MAP estimation

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Lecture 10 – Part II
and
Lecture 11 – Part I

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? $\hat{\theta}_{\text{MLE}} = \frac{n_1}{n} = \frac{2}{2} = 1$

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

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

$$\ell(y, p) = -y \log p - (1-y)\log(1-p)$$

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

$$E[\ell(Y, 1) \mid \theta = 0.5] = \frac{1}{2}\underbrace{\ell(1,1)}_{=0} + \frac{1}{2}\ell(0,1)$$

$$= \frac{1}{2}\left[\underbrace{-0 \log 1}_{0} - (1-0)\log(1-1)\right]$$

$$= \frac{1}{2}(-\log 0) = \frac{1}{2}(-(-\infty)) = +\infty$$

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?

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

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

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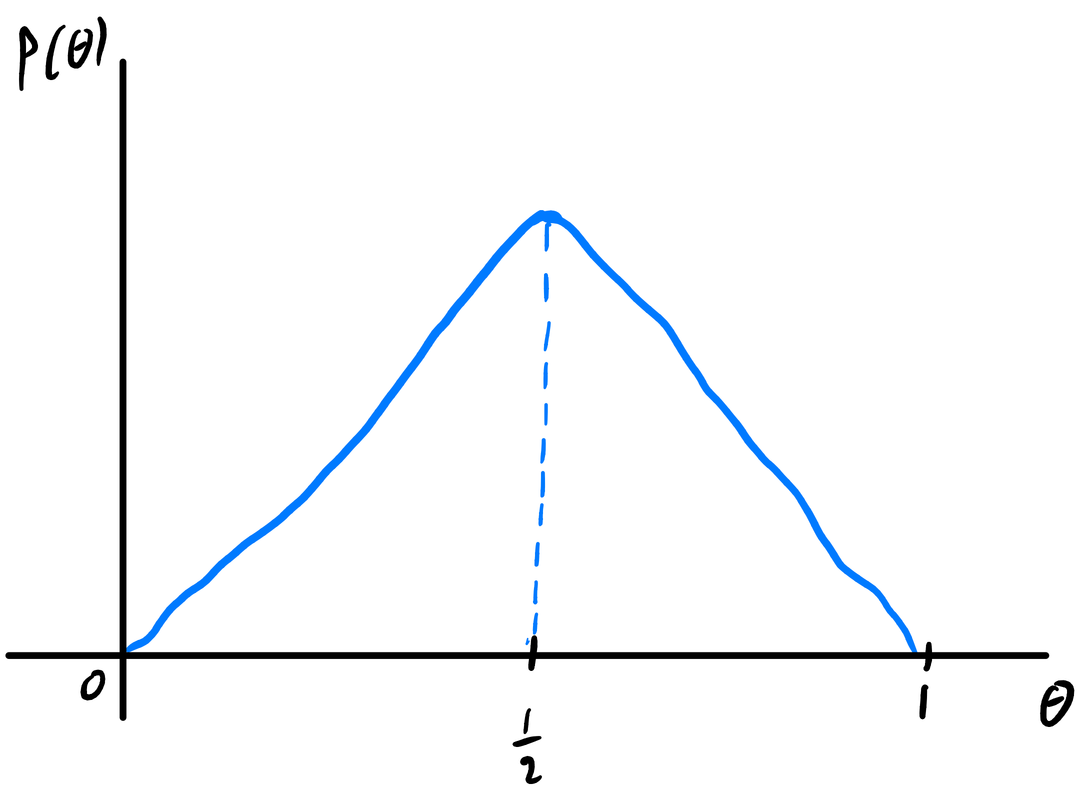
Prior distribution

