COMP90051 Statistical Machine Learning

Workshop Week 2

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https://github.com/HanXudong/COMP90051_Workshops

Your tutor

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- Slides https://github.com/HanXudong/COMP90051_Workshops

Learning Outcomes

At the end of this workshop you should:

- Be familiar with the Python ecosystem for ML
- Develop intuition about the role of the prior and posterior in Bayesian inference. See "worksheet02.ipynb".

The SciPy stack

NumPy

- Library for working with large multidimensional arrays
- High-level functions for arrays

SciPy

- Scientific computing library
- Functionality includes: statistics/random number generation, linear algebra, optimisation, special functions

scikit learn

- Machine learning library
- Includes implementations of most models covered in this course (exception: neural nets)

pandas

- Library for analysis and manipulation of tabular data
- Provides similar functionality to DataFrames and dplyr in R

matplotlib

- 2D plotting library
- Provides similar interface to MATLAB

Other libraries in the ecosystem

TensorFlow

- Library for numerical computations using data flow graphs
- Often used for neural nets
- Supports GPU, TPU acceleration

Apache Spark

- Cluster computing framework
- Supports scalable machine learning through Spark MLlib
- Has a Python API

Keras

- High-level neural net library written in Python
- Supports various backends: TensorFlow, CNTK and Theano

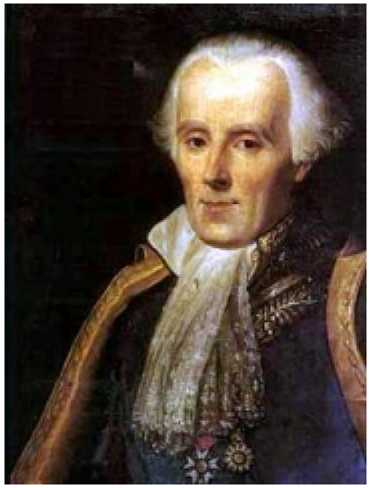
PyStan

- A probabilistic programming language written in C++
- Great for smaller-scale statistical modelling
- Has a Python API

PyMC3

- A probabilistic programming language written in Python and built on top of Theano
- More "Pythonic" than Stan

Bayesian statistics


Laplace

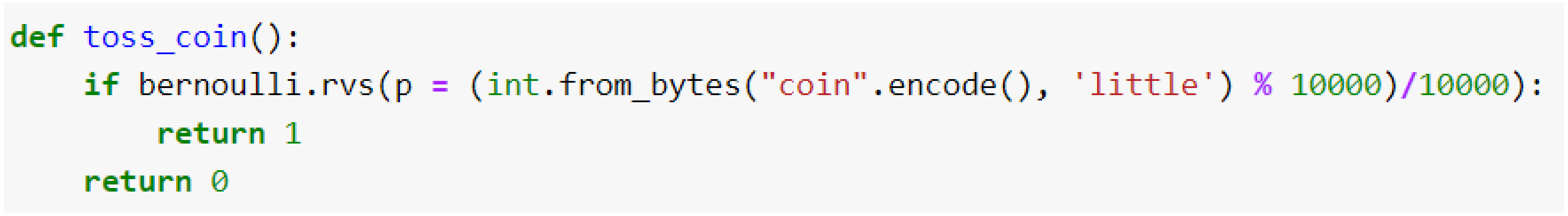
- Probabilities correspond to beliefs
- Parameters
  - Modeled as r.v.'s having distributions
  - Prior belief in θ encoded by prior distribution $P(\theta)$
    - Parameters are modeled like r.v.'s (even if not really random)
    - Thus: data likelihood $P_\theta(X)$ written as conditional $P(X|\theta)$
  - Rather than point estimate $\hat{\theta}$, Bayesians update belief $P(\theta)$ with observed data to $P(\theta|X)$ the posterior distribution)

1. A lucky find

You're interested in determining whether the coin is biased.

