Gaussian Process Regression

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1 Statistical and Machine Learning (01.113) - HW3 Question 5

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```
In [1]: import numpy as np
        from mpl_toolkits import mplot3d
        from matplotlib import cm
        import matplotlib.pyplot as plt
        from scipy.optimize import minimize
        from scipy.stats import norm
        from sklearn.gaussian_process import GaussianProcessRegressor
        from sklearn.gaussian_process.kernels import RBF, Matern
```

We will use Gaussian process regression to approximate the following function and find its global maximum (i.e) $y^* \approx 1$ at $((x_1^*, x_2^*) = (2.25, 2.65))$

```
In [2]: # function to predict
        def func(x1,x2):
            y = 0.5*np.exp(
                -0.5*((x1+1.25)**2+(x2+1.75)**2)
            )+np.exp(
                -0.5*((x1-2.25)**2+(x2-2.65)**2)
            )
            return y

        def calc_true_optimum(func):
            current_max = 0
            x1, x2 = 0, 0
            for x_1 in np.linspace(-10,10, 500):
                for x_2 in np.linspace(-10,10, 500):
                    y = func(x_1, x_2)
                    if y > current_max:
                        current_max = y
                        x1 , x2 = x_1, x_2

            print(f"True Global Optimum: {current_max}")
            print(f"Corresponding x1, x2: {x1, x2}")
```

Next, we define our "true" and "noisy" functions as follows:

```
In [3]: def noisy_func(x1,x2):
            output = func(x1,x2)
            noise = np.random.normal(0,0.1,np.shape(output))
            return output + noise
```

1.1 Write code for the following acquisition functions:

- probability of improvement:

$$A(x, f^*) = P(f_x > f^*) = \Phi(\gamma_x)$$

- expected improvement:

$$\mathbb{E}[\max\{f_x - f^*, 0\}] = \sigma_x[\gamma_x \Phi(\gamma_x) + \phi(\gamma_x)]$$

- upper confidence bound:

$$A(x) = \mu_x + \kappa\sigma_x$$

```
In [4]: def probability_of_improvement(mu_x,sigma_x,opt_val):
            gamma = (mu_x - opt_val)/sigma_x
            return norm.cdf(gamma)

        def expected_improvement(mu_x,sigma_x,opt_val):
            gamma = (mu_x - opt_val)/sigma_x
            return sigma_x * gamma * norm.cdf(gamma) + sigma_x * norm.pdf(gamma)

        def upper_confidence_bound(mu_x,sigma_x,k):
            return mu_x + k * sigma_x
```

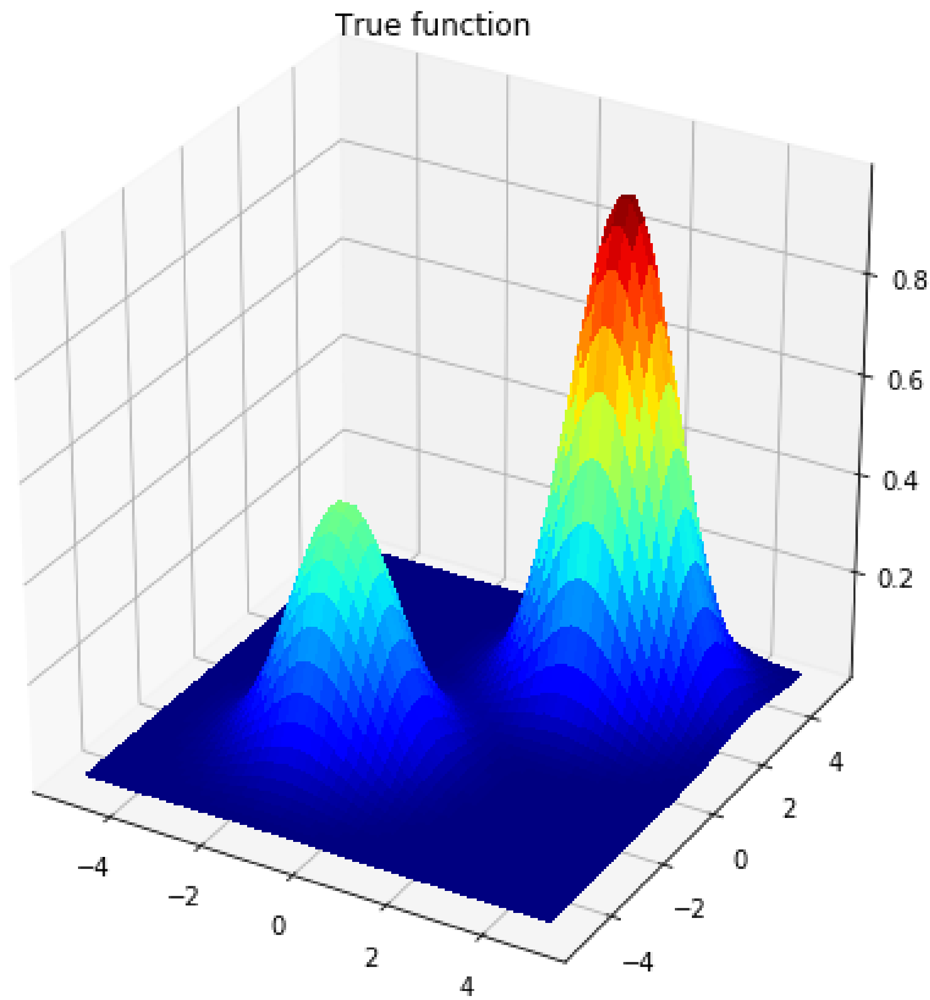
1.2 Define a query function using `scipy.optimize.minimize`

and the acquisition function of your choice.

