Gaussian processes in python

John Reid

17th March 2009

1 What are Gaussian processes?

Often we have an inference problem involving n data,

$$\mathcal{D} = \{(\boldsymbol{x_i}, y_i) | i = 1, \ldots, n, \boldsymbol{x_i} \in \mathcal{X}, y_i \in \mathbb{R}\}$$

where the $\boldsymbol{x_i}$ are the inputs and the y_i are the targets. We wish to make predictions, y_*, for new inputs $\boldsymbol{x_*}$. Taking a Bayesian perspecitve we might build a model that defines a distribution over all possible functions, $f : \mathcal{X} \to \mathbb{R}$. We can encode our initial beliefs about our particular problem as a prior over these functions. Given the data, $\mathcal{D}$, and applying Bayes' rule we can infer a posterior distribution. In particular, for any given $\boldsymbol{x_*}$ we can calculate or approximate a predictive distribution over y_* under this posterior.

Gaussian processes (GPs) are probability distributions over functions for which this inference task is tractable. They can be seen as a generalisation of the Gaussian probability distribution to the space of functions. I.e. a multivariate Gaussian *distribution* defines a distribution over a finite set of random variables, a Gaussian *process* defines a distribution over an infinite set of random variables, e.g. the real numbers. GP domains are not restricted to the real numbers, any space with a dot product is suitable. Analagously to a multivariate Gaussian distribution, a GP is defined by its mean, μ, and covariance, k. However for a GP these are themselves functions, $\mu : \mathcal{X} \to \mathbb{R}$ and $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. In all that follows we assume $\mu(\boldsymbol{x}) = 0$ without loss of generality as we can always shift the data to accomodate any given mean. See figure 1 for samples from two Gaussian processes with $\mathcal{X} = \mathbb{R}$.

1.1 The covariance function, k

Assuming the mean function, μ, is 0 everywhere then our GP is defined by 2 quantities, the data, If the mean is not 0 everywhere we can trivially shift the data to make it so. $\mathcal{D}$, and its covariance function (sometimes referred to as its *kernel*), k. The data is fixed so our modelling problem is exactly that of choosing a suitable covariance function. Given different problems we certainly wish to specify different priors over possible functions. Fortunately we have available a large library of possible covariance functions each of which represents a different prior on the space of functions. See figure 2 for some examples.

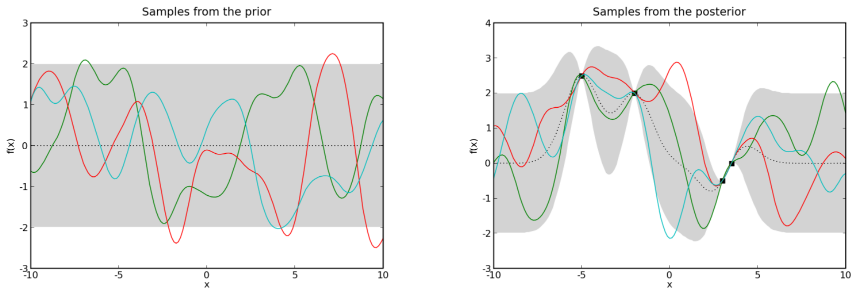


Figure 1: Samples from 2 Gaussian processes with the same mean and covariance functions. The prior samples are taken from a Gaussian process without any data and the posterior samples are taken from a Gaussian process where the data are shown as black squares. The black dotted line represents the mean of the process and the gray shaded area covers twice the standard deviation at each input, x. The coloured lines are samples from the process, or more accurately samples at a finite number of inputs, x, joined by lines.

Furthermore the point-wise product and sum of covariance functions are themselves covariance functions. In this way we can combine simple covariance functions to represent more complicated beliefs we have about our functions.