Bernoulli Distribution

- Let x_n denote the result of nth flip.
- $x_n = \begin{cases} 1, if\ heads \\ 0, if\ tails \end{cases}$
- $x_n \sim Bernoulli(\theta)$
- $f(x_n|\theta) = \ \theta^{x_n}(1-\theta)^{(1-x_n)}$
- For a fair coin,$\theta = 0.5$.



```
def toss_coin():
    if bernoulli.rvs(p = (int.from_bytes("coin".encode(), 'little') % 10000)/10000):
        return 1
    return 0
```

https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.bernoulli.html#scipy.stats.bernoulli

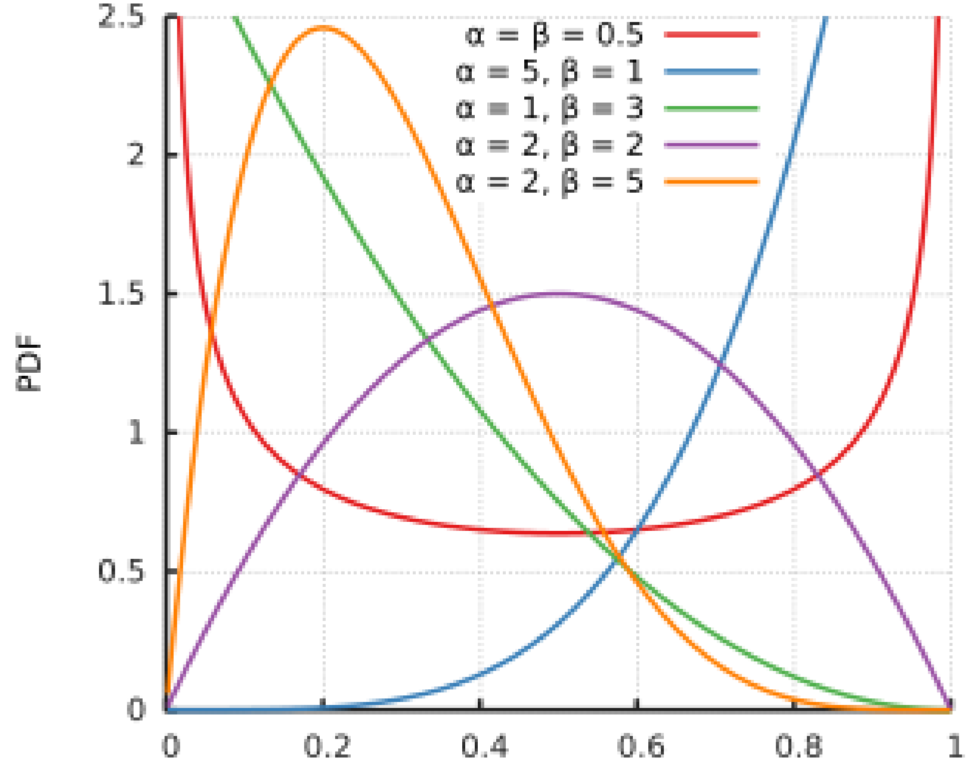
2. Prior belief

- How could we estimate the parameterθ?
  θ = the number of heads / total number
- In a Bayesian way:
  1) Prior belief in θ encoded by prior distribution $P(\theta)$.

