YG390_lab_week7-student

November 11, 2019

1 DS-GA 3001.001 Special Topics in Data Science: Probabilistic Time Series Analysis

2 Gaussian Processes

$$GP(\mu(x), K(x_1, x_2))$$

mean usually to $\mu(x) = 0$

structure defined through covariance $K(x_1, x_2)$

[1]:
```
%matplotlib inline
import numpy as np
import pandas as pd
import matplotlib.pylab as plt
from sklearn.metrics import mean_squared_error
import time
np.random.seed(12)
```

2.1 Part I: Data Generation

Visualization functions

[2]:
```
def plot_gp(x_pred, y_pred, sigmas, x_train, y_train, true_y=None,␣
↪samples=None):
    """
    Function that plots the GP mean & std on top of given points.
    x_pred: points for prediction
    y_pred: means
    sigmas: std
    x, y: given data
    true_y:
    samples: 2D numpy array with shape (# of points, # of samples)
    """
    if samples is not None:
        plt.plot(all_x.reshape(-1, 1), samples)
```

```
    plt.errorbar(x_pred, y_pred, yerr=sigmas, capsize=0,
                 ecolor=(0.85, 0.85, 0.85), fmt = "r-",
                 label="pred mean")
    plt.plot(x_train, y_train, "ko", label="training set")
    if true_y is not None:
        plt.plot(x_pred, true_y, "b-", label="truth function")
    plt.legend()
```

Various generative functions for GP to approximate.

Here we assume that y = 0 when x = 0.

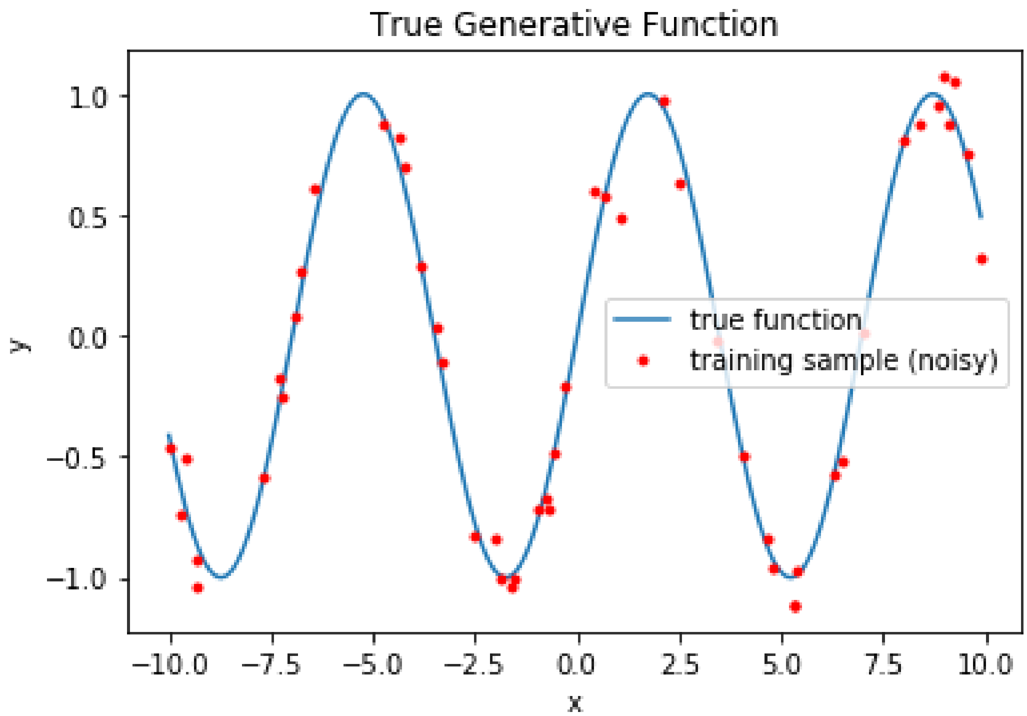
[3]:
```
def linear_func(x):
    return 1.2 * x

def sin_wave(x):
    return np.sin(0.9*x).flatten()
```

Generate train and test data.

[4]:
```
x_min = -10
x_max = 10
n_train = 50
generative_func = sin_wave

# X2: we want x in the range of (x_min, x_max)
all_x = np.arange(x_min, x_max, step=0.1)
# Y2: this is the true values of f(x) for x in (x_min, x_max)
# (we are NOT using them to train GP. true_y is only used for evaluation)
true_y = generative_func(all_x)
# X1, Y1: a randomly given training set of: n_train training points
X_train = np.random.uniform(x_min, x_max, n_train)
beta_inv = .01
# noisy data points
y_train = generative_func(X_train)+np.random.randn(len(X_train))*np.
 ↪sqrt(beta_inv)
```

[5]:
```
plt.figure()
plt.plot(all_x, true_y, label='true function')
plt.plot(X_train, y_train, '.r', label='training sample (noisy)')
plt.title("True Generative Function")
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
```

[5]: <matplotlib.legend.Legend at 0x7fc07830c470>



2.2 Part II GP with sklearn

Sklearn has a very handy API for Gaussian Process regression.

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

2.2.1 Kernel functions

Kernels to parametrize covariance structure

Constant Kernel: covariance is defined by a constant value

RBF (squared exponential) Kernel:

$$K(x_m, x_n) = exp\left(-\frac{||x_m - x_n||^2}{2 * l^2}\right)$$

White Kernel: accords for noise-component

$$K(x_m, x_n) = noise$$

where if $x_m = x_n$ else 0

[6]:
```
from sklearn import gaussian_process
```

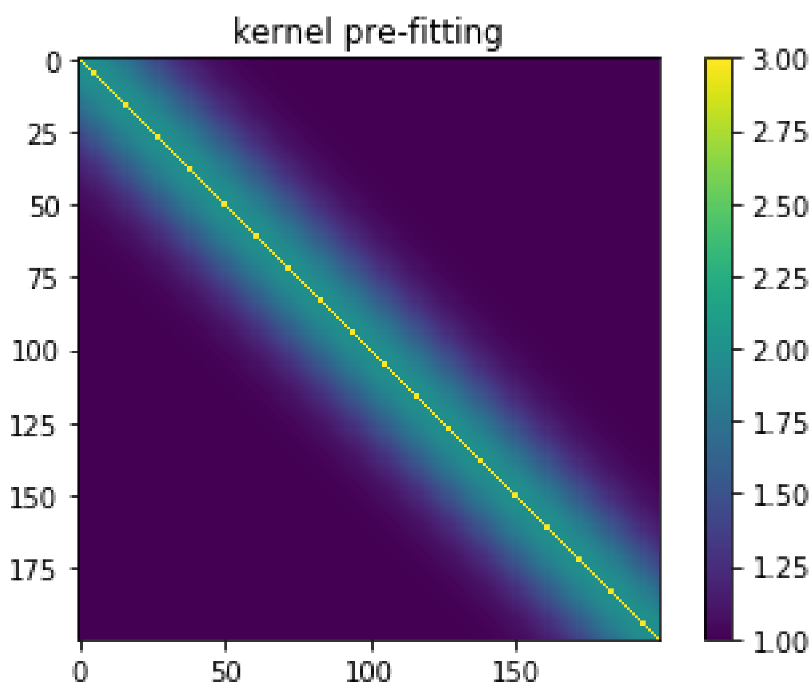
```
from sklearn.gaussian_process.kernels import RBF, Matern, WhiteKernel,␣
↪ConstantKernel
```

There are plenty pre-built kernels defined by the API. Moreover, you can construct you own kernels by combining the pre-built ones.

[7]:
```
kernel = ConstantKernel(constant_value=1, constant_value_bounds=(1e-5, 1e5)) +␣
↪RBF(length_scale=2) + WhiteKernel(noise_level=1)
```

[8]:
```
plt.figure()
plt.imshow(kernel(np.array([all_x]).T))
plt.colorbar()
plt.title('kernel pre-fitting')
```

[8]:
```
Text(0.5, 1.0, 'kernel pre-fitting')
```



fitting the GP model The fit() method automatically selects the hyper-parameters of given kernels.

[9]:
```
gp = gaussian_process.GaussianProcessRegressor(kernel=kernel)
gp.fit(X_train.reshape(-1,1), y_train.reshape(-1,1))
```

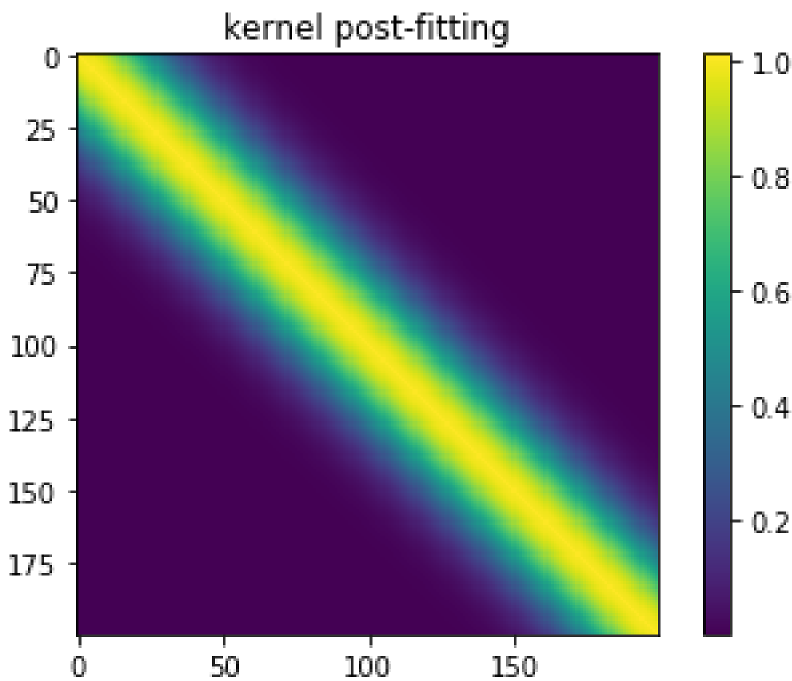
[9]:
```
GaussianProcessRegressor(alpha=1e-10, copy_X_train=True,
                         kernel=1**2 + RBF(length_scale=2) +
```

```
WhiteKernel(noise_level=1),
                         n_restarts_optimizer=0, normalize_y=False,
                         optimizer='fmin_l_bfgs_b', random_state=None)
```

[10]:
```
# print the kernel with fitted parameters
print(gp.kernel_)
plt.figure()
plt.imshow(gp.kernel_(np.array([all_x]).T))
plt.colorbar()
plt.title('kernel post-fitting')
```

```
0.00316**2 + RBF(length_scale=2.02) + WhiteKernel(noise_level=0.011)
```

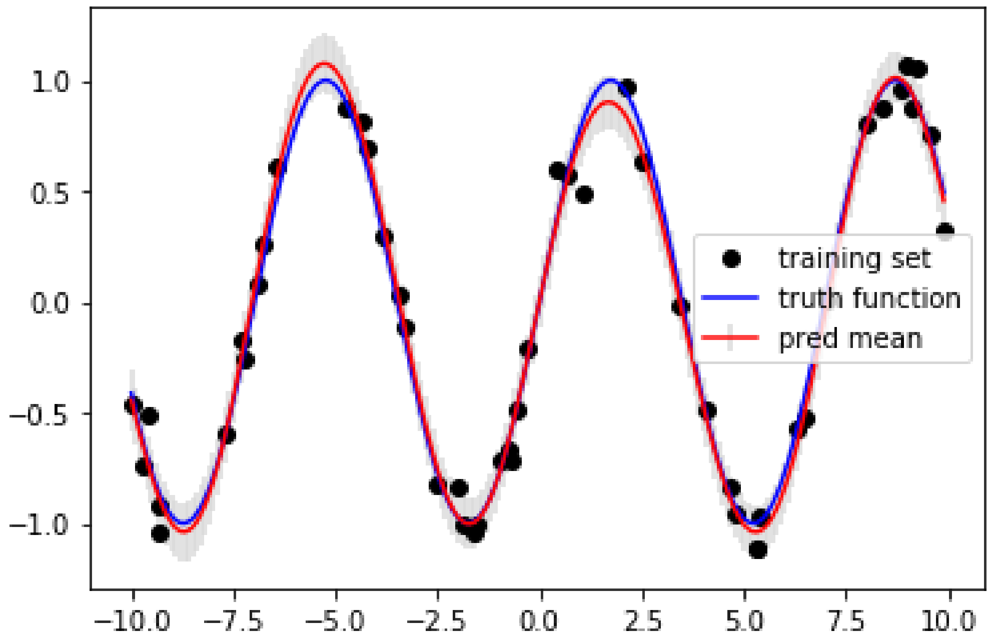
[10]:
```
Text(0.5, 1.0, 'kernel post-fitting')
```



