

# Probabilistic Machine Learning:

## 4. Beta-binomial model

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HR EXCELLENCE IN RESEARCH



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The presentation was inspired by Chapter 3 of Kevin Murphy book "Machine Learning A Probabilistic Perspective", 2012, MIT.  
Appropriate agreements to propagate his ideas has been acquired.



# Beta-binomial model

## "Number game"

- ▶ inferring a distribution over a discrete variable drawn from a finite hypothesis space
- ▶ given a series of discrete observations
- ▶ computations particularly simple: sum, multiplication and division

What if, like in many applications, the unknown parameters are continuous?

- ▶ the hypothesis space is subset of  $\mathbb{R}^K$ , where  $K$  is the number of parameters
- ▶ replace sums with integrals

# Coin toss example

The problem:

- ▶ inferring the probability that a coin shows up heads
- ▶ given a series of observed coin tosses

Might seem trivial, but

- ▶ this model forms the basis of many of the methods
- ▶ historically important, since it was the example which was analyzed in Bayes' original paper of 1763

# Recipe of specifying the model

Define

- ▶ likelihood
- ▶ prior

and derive

- ▶ posterior
- ▶ posterior predictive

# The problem

Let's consider a single binary random variable:

- ▶  $X_i \sim \text{Bern}(\theta)$
- ▶  $X_i = 1$  represents "heads",  $X_i = 0$  represents "tails"
- ▶  $\theta \in [0, 1]$  is the parameter (probability of heads)
- ▶  $p(X_i = 1|\theta) = \theta$ ,  $p(X_i = 0|\theta) = 1 - \theta$

Probability distribution over  $X$

- ▶  $\text{Bern}(X|\theta) = \theta^{N_1}(1 - \theta)^{N_0}$
- ▶ if the data are iid, the likelihood has the same shape
- ▶ there are  $N_1 = \sum_{i=1}^N \mathbb{1}(X_i = 1)$  heads and  $N_0 = \sum_{i=1}^N \mathbb{1}(X_i = 0)$  tails
- ▶  $N_0$  and  $N_1$  are called **sufficient statistics** (this is **all** we need to know about data to infer  $\theta$ )

# Bernoulli distribution recap

$$\text{Bern}(X|\theta) = \theta^{N_1}(1 - \theta)^{N_0}$$

$$N = N_0 + N_1$$

Mean:

$$\triangleright \mathbb{E}(X) = \theta$$

Variance:

$$\triangleright \text{var}(X) = \theta(1 - \theta)$$

# The problem: continuing

Let's demistify the exemplary problem more:

- ▶ suppose the data consists of the count of the number of heads  $N_1$  observed in a fixed number  $N = N_1 + N_0$  of trials
- ▶  $N_1 \sim \text{Bin}(N, \theta)$
- ▶ binomial pmf:  $\text{Bin}(k|n, \theta) = \binom{n}{k} \theta^k (1 - \theta)^{n-k}$
- ▶ term  $\binom{n}{k}$  is constant independent of  $\theta$ , thus the **binomial sampling model is the same as the likelihood for the Bernoulli model**



# Likelihood: in general

## Likelihood:

- ▶ a tool for summarizing the data's evidence about unknown parameter in the model
- ▶ as below: considered as a function of  $\theta$
- ▶ or: is the likelihood function (of  $\theta$ )
- ▶ the probability of "the value  $x$  of  $X$  for the parameter value  $\theta$ "

