

Introduction: Estimating Probabilities with Bayesian Inference

In this notebook, we'll look at solving the following statistics problem in a Bayesian Framework. (Problem courtesy of Allen Downey on Twitter: tweet link)

Today's Bayesian problem of the week: Suppose we visit a wild animal preserve where we know that the only animals are lions and tigers and bears, but we don't know how many of each there are. During the tour, we see 3 lions, 2 tigers, and 1 bear. Assuming that every animal had an equal chance to appear in our sample, estimate the prevalence of each species. What is the probability that the next animal we see is a bear?

Solution next week!

Our goal is to estimate the percentage of each species and determine the probability that the next animal is a bear.

Bayesian Approach

In a frequentist view, we would just use the observed animals to estimate the

prevalence and let the data completely speak for itself. In contrast, in a Bayesian framework, we incorporate priors, which here are set to be equal for all species. In the case of infinite observations, the effect of the priors disappear and we only use the data. Due to the limited number of observations, the *priors* will still have an large effect on the prevalence we obtain, and the *uncertainty* will be large. We can alter the weight of the priors depending on our confidence in them (we'll see this in the notebook).

Model

The overall system is as follows (each part will be explained):

- 1. The underlying model is a multinomial distribution with parameters p_k
- 2. The *prior* distribution of p_k is a Dirichlet Distribution
- 3. The α vector is a parameter of the prior Dirichlet Distribution, hence a *hyperparameter*

A Multinomial Distribution with a Dirichlet Prior is referred to as a Dirichlet-Multinomial Distribution.

Our model can be expressed in equations as:

$$oldsymbol{lpha} = (lpha_1, \ldots, lpha_K) = ext{concentration hyperparameter} \ oldsymbol{\mathrm{p}} \mid oldsymbol{lpha} = (p_1, \ldots, p_K) \sim ext{Dir}(K, oldsymbol{lpha}) \ \mathbb{X} \mid oldsymbol{\mathrm{p}} = (x_1, \ldots, x_K) \sim ext{Mult}(K, oldsymbol{\mathrm{p}})$$

Our goal is to find $p_{
m lions}$, $p_{
m tigers}$, $p_{
m bears}$ given the observation vector $c=[c_{lions},c_{tigers},c_{bears}]$

Multinomial Distribution

This problem is a classic example of the multinomial distribution which describes a situation in which we have n independent trials, each with k possible outcomes. With the wildlife preserve problem, n = 6 and k = 3. It is characterized by the probability of each outcome, p_k which must sum to 1. Our goal is to find $p_{\rm lions}$, $p_{\rm tigers}$, $p_{\rm bears}$ given the observations lions: 3, tigers: 2, and bears: 1.

Dirichlet Distribution

The prior for a multinomial distribution in Bayesian statistics is a Dirichlet distribution. (Together a multinomial distribution with a dirichlet prior is

called, not surprisingly, a Dirichlet-Multinomial Distribution. The Dirichlet distribution is characterized by α , the concentration hyperparameter vector.

Hyperparameters and Prior Beliefs

The α vector is a hyperparameter, a parameter of a prior distribution. This vector in turn could have its *own prior* distribution which is called a *hyperprior*. We won't use a hyperprior, but instead will only specify the hyperparameters.

The hyperparameter vector can be thought of as pseudo-counts, which we use to show our prior belief for the prevalence of each species. If want a uniform hyperparameter reflecting that we believe the chance of observing any species is the same we set each element of alpha equal such as $\alpha=[1,1,1]$. We can increase our decrease the effect of the priors by increasing or decreasing the values. This can be useful when we have more or less confidence in our prior beliefs. We'll see the effects of adjusting the hyperparameters in the notebook, but will mainly work with $\alpha=[1,1,1]$.

The most helpful way to think of the α vector is as our prior beliefs. We encode these using pseudocounts, and, if we initially think each species has the same prevalence, then we set the pseudocounts to be equal.

