MAP estimation

Nishant Mehta

Lecture 16

The perils of maximum likelihood estimation

wins = n_1

wins = n_0

Consider betting on two top chess players

Suppose the true probability that Kasparov wins is $\theta = 0.5$ (unknown to us), so Kasparov and Karpov are evenly matched

Instead, we have observed two games. Kasparov won both games.
What is the MLE? $\hat{\theta}_{\text{MLE}} =$

So, how much money should we bet on the next game?

Expected cross-entropy loss of $\hat{\theta}_{\mathrm{MLE}}$

What is risk under cross-entropy loss when true parameter is $\theta = 0.5$ and our estimate is $\hat{\theta} = 1$?

$\hat{\theta}$

$$\mathrm{E}\left[\ell(Y, 1) \mid \theta = 0.5\right] =$$

Intuition: Imaginary examples

Suppose we imagine that we have extra examples, one example for each class:

$$\tilde{n}_1 = n_1 + 1 \qquad\qquad \tilde{n}_0 = n_0 + 1$$

This is called *add-one smoothing*, a special case of a more general technique called *additive smoothing*.

Why might this be a good idea?

What happens to the MLE when we include these imaginary examples?

$$\hat{\theta} =$$

* add-one smoothing is also called Laplace's rule of succession

Intuition: Imaginary examples

Suppose we imagine that we have extra examples, one example for each class:

$$\tilde{n}_1 = n_1 + 1 \qquad \tilde{n}_0 = n_0 + 1$$

This is called *add-one smoothing*, a special case of a more general technique called *additive smoothing*.

Why might this be a good idea?

What happens to the MLE when we include these imaginary examples?

$$\hat{\theta} = \frac{\tilde{n}_1}{\tilde{n}_1 + \tilde{n}_0} = \frac{n_1 + 1}{n_1 + n_0 + 2}$$

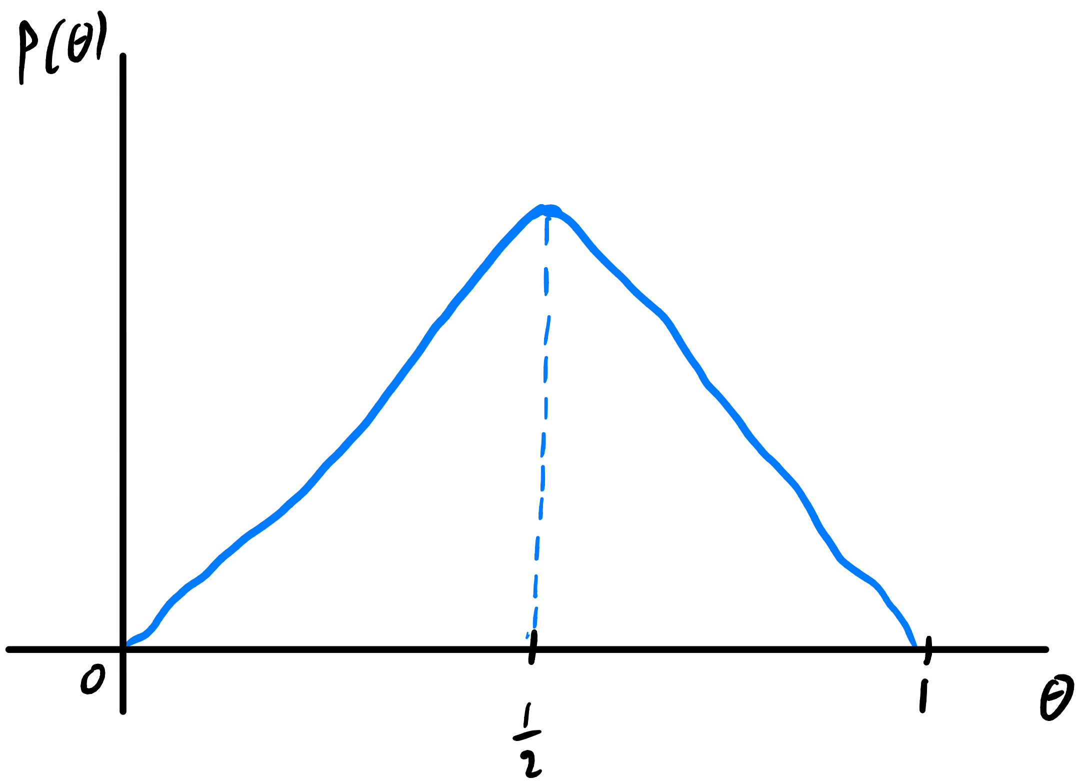
* add-one smoothing is also called Laplace's rule of succession

Prior distribution

Prior distribution $P(\theta)$

Indicates our probability of belief that θ is the true parameter, prior to seeing any evidence at all