prediction of new values The predict method returns both mean and std.

[11]:
```
mus, sigmas = gp.predict(all_x.reshape(-1,1), return_std=True)
```

[12]:
```
plot_gp(all_x, mus, sigmas, X_train, y_train, true_y=true_y)
```



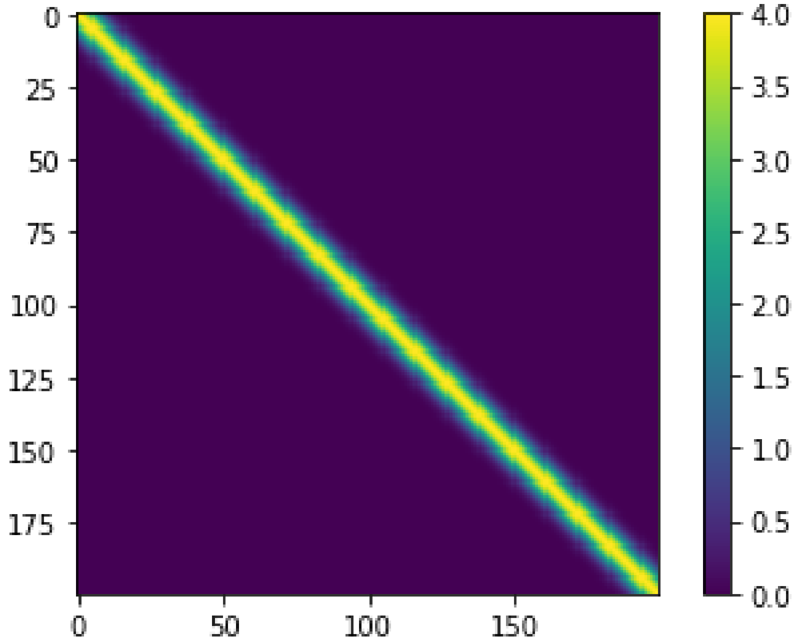
below we will use this form of the Squared Exponential Kernel:

$$k(x, x') = \sigma^2 exp(-\frac{(x - x')^2}{2\sigma^2})$$

[13]:
```
def exponential_cov(x, y, params):
    """
    Function that implements the squared exponential kernel
    """
    sigma, l = params
    return np.power(sigma,2) * np.exp( - np.subtract.outer(x, y)**2/(2 * np.
 ↪power(l,2)))
```

[14]:
```
plt.figure()
plt.imshow(exponential_cov(all_x, all_x, (2,.5)))
plt.colorbar()
```

[14]: <matplotlib.colorbar.Colorbar at 0x7fc0c8f686a0>



2.3 Part III: GP Inference

In this part, we implement the predict_cholesky function.

(Bishop chapter 6.4 on Gaussian Processes)

2.3.1 noisy observations

- in our training data the true generative function is hidden by Gaussian noise
- we take this noise into account by expressing the observed target value as

$$t_n = y_n + \epsilon_n$$

where y_n is the true function value of $y(x_n)$ and $\epsilon \sim N(0, \beta^{-1})$

- therefore the probability of an observation t_n given y_n is:

$$p(t_n|y_n) = N(t_n|y_n, \beta^{-1})$$

- marginalizing over the possible y_n gives us the marginal distribution for the observation vector $\mathbf{t}$:

$$p(\mathbf{t}) = N(0, C(x))$$

where C is made up of the GP covariance and the noise variance:

$$C(x_n, x_m) = K(x_n, x_m) + \beta^{-1}\delta_{nm}$$

2.3.2 inference

predict new data points/trajectories given fixed (noisy, observed) data points

define the probability for a new points $\mathbf{t}^{pred}$ given old observed values $\mathbf{t}^{train}$

$$p(\mathbf{t}^{pred}|\mathbf{t}^{train}) = N\left(\mu_{\mathbf{t}^{pred}|\mathbf{t}^{train}}, V_{\mathbf{t}^{pred}|\mathbf{t}^{train}}\right)$$

where

$$\mathbf{t}^{train} = y(\mathbf{x}^{train}) + \epsilon$$

remember Gaussian properties Using Gaussian properties:

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \sim N\left(\begin{bmatrix} a \\ b \end{bmatrix}, \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}\right)$$

translate this to our (observed/predicted) data points $\mathbf{t}$

$$p(\mathbf{t}^{train}, \mathbf{t}^{pred}) = N(0, \Sigma)$$

where

$$\Sigma = \begin{bmatrix} C^{train} & K \\ K^T & C^{pred} \end{bmatrix}$$

where K stands for $K(x_n, x_m)$

from this we get

$$p(\mathbf{t}^{pred}|\mathbf{t}^{train}) = N\left(\mu_{\mathbf{t}^{pred}|\mathbf{t}^{train}}, V_{\mathbf{t}^{pred}|\mathbf{t}^{train}}\right)$$

$$\mu_{\mathbf{t}^{pred}|\mathbf{t}^{train}} = K^T(C^{train})^{-1}\mathbf{t}^{train}$$

$$V_{\mathbf{t}^{pred}|\mathbf{t}^{train}} = C^{pred} - K^T(C^{train})^{-1}K$$

Note that here, we assume zero mean

2.3.3 inference using the Cholesky Decomposition

- faster and more stable way to compute $\mu_{\mathbf{t}^{pred}|\mathbf{t}^{train}}$ and $V_{\mathbf{t}^{pred}|\mathbf{t}^{train}}$ given that $(C^{train})^{-1}$ is not guaranteed to be non-singular
- The Cholesky decomposition converts a (Hermitian, positive-definite) matrix A into the product of a lower triangular matrix L and its conjugate transpose L^*
- We use the Cholesky decomposition to get $C^{train} = LL^T$