Normally we are modelling a system where we do not actually have access to the target values, y, but only noisy versions of them, $y + \epsilon$. If we assume ϵ has a Gaussian distribution with variance σ_n^2 we can incorporate this noise term into our covariance function. This requires that our noisy GP's covariance function, $k_{\text{noise}}(x_1, x_2)$ is aware of whether x_1 and x_2 are the same input.

$$k_{\text{noise}}(x_1, x_2) = k(x_1, x_2) + \delta(x_1 = x_2)\sigma_n^2$$

The effects of different noise levels can be seen in figure 3.

Most of the commonly used covariance functions are parameterised. These can be fixed if we are confident in our understanding of the problem. Alternatively we can treat them as hyper-parameters in our Bayesian inference task and optimise them through some technique such as maximum likelihood estimation or conjugate gradient descent. Figure 4 shows how optimising the hyper-parameters can help us model the data more accurately.

2 Installation

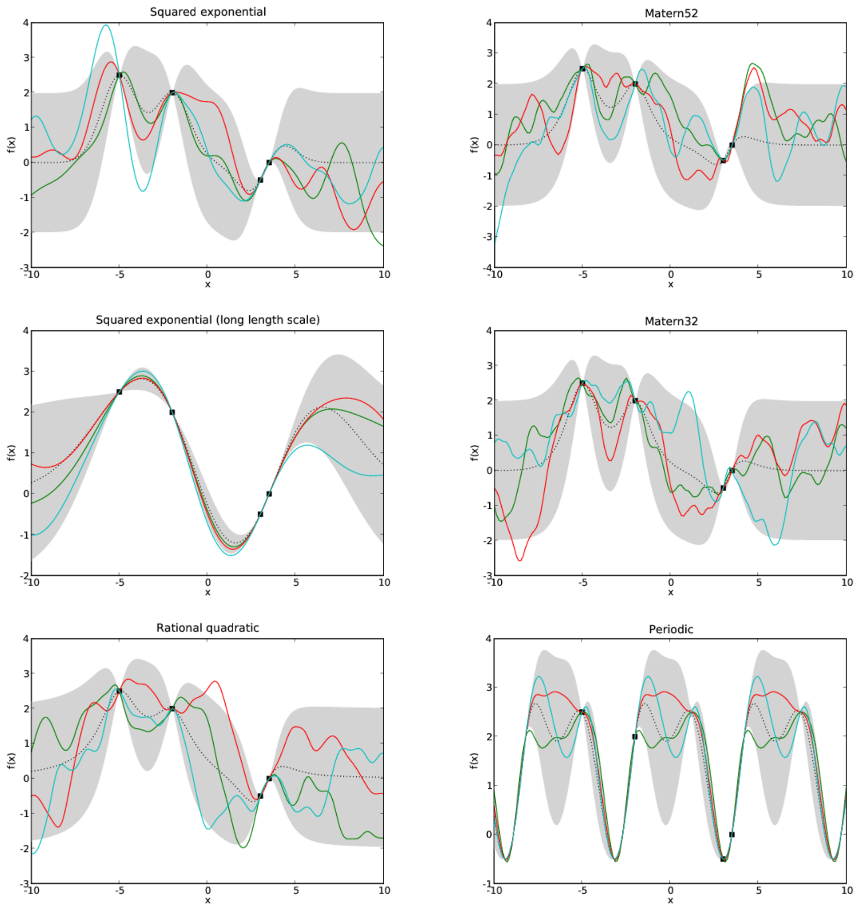


Figure 2: Samples drawn from GPs with the same data and different covariance functions. Typical samples from the posterior of GPs with different covariance functions have different characteristics. The periodic covariance function's primary characteristic is self explanatory. The other covariance functions affect the smoothness of the samples in different ways.

