EECS 553 HW8

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1 Problem 1

(a): To avoid confusion, I will still use the original notation. We first notice that :

$$\begin{aligned} P(y=k|\mathbf{x},\pi^{'}) &= \frac{P(\mathbf{x}|y=k,\pi^{'})P(y=k|\pi^{'})}{P(\mathbf{x}|\pi^{'})} && (1) \\ &= \frac{P(\mathbf{x}|y=k,\pi)\pi_k^{'}}{P(\mathbf{x}|\pi^{'})} && (2) \end{aligned}$$

because we know that $\phi_k(\mathbf{x})$ is unaffected by the shift. Now we also know that

$$P(\mathbf{x}|y=k,\pi) = \frac{P(y=k|\mathbf{x},\pi)P(\mathbf{x}|\pi)}{\pi_k}$$

Now if we substitute this term into (1), we will observe that

$$P(y=k|\mathbf{x},\pi^{'}) = P(y=k|\mathbf{x},\pi)\cdot\frac{\pi_k^{'}}{\pi_k}\cdot\frac{P(\mathbf{x}|\pi)}{P(\mathbf{x}|\pi^{'})}$$

Observe that

$$\begin{aligned} P(\mathbf{x}|\pi^{'}) &= \sum_{j=0}^{1} P(\mathbf{x}|y=j,\pi^{'})\pi_j^{'} && (3) \\ &= \sum_{j=0}^{1} P(\mathbf{x}|y=j,\pi)\pi_j^{'} \quad \text{(because } \phi_k(\mathbf{x}) \text{ is unaffected by shift)} && (4) \\ &= P(\mathbf{x}|\pi)\sum_{j=0}^{1}\frac{P(y=j|\mathbf{x},\pi)\pi_j^{'}}{\pi_j} && (5) \end{aligned}$$

Therefore, we finally conclude that

$$P(y=k|\mathbf{x},\pi^{'}) = \frac{\frac{\pi_k^{'}}{\pi_k}P(y=k|\mathbf{x},\pi)}{\frac{\pi_0^{'}}{\pi_0}P(y=0|\mathbf{x},\pi)+\frac{\pi_1^{'}}{\pi_1}P(y=1|\mathbf{x},\pi)}$$

which is exactly the same expression if we use the shorthand notation. This completes the proof.
(b) & (c): For the incomplete data likelihood function, we have that

$$\begin{aligned} l(\pi^{'}) &= \log p(\mathbb{X}|\pi^{'}) && (6) \\ &= \log\prod_{i=1}^{m}[\phi_1(\mathbf{x}_i)\pi^{'}+\phi_0(\mathbf{x}_i)(1-\pi^{'})] && (7) \\ &= \sum_{i=1}^{m}\log\left(\phi_1(\mathbf{x}_i)\pi^{'}+\phi_0(\mathbf{x}_i)(1-\pi^{'})\right) && (8) \end{aligned}$$

Now for the complete data log likelihood function, we have that

$$\log P(\mathbb{X}, \mathbb{Z}|\pi^{'}) = \log P(\mathbb{Z}|\mathbb{X}, \pi^{'}) + \log P(\mathbb{X}|\pi^{'})$$

Now we need to find $\log P(\mathbb{Z}|\mathbb{X}, \pi^{'})$, that is :

$$\log P(\mathbb{Z}|\mathbb{X}, \pi^{'}) = \sum_{i=1}^{m} y_i \log P(y_i = 1|\mathbb{X}, \pi^{'}) + (1 - y_i) \log P(y_i = 0|\mathbb{X}, \pi^{'})$$

Thus, combine the $\log P(\mathbb{Z}|\mathbb{X}, \pi^{'})$ and $\log P(\mathbb{X}|\pi^{'})$ will give us the full log-likelihood.

E-Step

Now to compute $Q(\pi^{'}; \pi^{'(t)})$, we observe that we need to compute that

$$E(y_i|\mathbb{X}, \pi^{'(t)}) = P^{(t)}(y = 1|\mathbb{X}, \pi^{'(t)})$$

that denote the randomness of $Q(\pi; \pi^{'(t)})$. We also notice that by Bayes rule, we have that

$$P(y_i = 1|\mathbb{X}, \pi^{'}) = \frac{\phi_1(\mathbf{x}_i)\pi^{'}}{(1 - \pi^{'})\phi_0(\mathbf{x}_i) + \pi^{'}\phi_1(\mathbf{x}_i)}$$

