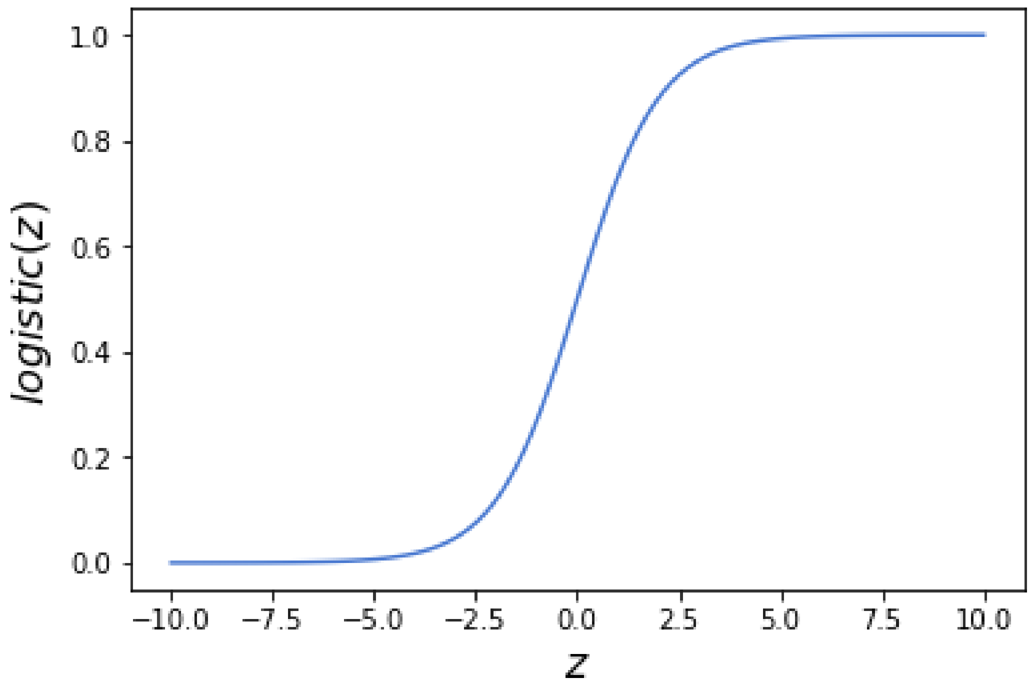
Bayesian Data Analysis Chapter 5

January 20, 2019

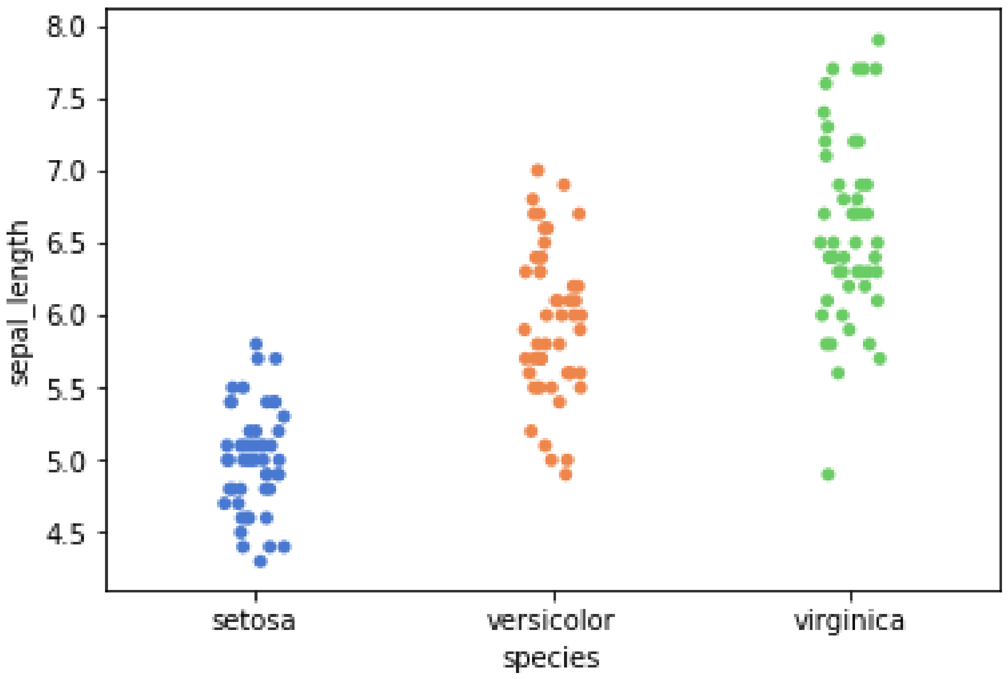
1 Logistic Regression

```
In [1]: %matplotlib inline
        import pymc3 as pm
        import numpy as np
        import pandas as pd
        import scipy.stats as stats
        import matplotlib.pyplot as plt
        import seaborn as sns
        import theano.tensor as tt
        palette = 'muted'
        sns.set_palette(palette); sns.set_color_codes(palette)
        np.set_printoptions(precision=2)
        pd.set_option('display.precision', 2)
```