Example: “probably” fair coin

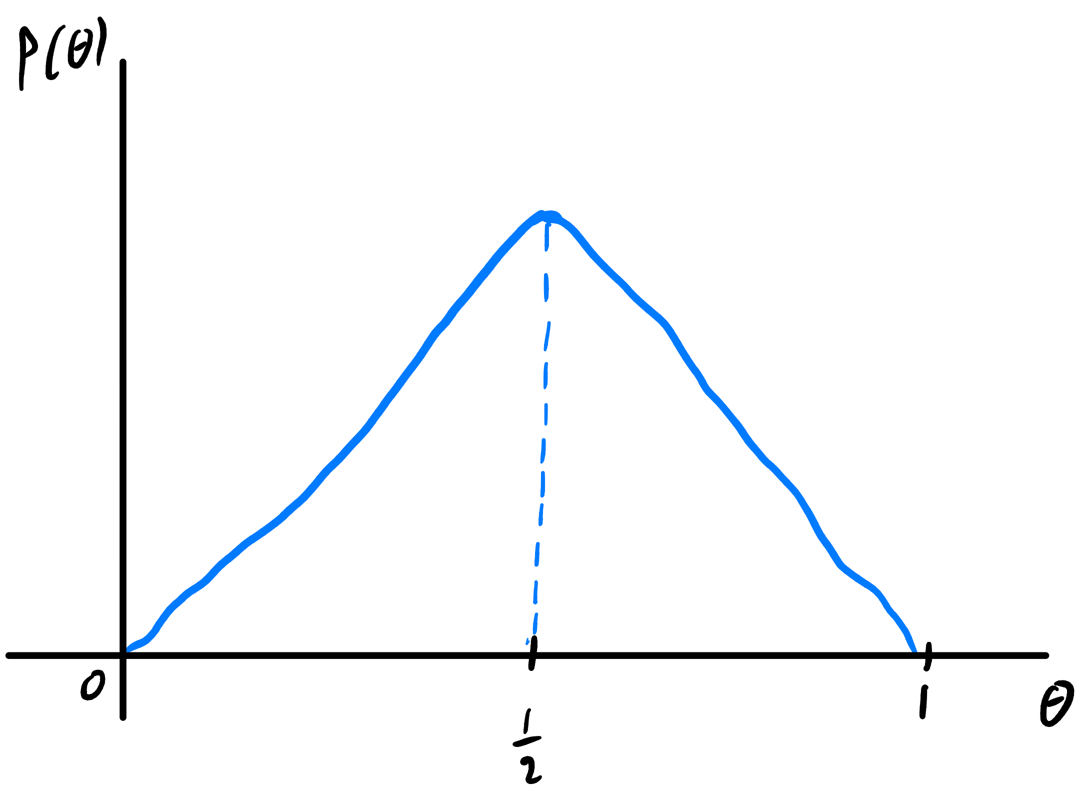


Prior distribution

Prior distribution $P(\theta)$

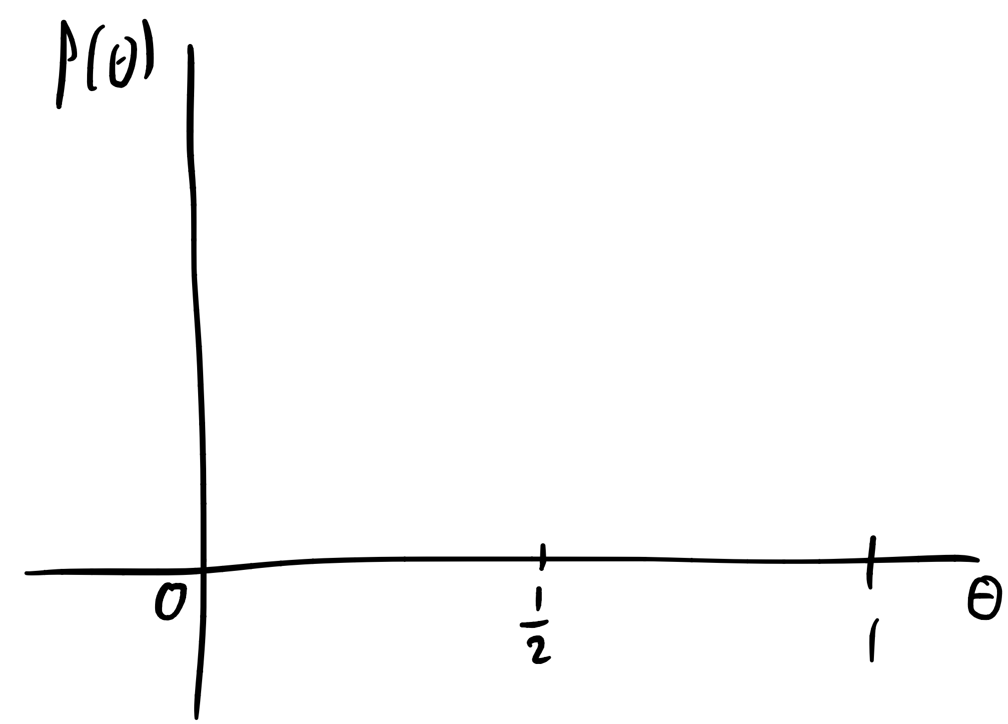
Indicates our probability of belief that θ is the true parameter, prior to seeing any evidence at all

Example: "probably" fair coin



Another example:

"probably unfair coin"!



