Gaussian_process_regression

October 20, 2016

1 Gaussian Process Regression

At times you don't care about the underlying model for your data points and just want a model that describes the data. One such fitting technique is know as Gaussian process regression (also know as kriging). This kind of regression assumes all the data points are drawn from a common covariance function. This function is used to generate an (infinite) set of functions and only keeps the ones that pass through the observed data.

1.1 Packages being used

- `sklearn`: has a Gaussian process regression function

1.2 Relevant documentation

- `sklearn`: http://scikit-learn.org/stable/modules/gaussian_process.html

```
In [1]: import numpy as np
        from sklearn.gaussian_process import GaussianProcessRegressor
        from sklearn.gaussian_process.kernels import RBF, ConstantKernel
        from matplotlib import pyplot as plt
        import mpl_style
        %matplotlib inline
        plt.style.use(mpl_style.style1)
```

1.3 The squared exponential covariance

As an example we will use the squared exponential covariance function:

$$\mathrm{Cov}\left(x_1, x_2; h\right) = \exp\left(\frac{-(x_1 - x_2)^2}{2h^2}\right)$$

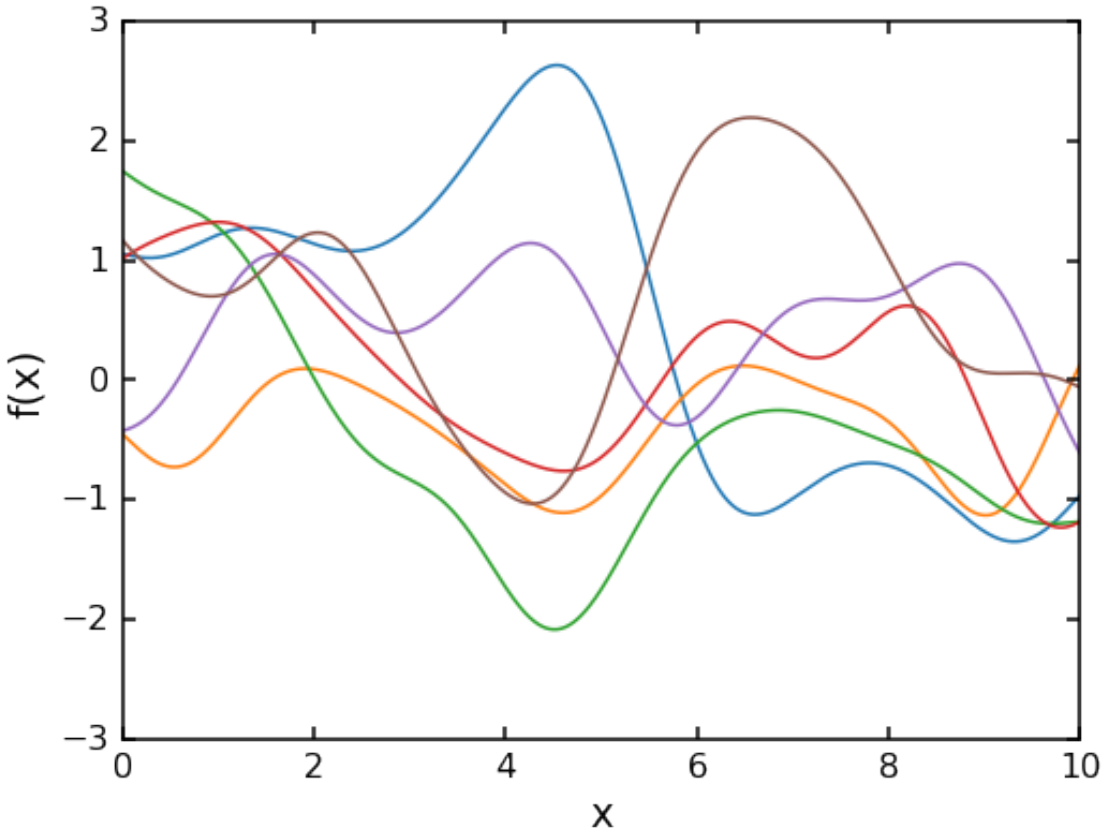
Lets using this function to draw some *unconstraned* functions:

```
In [2]: # define the function
        def squared_exponential(x1, x2, h):
            return np.exp(-0.5 * (x1 - x2)**2 / h**2)

        # draw samples from it
        x = np.linspace(0, 10, 1000)
        h = 1

        mu = np.zeros(len(x))
        C = squared_exponential(x, x[:, None], h)
        draws = np.random.multivariate_normal(mu, C, 6)
```

```
plt.figure(1)
plt.plot(x, draws.T)
plt.xlabel('x')
plt.ylabel('f(x)')
```

```
/Users/coleman/anaconda/envs/python3/lib/python3.5/site-packages/ipykernel/__main__.py:11: RuntimeWarning
```

```
Out[2]: <matplotlib.text.Text at 0x1031a2320>
```