Thus, plug the above term into $Q(\pi^{'}; \pi^{'(t)})$ and after some simplification, we find that

$$\begin{aligned} Q(\pi^{'}; \pi^{'(t)}) = \sum_{i=1}^{m} & P^{(t)}(y_i = 1|\mathbb{X}, \pi^{'(t)}) \cdot [\log \phi_1(\mathbf{x}_i) + \log \pi^{'} - \log((1 - \pi^{'})\phi_0(\mathbf{x}_i) + \pi^{'}\phi_1(\mathbf{x}_i))] && (9) \\ & + (1 - P^{(t)}(y_i = 1|\mathbb{X}, \pi^{'(t)})) \cdot [\log \phi_0(\mathbf{x}_i) + \log(1 - \pi^{'}) - \log((1 - \pi^{'})\phi_0(\mathbf{x}_i) + \pi^{'}\phi_1(\mathbf{x}_i))] && (10) \\ & + \sum_{i=1}^{m} \log\left(\phi_1(\mathbf{x}_i)\pi^{'} + \phi_0(\mathbf{x}_i)(1 - \pi^{'})\right) && (11) \end{aligned}$$

M-Step

Now take derivative respect to $\pi^{'}$, we will finally simplify to the below expression that:

$$\frac{\partial Q}{\partial \pi^{'}} = \frac{1}{\pi^{'}(1 - \pi^{'})} \sum_{i=1}^{m} P^{(t)}(y_i = 1|\mathbf{x}_i, \pi^{'(t)}) - \frac{m}{1 - \pi^{'}} = 0$$

Thus, we can then conclude that the final M-step update reduces to:

$$\pi^{'(t+1)} = \frac{1}{m} \sum_{i=1}^{m} P^{(t)}(y_i = 1|\mathbf{x}_i, \pi^{'(t)})$$

where $P^{(t)}(y_i = 1|\mathbf{x}_i, \pi^{'(t)})$ is obtained after we replacing $\pi^{'}_k$ with $\pi^{'(t)}$ and $\mathbf{x}$ with $\mathbf{x}_i$. This completes part(b) and part(c).

(d) Please check the py and ipynb file I uploaded on canvas to see the code, or you can see it in the end of the file. The unadjust LR has accuracy of 0.83, the EM-adjusted LR has accuracy of 0.9, the accuracy of Clairvoyant adjusted LR is 0.9.

2 Problem 2

Given that $\epsilon_i \sim Laplacian(\beta)$, we conclude that $y_i \sim Laplacian(w^T x_i, \beta)$ that is

$$p(y_i) = \frac{\beta}{2} \exp(-\beta|y_i - w^T x_i|)$$

Thus, the likelihood can be written as

$$\begin{aligned} L(\mathbf{y}|w) &= \prod_{i=1}^{n} \frac{\beta}{2} \exp(-\beta|y_i - w^T x_i|) && (12) \\ &= \left(\frac{\beta}{2}\right)^n \exp\left(-\beta \sum_{i=1}^{n} |y_i - w^T x_i|\right) && (13) \end{aligned}$$

so the log-likelihood could be written as

$$l(w|\mathbf{y}) = -\beta \sum_{i=1}^{n} |y_i - w^T x_i| + n \log\left(\frac{\beta}{2}\right)$$

Thus, to maximize the likelihood and find w to achieve this, it is same to solve the minimization problem that

$$\min_{w} \frac{1}{n} \sum_{i=1}^{n} |y_i - w^T x_i| - \frac{1}{\beta} \log\left(\frac{\beta}{2}\right)$$

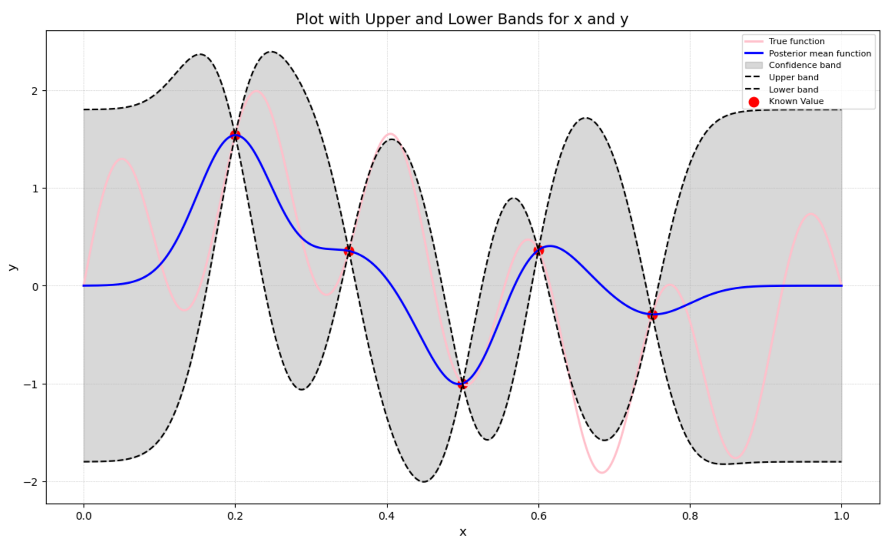
and notice the last term is unrelated to w, therefore, it is same to solve problem of empirical risk minimization that

$$\min_{w} \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i))$$

that the loss function is $L(y, t) = |y - t|$ and $f(x_i) = w^T x_i$. This completes the proof.

3 Problem 3

(a): please check the below picture.