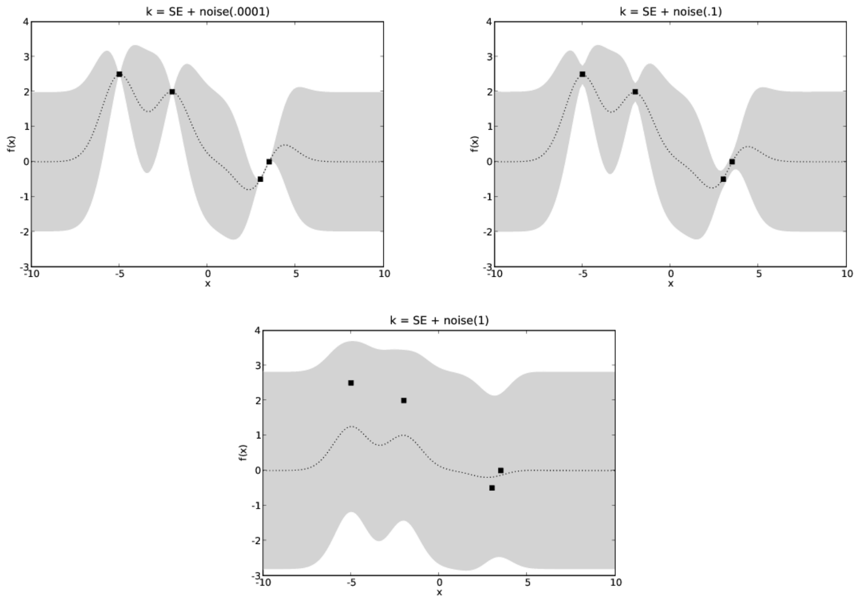


Figure 3: GP predictions with varying levels of noise. The covariance function is a squared exponential with additive noise of levels 0.0001, 0.1 and 1.

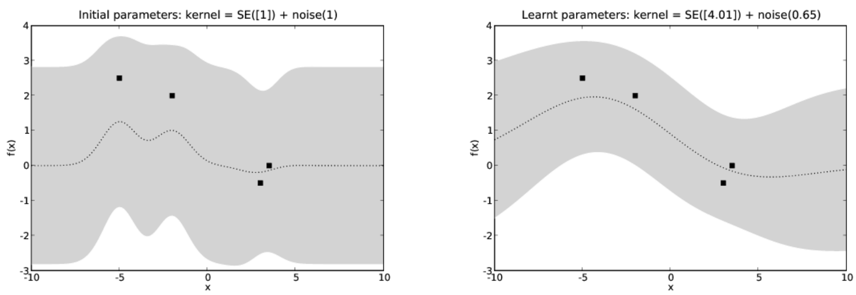


Figure 4: The effects of learning covariance function hyper-parameters. We see the predictions in the figure on the right seem to fit the data more accurately.

3 Examples

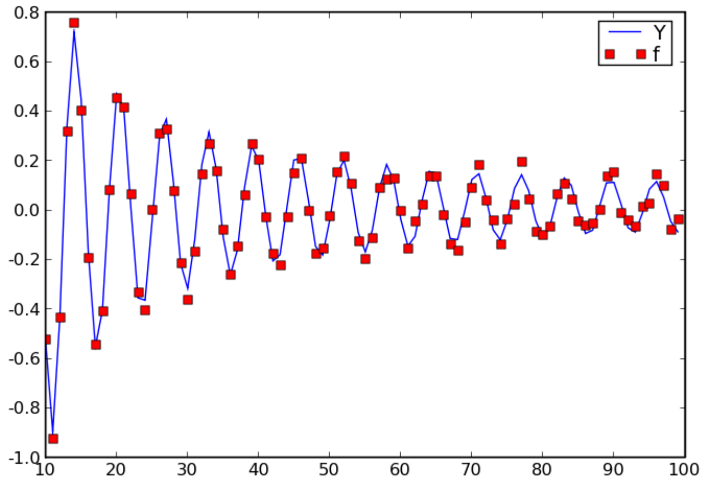
We generate some test data using

```
import numpy, pylab, infpy.gp

# Generate some noisy data from a modulated sin curve
x_min, x_max = 10.0, 100.0
X = infpy.gp.gp_1D_X_range(x_min, x_max) # input domain
Y = 10.0 * numpy.sin(X[:,0]) / X[:,0] # noise free output
Y = infpy.gp.gp_zero_mean(Y) # shift so mean=0.
e = 0.03 * numpy.random.normal(size = len(Y)) # noise
f = Y + e # noisy output

# a function to save plots
def save_fig(prefix):
  "Save current figure in extended postscript and PNG formats."
  pylab.savefig('%s.png' % prefix, format='PNG')
  pylab.savefig('%s.eps' % prefix, format='EPS')

# plot the noisy data
pylab.figure()
pylab.plot(X[:,0], Y, 'b-', label='Y')
pylab.plot(X[:,0], f, 'rs', label='f')
pylab.legend()
save_fig('simple-example-data')
pylab.close()
```



