Assignment 5

In [1]:

```
%matplotlib inline

import numpy as np
import pandas as pd

from scipy import stats

import pystan

import matplotlib
import matplotlib.pyplot as plt

font = {'size': 16}

matplotlib.rc('font', **font)
```

1. Generalized linear model with Metropolis

We use the same data as given in the book (table 3.1)

In [2]:

```
# data
x = np.array([-0.86, -0.30, -0.05, 0.73])
n = np.array([5, 5, 5, 5])
y = np.array([0, 1, 3, 5])

df = pd.DataFrame({
    'Sample': np.arange(4) + 1,
    'Dose (log g/ml)': x,
    'Number of animals': n,
    'Number of deaths': y
}).set_index('Sample')
df
```

Out[2]:

	Dose (log g/ml)	Number of animals	Number of deaths
Sample			
1	-0.86	5	0
2	-0.30	5	1
3	-0.05	5	3
4	0.73	5	5

We define the unnormalized distribution $q(X)$ of a single sample:

In [3]:

```
def q(X):
    a, b = X[0], X[1]
    ilogit_abx = 1 / (np.exp(-(a + b * x)) + 1)
    log_likelihood = np.sum(np.log(ilogit_abx**y) + np.log((1 - ilogit_abx)**(n - y)))
    return np.exp(log_likelihood)
```

Parameters for Metropolis-algorithm. We sample 4000 sampeles with a warm-up of 4000 (so in total 8000 samples will be taken, but we drop the first 1000). Since the starting point is arbitrary we can choose $(a, b) = (0, 0)$.

In [12]:

```
num_samp = 4000            # Number of samplte to pick
samp = np.array([0, 0])  # Initial proposal at start
samps = [samp]             # List of accepted samples
bootstrap_size = 4000     # Number of samples to skip for warm up
```

The Metropolis algorithm runs iterations until number of samples to pick is achieved. For each iteration t it does the following [1]:

- Generate : Generate a candidate prop_t for the next sample by picking from the distribution $g(\mathrm{prop}_t \mid \mathrm{samp}_{t-1})$. Here we use a gausian distribution for g with mean samp_{t-1} and scale 1.
- Calculate : Calculate the acceptance ratio $r = q(\mathrm{prop}_t)/q(samp_{t-1})$, which will be used to decide whether to accept or reject the candidate.
- Accept or Reject :
  - Generate a uniform random number u on $[0, 1[$.
  - If $u \leq r$ accept the candidate by setting $\mathrm{samp}_t = \mathrm{prop}_t$,
  - If $u > r$ reject the candidate and set $\mathrm{samp}_t = \mathrm{samp}_{t-1}$, instead.

In [13]:

```
# keep sampling until we have the desired number of samples
while len(samps) < bootstrap_size + num_samp:
    # get new proposal
    prop = np.random.normal(loc=samps[-1])
    r = np.divide(q(prop), q(samps[-1]))
    u = np.random.uniform()
    if u <= r:
        samps.append(prop)

# remove warm-up samples
samps = np.array(samps)[bootstrap_size:]
```

We check the mean of the samples:

In [14]:

```
np.mean(samps, axis = 0)
```

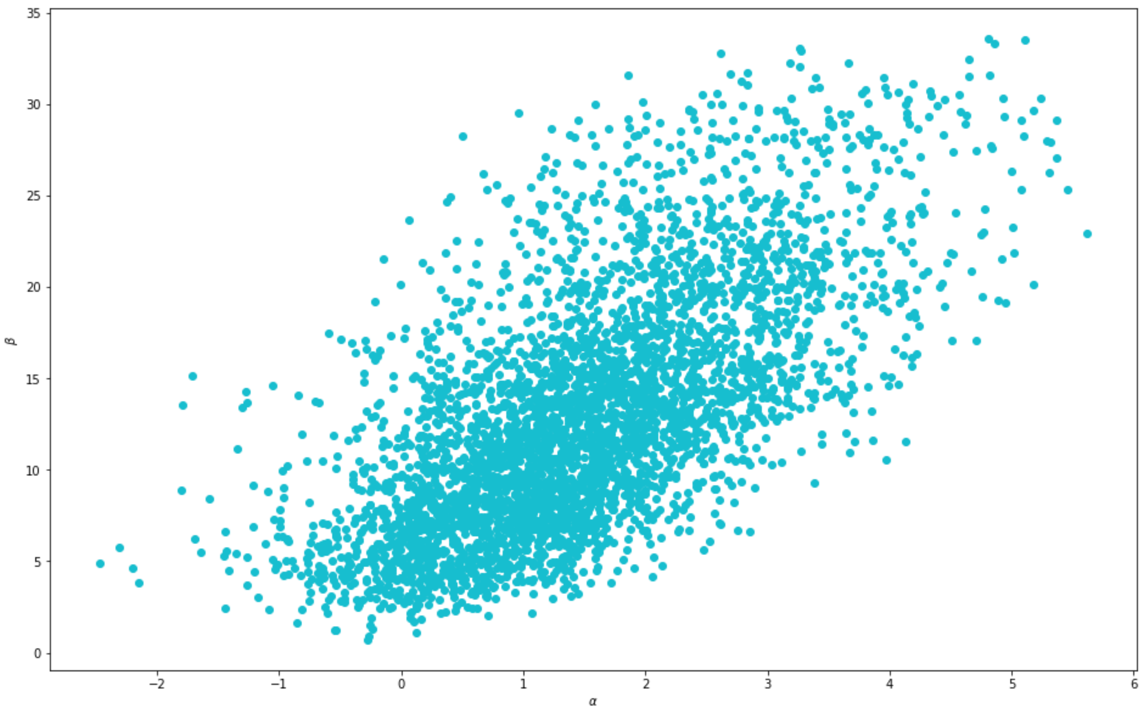
Out[14]:

```
array([ 1.50496811, 13.10736905])
```