(b): Please check the code I uploaded in canvas, or at the end of the page. The next value of x that going to evaluate is 0.2474.

(c): The next point that PI method suggest to evaluate is 0.2004.

(d): The next point that EI method suggest to evaluate is 0.234. Notice here I did not use the exact formula for calculating expectation, instead, I sample points from the normal distribution and then average them to get the EI for each point, which make sense by law of large number.(Monte-Carlo)

(e): All three method will approximately converge to 0.2276 with function value of 1.99. The detail of algorithm, number of iteration, epsilon can be seen in the below code I attached.

In [1]:
```
import numpy as np
import sklearn
import sklearn.linear_model as sk_linear
import matplotlib.pyplot as plt
from scipy.stats import norm
```

Problem 1 Code

In [2]:
```
def load_data():
    # Label 0 are pullovers, label 1 are coats
    # X matrices are shape (num samples, num pixels)
    data = np.load("p3f_data.npy", allow_pickle=True).item()
    X_train = data["X_train"] # (1500, 784)
    X_val = data["X_val"]     # (1400, 784)
    X_test = data["X_test"]   # (700, 784)
    y_train = data["y_train"] # (1500,)
    y_val = data["y_val"]     # (1400,)
    y_test = data["y_test"]   # (700,)
    return X_train, X_val, X_test, y_train, y_val, y_test
```

In [3]:
```
def prediction_metrics(y_true, y_pred):
    acc = sklearn.metrics.accuracy_score(y_true, y_pred)
    f1 = sklearn.metrics.f1_score(y_true, y_pred)
    prec = sklearn.metrics.precision_score(y_true, y_pred)
    recall = sklearn.metrics.recall_score(y_true, y_pred)
    return acc, f1, prec, recall
```

In [4]:
```
def EM_adjust_posterior(classifier, X_train, y_train, train_prior, X_val):
    # classifier is an sklearn.linear_model.LogisticRegression class
    # TODO: complete this function for estimating class priors after
    # the label shift.
    # X_val contains sample feature vectors from after the shift.
    # Hint: the method LogisticRegression.predict_proba()
    # may be useful.
    pred_prob = classifier.predict_proba(X_val)
    new_prior = train_prior.copy()

    for t in range(100):
        prob = []
        for i in range(X_val.shape[0]):
            prob_1 = ((new_prior[1]/train_prior[1]) * pred_prob[i][1]) / ((new_p
            prob.append(prob_1)

        new_prior[1] = sum(prob)/len(prob)
        new_prior[0] = 1 - new_prior[1]

    return new_prior
```

In [5]:
```
def update_predictions(classifier, train_prior, new_prior, X_test):
    # TODO: complete this function for updating the predictions
    # on X_test using new_prior, an estimate of the after-shift priors.
    # This function should return class predictions, not class probabilities.

    # default return so code runs
    pred_origin_prob = classifier.predict_proba(X_test)
    after_prob = []
```

```
    for i in range(X_test.shape[0]):
        prob_1 = ((new_prior[1]/train_prior[1]) * pred_origin_prob[i][1]) / ((ne
        after_prob.append(prob_1)

    predicted_labels = [1 if prob >= 0.5 else 0 for prob in after_prob]

    return np.array(predicted_labels)
```

In [6]:
```
if __name__ == "__main__":
    X_train, X_val, X_test, y_train, y_val, y_test = load_data()

    classifier = sk_linear.LogisticRegression(max_iter=500)
    classifier.fit(X_train, y_train)

    pi0 = (y_train == 0).mean()
    pi1 = (y_train == 1).mean()
    train_prior = np.asarray([pi0, pi1])

    y_pred_unadjust = classifier.predict(X_test)
    acc, f1, prec, recall = prediction_metrics(y_test, y_pred_unadjust)
    print(f"Unadjusted LR: Accuracy: {acc:.2f}, F1-score: {f1:.2f}, Precision: {

    EM_prior = EM_adjust_posterior(classifier, X_train, y_train, train_prior, X_
    y_pred_EM = update_predictions(classifier, train_prior, EM_prior, X_test)

    acc, f1, prec, recall = prediction_metrics(y_test, y_pred_EM)
    print(f"EM-adjusted LR: Accuracy: {acc:.2f}, F1-score: {f1:.2f}, Precision:

    test_ML_priors = np.asarray([(y_test==0).mean(), (y_test==1).mean()])
    y_pred_ML = update_predictions(classifier, train_prior, test_ML_priors, X_te

    acc, f1, prec, recall = prediction_metrics(y_test, y_pred_ML)
    print(f"CLairvoyant (ML) adjusted LR: Accuracy: {acc:.2f}, F1-score: {f1:.2f
```

```
Unadjusted LR: Accuracy: 0.83, F1-score: 0.59, Precision: 0.46, Recall: 0.85
EM-adjusted LR: Accuracy: 0.90, F1-score: 0.65, Precision: 0.65, Recall: 0.64
CLairvoyant (ML) adjusted LR: Accuracy: 0.90, F1-score: 0.63, Precision: 0.65, Re
call: 0.60
```