With the basic model in place, let's get to working through this problem!

```
In [1]:
         import pandas as pd
         import numpy as np
         # Visualizations
         import matplotlib.pyplot as plt
         import seaborn as sns
         plt.style.use('fivethirtyeight')
         plt.rcParams['font.size'] = 22
         %matplotlib inline
         from matplotlib import MatplotlibDeprecationWarning
         import warnings
         warnings.filterwarnings('ignore', category=FutureWarning)
         warnings.filterwarnings('ignore', category=MatplotlibDeprecation
         import pymc3 as pm
         # Helper functions
         from utils import draw pdf contours, Dirichlet, plot points, ann
```

Droblom Specifics

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We'll mainly use one version of the hyperparameters, $\alpha=[1,1,1]$. We'll also try some other values to see how that changes the problem. Remember, altering the hyperparameters is like chaning our confidence in our initial beliefs.

Expected Value

Source: http://users.cecs.anu.edu.au/~ssanner/MLSS2010/Johnson1.pdf

One way to get a single point estimate of the prevalence is to use the **expected value** of the posterior for p_k . The expected value of a Dirichlet-Multinomial Distribution is:

$$\mathrm{E}[p_i \mid \mathbb{X}, oldsymbol{lpha}] = rac{c_i + lpha_i}{N + \sum_k lpha_k}$$

Using $\alpha=[1,1,1]$, and the observation vector c=[3,2,1] we get the expected prevalances:

$$p_{lions}=rac{4}{9}=44.4\%$$

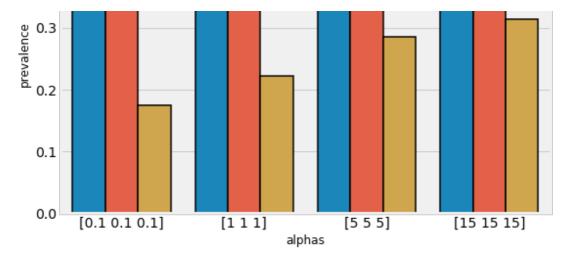
$$p_{tigers}=rac{3}{9}=33.3\%$$

$$p_{bears}=rac{2}{9}=22.2\%$$

However, at least to me, this result is unsatisfying because it does not show our uncertainty due to the limited amount of data. For that, we turn to Bayesian modeling and sampling from the posterior with MCMC (in a little bit). The expected value represents our best guess for a single trial. We can also alter the expected value by adjusting the weight of the hyperparameter vector.

First, let's confirm our math using the default alpha vector.

```
In [3]:
         display probs(dict(zip(animals, (alphas + c) / (c.sum() + alphas
                           Prevalence: 44.44%.
        Species: lions
        Species: tigers
                           Prevalence: 33.33%.
        Species: bears
                           Prevalence: 22.22%.
        This is as expected.
In [4]:
         display probs(dict(zip(animals, (4/9, 3/9, 2/9))))
        Species: lions
                           Prevalence: 44.44%.
        Species: tigers
                           Prevalence: 33.33%.
                           Prevalence: 22.22%.
        Species: bears
        Now, let's try a few different hyperparameter values (our previous beliefs)
        and see how that affects the expected value.
In [5]:
         values = []
         for alpha new in alpha list:
             values.append((alpha_new + c) / (c.sum() + alpha_new.sum()))
         value_df = pd.DataFrame(values, columns = animals)
         value df['alphas'] = [str(x) for x in alpha list]
         value df
Out[5]:
               lions
                       tigers
                                bears
                                          alphas
         0 0.492063 0.333333 0.174603 [0.1 0.1 0.1]
         1 0.444444 0.333333 0.222222
                                           [1 1 1]
         2 0.380952 0.333333 0.285714
                                          [5555]
         3 0.352941 0.333333 0.313725 [15 15 15]
In [6]:
         melted = pd.melt(value df, id vars = 'alphas', value name='preva
                  var_name = 'species')
         plt.figure(figsize = (8, 6))
         sns.barplot(x = 'alphas', y = 'prevalence', hue = 'species', dat
                      edgecolor = 'k', linewidth = 1.5);
         plt.xticks(size = 14); plt.yticks(size = 14)
         plt.title('Expected Value');
                                      Expected Value
           0.5
                                                                     species
                                                                       tigers
                                                                      bears
           0.4
```



We see that as the weight of the hyperparameters increases, the expected prevalence of the species converges to around 1/3. Intuitively, this makes sense: as we increase the number of pseudocounts, we express more strongly our initial belief of the equal prevalence. With heavier priors, the data (observations) matters less.

On the other hand, when we decrease the weight of the hyperparameters, the data matters more and the expected value converges on the counts. The ultimate choice of the hyperparameters depends on our confidence in our prior belief.

