

# Bayesian Data Analysis Chapter 4

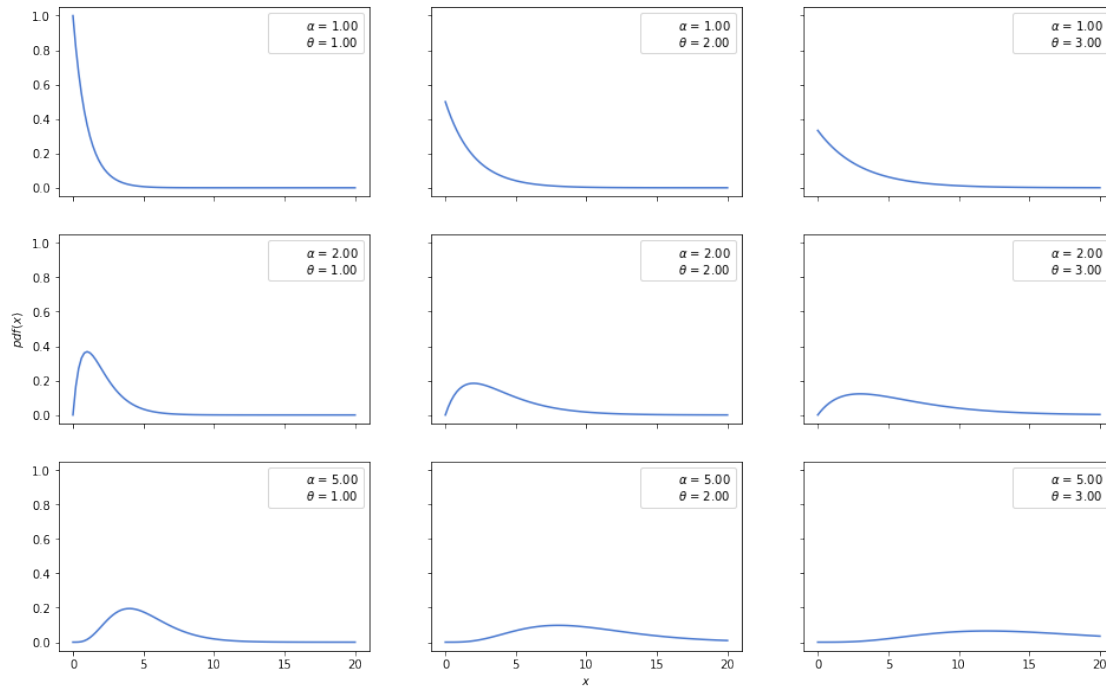
January 20, 2019

```
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 matplotlib
palette = 'muted'
sns.set_palette(palette); sns.set_color_codes(palette)
np.set_printoptions(precision=2)
pd.set_option('display.precision', 2)
```

## 0.1 The gamma distribution

```
In [2]: rates = [1, 2, 5]
scales = [1, 2, 3]

x = np.linspace(0, 20, 100)
f, ax = plt.subplots(len(rates), len(scales), sharex=True, sharey=True, figsize=(16,10))
for i in range(len(rates)):
    for j in range(len(scales)):
        rate = rates[i]
        scale = scales[j]
        rv = stats.gamma(a=rate, scale=scale)
        ax[i,j].plot(x, rv.pdf(x));
        ax[i,j].plot(0, 0,
            label="$\\alpha$ = {:.3f}\\n$\\theta$ = {:.3f}".format(rate, scale), alpha=0)
        ax[i,j].legend();
ax[2,1].set_xlabel('$x$');
ax[1,0].set_ylabel('$pdf(x)$');
```



## 0.2 Simple linear regression

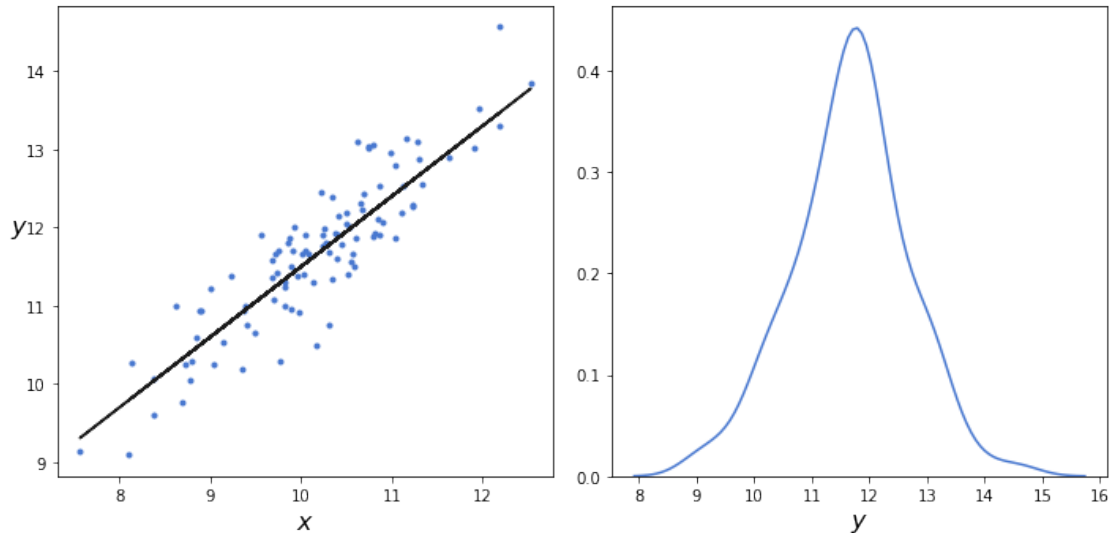
```
In [3]: np.random.seed(1)
        N = 100
        alfa_real = 2.5
        beta_real = 0.9
        eps_real = np.random.normal(0, 0.5, size=N)

        x = np.random.normal(10, 1, N)
        y_real = alfa_real + beta_real * x
        y = y_real + eps_real
```

```
# we can center the data
#x = x - x.mean()
# or standardize the data
#x = (x - x.mean())/x.std()
#y = (y - y.mean())/y.std()
```

```
In [4]: plt.figure(figsize=(10,5))
        plt.subplot(1,2,1)
        plt.plot(x, y, 'b.')
        plt.xlabel('$x$', fontsize=16)
        plt.ylabel('$y$', fontsize=16, rotation=0)
        plt.plot(x, y_real, 'k')
        plt.subplot(1,2,2)
```

```
sns.kdeplot(y)
plt.xlabel('$y$', fontsize=16)
plt.tight_layout()
```



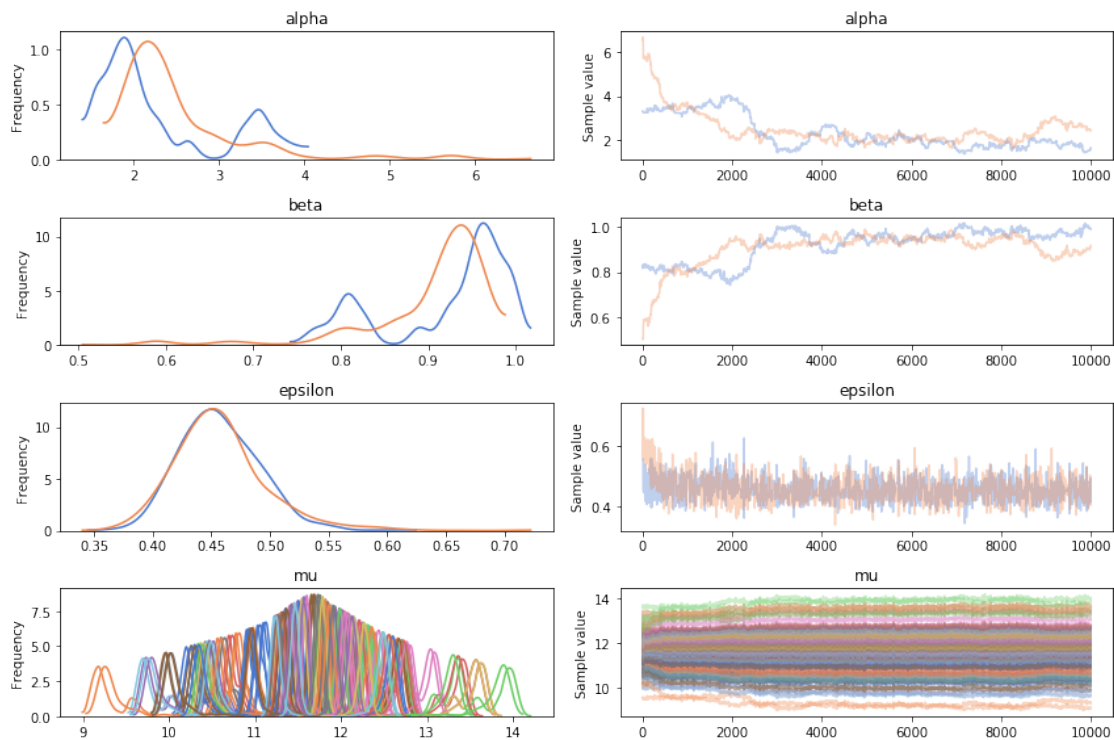
```
In [5]: with pm.Model() as model:
        alpha = pm.Normal('alpha', mu=0, sd=10)
        beta = pm.Normal('beta', mu=0, sd=1)
        epsilon = pm.HalfCauchy('epsilon', 5)

        mu = pm.Deterministic('mu', alpha + beta * x)
        y_pred = pm.Normal('y_pred', mu=mu, sd=epsilon, observed=y)

        start = pm.find_MAP()
        step = pm.Metropolis()
        trace = pm.sample(10000, step, start, njobs=1)
```

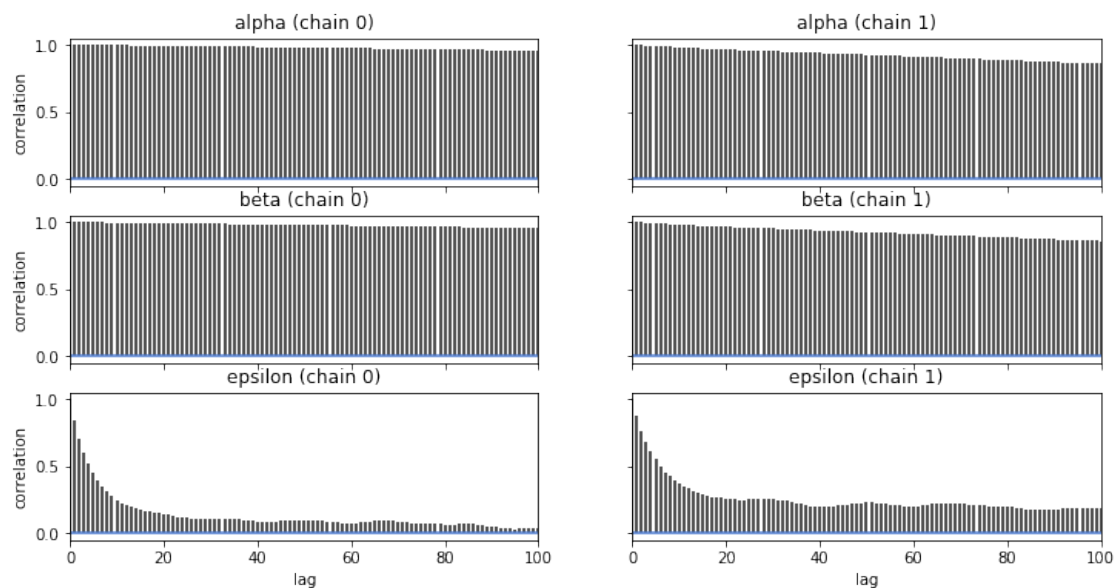
```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/pymc3/tuning/starting.py:61: U
    warnings.warn('find_MAP should not be used to initialize the NUTS sampler, simply call pymc3
logp = -66.676, ||grad|| = 48.412: 100%|| 38/38 [00:00<00:00, 2960.26it/s]
Sequential sampling (2 chains in 1 job)
CompoundStep
>Metropolis: [epsilon]
>Metropolis: [beta]
>Metropolis: [alpha]
100%|| 10500/10500 [00:02<00:00, 3914.10it/s]
100%|| 10500/10500 [00:02<00:00, 3926.04it/s]
The estimated number of effective samples is smaller than 200 for some parameters.
```

```
In [6]: pm.traceplot(trace);
```



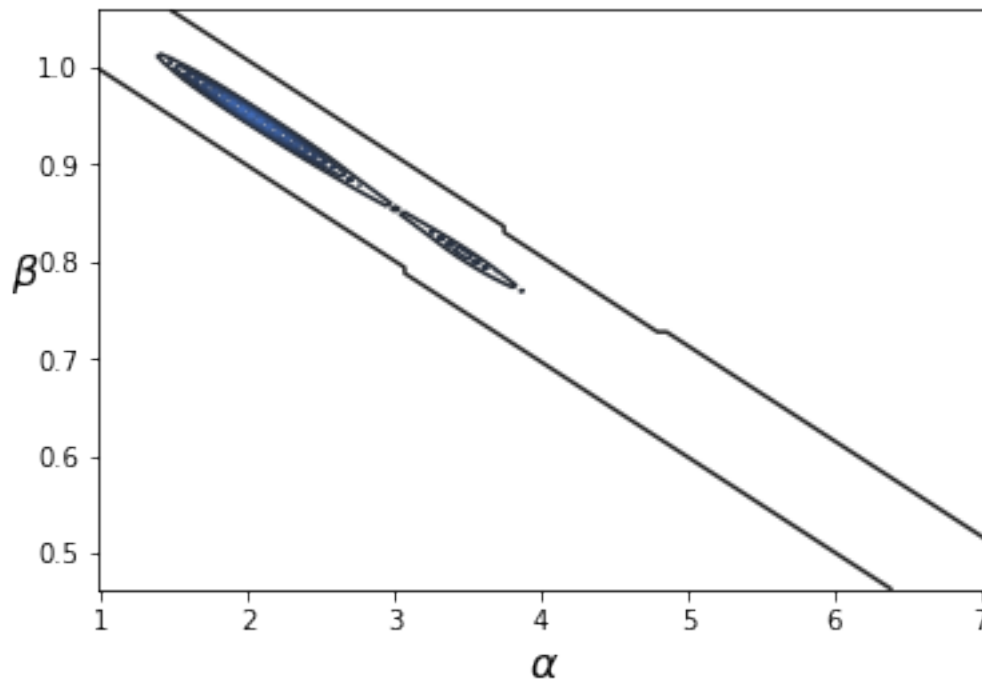
```
In [7]: #pm.summary(trace)
```

```
In [8]: varnames = ['alpha', 'beta', 'epsilon']
        pm.autocorrplot(trace, varnames);
```



We have a bad model we bad mixing and lots of autocorrelation for  $\alpha$  and  $\beta$ . This is because  $\alpha$  and  $\beta$  are correlated by definition since no matter what line we fit on our data it needs to pass through the means of  $y$  and  $x$ . So if that's true we are essentially spinning a line around the means of  $x$  and  $y$ , thus an increase in the slope  $\beta$  means a decrease in the intercept  $\alpha$ . This is obvious from the joint probability distribution below how correlated they are.

```
In [9]: sns.kdeplot(trace['alpha'], trace['beta']);
plt.xlabel(r'$\alpha$', fontsize=16);
plt.ylabel(r'$\beta$', fontsize=16, rotation=0);
```



To fix this we could centre the data before fitting (see commented code in the creation of the data above) or change our sampling method.