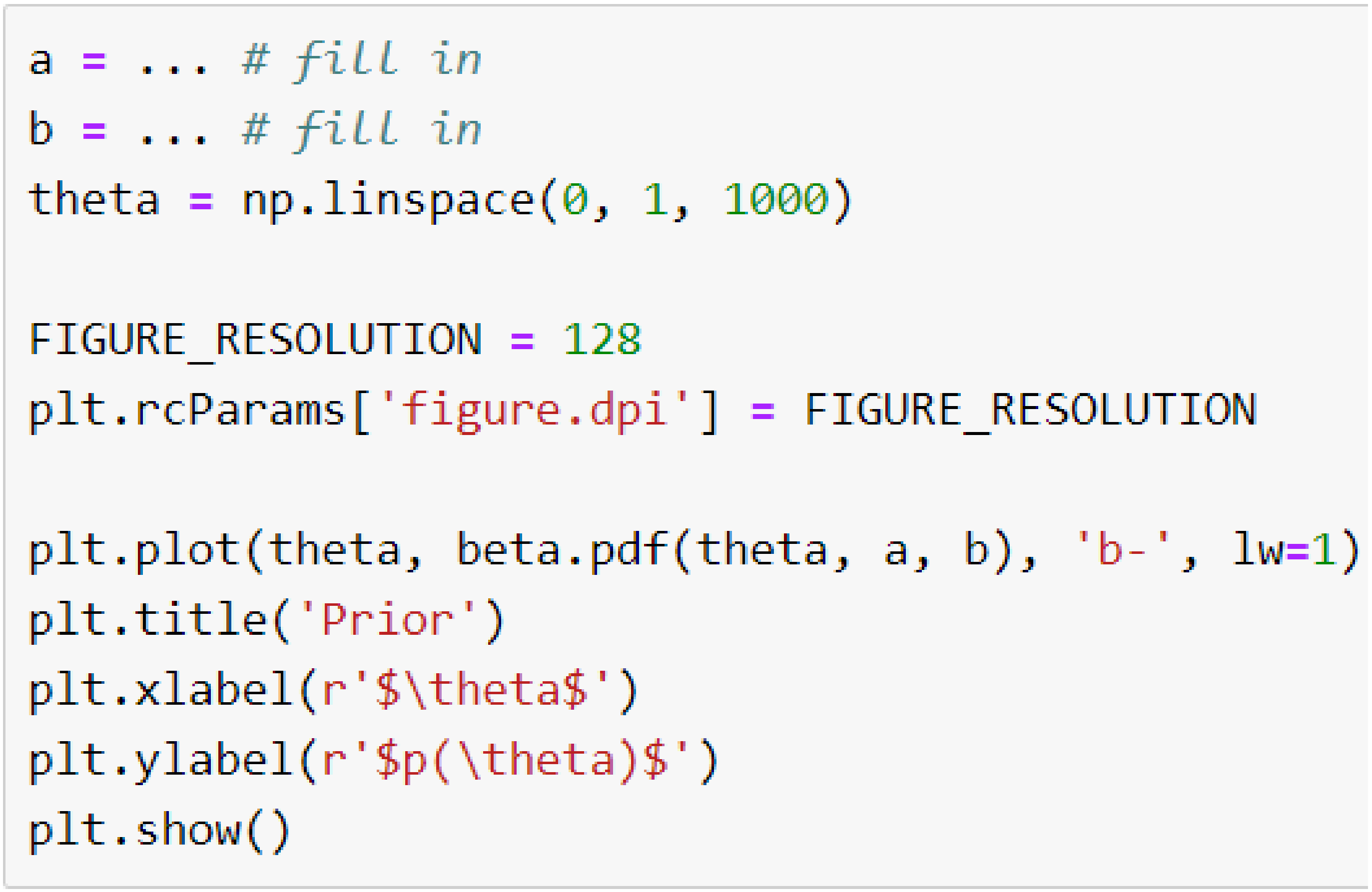
  2) Beliefs (prior) + New observations (likelihood) = New beliefs (posterior)

Parameter θ and Beta distribution

- θ is a probability, thus $0 \leq \theta \leq 1$
- https://en.wikipedia.org/wiki/Beta_distribution