Because our covariance matrix $(C^{train})^{-1}$ is positive-definite and a real matrix that mirrors itself along the diagonal, it is a Hermitian matrix

L will be a real-value matrix so its conjugate is itself

- From this we get:

$$\mu_{\mathbf{t}^{pred}|\mathbf{t}^{train}} = K^T(C^{train})^{-1}\mathbf{t}^{train} = K^T(LL^T)^{-1}\mathbf{t}^{train} = K^T(L^T)^{-1}L^{-1}\mathbf{t}^{train} = (L^{-1}K)^T(L^{-1}\mathbf{t}^{train})$$

$$V_{\mathbf{t}^{pred}|\mathbf{t}^{train}} = C^{pred} - K^T(C^{train})^{-1}K = C^{pred} - (L^{-1}K)^T(L^{-1}K)$$

where L=cholesky(C)

$L^{-1}K$ and $L^{-1}\mathbf{t}^{train}$ can be obtained by solving the linear system $Lx = K$ and $Lx = \mathbf{t}^{train}$ using np.linalg.solve

[15]:
```
def predict(x_pred, X_train, y_train, kernel, kernel_params, cholesky=True,␣
↪beta_inv = 0):
    """
    Top level wrapper function for GP prediction
    """
    if cholesky:
        return predict_cholesky(x_pred, X_train, y_train, kernel,␣
↪kernel_params, beta_inv)
    else:
        return predict_inverse(x_pred, X_train, y_train, kernel, kernel_params,␣
↪beta_inv)

def predict_inverse(x_pred, X_train, y_train, kernel, kernel_params, beta_inv):
    """
    GP inference using naive matrix inversion
    x_pred: X1, a numpy vector of size n
    X_train: X2, a numpy vector of size m
    y_train: Y2, a numpy vector of size m
    kernel: a kernel function, should be exponential_cov
    kernel_params: a numpy vector
    @return mu: E[y2]
    @return cov: covariance matrix, a numpy matrix that's n*n
    """
```

```
    C = kernel(X_train, X_train, kernel_params) + np.eye(len(X_train))*beta_inv
    B = kernel(x_pred, X_train, kernel_params)
    C_inv = np.linalg.inv(C)
    A = kernel(x_pred, x_pred, kernel_params) + np.eye(len(x_pred))*beta_inv
    mu = np.dot(B, C_inv).dot(y_train)
    cov = A - np.dot(B, C_inv).dot(B.T)
    return mu, cov

def predict_cholesky(x_pred, X_train, y_train, kernel, kernel_params, beta_inv):
    """
    GP inference using naive matrix inversion
    x_pred: X1, a numpy vector of size n
    X_train: X2, a numpy vector of size m
    y_train: Y2, a numpy vector of size m
    kernel: a kernel function, should be exponential_cov
    kernel_params: a numpy vector
    @return mu: E[y2]
    @return cov: covariance matrix, a numpy matrix that's n*n
    """
    ############################################
    ### TODO: please implement this function ###
    ######## (and replace current code) ########
    ############################################
    C_train = kernel(X_train, X_train, kernel_params) + np.
 ↪eye(len(X_train))*beta_inv
    B = kernel(x_pred, X_train, kernel_params)
    L = np.linalg.cholesky(C_train)
    L_inv_K = np.linalg.solve(L, B.T)
    t_L_inv = np.linalg.solve(L, y_train)
    mu = np.matmul(L_inv_K.T, t_L_inv)
    C_pred = kernel(x_pred, x_pred, kernel_params) + np.
 ↪eye(len(x_pred))*beta_inv
    cov = C_pred - np.matmul(L_inv_K.T, L_inv_K)
    return mu, cov

kernel_parameters = [2, 0.5]
```

2.3.4 prediction giving varying number of training data points

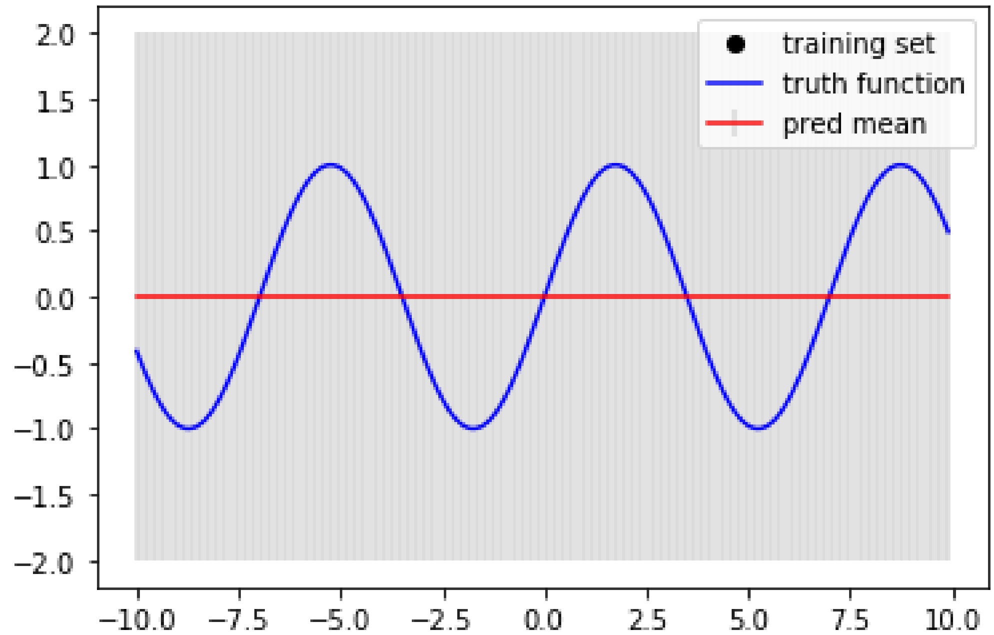
Prior distribution

$$y \sim N(\mu_0, \sigma_0^2)$$

Since we assume a zero mean function, we have $\mu_0 = E[y] = 0$.