Bernoulli distribution $\theta \in \Theta = [0,1]$

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



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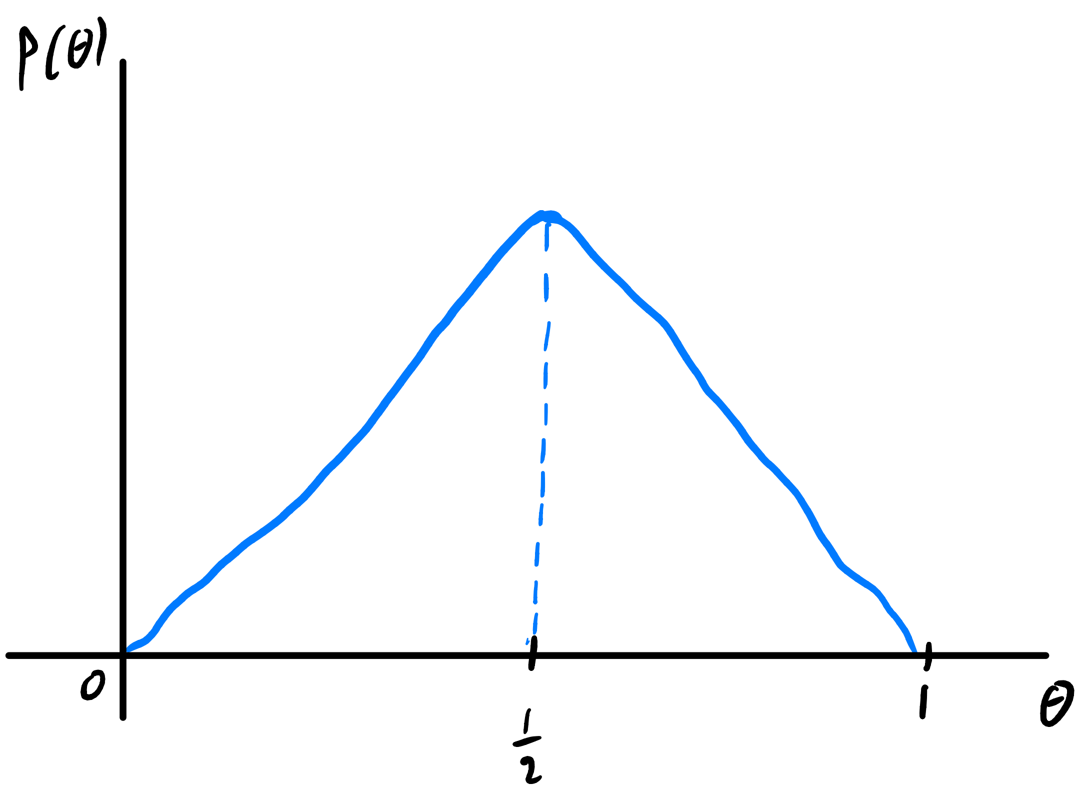
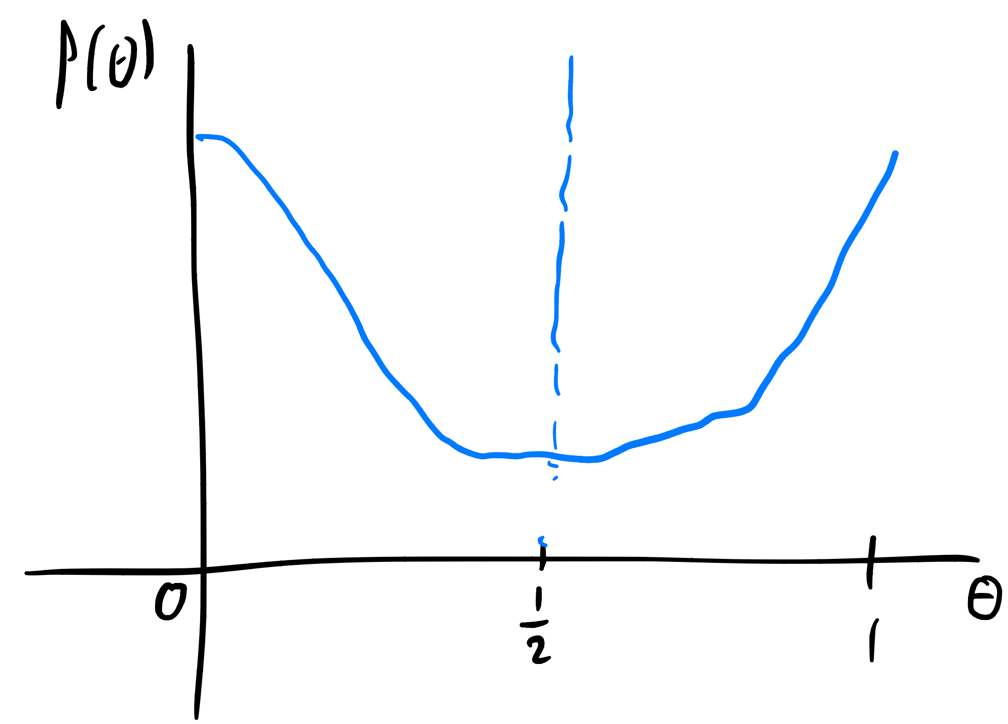


