Coursework 1: Gaussian processes

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In this assignment you will use Gaussian process modelling. This coursework uses the Python package `sklearn.gaussian_process` which is the rough equivalent of the GPML package for MATLAB. See the appendix at the end of this document for a walkthrough.

What to submit. Your answers should contain an explanation of what you do, and 2–4 central commands to achieve it. Complete listings are unnecessary. The focus of your answer should be *interpretation:* explain what the numerical values and graphs you produce *mean,* and why they are as they are. The text of your answer to each question should be no more than a paragraph or two.

```
# Standard imports for scientific and engineering work in Python:
import numpy as np                      # MATLAB-style matrix and vector manipulation
import matplotlib.pyplot as plt         # MATLAB-style plotting
import matplotlib                       # for more control over plotting
import scipy.io                         # some useful data input-output routines
import sklearn.gaussian_process as gp   # Gaussian process modeling
import requests                         # for retrieving data over the web
import io                               # also used for importing data
# Configure matplotlib to show its output right in the notebook
%matplotlib inline
```

Question (a)

Load data from `https://teachingfiles.blob.core.windows.net/probml/cw1a.mat`. Consider a Gaussian process with a squared exponential covariance function,

`v**2 * gp.kernels.RBF(length_scale=λ) + gp.kernels.WhiteKernel(noise_level=σ),`

and minimize the negative log marginal likelihood starting with hyperparameters `λ=np.exp(-1)`, `v=1`, `σ=1`. Show the 95% predictive error bars. Comment on the predictive error bars and the optimized hyperparameters.

```
# To import a .mat file from a URL:
r = requests.get('https://teachingfiles.blob.core.windows.net/probml/cw1a.mat')
with io.BytesIO(r.content) as f:
    data = scipy.io.loadmat(f)
    x,y = data['x'], data['y']
```

Question (b)

Show that by initializing the hyperparameters differently, you can find a different local optimum for the hyperparameters. Try a range of values. Show the fit. Explain what is going on. Which fit is best, and why?

Question (c)

Train instead a GP with a periodic covariance function, using `gp.kernels.ExpSineSquared`. Show the fit. Comment on the behaviour of the error-bars, compared to your fit from (a). Do you think the data generating mechanism was really periodic? Why, why not?

Question (d)

Generate 200 noise-free data points at `x = np.linspace(-5,5,200)` from a Gaussian process with the following covariance function:

```
1 * gp.kernels.ExpSineSquared(length_scale=np.exp(-0.5), periodicity=1)
    * gp.kernels.RBF(length_scale=np.exp(2)))
```

Don't add noise to the function values, i.e. don't add `gp.kernels.WhiteKernel()` to the kernel. Using `GaussianProcessRegressor.sample_y()`, plot some sample functions. Explain their behaviour.

Question (e)

Load `https://teachingfiles.blob.core.windows.net/probml/cw1e.mat`. This data has two-dimensional input and scalar output. Visualise the data, e.g. using the code snippets in the appendix. Consider two different Gaussian process models of the data, one using covariance function `RBF(length_scale=[l1,l2])` and the other using the sum of two such `RBF` terms. (Make sure to break symmetry, e.g. by choosing the initial hyperparameters randomly.)

Compare the two models. How do the data fits compare? How do the marginal likelihoods compare? What is your interpretation? Which of the two is better?

> When `length_scale` is a list, the `RBF` kernel uses separate length-scale parameters for each dimension of the input space. In GPML it is known as 'Squared Exponential with Automatic Relevance Determination', `covSEard`. It is a useful tool to learn which inputs are important for predictions: if length-scales are short, inputs are very important, and when they grow very long (compared to the spread of the data), the corresponding inputs will be largely ignored.

```
r = requests.get('https://teachingfiles.blob.core.windows.net/probml/cw1e.mat')
with io.BytesIO(r.content) as f:
    data = scipy.io.loadmat(f)
    x,y = data['x'], data['y']
```

Appendix

Gaussian processes in Python

Here is a simple example of how to use `sklearn.gaussian_process`. For full details, see the documentation.

Let's consider a simple Gaussian process model: a prior on the space of Gaussian processes, with mean 0, and with covariance function

$$k(x, x') = \nu^2 \exp\left(-\frac{(x - x')^2}{2\ell^2}\right)$$

(this function is called `RBF` in `sklearn.gaussian_process` and `covSEiso` in GPML). Suppose that the data model is

$$p(y \mid x, f) \sim \text{Normal}\big(f(x), \sigma^2 I\big)$$

where x and y are vectors and $f(x)$ means $(f(x_1), \ldots, f(x_n))$. In this model, ν, ℓ and σ are hyperparameters. Another way to write out this entire model is with a single covariance function,

$$k(x, x') = \nu^2 \exp\left(-\frac{(x - x')^2}{2\ell^2}\right) + \sigma^2 \delta_{xx'}.$$

In the `gaussian_process` package, a Gaussian process model is specified by a *kernel* object. (Kernel is another name for covariance function.) The package has a library of kernels, each implemented as a Python class, and we can create composite kernels by adding together and multiplying kernel objects.

```
l = np.exp(-1)
v = 0.5
σ = 1
kernel1 = v**2 * gp.kernels.RBF(length_scale=l) + gp.kernels.WhiteKernel(noise_level=σ)
kernel1
```

```
0.5**2 * RBF(length_scale=0.368) + WhiteKernel(noise_level=1)
```

To extract parameters from a kernel, use `get_params()`. You can also use `set_params` to set the parameters for a kernel.

```
kernel1.get_params()
```

```
{'k1': 0.5**2 * RBF(length_scale=0.368),
 'k1__k1': 0.5**2,
 'k1__k1__constant_value': 0.25,
 'k1__k1__constant_value_bounds': (1e-05, 100000.0),
 'k1__k2': RBF(length_scale=0.368),
 'k1__k2__length_scale': 0.36787944117144233,
 'k1__k2__length_scale_bounds': (1e-05, 100000.0),
 'k2': WhiteKernel(noise_level=1),
 'k2__noise_level': 1,
 'k2__noise_level_bounds': (1e-05, 100000.0)}
```

Machine learning functions are implemented via the class `GaussianProcessRegressor`, which is initialized with a kernel object. It has methods for learning hyperparameters and making predictions. We can access a model's kernel with `GaussianProcessRegressor.kernel`.

```
model1 = gp.GaussianProcessRegressor(kernel=kernel1)
model1.kernel
```

```
0.5**2 * RBF(length_scale=0.368) + WhiteKernel(noise_level=1)
```

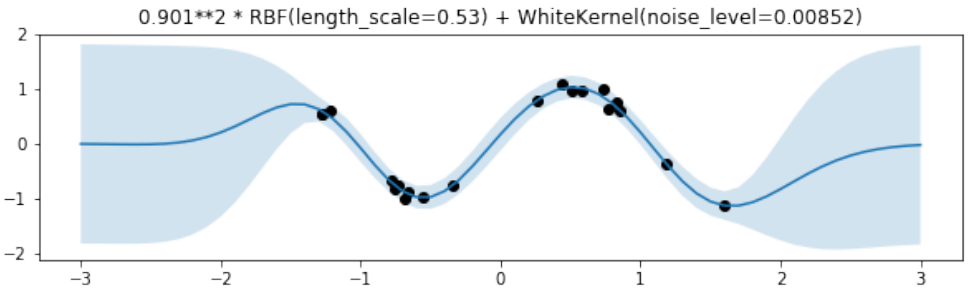
To learn hyperparameters, use `GaussianProcessRegressor.fit(x,y)`. It requires the parameters to be arrays with one row per observation. In the example below we start with one-dimensional input and output, so we have to reshape them to be column vectors. We can access the fitted kernel, and thence the fitted parameters, with `model.kernel_`.

```
# Training data
x = np.array([0.57650, 0.43504, 0.76607, -0.78369, -1.27129, -0.66034, 1.18100,
              0.25929, 0.50898, -0.73703, 0.83023, 1.60078, -0.34655, -0.68073,
              -1.21480, -0.55955, -1.28229, 0.85388, 0.73265, -0.75330])
y = np.array([ 0.96948, 1.08384, 0.62050, -0.65940, 0.54944, -0.88911, -0.37886,
              0.77166, 0.97753, -0.75901, 0.76003, -1.13327, -0.74600, -0.99293,
              0.60169, -0.98088, 0.55333, 0.60247, 0.99501, -0.83345])

model1.fit(x[..., np.newaxis], y[..., np.newaxis])
model1.kernel_
```

```
0.901**2 * RBF(length_scale=0.53) + WhiteKernel(noise_level=0.00852)
```

To make predictions with a fitted model, call `GaussianProcessRegressor.predict(x)`. As before, `x` should be a column vector.

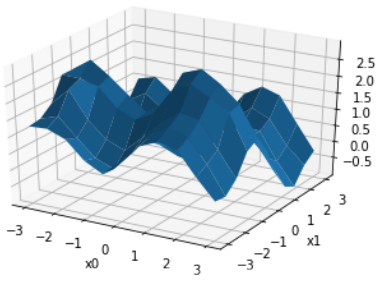
```
# New values of x where we want to make a prediction
newx = np.linspace(-3, 3, 61)
μ,σ = model1.predict(newx[..., np.newaxis], return_std=True)

# Plot the output.
# squeeze() is a numpy function that turns column vectors into simple 1d vectors.
with matplotlib.rc_context({'figure.figsize': [10,2.5]}):
    plt.fill_between(newx, μ.squeeze()-2*σ, μ.squeeze()+2*σ, alpha=.2)
    plt.plot(newx, μ.squeeze())
    plt.scatter(x, y, color='black')
    plt.title(model1.kernel_)
plt.show()
```



Plotting a function of two variables

Here are some ways we might plot the data from part (e).

```
from mpl_toolkits.mplot3d import axes3d   # import a library to allow 3d plots

# Reshape the data to be in array form
X = x[:,0].reshape((11,11))
Y = x[:,1].reshape((11,11))
Z = y.reshape((11,11))

# Optionally: use `%matplotlib notebook` to make the plots interactive.
# Get axes for a 3d plot, and then plot the surface
axes = plt.figure().gca(projection='3d')
axes.plot_surface(X, Y, Z)
axes.set_xlabel('x0')
axes.set_ylabel('x1')
plt.show()
```




```
# A heatmap
plt.imshow(y.reshape((11,11)), extent=np.array([-3,3,-3,3])*12/11, cmap=plt.get_cmap('coolwarm'))
plt.xlabel('x0')
```

```
plt.ylabel('x1')
plt.colorbar()
plt.show()
```