We plot the samples:

In [15]:

```
fig, ax = plt.subplots(nrows=1, ncols=1, figsize = (16, 10))
ax.plot(samps[:,0],samps[:,1], 'o', color = 'C9')
ax.set_xlabel(r'$\alpha$')
ax.set_ylabel(r'$\beta$')
None
```



We calculate $\hat{R}$ cf. BDA (p. 284-285):

In [59]:

```
# split chain into two equal parts
splitted_chains = np.array(np.split(samps, 2))
m = splitted_chains.shape[0]
n = splitted_chains.shape[1]
W = np.mean(np.var(splitted_samples, axis = 1, ddof = 1), axis = 0) # eq. is equal to m
ean of var.
psi_dot_j = np.mean(splitted_chains, axis = 1)
B = n * np.var(psi_dot_j, axis = 0, ddof = 1) # eq. is equal to var of mean of psi_dot_
j.
var_hat = (n - 1) / n * W + 1 / n * B # eq. (11.3)
R_hat = np.sqrt(var_hat / W) # eq. (11.4)
```

We get the following R hat values, which are acceptable:

In [60]:

```
print('R hat alpha : {:.3f}'.format(R_hat[0]))
print('R hat beta  : {:.3f}'.format(R_hat[1]))
```

```
R hat alpha : 1.015
R hat beta  : 1.037
```

To plot the sampled density we use kernel density estimation:

In [16]:

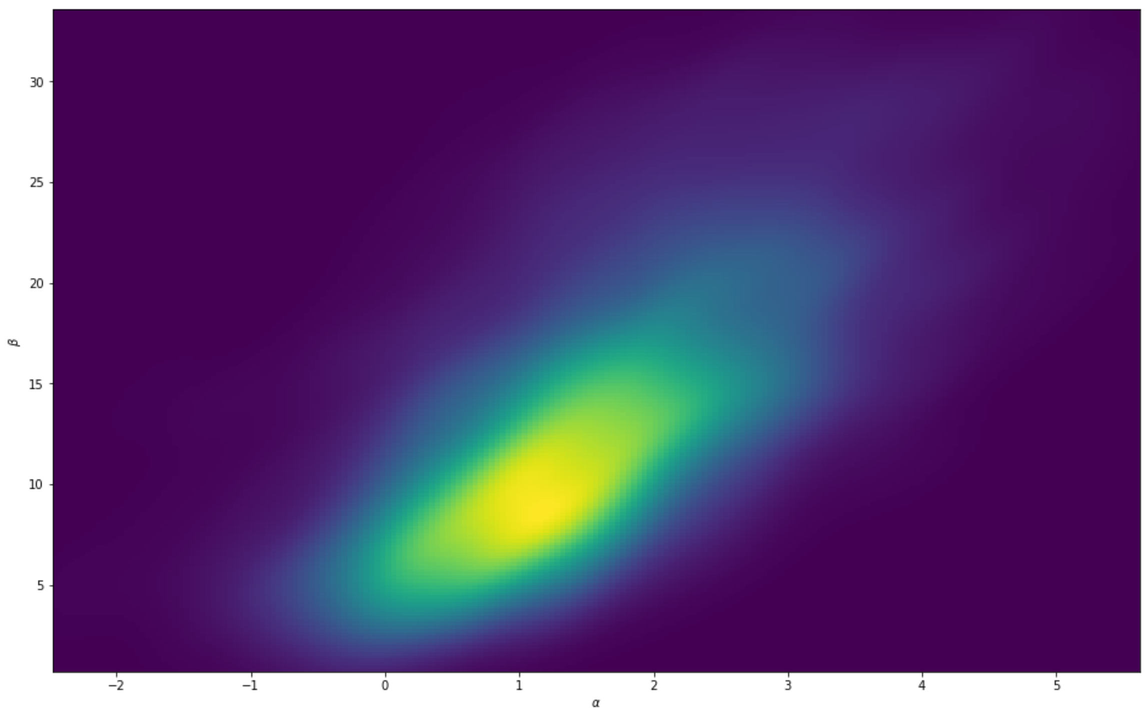
```
a = samps[:,0]
b = samps[:,1]
samp_kde = stats.kde.gaussian_kde([a, b])
```