Problem 3

(a)

In [2]:
```
## define the true function
def true_fun(x):
    values = []
    for i in range(len(x)):
        y = np.sin(2 * np.pi * x[i]) + np.sin(11 * np.pi * x[i])
        values.append(y)

    return values
```

In [3]:
```
x_train = [0.2, 0.35, 0.5, 0.6, 0.75]
y_train = true_fun(x_train)
y_train
```

Out[3]:
```
[1.5388417685876266,
 0.35502649463539787,
 -0.9999999999999999,
 0.36327126400268195,
 -0.2928932188134551]
```

In [4]:
```
## Now I need to define the kernel matrix
def gaussian_kernel_matrix(x1, x2, sigma_k, gamma):
    K = np.zeros((len(x1), len(x2)))
    for i in range(len(x1)):
        for j in range(len(x2)):
            K[i, j] = sigma_k**2 * np.exp(-gamma * (x1[i] - x2[j]) ** 2)

    return K
```

In [5]:
```
K_train = gaussian_kernel_matrix(x_train, x_train, sigma_k = 0.9, gamma = 200)
K_train
```

Out[5]:
```
array([[8.10000000e-01, 8.99828720e-03, 1.23362836e-08, 1.02579741e-14,
        4.30198472e-27],
       [8.99828720e-03, 8.10000000e-01, 8.99828720e-03, 3.01858907e-06,
        1.02579741e-14],
       [1.23362836e-08, 8.99828720e-03, 8.10000000e-01, 1.09621579e-01,
        3.01858907e-06],
       [1.02579741e-14, 3.01858907e-06, 1.09621579e-01, 8.10000000e-01,
        8.99828720e-03],
       [4.30198472e-27, 1.02579741e-14, 3.01858907e-06, 8.99828720e-03,
        8.10000000e-01]])
```

In [6]:
```
def sigma_eI(sigma_e, row_num, col_num):
    I = np.eye(row_num)
    return sigma_e ** 2 * I
```

In [7]:
```
row_num_K, col_num_K = K_train.shape
```

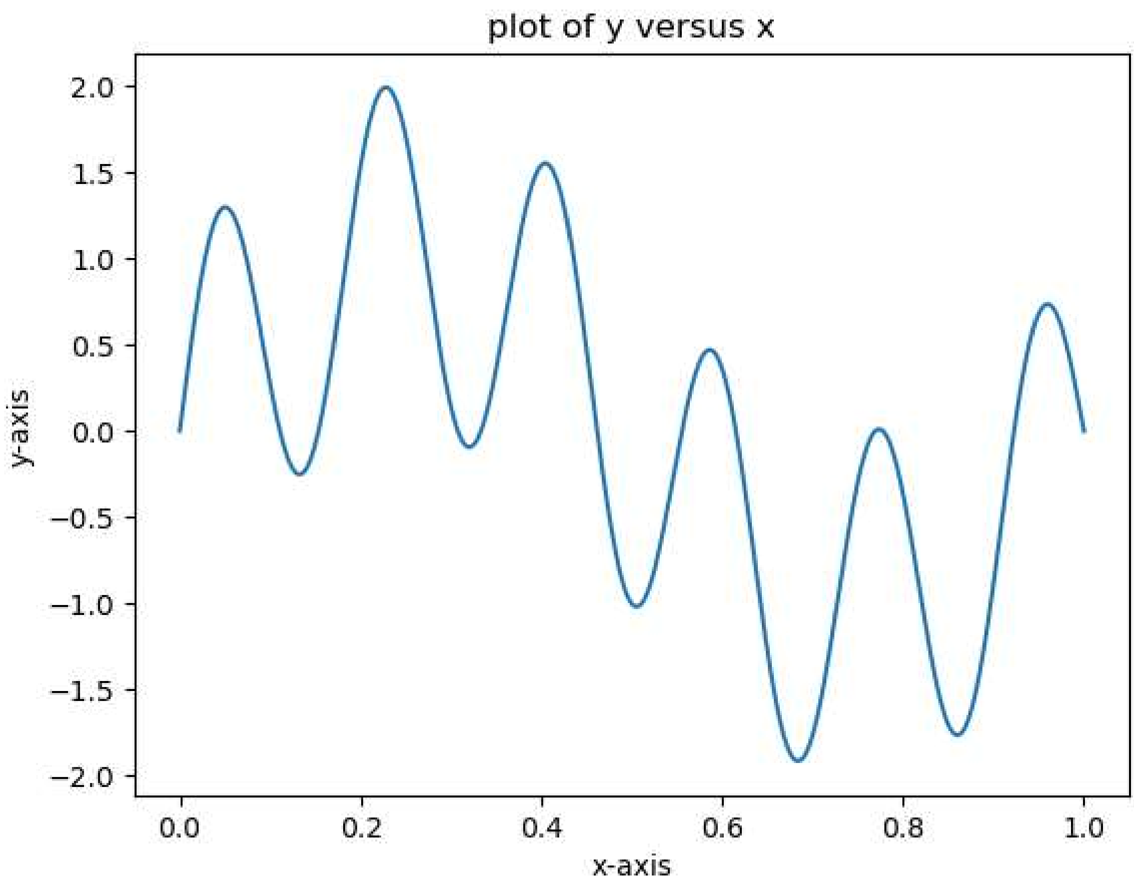
In [8]:
```
sigma_eI_train = sigma_eI(1e-10, row_num_K, col_num_K)
```