### 0.2.1 Changing the sampling method

```
In [10]: with pm.Model() as model_n:
    alpha = pm.Normal('alpha', mu=0, sd=10)
    beta = pm.Normal('beta', mu=0, sd=1)
    epsilon = pm.HalfCauchy('epsilon', 5)

    mu = pm.Deterministic('mu', alpha + beta * x)

    y_pred = pm.Normal('y_pred', mu=mu, sd=epsilon, observed=y)
```

```

start = pm.find_MAP()
step = pm.NUTS()
trace_n = pm.sample(2000, step=step, start=start, njobs=1)

```

```

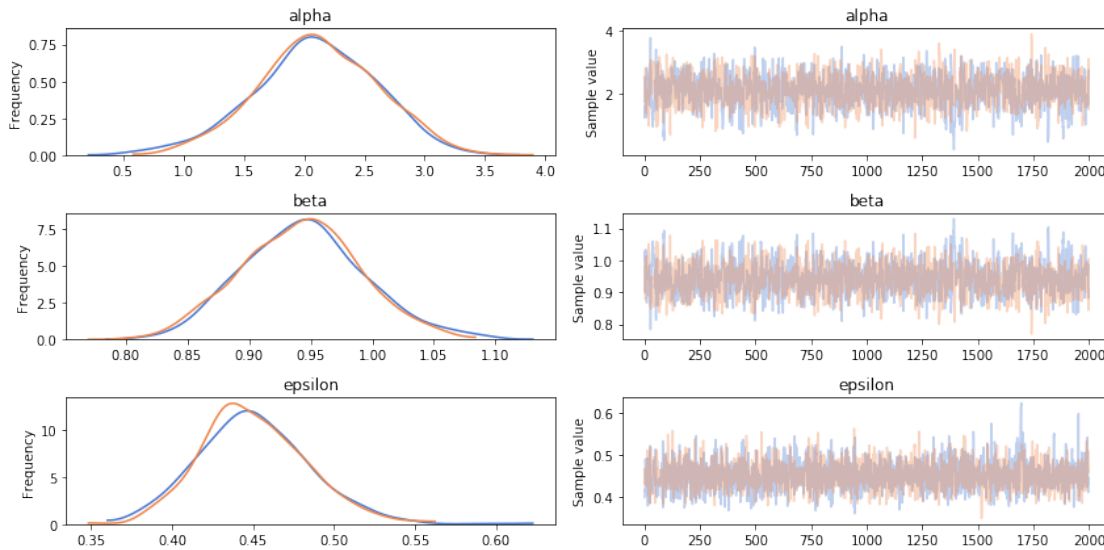
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/pymc3/tuning/starting.py:61: UserWarning: find_MAP should not be used to initialize the NUTS sampler, simply call pymc3
warnings.warn('find_MAP should not be used to initialize the NUTS sampler, simply call pymc3
logp = -66.676, ||grad|| = 48.412: 100%|| 38/38 [00:00<00:00, 3378.42it/s]
Sequential sampling (2 chains in 1 job)
NUTS: [epsilon, beta, alpha]
100%|| 2500/2500 [00:08<00:00, 284.84it/s]
100%|| 2500/2500 [00:08<00:00, 291.06it/s]

```

```

In [11]: pm.traceplot(trace_n, varnames);

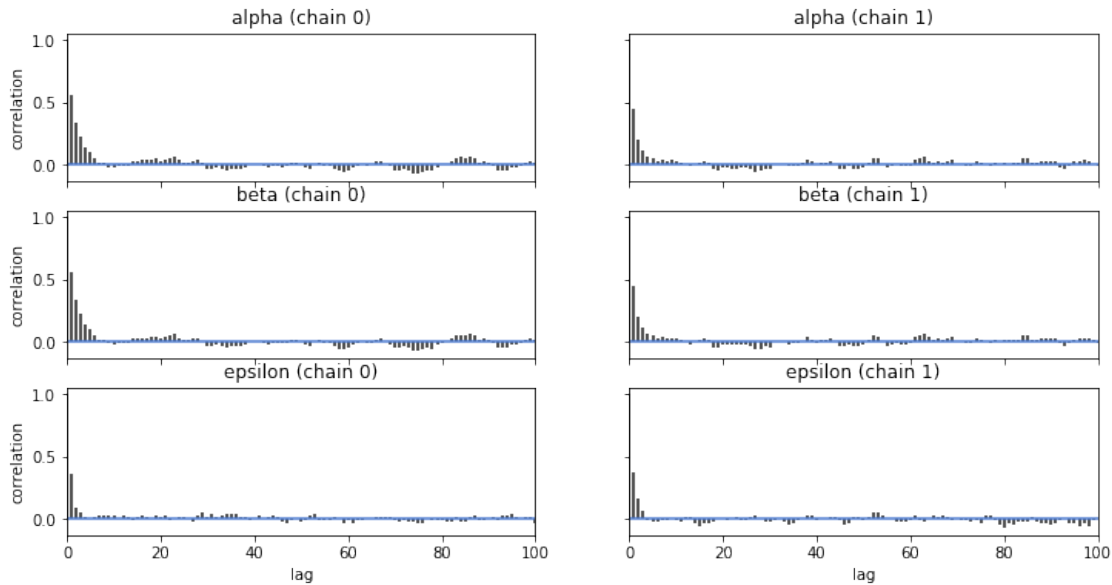
```



```

In [12]: pm.autocorrplot(trace_n, varnames);

```



```
In [13]: pm.summary(trace_n, varnames)
```

```
Out[13]:
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5	n_eff	Rhat
alpha	2.10	0.50	1.45e-02	1.11	3.07	1161.16	1.0
beta	0.94	0.05	1.43e-03	0.85	1.04	1148.15	1.0
epsilon	0.45	0.03	7.68e-04	0.38	0.51	1915.53	1.0

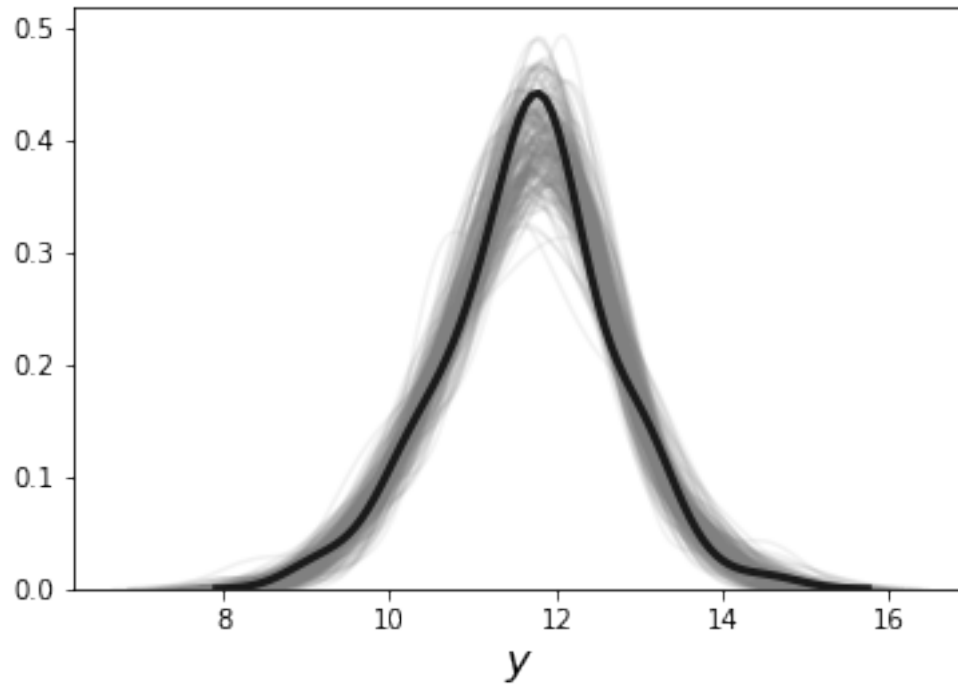
## 0.2.2 Posterior predictive checks

```
In [14]: ppc = pm.sample_ppc(trace_n, samples=231, model=model_n)
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/ipykernel_launcher.py:1: DeprecationWarning:
  """Entry point for launching an IPython kernel.
100%|| 231/231 [00:00<00:00, 2143.68it/s]
```

```
In [15]: # predicted data
for y_tilde in ppc['y_pred']:
    sns.kdeplot(y_tilde, alpha=0.1, c='gray')
# actual data
sns.kdeplot(y, linewidth=3, color='k')
plt.xlabel('$y$', fontsize=16);
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/matplotlib/cbook/__init__.py:
seen=seen, canon=canonical, used=seen[-1]))
```



### 0.3 Interpreting the posterior

#### 0.3.1 Plot the mean estimates of the model parameters

```
In [16]: plt.plot(x, y, 'b.');
```

```
         alpha_m = trace_n['alpha'].mean()
```

```
         beta_m = trace_n['beta'].mean()
```

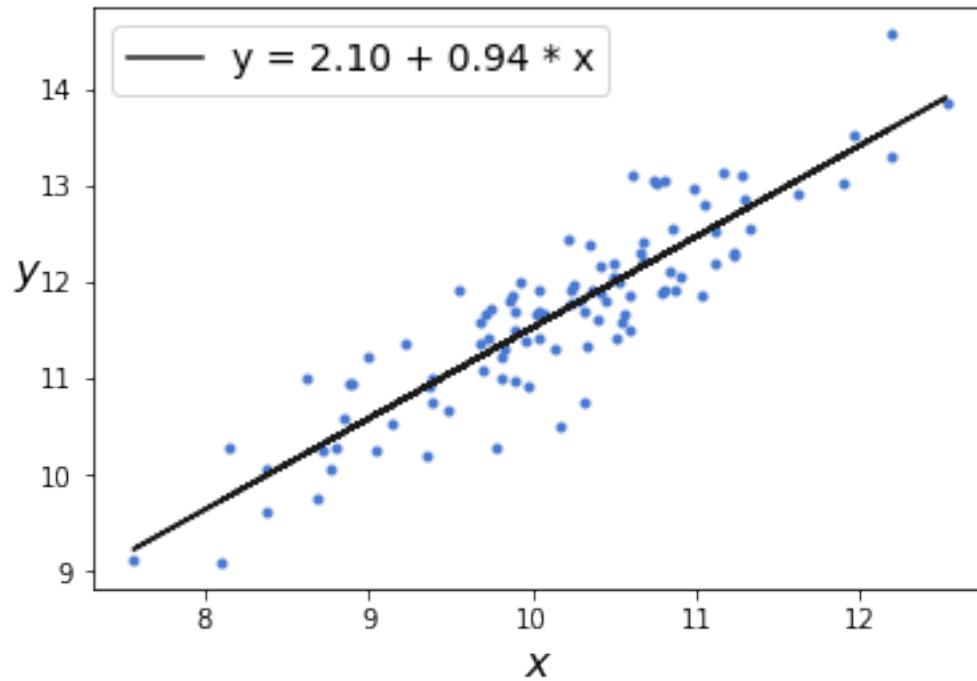
```
         plt.plot(x, alpha_m + beta_m * x, c='k', label='y = {:.2f} + {:.2f} * x'.format(alpha_m,
```

```
         plt.xlabel('$x$', fontsize=16);
```

```
         plt.ylabel('$y$', fontsize=16, rotation=0);
```

```
         plt.legend(loc=2, fontsize=14);
```





### 0.3.2 Plot the a sample of the lines from the parameters and the mean estimates

```
In [17]: plt.plot(x, y, 'b.');
```

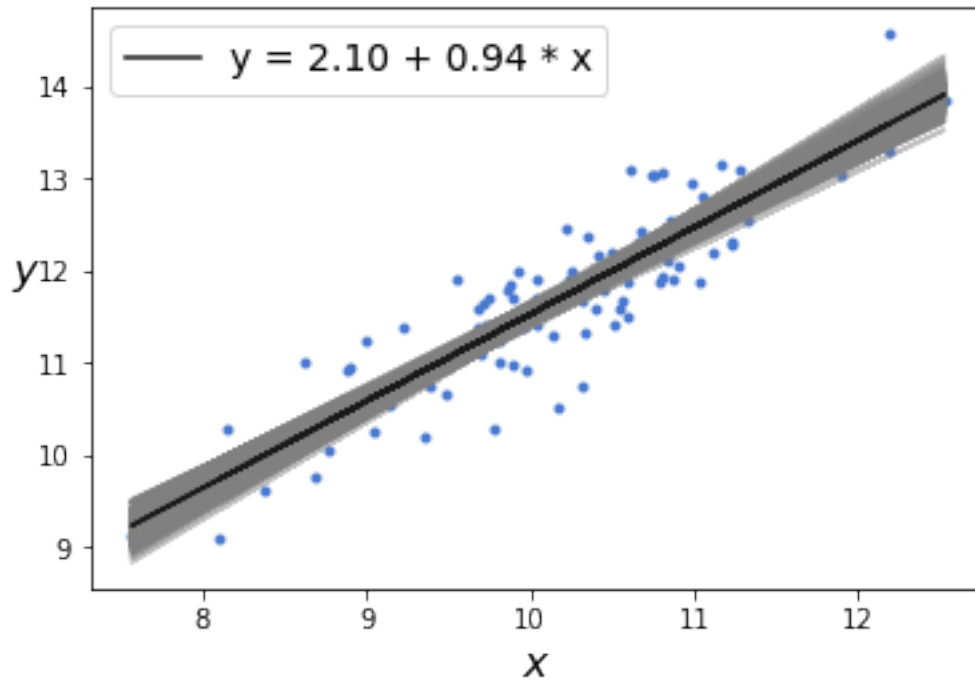
```

idx = range(0, len(trace_n['alpha']), 10)
plt.plot(x, trace_n['alpha'][idx] + trace_n['beta'][idx] * x[:,np.newaxis], c='gray'

plt.plot(x, alpha_m + beta_m * x, c='k', label='y = {:.2f} + {:.2f} * x'.format(alpha

plt.xlabel('$x$', fontsize=16);
plt.ylabel('$y$', fontsize=16, rotation=0);
plt.legend(loc=2, fontsize=14);

```

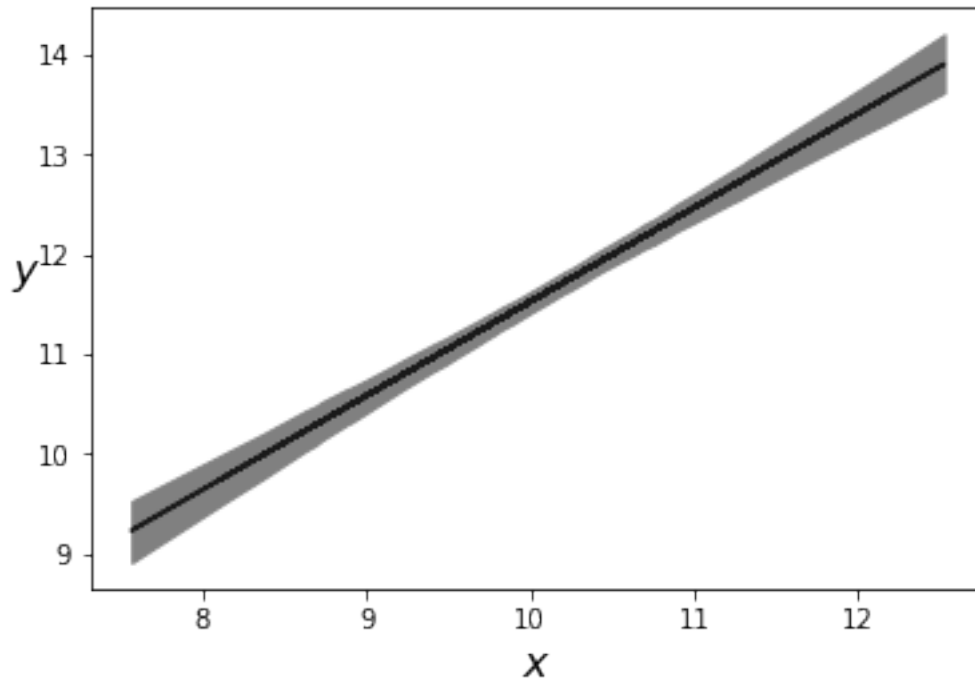


### 0.3.3 Plot the the HPD98% lines and the mean estimates

```
In [18]: plt.plot(x, alpha_m + beta_m * x, c='k', label='y = {:.2f} + {:.2f} * x'.format(alpha_m, beta_m))

idx = np.argsort(x)
x_ord = x[idx]
# note that `mu` is the deterministic variable that corresponds to the mean of the model
# (i.e. y_pred without the noise)
sig = pm.hpd(trace_n['mu'], alpha=.02)[idx]
plt.fill_between(x_ord, sig[:,0], sig[:,1], color='gray');

plt.xlabel('$x$', fontsize=16);
plt.ylabel('$y$', fontsize=16, rotation=0);
```



```
In [19]: ppc = pm.sample_ppc(trace_n, samples=1000, model=model_n)
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/ipykernel_launcher.py:1: DeprecationWarning:
  """Entry point for launching an IPython kernel.
100%|| 1000/1000 [00:00<00:00, 2792.48it/s]
```

### 0.3.4 Plot the the HPD95% lines of the prediction ( $y_{\text{pred}}$ ) and the mean estimates

```
In [20]: plt.plot(x, y, 'b.')
```

```
plt.plot(x, alpha_m + beta_m * x, c='k', label='y = {:.2f} + {:.2f} * x'.format(alpha_m, beta_m))
```

```
# note y_pred includes the noise (vs mu that doesn't)
```

```
# note that idx is used to order the samples according to the order of x
```

```
sig0 = pm.hpd(ppc['y_pred'], alpha=0.5)[idx]
```

```
sig1 = pm.hpd(ppc['y_pred'], alpha=0.05)[idx]
```

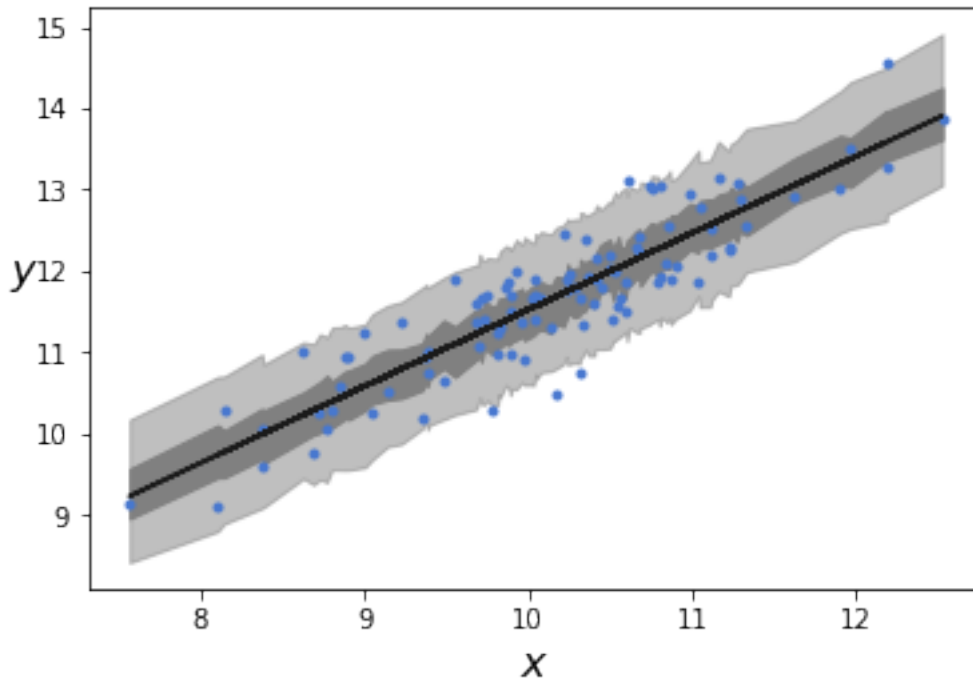
```
plt.fill_between(x_ord, sig0[:,0], sig0[:,1], color='gray', alpha=1)
```

