Sheet#04 Proposed Solution MLPH_W24

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November 17, 2024

1 Sheet 5

1.1 1 Bayes

The desired probability

$$p(\text{gamma ray}|\text{target direction})$$

is given by Bayes' theorem, stating that

$$p(A|B) = \frac{p(B|A) \cdot p(A)}{p(B)}.$$

Namely,

$$p(\text{gamma ray}|\text{target direction}) = \frac{p(\text{target direction}|\text{gamma ray}) \cdot p(\text{gamma ray})}{p(\text{target direction})}$$

$$= \frac{p(\text{target direction}|\text{gamma ray}) \cdot p(\text{gamma ray})}{p(\text{target direction } \cap \text{ background}) + p(\text{target direction } \cap \text{ gamma ray})}$$

$$= \frac{p(\text{target direction}|\text{gamma ray}) \cdot p(\text{gamma ray})}{p(\text{target direction}|\text{background}) \cdot p(\text{background}) + p(\text{target direction}|\text{gamma ray}) \cdot p(\text{gamma ray})}$$

$$= \frac{0.95 \cdot 0.1}{0.1 \cdot 0.9 + 0.95 \cdot 0.1} = 0.5\overline{13}.$$

We used that the probability of the intersection is given by $p(A \cap B) = p(A|B) \cdot p(B)$.

1.2 2 Bayes Classifiers

(a)

The optimal Bayes classifier $f(x)$ minimizes the risk $R(f)$ given evidence x:

$$f = \arg\min_f R(f) = \arg\min_f \mathbb{E}_X \mathbb{E}_{Y|X} \, L(Y = y|f(X = x))$$

$$= \arg\min_f \mathbb{E}_X \sum_{y \in \{0,1\}} L(y, f(x)) P(y|x)$$

The expected values are given by

$$L(0,0)P(y = 0 \mid x) + L(1,0)P(y = 1 \mid x) = 10 \cdot P(y = 1 \mid x) = 10 \cdot P(y = 1 \mid x)$$

and

$$L(0,1)P(y=0 \mid x) + L(1,1)P(y=1 \mid x) = 1 \cdot P(y=0|x)$$

The decision boundary is given by

$$10P(y=1|x) \leq P(y=0|x) = 1 - P(y=1|x) \implies P(y=1|x) \geq \frac{1}{11}$$

such that the estimator can be stated as

$$f(x) = \begin{cases} 0 & \text{if } P(y=1|x) < 1/11 \\ 1 & \text{if } P(y=1|x) \geq 1/11 \end{cases}.$$

Using this estimator could be useful when false negatives are much more costly than false positives, e.g. malignant cancer detection.

(b)

The derivation is identical to the k-class 0-1-loss with the exception of the added rejection risk:

For all $f(x) \in \{1, \dots, k\}$:

$$\mathbb{E}_{Y|X} L(y, \hat{y} = f(x)|x) = 1 - P(f(x)|x).$$

For $f(x) = 0$:

$$\mathbb{E}_{Y|X} L(y, \hat{y} = f(x)|x) = \alpha$$

The optimal classifier minimizes the risk, which means that it prefers to reject a classification if the class with the highest posterior fails to exceed the bound $1 - \alpha$:

$$P_{\max}(f(x)|x) < 1 - \alpha \implies \text{reject}$$

When the posterior probability of all classes are approximately equal, one might set $\alpha \geq (k-1)/k - \epsilon$ where $\epsilon > 0$ is some safety term in order to only allow classifications when the classifier is truly confident.

1.3 3

QDA ### (a)

[1]:
```
import numpy as np
from matplotlib import pyplot as plt
```

[2]:
```
pts = np.load('data/data1d.npy')
labels = np.load('data/labels1d.npy')
pts.shape, labels.shape
```