The fs are noisy observations of the underlying Ys. How can we model this using GPs?

Using the following function as an interface to the infpy GP library,

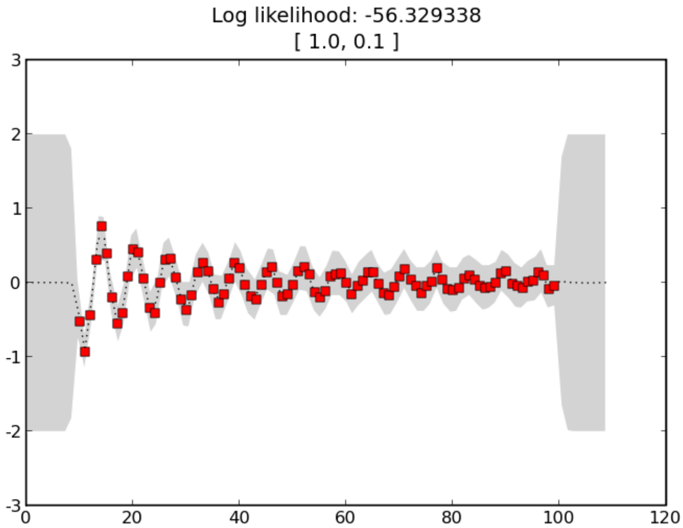
```
def predict_values(K, file_tag, learn=False):
  """
  Create a GP with kernel K and predict values.
  Optionally learn K's hyperparameters if learn==True.
  """
  gp = infpy.gp.GaussianProcess(X, f, K)
  if learn:
    infpy.gp.gp_learn_hyperparameters(gp)
  pylab.figure()
  infpy.gp.gp_1D_predict(gp, 90, x_min - 10., x_max + 10.)
  save_fig(file_tag)
  pylab.close()
```

we can test various different kernels to see how well they fit the data. For instance a simple squared exponential kernel with some noise

```
# import short forms of GP kernel names
import infpy.gp.kernel_short_names as kernels

# create a kernel composed of a squared exponential kernel
# and a small noise term
K = kernels.SE() + kernels.Noise(.1)
predict_values(K, 'simple-example-se')
```

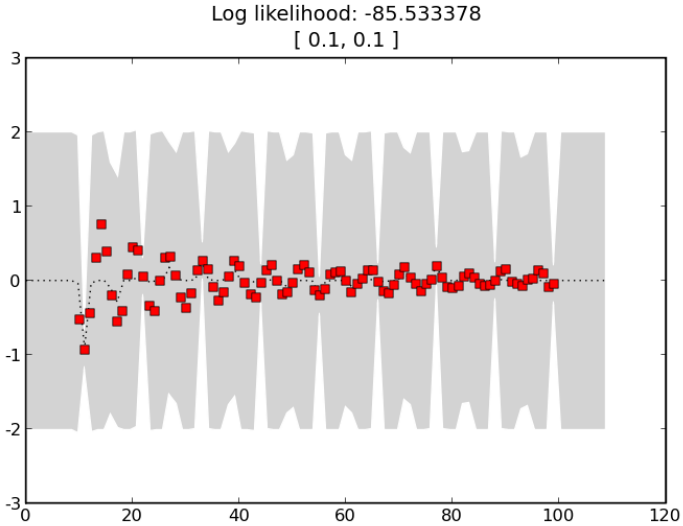
will generate



if we change the kernel so that the squared exponential term is given a shorter characteristic length scale

```
# Try a different kernel with a shorter characteristic length scale
K = kernels.SE([.1]) + kernels.Noise(.1)
predict_values(K, 'simple-example-se-shorter')
```

