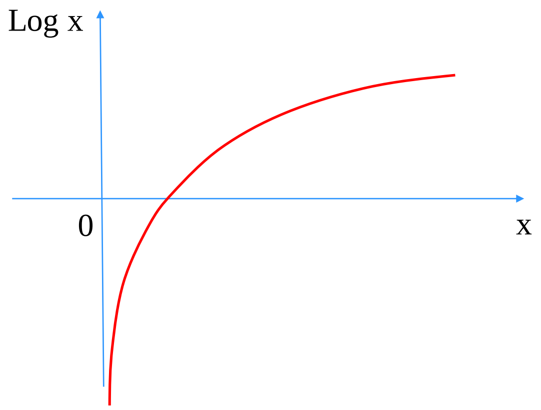
- **Maximum likelihood (ML)** $\max_{\Theta} p(D \mid \Theta, \xi)$
  - Find Θ that maximizes likelihood $p(D \mid \Theta, \xi)$

$$P(D \mid \Theta, \xi) = P(D_1, D_2, .., D_n \mid \Theta, \xi)$$
$$= P(D_1 \mid \Theta, \xi) P(D_2 \mid \Theta, \xi) \ldots P(D_n \mid \Theta, \xi)$$
$$= \prod_{i=1}^{n} P(D_i \mid \Theta, \xi)$$

Independent examples

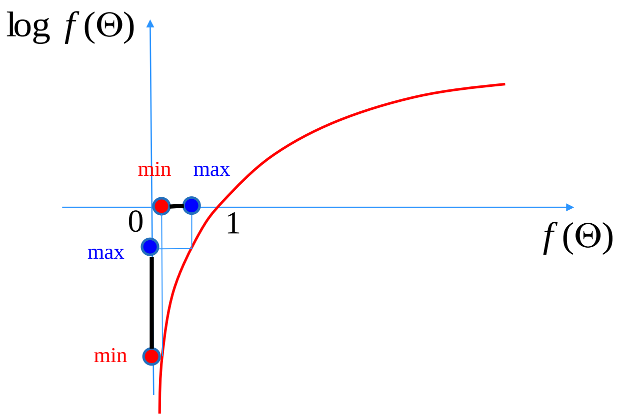
$$\Theta_{ML} = \arg\max_{\Theta} p(D \mid \Theta, \xi)$$

Logarithm function



Properties of the log function: ?

Logarithm



$$\Theta^* = \arg\max_\Theta f(\Theta) = \arg\max_\Theta \log f(\Theta)$$

ML Parameter estimation

Model $\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \boldsymbol{\Theta})$ **Data** $D = \{D_1, D_2, .., D_n\}$

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

- **Maximum likelihood (ML)**
  - Find Θ that maximizes likelihood $p(D \mid \Theta, \xi)$

$$P(D \mid \Theta, \xi) = P(D_1, D_2, .., D_n \mid \Theta, \xi)$$
$$= P(D_1 \mid \Theta, \xi) P(D_2 \mid \Theta, \xi) \dots P(D_n \mid \Theta, \xi)$$
$$= \prod_{i=1}^{n} P(D_i \mid \Theta, \xi)$$

Independent examples

log-likelihood $\log p(D \mid \Theta, \xi) = \sum_{i=1}^{n} \log P(D_i \mid \Theta, \xi)$

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

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

Parameter estimation. 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 would be your estimate of the probability of a head ?

$$\tilde{\theta} = ?$$

Parameter estimation. 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 would be your choice of the probability of a head ?

Solution: use frequencies of occurrences to do the estimate

$$\tilde{\theta} = \frac{15}{25} = 0.6$$

This is **the maximum likelihood estimate** of the parameter θ

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 $(1-\theta)$

Assume: we know the probability θ

Probability of an outcome of a coin flip x_i

$$P(x_i \mid \theta) = \theta^{x_i}(1-\theta)^{(1-x_i)}$$ ← **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 independent coin flips

D = H H T H T H (encoded as D= 110101)

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

$$P(D \mid \theta) = ?$$

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:**

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

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:**

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

likelihood of the data

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:**

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

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

Can be rewritten using the Bernoulli distribution:

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?

The solution to the "best": Maximize the likelihood

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

Intuition:

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

Note: Instead of an error function that measures how bad the data fit the model we have a measure that tells us how well the data fit :

$$Error(D, \theta) = -P(D \mid \theta)$$

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)

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

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)

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

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

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 $\theta = \dfrac{N_1}{N_1 + N_2}$

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

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