[16]:
```
mu_0 = np.zeros(len(all_x))
sigma_0 = np.sqrt(exponential_cov(0, 0, kernel_parameters))
plot_gp(all_x, mu_0, sigma_0, [], [], true_y)
print("rmse = {0}".format(np.sqrt(mean_squared_error(mu_0, true_y))))
```

```
rmse = 0.7216677922512522
```



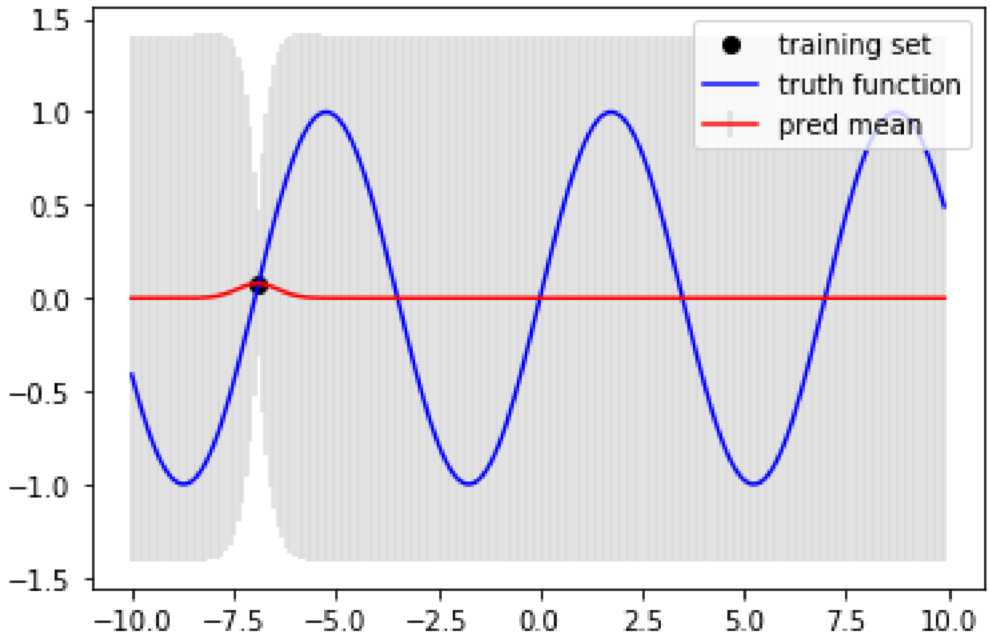
Posterior Distribution - single points

Now we start by feeding our GP with a single datum.

[17]:
```
cholesky = True
```

[18]:
```
training_data_num = 1
need_X_train = X_train[:training_data_num]
need_y_train = y_train[:training_data_num]
C = exponential_cov(need_X_train, need_X_train, kernel_parameters)
mus, cov = predict(all_x, X_train[:training_data_num], y_train[:
↪training_data_num], exponential_cov,
                   kernel_parameters, cholesky=cholesky, beta_inv=beta_inv)
sigmas = np.sqrt(np.diag(cov))
plot_gp(all_x, mus, np.sqrt(sigmas), need_X_train, need_y_train, true_y)
print("rmse = {0}".format(np.sqrt(mean_squared_error(mus, true_y))))
```

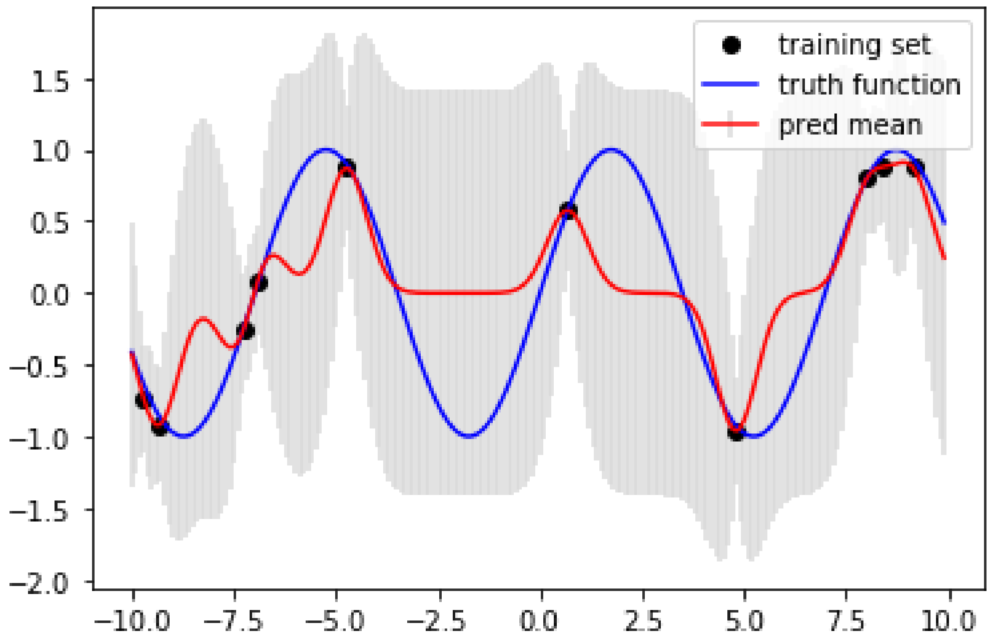
```
rmse = 0.7214994093740607
```



With 10 points

[19]:
```
training_data_num = 10
need_X_train = X_train[:training_data_num]
need_y_train = y_train[:training_data_num]
C = exponential_cov(need_X_train, need_X_train, kernel_parameters)
mus, cov = predict(all_x, X_train[:training_data_num], y_train[:
 ↪training_data_num], exponential_cov,
                    kernel_parameters, cholesky=cholesky, beta_inv=beta_inv)
sigmas = np.sqrt(np.diag(cov))
plot_gp(all_x, mus, np.sqrt(sigmas), need_X_train, need_y_train, true_y)
print("rmse = {0}".format(np.sqrt(mean_squared_error(mus, true_y))))
```