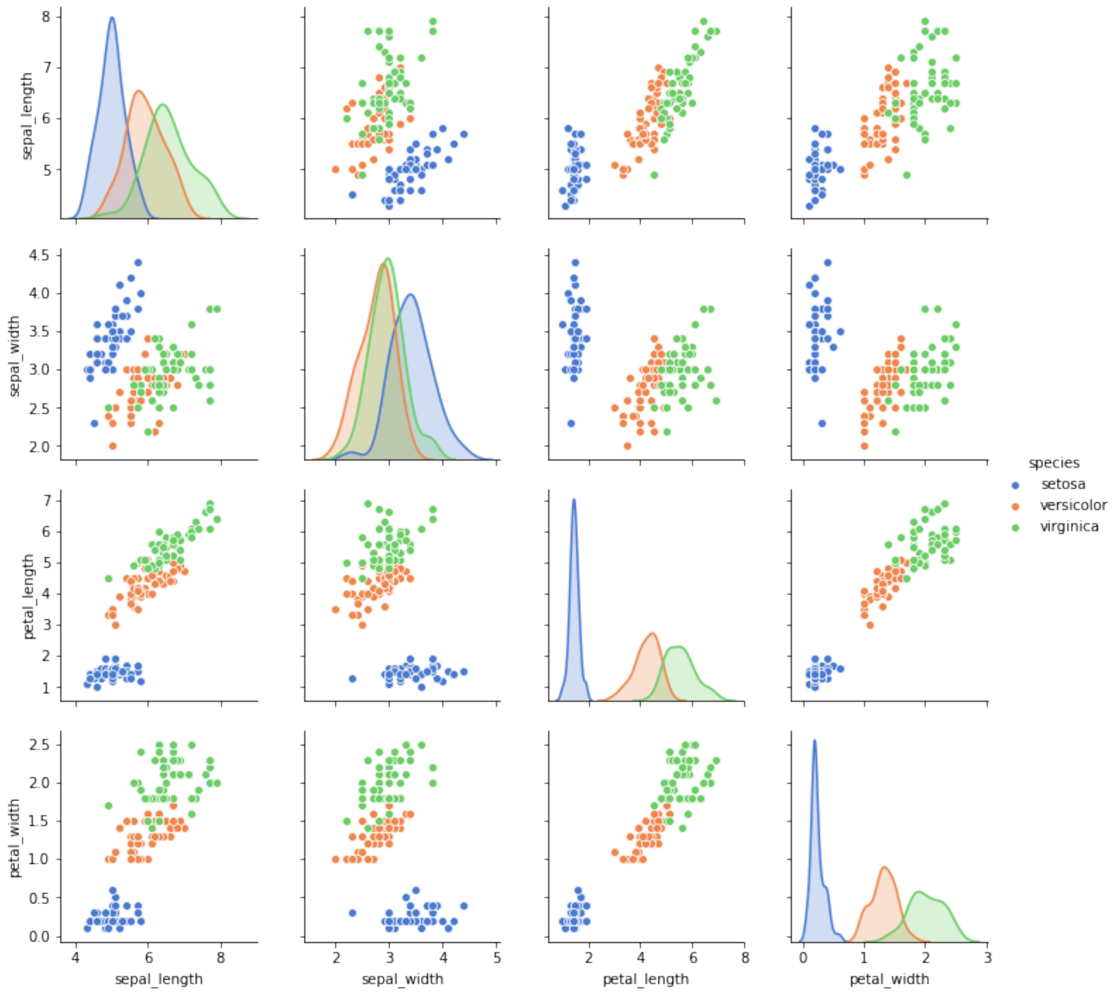
```
In [2]: z = np.linspace(-10, 10, 100)
        logistic = 1 / (1 + np.exp(-z))
        plt.plot(z, logistic);
        plt.xlabel('$z$', fontsize=16);
        plt.ylabel('$logistic(z)$', fontsize=16);
```



```
In [3]: iris = sns.load_dataset("iris")
        iris.head()

Out[3]:    sepal_length  sepal_width  petal_length  petal_width species
        0           5.1          3.5           1.4          0.2  setosa
        1           4.9          3.0           1.4          0.2  setosa
        2           4.7          3.2           1.3          0.2  setosa
        3           4.6          3.1           1.5          0.2  setosa
        4           5.0          3.6           1.4          0.2  setosa

In [4]: sns.stripplot(x="species", y="sepal_length", data=iris, jitter=True);
```



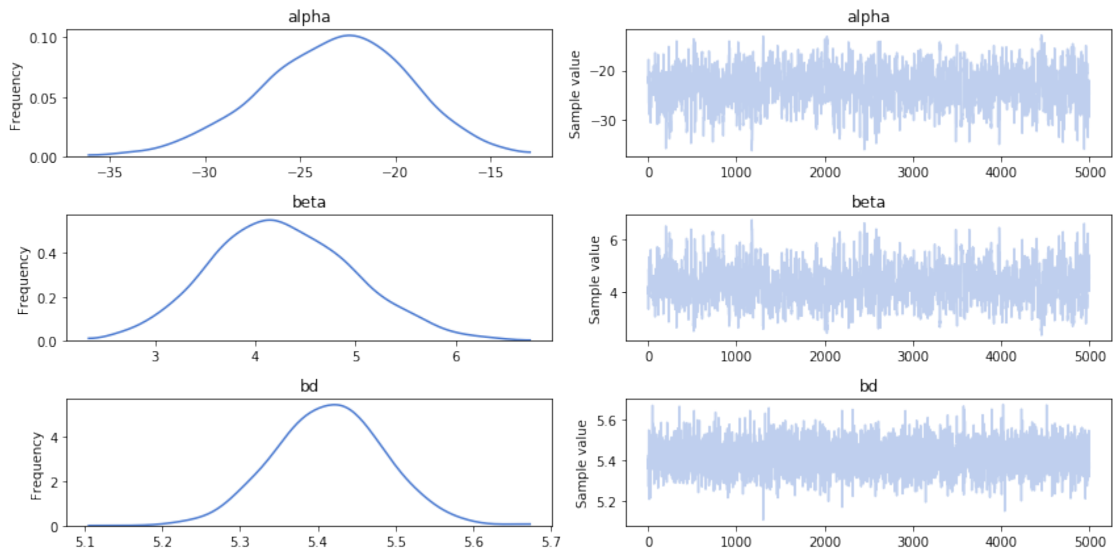
```
In [5]: sns.pairplot(iris, hue='species', diag_kind='kde');
```



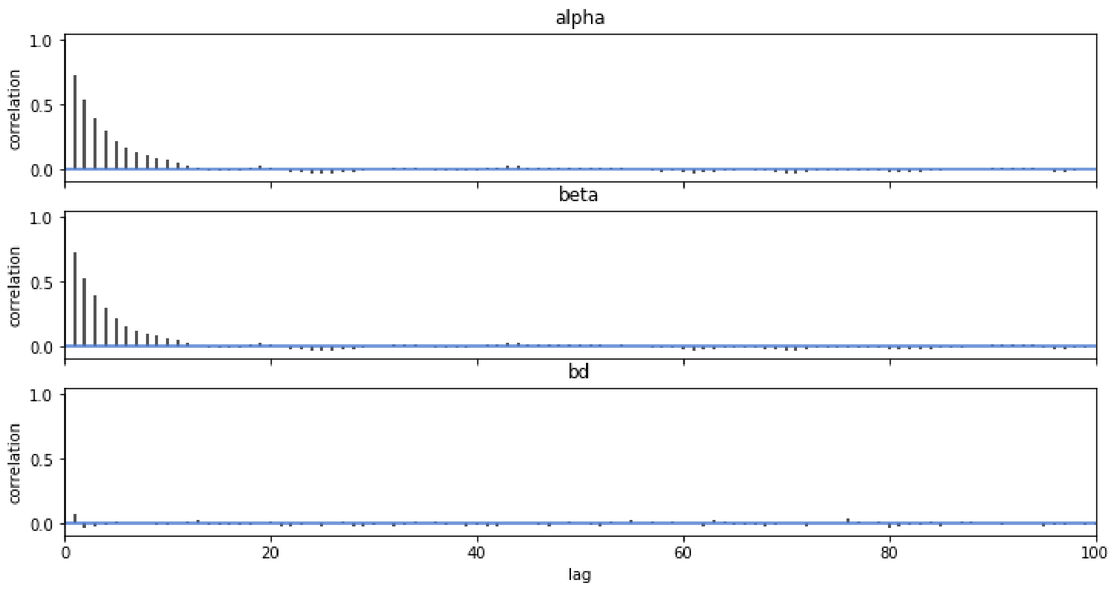
```
In [6]: df = iris.query("species == ('setosa', 'versicolor')")
        y_0 = pd.Categorical(df['species']).codes
        x_n = 'sepal_length'
        x_0 = df[x_n].values

In [7]: with pm.Model() as model_0:
            alpha = pm.Normal('alpha', mu=0, sd=10)
            beta = pm.Normal('beta', mu=0, sd=10)

            mu = alpha + pm.math.dot(x_0, beta)
            #theta = pm.Deterministic('theta', tt.nnet.sigmoid(mu))
            # the theta of the Bernoulli is derived from the logistic inverse link function
            theta = pm.Deterministic('theta', 1 / (1 + pm.math.exp(-mu)))

            bd = pm.Deterministic('bd', -alpha/beta)
            yl = pm.Bernoulli('yl', p=theta, observed=y_0)

        #     start = pm.find_MAP()
            step = pm.NUTS()
            trace_0 = pm.sample(5000, step, chains=1, njobs=1)
```

```
Sequential sampling (1 chains in 1 job)
NUTS: [beta, alpha]
100%|| 5500/5500 [00:14<00:00, 367.59it/s]
Only one chain was sampled, this makes it impossible to run some convergence checks
```