### Discrete probability distribution

$$\mathcal{L}(x \mid \theta) = p_{\theta}(x) = P_{\theta}(X = x)$$

### Continuous probability distribution

$$\mathcal{L}(x \mid \theta) = f_{\theta}(x)$$

# Likelihood of our problem

$$\mathcal{L}(\mathcal{D} \mid \theta) = \theta^{N_1}(1 - \theta)^{N_0}$$

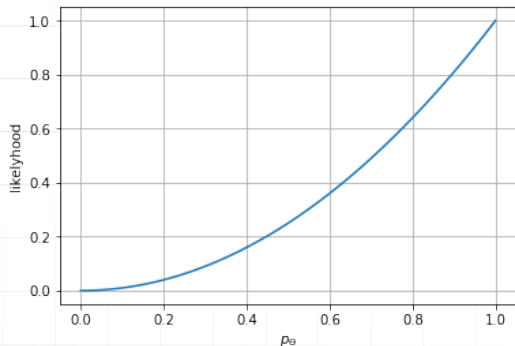


Figure: Likelihood  $\mathcal{D}=\{HH\}$

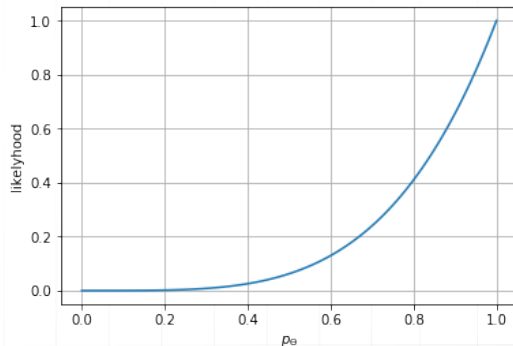


Figure: Likelihood  $\mathcal{D}=\{HHHH\}$

# What about prior?

- ▶ need of prior with support over  $[0,1]$  interval
- ▶ easier, if it would have the same form as likelihood, for some prior parameters  $\gamma_1$  and  $\gamma_2$ :

$$p(\theta) \propto \theta^{\gamma_1} (1 - \theta)^{\gamma_2}$$

- ▶ easy evaluation of posterior: adding exponents

$$\mathcal{L}(\theta | \mathcal{D})p(\theta) = \theta^{N_1} (1 - \theta)^{N_0} \theta^{\gamma_1} (1 - \theta)^{\gamma_2} = \theta^{N_1 + \gamma_1} (1 - \theta)^{N_0 + \gamma_2}$$

## Conjugate priors

When the prior and the posterior have the same form, we say that the prior is a conjugate prior for the corresponding likelihood.