Another example:
"probably unfair coin"!



Posterior distribution

$$P(x \mid y) = \frac{P(y \mid x)\, P(x)}{P(y)} = \frac{P(x, y)}{P(y)}$$

From Bayes rule, we have

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

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

$\Theta = [0,1]$

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Maximum A Posteriori estimate

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

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

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

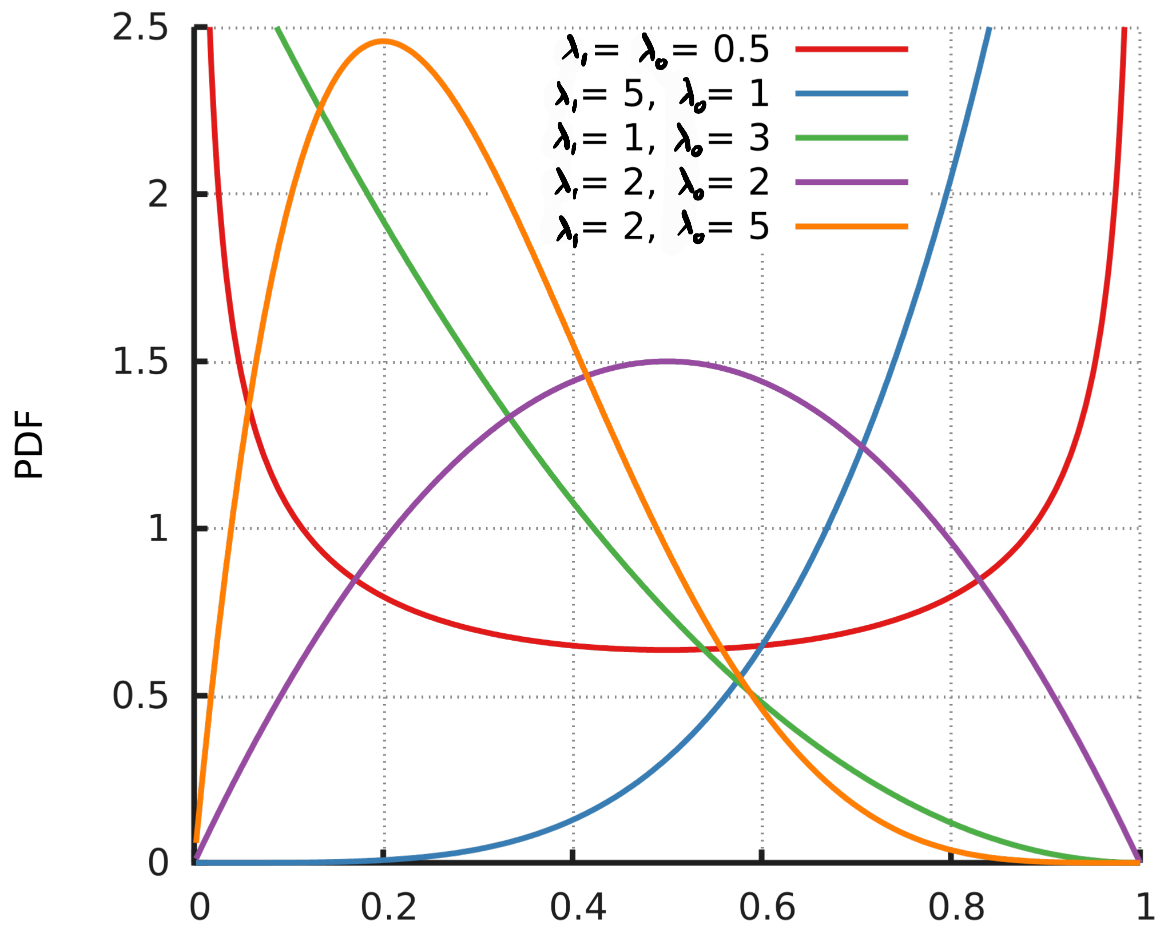
Beta prior distribution

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

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

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

normalization constant



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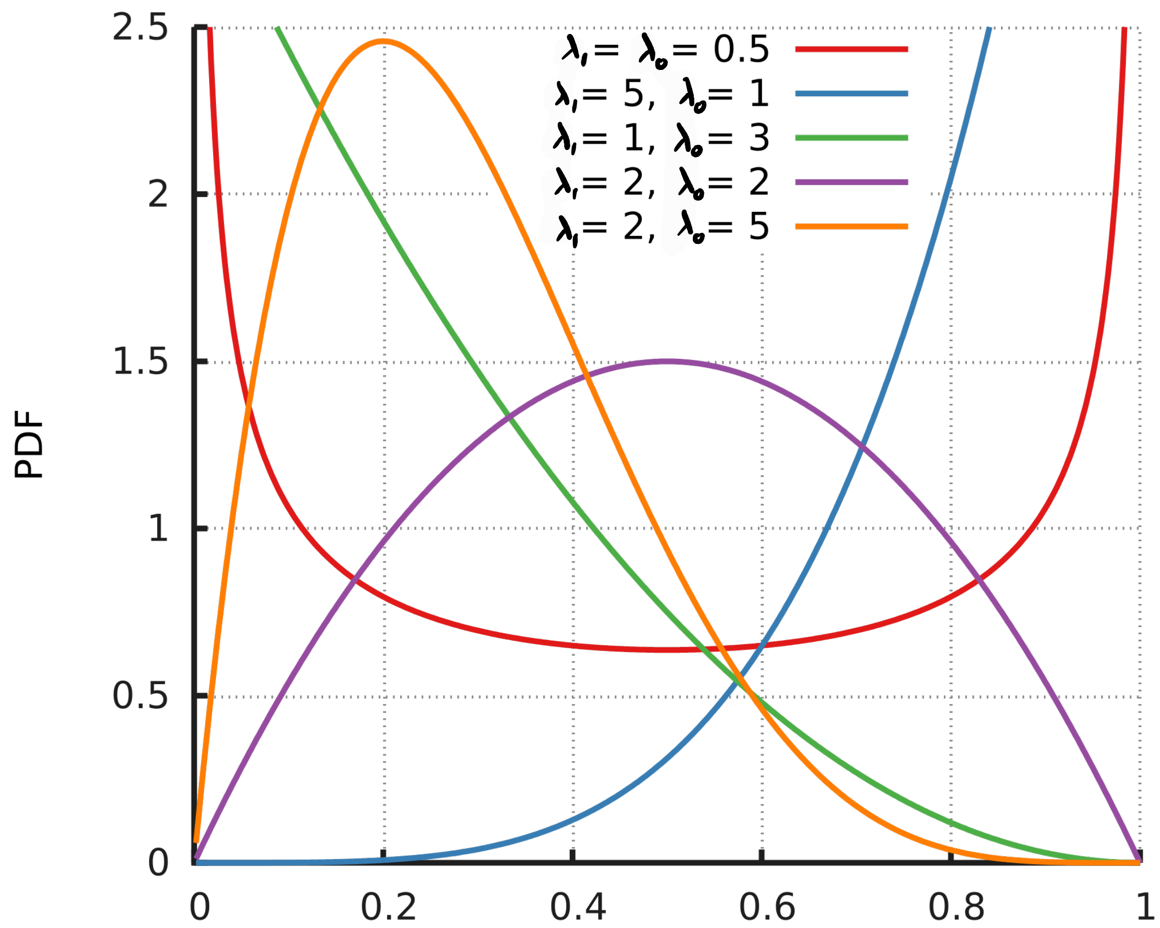

