10-301/601: Introduction to Machine Learning Lecture 9 – MLE & MAP

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6/5/23

Front Matter

- Announcements:
  - Quiz 3: Linear Regression & Optimization on 6/6 (tomorrow!)
- Recommended Readings:
  - Mitchell, Estimating Probabilities

Probabilistic Learning

- Previously:
  - (Unknown) Target function, $c^*: \mathcal{X} \rightarrow \mathcal{Y}$
  - Classifier, $h : \mathcal{X} \rightarrow \mathcal{Y}$
  - Goal: find a classifier, h, that best approximates c^*
- Now:
  - (Unknown) Target *distribution*, $y \sim p^*(Y|\boldsymbol{x})$
  - Distribution, $p(Y|\boldsymbol{x})$
  - Goal: find a distribution, p, that best approximates p^*

Likelihood

- Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$ of a random variable X
  - If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *likelihood* of $\mathcal{D}$ is

$$L(\theta) = \prod_{n=1}^{N} p\left(x^{(n)}|\theta\right)$$

  - If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *likelihood* of $\mathcal{D}$ is

$$L(\theta) = \prod_{n=1}^{N} f\left(x^{(n)}|\theta\right)$$

Log-Likelihood

- Given N independent, identically distribution (iid) samples $\mathcal{D} = \{x^{(1)}, \ldots, x^{(N)}\}$ of a random variable X
  - If X is discrete with probability mass function (pmf) $p(X|\theta)$, then the *log-likelihood* of $\mathcal{D}$ is

$$\ell(\theta) = \log \prod_{n=1}^{N} p\left(x^{(n)}|\theta\right) = \sum_{n=1}^{N} \log p\left(x^{(n)}|\theta\right)$$

  - If X is continuous with probability density function (pdf) $f(X|\theta)$, then the *log-likelihood* of $\mathcal{D}$ is

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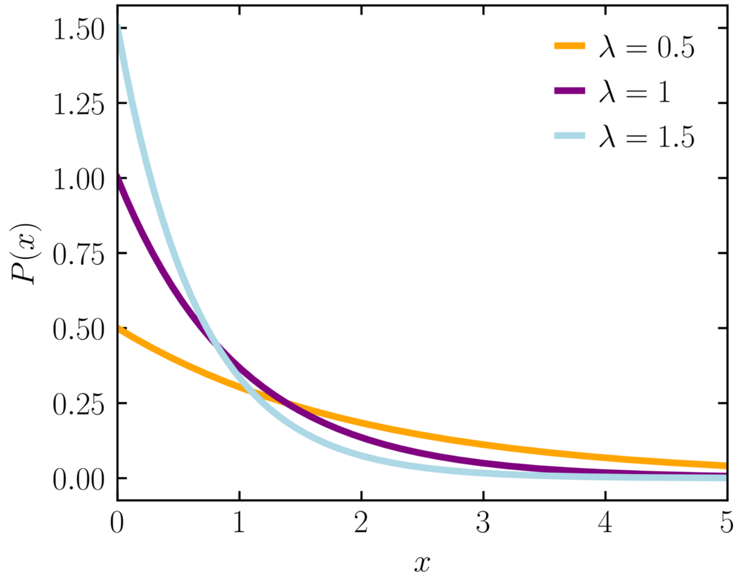
Maximum Likelihood Estimation (MLE)

- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
- Idea: set the parameter(s) so that the likelihood of the samples is maximized
- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*
- Example: the exponential distribution



Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

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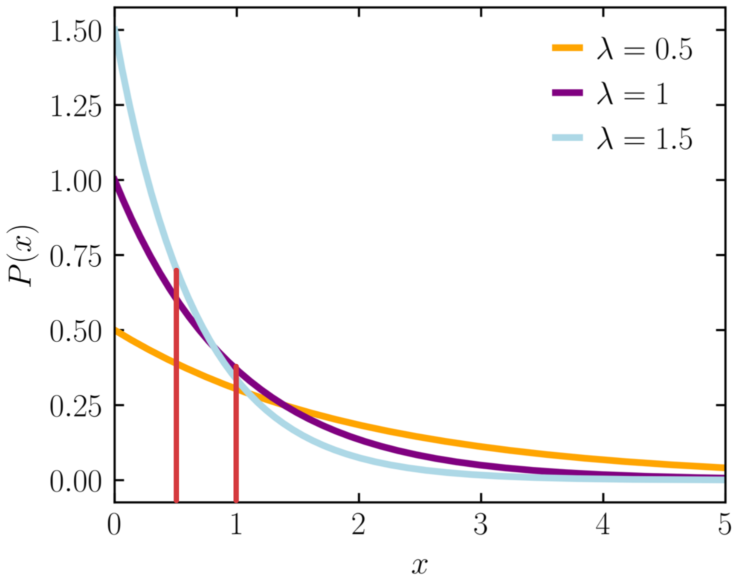