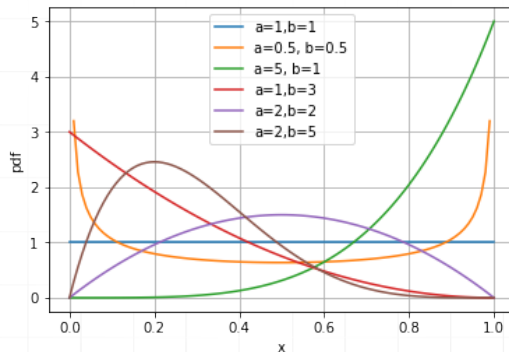
# Conjugate priors

Likelihood	Model parameters	Conjugate prior distribution	Prior hyperparameters	Posterior hyperparameters	Interpretation of hyperparameters <sup>[note 1]</sup>	Posterior predictive <sup>[note 2]</sup>
Bernoulli	$p$ (probability)	Beta	$\alpha, \beta$	$\alpha + \sum_{i=1}^n x_i, \beta + n - \sum_{i=1}^n x_i$	$\alpha - 1$ successes, $\beta - 1$ failures <sup>[note 1]</sup>	$p(\tilde{x} = 1) = \frac{\alpha'}{\alpha' + \beta'}$
Binomial	$p$ (probability)	Beta	$\alpha, \beta$	$\alpha + \sum_{i=1}^n x_i, \beta + \sum_{i=1}^n N_i - \sum_{i=1}^n x_i$	$\alpha - 1$ successes, $\beta - 1$ failures <sup>[note 1]</sup>	BetaBin( $\tilde{x} \alpha', \beta'$ ) (beta-binomial)
Negative binomial with known failure number, $r$	$p$ (probability)	Beta	$\alpha, \beta$	$\alpha + \sum_{i=1}^n x_i, \beta + rn$	$\alpha - 1$ total successes, $\beta - 1$ failures <sup>[note 1]</sup> (i.e., $\frac{\beta - 1}{r}$ experiments, assuming $r$ stays fixed)	
Poisson	$\lambda$ (rate)	Gamma	$k, \theta$	$k + \sum_{i=1}^n x_i, \frac{\theta}{n\theta + 1}$	$k$ total occurrences in $\frac{1}{\theta}$ intervals	NB( $\tilde{x} k', \theta'$ ) (negative binomial)
			$\alpha, \beta$ <sup>[note 3]</sup>	$\alpha + \sum_{i=1}^n x_i, \beta + n$	$\alpha$ total occurrences in $\beta$ intervals	NB( $\tilde{x} \alpha', \frac{1}{1 + \beta'}$ ) (negative binomial)
Categorical	$\mathbf{p}$ (probability vector), $k$ (number of categories; i.e., size of $\mathbf{p}$ )	Dirichlet	$\boldsymbol{\alpha}$	$\boldsymbol{\alpha} + (c_1, \dots, c_k)$ , where $c_i$ is the number of observations in category $i$	$\alpha_i - 1$ occurrences of category $i$ <sup>[note 1]</sup>	$p(\tilde{x} = i) = \frac{\alpha_i'}{\sum_i \alpha_i'}$ $= \frac{\alpha_i + c_i}{\sum_i \alpha_i + n}$
Multinomial	$\mathbf{p}$ (probability vector), $k$ (number of categories; i.e., size of $\mathbf{p}$ )	Dirichlet	$\boldsymbol{\alpha}$	$\boldsymbol{\alpha} + \sum_{i=1}^n \mathbf{x}_i$	$\alpha_i - 1$ occurrences of category $i$ <sup>[note 1]</sup>	DirMult( $\tilde{\mathbf{x}} \boldsymbol{\alpha}'$ ) (Dirichlet-multinomial)
Hypergeometric with known total population size, $N$	$M$ (number of target members)	Beta-binomial <sup>[4]</sup>	$n = N, \alpha, \beta$	$\alpha + \sum_{i=1}^n x_i, \beta + \sum_{i=1}^n N_i - \sum_{i=1}^n x_i$	$\alpha - 1$ successes, $\beta - 1$ failures <sup>[note 1]</sup>	
Geometric	$p_0$ (probability)	Beta	$\alpha, \beta$	$\alpha + n, \beta + \sum_{i=1}^n x_i - n$	$\alpha - 1$ experiments, $\beta - 1$ total failures <sup>[note 1]</sup>	

please check: [https://en.wikipedia.org/wiki/Conjugate\\_prior](https://en.wikipedia.org/wiki/Conjugate_prior) (source)

# Beta distribution

- ▶ conjugate prior for the Bernoulli, binomial, negative binomial and geometric distributions
- ▶  $\text{Beta}(\theta|a, b) \sim \theta^{a-1}(1 - \theta)^{b-1}$



# Beta distribution

- ▶ required  $a, b > 0$
- ▶ if  $a = b = 1$ , we get the uniform distribution
- ▶ if  $a$  and  $b$  are both less than 1, we get a bimodal distribution with “spikes” at 0 and 1
- ▶ if  $a$  and  $b$  are both greater than 1, the distribution is unimodal

## Distribution properties

$$\text{mean} = \frac{a}{a+b}, \text{ mode} = \frac{a-1}{a+b-2}, \text{ var} = \frac{ab}{(a+b)^2(a+b+1)}$$

# Beta prior

$$\text{Beta}(\theta|a, b) \sim \theta^{a-1}(1 - \theta)^{b-1}$$

- ▶ prior parameters  $a$  and  $b$  are called **hyper-parameters**
- ▶ set  $a$  and  $b$  to encode your prior belief

## Example

- ▶ to encode our beliefs that  $\theta$  has mean 0.7 and standard deviation 0.2, we set  $a = 2.975$  and  $b = 1.275$
- ▶ to encode our beliefs that  $\theta$  has mean 0.15 and that we think it lives in the interval (0.05, 0.30), we find  $a = 4.5$  and  $b = 25.5$

# Posterior

Multiply the likelihood by the beta prior:

$$p(\theta|\mathcal{D}) \propto \text{Bin}(N_1|\theta, N_0 + N_1)\text{Beta}(\theta|a, b) \propto \text{Beta}(\theta|N_1 + a, N_0 + b)$$