Now I am going to construct a sequence of x's

In [87]:
```
x_points = np.linspace(0, 1, 15000)
y_points = true_fun(x_points)
```

In [88]:
```
## first visualize y versus x
plt.plot(x_points, y_points)
plt.xlabel("x-axis")
plt.ylabel("y-axis")
plt.title("plot of y versus x")
```

Out[88]:
```
Text(0.5, 1.0, 'plot of y versus x')
```



I will first compute the posterior mean function

In [89]:
```
x_1 = gaussian_kernel_matrix([x_points[0]], x_train, 0.9, 200)
```

In [90]:
```
def compute_mean_posterior(x, x_train, y_train):
    posterior_mean = []
    for i in range(len(x)):
        k_x = gaussian_kernel_matrix([x[i]], x_train, 0.9, 200)
        inv_K_sigma_e_I = np.linalg.inv(K_train + sigma_eI_train)
        f_x = np.dot(k_x, np.dot(inv_K_sigma_e_I, y_train))

        posterior_mean.append(f_x.item(0))

    return posterior_mean
```

In [91]:
```
def compute_band_sigma(x, x_train):
    sigma_x = []
    for i in range(len(x)):
        k_xx = 0.9**2 * np.exp(- 200 * (x[i] - x[i]) ** 2)
        k_x = gaussian_kernel_matrix([x[i]], x_train, 0.9, 200)
        inv_K_sigma_e_I = np.linalg.inv(K_train + sigma_eI_train)
        value = k_xx - np.dot(k_x, np.dot(inv_K_sigma_e_I, k_x.T))

        sigma_x.append(np.sqrt(value.item(0)))

    return sigma_x
```

In [92]:
```
x_posterior_mean = compute_mean_posterior(x_points, x_train, y_train)
x_band_sigma = compute_band_sigma(x_points, x_train)
```

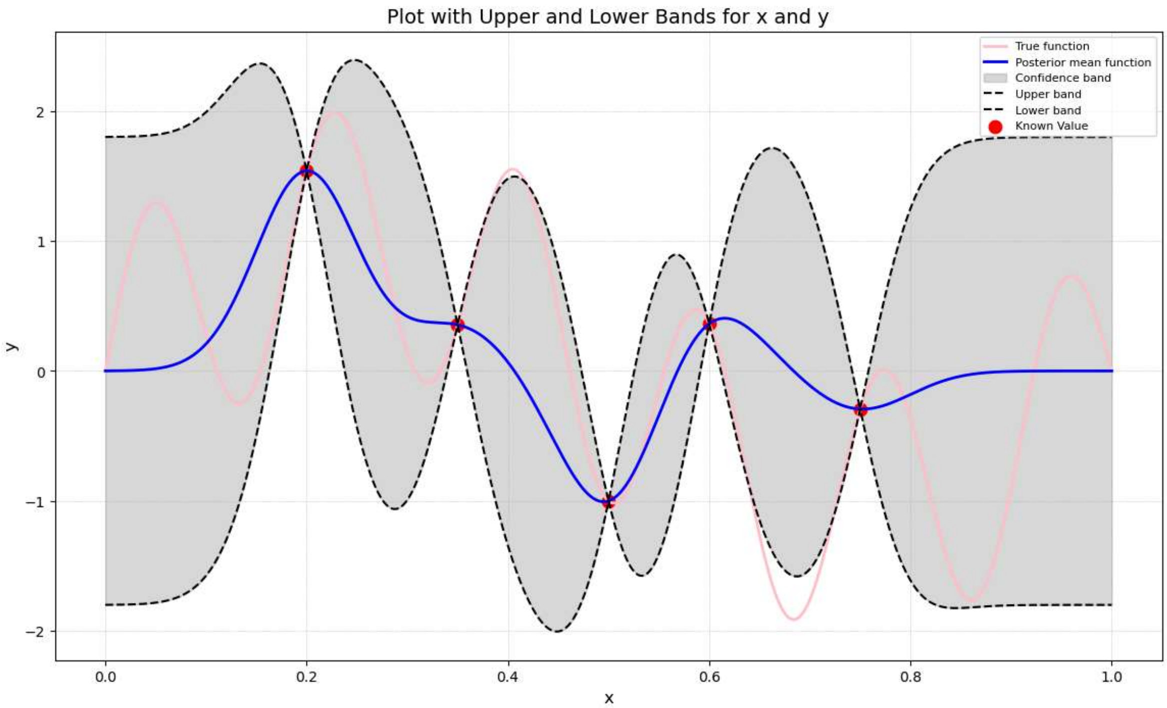
In [93]:
```
### define the upper band
upper_band = np.array(x_posterior_mean) + 2 * np.array(x_band_sigma)
upper_band = upper_band.tolist()

### define the lower band
lower_band = np.array(x_posterior_mean) - 2 * np.array(x_band_sigma)
lower_band = lower_band.tolist()
```