Posterior distribution

From Bayes rule, we have

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

This quantity is our probability of belief θ is the true parameter, *a posteriori of the data*.

We call $\theta \mapsto P(\theta \mid D)$ the *posterior distribution* over Θ

Posterior distribution

Bernoulli

$\Theta = [0,1]$

From Bayes rule, we have

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)} = \frac{P(D \mid \theta)P(\theta)}{\int_{\Theta} P(D \mid \theta)P(\theta)d\theta}$$

This quantity is our probability of belief that θ is the true parameter, *a posteriori of the data*.

We call $\theta \mapsto P(\theta \mid D)$ the *posterior distribution* over Θ

Maximum A Posteriori estimate

From Bayes rule, we have

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)} = \frac{P(D \mid \theta)P(\theta)}{\int_{\Theta} P(D \mid \theta)P(\theta)d\theta}$$

This quantity is our probability of belief that θ is the true parameter, *a posteriori of the data*.

We call $\theta \mapsto P(\theta \mid D)$ the *posterior distribution* over Θ

The *Maximum a Posteriori estimate* (*MAP estimate*) of θ is

$$\hat{\theta}_{\mathrm{MAP}} = \arg\max_{\theta} P(\theta \mid D) = \arg\max_{\theta} \frac{P(D \mid \theta)P(\theta)}{P(D)}$$

ignore

Maximum A Posteriori estimate

From Bayes rule, we have

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)} = \frac{P(D \mid \theta)P(\theta)}{\int_\Theta P(D \mid \theta)P(\theta)d\theta}$$

This quantity is our probability of belief that θ is the true parameter, *a posteriori of the data*.

We call $\theta \mapsto P(\theta \mid D)$ the *posterior distribution* over Θ

The *Maximum a Posteriori estimate* (*MAP estimate*) of θ is

$$\hat{\theta}_{\mathrm{MAP}} = \arg\max_\theta P(\theta \mid D) = \arg\max_\theta \frac{P(D \mid \theta)P(\theta)}{P(D)}$$