And calculate grid for plotting heatmap

In [17]:

```
nbins = 200
ai, bi = np.mgrid[a.min():a.max():nbins*1j, b.min():b.max():nbins*1j]
pi = samp_kde(np.vstack([ai.flatten(), bi.flatten()]))

# Make the plot
fig, ax = plt.subplots(nrows=1, ncols=1, figsize = (16, 10))
ax.pcolormesh(ai, bi, pi.reshape(ai.shape))
ax.set_xlabel(r'$\alpha$')
ax.set_ylabel(r'$\beta$')
plt.show()
```



We see that the heatmap looks similar to the one produced in the previous assignment

Generalized linear model: Bioassay with Stan

In [18]:

```
stan_code = """
data {
    real x[4];
    int n[4];
    int y[4];
}
parameters {
    real alpha;
    real beta;
}
transformed parameters {
    real logits[4];
    logits[1] <- alpha + beta * x[1];
    logits[2] <- alpha + beta * x[2];
    logits[3] <- alpha + beta * x[3];
    logits[4] <- alpha + beta * x[4];
}
model {
    y ~ binomial_logit(n, logits);
}
"""

stan_data = {
    'x': x,
    'n': n,
    'y': y
}

fit = pystan.stan(model_code=stan_code, data=stan_data, iter=4000)
params = fit.extract()
print(fit)
```

```
INFO:pystan:COMPILING THE C++ CODE FOR MODEL anon_model_4c2104d3a845be14e7
c630b78c1594f9 NOW.
c:\users\ncp\appdata\local\continuum\anaconda3\envs\stan_env\lib\site-pack
ages\pystan\misc.py:399: FutureWarning: Conversion of the second argument
of issubdtype from `float` to `np.floating` is deprecated. In future, it w
ill be treated as `np.float64 == np.dtype(float).type`.
  elif np.issubdtype(np.asarray(v).dtype, float):
```

```
Inference for Stan model: anon_model_4c2104d3a845be14e7c630b78c1594f9.
4 chains, each with iter=4000; warmup=2000; thin=1;
post-warmup draws per chain=2000, total post-warmup draws=8000.

            mean se_mean     sd   2.5%    25%    50%    75%  97.5%  n_eff
  Rhat
alpha       1.32    0.02    1.1  -0.52   0.54   1.23   1.96   3.86   2202
   1.0
beta        11.6    0.13   5.84   3.43   7.36  10.55  14.75  25.48   1955
   1.0
logits[0]  -8.66    0.09   4.38  -19.2  -11.0  -7.86  -5.51  -2.53   2132
   1.0
logits[1]  -2.16    0.02   1.33  -5.26  -2.86  -1.96  -1.26  -0.16   3079
   1.0
logits[2]   0.74    0.02   0.94  -0.93    0.1   0.67   1.31   2.83   2618
   1.0
logits[3]   9.78    0.12   5.05   2.55   6.06   8.91  12.59  21.95   1873
   1.0
lp__        -7.0    0.03   1.16 -10.09  -7.42  -6.64  -6.19  -5.92   1956
   1.0

Samples were drawn using NUTS at Mon Mar  5 09:48:14 2018.
For each parameter, n_eff is a crude measure of effective sample size,
and Rhat is the potential scale reduction factor on split chains (at
convergence, Rhat=1).
```

We plot the samples from the stan-model side by side with the Metropolis draws:

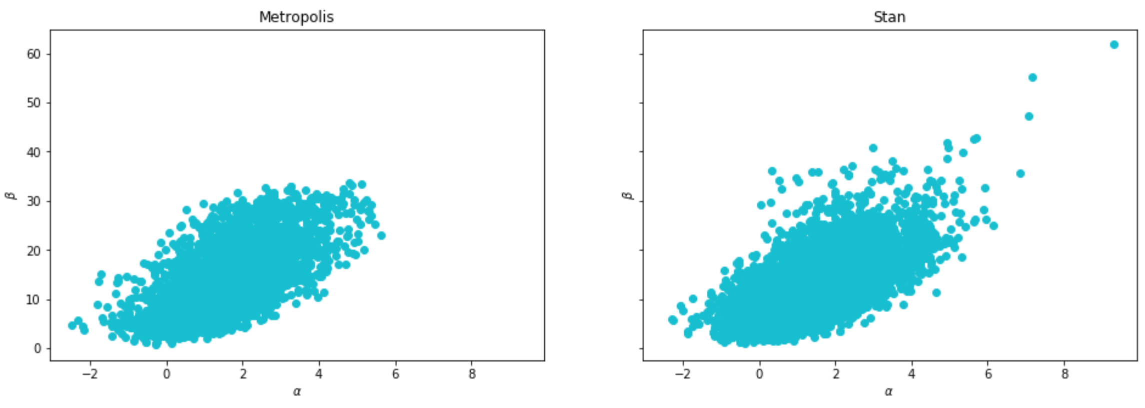
In [19]:

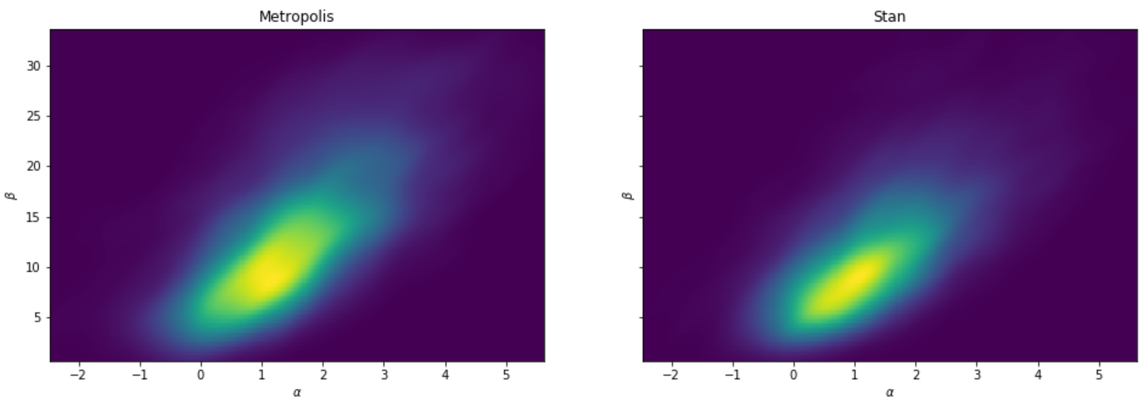
```
fig, ax = plt.subplots(nrows=1, ncols=2, figsize = (16, 5), sharex = True, sharey = Tru
e)
ax[0].set_title('Metropolis')
ax[0].plot(samps[:,0],samps[:,1], 'o', color = 'C9')
ax[0].set_xlabel(r'$\alpha$')
ax[0].set_ylabel(r'$\beta$')
ax[1].set_title('Stan')
ax[1].plot(params['alpha'], params['beta'], 'o', color = 'C9')
ax[1].set_xlabel(r'$\alpha$')
ax[1].set_ylabel(r'$\beta$')
[(
    [tk.set_visible(True) for tk in ax.get_yticklabels()],
    [tk.set_visible(True) for tk in ax.get_yticklabels()]
 ) for ax in ax.flatten()]

stan_kde = stats.kde.gaussian_kde([params['alpha'], params['beta']])
stan_p = stan_kde(np.vstack([ai.flatten(), bi.flatten()]))

fig, ax = plt.subplots(nrows=1, ncols=2, figsize = (16, 5), sharex = True, sharey = Tru
e)
ax[0].set_title('Metropolis')
ax[0].pcolormesh(ai, bi, pi.reshape(ai.shape))
ax[0].set_xlabel(r'$\alpha$')
ax[0].set_ylabel(r'$\beta$')
ax[1].set_title('Stan')
ax[1].pcolormesh(ai, bi, stan_p.reshape(ai.shape))
ax[1].set_xlabel(r'$\alpha$')
ax[1].set_ylabel(r'$\beta$')

None
```





We see the to models looks similar, even though the Stan-model seems more smooth, and closer to the grid-reference.

References

[1] Metropolis–Hastings algorithm, Wikipedia (https://en.wikipedia.org/wiki/Metropolis%E2%80%93Hastings_algorithm)