In [94]:
```
max(upper_band)
```

Out[94]:
```
2.3925129058814223
```

We can now start the drawing

In [95]:
```
plt.figure(figsize=(14, 8))
plt.plot(x_points, y_points, color="pink", linestyle="-", linewidth=2, label="Tr

# Plot the posterior mean function
plt.plot(x_points, x_posterior_mean, color="blue", linestyle="-", linewidth=2, l

# Plot the confidence band as a filled area between upper and lower bands
plt.fill_between(x_points, lower_band, upper_band, color="gray", alpha=0.3, labe

# Plot the upper and lower band lines
plt.plot(x_points, upper_band, color="black", linestyle="--", linewidth=1.5, lab
plt.plot(x_points, lower_band, color="black", linestyle="--", linewidth=1.5, lab

plt.xlabel("x", fontsize=12)
plt.ylabel("y", fontsize=12)
plt.title("Plot with Upper and Lower Bands for x and y", fontsize=14)

plt.scatter(x_train, y_train, color = "red", marker = "o", s = 80, label = "Know

plt.grid(True, which='both', linestyle=':', linewidth=0.5)
plt.legend(loc="best", fontsize=8)

plt.show()
```



(b)

In [96]:
```
max_ucb_index = upper_band.index(max(upper_band))
x_ucb_next = x_points[max_ucb_index]
```

In [97]:
```
### Get the next value of x going to evalutate the function
print("The next value of x going to evaluate the function is:", x_ucb_next)
```

```
The next value of x going to evaluate the function is: 0.2474831655443696
```

In [99]:
```
y_ucb_next = y_points[max_ucb_index]
print("The next value of y_ucb_next is:", y_ucb_next)
```

```
The next value of y_ucb_next is: 1.7657323843674873
```

Thus, the next value of x we are going to evaluate the function is 0.2474.

(c)

In [100...
```
max_pi_index = x_posterior_mean.index(max(x_posterior_mean))
x_star = x_points[max_pi_index]
print("The point with highest function value is:", x_star)
```

```
The point with highest function value is: 0.20041336089072603
```

In [104...
```
max_pi_index
```

Out[104...
```
3006
```

In [105...
```
### Determine the point that with highest probability of f(x) will exceed f(x*)
def PI_method(list_x, x_posterior_mean_list, x_band_sigma_list):

    f_x_star = max(x_posterior_mean_list)

    # Calculate PI for each point in list_x
    prob_exceed_x_star = []
```

```
    for i in range(len(list_x)):
        # Calculate the probability of improvement
        prob_exceed = 1 - norm.cdf((f_x_star - x_posterior_mean_list[i]) / x_ban
        prob_exceed_x_star.append(prob_exceed)

    # Find the index of the point with the highest PI value
    max_pi_index_after = prob_exceed_x_star.index(max(prob_exceed_x_star))

    return list_x[max_pi_index_after], max_pi_index_after
```

In [109…

```
x_pi_next, index  = PI_method(x_points, x_posterior_mean, x_band_sigma)
print("The point with highest probability of f(x) will exceed f(x*) using PI met
```

```
The point with highest probability of f(x) will exceed f(x*) using PI method is :
0.20041336089072603
```

In [110…

```
y_pi_next = y_points[index]
print("The next value of y_ucb_next is:", y_pi_next)
```

```
The next value of y_ucb_next is: 1.5511373710809984
```

(d)

I will use sampling method to simulate the EI, that I will not get a precise formula for calculating EI

In [117…

```
def EI_method(list_x, x_posterior_mean_list, x_band_sigma_list):

    f_x_star = max(x_posterior_mean_list)

    EI_exceed_x_star = []
    for i in range(len(list_x)):
        mean_x = x_posterior_mean_list[i] - f_x_star
        sigma_x = x_band_sigma_list[i]
        ### sampling from the distribution
        samples = np.random.normal(loc = mean_x, scale= sigma_x, size = 20000).t
        ### calculate E(max(0, f(x) - f(x_star)))
        samples_alter = [sample if sample > 0 else 0 for sample in samples]
        EI_value = sum(samples_alter)/len(samples_alter)

        ### append to the emtpy list
        EI_exceed_x_star.append(EI_value)

    max_EI_index_after = EI_exceed_x_star.index(max(EI_exceed_x_star))
    return list_x[max_EI_index_after], max_EI_index_after
```