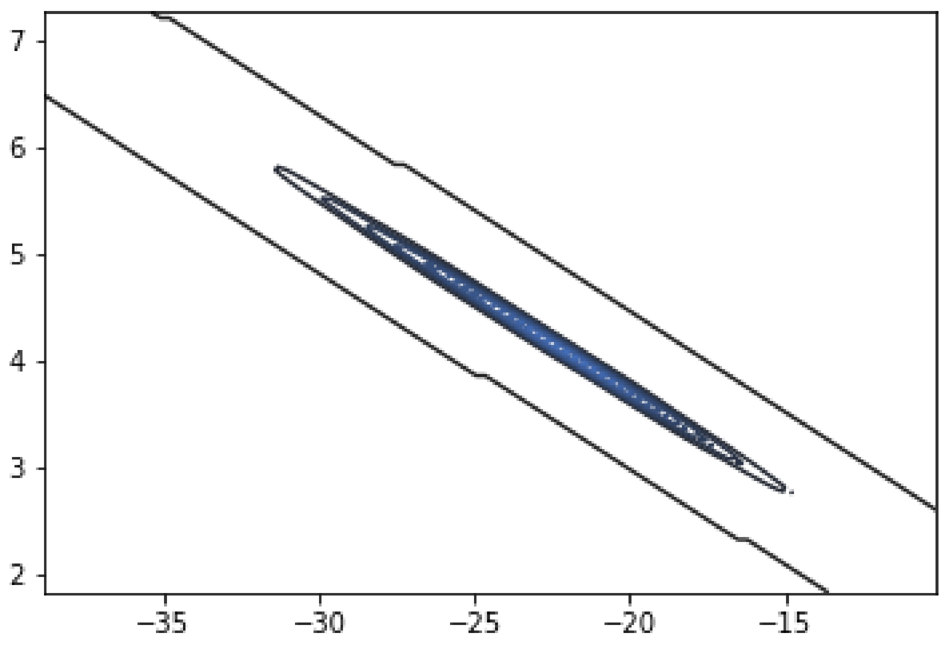
```
In [8]: varnames = ['alpha', 'beta', 'bd']
        pm.traceplot(trace_0, varnames);
```



```
In [9]: pm.autocorrplot(trace_0, varnames);
```



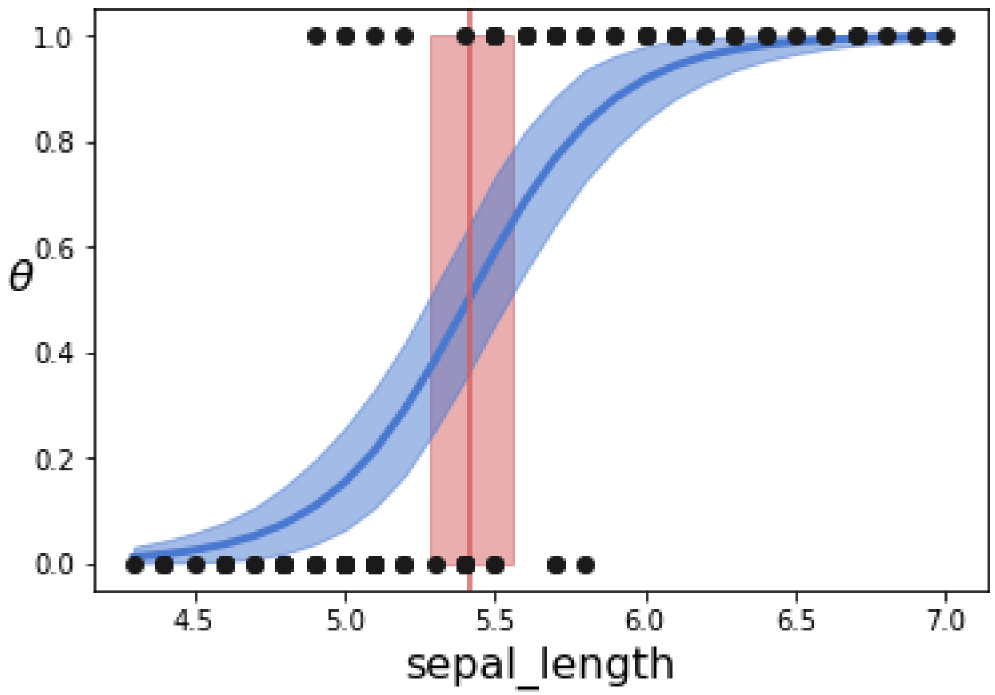
```
In [10]: sns.kdeplot(trace_0['alpha'], trace_0['beta']);
```



```
In [11]: pm.summary(trace_0, varnames)

Out[11]:        mean    sd  mc_error  hpd_2.5  hpd_97.5
         alpha -23.17  3.84  1.31e-01   -30.82    -15.89
```

```
beta     4.28   0.71   2.42e-02     2.94       5.70
bd       5.42   0.07   9.42e-04     5.28       5.55
```

```
In [12]: theta = trace_0['theta'].mean(axis=0)
         idx = np.argsort(x_0)
         plt.plot(x_0[idx], theta[idx], color='b', lw=3);
         plt.axvline(trace_0['bd'].mean(), ymax=1, color='r');
         bd_hpd = pm.hpd(trace_0['bd'])
         plt.fill_betweenx([0, 1], bd_hpd[0], bd_hpd[1], color='r', alpha=0.5);

         plt.plot(x_0, y_0, 'o', color='k');
         theta_hpd = pm.hpd(trace_0['theta'])[idx]
         plt.fill_between(x_0[idx], theta_hpd[:,0], theta_hpd[:,1], color='b', alpha=0.5);

         plt.xlabel(x_n, fontsize=16);
         plt.ylabel(r'$\theta$', rotation=0, fontsize=16);
```