ignore

$$= \arg\max_\theta P(D \mid \theta)P(\theta)$$

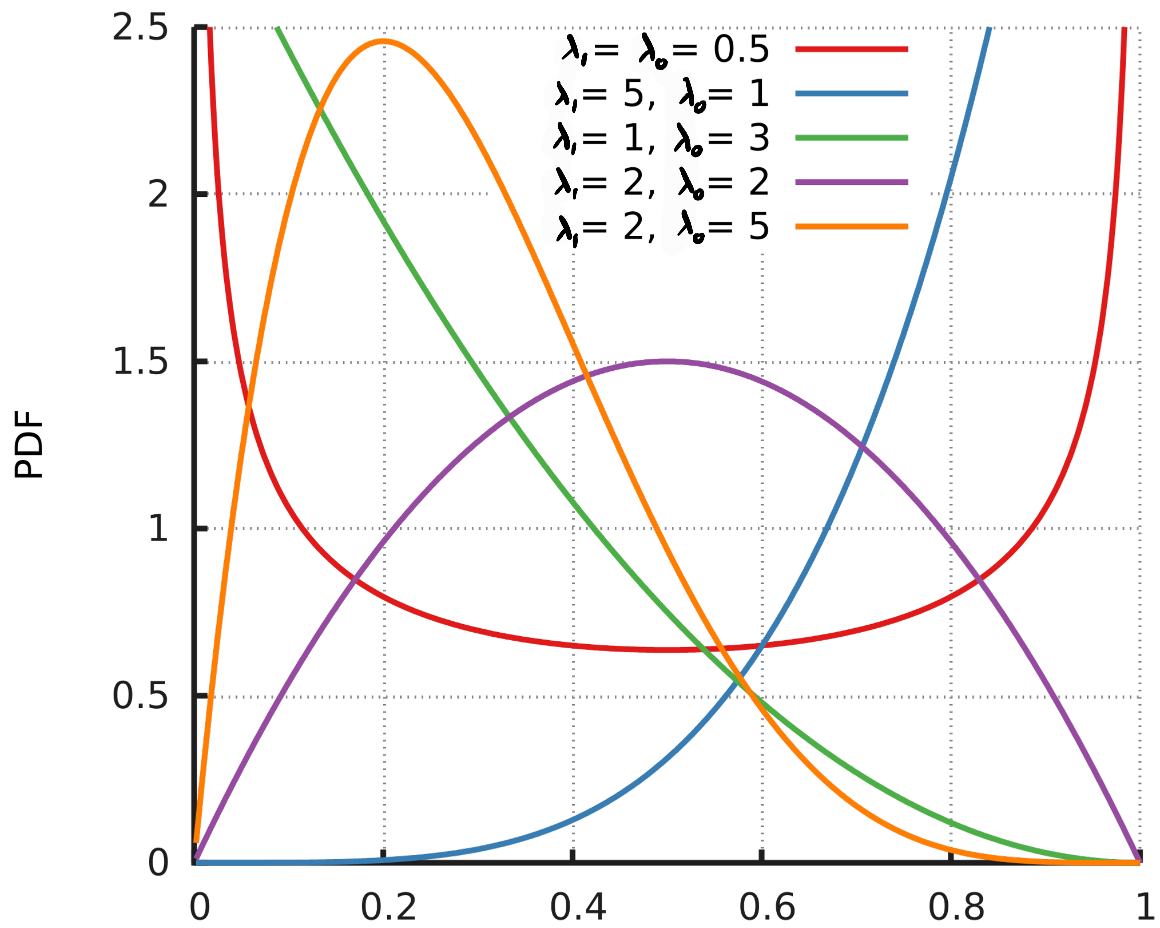
Beta prior distribution

Suppose the examples are drawn i.i.d. from a Bernoulli distribution

A common choice of prior distribution is the *Beta distribution*

$$P(\theta) = \text{Beta}(\lambda_1, \lambda_0) = \frac{\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}}{B(\lambda_1, \lambda_0)}$$

normalization constant



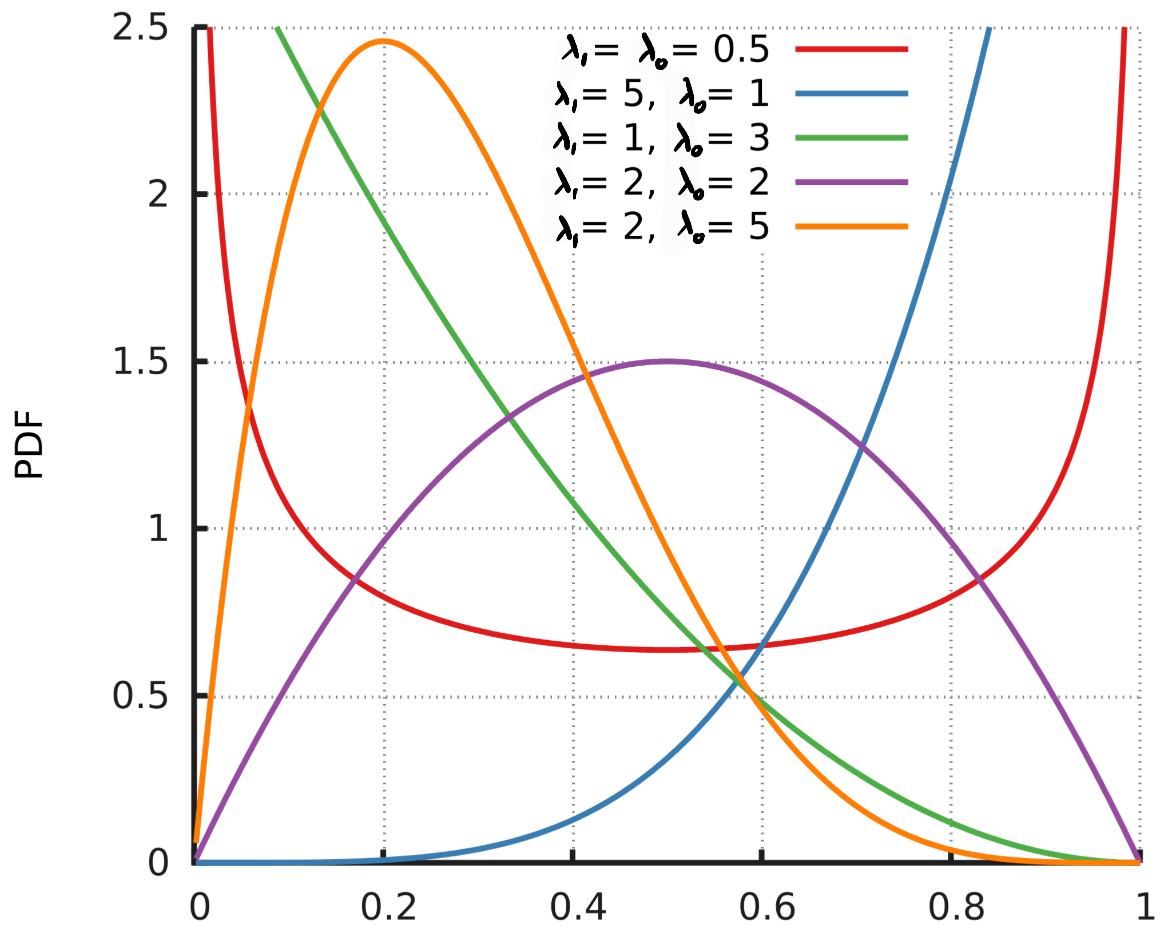
Beta prior distribution

Suppose the examples are drawn i.i.d. from a Bernoulli distribution

A common choice of prior distribution is the *Beta distribution*

$$P(\theta) = \text{Beta}(\lambda_1, \lambda_0) = \frac{\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}}{B(\lambda_1, \lambda_0)}$$