If λ_1 and λ_0 are positive integers, then

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

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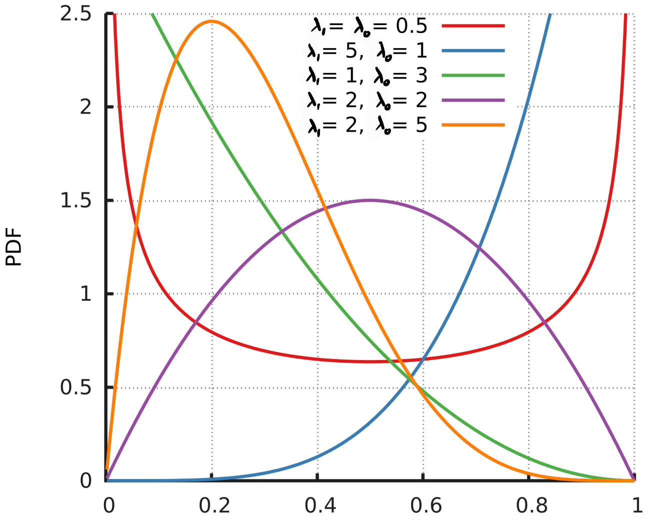

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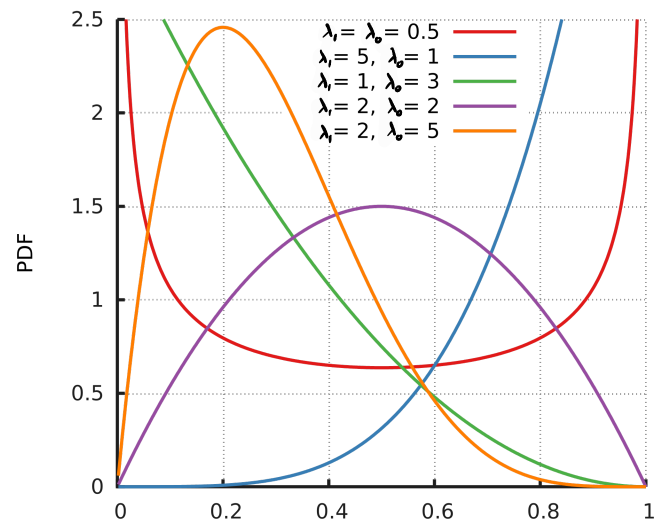

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$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta \in [0,1]} P(D \mid \theta) P(\theta) = \arg\max_{\theta \in [0,1]} \theta^{n_1}(1-\theta)^{n_0}\theta^{\lambda_1 - 1}(1-\theta)^{\lambda_0 - 1}$$

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

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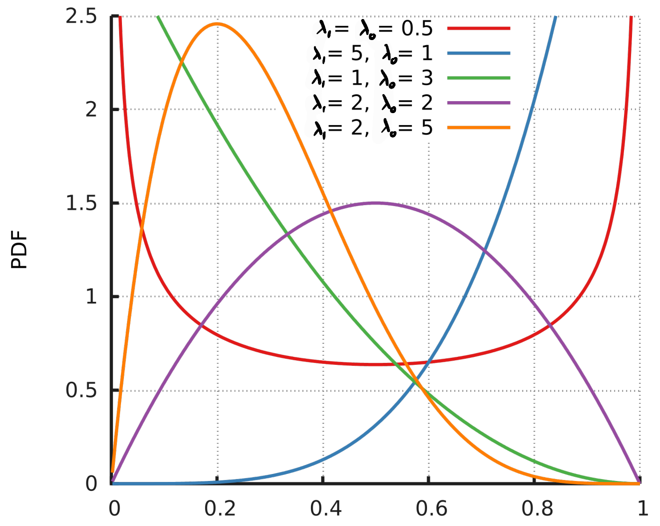