we will generate

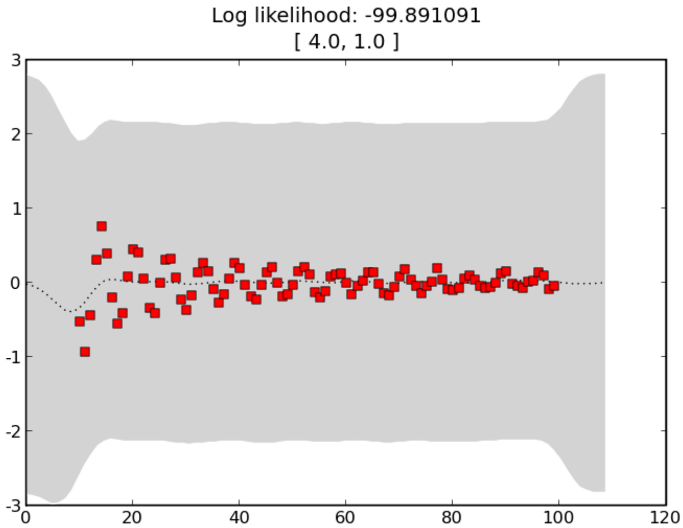


Here the shorter length scale means that data points are less correlated as the GP allows more variation over the same distance. The estimates of the noise between the training points is now much higher.

If we try a kernel with more noise

```
# Try another kernel with a lot more noise
K = kernels.SE([4.]) + kernels.Noise(1.)
predict_values(K, 'simple-example-more-noise')
```

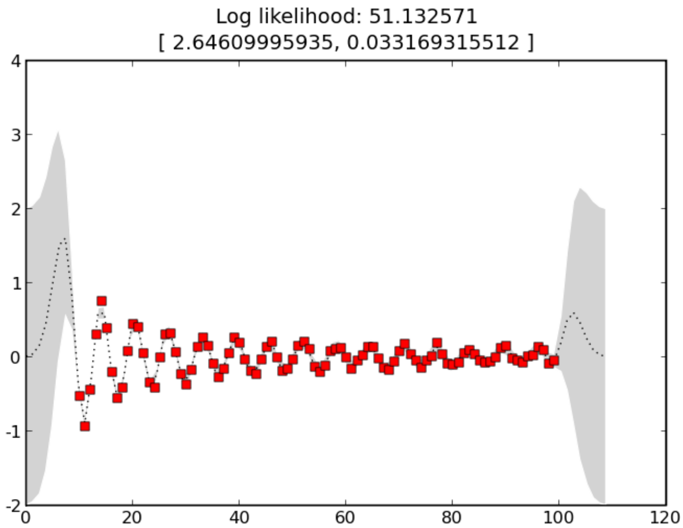
we get the following estimates showing that the training data does not affect the predictions as much



Perhaps we are really interested in learning the hyperparameters. We can acheive this as follows

```
# Try to learn kernel hyper-parameters
K = kernels.SE([4.0]) + kernels.Noise(.1)
predict_values(K, 'simple-example-learnt', learn=True)
```

and the result is



where the learnt length-scale is about 2.6 and the learnt noise level is about 0.03.

4 Appendix A - Code for figures

We list the code that generated the figures in this document.