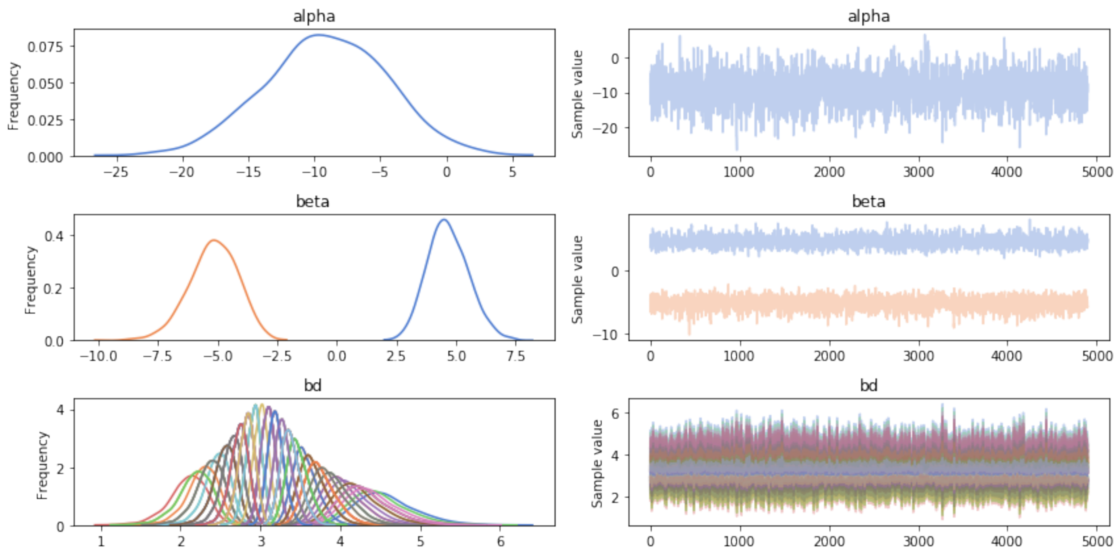


```
In [13]: def classify(n, threshold):
             """
             A simple classifying function
             """
             n = np.array(n)
             mu = trace_0['alpha'].mean() + trace_0['beta'].mean() * n
             prob = 1 / (1 + np.exp(-mu))
```

```
            return prob, prob >= threshold

        classify([5, 5.5, 6], 0.5)

Out[13]: (array([0.15, 0.59, 0.92]), array([False,  True,  True]))
```

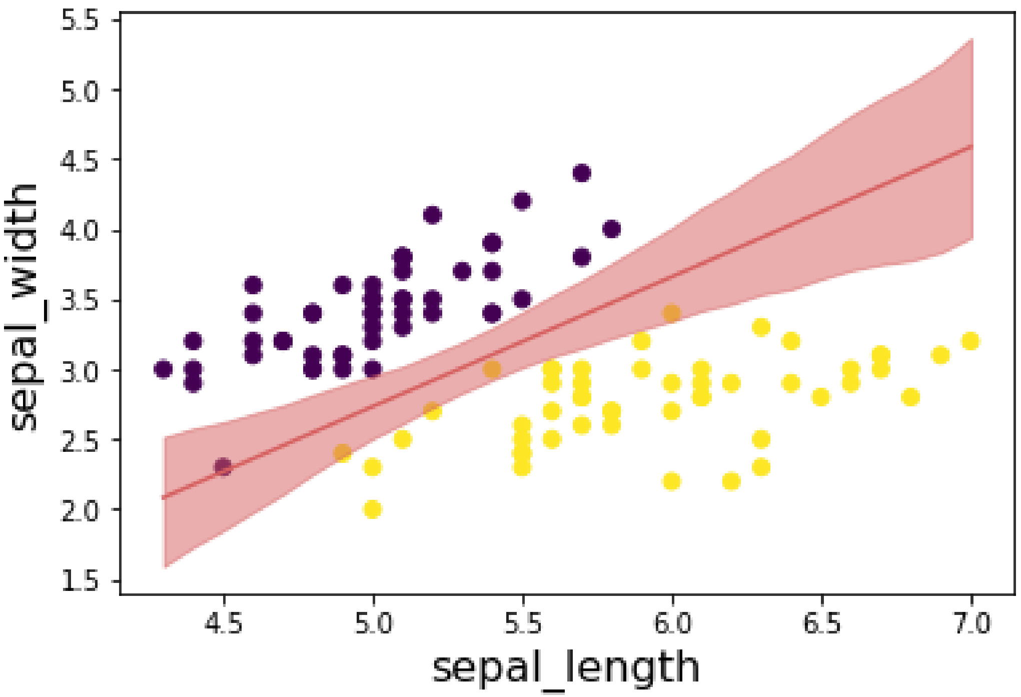
1.1 Multiple logistic regression

```
In [14]: df = iris.query("species == ('setosa', 'versicolor')")
         y_1 = pd.Categorical(df['species']).codes
         x_n = ['sepal_length', 'sepal_width'] #['petal_length', 'petal_width']
         x_1 = df[x_n].values

         #x_1 = (x_1 - x_1.mean(axis=0))/x_1.std(axis=0) #
         #x_1 = (x_1 - x_1.mean(axis=0))

In [15]: with pm.Model() as model_1:
             # We define the prioris
             alpha = pm.Normal('alpha', mu=0, sd=10)
             beta = pm.Normal('beta', mu=0, sd=2, shape=len(x_n))

             mu = alpha + pm.math.dot(x_1, beta)
             # Apply the logistic linking function
             theta = 1 / (1 + pm.math.exp(-mu))
             # Compute the boundary decision
             bd = pm.Deterministic('bd', -alpha/beta[1] - beta[0]/beta[1] * x_1[:,0])

             # Define the likelihood
             yl = pm.Bernoulli('yl', p=theta, observed=y_1)
             # Sampling
             trace_1 = pm.sample(5000,chains=1, njobs=1)

Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Sequential sampling (1 chains in 1 job)
NUTS: [beta, alpha]
100%|| 5500/5500 [00:20<00:00, 272.09it/s]
The acceptance probability does not match the target. It is 0.8931604002334997, but should be c
Only one chain was sampled, this makes it impossible to run some convergence checks


In [16]: chain_1 = trace_1[100:]
         pm.traceplot(chain_1);
```