1.4 Constrain the model

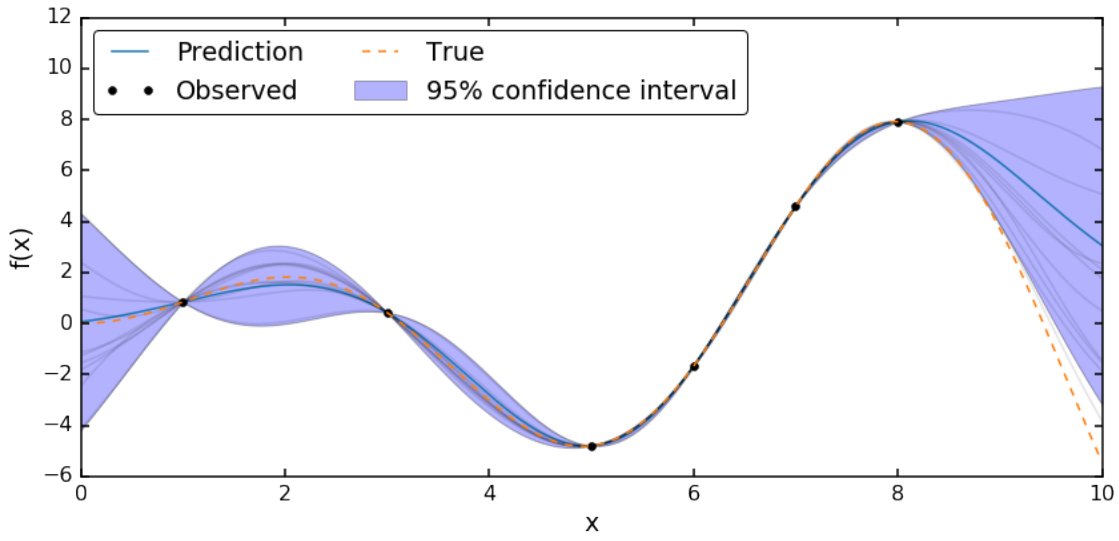
Assume we have some data points, we can use Gaussian process regression to only pick the models that pass through those points:

```
In [3]: x1 = np.array([1, 3, 5, 6, 7, 8])
        y1 = x1 * np.sin(x1)

        kernel = ConstantKernel(1, (1e-3, 1e3)) * RBF(10, (1e-2, 1e2))
        gp1 = GaussianProcessRegressor(kernel=kernel, n_restarts_optimizer=9)
        gp1.fit(x1[:, None], y1)
        f1, f1_err = gp1.predict(x[:, None], return_std=True)
        print('Coefficient of determination R^2 of the prediction: {0}'.format(gp1.score(x1[:, None], y
        print('Best fit kernel: {0}'.format(gp1.kernel_))
```

```
        plt.figure(2, figsize=(12, 6))
        plt.plot(x, f1, '-', label='Prediction')
        plt.fill_between(x, f1 - 1.96 * f1_err, f1 + 1.96 * f1_err, alpha=0.3, label='95% confidence int
        plt.plot(x, gp1.sample_y(x[:, None], n_samples=10), color='k', alpha=0.1)
        plt.plot(x1, y1, 'ok', ms=6, label='Observed')
        plt.plot(x, x * np.sin(x), '--', label='True')
        plt.xlabel('x')
        plt.ylabel('f(x)')
        plt.ylim(-6, 12)
        plt.legend(loc='upper left', ncol=2)
        plt.tight_layout()
```

```
Coefficient of determination R^2 of the prediction: 1.0
Best fit kernel: 4.71**2 * RBF(length_scale=1.68)
```

```
/Users/coleman/anaconda/envs/python3/lib/python3.5/site-packages/sklearn/gaussian_process/gpr.py:339: Ru
  y_samples = rng.multivariate_normal(y_mean, y_cov, n_samples).T
```