$\{x^{(1)} = 0.5, x^{(2)} = 1\}$

Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

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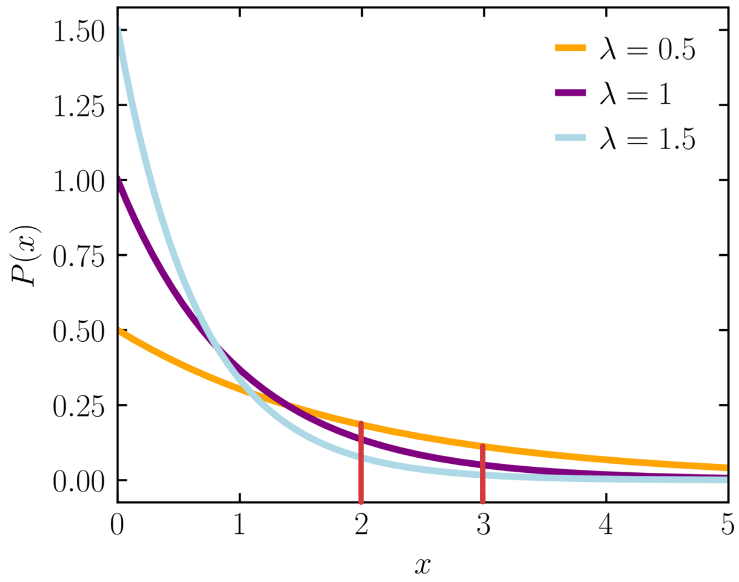


$\{x^{(1)} = 2, x^{(2)} = 3\}$

Source: https://en.wikipedia.org/wiki/Exponential_distribution#/media/File:Exponential_probability_density.svg

General Recipe for Machine Learning

- Define a model and model parameters
- Write down an objective function
- Optimize the objective w.r.t. the model parameters

Recipe for MLE

- Define a model and model parameters
  - Specify the *generative story*, i.e., the data generating distribution
- Write down an objective function
  - Maximize the log-likelihood of $\mathcal{D} = \left\{x^{(1)}, \dots, x^{(N)}\right\}$

$$\ell(\theta) = \sum_{n=1}^{N} \log p\left(x^{(n)} | \theta\right)$$

- Optimize the objective w.r.t. the model parameters
  - Solve in *closed form*: take partial derivatives, set to 0 and solve

Exponential Distribution MLE

- The pdf of the exponential distribution is

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

- Given N iid samples $\{x^{(1)}, \ldots, x^{(N)}\}$, the likelihood is

$$L(\lambda) = \prod_{n=1}^{N} f\left(x^{(n)}|\lambda\right) = \prod_{n=1}^{N} \lambda e^{-\lambda x^{(n)}}$$

Exponential Distribution MLE

- The pdf of the exponential distribution is
$$f(x|\lambda) = \lambda e^{-\lambda x}$$
- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is
$$\ell(\lambda) = \sum_{n=1}^{N} \log f(x^{(n)}|\lambda) = \sum_{n=1}^{N} \log \lambda e^{-\lambda x^{(n)}}$$
$$= \sum_{n=1}^{N} \log \lambda + \log e^{-\lambda x^{(n)}} = N \log \lambda - \lambda \sum_{n=1}^{N} x^{(n)}$$
- Taking the partial derivative and setting it equal to 0 gives
$$\frac{\partial \ell}{\partial \lambda} = \frac{N}{\lambda} - \sum_{n=1}^{N} x^{(n)}$$

Exponential Distribution MLE

- The pdf of the exponential distribution is

$$f(x|\lambda) = \lambda e^{-\lambda x}$$

- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is

$$\ell(\lambda) = \sum_{n=1}^{N} \log f\left(x^{(n)}|\lambda\right) = \sum_{n=1}^{N} \log \lambda e^{-\lambda x^{(n)}}$$

$$= \sum_{n=1}^{N} \log \lambda + \log e^{-\lambda x^{(n)}} = N \log \lambda - \lambda \sum_{n=1}^{N} x^{(n)}$$