normalization constant



If λ_1 and λ_0 are positive integers, then

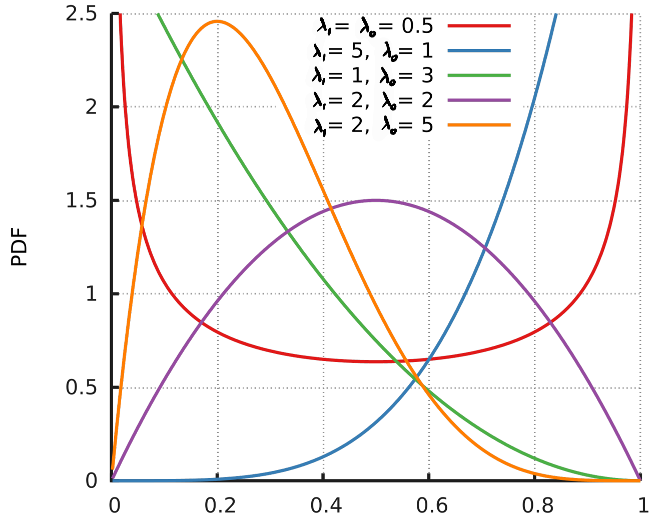
$$B(\lambda_1, \lambda_2) = \frac{(\lambda_1 - 1)!(\lambda_0 - 1)!}{(\lambda_1 + \lambda_0 - 1)!}$$

Beta prior distribution

Suppose the examples are drawn i.i.d. from a Bernoulli distribution

A common choice of prior distribution is the *Beta distribution*

$$P(\theta) = \mathrm{Beta}(\lambda_1, \lambda_0) = \frac{\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}}{B(\lambda_1, \lambda_0)}$$



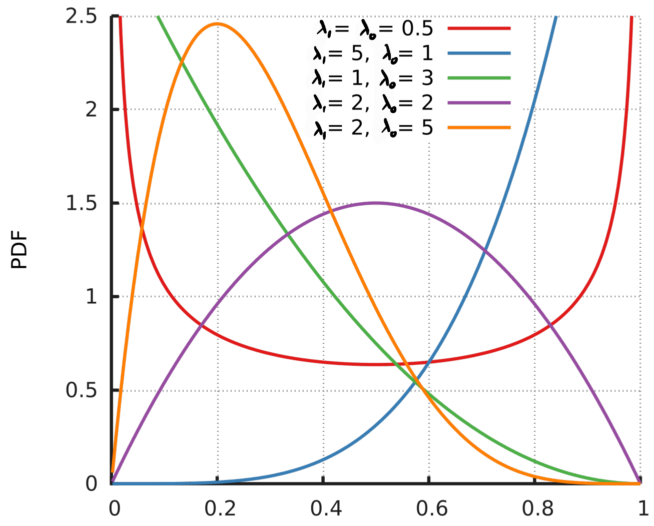
What is the MAP estimate when using a Beta prior?

Beta prior distribution

Suppose the examples are drawn i.i.d. from a Bernoulli distribution

A common choice of prior distribution is the *Beta distribution*

$$P(\theta) = \text{Beta}(\lambda_1, \lambda_0) = \frac{\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}}{B(\lambda_1, \lambda_0)}$$



What is the MAP estimate when using a Beta prior?

$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta \in [0,1]} P(D \mid \theta) P(\theta) = \arg\max_{\theta \in [0,1]} \theta^{n_1}(1-\theta)^{n_0} \theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}$$

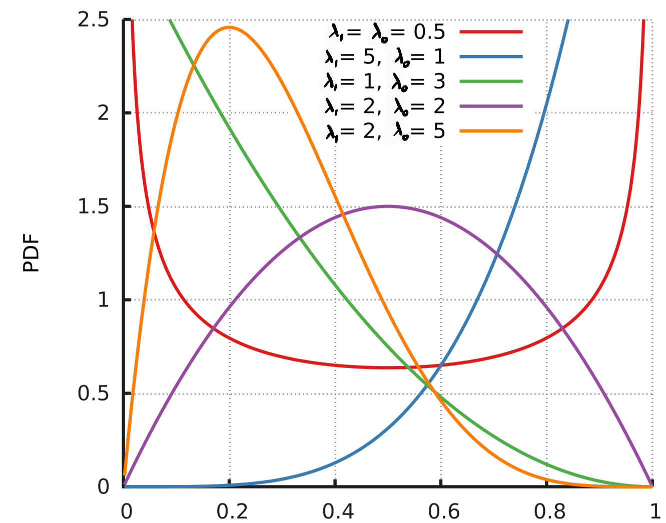
$$= \arg\max_{\theta \in [0,1]} \theta^{n_1 + \lambda_1 - 1}(1-\theta)^{n_0 + \lambda_0 - 1}$$

Beta prior distribution

Suppose the examples are drawn i.i.d. from a Bernoulli distribution

A common choice of prior distribution is the *Beta distribution*

$$P(\theta) = \text{Beta}(\lambda_1, \lambda_0) = \frac{\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}}{B(\lambda_1, \lambda_0)}$$



What is the MAP estimate when using a Beta prior?