In [118…

```
x_ei_next, index = EI_method(x_points, x_posterior_mean, x_band_sigma)
print("The point with highest EI is :", x_ei_next)
```

```
The point with highest EI is : 0.23401560104006933
```

In [119…

```
y_ei_next = y_points[index]
print("The next value of y_EI_next is:", y_ei_next)
```

```
The next value of y_EI_next is: 1.967935009047609
```

(e)

In [ ]:
```
### Algorithm for UCB method
def UCB_algorithm(list_x, list_y, x_train, y_train, sigma_e, sigma_k, gamma, num
    result_x = x_train.copy()
    result_y = y_train.copy()

    result_x.append(x_ucb_next)
    result_y.append(y_ucb_next)

    error = 1
    iter = 0

    while iter < num_iter and error > epsilon:

        ### calculating the related matrix
        K_train = np.zeros((len(result_x), len(result_x)))
        for i in range(len(result_x)):
            for j in range(len(result_x)):
                K_train[i, j] = sigma_k ** 2 * np.exp(-gamma * (result_x[i] - re

        sigma_eI = sigma_e ** 2 * np.eye(K_train.shape[0])
        inv_K_sigma_e_I = np.linalg.inv(K_train + sigma_eI)

        ### calculate the posterior mean
        posterior_mean = []
        sigma_x = []
        for i in range(len(list_x)):
            k_x = gaussian_kernel_matrix([list_x[i]], result_x, sigma_k, gamma)
            k_xx = sigma_k ** 2
            f_x = np.dot(k_x, np.dot(inv_K_sigma_e_I, result_y))
            sigma = k_xx - np.dot(k_x, np.dot(inv_K_sigma_e_I, k_x.T))

            posterior_mean.append(f_x.item(0))
            sigma_x.append(np.sqrt(sigma.item(0)))

        ### Now calculating the upper band
        upper_band = np.array(posterior_mean) + 2 * np.array(sigma_x)
        upper_band = upper_band.tolist()

        max_ucb_index = upper_band.index(max(upper_band))
        x_next = list_x[max_ucb_index]

        ### now compute y_next
        # k_x_next = gaussian_kernel_matrix([x_next], result_x, sigma_k, gamma)
        # f_x_next = np.dot(k_x_next, np.dot(inv_K_sigma_e_I, result_y))
        # y_next = f_x_next.item(0)

        y_next = list_y[max_ucb_index]

        error = abs(x_next - result_x[-1])
        iter = iter + 1

        result_x.append(x_next)
        result_y.append(y_next)


    return result_x[-1], result_y[-1], iter
```

In [103…
```
UCB_algorithm(x_points, y_points, x_train, y_train, 1e-10, 0.9, 200, 30, 1e-3)
```

```
C:\Users\16343\AppData\Local\Temp\ipykernel_18764\3433594492.py:33: RuntimeWarnin
g: invalid value encountered in sqrt
  sigma_x.append(np.sqrt(sigma.item(0)))
0.282352156810454 0.6528976697204256
0.22594839655977064 1.9875559229645572
0.22948196546436428 1.9887885739534292
0.2280152010134009 1.9901454319170737
0.22768184545636375 1.9900840593941038
```

Out[103…

```
(0.22768184545636375, 1.9900840593941038, 5)
```

Thus, we conclude that the UCB algorithm will finally reach x at 0.2276 and the maximized function value is 1.99, with 5 iterations using epsilon of 1e-3.

In [115…

```python
### Algorithm for PI method
def PI_algorithm(list_x, list_y, x_train, y_train, sigma_e, sigma_k, gamma, num_
    result_x = x_train.copy()
    result_y = y_train.copy()

    result_x.append(x_pi_next)
    result_y.append(y_pi_next)

    error = 1
    iter = 0

    while iter < num_iter and error > epsilon:
        ### calculating the related matrix
        K_train = np.zeros((len(result_x), len(result_x)))
        for i in range(len(result_x)):
            for j in range(len(result_x)):
                K_train[i, j] = sigma_k ** 2 * np.exp(-gamma * (result_x[i] - re

        sigma_eI = sigma_e * np.eye(K_train.shape[0])
        inv_K_sigma_e_I = np.linalg.inv(K_train + sigma_eI)

        ### calculate the posterior mean
        posterior_mean = []
        sigma_x = []
        for i in range(len(list_x)):
            k_x = gaussian_kernel_matrix([list_x[i]], result_x, sigma_k, gamma)
            k_xx = sigma_k ** 2
            f_x = np.dot(k_x, np.dot(inv_K_sigma_e_I, result_y))
            sigma = k_xx - np.dot(k_x, np.dot(inv_K_sigma_e_I, k_x.T))

            posterior_mean.append(f_x.item(0))
            sigma_x.append(np.sqrt(sigma.item(0)))


        f_x_star = max(posterior_mean)
        prob_exceed_x_star = []

        for i in range(len(list_x)):
            prob_exceed = 1 - norm.cdf((f_x_star - posterior_mean[i]) / sigma_x[
            prob_exceed_x_star.append(prob_exceed)

        max_pi_index_after = prob_exceed_x_star.index(max(prob_exceed_x_star))
        x_next = list_x[max_pi_index_after]

        ## calculating y_next
```

```
        # k_x_next = gaussian_kernel_matrix([x_next], result_x, sigma_k, gamma)
        # f_x_next = np.dot(k_x_next, np.dot(inv_K_sigma_e_I, result_y))
        y_next = list_y[max_pi_index_after]

        error = abs(x_next - result_x[-1])
        iter = iter + 1

        result_x.append(x_next)
        result_y.append(y_next)

    return result_x[-1], result_y[-1], iter
```