Try

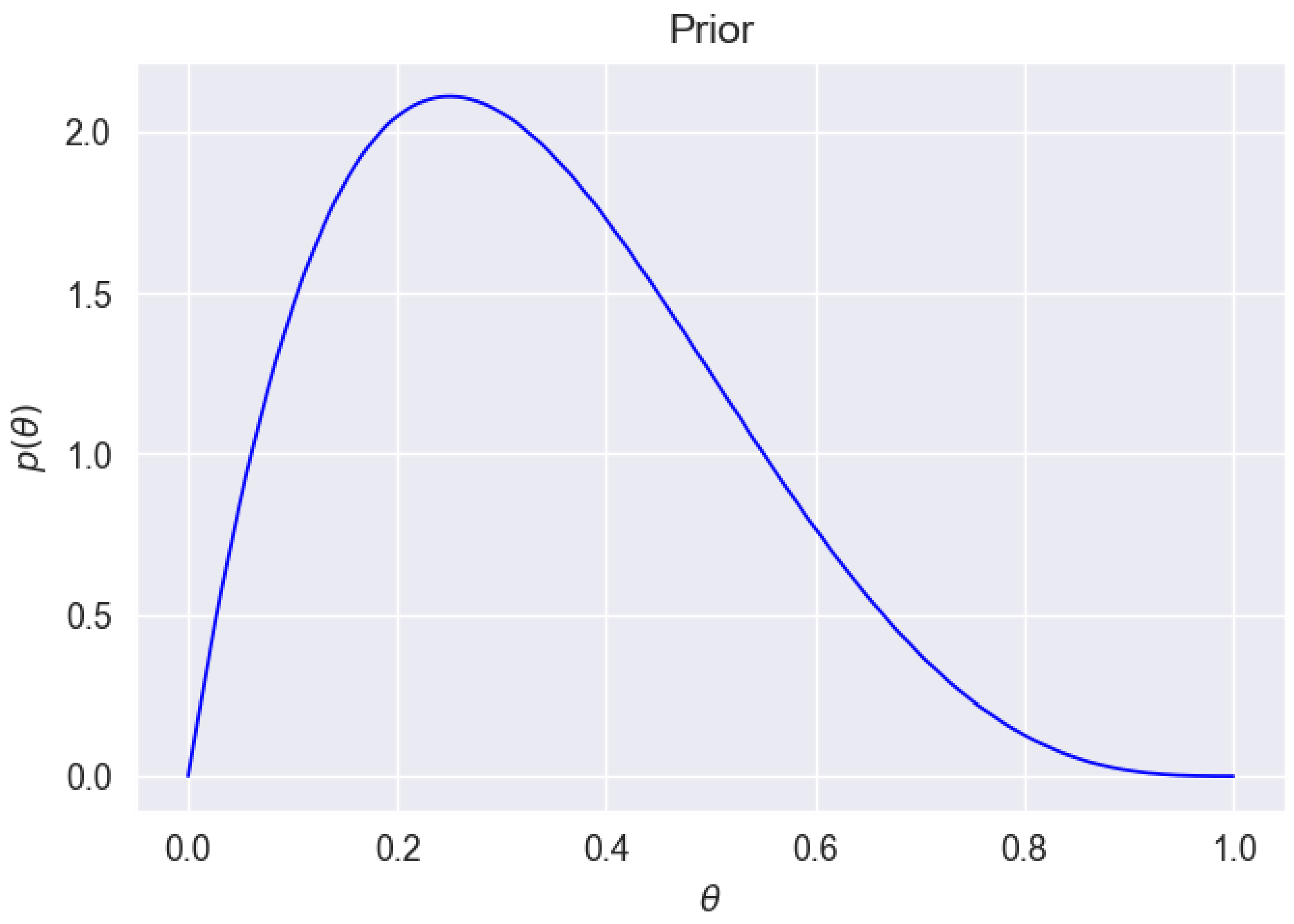


```python
a = ... # fill in
b = ... # fill in
theta = np.linspace(0, 1, 1000)

FIGURE_RESOLUTION = 128
plt.rcParams['figure.dpi'] = FIGURE_RESOLUTION

plt.plot(theta, beta.pdf(theta, a, b), 'b-', lw=1)
plt.title('Prior')
plt.xlabel(r'$\theta$')
plt.ylabel(r'$p(\theta)$')
plt.show()
```

We expect tails are more likely.