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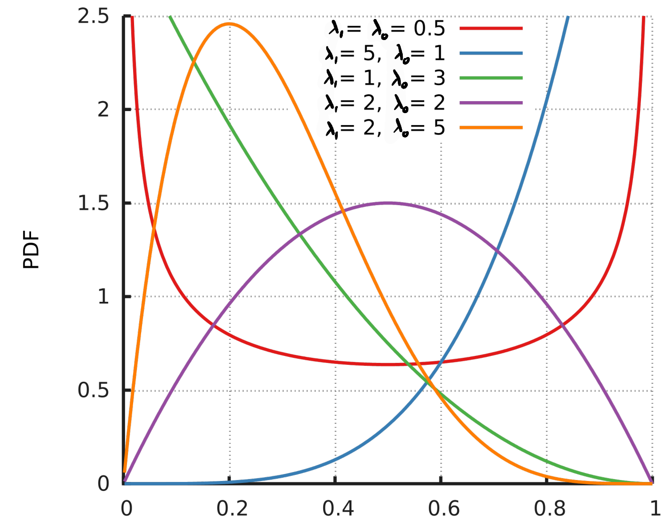

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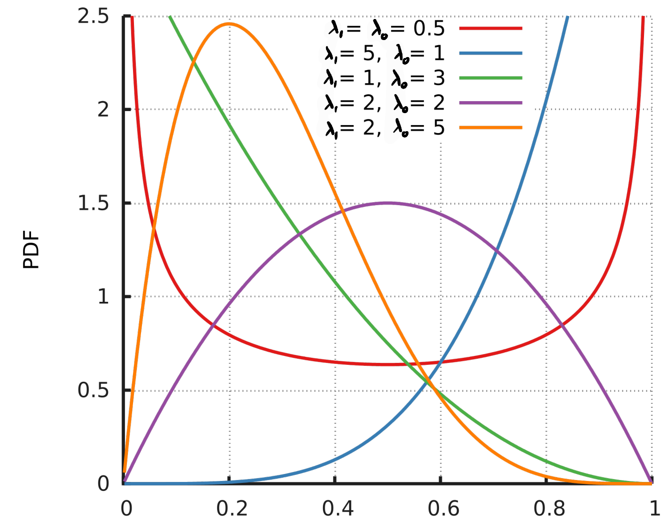

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$\tilde{n}_1 = n_1 + \lambda_1 - 1$

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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?

$\lambda_1 - 1 = c$ $\lambda_1 = c + 1$

$\lambda_0 = c + 1$

MAP estimation ⟺ 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!

$$\max_{\theta \in \Theta} \; P(\theta \mid D)$$

$$\equiv \max_{\theta} \; P(D \mid \theta)\, P(\theta)$$

$$\equiv \max_{\theta} \; \log P(D \mid \theta) + \log P(\theta)$$

NLL — negative log likelihood

$$\theta^{-(\lambda_1 - 1)} \quad (1-\theta)^{-(\lambda_0 - 1)}$$

$$\equiv \min_{\theta} \; -\log P(D \mid \theta) - \log P(\theta)$$

$$\equiv \min_{\theta} \; \sum_{i=1}^{n} \ell_{c-e}(y_i, \theta) + \log \left(\frac{1}{\theta^{\lambda_1 - 1} (1-\theta)^{\lambda_0 - 1}} \right)$$

$$\equiv \min_{\theta} \; \sum_{i=1}^{n} \ell_{c-e}(y_i, \theta) + (\lambda_1 - 1) \log \frac{1}{\theta} + (\lambda_0 - 1) \log \frac{1}{1-\theta}$$

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 $\sum_{j=1}^{K} \theta_j = 1$ $\theta_j = \Pr(y = j)$

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

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

$$y = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

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Multiclass cross-entropy loss

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

suppose n_j is # of times we observed label j

What is the MLE?