- Taking the partial derivative and setting it equal to 0 gives

$$\frac{N}{\hat{\lambda}} - \sum_{n=1}^{N} x^{(n)} = 0 \rightarrow \frac{N}{\hat{\lambda}} = \sum_{n=1}^{N} x^{(n)} \rightarrow \hat{\lambda} = \frac{N}{\sum_{n=1}^{N} x^{(n)}}$$

Bernoulli Distribution MLE

- A Bernoulli random variable takes value 1 with probability ϕ and value 0 with probability $1-\phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x(1-\phi)^{1-x}$$

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x (1-\phi)^{1-x}$$

- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is

$$\ell(\phi) = \sum_{n=1}^{N} \log p\left(x^{(n)}|\phi\right) = \sum_{n=1}^{N} \log \phi^{x^{(n)}} (1-\phi)^{1-x^{(n)}}$$

$$= \sum_{n=1}^{N} x \log \phi + (1-x) \log(1-\phi)$$

$$= N_1 \log \phi + N_0 \log(1-\phi)$$

- where N_1 is the number of 1's in $\{x^{(1)}, \dots, x^{(N)}\}$ and N_0 is the number of 0's

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$

- The partial derivative of the log-likelihood is

$$\frac{\partial \ell}{\partial \phi} = \frac{N_1}{\phi} - \frac{N_0}{1 - \phi}$$

- where N_1 is the number of 1's in $\{x^{(1)}, \ldots, x^{(N)}\}$ and N_0 is the number of 0's

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

$$p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$

- The partial derivative of the log-likelihood is

$$\frac{N_1}{\hat{\phi}} - \frac{N_0}{1 - \hat{\phi}} = 0 \rightarrow \frac{N_1}{\hat{\phi}} = \frac{N_0}{1 - \hat{\phi}}$$

$$\rightarrow N_1\left(1 - \hat{\phi}\right) = N_0 \hat{\phi} \rightarrow N_1 = \hat{\phi}(N_0 + N_1)$$

$$\rightarrow \hat{\phi} = \frac{N_1}{N_0 + N_1}$$

- where N_1 is the number of 1's in $\left\{x^{(1)}, \dots, x^{(N)}\right\}$ and N_0 is the number of 0's

Given the result of your 5 coin flips, what is the MLE of ϕ for your coin?

- 0/5
- 1/5
- 2/5
- 3/5
- 4/5
- 5/5

Maximum a Posteriori (MAP) Estimation

- Insight: sometimes we have *prior* information we want to incorporate into parameter estimation
- Idea: use Bayes rule to reason about the *posterior* distribution over the parameters
  - MLE finds $\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\ p(\mathcal{D}|\theta)$
  - MAP finds $\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\ p(\theta|\mathcal{D})$

$$= \underset{\theta}{\operatorname{argmax}}\ p(\mathcal{D}|\theta)p(\theta)/p(\mathcal{D})$$

$$= \underset{\theta}{\operatorname{argmax}}\ \underbrace{p(\mathcal{D}|\theta)}_{\text{likelihood}}\underbrace{p(\theta)}_{\text{prior}}$$

$$= \underset{\theta}{\operatorname{argmax}}\ \underbrace{\log p(\mathcal{D}|\theta) + \log p(\theta)}_{\text{log-posterior}}$$

Recipe for MAP

- Define a model and model parameters
  - Specify the *generative story*, i.e., the data generating distribution, including a *prior distribution*

    (how do we pick a prior???)

- Write down an objective function
  - Maximize the log-posterior of $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$

$$\ell_{MAP}(\theta) = \log p(\theta) + \sum_{n=1}^{N} \log p\left(x^{(n)} | \theta\right)$$

- Optimize the objective w.r.t. the model parameters
  - Solve in *closed form*: take partial derivatives, set to 0 and solve