3. Posterior updates

- Now toss the coin once and denote the outcome by x_1
- Update beliefs:

$$p(\theta|x_1) = \frac{p(\theta, x_1)}{p(x_1)} = \frac{p(x_1|\theta)p(\theta)}{p(x_1)} \propto p(x_1|\theta)p(\theta)$$

- Now the likelihood:

$$p(x_1|\theta) = \theta^{x_1}(1-\theta)^{(1-x_1)}$$

- $p(\theta)$ is our prior distribution. Beta(a, b)

$$p(\theta) = \frac{1}{B(a,b)}\theta^{a-1}(1-\theta)^{b-1}$$

Exercise: Show (on paper) that the posterior takes the form of a Beta distribution.

$$\theta|x_1 \sim \text{Beta}[x_1 + a, (1 - x_1) + b]$$

If the posterior and prior have the same function form, we say that the prior (in this case Beta) is *conjugate* to the likelihood function (in this case Bernoulli). This is convenient because the prior and posterior distributions have the same functional form, which admits a closed form expression for all posterior updates. This also allows us to ignore constant factors in intermediate calculations, as we may recover the normalizing factors by comparison with the standard form of the relevant density for the posterior.

[Hint: a similar calculation was performed in L2, slide 20 for the case of a normal prior and posterior.]

Exercise: Show that for N coin tosses, the posterior $p(\theta|x_1, \ldots, x_N) = \mathrm{Beta}[N_H + a, N - N_H + b]$ where $N_H = \sum_{n=1}^{N} x_n$ is the number of heads observed.

- We assume the tosses are independent.
- Likelihood now is the product of all the pdf of each x.

$$p(\theta|x_1, x_2, \ldots, x_n) = \prod f(x_i|\theta)$$

- Remember

$$p(x_1|\theta) = \theta^{x_1}(1-\theta)^{(1-x_1)}$$

4. MAP estimator and MLE estimator

The posterior $\theta|x_1, \ldots, x_N$ contains all the information we know about θ after observing N coin tosses. One way of obtaining a point estimate of θ from the posterior, is to take the value with the maximum a posteriori probability (MAP):