$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta \in [0,1]} P(D \mid \theta) P(\theta) = \arg\max_{\theta \in [0,1]} \theta^{n_1}(1-\theta)^{n_0}\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}$$

$$= \arg\max_{\theta \in [0,1]} \theta^{n_1 + \lambda_1 - 1}(1-\theta)^{n_0 + \lambda_0 - 1}$$

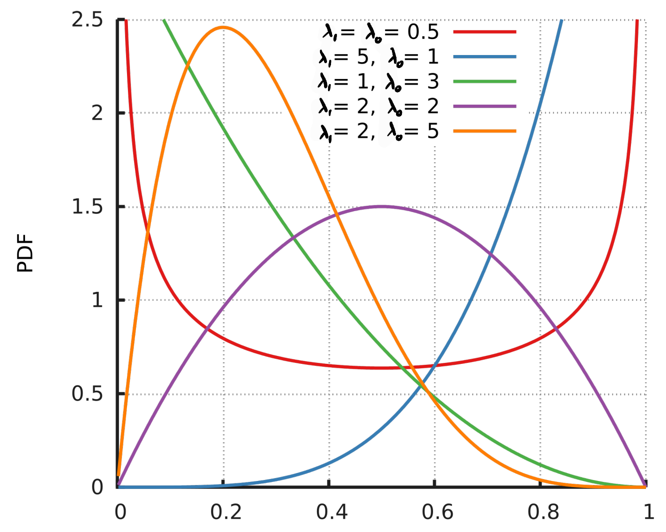
$$\tilde{n}_1 = n_1 + \lambda_1 - 1$$
$$\tilde{n}_0 = n_0 + \lambda_0 - 1$$

Beta prior distribution

Suppose the examples are drawn i.i.d. from a Bernoulli distribution

A common choice of prior distribution is the *Beta distribution*

$$P(\theta) = \text{Beta}(\lambda_1, \lambda_0) = \frac{\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}}{B(\lambda_1, \lambda_0)}$$



What is the MAP estimate when using a Beta prior?

$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta \in [0,1]} P(D \mid \theta) P(\theta) = \arg\max_{\theta \in [0,1]} \theta^{n_1}(1-\theta)^{n_0} \theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}$$

$$= \arg\max_{\theta \in [0,1]} \theta^{n_1 + \lambda_1 - 1}(1-\theta)^{n_0 + \lambda_0 - 1} = \arg\max_{\theta \in [0,1]} \theta^{\tilde{n}_1}(1-\theta)^{\tilde{n}_0}$$

$$\tilde{n}_1 = n_1 + \lambda_1 - 1$$

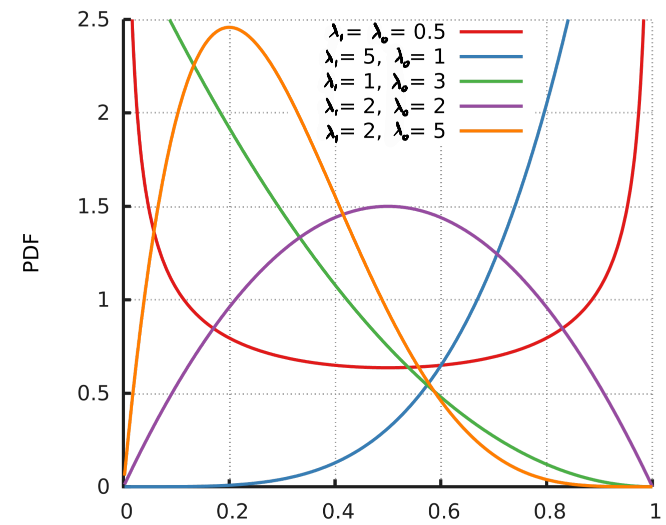
$$\tilde{n}_0 = n_0 + \lambda_0 - 1$$

Beta prior distribution

Suppose the examples are drawn i.i.d. from a Bernoulli distribution

A common choice of prior distribution is the *Beta distribution*

$$P(\theta) = \text{Beta}(\lambda_1, \lambda_0) = \frac{\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}}{B(\lambda_1, \lambda_0)}$$



What is the MAP estimate when using a Beta prior?