Coin Flipping MAP

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

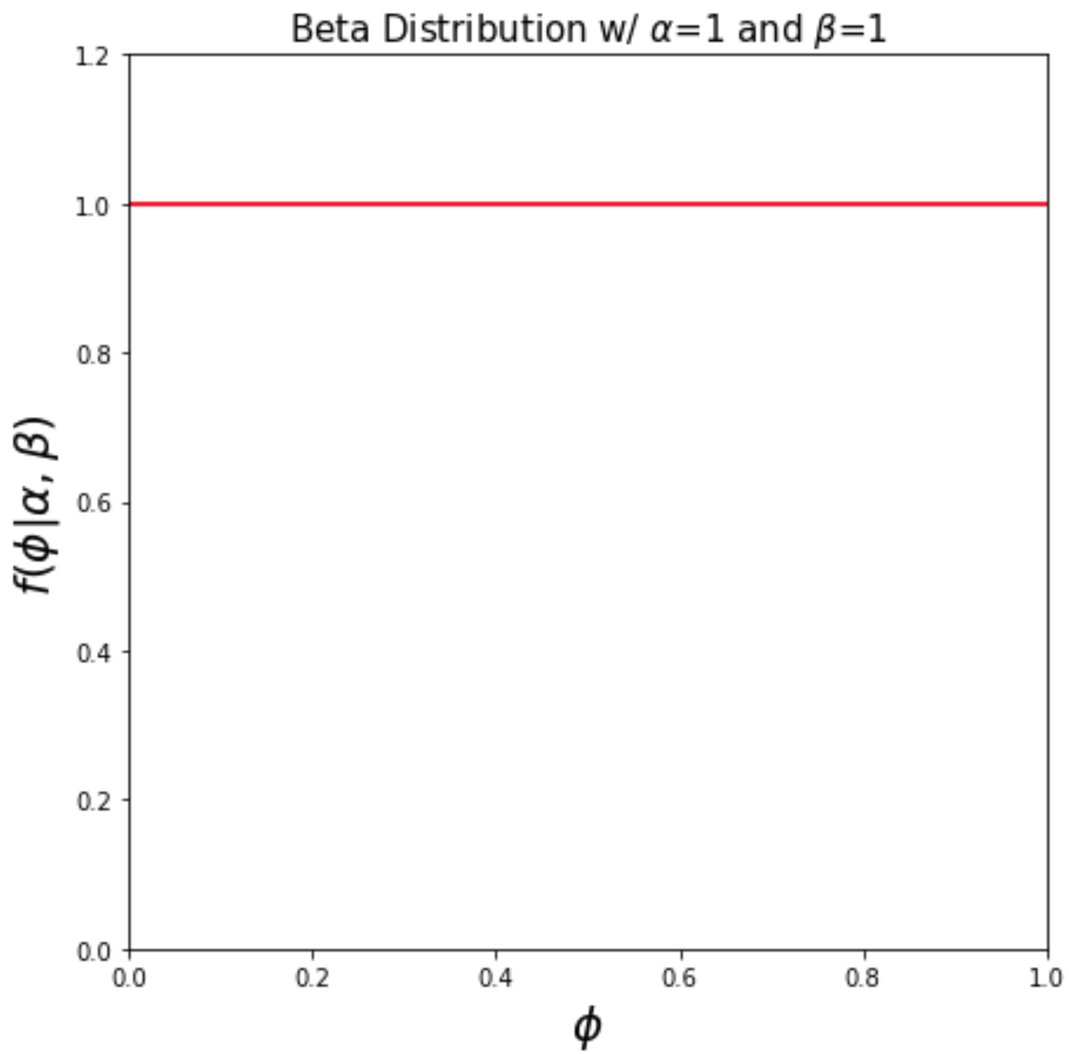
$$p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$