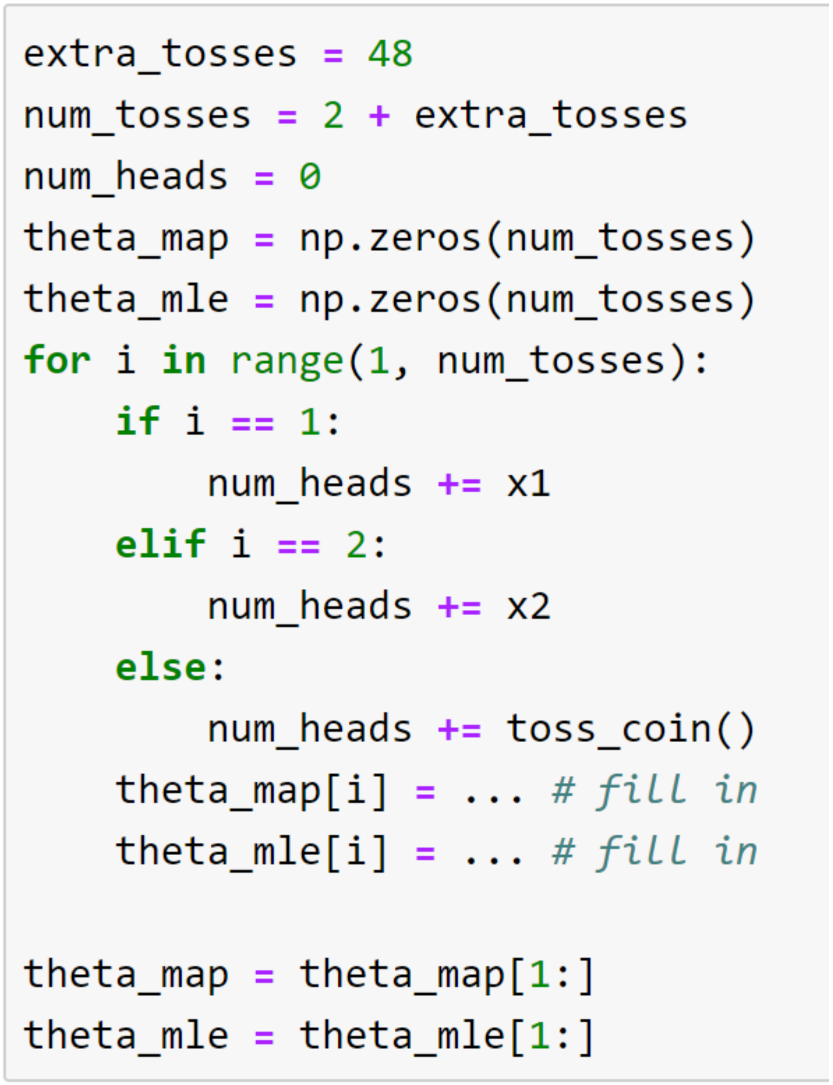
Mode

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg\max_{\theta} p(\theta|x_1, \ldots, x_N) \\ &= \frac{N_H + a - 1}{N + a + b - 2}\end{aligned}$$

In general, the MAP estimator gives a different result to the maximum likelihood estimator (MLE) for θ:

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg\max_{\theta} p(x_1, \ldots, x_N|\theta) \\ &= \frac{N_H}{N}\end{aligned}$$

5. Convergence of the estimates



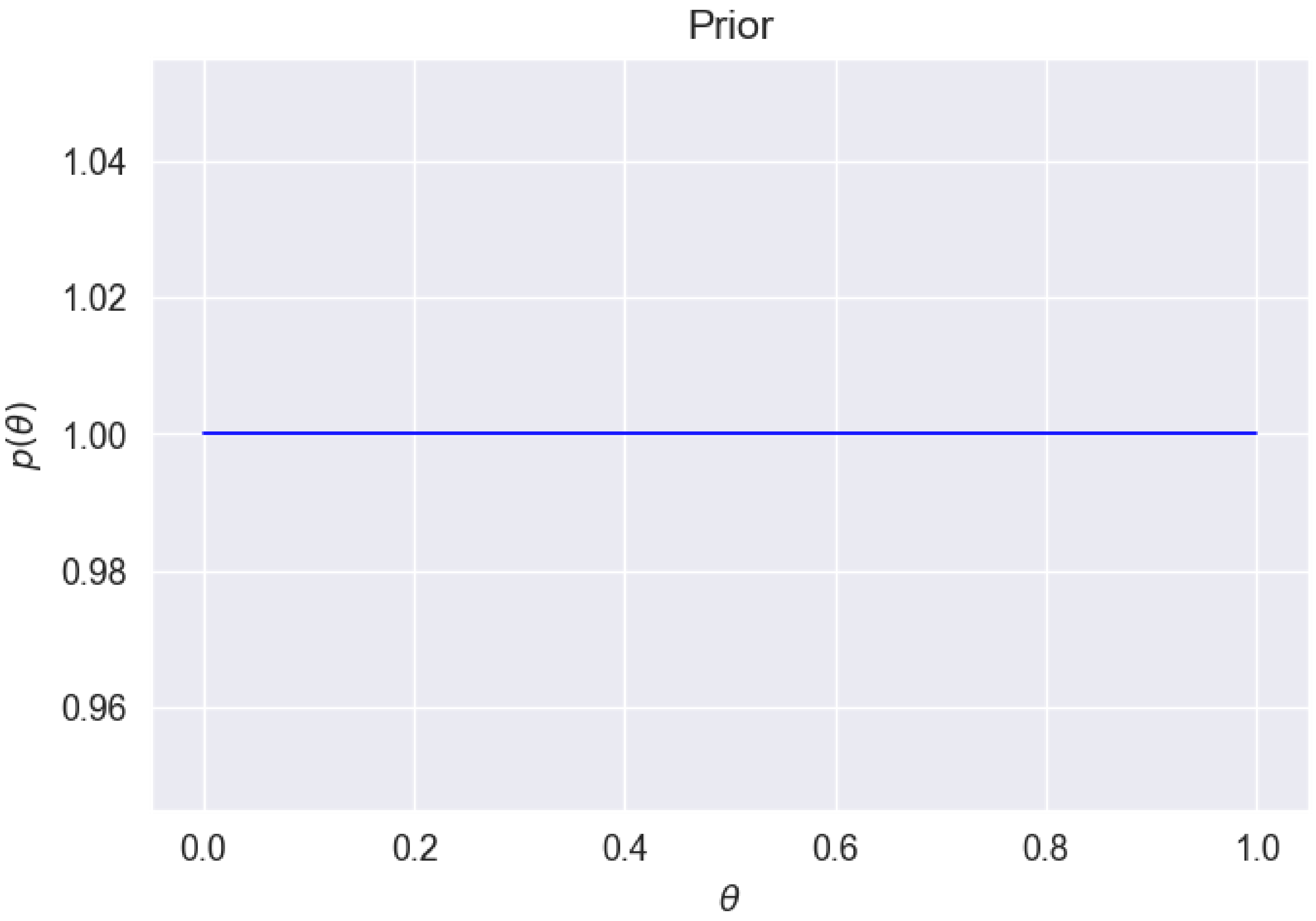
```
extra_tosses = 48
num_tosses = 2 + extra_tosses
num_heads = 0
theta_map = np.zeros(num_tosses)
theta_mle = np.zeros(num_tosses)
for i in range(1, num_tosses):
    if i == 1:
        num_heads += x1
    elif i == 2:
        num_heads += x2
    else:
        num_heads += toss_coin()
    theta_map[i] = ... # fill in
    theta_mle[i] = ... # fill in

theta_map = theta_map[1:]
theta_mle = theta_mle[1:]
```

