CS 2750 Machine Learning
Lecture 5

Density estimation

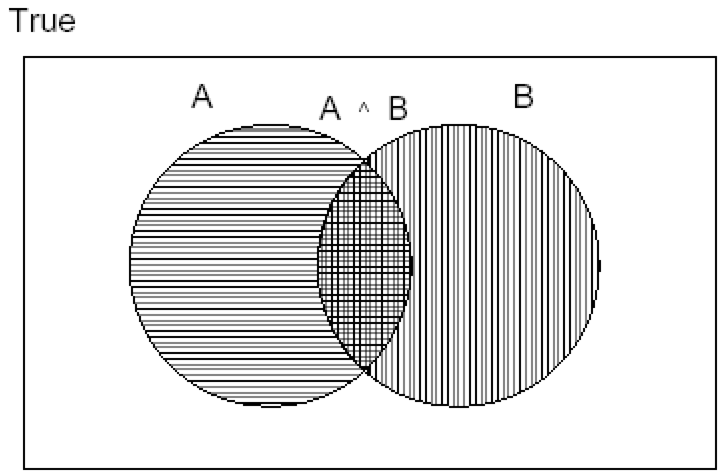
Milos Hauskrecht
milos@cs.pitt.edu
5329 Sennott Square

Probability

- Well-defined theory for representing and manipulating uncertainty
- **Axioms of probability:**

  Let A and B be two events. Then:

  1. $0 \leq P(A) \leq 1$
  2. $P(True) = 1$ and $P(False) = 0$
  3. $P(A \vee B) = P(A) + P(B) - P(A \wedge B)$



Probability

- **Let A be an event, and ¬A its complement.**
  - **Then**

$$P(A) + P(\neg A) = 1$$

$$P(A \wedge \neg A) = 0$$

$$P(False) = 0$$

$$P(A \vee \neg A) = 1$$

$$P(True) = 1$$

Joint probability

Joint probability:

- **Let A and B be two events.** The probability of an event A, B occurring jointly

$$P(A \wedge B) = P(A, B)$$

We can add more events, say, A,B,C

$$P(A \wedge B \wedge C) = P(A, B, C)$$

Independence

Independence :

- Let A, B be two events. The events are independent if:

$$P(A,B) = P(A)P(B)$$

Conditional probability

Conditional probability :

- Let A, B be two events. The conditional probability of A given B is defined as:

$$P(A \mid B) = \frac{P(A,B)}{P(B)}$$

Product rule:

- A rewrite of the conditional probability

$$P(A,B) = P(A \mid B)P(B)$$

Bayes theorem

Bayes theorem

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

Why?

$$P(A \mid B) = \frac{P(A,B)}{P(B)} \qquad P(A,B) = P(B \mid A)P(A)$$

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

Random variable

A function that maps observed quantities to real valued outcomes

Binary random variables:

Mapped to **0,1**

Example: Tail mapped to 0, Head mapped to 1

Note: Only one value for each outcome: either 0 or 1

$P(x=0)$ **probability of tail**

$P(x=1)$ **probability of head**

- **Probability distribution:**

$P(\mathrm{x}) =$

0.45
0.55

Assigns a probability to each possible outcome

Random variable

Discrete

- x=0,1 based on tail/head coin toss
- x=1,2,3,4,5,6 based on the roll of a dice
- p(x) – assigns a probability to each possible outcomes

- **Continuous**
  - x height of a person
  - p(x) defined in terms of the probability density function

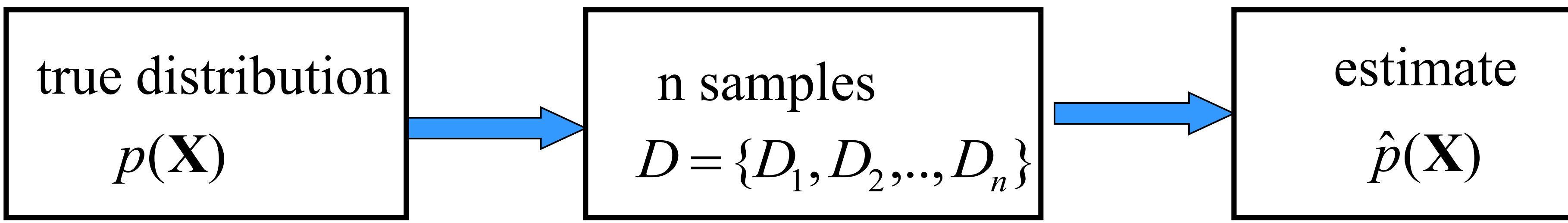
$$\int p(x)dx = 1$$

Density estimation

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

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

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



Standard (iid) assumptions: Samples

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

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 $\boldsymbol{X}$ with parameters Θ : $\hat{p}(\mathbf{X} \mid \Theta)$
- **Data** $D = \{D_1, D_2, .., D_n\}$