- Assume a Beta prior over the parameter ϕ, which has pdf

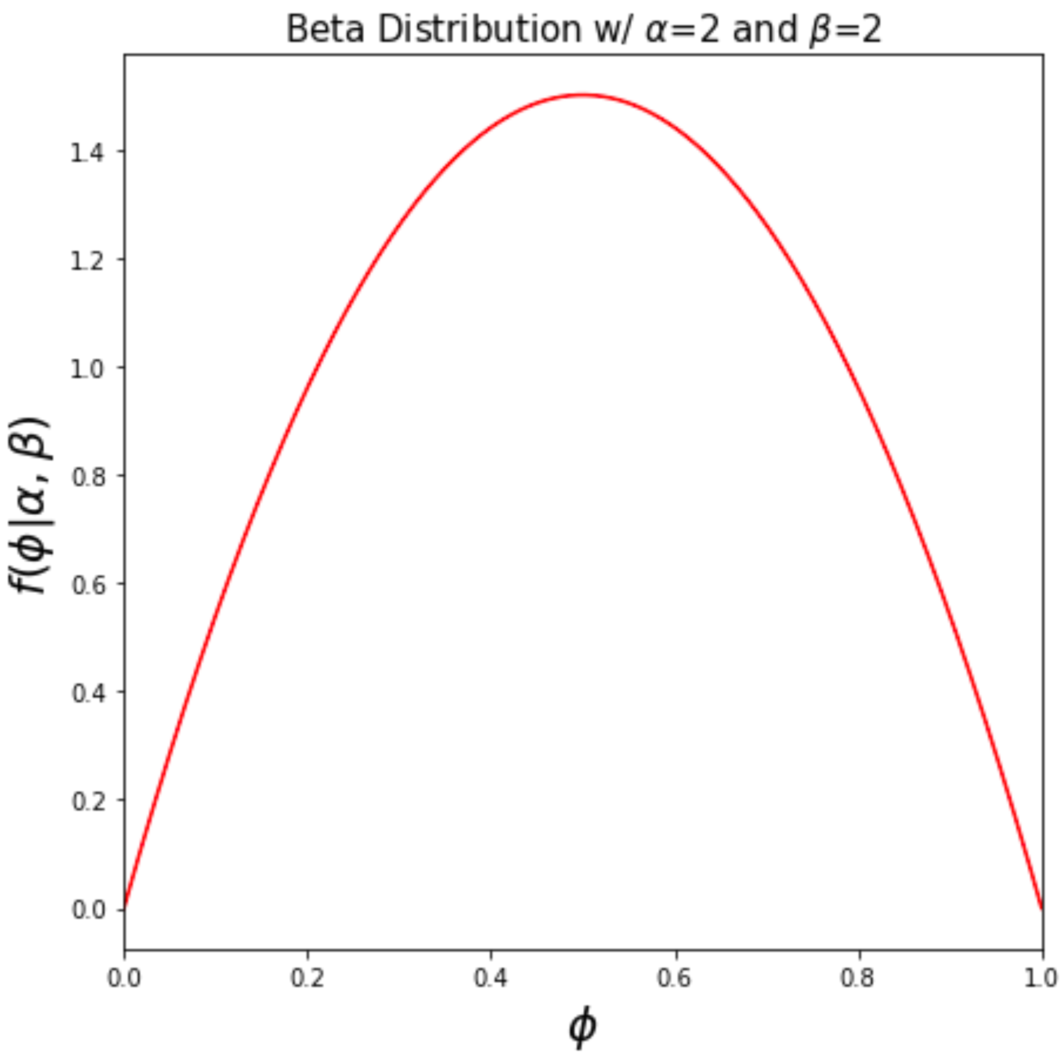
$$f(\phi|\alpha, \beta) = \frac{\phi^{\alpha-1}(1 - \phi)^{\beta-1}}{\mathrm{B}(\alpha, \beta)}$$

where $\mathrm{B}(\alpha, \beta) = \int_0^1 \phi^{\alpha-1}(1 - \phi)^{\beta-1} d\phi$ is a normalizing constant to ensure the distribution integrates to 1