$\frac{n_j}{n}$

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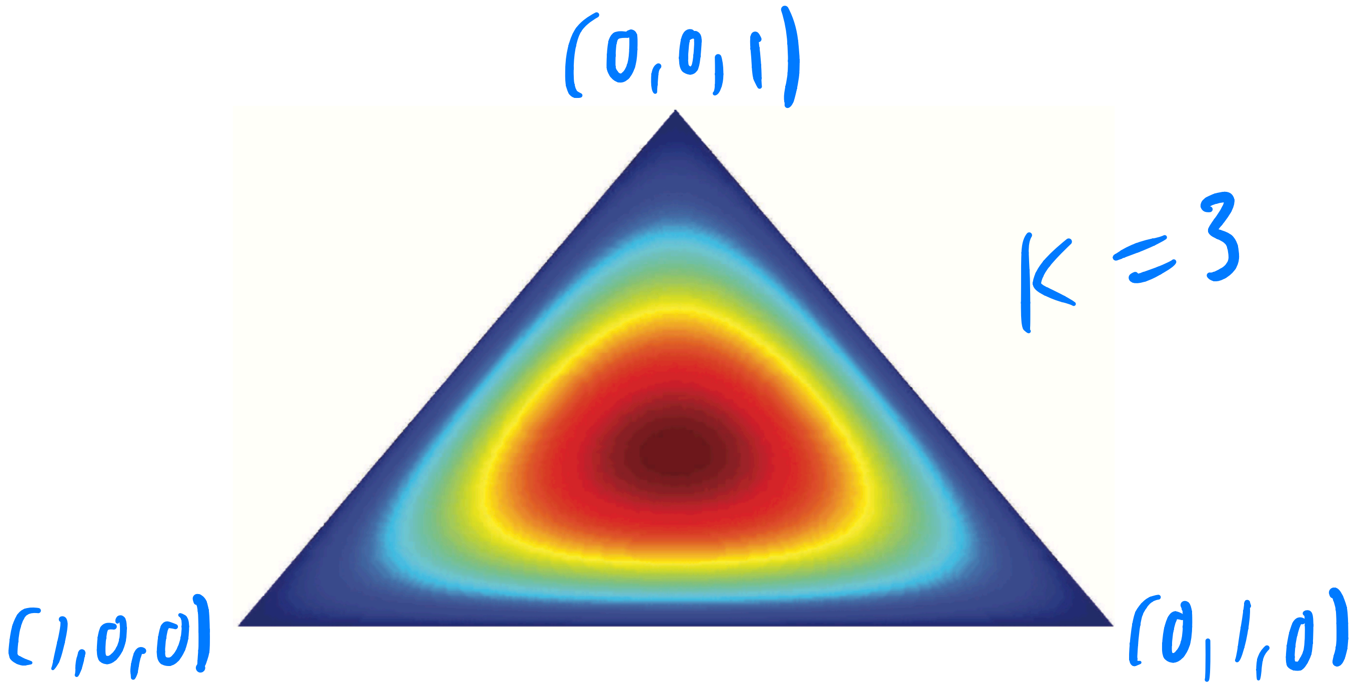
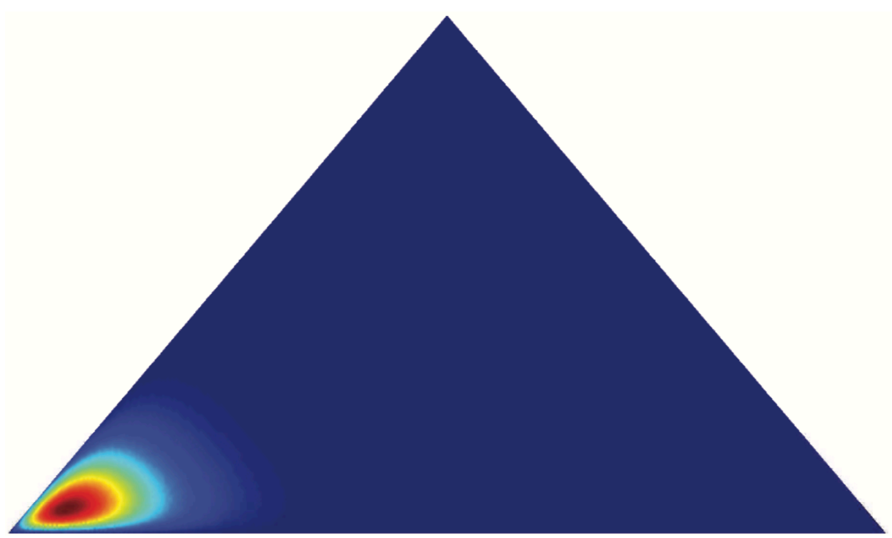
What is the MLE? $\hat{\theta}_j = \frac{n_j}{n}$ ← number of examples with label j