4.1 Code for figure 1

```
from numpy.random import seed
from infpy.gp import GaussianProcess, gp_1D_X_range, gp_plot_samples_from
from pylab import plot, savefig, title, close, figure, xlabel, ylabel

# seed RNG to make reproducible and close all existing plot windows
seed(2)
close('all')

#
# Kernel
#
from infpy.gp import SquaredExponentialKernel as SE
```

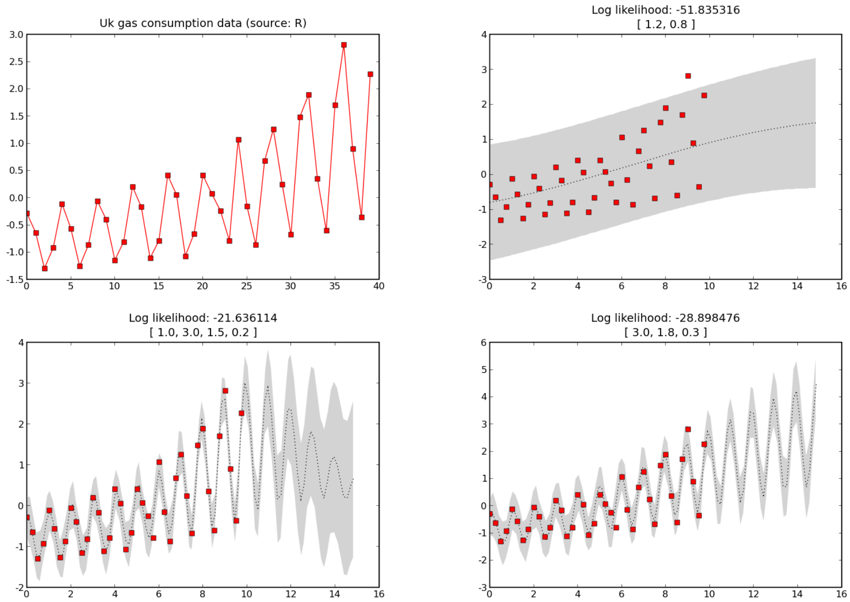


Figure 5: An application of GPs with periodic covariance functions to UK gas consumption data. *Top left*: The data which has been shifted to have a mean of 0. *Top right*: A GP incorporating some noise and a fixed long length scale squared exponential kernel. *Bottom left*: As top right but with a periodic term. *Bottom right*: As bottom left but with a periodic term with a reasonable period.

```
kernel = SE([1])

#
# Part of X-space we will plot samples from
#
support = gp_1D_X_range(-10.0, 10.01, .125)

#
# Plot samples from prior
#
figure()
gp = GaussianProcess([], [], kernel)
gp_plot_samples_from(gp, support, num_samples=3)
xlabel('x')
ylabel('f(x)')
title('Samples from the prior')
savefig('samples_from_prior.png')
savefig('samples_from_prior.eps')

#
# Data
#
```

```
X = [[-5.], [-2.], [3.], [3.5]]
Y = [2.5, 2, -.5, 0.]

#
# Plot samples from posterior
#
figure()
plot([x[0] for x in X], Y, 'ks')
gp = GaussianProcess(X, Y, kernel)
gp_plot_samples_from(gp, support, num_samples=3)
xlabel('x')
ylabel('f(x)')
title('Samples from the posterior')
savefig('samples_from_posterior.png')
savefig('samples_from_posterior.eps')
```