```
plt.fill_between(x_ord, sig1[:,0], sig1[:,1], color='gray', alpha=0.5)
```

```
plt.xlabel('$x$', fontsize=16)
```

```
plt.ylabel('$y$', fontsize=16, rotation=0)
```

```
Out[20]: Text(0, 0.5, '$y$')
```



#### 0.4 Pearson correlation coefficient

```
In [21]: with pm.Model() as model_n:
          alpha = pm.Normal('alpha', mu=0, sd=10)
          beta = pm.Normal('beta', mu=0, sd=1)
          epsilon = pm.HalfCauchy('epsilon', 5)

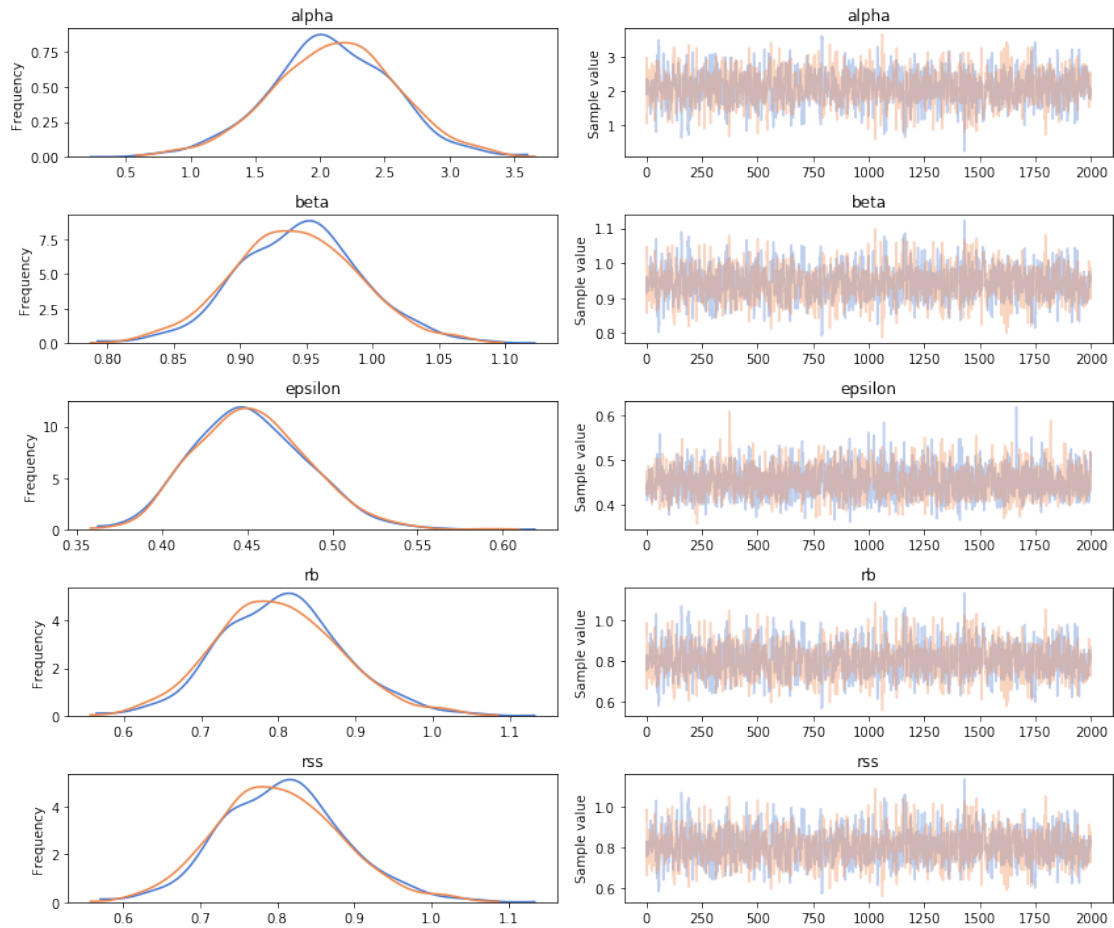
          mu = alpha + beta * x
          y_pred = pm.Normal('y_pred', mu=mu, sd=epsilon, observed=y)
          # coefficient of determination, i.e.  $r^2$  can be calculated like this
          rb = pm.Deterministic('rb', (beta * x.std() / y.std()) ** 2)
          # or like this `rss`
          y_mean = y.mean()
          ss_reg = pm.math.sum((mu - y_mean) ** 2)
          ss_tot = pm.math.sum((y - y_mean) ** 2)
          rss = pm.Deterministic('rss', ss_reg/ss_tot)

          start = pm.find_MAP()
          step = pm.NUTS()
          trace_n = pm.sample(2000, step=step, start=start, njobs=1)
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/pymc3/tuning/starting.py:61: UserWarning: find_MAP should not be used to initialize the NUTS sampler, simply call pymc3
logp = -66.676, ||grad|| = 48.412: 100%| 38/38 [00:00<00:00, 4219.96it/s]
```

```
Sequential sampling (2 chains in 1 job)
NUTS: [epsilon, beta, alpha]
100%|| 2500/2500 [00:08<00:00, 296.38it/s]
100%|| 2500/2500 [00:08<00:00, 302.33it/s]
```

```
In [22]: pm.traceplot(trace_n);
```



```
In [23]: pm.summary(trace_n)
```

```
Out [23]:
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5	n_eff	Rhat
alpha	2.09	0.48	1.20e-02	1.13	3.03	1231.79	1.0
beta	0.94	0.05	1.17e-03	0.85	1.04	1230.75	1.0
epsilon	0.45	0.03	7.54e-04	0.39	0.51	1728.19	1.0
rb	0.80	0.08	1.99e-03	0.65	0.97	1228.96	1.0
rss	0.80	0.08	2.00e-03	0.65	0.96	1228.58	1.0

## 0.4.1 The multivariate normal distribution

Actually the bivariate

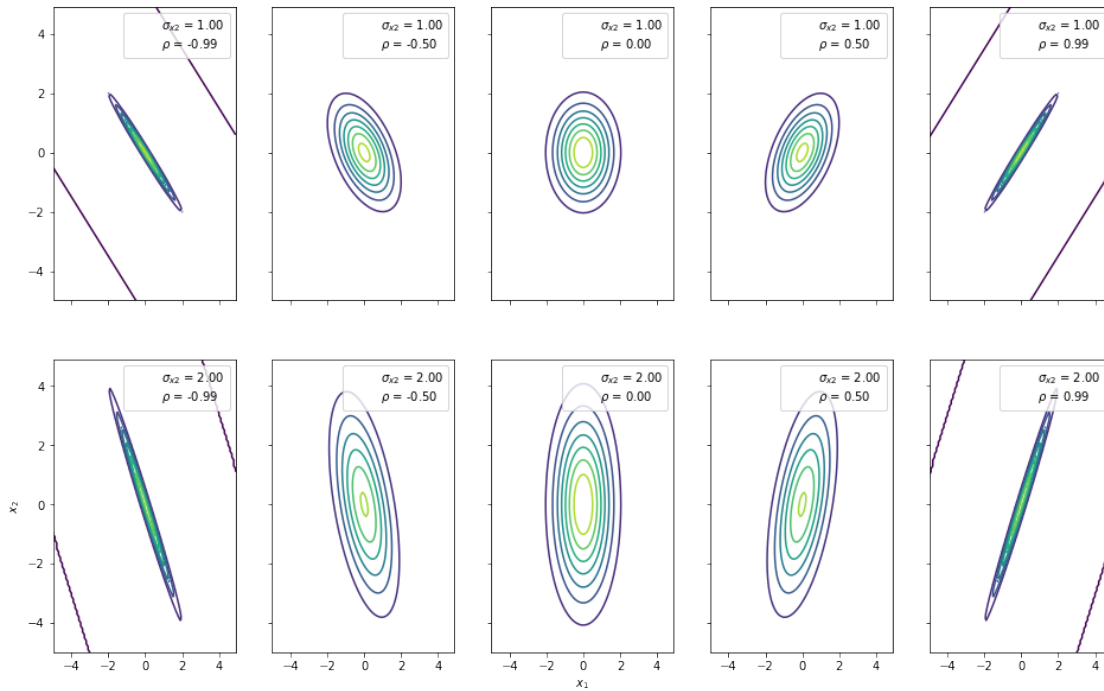
```

In [24]: sigma_x1 = 1
        sigmas_x2 = [1, 2]
        rhos = [-0.99, -0.5, 0, 0.5, 0.99]

        k, l = np.mgrid[-5:5:.1, -5:5:.1]
        pos = np.empty(k.shape + (2,))
        pos[:, :, 0] = k; pos[:, :, 1] = l

        f, ax = plt.subplots(len(sigmas_x2), len(rhos), sharex=True, sharey=True)
        #f.figure(figsize=(5, 1))
        for i in range(2):
            for j in range(5):
                sigma_x2 = sigmas_x2[i]
                rho = rhos[j]
                cov = [[sigma_x1**2, sigma_x1*sigma_x2*rho], [sigma_x1*sigma_x2*rho, sigma_x2**2]]
                rv = stats.multivariate_normal([0, 0], cov)
                ax[i,j].contour(k, l, rv.pdf(pos))
                ax[i,j].plot(0, 0,
                    label="$\\sigma_{x2} = {:.2f} \\rho = {:.2f}".format(sigma_x2, rho),
                    ax[i,j].legend()
                ax[1,2].set_xlabel('$x_1$')
                ax[1,0].set_ylabel('$x_2$')
                fig = matplotlib.pyplot.gcf()
                fig.set_size_inches(16,10)

```



```
In [25]: data = np.stack((x, y)).T
         print('Stacked x(column 1) and y(column 2): \n{}'.format(data[:5,:]))
```

Stacked x(column 1) and y(column 2):

```
[[ 9.55 11.91]
 [11.22 12.3 ]
 [10.4  11.6 ]
 [10.59 11.5 ]
 [ 8.91 10.95]]
```

```
In [26]: with pm.Model() as pearson_model:
         # 2-d vector of the means of each variable
         # we initialise at the calculated means from the data (data.mean(axis=0))
         mu = pm.Normal('mu', mu=data.mean(axis=0), sd=10, shape=2)
         # priors on the elements that make up the covariance matrix
         # there are other ways of putting a prior on a covariance matrix
         # see page 112 of the book
         sigma_1 = pm.HalfNormal('sigma_1', 10)
         sigma_2 = pm.HalfNormal('sigma_2', 10)
         rho = pm.Uniform('rho', -1, 1)

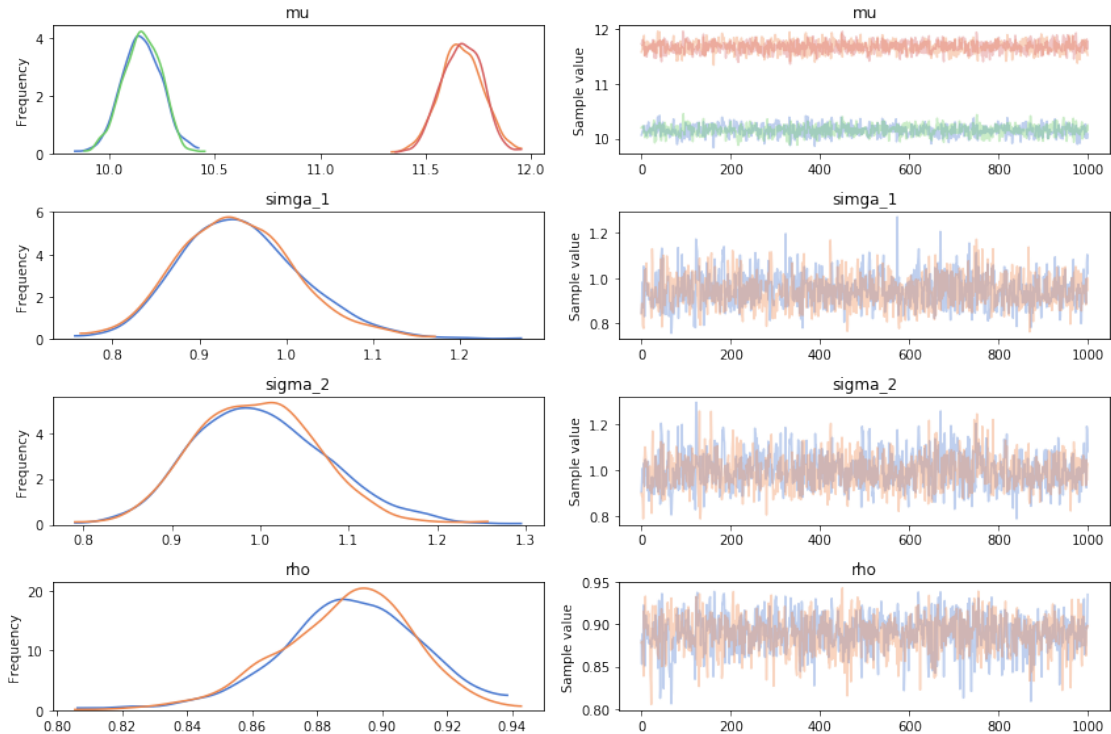
         cov = pm.math.stack([sigma_1**2, sigma_1*sigma_2*rho], [sigma_1*sigma_2*rho, sigma_2**2])

         y_pred = pm.MvNormal('y_pred', mu=mu, cov=cov, observed=data)

         # start = pm.find_MAP()
         step = pm.NUTS()#scaling=start
         trace_p = pm.sample(1000, step=step, start=start, njobs=1)
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: I
result[diagonal_slice] = x
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: I
result[diagonal_slice] = x
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: I
result[diagonal_slice] = x
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: I
result[diagonal_slice] = x
Sequential sampling (2 chains in 1 job)
NUTS: [rho, sigma_2, sigma_1, mu]
0%|          | 0/1500 [00:00<?, ?it/s]/home/damianos/miniconda3/envs/pymc3/lib/python3.7/sit
result[diagonal_slice] = x
100%|| 1500/1500 [00:09<00:00, 165.60it/s]
100%|| 1500/1500 [00:07<00:00, 204.79it/s]
```

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



```
In [28]: print(pm.summary(trace_p))
          print('R^2 = {:.2f}'.format(np.square(trace_p['rho'].mean()))+ ' (for comparison with
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5	n_eff	Rhat
mu__0	10.15	0.09	2.58e-03	9.96	10.32	1123.01	1.0
mu__1	11.67	0.10	2.65e-03	11.48	11.85	1092.48	1.0
sigma_1	0.95	0.07	2.11e-03	0.82	1.08	1063.89	1.0
sigma_2	1.00	0.07	2.33e-03	0.86	1.14	921.04	1.0
rho	0.89	0.02	6.92e-04	0.85	0.93	1118.32	1.0

R^2 = 0.79 (for comparison with previous)

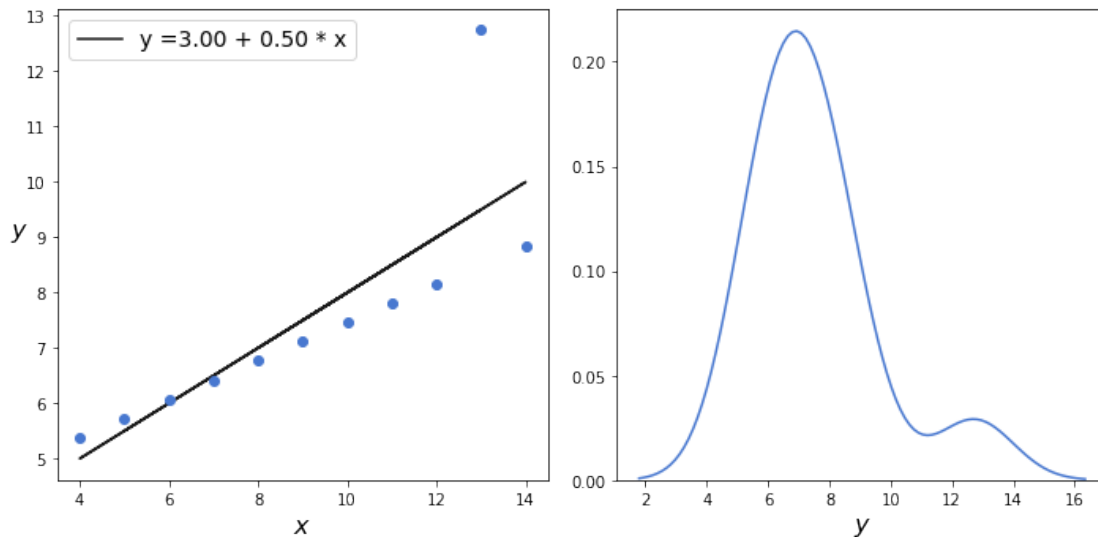
## 0.5 Robust linear regression

