CS 2750 Machine Learning
Lecture 3

Density estimation

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**

Density estimation

Density estimation: is an unsupervised learning

- Learn relations among attributes in the data

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

$D_i = \mathbf{x}_i$ 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 attempts to learn the underlying probability distribution: $p(\mathbf{X}) = p(X_1, X_2, \ldots, X_d)$

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

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

Density estimation

Types of density estimation:

Parametric

- the distribution is modeled using a set of parameters Θ

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

- **Example:** mean and covariances of a multivariate normal
- **Estimation:** find parameters Θ describing data D

Non-parametric

- The model of the distribution utilizes all examples in D
- As if all examples were parameters of the distribution
- **Examples:** Nearest-neighbor

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

Parameter estimation

- **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

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?

One 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 :

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

Example: Bernoulli distribution

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** $\hat{\theta}$

Probability of an outcome x_i

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

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

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

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 **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 $\Gamma(x) = (x-1)\Gamma(x-1)$

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

Why to use Beta distribution?

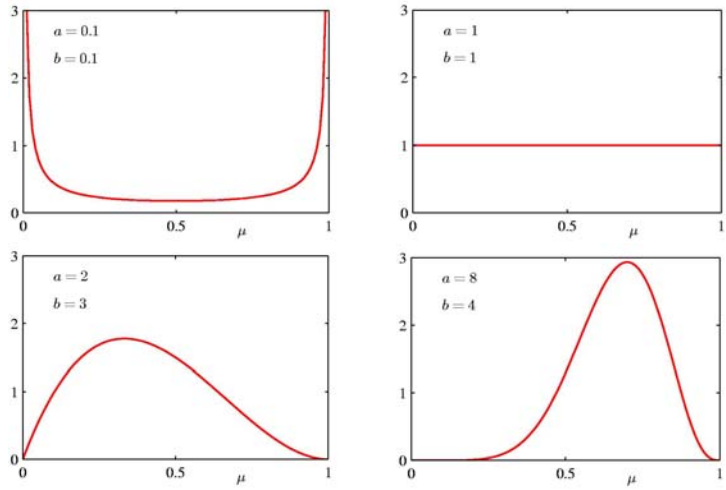
Beta distribution "**fits**" Bernoulli trials - **conjugate choices**

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

Posterior distribution is again a Beta distribution

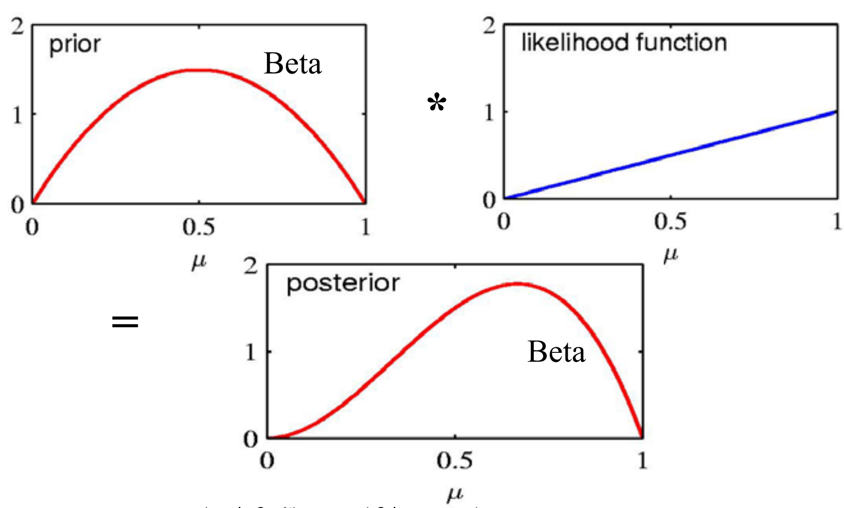
$$p(\theta \mid D, \xi) = \frac{P(D \mid \theta, \xi) Beta(\theta \mid \alpha_1, \alpha_2)}{P(D \mid \xi)} = Beta(\theta \mid \alpha_1 + N_1, \alpha_2 + N_2)$$

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

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

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

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

- **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

- **Predictive 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:

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

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

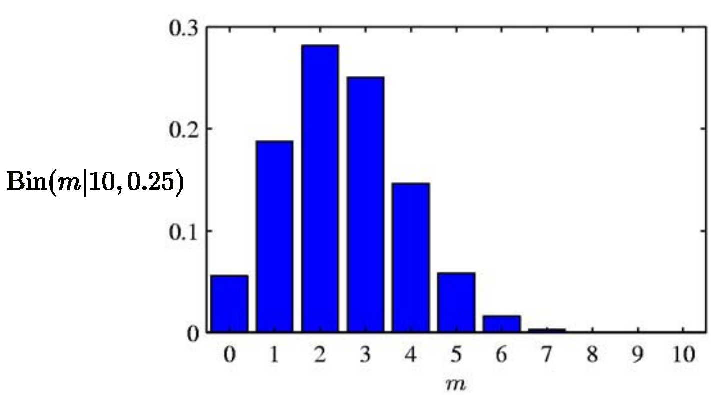
$$P(N_1 \mid N, \theta) = \binom{N}{N_1} \theta^{N_1} (1-\theta)^{N-N_1}$$ **Binomial distribution**

Objective:

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

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 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

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