Beta Distribution



Beta Distribution



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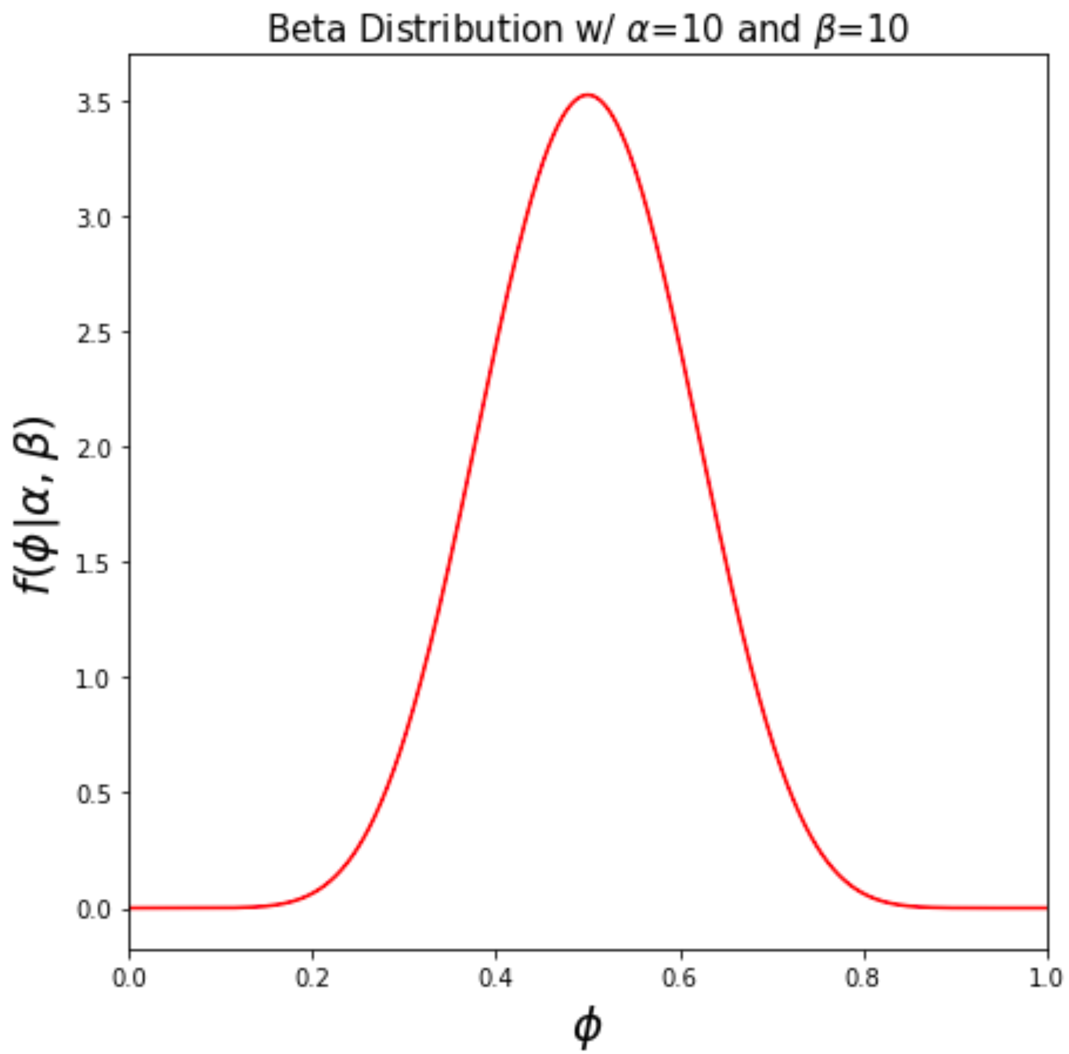

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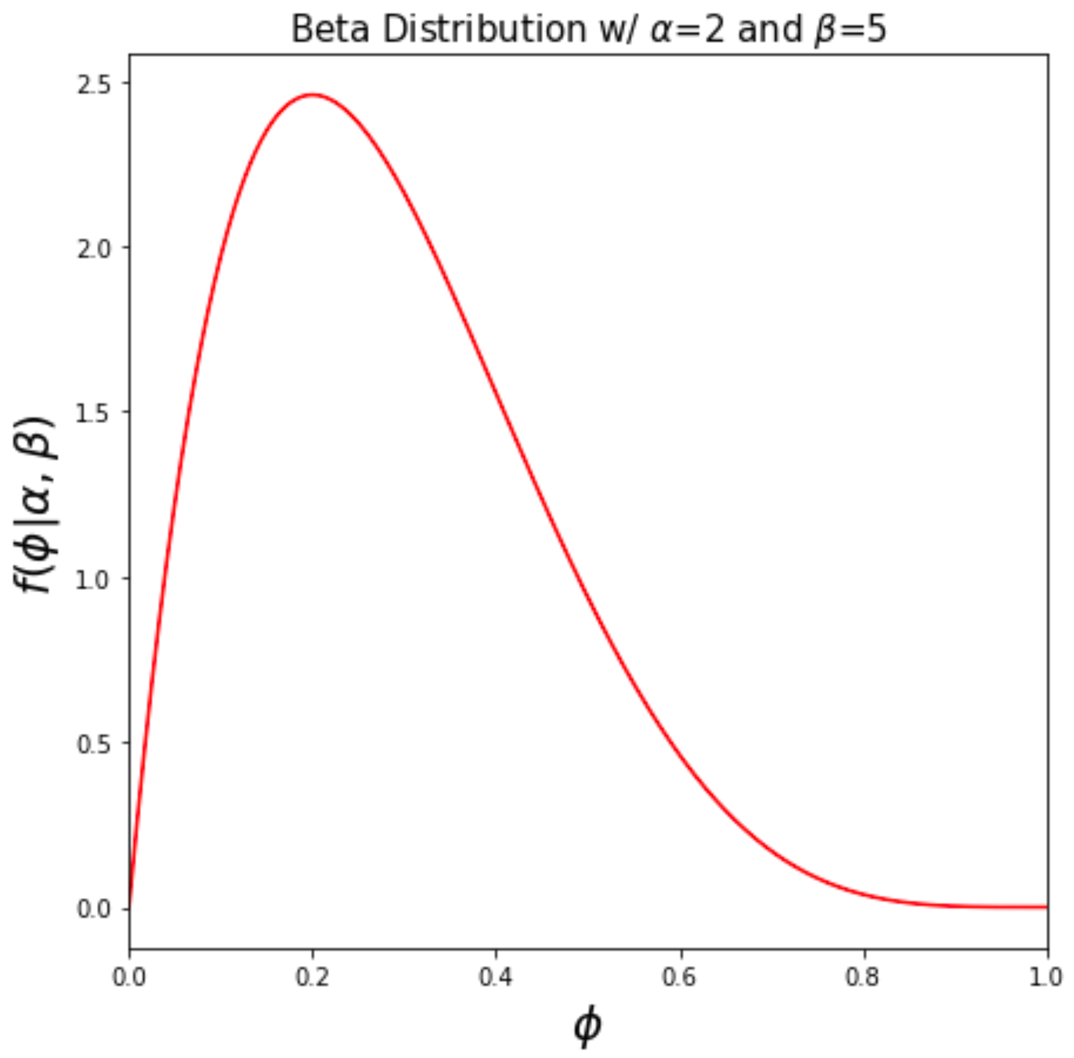