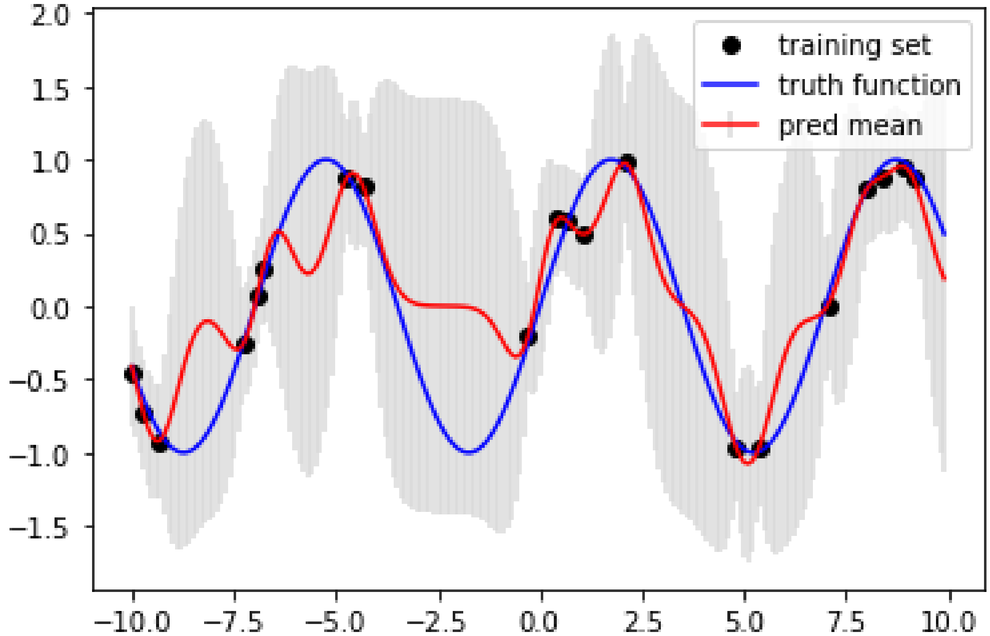
```
rmse = 0.47857176130581947
```



With 20 points

[20]:
```
training_data_num = 20
need_X_train = X_train[:training_data_num]
need_y_train = y_train[:training_data_num]
C = exponential_cov(need_X_train, need_X_train, kernel_parameters)
mus, cov = predict(all_x, X_train[:training_data_num], y_train[:
 ↪training_data_num], exponential_cov,
                   kernel_parameters, cholesky=cholesky, beta_inv=beta_inv)
sigmas = np.sqrt(np.diag(cov))
plot_gp(all_x, mus, np.sqrt(sigmas), need_X_train, need_y_train, true_y)
print("rmse = {0}".format(np.sqrt(mean_squared_error(mus, true_y))))
```

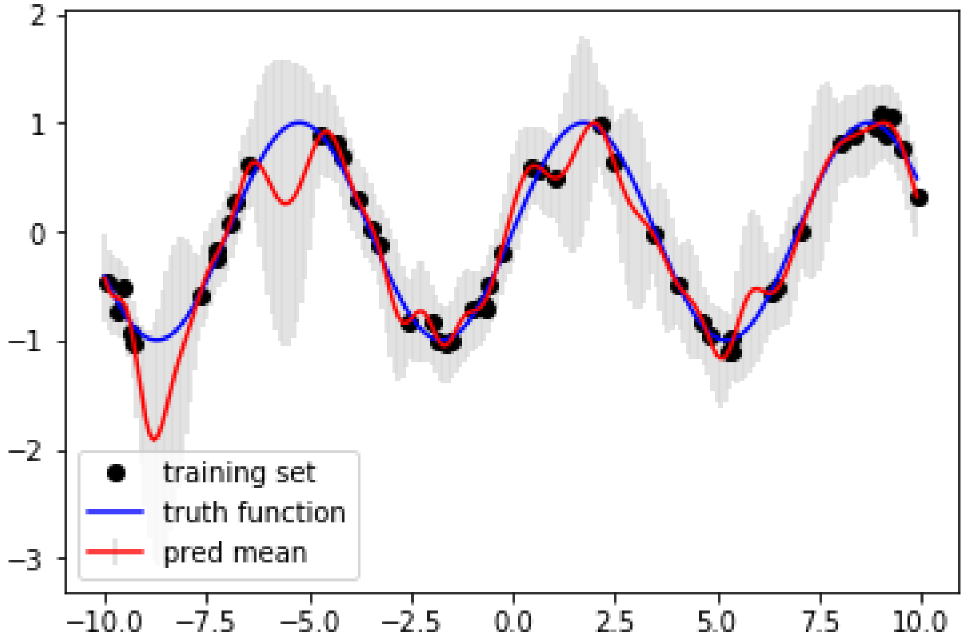
```
rmse = 0.3799906094256711
```



50 points

[21]:
```
training_data_num = 50
need_X_train = X_train[:training_data_num]
need_y_train = y_train[:training_data_num]
mus, cov = predict(all_x, need_X_train, need_y_train, exponential_cov,
 ↪kernel_parameters, cholesky=cholesky, beta_inv=beta_inv)
sigmas = np.sqrt(np.diag(cov))
plot_gp(all_x, mus, np.sqrt(sigmas), need_X_train, need_y_train, true_y)
print("rmse = {0}".format( np.sqrt(mean_squared_error(mus, true_y))))
```

```
rmse = 0.23905184880329788
```



2.4 Part IV: Sampling

For this part, we implement the sample_cholesky function.