Maximum A Posterior Estimation

Source: http://users.cecs.anu.edu.au/~ssanner/MLSS2010/Johnson1.pdf

The maximum a posterior (MAP) is another point estimate that is equal to the mode of the posterior distribution. The MAP for a Dirichlet-Multinomial is:

$$rg \max_{\mathbf{p}} p(\mathbf{p} \mid \mathbb{X}) = rac{lpha_i + c_i - 1}{\sum_i (lpha_i + c_i - 1)}, \qquad orall i \; lpha_i + c_i > 1$$

In the case of lpha=[1,1,1] this becomes the frequency observed in the data.

```
Species: tigers Prevalence: 33.33%.
Species: bears Prevalence: 16.67%.
```

Again, this estimate is reasonable because with our choice of hyperparameters, we are considering only the data for the MAP. Let's look at what happens when we change the hyperparameters.

```
In [9]:
    values = []
    for alpha_new in alpha_list:
        values.append((alpha_new + c - 1) / sum(alpha_new + c - 1))

    value_df = pd.DataFrame(values, columns = animals)
    value_df['alphas'] = [str(x) for x in alpha_list]
    value_df
```

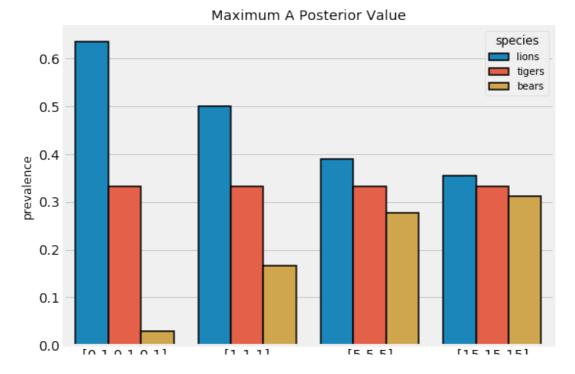
```
        Out[9]:
        lions
        tigers
        bears
        alphas

        0
        0.636364
        0.333333
        0.030303
        [0.1 0.1 0.1]

        1
        0.500000
        0.333333
        0.166667
        [111]

        2
        0.388889
        0.333333
        0.277778
        [5 5 5]

        3
        0.354167
        0.333333
        0.312500
        [15 15 15]
```



The same effect occurs, representing our decreased or increased confidence in the prior belief.

Both the Expected Value and Maximum A Posterior only provide a point estimate with no uncertainty. Given the relatively few observations, there should be a large amount of uncertainty; to capture that, we turn to Bayesian Modeling.

Bayesian Model

Now we'll get into building and sampling from a Bayesian model. As a reminder, we are using a multinomial as our model, a Dirichlet distribution as the prior, and a specified hyperparameter vector. The objective is to find the parameters of the multinomial, p_k which are the probability of each species given the evidence.

$$(\mathbf{p} \mid \mathbb{X}, \boldsymbol{\alpha})$$

PyMC3 and MCMC

To solve the problem, we'll build a model in PyMC3 and then use a variant of Markov Chain Monte Carlo (the No-UTurn Sampler specifically) to draw samples from the posterior. With enough samples, the estimate will converge on the true posterior. Along with single point estimates (such as the mean of sampled values), MCMC also gives us built in uncertainty because we get thousands of possible values from the posterior.

Building a model in PyMC3 is simple. Each distribution is specified, along with the required parameters. We assign the observed counts to the observed parameter of the multinomial which in turn has the Dirichlet as the prior.

We'll use lpha=[1,1,1] for our main model.

```
Out [12]: parameters \sim \text{Dirichlet}(a = array) observed_data \sim \text{Multinomial}(n = 6, p = f(parameters, f(f(parameters))))
```

Sampling from the Model

The cell below samples 1000 draws from the posterior in 2 chains. We use 500 samples for tuning which are discarded. This means that for each random variable in the model - the parameters - we will have 2000 values drawn from the posterior distribution.