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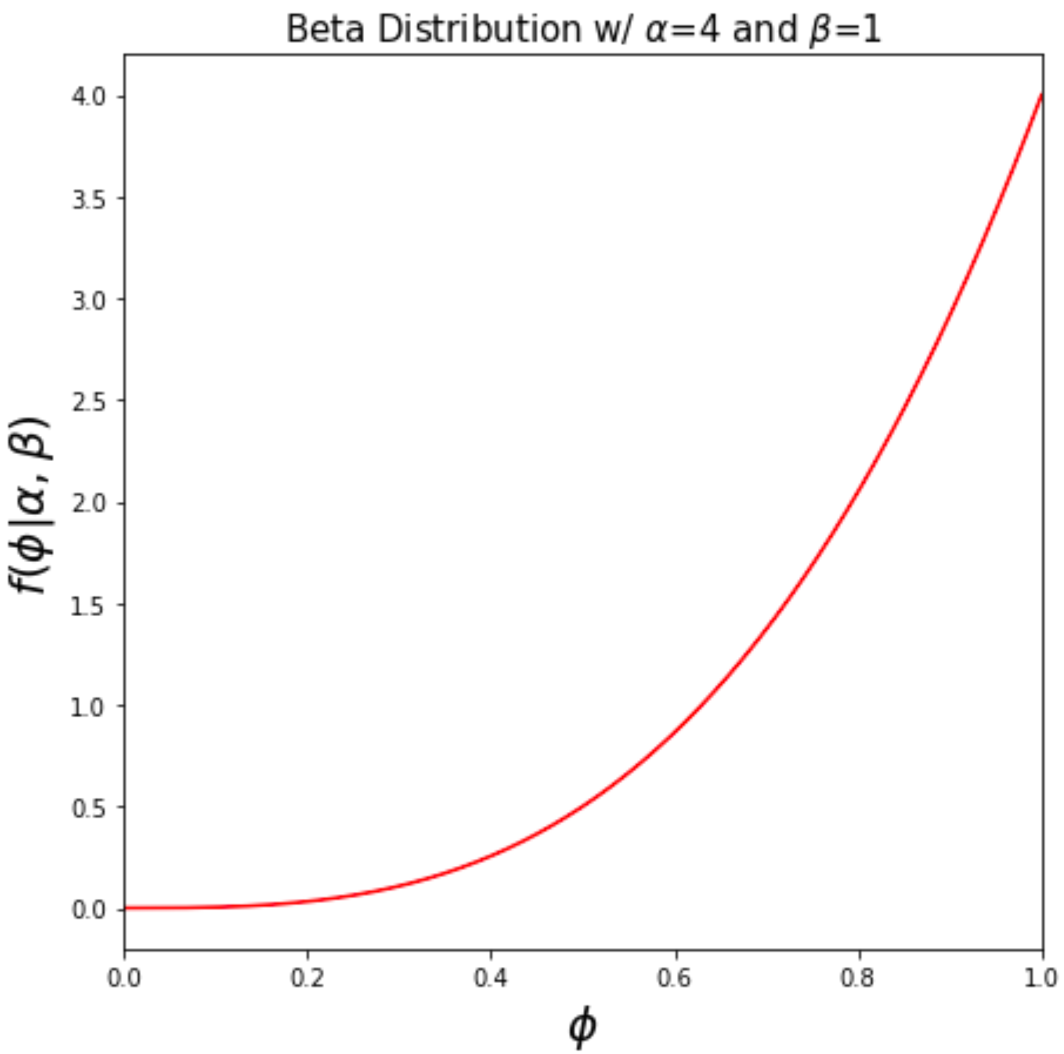