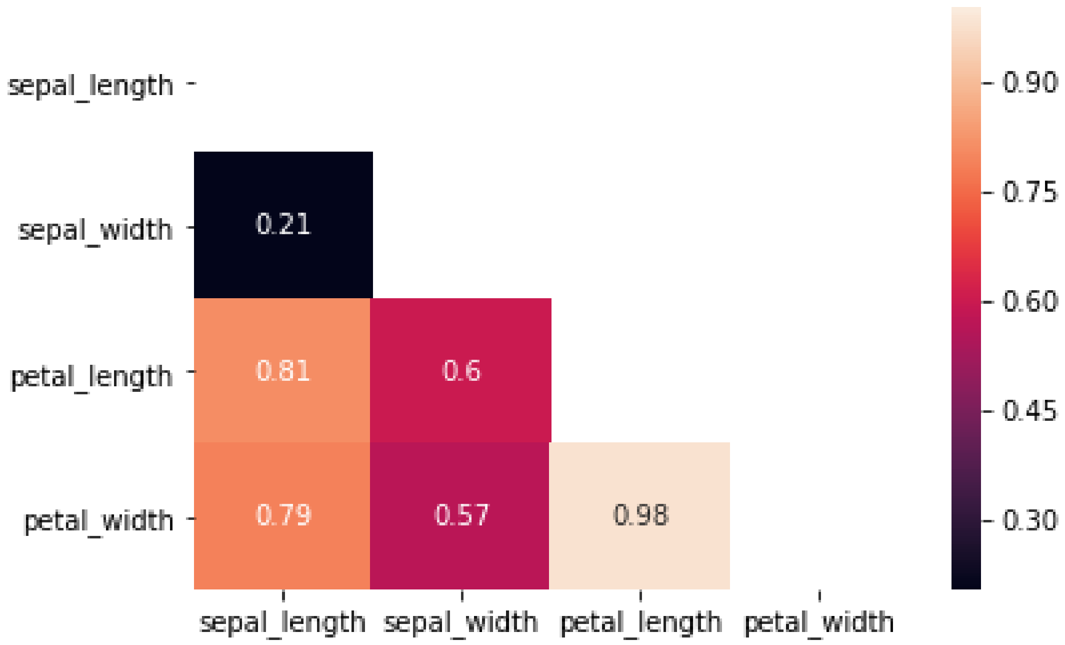
Note that now the boundary decision has 100 parameters, one for each data point

```
In [17]: pm.summary(chain_1, ['alpha', 'beta'])

Out[17]:          mean    sd  mc_error  hpd_2.5  hpd_97.5
         alpha   -9.12  4.67      0.11   -18.29     -0.17
         beta__0  4.67  0.86      0.02     3.06      6.39
         beta__1 -5.18  1.03      0.02    -7.18     -3.20

In [18]: idx = np.argsort(x_1[:,0])
         ld = chain_1['bd'].mean(0)[idx]
         plt.scatter(x_1[:,0], x_1[:,1], c=y_0);
         plt.plot(x_1[:,0][idx], ld, color='r');

         ld_hpd = pm.hpd(chain_1['bd'])[idx]
         plt.fill_between(x_1[:,0][idx], ld_hpd[:,0], ld_hpd[:,1], color='r', alpha=0.5);

         plt.xlabel(x_n[0], fontsize=16);
         plt.ylabel(x_n[1], fontsize=16);
```



1.2 Correlated variables

```
In [19]: corr = iris[iris['species'] != 'virginica'].corr()
         mask = np.tri(*corr.shape).T
         sns.heatmap(corr.abs(), mask=mask, annot=True);
```



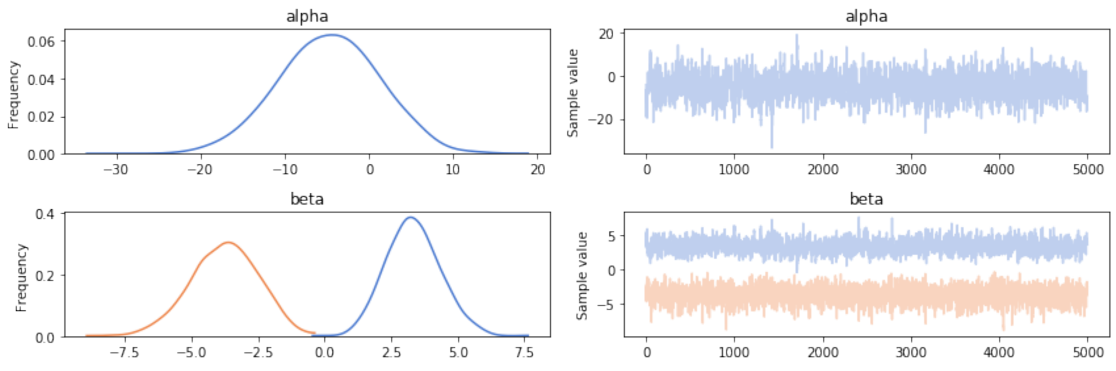
1.3 Unbalanced Classes

```
In [20]: df = iris.query("species == ('setosa', 'versicolor')")
         df = df[45:] #df[22:78]
         y_3 = pd.Categorical(df['species']).codes
         x_n = ['sepal_length', 'sepal_width']
         x_3 = df[x_n].values
```

```
In [21]: with pm.Model() as model_3:
             # We define the a prioris
             alpha = pm.Normal('alpha', mu=0, sd=10)
             beta = pm.Normal('beta', mu=0, sd=2, shape=len(x_n))

             mu = alpha + pm.math.dot(x_3, beta)
             # Aplly the logistic linking function
             p = 1 / (1 + pm.math.exp(-mu))
             # Compute the boundary decision
             ld = pm.Deterministic('ld', -alpha/beta[1] - beta[0]/beta[1] * x_3[:,0])

             # Define the likelihood
             yl = pm.Bernoulli('yl', p=p, observed=y_3)
             trace_3 = pm.sample(5000,chains=1, njobs=1)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Sequential sampling (1 chains in 1 job)
NUTS: [beta, alpha]
100%|| 5500/5500 [00:14<00:00, 383.43it/s]
There were 112 divergences after tuning. Increase `target_accept` or reparameterize.
Only one chain was sampled, this makes it impossible to run some convergence checks
```