$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta \in [0,1]} P(D \mid \theta) P(\theta) = \arg\max_{\theta \in [0,1]} \theta^{n_1}(1-\theta)^{n_0} \theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}$$

$$= \arg\max_{\theta \in [0,1]} \theta^{n_1 + \lambda_1 - 1}(1-\theta)^{n_0 + \lambda_0 - 1} = \arg\max_{\theta \in [0,1]} \theta^{\tilde{n}_1}(1-\theta)^{\tilde{n}_0} = \frac{\tilde{n}_1}{\tilde{n}_1 + \tilde{n}_0}$$

$$\tilde{n}_1 = n_1 + \lambda_1 - 1$$
$$\tilde{n}_0 = n_0 + \lambda_0 - 1$$

Conjugate prior

Note that the form of the posterior is again a Beta distribution

When the prior and posterior distributions have the same form, the prior is known as a *conjugate prior*

Benefits of a conjugate prior:

- Posterior is easy to interpret (if prior was easy to interpret)
- Computationally friendly (updating is easier)

Additive smoothing

In *additive smoothing*, we add c imaginary positive examples and c imaginary negative examples, for parameter $c > 0$

How should we set λ_1 and λ_0 to get additive smoothing?

$$\tilde{n}_1 = n_1 + c$$

$$\tilde{n}_0 = n_0 + c$$

$$\hat{\theta}_{MAP} = ?$$

MAP estimation $\Longleftrightarrow$ regularized training

Just like with the MLE, we can write MAP estimation as the minimization of training error under cross-entropy loss…

… but now, we also have regularization!

Multiclass - One-hot encoding

In the multiclass case with K classes, there are two common choices of representation of the label

1) Standard representation:

$$Y \in \{1, 2, \ldots, K\}$$

2) One-hot encoding (also called one-of-K encoding):

$$Y \in \{0, 1\}^K \text{ with } Y_j = 1 \text{ if label is } j \text{ and } Y_j = 0 \text{ otherwise}$$

MLE - Extension to multinoulli distribution

Suppose we have K classes. We use parameter vector $\theta = \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_K \end{pmatrix}$

satisfying $\theta_j \in [0, 1]$ and $\displaystyle\sum_{j=1}^{K} \theta_j = 1$

Log likelihood for *Multinoulli* (or *categorical*) distribution

$$\log P(Y = y) = \begin{cases} \log \theta_y & \text{(standard representation)} \\ \log \prod_{j=1}^{K} \theta_j^{y_j} = \sum_{j=1}^{K} y_j \log \theta_j & \text{(one-hot encoding)} \end{cases}$$

MLE - Extension to multinoulli distribution

Suppose we have K classes. We use parameter vector $\theta = \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_K \end{pmatrix}$

satisfying $\theta_j \in [0, 1]$ and $\sum_{j=1}^{K} \theta_j = 1$

Log likelihood for *Multinoulli* (or *categorical*) distribution

$$\log P(Y = y) = \begin{cases} \log \theta_y & \text{(standard representation)} \\ \log \prod_{j=1}^{K} \theta_j^{y_j} = \sum_{j=1}^{K} y_j \log \theta_j & \text{(one-hot encoding)} \end{cases}$$

Multiclass cross-entropy loss

$$\log P(Y = y) = \begin{cases} -\log \theta_y & \text{(standard representation)} \\ \sum_{j=1}^{K} -y_j \log \theta_j & \text{(one-hot encoding)} \end{cases}$$

What is the MLE?

MLE - Extension to multinoulli distribution

Suppose we have K classes. We use parameter vector $\theta = \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_K \end{pmatrix}$

satisfying $\theta_j \in [0, 1]$ and $\sum_{j=1}^{K} \theta_j = 1$

Log likelihood for *Multinoulli* (or *categorical*) distribution

$$\log P(Y = y) = \begin{cases} \log \theta_y & \text{(standard representation)} \\ \log \prod_{j=1}^{K} \theta_j^{y_j} = \sum_{j=1}^{K} y_j \log \theta_j & \text{(one-hot encoding)} \end{cases}$$

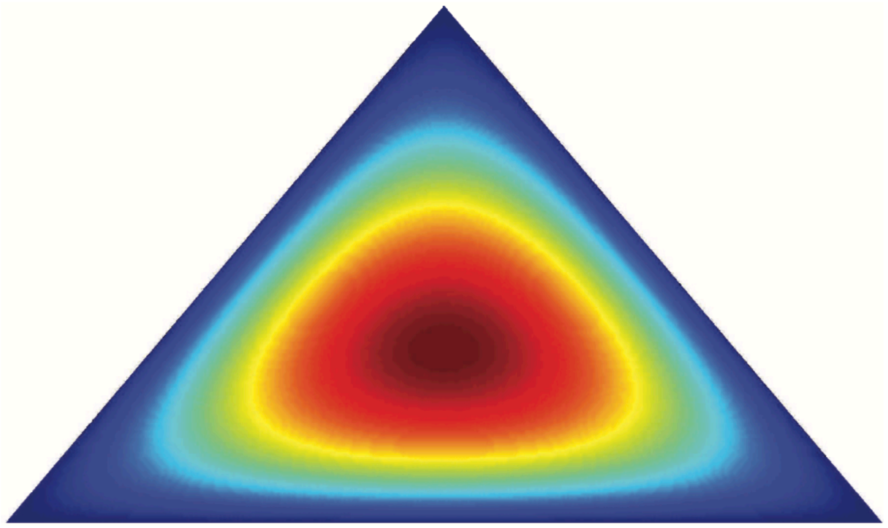
Multiclass cross-entropy loss

$$\log P(Y = y) = \begin{cases} -\log \theta_y & \text{(standard representation)} \\ \sum_{j=1}^{K} -y_j \log \theta_j & \text{(one-hot encoding)} \end{cases}$$