$$\hat{\theta}_{MAP} = \arg\max_{\theta} p(\theta | x_1, \ldots, x_N) = \frac{N_H + a - 1}{N + a + b - 2}$$

$$\hat{\theta}_{MLE} = \arg\max_{\theta} p(x_1, \ldots, x_N | \theta) = \frac{N_H}{N}$$

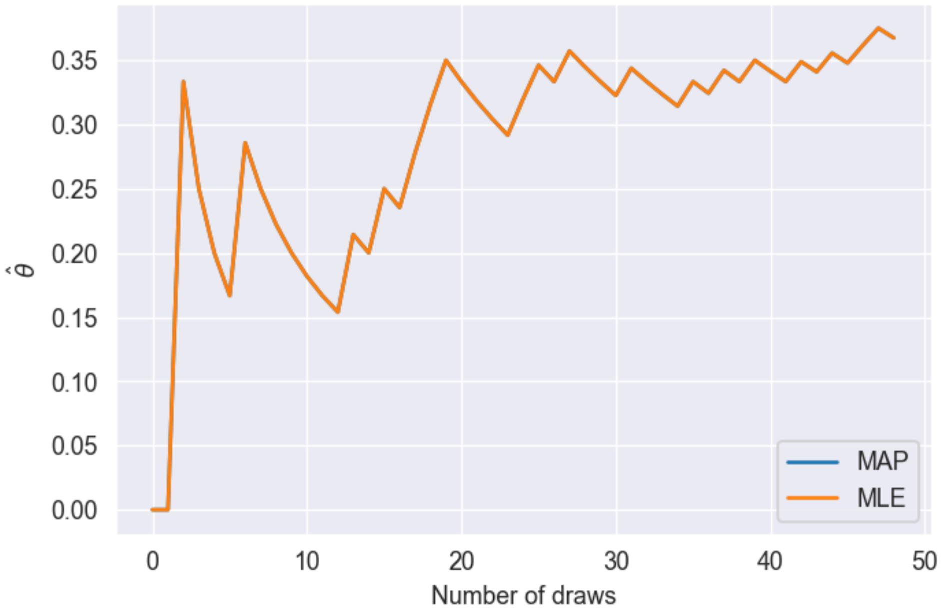
What happens if you set a=b=1?



What happens if you set a=b=1?

$$\hat{\theta}_{MAP} = \arg\max_{\theta} p(\theta | x_1, \ldots, x_N) = \frac{N_H + a - 1}{N + a + b - 2}$$

$$\hat{\theta}_{MLE} = \arg\max_{\theta} p(x_1, \ldots, x_N | \theta) = \frac{N_H}{N}$$


$\hat{\theta}$
Number of draws
MAP
MLE