Inspecting Results

PyMC3 offers comprehensive tools for inspecting the results of a trace. We can start by getting the stats in a dataframe.

```
In [14]:
    summary = pm.summary(trace)
    summary.index = animals
    summary
```

```
        Out[14]:
        mean
        sd
        mc_error
        hpd_2.5
        hpd_97.5
        n_eff
        R

        lions
        0.449862
        0.158911
        0.003371
        0.170494
        0.761727
        1790.050932
        0.999

        tigers
        0.330618
        0.148583
        0.003256
        0.047436
        0.596449
        1747.828016
        1.000

        bears
        0.219520
        0.134556
        0.003160
        0.011707
        0.479332
        1763.772811
        0.999
```

We can see that the mean of the samples is very close to the expected value. However, instead of just getting one number, we get a range of uncertainty as indicated by the large standard deviation and 95% highest probability interval.

```
In [15]: # Samples
    trace df = pd.DataFrame(trace['parameters'], columns = animals)
```

trace df.head()

```
Out[15]:
                lions
                         tigers
                                   bears
             0.521821 0.387095 0.091084
          1 0.425729 0.538425 0.035846
          2 0.608407 0.369802
                                0.021791
            0.613399 0.326226 0.060375
          4 0.265605 0.252913 0.481482
In [16]:
           trace df.shape
          (2000, 3)
Out[16]:
         For a single point estimate, we can use the mean of the samples.
In [17]:
           # For probabilities use samples after burn in
           pvals = trace df.iloc[:, :3].mean(axis = 0)
           display_probs(dict(zip(animals, pvals)))
          Species: lions
                             Prevalence: 44.99%.
          Species: tigers
                             Prevalence: 33.06%.
                             Prevalence: 21.95%.
          Species: bears
         These numbers align nearly exactly with the expected values! However, we
         also get a range of uncertainty.
In [18]:
           summary.iloc[:, 3:5]
Out[18]:
                 hpd_2.5 hpd_97.5
           lions 0.170494 0.761727
          tigers 0.047436 0.596449
                0.011707 0.479332
          bears
```

We can see the large amount of uncertainty in the estimates due to the limited amount of data. To see the estimates and uncertainty visually, we can use some of PyMC3's built in plots.

Diagnostic Plots

PyMC3 offers a number of plotting options for inspecting our samples.

Posterior Plot

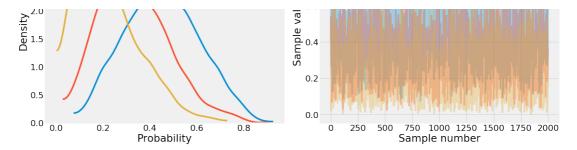
What we see hear is a histogram of the sampled values.

The 95% HPD is the same idea as a 95% confidence interval in frequentist statistics. In Bayesian stats, this is called the Highest Posterior Density.

Traceplot

The traceplot shows a kernel density estimate (a smoothed histogram) on the left and all the samples that were drawn on the right. We collapse the chains on th plots (combined = True) but in reality we drew 2 independent chains.

```
In [20]:
           prop cycle = plt.rcParams['axes.prop cycle']
           cs = [x['color'] for x in list(prop_cycle)]
           ax = pm.traceplot(trace, varnames = ['parameters'], figsize = (2
           ax[0][0].set title('Posterior Probability Distribution'); ax[0][
           ax[0][0].set xlabel('Probability'); ax[0][0].set ylabel('Density')
           ax[0][1].set xlabel('Sample number');
           add_legend(ax[0][0])
           add_legend(ax[0][1])
                Posterior Probability Distribution
                                                           Trace Samples
           3.0
                                        tiaers
                                                                            tiaers
                                        bears
                                                                            bears
           2.5
```



Even here we see a large amount of uncertainty although the model is clear that $p_{bears} < p_{tigers} < p_{lions}$.

Maximum A Posteriori Result with PyMC3

PyMC3 has a method for directly finding the MAP.

The MAP estimates are exactly the same as the observations. These are also the results that a frequentist would come up with!

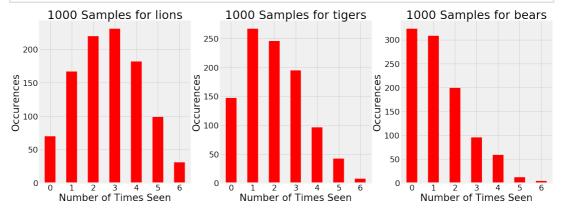
Sample From Posterior

We can now use the posterior (contained in the trace) to draw samples of data. For example, we can simulate 1000 trips to the wildlife preserve as follows.