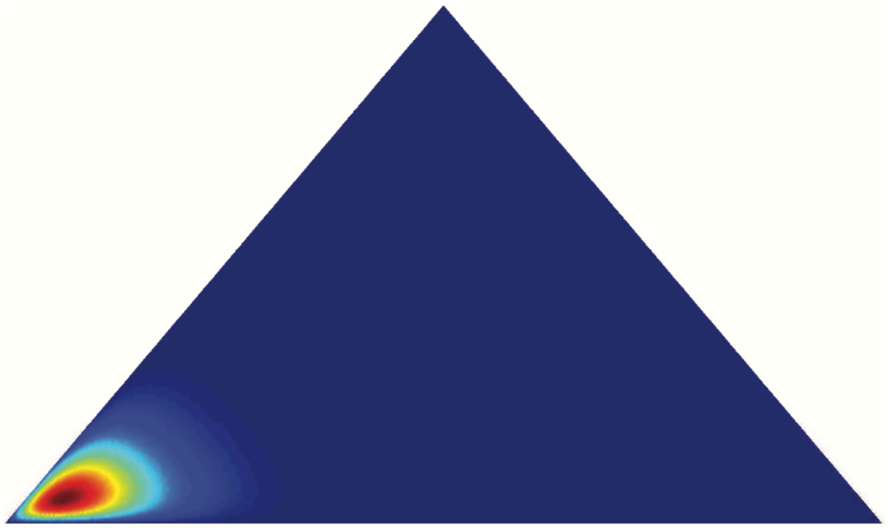
What is the MLE? $\hat{\theta}_j = \frac{n_j}{n}$ number of examples with label j

MAP - Extension to multinoulli distribution

- Conjugate prior? *Dirichlet distribution*
- $$P(\theta \mid \alpha) = \frac{1}{B(\alpha)} \prod_{j=1}^{K} \theta_j^{\alpha_j - 1}$$ if θ is probability vector (zero otherwise)



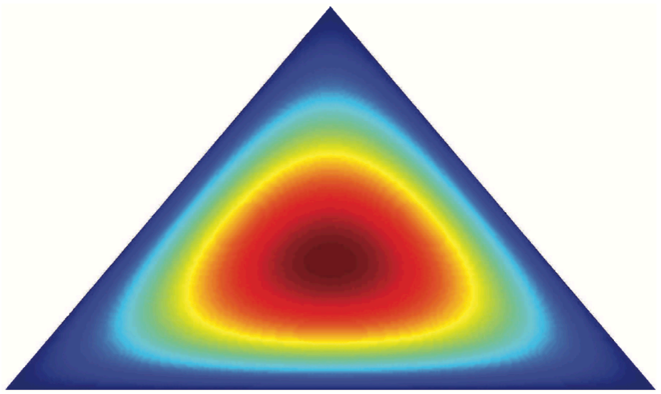
$\alpha = (2, 2, 2)$



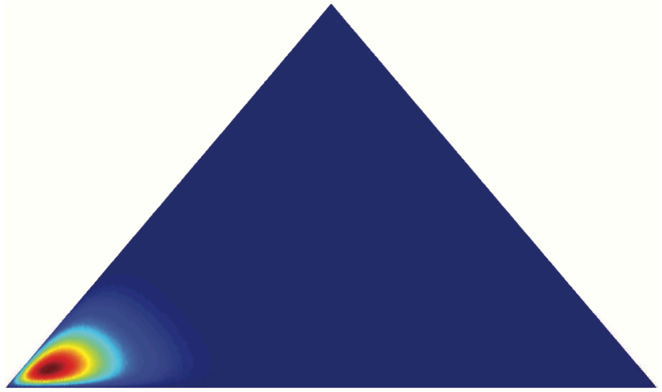
$\alpha = (20, 2, 2)$

MAP - Extension to multinoulli distribution

- Conjugate prior? *Dirichlet distribution*
- $$P(\theta \mid \alpha) = \frac{1}{B(\alpha)} \prod_{j=1}^{K} \theta_j^{\alpha_j - 1}$$ if θ is probability vector (zero otherwise)



$\alpha = (2, 2, 2)$



$\alpha = (20, 2, 2)$

- If we have N_j occurrences of class j, then posterior distribution is

$$P(\theta \mid D) = \frac{P(D \mid \theta) p(\theta)}{P(D)} \propto \prod_{j=1}^{K} \theta_j^{\alpha_j + n_j - 1}$$