```
In [5]: def my_acquisition_function(mu_x, sigma_x, k):
        #     return expected_improvement(mu_x,sigma_x,opt_val=1)
            return upper_confidence_bound(mu_x,sigma_x,k=1)
        def query(opt_val,gp):
            def obj(x):
                #do gaussian process prediction
                mu_x,sigma_x = gp.predict(x.reshape(1,-1),return_std=True)

                return -my_acquisition_function(mu_x,sigma_x,opt_val)

            x0 = np.random.uniform(-5,5,2)
            res = minimize(obj, x0=x0.reshape(1,-1), bounds=([-5, 5], [-5, 5]))
            return res.x
```

Use the next few lines of code to visualize the true function.

```
In [6]: def add_subplot(gp, subplt):
            mu = gp.predict(meshpts, return_std=False)
            ax = fig.add_subplot(2, 5, subplt, projection = '3d')
            ax.plot_surface(meshX, meshY, np. reshape (mu, (50 , 50)) ,
                            rstride=1, cstride =1, cmap=cm. jet,
                            linewidth=0, antialiased=False)

        res = 50
        lin = np.linspace(-5, 5, res)
        meshX, meshY = np.meshgrid(lin, lin)
        meshpts = np.vstack((meshX.flatten(), meshY.flatten())).T
        true_y = func(meshX, meshY)

        fig = plt.figure(figsize=(8,8))
        ax = fig.add_subplot(111, projection='3d')
        ax.plot_surface(meshX, meshY, true_y, rstride=1, cstride=1,
                        cmap=cm.jet, linewidth=0, antialiased=False)
        plt.title('True function')
        plt.show()
```



1.3 Initialize 4 random points and evaluate the noisy function at these points:

```
In [7]: xi = np.random.uniform(-5,5,(4,2))
        yi = noisy_func(xi[:,0], xi[:,1])
```

1.4 Initialize the Gaussian process regressor with a kernel of your choice:

```
In [8]: gp = GaussianProcessRegressor(kernel=RBF(length_scale=1.0) ,
                                      n_restarts_optimizer=10)
```

Finally, use the following code to perform Bayesian optimization and plot the evolution of the mean of the Gaussian process over 10 iterations:

```
In [9]: fig=plt.figure(figsize=plt.figaspect(0.5))
```

```python
for i in range(10):
    gp.fit(xi,yi)

    #find the current optimal value and its location
    opt_val = max(yi)
    opt_x = xi[np.where(yi == opt_val)]

    print('Best value: ', opt_val)
    print('at ', opt_x)

    next_x = query(opt_val, gp)

    # add next_x to the list of data points
    xi = np.append(xi, [next_x],axis=0)

    next_y = noisy_func(xi[-1][0], xi[-1][1]).reshape(1)

    # add next_y to the list of observations
    yi = np.append(yi,next_y)

    add_subplot(gp, i+1)

plt.show()
```

```
Best value:  0.558733394676865
at  [[2.91550841 1.71240961]]
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at  [[2.91550841 1.71240961]]
Best value:  1.137380594252116
at  [[2.27975136 2.25997191]]
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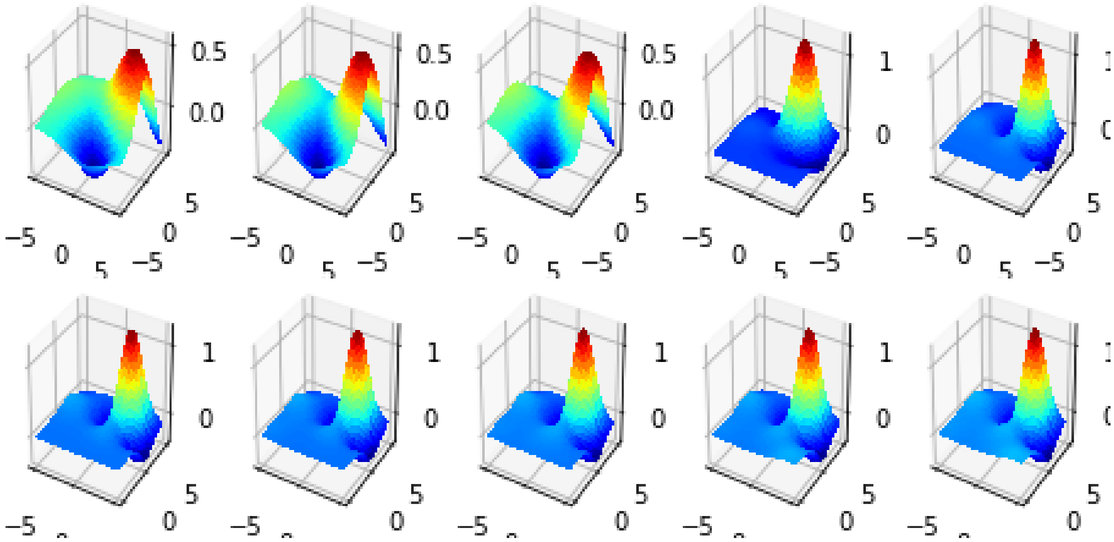

```
In [10]: print(f"Final value: {opt_val} at {opt_x[0]} \n")
         calc_true_optimum(func)
```

```
Final value: 1.137380594252116 at [2.27975136 2.25997191]

True Global Optimum: 0.999777024262348
Corresponding x1, x2: (2.2645290581162314, 2.6653306613226455)
```