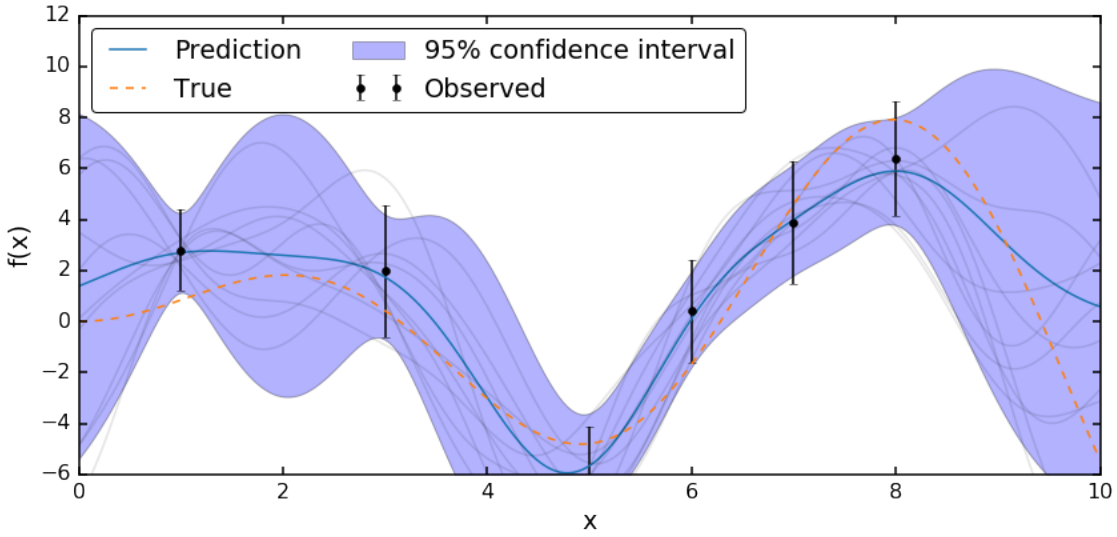
1.5 Lets add some noise to the data

In [4]:
```
dy = 0.5 + np.random.random(y1.shape)
noise = np.random.normal(0, dy)
y2 = y1 + noise
gp2 = GaussianProcessRegressor(kernel=kernel, alpha=dy**2, n_restarts_optimizer=10)
gp2.fit(x1[:, None], y2)
f2, f2_err = gp2.predict(x[:, None], return_std=True)
print('Coefficient of determination R^2 of the prediction: {0}'.format(gp2.score(x1[:, None], y
print('Best fit kernel: {0}'.format(gp2.kernel_))

plt.figure(3, figsize=(12, 6))
plt.plot(x, f2, '-', label='Prediction')
plt.fill_between(x, f2 - 1.96 * f2_err, f2 + 1.96 * f2_err, alpha=0.3, label='95% confidence int
plt.plot(x, gp2.sample_y(x[:, None], n_samples=10), color='k', alpha=0.1)
plt.errorbar(x1, y2, yerr=1.96*dy, fmt='ok', ms=6, label='Observed')
```

```
    plt.plot(x, x * np.sin(x), '--', label='True')
    plt.xlabel('x')
    plt.ylabel('f(x)')
    plt.ylim(-6, 12)
    plt.legend(loc='upper left', ncol=2)
    plt.tight_layout()
```

```
Coefficient of determination R^2 of the prediction: 0.9913661214942777
Best fit kernel: 4.11**2 * RBF(length_scale=0.919)
```

```
/Users/coleman/anaconda/envs/python3/lib/python3.5/site-packages/sklearn/gaussian_process/gpr.py:339: Ru
  y_samples = rng.multivariate_normal(y_mean, y_cov, n_samples).T
```



1.6 Other notes

- There are many covariance kernels you can pick;
  - `ConstantKernel`: a constant value that can be multiplied or added to any of the other kernels
  - `WhiteKernel`: a white noise kernel
  - `RBF`: Radial-based function, smooth kernel parameterized by a length-scale
  - `Marten`: non-smooth generalization of `RBF`, parameterized by length-scale and smoothness
  - `RationalQuadratic`: a (infinite sum) mixture of different `RBF`'s each with different length-scales
  - `ExpSineSquared`: periodic function kernel, parameterized by a length-scale and periodicity
  - `DotProduct`: a non-stationary kernel commonly combined with exponentiation to produce a 'polynomial like' fit (e.g. raising `DotProduct` to the power of 2 will give a quadratic like fit)
- The kernel parameter (e.g. the first parameter in the `RBF` function) is automatically fit within the bounds provided (e.g. the second parameter in `RBF`)
- `n_restarts_optimizer` indicates the number of times to re-run the optimizer starting at different locations (e.g. to find a global max instead of a local max)
- All `X` positions must be unique
- The computational complexity is $O(N^3)$ where N is the number of data point

In [ ]: