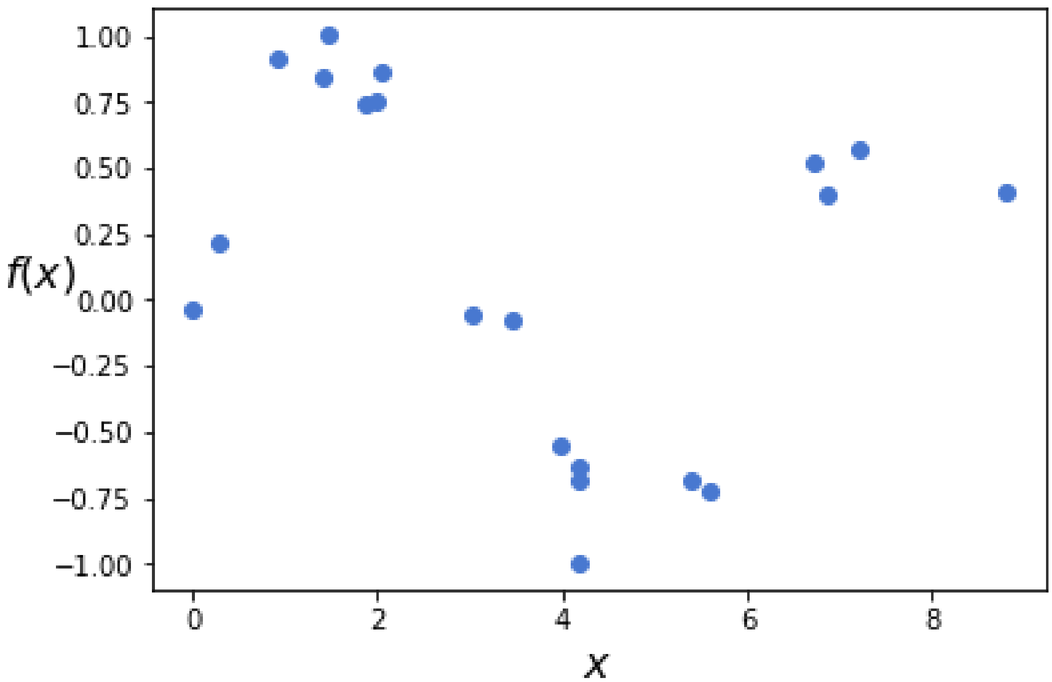
Bayesian Data Analysis Chapter 8

January 20, 2019

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

0.1 Kernelized Regression

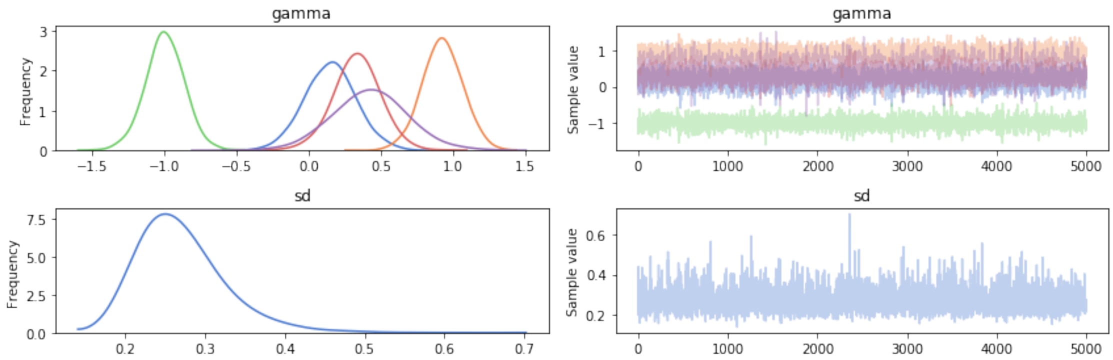
In [2]:
```
np.random.seed(1)
x = np.random.uniform(0, 10, size=20)
y = np.random.normal(np.sin(x), 0.2)
plt.plot(x, y, 'o')
plt.xlabel('$x$', fontsize=16);
plt.ylabel('$f(x)$', fontsize=16, rotation=0);
```




```
In [3]: def gauss_kernel(x, n_knots):
            """
            Simple Gaussian radial kernel
            """
            knots = np.linspace(x.min(), x.max(), n_knots)
            w = 2
            return np.array([np.exp(-(x-k)**2/w) for k in knots])

In [4]: n_knots = 5

In [5]: with pm.Model() as kernel_model:
            gamma = pm.Cauchy('gamma', alpha=0, beta=1, shape=n_knots)
            sd = pm.Uniform('sd',0,  10)
            mu = pm.math.dot(gamma, gauss_kernel(x, n_knots))
            yl = pm.Normal('yl', mu=mu, sd=sd, observed=y)
            kernel_trace = pm.sample(10000, chains=1,njobs=1)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Sequential sampling (1 chains in 1 job)
NUTS: [sd, gamma]
100%|| 10500/10500 [00:08<00:00, 1168.71it/s]
Only one chain was sampled, this makes it impossible to run some convergence checks
```

In [6]:
```
chain = kernel_trace[5000:]
pm.traceplot(chain);
```



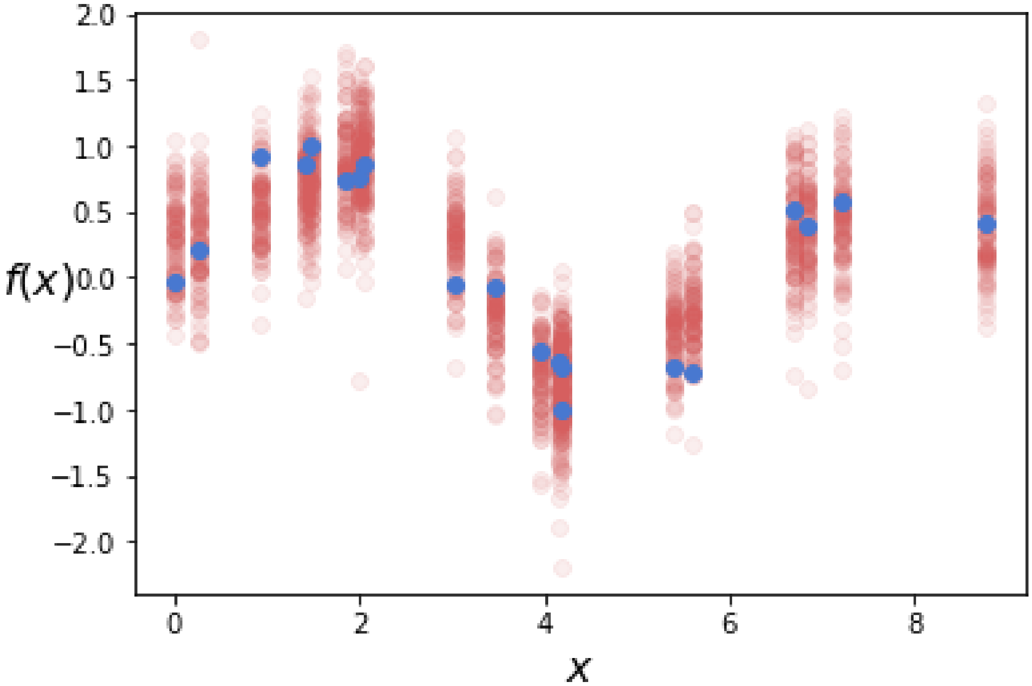
In [7]:
```
pm.summary(chain)
```

Out[7]:

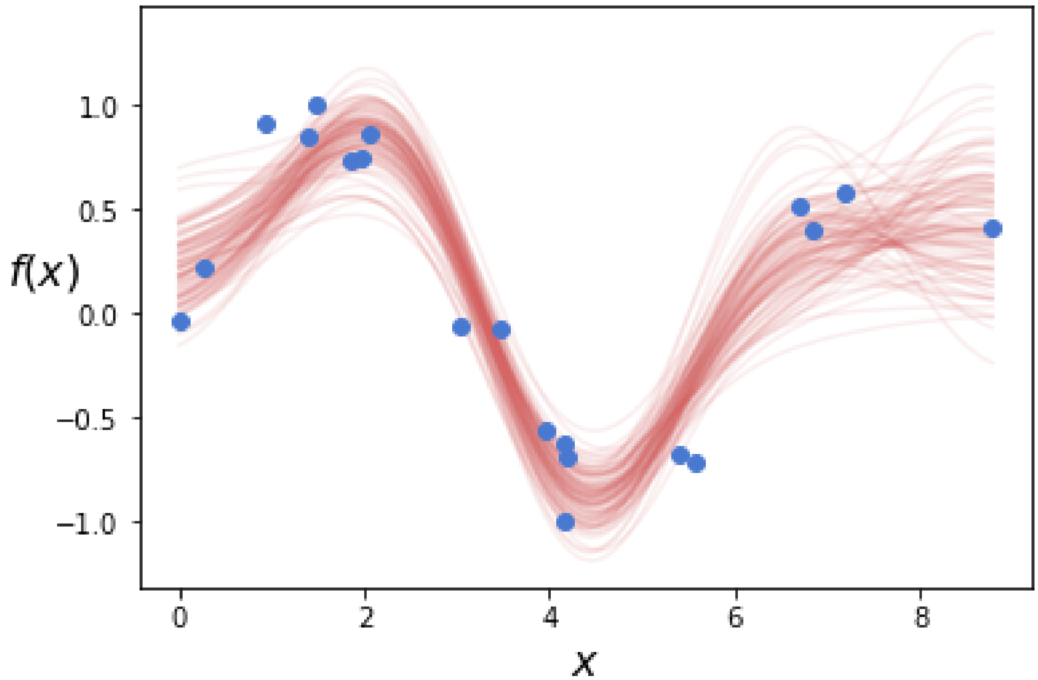
	mean	sd	mc_error	hpd_2.5	hpd_97.5
gamma__0	0.149587	0.178287	0.002675	-0.188123	0.513712
gamma__1	0.927369	0.140474	0.002009	0.640079	1.194028
gamma__2	-0.997580	0.135827	0.002167	-1.271611	-0.731901
gamma__3	0.335250	0.165045	0.002291	-0.006687	0.649435
gamma__4	0.425855	0.261586	0.003824	-0.108575	0.927639
sd	0.270219	0.054199	0.000974	0.185070	0.385145

In [8]:
```
ppc = pm.sample_posterior_predictive(chain, model=kernel_model, samples=100)
plt.plot(x, ppc['yl'].T, 'ro', alpha=0.1);
plt.plot(x, y, 'bo');
plt.xlabel('$x$', fontsize=16);
plt.ylabel('$f(x)$', fontsize=16, rotation=0);
```

```
100%|| 100/100 [00:00<00:00, 1341.11it/s]
```



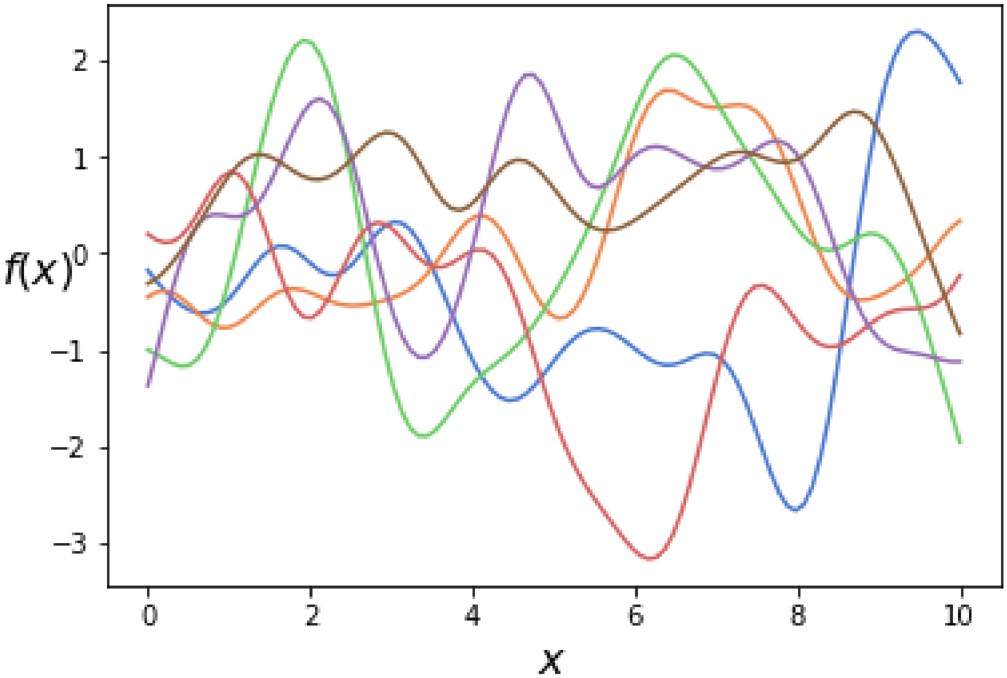

```
In [9]: new_x = np.linspace(x.min(), x.max(), 100)
        k = gauss_kernel(new_x, n_knots)
        gamma_pred = chain['gamma']
        for i in range(100):
            idx = np.random.randint(0, len(gamma_pred))
            # grap a random set of gammas from the MCMC chain
            # e.g. gamma_pred[3642]=[-0.04  0.93 -0.97  0.32  0.05]
            # to get an idea of the uncertainty
            y_pred = np.dot(gamma_pred[idx], k)
            plt.plot(new_x, y_pred, 'r-', alpha=0.1)
        plt.plot(x, y, 'bo')
        plt.xlabel('$x$', fontsize=16)
        plt.ylabel('$f(x)$', fontsize=16, rotation=0);
```



0.2 Gaussian Processes

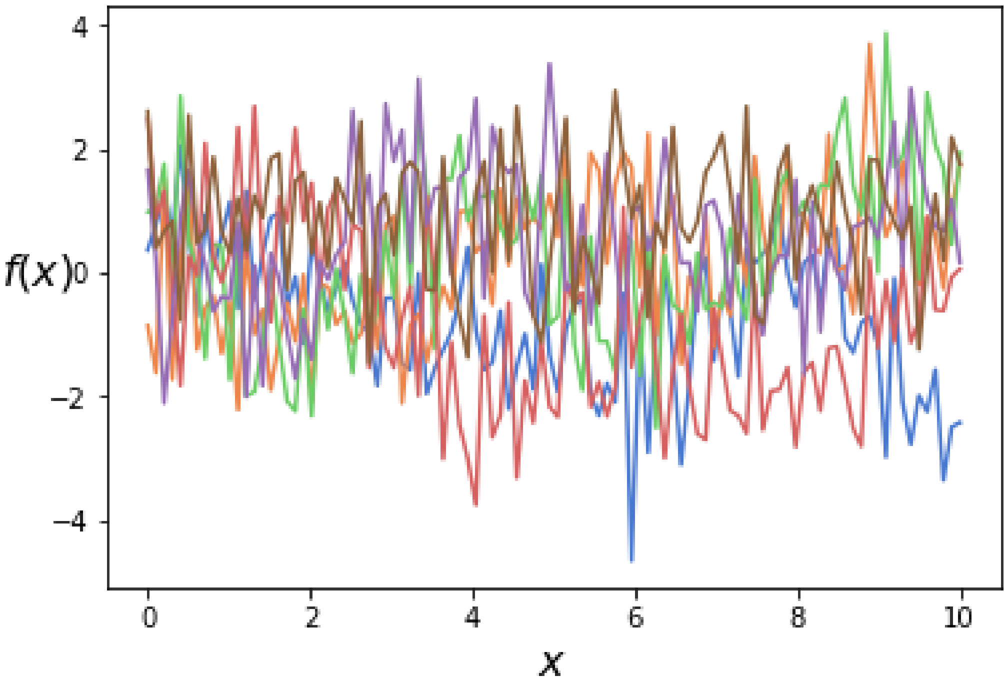
```
In [10]: squared_distance = lambda x, y: np.array([[(x[i] - y[j])**2 for i in range(len(x))] fo
```

```
In [11]: np.random.seed(1)
         test_points = np.linspace(0, 10, 100)
         cov = np.exp(-squared_distance(test_points, test_points))
         plt.plot(test_points, stats.multivariate_normal.rvs(cov=cov, size=6).T);
         plt.xlabel('$x$', fontsize=16);
         plt.ylabel('$f(x)$', fontsize=16, rotation=0);
```



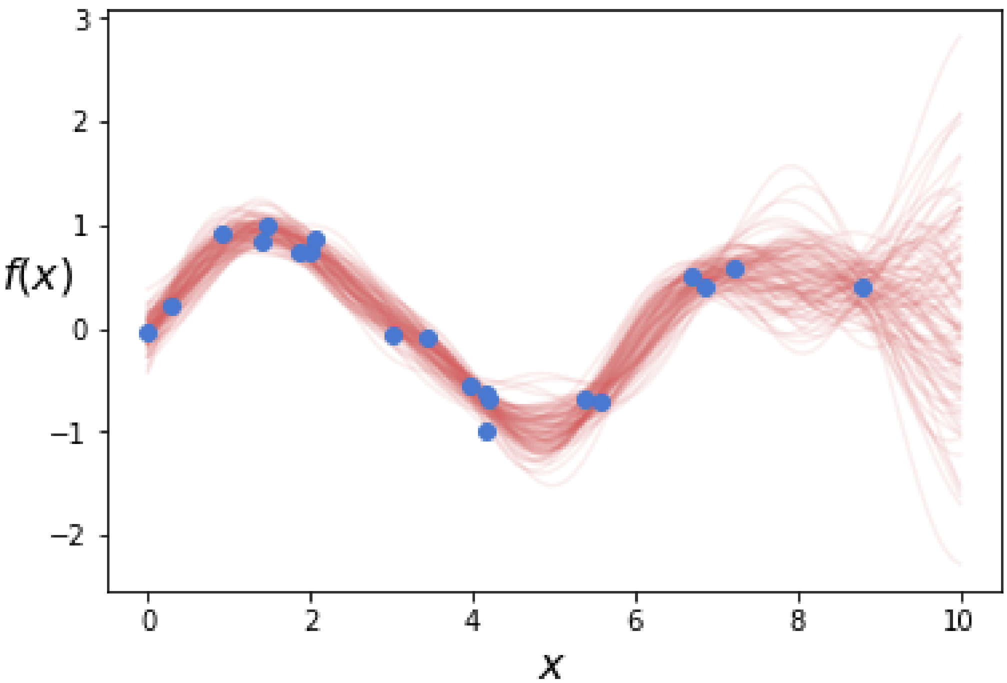

```
In [12]: np.random.seed(1)
         eta = 1
         rho = 0.5
         sigma = 0.03
         D = squared_distance(test_points, test_points)

         cov = eta * np.exp(-rho * D)
         diag = eta * sigma

         np.fill_diagonal(cov, diag)

         for i in range(6):
             plt.plot(test_points, stats.multivariate_normal.rvs(cov=cov))
         plt.xlabel('$x$', fontsize=16);
         plt.ylabel('$f(x)$', fontsize=16, rotation=0);
```

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/scipy/stats/_multivariate.py:6
  out = random_state.multivariate_normal(mean, cov, size)
```




```
In [13]: np.random.seed(1)
         # K_{**}
         K_oo = eta * np.exp(-rho * D)

         D_x = squared_distance(x, x)
         # K
         K = eta * np.exp(-rho * D_x)
         diag_x = eta + sigma
         np.fill_diagonal(K, diag_x)

         D_off_diag = squared_distance(x, test_points)
         # K_{*}
         K_o = eta * np.exp(-rho * D_off_diag)

         # Posterior mean
         mu_post = np.dot(np.dot(K_o, np.linalg.inv(K)), y)
         # Posterior covariance
         SIGMA_post = K_oo - np.dot(np.dot(K_o, np.linalg.inv(K)), K_o.T)


         for i in range(100):
             fx = stats.multivariate_normal.rvs(mean=mu_post, cov=SIGMA_post)
             plt.plot(test_points, fx, 'r-', alpha=0.1)
```

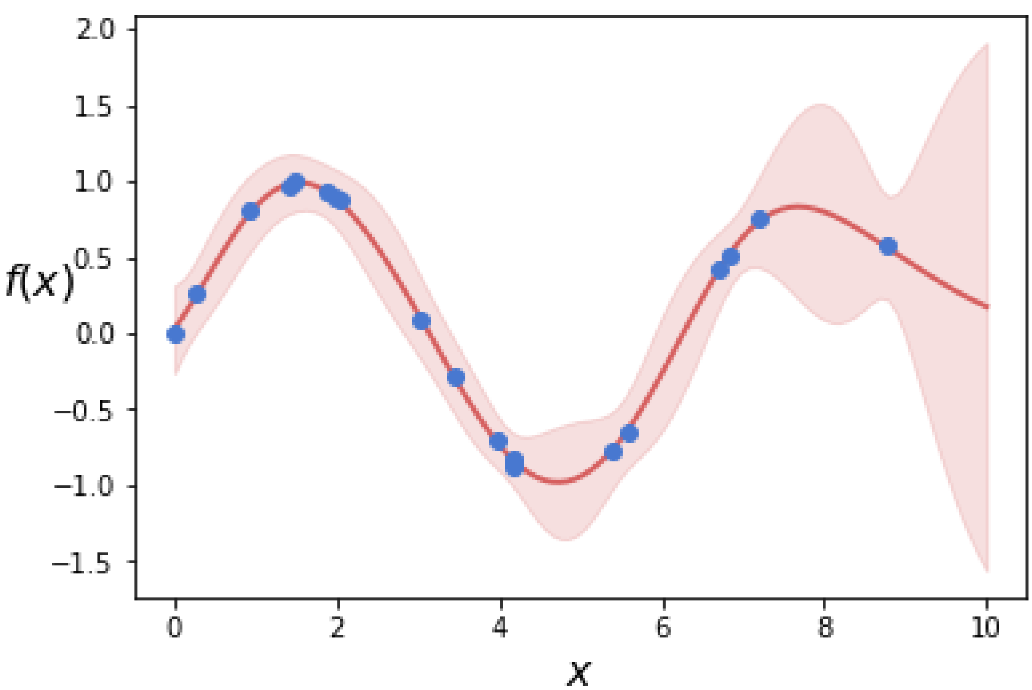
```
plt.plot(x, y, 'o')

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



Posterior of GP model using Cholesky decomposition

In [14]:
```
np.random.seed(1)
eta = 1
rho = 0.5
sigma = 0.03

# This is the true unknown function we are trying to approximate
f = lambda x: np.sin(x).flatten()

# Define the kernel
def kernel(a, b):
    """ GP squared exponential kernel """
    D = np.sum(a**2,1).reshape(-1,1) + np.sum(b**2,1) - 2*np.dot(a, b.T)
    return eta * np.exp(- rho * D)

N = 20          # number of training points.
n = 100          # number of test points.
```

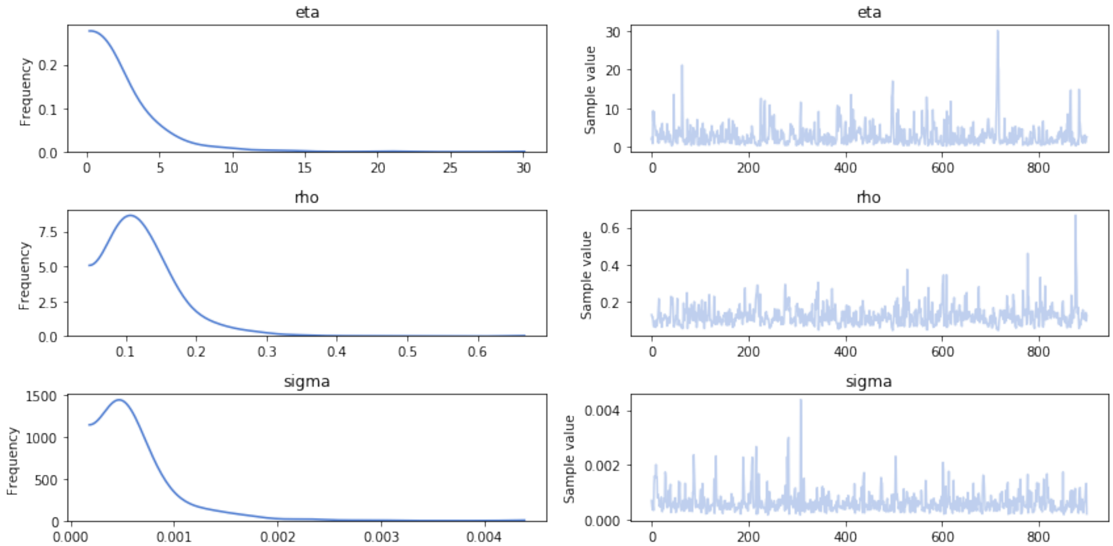
```
# Sample some input points and noisy versions of the function evaluated at
# these points.
X = np.random.uniform(0, 10, size=(N,1))
y = f(X) + sigma * np.random.randn(N)

K = kernel(X, X)
L = np.linalg.cholesky(K + sigma * np.eye(N))

# points we're going to make predictions at.
Xtest = np.linspace(0, 10, n).reshape(-1,1)

# compute the mean at our test points.
Lk = np.linalg.solve(L, kernel(X, Xtest))
mu = np.dot(Lk.T, np.linalg.solve(L, y))

# compute the variance at our test points.
K_ = kernel(Xtest, Xtest)
sd_pred = (np.diag(K_) - np.sum(Lk**2, axis=0))**0.5


plt.fill_between(Xtest.flat, mu - 2 * sd_pred, mu + 2 * sd_pred, color="r", alpha=0.2)
plt.plot(Xtest, mu, 'r', lw=2)
plt.plot(x, y, 'o')
plt.xlabel('$x$', fontsize=16)
plt.ylabel('$f(x)$', fontsize=16, rotation=0);
```



In [15]:
```
with pm.Model() as GP:
    mu = np.zeros(N)
    eta = pm.HalfCauchy('eta', 5)
    rho = pm.HalfCauchy('rho', 5)
    sigma = pm.HalfCauchy('sigma', 5)

    D = squared_distance(x, x)

    K = tt.fill_diagonal(eta * pm.math.exp(-rho * D), eta + sigma)

    obs = pm.MvNormal('obs', mu, cov=K, observed=y)

    test_points = np.linspace(0, 10, 100)
    D_pred = squared_distance(test_points, test_points)
    D_off_diag = squared_distance(x, test_points)

    K_oo = eta * pm.math.exp(-rho * D_pred)
    K_o = eta * pm.math.exp(-rho * D_off_diag)

    mu_post = pm.Deterministic('mu_post', pm.math.dot(pm.math.dot(K_o, tt.nlinalg.matr
    SIGMA_post = pm.Deterministic('SIGMA_post', K_oo - pm.math.dot(pm.math.dot(K_o, tt

    #start = pm.find_MAP()
    trace = pm.sample(1000, chains=1,njobs=1)
```

```
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: F
  result[diagonal_slice] = x
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: F
  result[diagonal_slice] = x
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: F
  result[diagonal_slice] = x
Sequential sampling (1 chains in 1 job)
NUTS: [sigma, rho, eta]
  0%|          | 0/1500 [00:00<?, ?it/s]/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site
  result[diagonal_slice] = x
100%|| 1500/1500 [00:18<00:00, 80.84it/s]
Only one chain was sampled, this makes it impossible to run some convergence checks
```

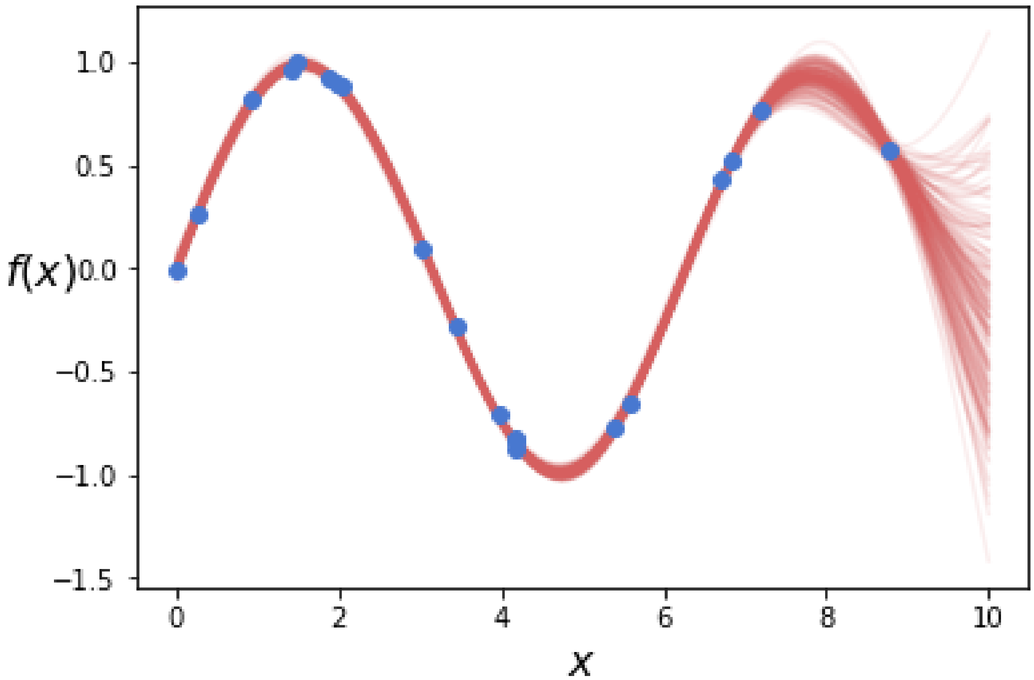
In [16]:
```
varnames = ['eta', 'rho', 'sigma']
chain = trace[100:]
pm.traceplot(chain, varnames);
```




```
In [17]: pm.summary(chain, varnames).round(4)
```

```
Out[17]:          mean      sd  mc_error  hpd_2.5  hpd_97.5
         eta    2.8176  2.8098    0.1533   0.2049    7.8822
         rho    0.1272  0.0537    0.0028   0.0510    0.2265
         sigma  0.0006  0.0004    0.0000   0.0002    0.0014
```

```
In [18]: y_pred = [np.random.multivariate_normal(m, S) for m,S in zip(chain['mu_post'][::5], c

         for yp in y_pred:
             plt.plot(test_points, yp, 'r-', alpha=0.1)

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



1 Periodic Kernel

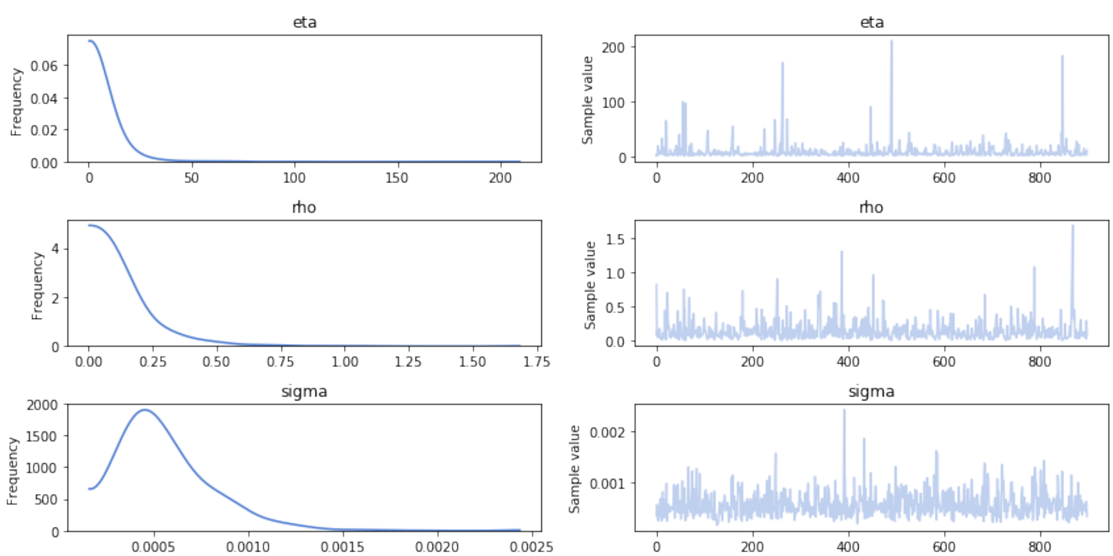
```
In [19]: periodic = lambda x, y: np.array([[np.sin((x[i] - y[j])/2)**2 for i in range(len(x))]
```

```
In [20]: with pm.Model() as GP_periodic:
             mu = np.zeros(N)
             eta = pm.HalfCauchy('eta', 5)
             rho = pm.HalfCauchy('rho', 5)
             sigma = pm.HalfCauchy('sigma', 5)