```
In [29]: ans = sns.load_dataset('anscombe')
          x_3 = ans[ans.dataset == 'III']['x'].values
          y_3 = ans[ans.dataset == 'III']['y'].values

In [30]: plt.figure(figsize=(10,5))
          plt.subplot(1,2,1)
          beta_c, alpha_c = stats.linregress(x_3, y_3)[:2]
          plt.plot(x_3, (alpha_c + beta_c* x_3), 'k', label='y = {:.2f} + {:.2f} * x'.format(alpha_c, beta_c))
          plt.plot(x_3, y_3, 'bo')
          plt.xlabel('$x$', fontsize=16)
```



```
plt.ylabel('$y$', rotation=0, fontsize=16)
plt.legend(loc=0, fontsize=14)
plt.subplot(1,2,2)
sns.kdeplot(y_3);
plt.xlabel('$y$', fontsize=16)
plt.tight_layout()
```



```
In [31]: with pm.Model() as model_t:
          alpha = pm.Normal('alpha', mu=0, sd=100)
          beta = pm.Normal('beta', mu=0, sd=1)
          epsilon = pm.HalfCauchy('epsilon', 5)
          nu = pm.Deterministic('nu', pm.Exponential('nu_', 1/29) + 1)

          y_pred = pm.StudentT('y_pred', mu=alpha + beta * x_3, sd=epsilon, nu=nu, observed=

          # start = pm.find_MAP() -> pymc3 warns against using MAP to initialise NUTS
          step = pm.NUTS() #scaling=start
          trace_t = pm.sample(2000, step=step, start=start, njobs=1)
```

Sequential sampling (2 chains in 1 job)

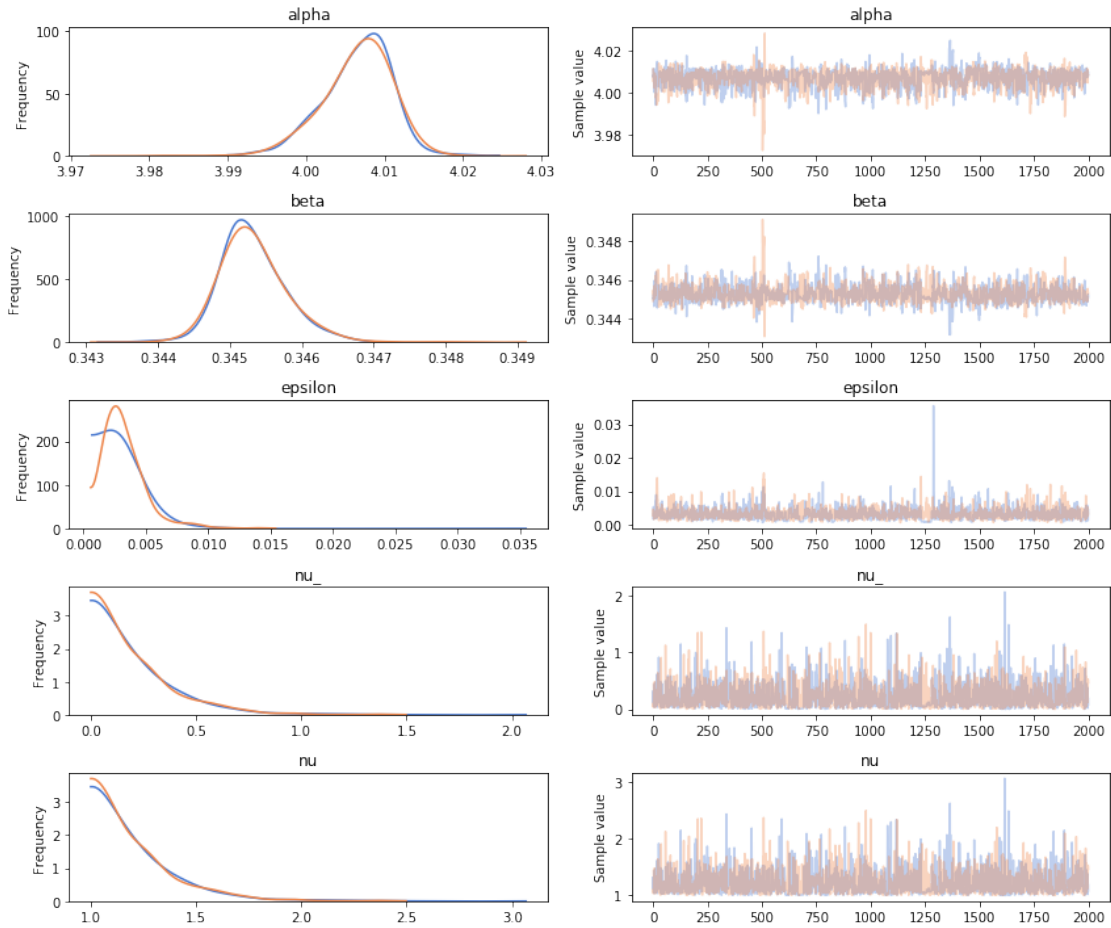
NUTS: [nu\_, epsilon, beta, alpha]

100%|| 2500/2500 [00:08<00:00, 286.47it/s]

100%|| 2500/2500 [00:10<00:00, 230.80it/s]

The acceptance probability does not match the target. It is 0.8922604997825845, but should be 0.8

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

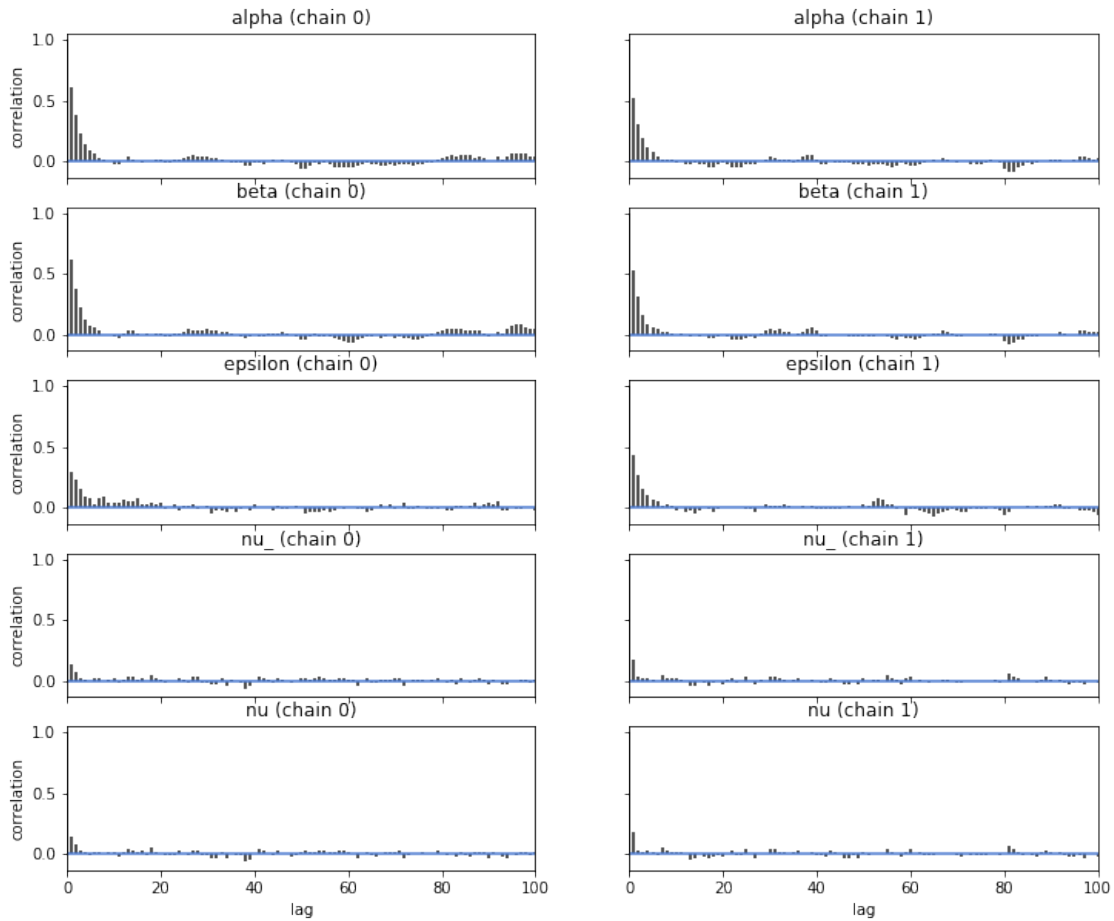


```
In [33]: pm.summary(trace_t)
```

```
Out[33]:
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5	n_eff	Rhat
alpha	4.01e+00	4.38e-03	1.31e-04	4.00e+00	4.01e+00	1035.04	1.0
beta	3.45e-01	4.55e-04	1.37e-05	3.45e-01	3.46e-01	1069.23	1.0
epsilon	3.24e-03	1.79e-03	5.53e-05	6.67e-04	6.39e-03	1114.93	1.0
nu <sub>-</sub>	2.11e-01	2.09e-01	4.23e-03	7.57e-05	6.20e-01	2590.24	1.0
nu	1.21e+00	2.09e-01	4.23e-03	1.00e+00	1.62e+00	2590.24	1.0

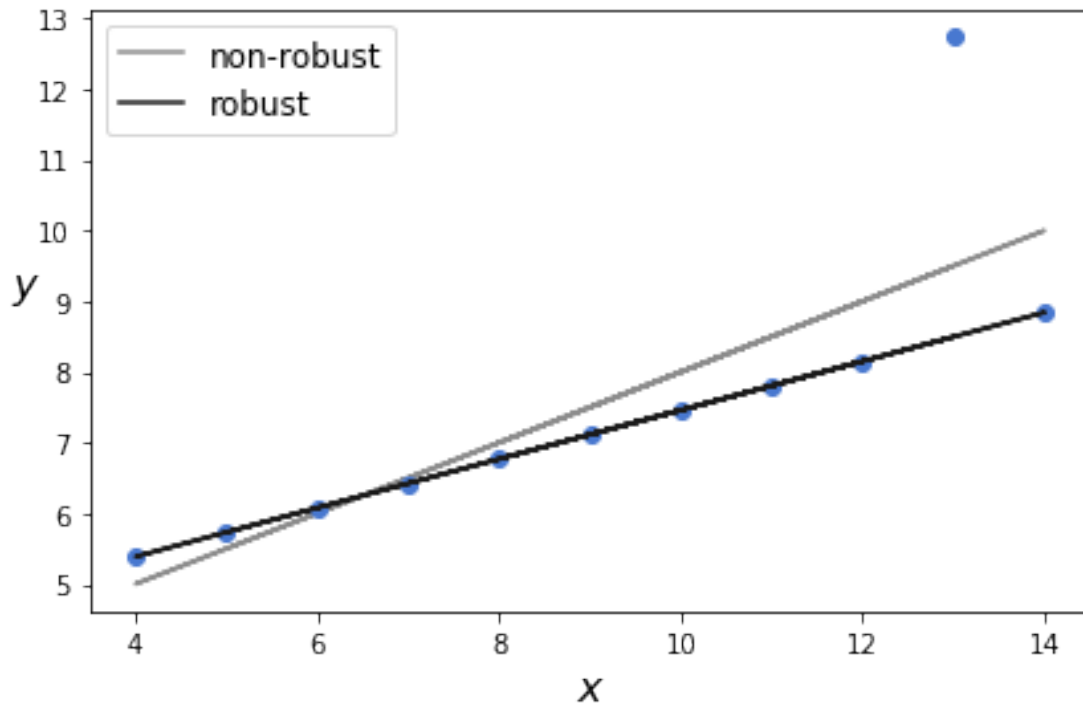
```
In [34]: pm.autocorrplot(trace_t);
```



```
In [35]: beta_c, alpha_c = stats.linregress(x_3, y_3)[:2]
```

```
plt.plot(x_3, (alpha_c + beta_c * x_3), 'k', label='non-robust', alpha=0.5)
plt.plot(x_3, y_3, 'bo')
alpha_m = trace_t['alpha'].mean()
beta_m = trace_t['beta'].mean()
plt.plot(x_3, alpha_m + beta_m * x_3, c='k', label='robust')

plt.xlabel('$x$', fontsize=16)
plt.ylabel('$y$', rotation=0, fontsize=16)
plt.legend(loc=2, fontsize=12)
plt.tight_layout()
```



```
In [36]: ppc = pm.sample_ppc(trace_t, samples=200, model=model_t, random_seed=2)
```

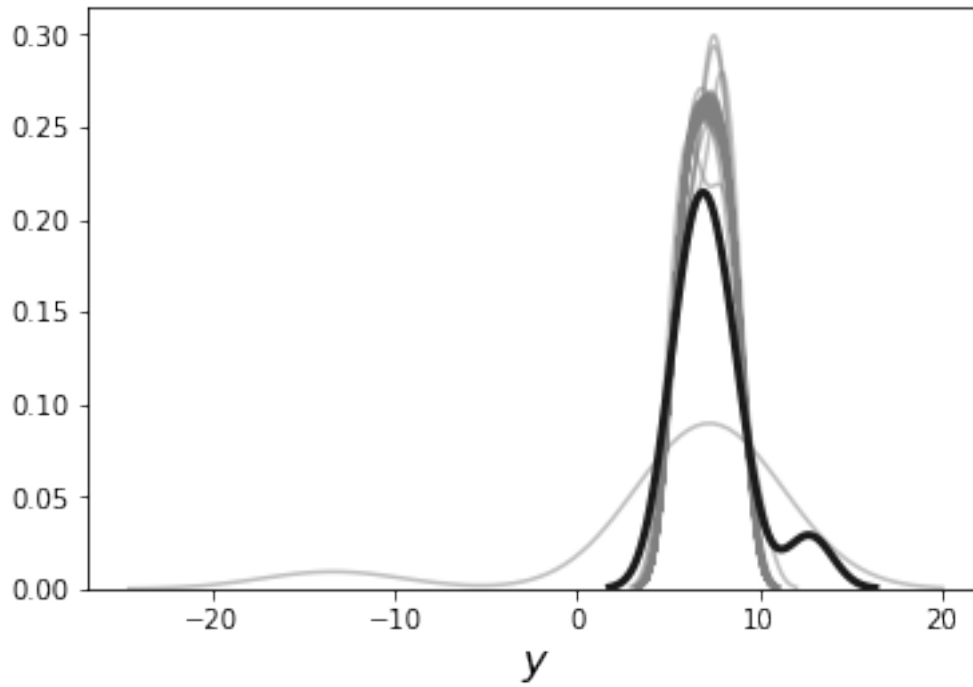
```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/ipykernel_launcher.py:1: DeprecationWarning:
  """Entry point for launching an IPython kernel.
100%|| 200/200 [00:00<00:00, 1524.18it/s]
```

```
In [37]: # predicted data
for y_tilde in ppc['y_pred']:
    sns.kdeplot(y_tilde, alpha=0.5, c='gray')

# actual data
sns.kdeplot(y_3, linewidth=3, color='k')
plt.xlabel('$y$', fontsize=16)
```

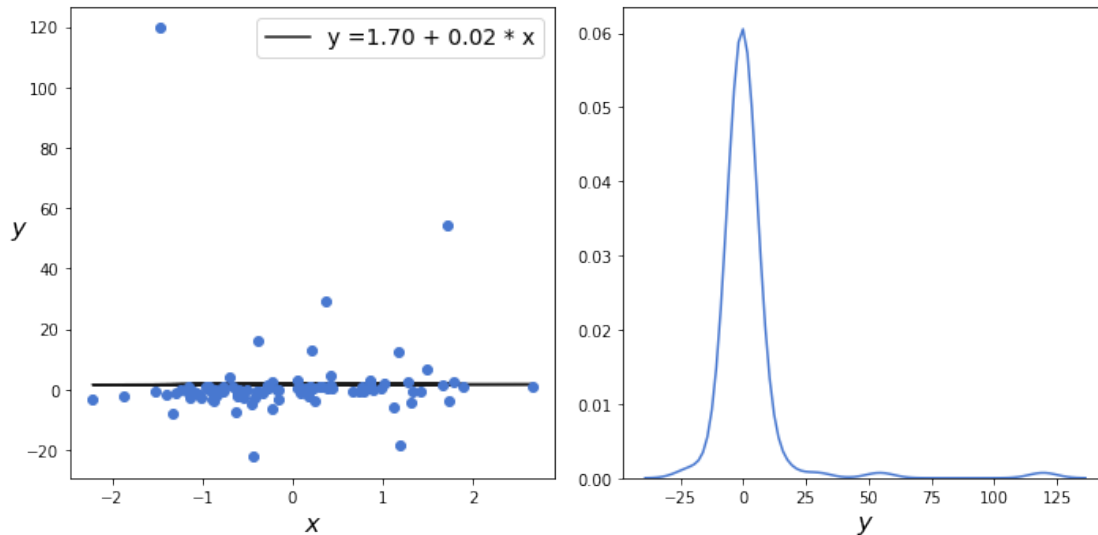
```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/matplotlib/cbook/__init__.py:
seen=seen, canon=canonical, used=seen[-1]))
```

```
Out[37]: Text(0.5, 0, '$y$')
```



```
In [38]: np.random.seed(314)
x_4 = np.random.normal(size=100)
y_4 = x_4 + np.random.standard_t(df=1, size=100) # experiments with different values

plt.figure(figsize=(10,5))
plt.subplot(1,2,1)
beta_c, alpha_c = stats.linregress(x_4, y_4)[:2]
plt.plot(x_4, (alpha_c + beta_c* x_4), 'k', label='y ={: .2f} + {: .2f} * x'.format(alpha_c, beta_c))
plt.plot(x_4, y_4, 'bo')
plt.xlabel('$x$', fontsize=16)
plt.ylabel('$y$', rotation=0, fontsize=16)
plt.legend(loc=0, fontsize=14)
plt.subplot(1,2,2)
sns.kdeplot(y_4);
plt.xlabel('$y$', fontsize=16)
plt.tight_layout()
```



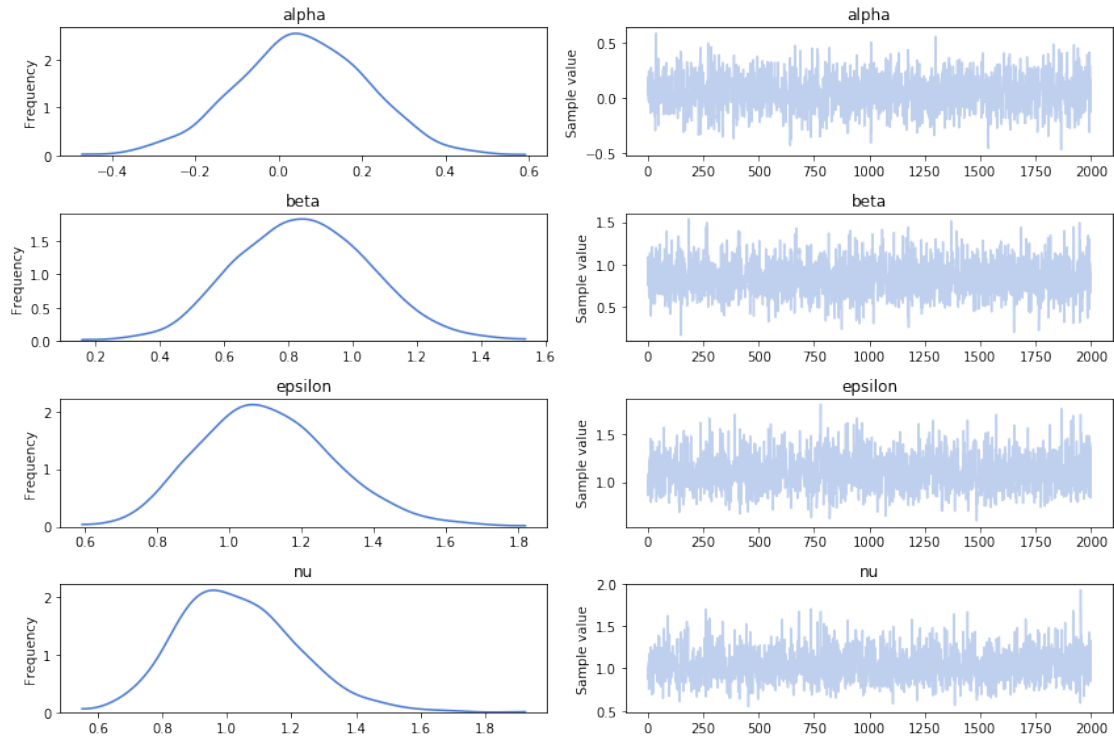
```
In [39]: with pm.Model() as model_t2:
          alpha = pm.Normal('alpha', mu=0, sd=100)
          beta = pm.Normal('beta', mu=0, sd=1)
          epsilon = pm.HalfCauchy('epsilon', 5)
          nu = pm.Exponential('nu', 1/30)
          #nu = pm.Gamma('nu', mu=20, sd=15)
          #nu = pm.Gamma('nu', 2, 0.1)

          y_pred = pm.StudentT('y_pred', mu=alpha + beta * x_4, sd=epsilon, nu=nu, observed=

          #      start = pm.find_MAP()
          step = pm.NUTS() #scaling=start
          trace_t2 = pm.sample(2000, step=step, start=start, njobs=1, chains=1)

Sequential sampling (1 chains in 1 job)
NUTS: [nu, epsilon, beta, alpha]
100%|| 2500/2500 [00:02<00:00, 1113.72it/s]
Only one chain was sampled, this makes it impossible to run some convergence checks

In [40]: pm.traceplot(trace_t2);
```



```
In [41]: pm.summary(trace_t2)
```

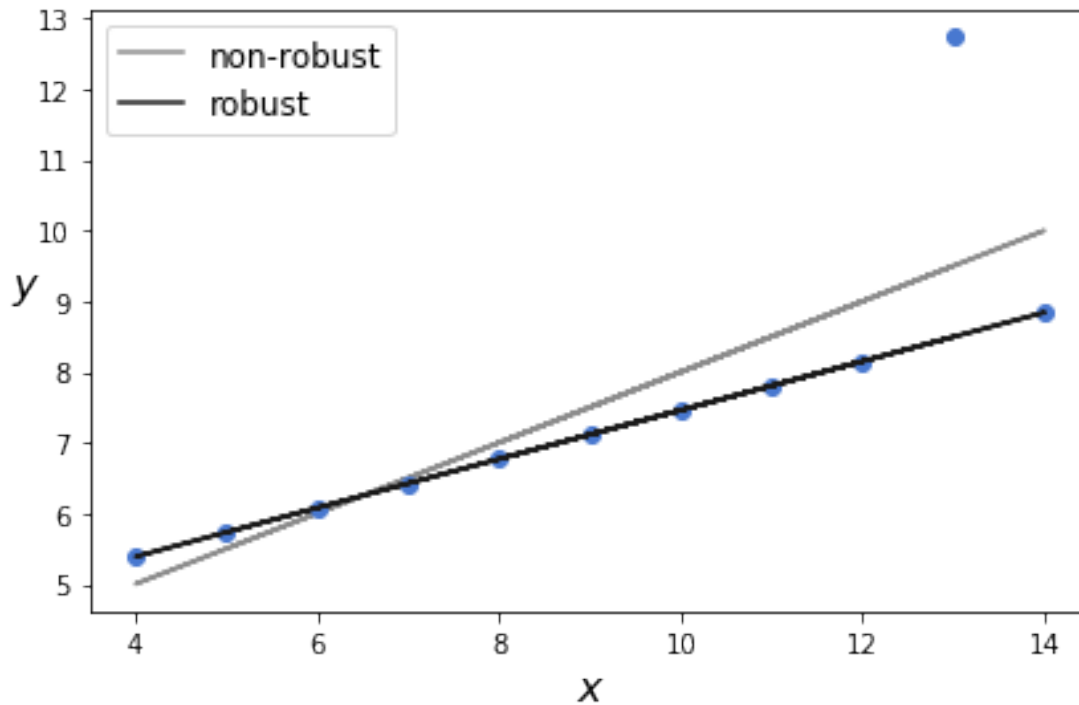
```
Out[41]:
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5
alpha	0.05	0.15	3.23e-03	-0.27	0.33
beta	0.84	0.21	4.84e-03	0.44	1.24
epsilon	1.10	0.18	4.96e-03	0.76	1.46
nu	1.03	0.18	4.84e-03	0.69	1.39

```
In [42]: beta_c, alpha_c = stats.linregress(x_3, y_3)[:2]
```

```
plt.plot(x_3, (alpha_c + beta_c * x_3), 'k', label='non-robust', alpha=0.5)
plt.plot(x_3, y_3, 'bo')
alpha_m = trace_t['alpha'].mean()
beta_m = trace_t['beta'].mean()
plt.plot(x_3, alpha_m + beta_m * x_3, c='k', label='robust')

plt.xlabel('$x$', fontsize=16)
plt.ylabel('$y$', rotation=0, fontsize=16)
plt.legend(loc=2, fontsize=12)
plt.tight_layout()
```



## 0.6 Hierarchical linear regression

In [43]: `N = 20`

`M = 8`

`idx = np.repeat(range(M-1), N)`

`idx = np.append(idx, 7)`

`np.random.seed(314)`

`print('alpha and beta are drawn from the same distributions justifying the use of hierarchical models')`

`alpha_real = np.random.normal(2.5, 0.5, size=M)`

`beta_real = np.random.beta(6, 1, size=M)`

`eps_real = np.random.normal(0, 0.5, size=len(idx))`

`y_m = np.zeros(len(idx))`

`x_m = np.random.normal(10, 1, len(idx))`

`y_m = alpha_real[idx] + beta_real[idx] * x_m + eps_real`

`print('alpha of each group:\n {}'.format(alpha_real))`

`print('beta of each group:\n {}'.format(beta_real))`

`print('Indices of the groups to identify each point in x_m and y_m:\n {}'.format(idx))`

alpha and beta are drawn from the same distributions justifying the use of hierarchical models

alpha of each group:

[2.58 2.89 2.93 2.15 2.03 2.94 2.39 2.69]



[0.89 0.96 0.88 0.79 0.78 0.7 0.92 0.94]

[illegible]

```
1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 5 5 5 5 5 5 5 5 5 5 5 5 5
5 5 5 5 5 5 5 5 5 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 7]
```

Figure 1 displays eight scatter plots showing the relationship between  $y$  and  $x_0$  through  $x_7$ . The plots are arranged in a 2x4 grid. The y-axis for all plots ranges from 8 to 16. The x-axes range from 7.5 to 15.0. The plots show varying degrees of correlation and data density.

### Non-hierarchical model

25

```

beta = pm.Normal('beta', mu=0, sd=10, shape=M)
epsilon = pm.HalfCauchy('epsilon', 5)
nu = pm.Exponential('nu', 1/30)

y_pred = pm.StudentT('y_pred', mu= alpha_tmp[idx] + beta[idx] * x_centered,
                      sd=epsilon, nu=nu, observed=y_m)

alpha = pm.Deterministic('alpha', alpha_tmp - beta * x_m.mean())

# start = pm.find_MAP()
step = pm.NUTS()# scaling=start
trace_up = pm.sample(2000, step=step, chains=1,njobs=1)

```

Sequential sampling (1 chains in 1 job)

NUTS: [nu, epsilon, beta, alpha\_tmp]

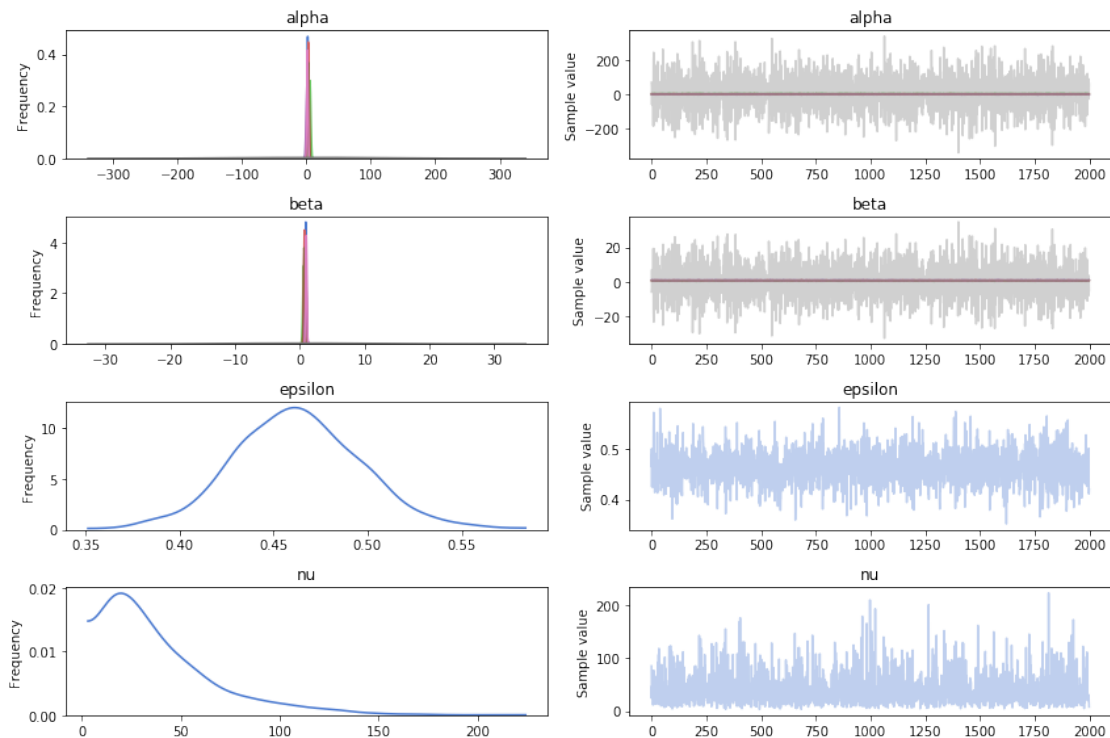
100%|| 2500/2500 [00:04<00:00, 558.31it/s]

Only one chain was sampled, this makes it impossible to run some convergence checks

```

In [47]: varnames=['alpha', 'beta', 'epsilon', 'nu']
         _=pm.traceplot(trace_up, varnames)

```



we can see that everything is converging except one  $\beta$  and one  $\alpha$

```
In [48]: # pm.autocorrplot(trace_up, varnames);
```

```
In [49]: pm.summary(trace_up, varnames)
```

```
Out[49]:
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5
alpha__0	2.42	0.80	1.13e-02	0.91	3.95
alpha__1	3.70	1.16	1.77e-02	1.42	6.00
alpha__2	5.63	1.30	2.22e-02	3.08	8.17
alpha__3	3.04	0.87	1.36e-02	1.22	4.63
alpha__4	1.29	1.35	2.12e-02	-1.36	3.95
alpha__5	3.22	1.03	1.56e-02	1.29	5.15
alpha__6	1.74	0.92	1.55e-02	-0.05	3.45
alpha__7	8.47	104.36	1.40e+00	-186.40	215.11
beta__0	0.90	0.08	1.10e-03	0.74	1.04
beta__1	0.88	0.12	1.81e-03	0.64	1.10
beta__2	0.60	0.13	2.18e-03	0.35	0.86
beta__3	0.70	0.09	1.35e-03	0.53	0.87
beta__4	0.87	0.13	2.05e-03	0.62	1.14
beta__5	0.68	0.10	1.51e-03	0.49	0.87
beta__6	0.99	0.09	1.49e-03	0.82	1.16
beta__7	0.33	10.38	1.39e-01	-20.20	19.69
epsilon	0.46	0.03	6.22e-04	0.39	0.53
nu	39.81	30.20	5.90e-01	3.90	103.33

note the massive sd on  $\alpha_7$   $\beta_7$

```
In [50]: with pm.Model() as hierarchical_model:
```

```
    # hyper-priors
```

```
    alpha_tmp_mu = pm.Normal('alpha_tmp_mu', mu=0, sd=10)
```

```
    alpha_tmp_sd = pm.HalfNormal('alpha_tmp_sd', 10)
```

```
    beta_mu = pm.Normal('beta_mu', mu=0, sd=10)
```

```
    beta_sd = pm.HalfNormal('beta_sd', sd=10)
```

```
    # priors
```

```
    alpha_tmp = pm.Normal('alpha_tmp', mu=alpha_tmp_mu, sd=alpha_tmp_sd, shape=M)
```

```
    beta = pm.Normal('beta', mu=beta_mu, sd=beta_sd, shape=M)
```

```
    epsilon = pm.HalfCauchy('epsilon', 5)
```

```
    nu = pm.Exponential('nu', 1/30)
```

```
    y_pred = pm.StudentT('y_pred', mu=alpha_tmp[idx] + beta[idx] * x_centered,
                          sd=epsilon, nu=nu, observed=y_m)
```

```
    alpha = pm.Deterministic('alpha', alpha_tmp - beta * x_m.mean())
```

```
    alpha_mu = pm.Deterministic('alpha_mu', alpha_tmp_mu - beta_mu * x_m.mean())
```

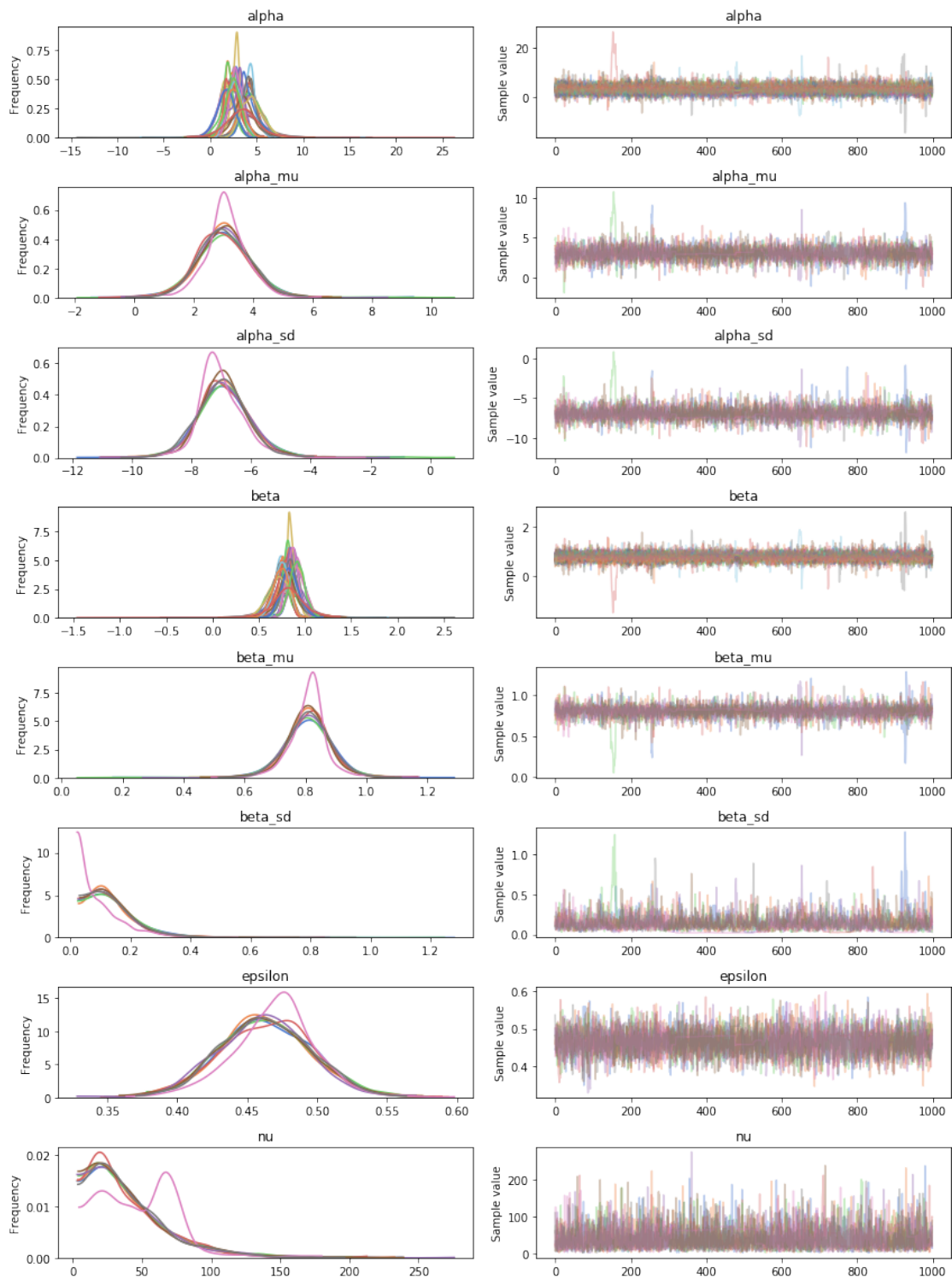
```
    alpha_sd = pm.Deterministic('alpha_sd', alpha_tmp_sd - beta_mu * x_m.mean())
```

```
    # use advi instead of MAP to provide initial values
```

```
    trace_hm = pm.sample(1000, advi_map=True, chains=8, njobs=8)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Multiprocess sampling (8 chains in 8 jobs)
NUTS: [nu, epsilon, beta, alpha_tmp, beta_sd, beta_mu, alpha_tmp_sd, alpha_tmp_mu]
Sampling 8 chains: 100%|| 12000/12000 [00:10<00:00, 1154.97draws/s]
There were 47 divergences after tuning. Increase `target_accept` or reparameterize.
There were 21 divergences after tuning. Increase `target_accept` or reparameterize.
There were 14 divergences after tuning. Increase `target_accept` or reparameterize.
There were 67 divergences after tuning. Increase `target_accept` or reparameterize.
There were 11 divergences after tuning. Increase `target_accept` or reparameterize.
There were 34 divergences after tuning. Increase `target_accept` or reparameterize.
There were 265 divergences after tuning. Increase `target_accept` or reparameterize.
The acceptance probability does not match the target. It is 0.5052073665905551, but should be 0.9.
There were 41 divergences after tuning. Increase `target_accept` or reparameterize.
The number of effective samples is smaller than 10% for some parameters.
```

```
In [51]: varnames=['alpha', 'alpha_mu', 'alpha_sd', 'beta', 'beta_mu', 'beta_sd', 'epsilon', 'nu']
         _=pm.traceplot(trace_hm, varnames)
```



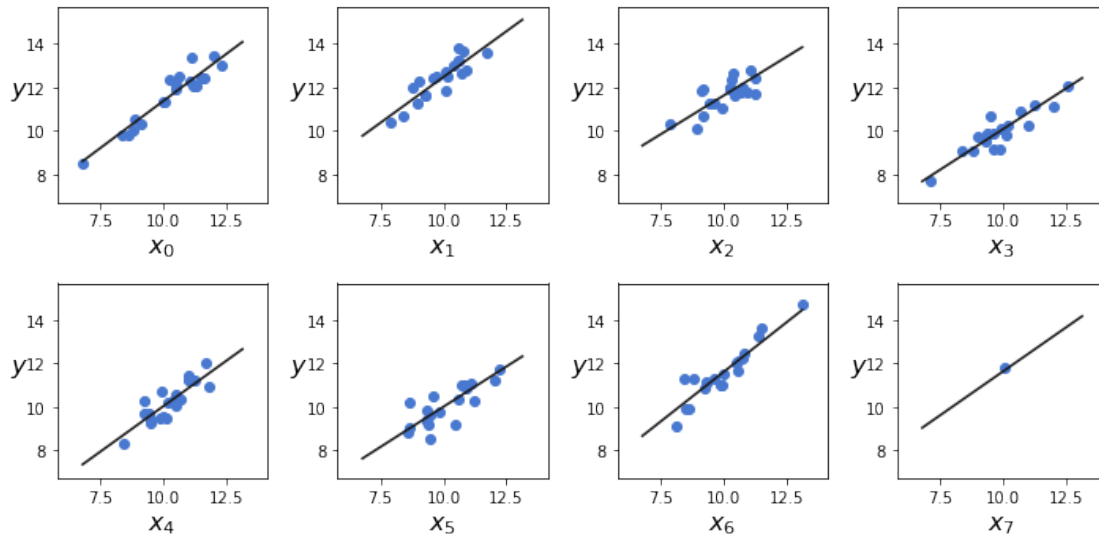
```
In [52]: pm.summary(trace_hm, varnames)
```

```
Out [52]:          mean      sd  mc_error  hpd_2.5  hpd_97.5    n_eff  Rhat
```

alpha__0	2.73	0.69	1.10e-02	1.42	4.11	5159.06	1.00
alpha__1	4.05	0.87	1.14e-02	2.29	5.81	7756.94	1.00
alpha__2	4.48	1.06	2.63e-02	2.50	6.54	1032.73	1.01
alpha__3	2.60	0.78	1.82e-02	1.13	4.16	1331.37	1.01
alpha__4	1.69	0.94	1.35e-02	-0.20	3.53	6819.79	1.00
alpha__5	2.61	0.89	2.18e-02	1.04	4.43	1186.52	1.00
alpha__6	2.48	0.84	2.42e-02	0.86	4.13	900.70	1.01
alpha__7	3.56	2.02	3.16e-02	-0.72	7.32	3242.79	1.00
alpha_mu	3.01	0.88	1.62e-02	1.36	4.78	3415.33	1.00
alpha_sd	-6.92	0.88	1.75e-02	-8.57	-5.15	2858.37	1.00
beta__0	0.86	0.07	1.16e-03	0.74	1.00	3457.79	1.00
beta__1	0.84	0.09	1.19e-03	0.65	1.01	7055.04	1.00
beta__2	0.71	0.10	2.71e-03	0.50	0.90	922.38	1.01
beta__3	0.75	0.08	1.96e-03	0.59	0.89	975.45	1.01
beta__4	0.84	0.09	1.23e-03	0.66	1.02	7527.17	1.00
beta__5	0.74	0.09	2.17e-03	0.56	0.89	1189.49	1.01
beta__6	0.91	0.08	2.34e-03	0.76	1.08	889.92	1.01
beta__7	0.81	0.20	2.99e-03	0.43	1.20	3218.63	1.00
beta_mu	0.81	0.08	1.46e-03	0.66	0.95	3175.61	1.00
beta_sd	0.14	0.09	3.36e-03	0.02	0.30	518.80	1.02
epsilon	0.46	0.03	6.25e-04	0.40	0.53	3621.11	1.00
nu	41.43	29.96	5.78e-01	3.67	97.97	2776.35	1.01

note the the reduced sd on  $\alpha_7$   $\beta_7$  compared to non-hierarchical model

```
In [53]: plt.figure(figsize=(10,5))
j, k = 0, N
x_range = np.linspace(x_m.min(), x_m.max(), 10)
for i in range(M):
    plt.subplot(2,4,i+1)
    plt.scatter(x_m[j:k], y_m[j:k])
    plt.xlabel('$x_{%d}$'.format(i), fontsize=16)
    plt.ylabel('$y$', fontsize=16, rotation=0)
    alfa_m = trace_hm['alpha'][:,i].mean()
    beta_m = trace_hm['beta'][:,i].mean()
    plt.plot(x_range, alfa_m + beta_m * x_range, c='k', label='y = {:.2f} + {:.2f} * x')
    plt.xlim(x_m.min()-1, x_m.max()+1)
    plt.ylim(y_m.min()-1, y_m.max()+1)
    j += N
    k += N
plt.tight_layout()
```

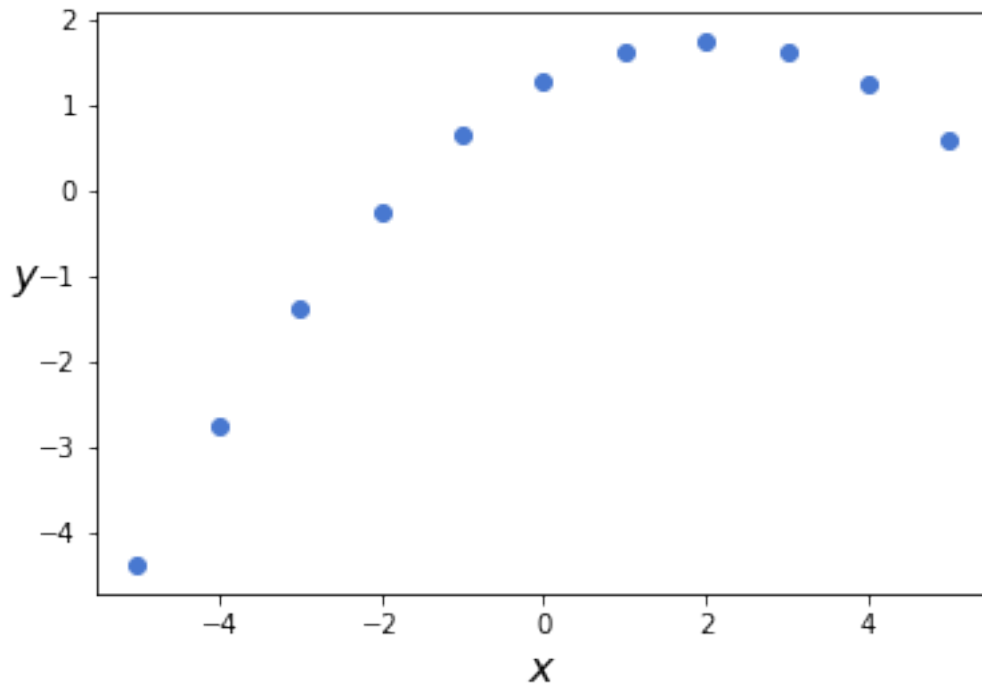


## 0.7 Polynomial regression

```
In [54]: ans = sns.load_dataset('anscombe')
x_2 = ans[ans.dataset == 'II']['x'].values
y_2 = ans[ans.dataset == 'II']['y'].values
x_2 = x_2 - x_2.mean()
y_2 = y_2 - y_2.mean()

plt.scatter(x_2, y_2)
plt.xlabel('$x$', fontsize=16)
plt.ylabel('$y$', fontsize=16, rotation=0)
```

```
Out[54]: Text(0, 0.5, '$y$')
```



```
In [55]: with pm.Model() as model_poly:
          alpha = pm.Normal('alpha', mu=0, sd=10)
          beta1 = pm.Normal('beta1', mu=0, sd=1)
          beta2 = pm.Normal('beta2', mu=0, sd=1)
          epsilon = pm.HalfCauchy('epsilon', 5)

          mu = alpha + beta1 * x_2 + beta2 * x_2**2

          y_pred = pm.Normal('y_pred', mu=mu, sd=epsilon, observed=y_2)

          # start = pm.find_MAP()
          step = pm.NUTS()# scaling=start
          trace_poly = pm.sample(2000, step=step, chains=1, njobs=1)
```

Sequential sampling (1 chains in 1 job)

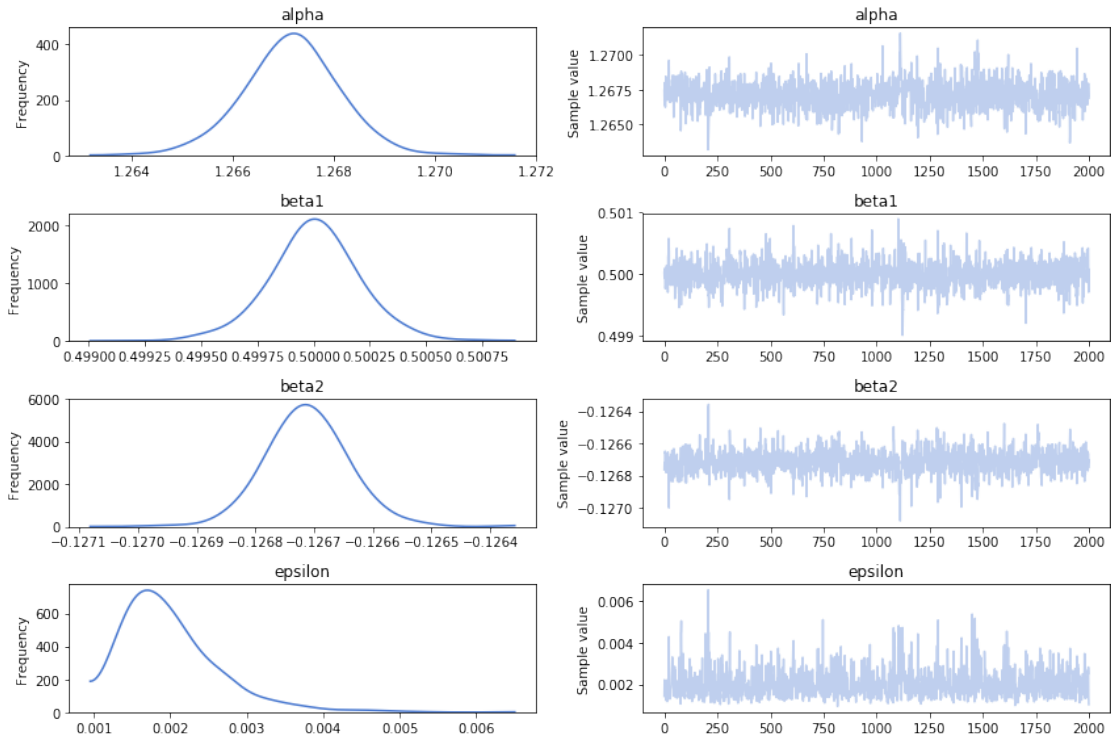
NUTS: [epsilon, beta2, beta1, alpha]

100%|| 2500/2500 [00:03<00:00, 659.32it/s]

The acceptance probability does not match the target. It is 0.9025982952476729, but should be 0.9. Only one chain was sampled, this makes it impossible to run some convergence checks

```
In [56]: pm.traceplot(trace_poly);
```