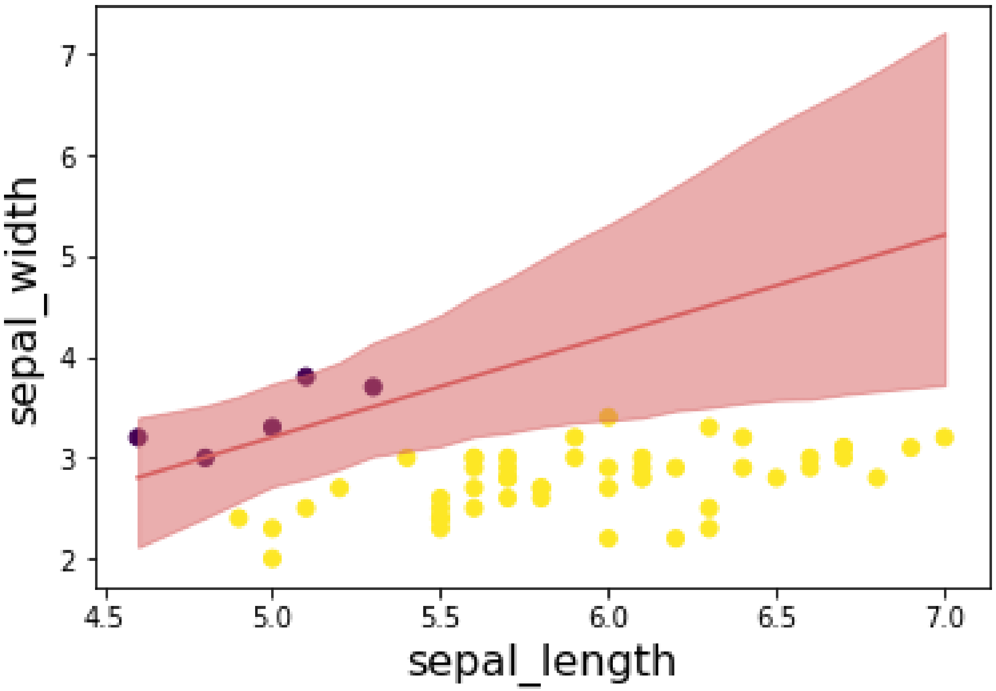
```
In [22]: cadena_3 = trace_3[:]
         varnames = ['alpha', 'beta']
         pm.traceplot(cadena_3, varnames);
```



```
In [23]: pm.summary(cadena_3, varnames)
```

```
Out[23]:          mean    sd  mc_error  hpd_2.5  hpd_97.5
         alpha   -4.70  5.94      0.18   -15.93      6.74
         beta__0  3.33  1.01      0.03     1.30      5.25
         beta__1 -3.77  1.27      0.03    -6.22     -1.36
```

```
In [24]: idx = np.argsort(x_3[:,0])
         ld = trace_3['ld'].mean(0)[idx]
         plt.scatter(x_3[:,0], x_3[:,1], c=y_3);
         plt.plot(x_3[:,0][idx], ld, color='r');

         ld_hpd = pm.hpd(trace_3['ld'])[idx]
         plt.fill_between(x_3[:,0][idx], ld_hpd[:,0], ld_hpd[:,1], color='r', alpha=0.5);

         plt.xlabel(x_n[0], fontsize=16);
         plt.ylabel(x_n[1], fontsize=16);
```



1.4 Softmax logistic regression (AKA multinomial regression)

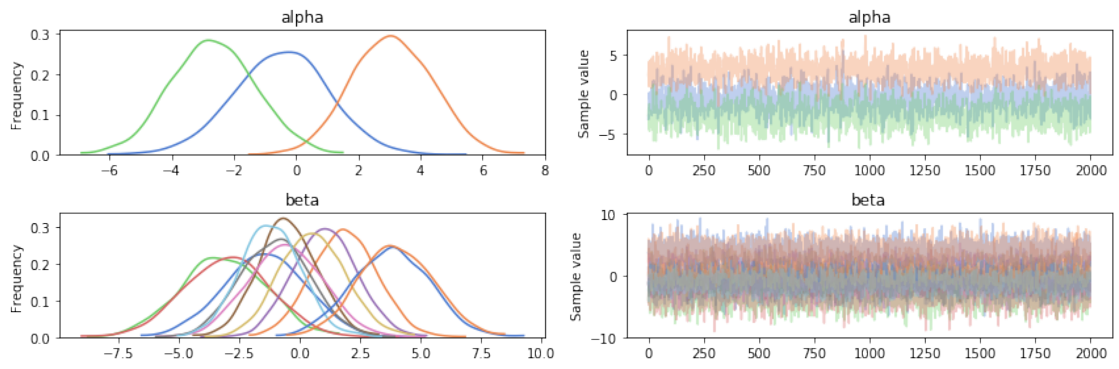
```
In [25]: iris = sns.load_dataset("iris")
         y_s = pd.Categorical(iris['species']).codes
```

```
        x_n = iris.columns[:-1]
        x_s = iris[x_n].values
        x_s = (x_s - x_s.mean(axis=0))/x_s.std(axis=0)
        #x_s = (x_s - x_s.mean(axis=0))
```

```
In [26]: with pm.Model() as model_s:
             alpha = pm.Normal('alpha', mu=0, sd=2, shape=3)
             beta = pm.Normal('beta', mu=0, sd=2, shape=(4,3))

             mu = alpha + pm.math.dot(x_s, beta)
             theta = tt.nnet.softmax(mu)

             yl = pm.Categorical('yl', p=theta, observed=y_s)
             step = pm.NUTS()
             trace_s = pm.sample(2000, step, chains=1, njobs=1)
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/subtensor.py:21
  rval = inputs[0].__getitem__(inputs[1:])
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/subtensor.py:21
  rval = inputs[0].__getitem__(inputs[1:])
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/subtensor.py:21
  rval = inputs[0].__getitem__(inputs[1:])
Sequential sampling (1 chains in 1 job)
NUTS: [beta, alpha]
100%|| 2500/2500 [00:12<00:00, 197.64it/s]
Only one chain was sampled, this makes it impossible to run some convergence checks
```