2.4.1 sampling from multivariate Gaussian

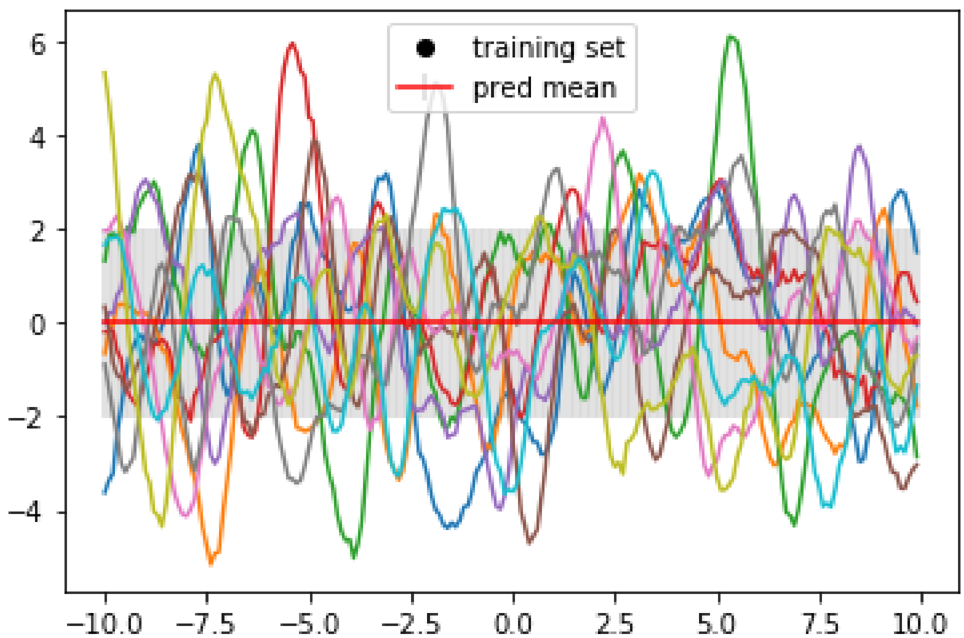
use property of multivariate Gaussian where if $z \sim N(0, I)$ then $x = \mu + Lz$ gives $x \sim N(\mu, LL^T)$ where $L = cholesky(LL^T)$

[22]:
```
def sample_cholesky(mu, cov, n_points, n_samples):
    """
    Function that performs sampling from multi-variate Gaussian using Cholesky␣
 ↪Decomposition
    @param mu: a numpy array of size n
    @param cov: a numpy matrix of size n*n
    @param n_points: how many points per sample
    @param n_samples: how many samples
    @return a numpy matrix with dimension (n_points, n_samples)
    """
    ############################################
    ### TODO: please implement this function ###
    ############################################
    return np.random.multivariate_normal(mus, cov, n_samples).T
    # OR
```

```
    # L = np.linalg.cholesky(cov)
    # z_samp = np.random.normal(size=(n_points, n_samples))
    # return mus.reshape(-1,1) + np.matmul(L, z_samp)
#    return np.zeros([n_points, n_samples])
```

Sample from prior

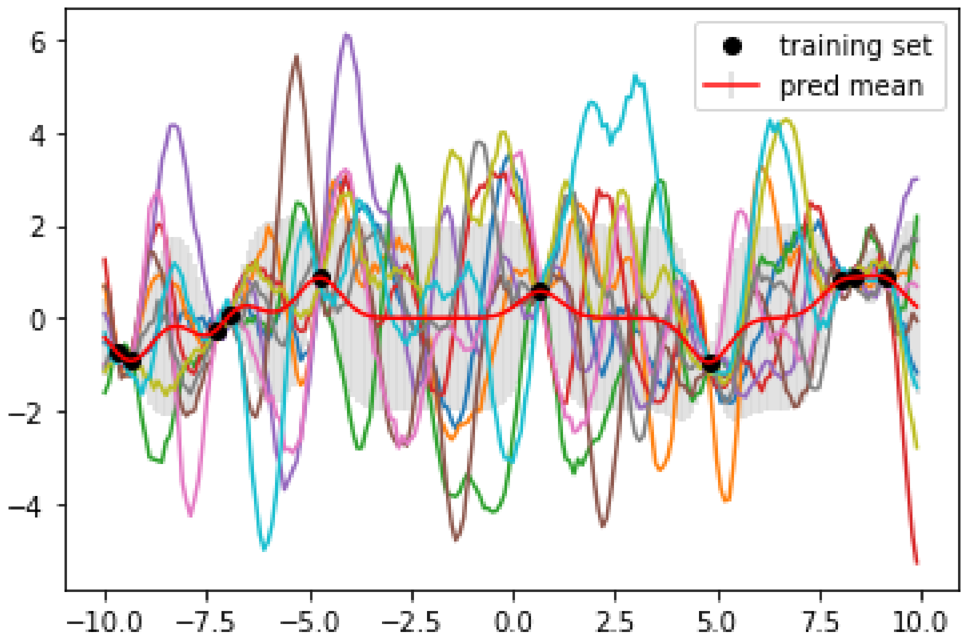
[23]:
```
training_data_num = 0
n_samples = 10
# fix mean and sigmas
mus, cov = predict(all_x, X_train[:training_data_num], y_train[:
 ↪training_data_num], exponential_cov,
                   kernel_parameters, cholesky=False, beta_inv=beta_inv)
sigmas = np.sqrt(np.diag(cov))

# sampling - using sample_cholesky
samples = sample_cholesky(mus, cov, len(all_x), n_samples)

# plot samples
plot_gp(all_x, mus, sigmas, X_train[:training_data_num], y_train[:
 ↪training_data_num], samples=samples)
```