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)



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



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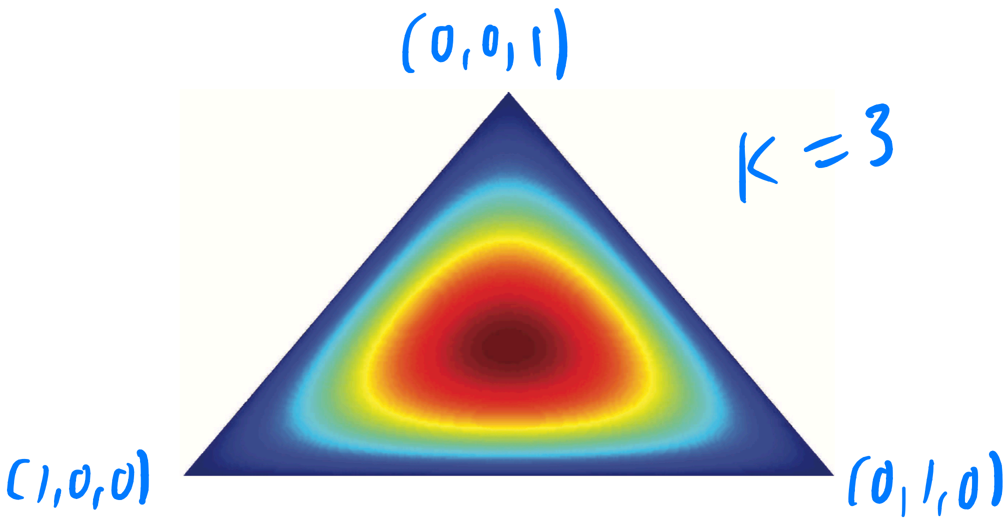

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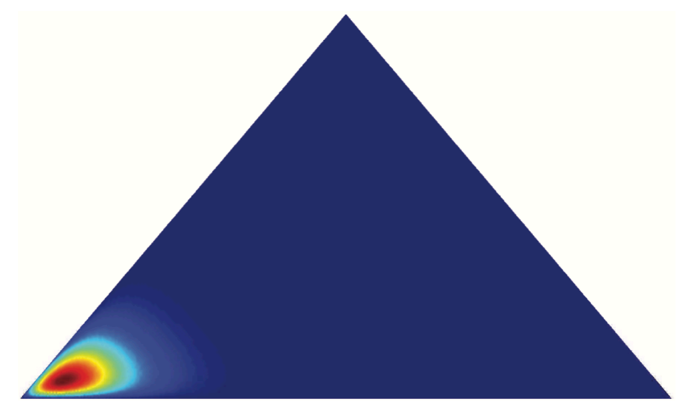

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- If we have N_j occurrences of class j, then posterior distribution is

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