4.2 Code for figure 2

```
from numpy.random import seed
from infpy.gp import GaussianProcess, gp_1D_X_range, gp_plot_samples_from
from pylab import plot, savefig, title, close, figure, xlabel, ylabel
from infpy.gp import SquaredExponentialKernel as SE
from infpy.gp import Matern52Kernel as Matern52
from infpy.gp import Matern52Kernel as Matern32
from infpy.gp import RationalQuadraticKernel as RQ
from infpy.gp import NeuralNetworkKernel as NN
from infpy.gp import FixedPeriod1DKernel as Periodic
from infpy.gp import noise_kernel as noise

# seed RNG to make reproducible and close all existing plot windows
seed(2)
close('all')

#
# Part of X-space we will plot samples from
#
support = gp_1D_X_range(-10.0, 10.01, .125)

#
# Data
#
X = [[-5.], [-2.], [3.], [3.5]]
Y = [2.5, 2, -.5, 0.]

def plot_for_kernel(kernel, fig_title, filename):
  figure()
  plot([x[0] for x in X], Y, 'ks')
  gp = GaussianProcess(X, Y, kernel)
  gp_plot_samples_from(gp, support, num_samples=3)
```

```
  xlabel('x')
  ylabel('f(x)')
  title(fig_title)
  savefig('%s.png' % filename)
  savefig('%s.eps' % filename)

plot_for_kernel(
  kernel=Periodic(6.2),
  fig_title='Periodic',
  filename='covariance_function_periodic'
)

plot_for_kernel(
  kernel=RQ(1., dimensions=1),
  fig_title='Rational quadratic',
  filename='covariance_function_rq'
)

plot_for_kernel(
  kernel=SE([1]),
  fig_title='Squared exponential',
  filename='covariance_function_se'
)

plot_for_kernel(
  kernel=SE([3.]),
  fig_title='Squared exponential (long length scale)',
  filename='covariance_function_se_long_length'
)

plot_for_kernel(
  kernel=Matern52([1.]),
  fig_title='Matern52',
  filename='covariance_function_matern_52'
)

plot_for_kernel(
  kernel=Matern32([1.]),
  fig_title='Matern32',
  filename='covariance_function_matern_32'
)
```

4.3 Code for figure 3

```
from numpy.random import seed
from infpy.gp import GaussianProcess, gp_1D_X_range, gp_plot_prediction
from pylab import plot, savefig, title, close, figure, xlabel, ylabel
from infpy.gp import SquaredExponentialKernel as SE
from infpy.gp import noise_kernel as noise
```

```
# close all existing plot windows
close('all')

#
# Part of X-space we are interested in
#
support = gp_1D_X_range(-10.0, 10.01, .125)

#
# Data
#
X = [[-5.], [-2.], [3.], [3.5]]
Y = [2.5, 2, -.5, 0.]

def plot_for_kernel(kernel, fig_title, filename):
  figure()
  plot([x[0] for x in X], Y, 'ks')
  gp = GaussianProcess(X, Y, kernel)
  mean, sigma, LL = gp.predict(support)
  gp_plot_prediction(support, mean, sigma)
  xlabel('x')
  ylabel('f(x)')
  title(fig_title)
  savefig('%s.png' % filename)
  savefig('%s.eps' % filename)

plot_for_kernel(
  kernel=SE([1.]) + noise(.1),
  fig_title='k = SE + noise(.1)',
  filename='noise_mid'
)

plot_for_kernel(
  kernel=SE([1.]) + noise(1.),
  fig_title='k = SE + noise(1)',
  filename='noise_high'
)

plot_for_kernel(
  kernel=SE([1.]) + noise(.0001),
  fig_title='k = SE + noise(.0001)',
  filename='noise_low'
)
```

4.4 Code for figure 4

```
from numpy.random import seed
from infpy.gp import GaussianProcess, gp_1D_X_range
```

```python
from infpy.gp import gp_plot_prediction, gp_learn_hyperparameters
from pylab import plot, savefig, title, close, figure, xlabel, ylabel
from infpy.gp import SquaredExponentialKernel as SE
from infpy.gp import noise_kernel as noise

# close all existing plot windows
close('all')

#
# Part of X-space we are interested in
#
support = gp_1D_X_range(-10.0, 10.01, .125)

#
# Data
#
X = [[-5.], [-2.], [3.], [3.5]]
Y = [2.5, 2, -.5, 0.]

def plot_gp(gp, fig_title, filename):
  figure()
  plot([x[0] for x in X], Y, 'ks')
  mean, sigma, LL = gp.predict(support)
  gp_plot_prediction(support, mean, sigma)
  xlabel('x')
  ylabel('f(x)')
  title(fig_title)
  savefig('%s.png' % filename)
  savefig('%s.eps' % filename)

#
# Create a kernel with reasonable parameters and plot the GP predictions
#
kernel = SE([1.]) + noise(1.)
gp = GaussianProcess(X, Y, kernel)
plot_gp(
  gp=gp,
  fig_title='Initial parameters: kernel = SE([1]) + noise(1)',
  filename='learning_first_guess'
)

#
# Learn the covariance function's parameters and replot
#
gp_learn_hyperparameters(gp)
plot_gp(
  gp=gp,
  fig_title='Learnt parameters: kernel = SE([%.2f]) + noise(%.2f)' % (
    kernel.k1.params[0],
    kernel.k2.params.o2[0]
```

```
  ),
  filename='learning_learnt'
)
```

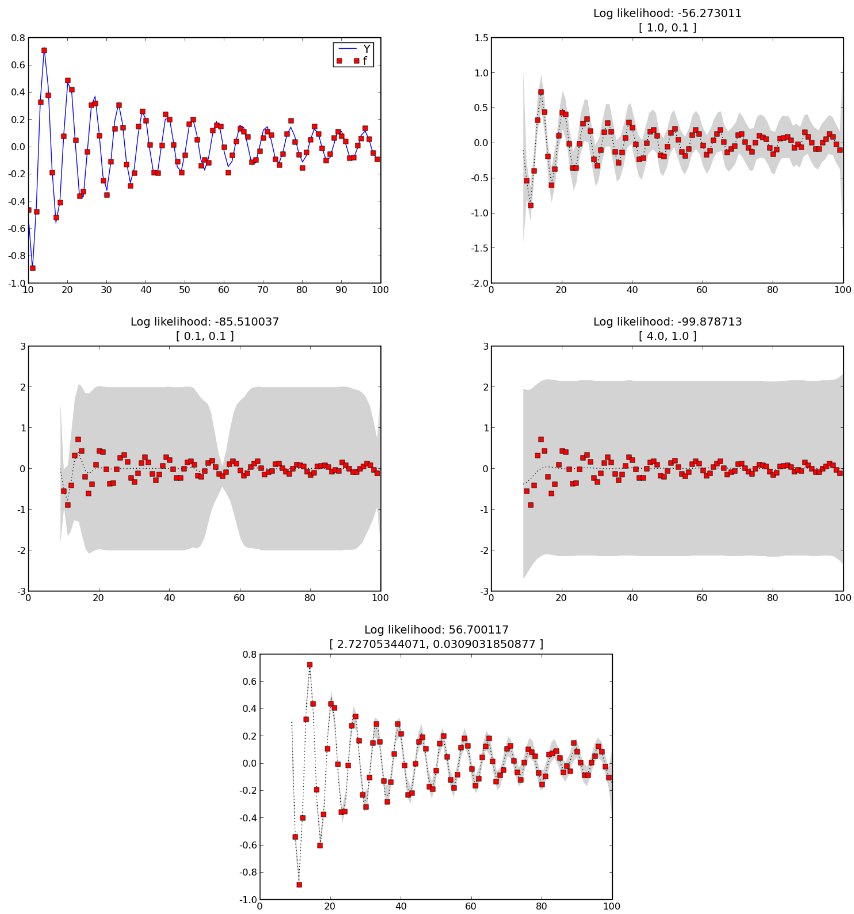


Figure 6: Modulated sine example: *Top left*: The data: a modulated noisy sine wave. *Top right*: GP with a squared exponential kernel. *Middle left*: GP with a squared exponential kernel with a shorter length scale. *Middle right*: GP with a squared exponential kernel with a larger noise term. *Bottom*: GP with a squared exponential kernel with learnt hyper-parameters.