These represent the estimate number of each species we'd see over 1000 trips to the preserve.

```
In [23]: sample_df = pd.DataFrame(samples['observed_data'], columns = ani
```

```
plt.figure(figsize = (22, 8))
for i, animal in enumerate(sample_df):
    plt.subplot(1, 3, i+1)
    sample_df[animal].value_counts().sort_index().plot.bar(color
    plt.xticks(range(7), range(7), rotation = 0);
    plt.xlabel('Number of Times Seen'); plt.ylabel('Occurences')
    plt.title(f'1000 Samples for {animal}');
```



Even though it's not very likely, it's possible we could see 6 bears and 0 lions and 0 tigers.

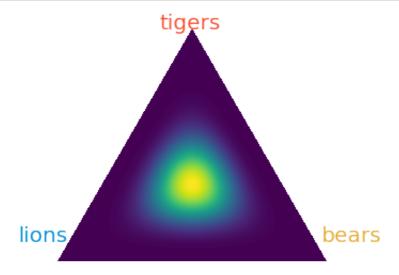
Dirichlet Distribution

We can plot the Dirichlet Distribution as a triangle with colors indicating the value of the hyperparameters. This code is taken from the following sources.

http://blog.bogatron.net/blog/2014/02/02/visualizing-dirichlet-distributions/

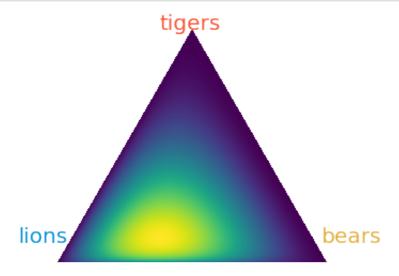
https://gist.github.com/tboggs/8778945

```
In [24]: draw_pdf_contours(Dirichlet(6 * alphas))
    annotate_plot()
```

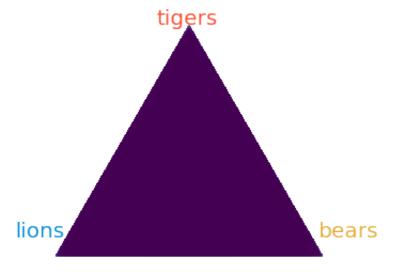


Initially, the probability for all species is equalvalent. After our sampling though we see the balance shift towards the lions.

```
In [25]: draw_pdf_contours(Dirichlet(6 * pvals))
    annotate_plot();
```



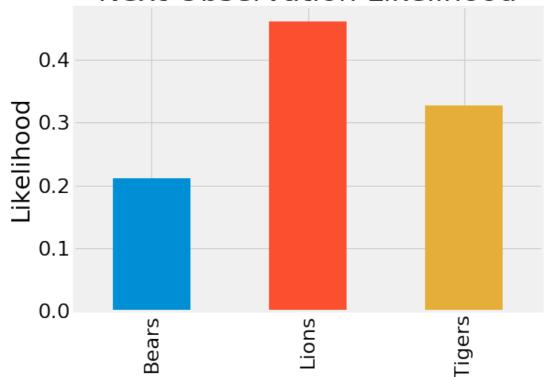
```
In [26]:
    draw_pdf_contours(Dirichlet([0.1, 0.1, 0.1]))
    annotate_plot();
```



Next Observation

In order to find what we can expect from the next observation, we draw a single sample 10000 times from a multinomial distribution. The probability of seeing each species is proportional to that obtained from the sampling.

Next Observation Likelihood



```
In [28]: next_obs.iloc[:, [0, 2]]
```

Out[28]:		variable	total
	1	Bears	0.2111
	3	Lions	0.4616
	5	Tigers	0.3273

More Observations

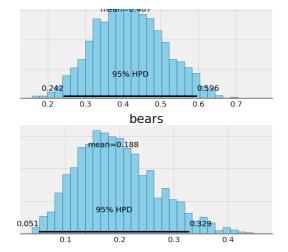
If we have additional observations, more trips to the preserve, we can easily