             P = periodic(x, x)

             K = tt.fill_diagonal(eta * pm.math.exp(-rho * P), eta + sigma)

             obs = pm.MvNormal('obs', mu, cov=K, observed=y)

             test_points = np.linspace(0, 10, 100)
             D_pred = periodic(test_points, test_points)
             D_off_diag = periodic(x, test_points)

             K_oo = eta * pm.math.exp(-rho * D_pred)
             K_o = eta * pm.math.exp(-rho * D_off_diag)
```

```
            mu_post = pm.Deterministic('mu_post', pm.math.dot(pm.math.dot(K_o, tt.nlinalg.mat
            SIGMA_post = pm.Deterministic('SIGMA_post', K_oo - pm.math.dot(pm.math.dot(K_o, t

            start = pm.find_MAP()
            trace = pm.sample(1000, start=start,chains=1,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
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: F
  result[diagonal_slice] = x
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/theano/tensor/basic.py:6611: F
  result[diagonal_slice] = x
  0%|          | 0/5000 [00:00<?, ?it/s]/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site
  result[diagonal_slice] = x
logp = 23.985, ||grad|| = 1.9188: 100%|| 18/18 [00:00<00:00, 839.37it/s]
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Sequential sampling (1 chains in 1 job)
NUTS: [sigma, rho, eta]
100%|| 1500/1500 [00:19<00:00, 75.12it/s]
There was 1 divergence after tuning. Increase `target_accept` or reparameterize.
Only one chain was sampled, this makes it impossible to run some convergence checks
```

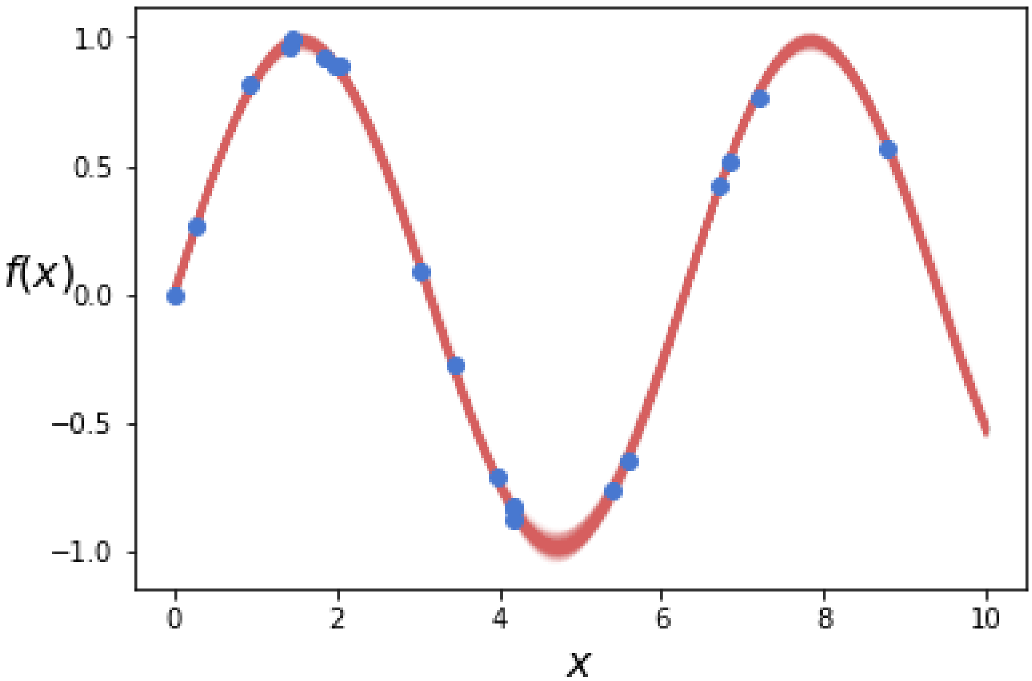
```
In [21]: varnames = ['eta', 'rho', 'sigma']
         chain = trace[100:]
         pm.traceplot(chain, varnames);
```




```
In [22]: y_pred = [np.random.multivariate_normal(m, S) for m,S in zip(chain['mu_post'][::5], cl
```

```
for yp in y_pred:
    plt.plot(test_points, yp, 'r-', alpha=0.1)

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

```
/home/damianos/miniconda3/envs/pymc3/lib/python3.7/site-packages/ipykernel_launcher.py:1: Runti
  """Entry point for launching an IPython kernel.
```




```
In [23]: import sys, IPython, scipy, matplotlib, platform
         print("This notebook was created on a computer %s running %s and using:\nPython %s\nIP
```

```
This notebook was created on a computer x86_64 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
Pandas 0.23.4
Matplotlib 3.0.2
Seaborn 0.9.0
```

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