Sample from posterior with 10 points

[24]:
```
training_data_num = 10
n_samples = 10
```

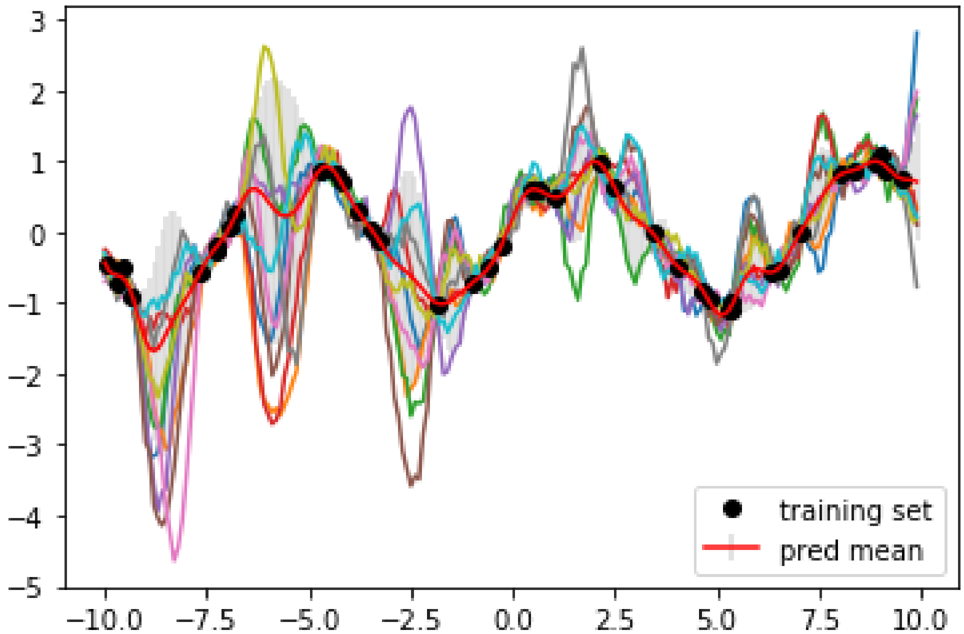
```
# fix mean and sigmas
mus, cov = predict(all_x, X_train[:training_data_num], y_train[:
 ↪training_data_num], exponential_cov, kernel_parameters, cholesky=False,␣
 ↪beta_inv=beta_inv)
sigmas = np.sqrt(np.diag(cov))

# sampling - using sample_cholesky
samples = sample_cholesky(mus, cov, len(all_x), n_samples)

# plot samples
plot_gp(all_x, mus, sigmas, X_train[:training_data_num], y_train[:
 ↪training_data_num], samples=samples)
```



Sample from posterior with 30 points

[25]:
```
training_data_num = 40
n_samples = 10
# fix mean and sigmas
mus, cov = predict(all_x, X_train[:training_data_num], y_train[:
 ↪training_data_num], exponential_cov,
                    kernel_parameters, cholesky=False, beta_inv=beta_inv)
sigmas = np.sqrt(np.diag(cov))

# sampling - using sample_cholesky
samples = sample_cholesky(mus, cov, len(all_x), n_samples)
```

```
# plot samples
plot_gp(all_x, mus, sigmas, X_train[:training_data_num], y_train[:
↪training_data_num], samples=samples)
```



2.4.2 What if observation noise is assumed to be 0

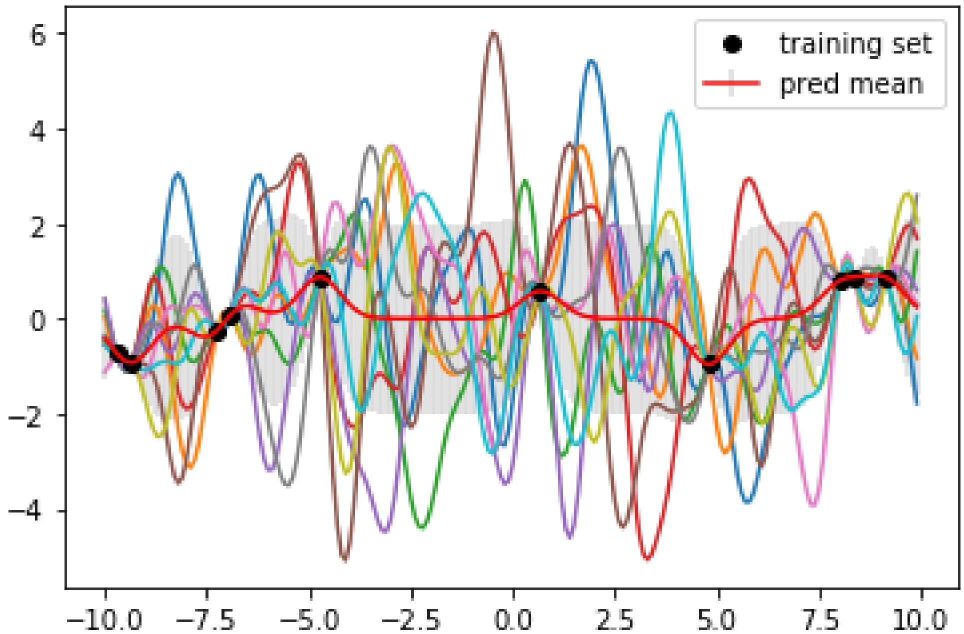
(this part is not graded)

[26]:
```
def is_pos_def(x):
    return np.all(np.linalg.eigvals(x) > 0)
```

[27]:
```
training_data_num = 10
n_samples = 10
# fix mean and sigmas
mus, cov = predict(all_x, X_train[:training_data_num], y_train[:
↪training_data_num], exponential_cov,
                   kernel_parameters, cholesky=True, beta_inv=0)
sigmas = np.sqrt(np.diag(cov))

print(is_pos_def(cov))

# sampling - using sample_cholesky
samples = sample_cholesky(mus, cov, len(all_x), n_samples)

# plot samples
```

```
plot_gp(all_x, mus, sigmas, X_train[:training_data_num], y_train[:
↪training_data_num], samples=samples)
```

```
False
```




```
[ ]:
```