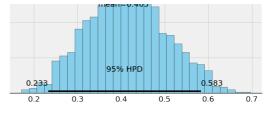
do the sampling taking into account this data.

```
In [29]:
          c = np.array([[3, 2, 1],
                        [2, 3, 1],
                        [3, 2, 1],
                        [2, 3, 1]])
         with pm.Model() as model:
              # Parameters are a dirichlet distribution
              parameters = pm.Dirichlet('parameters', a=alphas, shape=3)
              # Observed data is a multinomial distribution
              observed_data = pm.Multinomial(
                  'observed_data', n=6, p=parameters, shape=3, observed=c)
              trace = pm.sample(draws=1000, chains=2, tune=500, discard tu
         Auto-assigning NUTS sampler...
         Initializing NUTS using jitter+adapt diag...
         Multiprocess sampling (2 chains in 4 jobs)
         NUTS: [parameters]
         Sampling 2 chains: 100% 3000/3000 [00:14<00:00, 201.
         98draws/s]
In [30]:
          summary = pm.summary(trace)
          summary.index = animals
          summary
Out[30]:
                             sd mc_error
                                         hpd_2.5 hpd_97.5
                  mean
                                                               n_eff
          lions 0.406787 0.092886 0.001974
                                         tigers 0.405396 0.092945 0.002071 0.232870 0.582661 1935.575356 1.000
         bears
                The uncertainty of the prevalence of bears has decreased and the
        prevalence of the lions and tigers is nearly identical as expected from the
        data. As we gather more data, we can incorporate it into the model to get
        more accurate estimates. A larger amount of data will mean less uncertainty
        in the sampling as well.
In [31]:
          ax = pm.plot_posterior(trace, varnames = ['parameters'],
                                figsize = (20, 10), edgecolor = 'k');
          plt.rcParams['font.size'] = 22
          for i, a in enumerate(animals):
              ax[i].set_title(a);
```

```
plt.suptitle('Posterior with More Observations', y = 1.05);
                        Posterior with More Observations
```

lions tigers 107

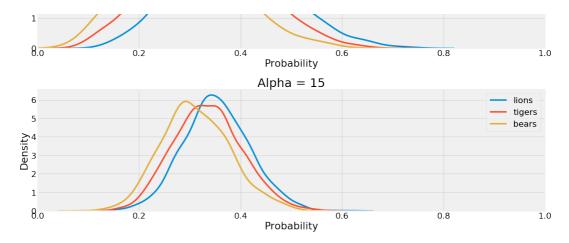




Increasing/Decreasing Confidence in Hyperparameters

As noted earlier, we can increase or decrease our confidence in our initial belief by changing the weighting of the hyperparameter vector. Initially we use all 1s, but we can reduce or increase this.

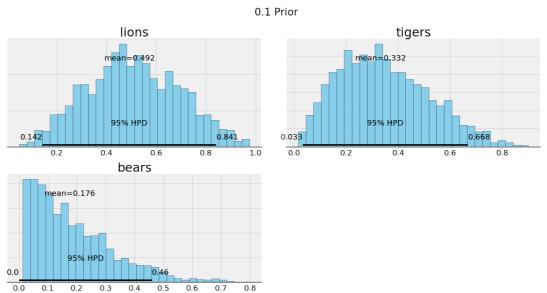
```
Multiprocess sampling (2 chains in 4 jobs)
          NUTS: [parameters]
          Sampling 2 chains: 100% 3000/3000 [00:07<00:00, 891.
          28draws/sl
          Auto-assigning NUTS sampler...
          Initializing NUTS using jitter+adapt diag...
          Multiprocess sampling (2 chains in 4 jobs)
          NUTS: [parameters]
                                      3000/3000 [00:03<00:00, 803.
          Sampling 2 chains: 100%
          25draws/s]
          Auto-assigning NUTS sampler...
          Initializing NUTS using jitter+adapt_diag...
          Multiprocess sampling (2 chains in 4 jobs)
          NUTS: [parameters]
          Sampling 2 chains: 100% 3000/3000 [00:03<00:00, 754.
          46draws/sl
In [34]:
          plt.figure(figsize = (20, 24))
          for ii, (alpha, trace) in enumerate(trace_dict.items()):
               plt.subplot(4, 1, ii + 1)
               array = trace['parameters']
               for jj, animal in enumerate(animals):
                   sns.kdeplot(array[:, jj], label = f'{animal}')
               plt.legend();
               plt.xlabel('Probability'); plt.ylabel('Density')
               plt.title(f'Alpha = {alpha}');
               plt.xlim((0, 1));
          plt.tight layout();
          plt.show();
                                        Alpha = 0.1
                                                                         lions
                                                                         tigers
            8.0
                         0.2
                                     0.4
                                         Probability
                                         Alpha = 1
           3.0
                                                                         tigers
           2.5
                                                                         bears
         Density
1.5
           1.0
           0.5
           0.8.0
                         0.2
                                                                            1.0
                                         Probability
                                         Alpha = 5
                                                                         lions
                                                                         tigers
                                                                        bears
```



As the weight increases, the estimated prevalence tends to collapse to 1/3 for each species. These results are intuitive: if we have a greater belief that the prevalences are equivalent, then the limited data we collected should not change our beliefs greatly.