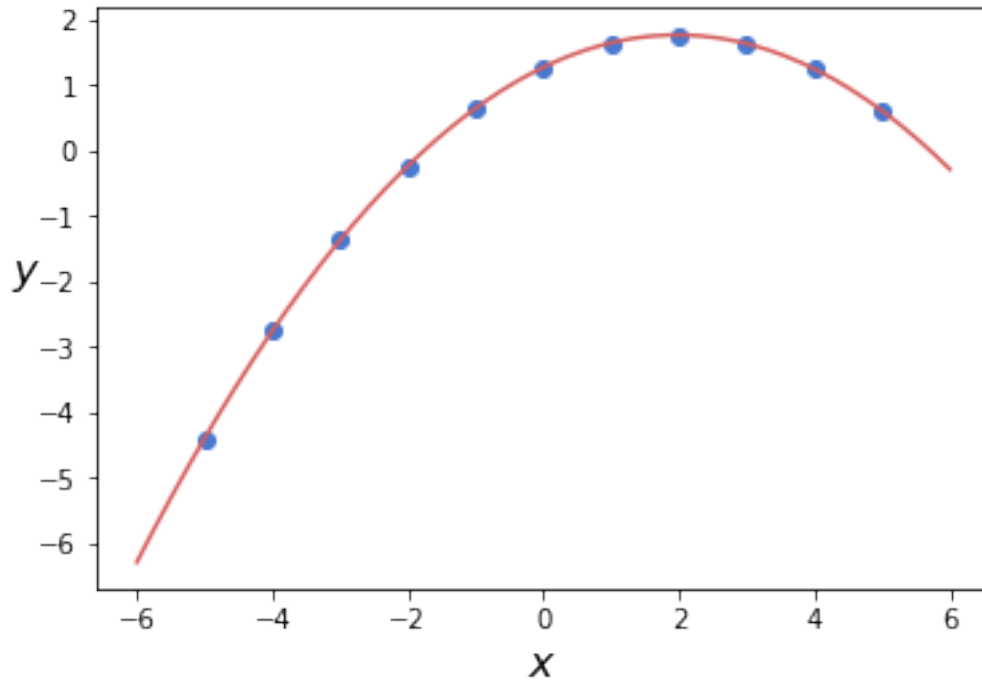
```
In [57]: pm.summary(trace_poly)
```

```
Out [57]:
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5
alpha	1.27e+00	9.49e-04	3.19e-05	1.27e+00	1.27e+00
beta1	5.00e-01	2.01e-04	5.54e-06	5.00e-01	5.00e-01
beta2	-1.27e-01	7.04e-05	2.38e-06	-1.27e-01	-1.27e-01
epsilon	2.02e-03	6.39e-04	2.41e-05	1.11e-03	3.29e-03

```
In [58]: x_p = np.linspace(-6, 6)
y_p = trace_poly['alpha'].mean() + trace_poly['beta1'].mean() * x_p + trace_poly['beta2'].mean() * x_p**2
plt.scatter(x_2, y_2)
plt.xlabel('$x$', fontsize=16)
plt.ylabel('$y$', fontsize=16, rotation=0)
plt.plot(x_p, y_p, c='r')
```

```
Out [58]: [<matplotlib.lines.Line2D at 0x7ff7771cfba8>]
```



## 0.8 Multiple Linear regression

```
In [59]: np.random.seed(314)
         N = 100
         alpha_real = 2.5
         beta_real = [0.9, 1.5]
         eps_real = np.random.normal(0, 0.5, size=N)

         X = np.array([np.random.normal(i, j, N) for i,j in zip([10, 2], [1, 1.5])])
         X_mean = X.mean(axis=1, keepdims=True)
         X_centered = X - X_mean
         y = alpha_real + np.dot(beta_real, X) + eps_real
         print('The features (independent variable) are across the columns. A sample:\n {}'.format(X_centered[0].tolist()))
```

The features (independent variable) are across the columns. A sample:

```
[[ 0.06 -1.66 -0.21 -0.12  0.53]
 [ 1.38  0.85 -1.49  0.2  -0.38]]
```

```
In [60]: def scatter_plot(x, y):
         plt.figure(figsize=(10, 10))
         for idx, x_i in enumerate(x):
             plt.subplot(2, 2, idx+1)
             plt.scatter(x_i, y)
```

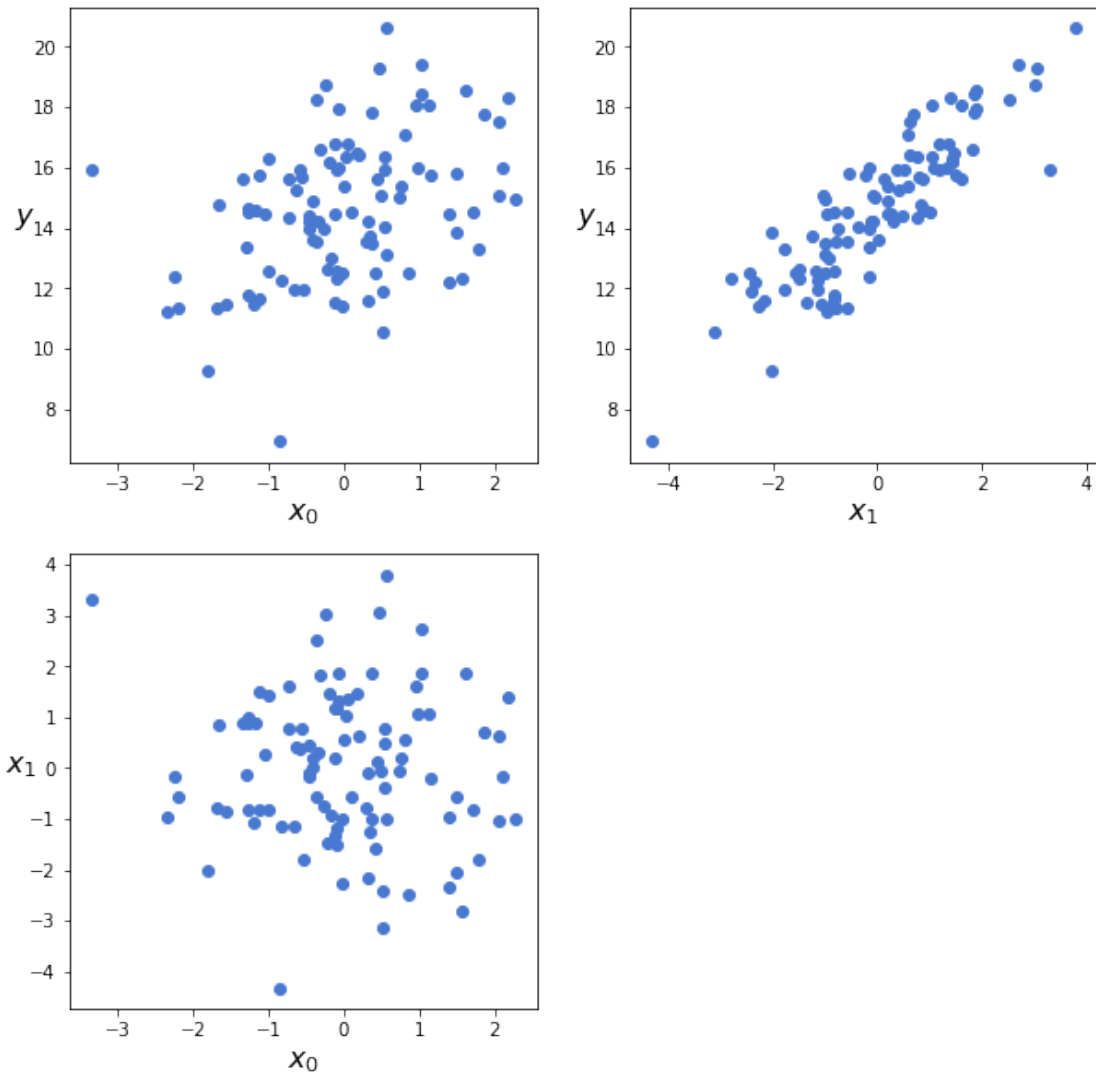
```

plt.xlabel('$x_{{}}$'.format(idx), fontsize=16)
plt.ylabel('$y$', rotation=0, fontsize=16)

plt.subplot(2, 2, idx+2)
plt.scatter(x[0], x[1])
plt.xlabel('$x_{{}}$'.format(idx-1), fontsize=16)
plt.ylabel('$x_{{}}$'.format(idx), rotation=0, fontsize=16)

scatter_plot(X_centered, y)

```



```

In [61]: with pm.Model() as model_mlr:
          alpha_tmp = pm.Normal('alpha_tmp', mu=0, sd=10)
          beta = pm.Normal('beta', mu=0, sd=1, shape=2)
          epsilon = pm.HalfCauchy('epsilon', 5)

```

```

mu = alpha_tmp + pm.math.dot(beta, X_centered)

alpha = pm.Deterministic('alpha', alpha_tmp - pm.math.dot(beta, X_mean))

y_pred = pm.Normal('y_pred', mu=mu, sd=epsilon, observed=y)

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

```

Sequential sampling (1 chains in 1 job)

NUTS: [epsilon, beta, alpha\_tmp]

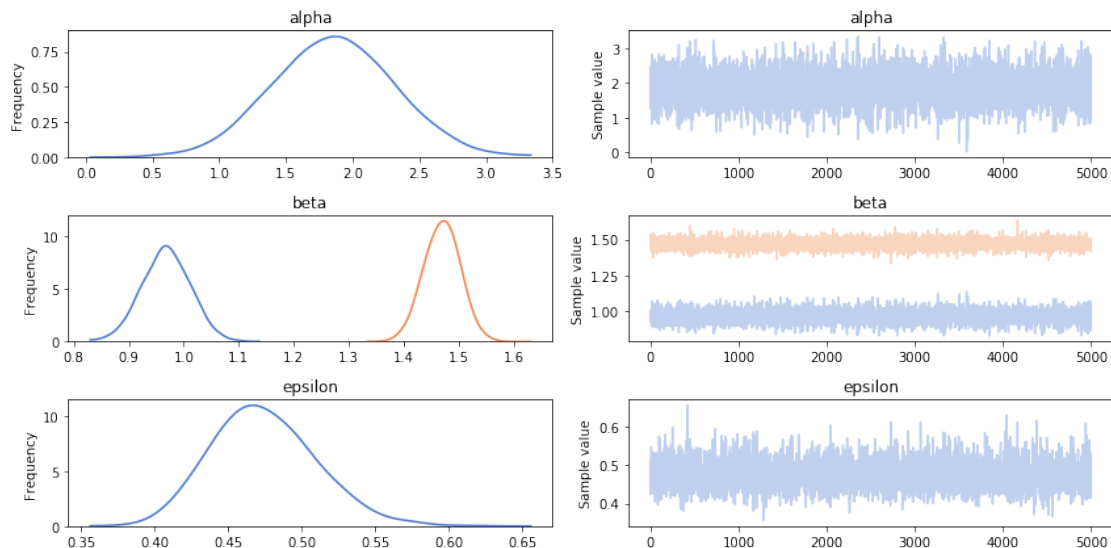
100%|| 5500/5500 [00:03<00:00, 1485.37it/s]

Only one chain was sampled, this makes it impossible to run some convergence checks

```

In [62]: varnames = ['alpha', 'beta', 'epsilon']
pm.traceplot(trace_mlr, varnames);

```



```

In [63]: pm.summary(trace_mlr, varnames)

```

```

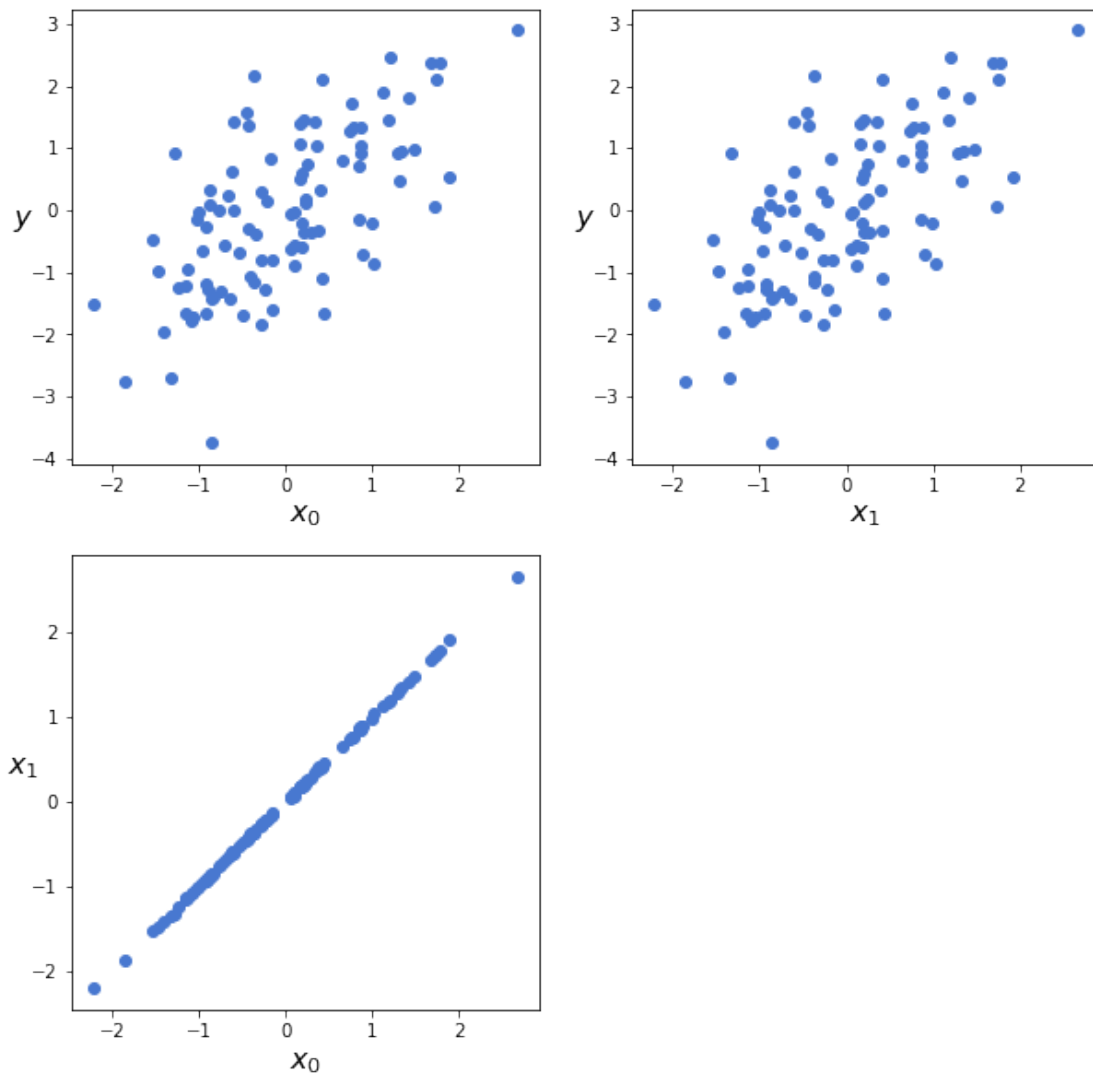
Out [63]:
          mean    sd  mc_error  hpd_2.5  hpd_97.5
alpha__0  1.86  0.45  5.91e-03    0.98    2.75
beta__0   0.97  0.04  5.55e-04    0.88    1.05
beta__1   1.47  0.03  4.05e-04    1.40    1.53
epsilon   0.47  0.04  4.74e-04    0.41    0.54

```

## 0.9 Confounding variables and redundant variables

```
In [64]: np.random.seed(314)
N = 100
x_1 = np.random.normal(size=N)
# x_2 = x_1 + np.random.normal(size=N, scale=1) lower correlation case
x_2 = x_1 + np.random.normal(size=N, scale=0.01)
y = x_1 + np.random.normal(size=N)
X = np.vstack((x_1, x_2))
```

```
In [65]: scatter_plot(X, y)
```



```
In [66]: with pm.Model() as model_red:
alpha = pm.Normal('alpha', mu=0, sd=1)
```

```

beta = pm.Normal('beta', mu=0, sd=10, shape=2)
#beta = pm.Normal('beta', mu=0, sd=10)
epsilon = pm.HalfCauchy('epsilon', 5)

mu = alpha + pm.math.dot(beta, X)
#mu = alpha + beta * X[0]

y_pred = pm.Normal('y_pred', mu=mu, sd=epsilon, observed=y)