Coin Flipping MAP

- Given N iid samples $\{x^{(1)}, \ldots, x^{(N)}\}$, the log-posterior is

$$\ell(\phi) = \log f(\phi|\alpha, \beta) + \sum_{n=1}^{N} \log p\left(x^{(n)}|\phi\right)$$

$$= \log \frac{\phi^{\alpha-1}(1-\phi)^{\beta-1}}{\mathrm{B}(\alpha, \beta)} + \sum_{n=1}^{N} \log \phi^{x^{(n)}}(1-\phi)^{1-x^{(n)}}$$

$$= (\alpha - 1)\log \phi + (\beta - 1)\log(1-\phi) - \log \mathrm{B}(\alpha, \beta)$$

$$+ \sum_{n=1}^{N} x^{(n)} \log \phi + \left(1 - x^{(n)}\right)\log(1-\phi)$$

$$= (\alpha - 1 + N_1)\log \phi + (\beta - 1 + N_0)\log(1-\phi)$$

$$- \log \mathrm{B}(\alpha, \beta)$$

Coin Flipping MAP

- Given N iid samples $\{x^{(1)}, \ldots, x^{(N)}\}$, the partial derivative of the log-posterior is

$$\frac{\partial \ell}{\partial \phi} = \frac{(\alpha - 1 + N_1)}{\phi} - \frac{(\beta - 1 + N_0)}{1 - \phi}$$

$$\vdots$$

$$\rightarrow \hat{\phi}_{MAP} = \frac{(\alpha - 1 + N_1)}{(\beta - 1 + N_0) + (\alpha - 1 + N_1)}$$

- $\alpha - 1$ is a "pseudocount" of the number of 1's (or heads) you've "observed"
- $\beta - 1$ is a "pseudocount" of the number of 0's (or tails) you've "observed"

Coin Flipping MAP: Example

- Suppose $\mathcal{D}$ consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$):

$$\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$$

- Using a Beta prior with $\alpha = 2$ and $\beta = 5$, then

$$\phi_{MAP} = \frac{(2-1+10)}{(2-1+10)+(5-1+2)} = \frac{11}{17} < \frac{10}{12}$$

Coin Flipping MAP: Example

- Suppose $\mathcal{D}$ consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$):

$$\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$$

- Using a Beta prior with $\alpha = 101$ and $\beta = 101$, then

$$\phi_{MAP} = \frac{(101-1+10)}{(101-1+10)+(101-1+2)} = \frac{110}{212} \approx \frac{1}{2}$$

Coin Flipping MAP: Example

- Suppose $\mathcal{D}$ consists of ten 1's or heads ($N_1 = 10$) and two 0's or tails ($N_0 = 2$):

$$\phi_{MLE} = \frac{10}{10+2} = \frac{10}{12}$$

- Using a Beta prior with $\alpha = 1$ and $\beta = 1$, then

$$\phi_{MAP} = \frac{(1-1+10)}{(1-1+10)+(1-1+2)} = \frac{10}{12} = \phi_{MLE}$$

Key Takeaways

- Probabilistic learning tries to learn a probability distribution as opposed to a classifier
- Two ways of estimating the parameters of a probability distribution given samples of a random variable:
  - Maximum likelihood estimation – maximize the (log-)likelihood of the observations
  - Maximum a posteriori estimation – maximize the (log-)posterior of the parameters conditioned on the observations
    - Requires a prior distribution, drawn from background knowledge or domain expertise