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

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

$$p(D \mid \Theta, \xi) = P(D_1, D_2, .., D_n \mid \Theta, \xi)$$

$$= P(D_1 \mid \Theta, \xi) P(D_2 \mid \Theta, \xi) \ldots P(D_n \mid \Theta, \xi)$$

$$= \prod_{i=1}^{n} P(D_i \mid \Theta, \xi)$$

Independent examples

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

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

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 coin flips D = H H T H T H

encoded as D= 110101

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

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

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

Maximum a posteriori estimate

Maximum a posteriori estimate

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

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

Likelihood of data → $P(D \mid \theta, \xi)$; **prior** → $p(\theta \mid \xi)$

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

Normalizing factor → $P(D \mid \xi)$

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

$p(\theta \mid \xi)$ - 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 $\Gamma(x) = (x-1)\Gamma(x-1)$

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

Why to use Beta distribution?

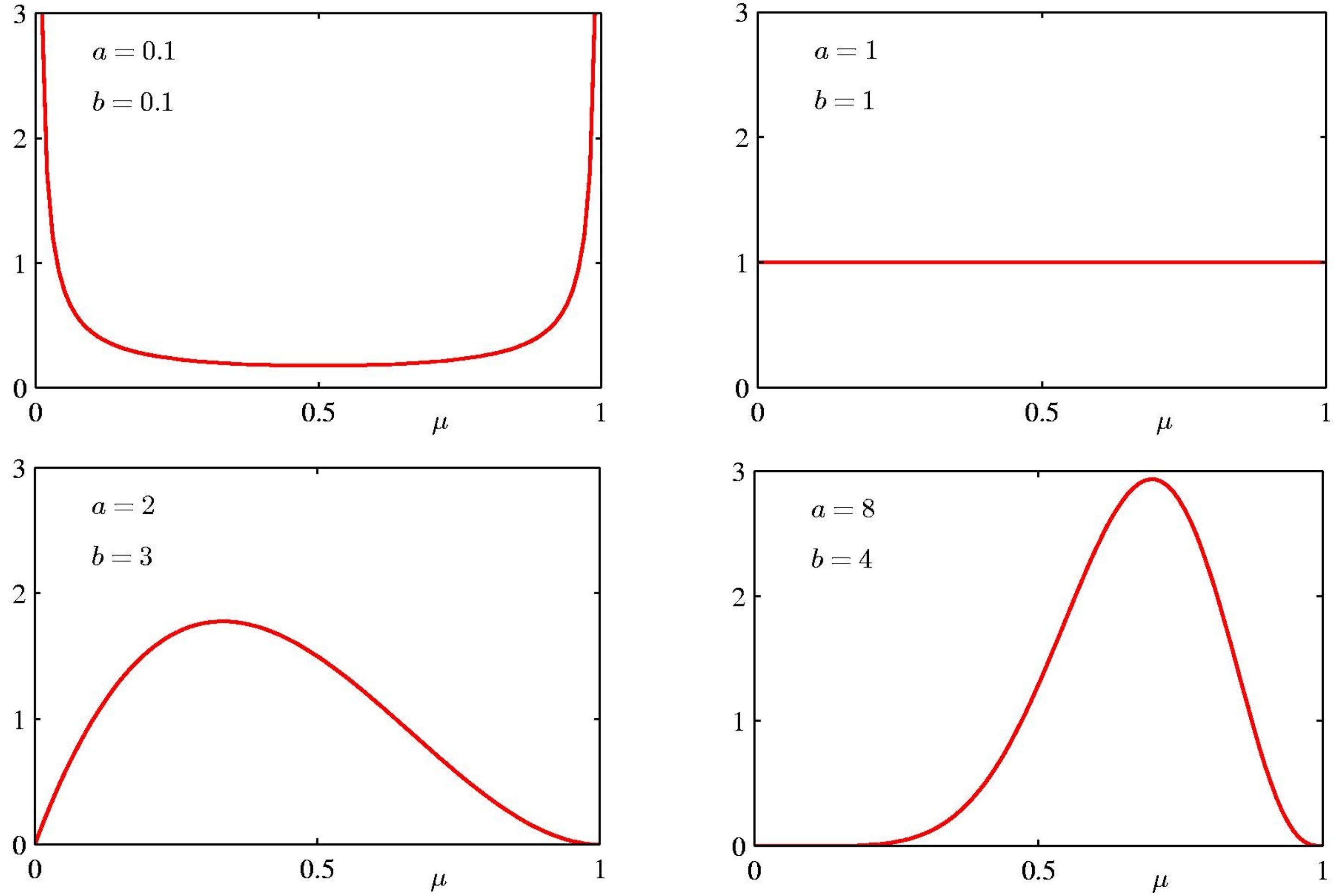
Beta distribution "**fits**" Bernoulli trials - **conjugate choices**