Comparison of Beliefs

Next we compare the hyperparameters lpha=[0.1,0.1,0.1] with lpha=[15,15,15]



```
In [36]:
         summary = pm.summary(trace)
         summary.index = animals
         summary
Out[36]:
                         sd mc_error
                                    hpd_2.5 hpd_97.5
                mean
                                                        n_eff
         lions 0.492304 0.186867
                            0.004179
                                    0.142102
                                           0.840901
                                                   1762.158016 0.999
        tigers
              bears
             0.175989
In [37]:
         prior = '15'
         trace = trace_dict[prior]
         ax = pm.plot_posterior(trace, varnames = ['parameters'],
                             figsize = (20, 10), edgecolor = 'k');
        plt.rcParams['font.size'] = 22
         for i, a in enumerate(animals):
            ax[i].set_title(a);
        plt.suptitle(f'{prior} Prior', y = 1.05);
                                  15 Prior
                   lions
                                                tigers
                   bears
```

```
In [38]: summary = pm.summary(trace)
    summary.index = animals
    summary
```

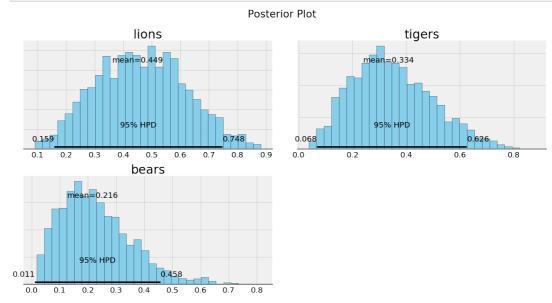
Out[38]:		mean	sd	mc_error	hpd_2.5	hpd_97.5	n_eff	R
	lions	0.352541	0.064846	0.001463	0.222414	0.477195	1975.877117	0.999
	tigers	0.335350	0.066687	0.001610	0.211996	0.466497	1814.916145	0.999
	bears	0.312108	0.067048	0.001612	0.183867	0.443939	1701.988778	0.9998

Overall, the choice of the hyperpriors depends on our confidence in our initial belief. If we have good reason to believe all the animals are represented at the same frequency, then we should increase the weight of the priors.

Conclusions

```
In [39]:
    prior = '1'
    trace = trace_dict[prior]
    summary = pm.summary(trace)
    summary.index = animals
    summary
```

```
Out[39]:
                    mean
                                 sd mc_error
                                               hpd_2.5 hpd_97.5
                                                                       n_eff
                                                                                  R
           lions 0.449412 0.156988
                                    0.003551
                                              0.158765
                                                        0.747843 1814.673630
                                                                              0.999
          tigers 0.334244 0.149916 0.003432 0.068359
                                                        0.625679
                                                                  1737.623151 0.9990
                                              0.011026  0.457694  1735.077325  0.999
           bears
                 0.216344 0.127805 0.002647
```



Given the question posed, we can provide the following answers:

Estimated Prevalence

Below are the means and 95% HPD for the estimates

Lions: 44.5% (16.9% - 75.8%)
Tigers: 32.7% (6.7% - 60.5%)
Bears: 22.7% (1.7% - 50.0%)

Probability Next Observation is a Bear

Based on the sampling, 22.9%.

(Results may change from one run to the next. This is due to the stochastic nature of MCMC).

The best parts about Bayesian Inference are the incorporation of priors and the uncertainty inherent in the methods. With the scant evidence, we can provide estimates, but only with a large amount of uncertainty. More visits to the wildlife preserve would certainly help to clear up the matter!

In this notebook, we were able to explore the basics of Bayesian modeling and probabilistic programming. Although this was only a simple problem, we can use the concepts here to build more complex models.

probabilistic-programming/Estimating Probabilities with Bayesian Inference.ipynb at master	· WillKoehrsen/probabilistic-programming	2022/01/09 18:46