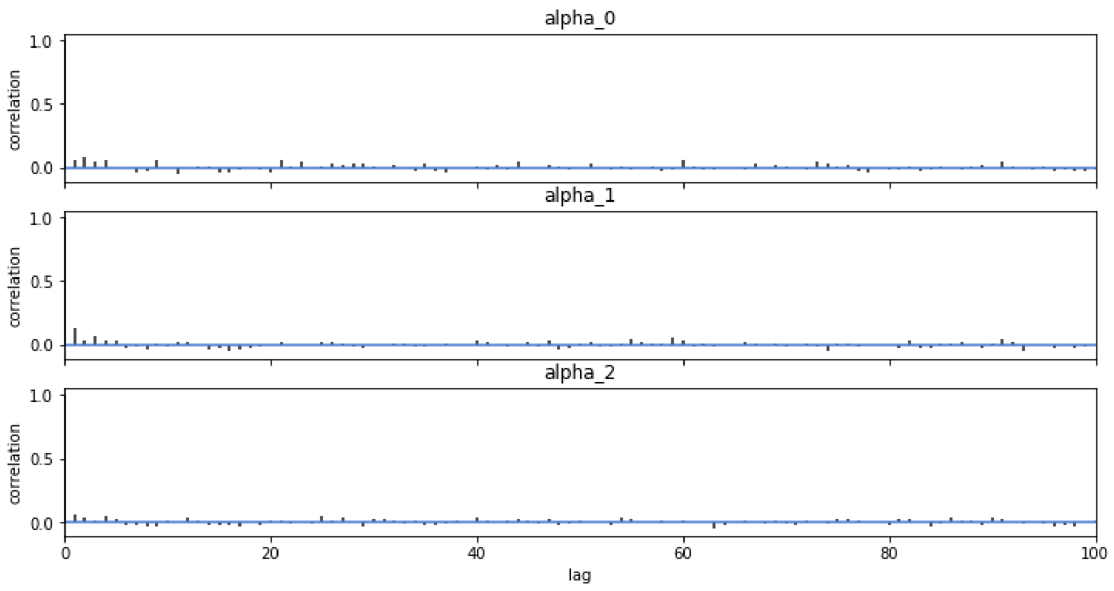
```
In [27]: pm.traceplot(trace_s);
```



```
In [28]: pm.summary(trace_s)

Out[28]:             mean    sd  mc_error  hpd_2.5  hpd_97.5
         alpha__0  -0.50  1.50      0.04    -3.64      2.20
         alpha__1   3.07  1.29      0.03     0.56      5.51
```

```
alpha__2  -2.68  1.35      0.03     -5.19      0.08
beta__0_0 -1.45  1.68      0.04     -4.87      1.64
beta__0_1  1.04  1.29      0.04     -1.41      3.52
beta__0_2  0.53  1.34      0.04     -2.24      3.02
beta__1_0  1.85  1.31      0.03     -0.64      4.39
beta__1_1 -0.50  1.21      0.03     -2.77      1.95
beta__1_2 -1.20  1.25      0.03     -3.55      1.31
beta__2_0 -3.17  1.73      0.04     -6.72     -0.08
beta__2_1 -0.59  1.53      0.03     -3.63      2.25
beta__2_2  3.77  1.60      0.03      0.45      6.67
beta__3_0 -3.00  1.76      0.03     -6.57      0.26
beta__3_1 -1.02  1.42      0.03     -3.72      1.80
beta__3_2  3.98  1.52      0.03      1.23      7.22
```

```
In [29]: pm.autocorrplot(trace_s, varnames=['alpha']);
```



```
In [30]: probs = trace_s['alpha'].mean(axis=0) + np.dot(x_s, trace_s['beta'].mean(axis=0))
         y_pred = []
         for point in probs:
             # each array appended contains the softmax estimates of each class
             y_pred.append(np.exp(point)/np.sum(np.exp(point), axis=0))
         print('Accuracy on training data is {0:.2%}'.format(np.sum(y_s == np.argmax(y_pred, a
```

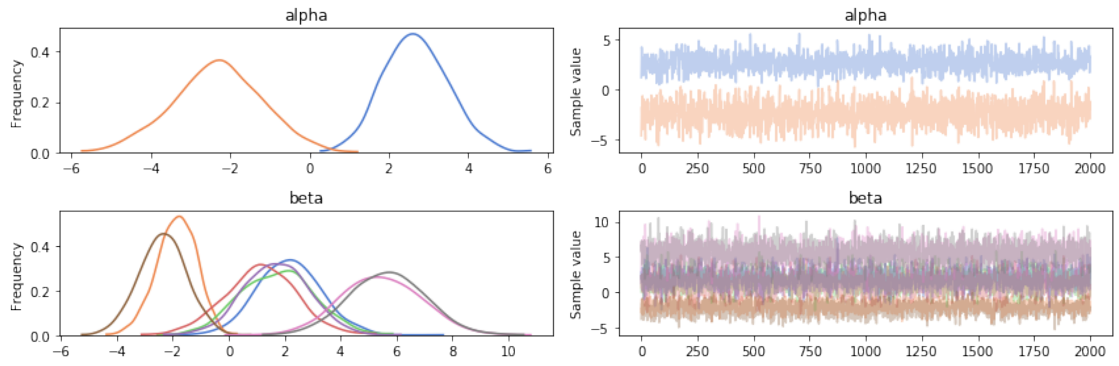
```
Accuracy on training data is 97.33%
```

```
In [31]: with pm.Model() as model_sf:
             alpha = pm.Normal('alpha', mu=0, sd=2, shape=2)
```

```
            beta = pm.Normal('beta', mu=0, sd=2, shape=(4,2))

            alpha_f = tt.concatenate([[0] , alpha])
            beta_f = tt.concatenate([np.zeros((4,1)) , beta], axis=1)

            mu = alpha_f + pm.math.dot(x_s, beta_f)
            theta = tt.nnet.softmax(mu)

            yl = pm.Categorical('yl', p=theta, observed=y_s)
            step = pm.NUTS()
            trace_sf = pm.sample(2000, step, chains=1, njobs=1)
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/subtensor.py:21
  rval = inputs[0].__getitem__(inputs[1:])
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/subtensor.py:21
  rval = inputs[0].__getitem__(inputs[1:])
Sequential sampling (1 chains in 1 job)
NUTS: [beta, alpha]
100%|| 2500/2500 [00:11<00:00, 222.00it/s]
The acceptance probability does not match the target. It is 0.8851232083982429, but should be
Only one chain was sampled, this makes it impossible to run some convergence checks
```

```
In [32]: pm.traceplot(trace_sf);
```



we get much better defined α's and β's than before because we didn't parametrize the problem correctly. We need to fix the number of parameters to $num_{classes} - 1$, since all probabilities must sum to one we had too many parameters in the first instance of the model. We do this by setting the first α and first β's to zero (see code).

```
In [33]: pm.summary(trace_sf)
```

```
Out[33]:            mean    sd  mc_error    hpd_2.5  hpd_97.5
         alpha__0   2.68  0.82      0.02  1.12e+00      4.35
```

```
alpha__1  -2.34  1.12      0.03 -4.49e+00     -0.09
beta__0_0  2.14  1.12      0.03  2.37e-03      4.47
beta__0_1  1.69  1.16      0.03 -5.15e-01      4.04
beta__1_0 -1.88  0.70      0.02 -3.23e+00     -0.52
beta__1_1 -2.37  0.84      0.02 -3.99e+00     -0.71
beta__2_0  1.73  1.30      0.03 -6.13e-01      4.34
beta__2_1  5.43  1.42      0.04  2.49e+00      7.98
beta__3_0  1.12  1.27      0.03 -1.38e+00      3.65
beta__3_1  5.66  1.35      0.03  3.11e+00      8.40
```