In [116…

```
PI_algorithm(x_points, y_points, x_train, y_train, 1e-10, 0.9, 200, 20, 1e-3)
```

```
C:\Users\16343\AppData\Local\Temp\ipykernel_18764\1883482178.py:32: RuntimeWarnin
g: invalid value encountered in sqrt
  sigma_x.append(np.sqrt(sigma.item(0)))
```

Out[116…

```
(0.22794852990199346, 1.990144119333211, 3)
```

In [124…

```
def EI_algorithm(list_x, list_y, x_train, y_train, sigma_e, sigma_k, gamma, num_
    result_x = x_train.copy()
    result_y = y_train.copy()

    result_x.append(x_ei_next)
    result_y.append(y_ei_next)

    error = 1
    iter = 0

    while iter < num_iter and error > epsilon:
        ### calculating the related matrix
        K_train = np.zeros((len(result_x), len(result_x)))
        for i in range(len(result_x)):
            for j in range(len(result_x)):
                K_train[i, j] = sigma_k ** 2 * np.exp(-gamma * (result_x[i] - re

        sigma_eI = sigma_e * np.eye(K_train.shape[0])
        inv_K_sigma_e_I = np.linalg.inv(K_train + sigma_eI)

        ### calculate the posterior mean
        posterior_mean = []
        sigma_x = []
        for i in range(len(list_x)):
            k_x = gaussian_kernel_matrix([list_x[i]], result_x, sigma_k, gamma)
            k_xx = sigma_k ** 2
            f_x = np.dot(k_x, np.dot(inv_K_sigma_e_I, result_y))
            sigma = k_xx - np.dot(k_x, np.dot(inv_K_sigma_e_I, k_x.T))

            posterior_mean.append(f_x.item(0))
            sigma_x.append(np.sqrt(sigma.item(0)))

        f_x_star = max(posterior_mean)

        EI_exceed_x_star = []
        for i in range(len(list_x)):
```

```
            mean_x = posterior_mean[i] - f_x_star
            sigma_x1 = sigma_x[i]
            samples = np.random.normal(loc = mean_x, scale= sigma_x1, size = 20(
            samples_alter = [sample if sample > 0 else 0 for sample in samples]
            EI_value = sum(samples_alter)/len(samples_alter)

            EI_exceed_x_star.append(EI_value)

        max_EI_x_after = EI_exceed_x_star.index(max(EI_exceed_x_star))
        x_next = list_x[max_EI_x_after]

        # ## calculating y_next
        # k_x_next = gaussian_kernel_matrix([x_next], result_x, sigma_k, gamma)
        # f_x_next = np.dot(k_x_next, np.dot(inv_K_sigma_e_I, result_y))
        # y_next = f_x_next.item(0)

        # error = abs(x_next - result_x[-1])
        # iter = iter + 1

        # result_x.append(x_next)
        # result_y.append(y_next)
        y_next = list_y[max_EI_x_after]
        print(x_next)
        print(y_next)

        error = abs(x_next - result_x[-1])
        iter = iter + 1

        result_x.append(x_next)
        result_y.append(y_next)

    return result_x[-1], result_y[-1], iter
```

In [126…

```
EI_algorithm(x_points, y_points, x_train, y_train, 1e-10, 0.9, 200, 15, 1e-3)
```

```
0.2648843256217081
1.2633567720212657
0.22648176545103008
1.988728408984246
0.9849323288219214
0.4029570399788028
0.8775918394559638
-1.5814442557226136
0.01946796453096873
0.7451665531930954
0.08647243149543303
0.6697026903238498
0.6763117541169411
-1.8766677178766764
0.41202746849789984
1.5198830503593794
0.8015867724514968
-0.4053667808506922
0.22814854323621575
1.9901316161318523
```

```
C:\Users\16343\AppData\Local\Temp\ipykernel_18764\2329107945.py:31: RuntimeWarnin
g: invalid value encountered in sqrt
  sigma_x.append(np.sqrt(sigma.item(0)))
```

```
0.4382292152810187
0.9128895340318135
0.5526368424561637
-0.07906893773473087
0.9387959197279818
0.48036003692442064
0.22808187212480832
1.9901412640773704
0.2278151876791786
1.9901250517647835
```

Out[126…

```
(0.2278151876791786, 1.9901250517647835, 15)
```