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

```

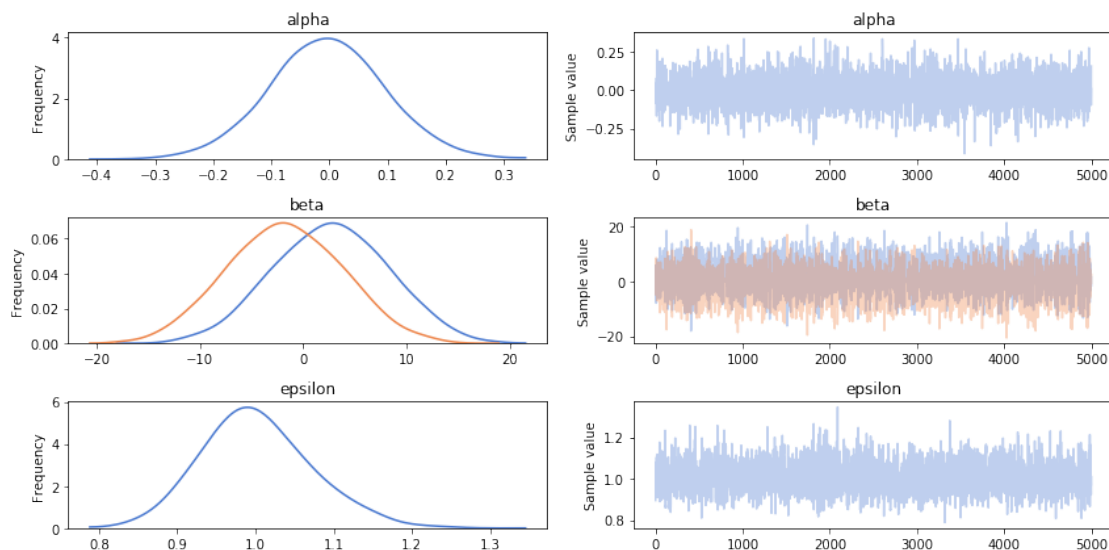
Sequential sampling (1 chains in 1 job)

NUTS: [epsilon, beta, alpha]

100%|| 5500/5500 [01:30<00:00, 67.64it/s]

Only one chain was sampled, this makes it impossible to run some convergence checks

In [67]: pm.traceplot(trace\_red);



In [68]: pm.summary(trace\_red)

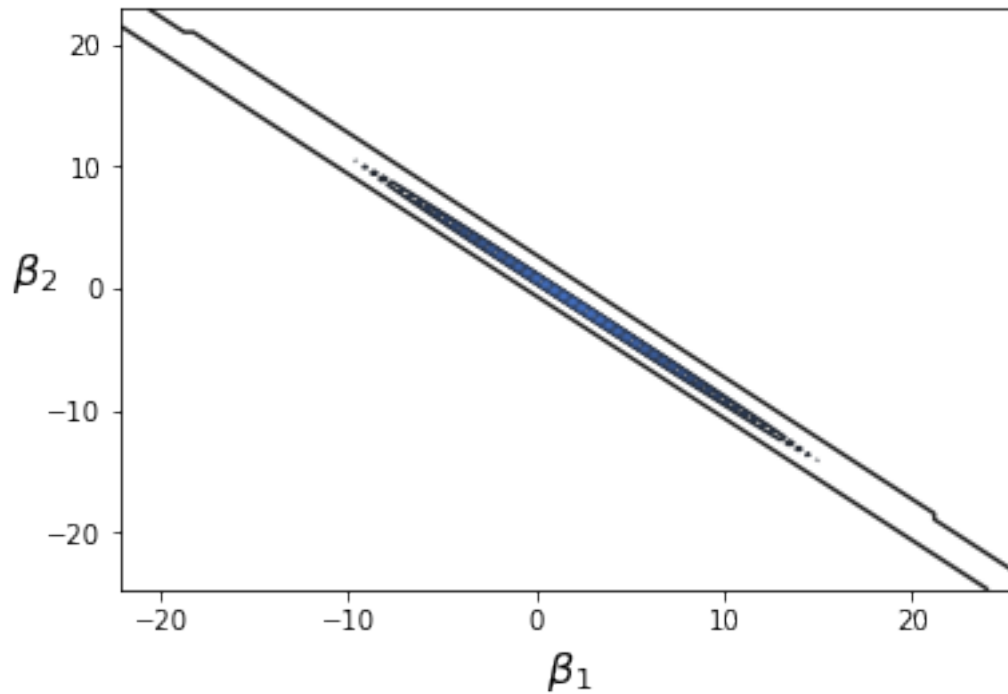
```

Out [68]:
          mean      sd  mc_error  hpd_2.5  hpd_97.5
alpha   -3.67e-03  0.10  1.82e-03   -0.20    0.19
beta__0   2.67e+00  5.59  1.29e-01   -7.42   14.26
beta__1  -1.77e+00  5.57  1.29e-01  -13.08    8.51
epsilon   1.00e+00  0.07  1.39e-03    0.87    1.15

```

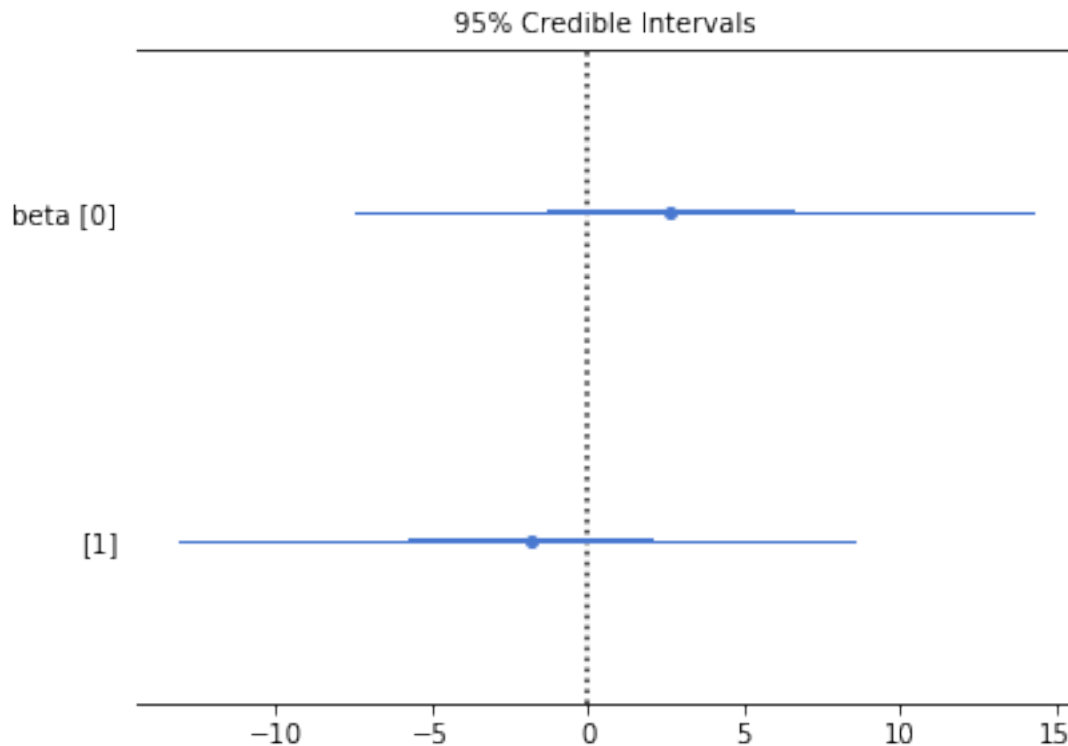
```
In [69]: sns.kdeplot(trace_red['beta'][:,0], trace_red['beta'][:,1])  
plt.xlabel(r'$\beta_1$', fontsize=16)  
plt.ylabel(r'$\beta_2$', fontsize=16, rotation=0)
```

```
Out[69]: Text(0, 0.5, '$\beta_2$')
```



```
In [70]: pm.forestplot(trace_red, varnames=['beta'])
```

```
Out[70]: GridSpec(1, 1)
```



**When two variables are highly correlated they are masking the effects of each other** We can: - Eliminate a variable - Combine them (average them, PCA) - Add stronger priors, i.e. regularizing priors that restrict the plausible values the coefficient can take

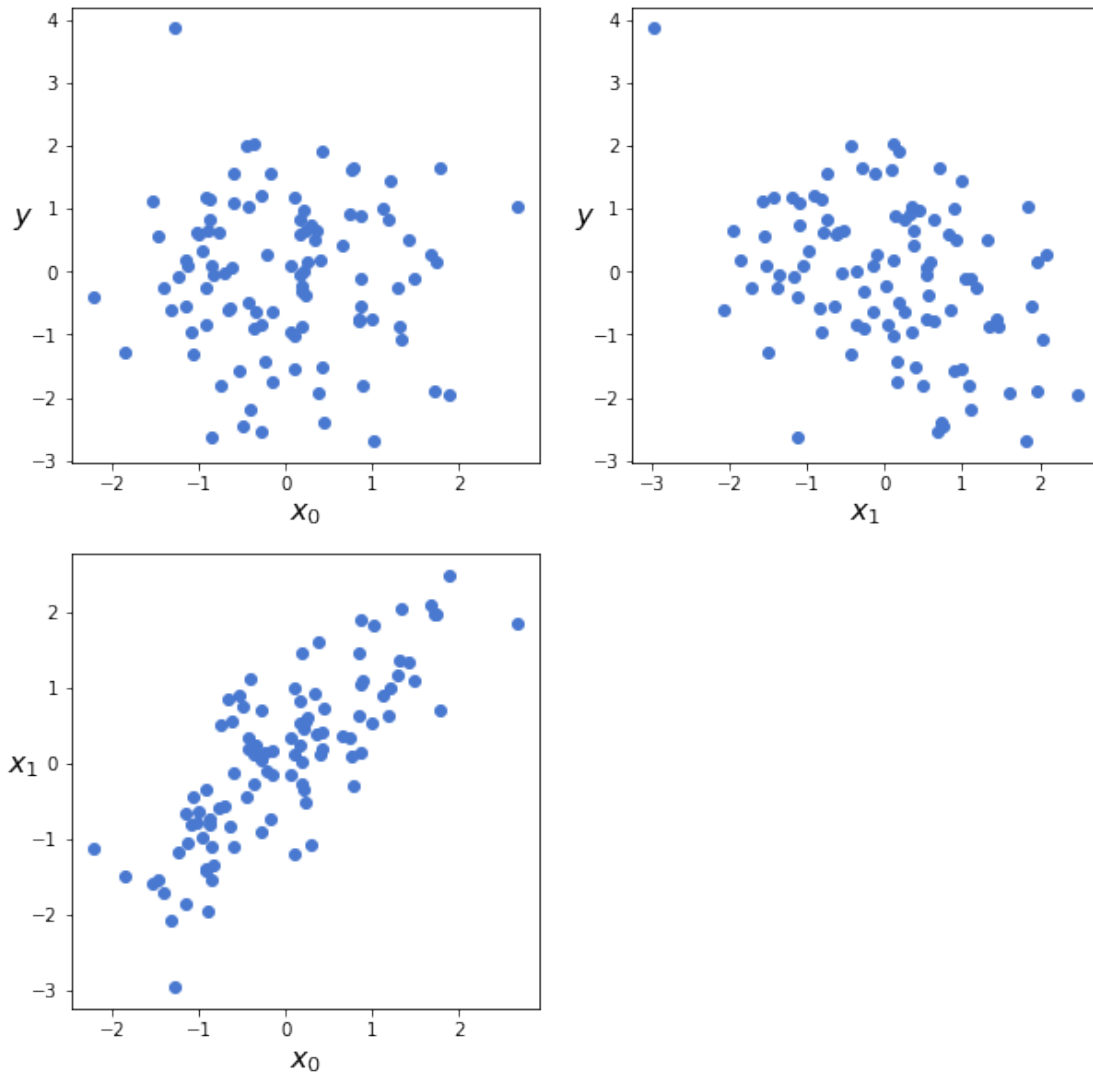
## 0.10 Masking effect variables

In this case the dependent variable  $y$  is the difference of two correlated variables and omitting one from the analysis will be a mistake since their individual effects are negligible.

```
In [71]: np.random.seed(314)
         N = 100
         r = 0.8
         x_0 = np.random.normal(size=N)
         x_1 = np.random.normal(loc=x_0 * r, scale=(1 - r ** 2) ** 0.5)
         y = np.random.normal(loc=x_0 - x_1)
         X = np.vstack((x_0, x_1))
```

```
In [72]: scatter_plot(X, y)
```





```
In [73]: with pm.Model() as model_ma:
          alpha = pm.Normal('alpha', mu=0, sd=10)
          beta = pm.Normal('beta', mu=0, sd=10, shape=2)
          #beta = pm.Normal('beta', mu=0, sd=10)
          epsilon = pm.HalfCauchy('epsilon', 5)

          mu = alpha + pm.math.dot(beta, X)
          #mu = alpha + beta * X[0]

          y_pred = pm.Normal('y_pred', mu=mu, sd=epsilon, observed=y)

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

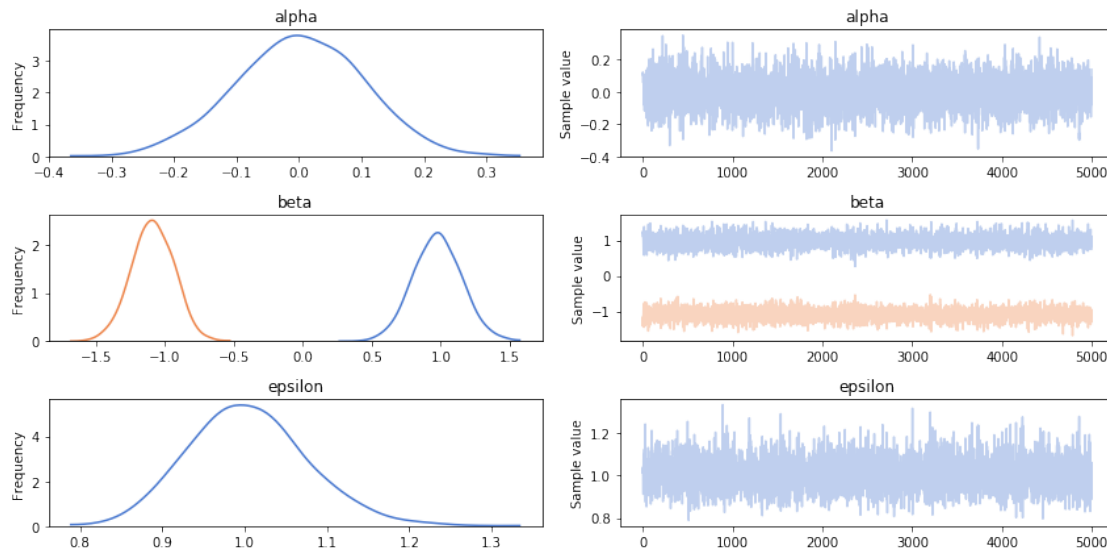
Sequential sampling (1 chains in 1 job)

NUTS: [epsilon, beta, alpha]

100%| 5500/5500 [00:04<00:00, 1207.37it/s]

Only one chain was sampled, this makes it impossible to run some convergence checks

```
In [74]: pm.traceplot(trace_ma);
```

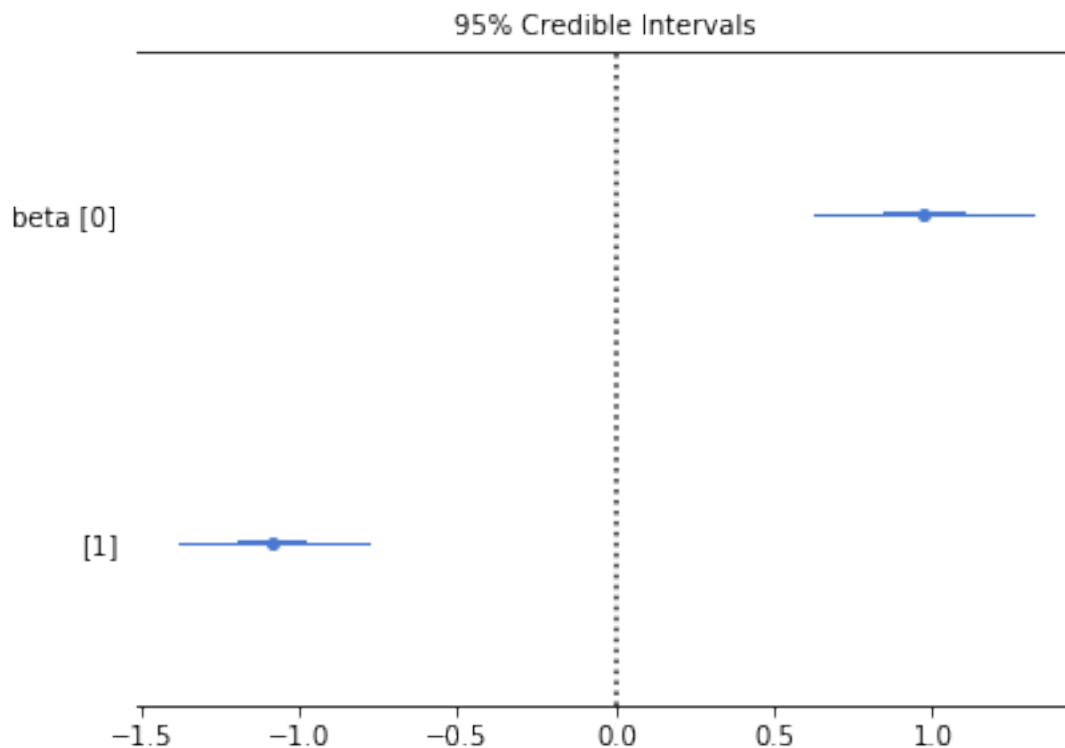


```
In [75]: pm.summary(trace_ma)
```

```
Out[75]:
```

	mean	sd	mc_error	hpd_2.5	hpd_97.5
alpha	1.29e-03	0.10	1.71e-03	-0.20	0.19
beta__0	9.75e-01	0.18	2.53e-03	0.62	1.32
beta__1	-1.09e+00	0.15	2.32e-03	-1.38	-0.78
epsilon	1.00e+00	0.07	1.03e-03	0.87	1.15

```
In [76]: pm.forestplot(trace_ma, varnames=['beta']);
```



```
In [77]: import sys, IPython, scipy, matplotlib, platform
         print("This notebook was created on a %s computer running %s and using:\nPython %s\nIP
```

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: DeprecationWarning: The 'warn' method is deprecated, use 'warn' instead.