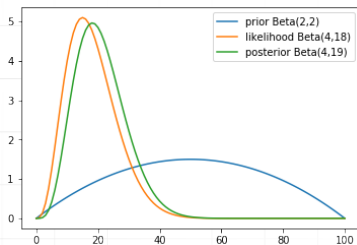


Figure: Beta(2,2) prior updated with Binomial likelihood with sufficient statistics  $N_1 = 3, N_0 = 17$  yields Beta(5,19)

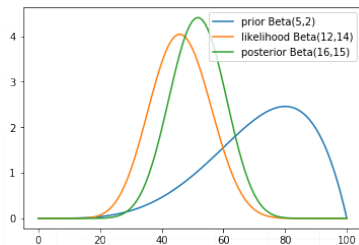


Figure: Beta(5,2) prior updated with Binomial likelihood with sufficient statistics  $N_1 = 11, N_0 = 13$  yields Beta(16,15)



## Remark: two ways of updating posterior

Updating the posterior **sequentially** is equivalent to updating in a **single batch**

Let  $D_a$  and  $D_b$  be two datasets with sufficient statistics  $N_1^a, N_0^a$  and  $N_1^b, N_0^b$ ; let  $N_1 = N_1^a + N_1^b$  and  $N_0 = N_0^a + N_0^b$  be the sufficient statistics of the combined datasets

► Batch mode:

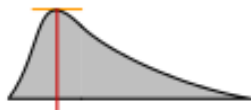
$$p(\theta|\mathcal{D}_a, \mathcal{D}_b) \propto \text{Bin}(N_1|\theta, N_1 + N_0)\text{Beta}(\theta|a, b) \propto \text{Beta}(\theta|N_1 + a, N_0 + b)$$

► Sequential mode:

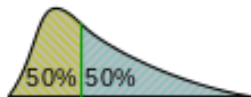
$$\begin{aligned} p(\theta|\mathcal{D}_a, \mathcal{D}_b) &\propto p(\theta|\mathcal{D}_b)p(\theta|\mathcal{D}_a) \\ &\propto \text{Bin}(N_1^b|\theta, N_1^b + N_0^b)\text{Beta}(\theta|N_1^a + a, N_0^a + b) \\ &\propto \text{Beta}(\theta|N_1^a + N_1^b + a, N_0^a + N_0^b + b) \end{aligned}$$

**REMARK! Online learning**

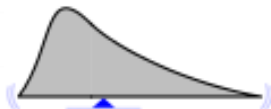
# Mean, mode, median



mode



median



mean

## Posterior mean and mode

### MAP

$$\hat{\theta}_{MAP} = \frac{a + N_1 - 1}{a + b + N - 2}$$

When we use a uniform prior, then the MAP estimate reduces to the MLE, which is just the empirical fraction of heads:

$$\hat{\theta}_{MLE} = \frac{N_1}{N}$$

### Posterior mean

$$\bar{\theta} = \frac{a + N_1}{a + b + N}$$

# Posterior predictive distribution

How to make prediction of future observable data?

Predicting the probability of heads in a single future trial under a Beta(a, b) posterior:

$$\begin{aligned} p(\tilde{x} = 1|\mathcal{D}) &= \int_0^1 p(x = 1|\theta)p(\theta|\mathcal{D})dx \\ &= \int_0^1 \theta \text{Beta}(\theta|a, b)d\theta = \mathbb{E}(\theta|\mathcal{D}) = \frac{a}{a+b} \end{aligned}$$

The mean of the posterior predictive distribution is equivalent (in this case) to plugging in the posterior mean parameters:  $p(\tilde{x}|\mathcal{D}) = \text{Ber}(\tilde{x}|\mathbb{E}[\theta|\mathcal{D}])$

# Overfitting

- ▶ let assume  $p(\tilde{x}|\mathcal{D}) = \text{Ber}(\tilde{x}|\hat{\theta}_{MLE})$
- ▶ and  $N = 3$  with 3 tails in a row
- ▶ MLE is  $\hat{\theta} = 0/3 = 0$
- ▶ this makes the observed data as probable as possible
- ▶ **BUT** we predict that heads are impossible

This is called: **zero count problem** or the **sparse data problem**. Approximation can perform quite poorly.