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

Posterior distribution is again a Beta distribution

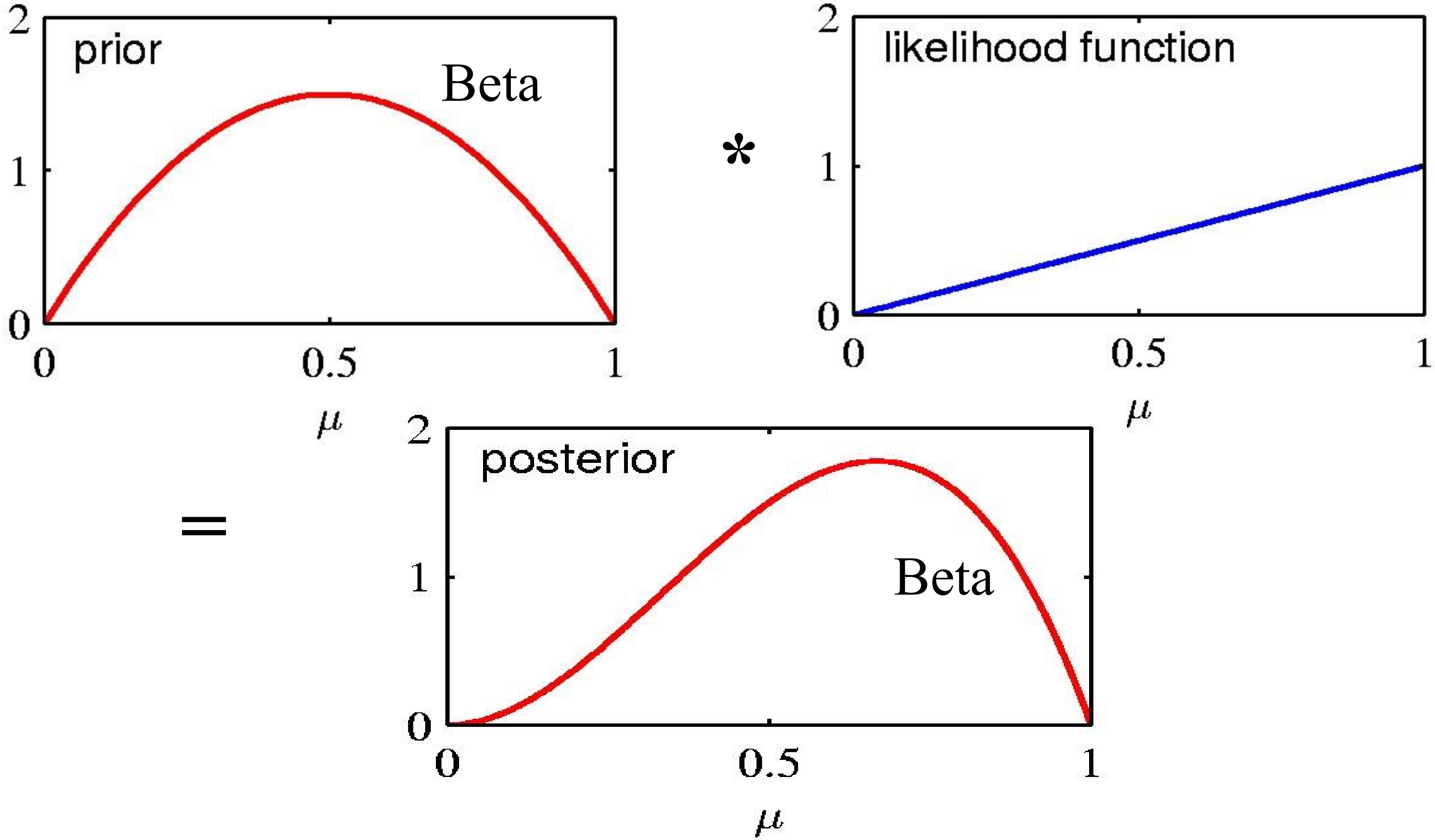
$$p(\theta \mid D, \xi) = \frac{P(D \mid \theta, \xi) Beta(\theta \mid \alpha_1, \alpha_2)}{P(D \mid \xi)} = Beta(\theta \mid \alpha_1 + N_1, \alpha_2 + N_2)$$

Beta distribution



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

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**

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

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

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

MAP Solution:

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

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

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

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