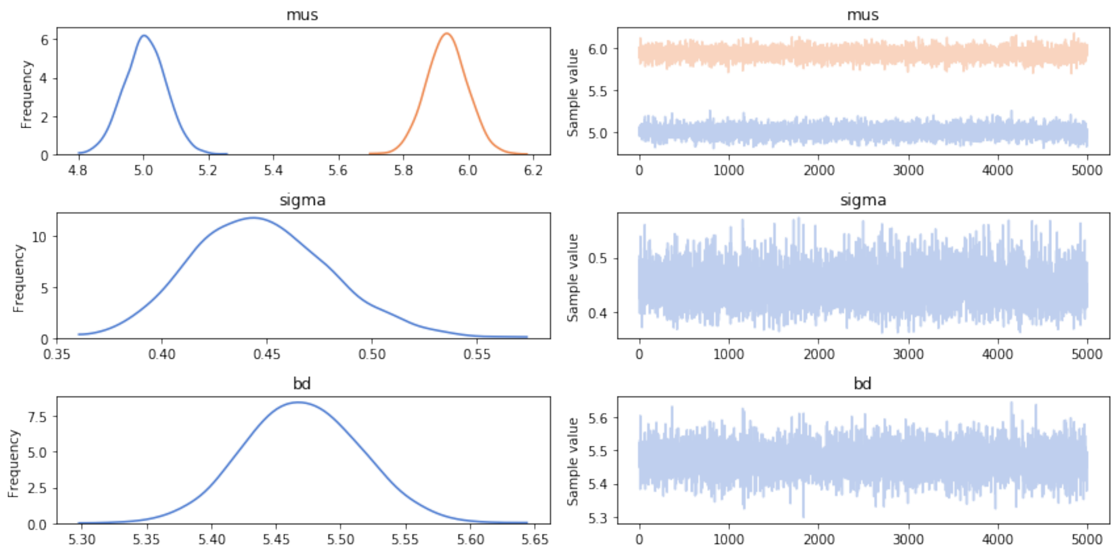
1.5 Linear discriminat Analysis

```
In [34]: iris = sns.load_dataset("iris")
         df = iris.query("species == ('setosa', 'versicolor')")
         y_0 = pd.Categorical(df['species']).codes
         x_n = 'sepal_length'
         x_0 = df[x_n].values
```

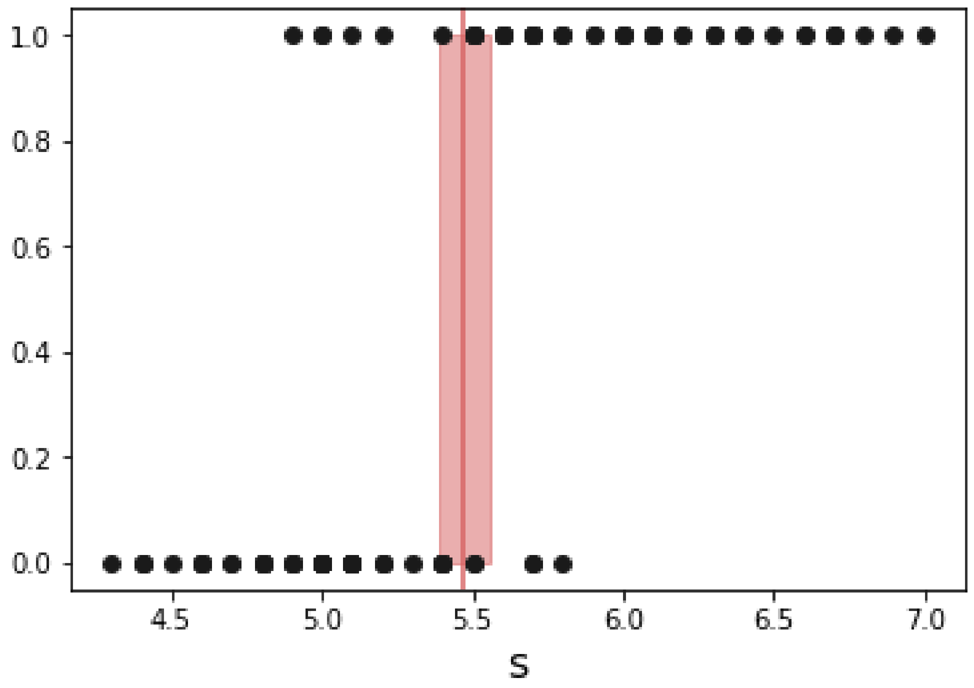
```
In [35]: with pm.Model() as model_lda:

             mus = pm.Normal('mus', mu=0, sd=10, shape=2)
             sigma = pm.HalfCauchy('sigma', 5)

             setosa = pm.Normal('setosa', mu=mus[0], sd=sigma, observed=x_0[:50])
             versicolor = pm.Normal('versicolor', mu=mus[1], sd=sigma, observed=x_0[50:])

             bd = pm.Deterministic('bd', (mus[0]+mus[1])/2)

             trace_lda = pm.sample(5000, chains=1, njobs=1)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Sequential sampling (1 chains in 1 job)
NUTS: [sigma, mus]
100%|| 5500/5500 [00:03<00:00, 1703.58it/s]
Only one chain was sampled, this makes it impossible to run some convergence checks
```

```
In [36]: pm.traceplot(trace_lda);
```



```
In [37]: pm.summary(trace_lda)

Out[37]:         mean    sd  mc_error  hpd_2.5  hpd_97.5
         mus__0  5.01  0.06  9.93e-04     4.88      5.13
         mus__1  5.93  0.06  9.24e-04     5.81      6.06
         sigma   0.45  0.03  4.35e-04     0.38      0.51
         bd      5.47  0.04  6.29e-04     5.39      5.56

In [38]: plt.axvline(trace_lda['bd'].mean(), ymax=1, color='r');
         bd_hpd = pm.hpd(trace_lda['bd']);
         plt.fill_betweenx([0, 1], bd_hpd[0], bd_hpd[1], color='r', alpha=0.5);
         plt.plot(x_0, y_0, 'o', color='k');
         plt.xlabel(x_n[0], fontsize=16);
```



```
In [39]: import sys, IPython, scipy, matplotlib, platform
         print("This notebook was created on a %s computer running %s and using:\nPython %s\nI
```

```
This notebook was created on a x86_64 computer running debian buster/sid and using:
Python 3.7.2
IPython 7.2.0
PyMC3 3.6
NumPy 1.16.0
SciPy 1.2.0
Matplotlib 3.0.2
Seaborn 0.9.0
Pandas 0.23.4


/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/ipykernel_launcher.py:2: Depre
```