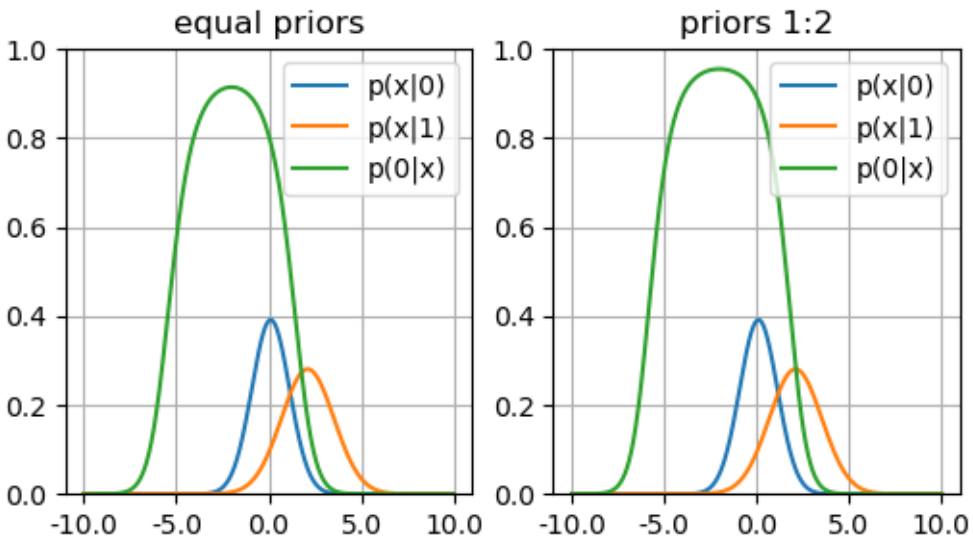
[2]:
```
((300,), (300,))
```

[3]:
```
mu = []
sigma = []
```

```
for label in sorted(np.unique(labels).astype(int)):
    mask = labels == label
    selection = pts[mask]
    mu.append(selection.sum()/len(selection))
    sigma.append(
        (
            (selection**2).sum()/len(selection) - mu[-1]**2
        )**0.5
    )
```

1.3.1 (b)

[4]:
```
def normal1d(x, mu, sigma):
    return (2*3.14159265*sigma**2)**-0.5 * np.exp( - (x-mu)**2 / (2*sigma**2))

fig, axes = plt.subplots(1,2, figsize=(6,3))
axes = axes.flatten()
x = np.linspace(-10, 10, 2001)
y0 = normal1d(x, mu[0], sigma[0])
y1 = normal1d(x, mu[1], sigma[1])
prior0 = 1 # arbitrary scaling cancels out in fraction
prior1 = 1
p1 = y0*prior0/(y0*prior0 + y1 * prior1)
axes[0].plot(y0, label="p(x|0)")
axes[0].plot(y1, label="p(x|1)")
axes[0].plot(p1, label="p(0|x)")
axes[0].set_title("equal priors")
axes[0].set_xticks(np.linspace(0, 2000,5), np.linspace(-10, 10, 5))
prior0 = 2
prior1 = 1
p1 = y0*prior0/(y0*prior0 + y1 * prior1)
axes[1].plot(y0, label="p(x|0)")
axes[1].plot(y1, label="p(x|1)")
axes[1].plot(p1, label="p(0|x)")
axes[1].set_title("priors 1:2")
axes[1].set_xticks(np.linspace(0, 2000,5), np.linspace(-10, 10, 5))
axes[0].grid()
axes[1].grid()
axes[0].set_ylim(0, 1)
axes[1].set_ylim(0, 1)
axes[0].legend()
axes[1].legend();
```



We observe that a higher prior of class 0 indeed changes the posterior distribution of that class. The resulting posterior distribution favors class 0 but is still symmetric.

1.4 4 Trees and Random Forests

(a)

1. Parent node impurity:

- $H_{P,\text{Gini}} = 1 - 2 * \frac{400}{800}^2 = 1/2$
- $H_{P,\text{Entropy}} = -2 * \frac{400}{800} \log_2 \frac{400}{800} = 1$

3. Misclassification error:

- $\text{E} = 1 - \max_c p(c|\text{node})$
- $E_{A1} = E_{A2} = 1 - \frac{300}{300+100} = 1/4$
- $E_{B1} = 1 - \frac{200}{200+0} = 0$
- $E_{B2} = 1 - \frac{400}{200+400} = 1/3$

3. Gini

- $H_{A1} = H_{A2} = 1 - \frac{300}{400}^2 - \frac{100}{400}^2 = 6/16$
- $H_{B1} = 1 - \frac{200}{200}^2 = 0$
- $H_{B2} = 1 - \frac{200}{600}^2 - \frac{400}{600}^2 = 4/9$

4. Entropy

- $H_{A1} = H_{A2} = -\frac{100}{400} \log_2 \frac{100}{400} - \frac{300}{400} \log_2 \frac{300}{400} \approx 0.81$
- $H_{B1} = 0$
- $H_{B2} = -\frac{200}{600} \log_2 \frac{200}{600} - \frac{400}{600} \log_2 \frac{400}{600} \approx 0.92$

The resulting uncertainty decreases are * Gini, A: $\Delta H_A = \frac{400}{800}(H_{A1}+H_{A2}) - H_{P,\text{Gini}} = \frac{1 \cdot 2 \cdot 6}{2 \cdot 16} - 8/16 =$

$-1/8$ * Gini, B: $\Delta H_B = \frac{200}{800} H_{B1} + \frac{600}{800} H_{B2} - H_{P,\text{Gini}} = \frac{3 \cdot 4}{4 \cdot 9} - 1/2 = -1/6 < -1/8$ * Entropy, A: $\Delta H_A = -0.19$ $\Delta H_B = -0.31 < 0.19$ Thus, both uncertainty criteria prefer split B.

(b)

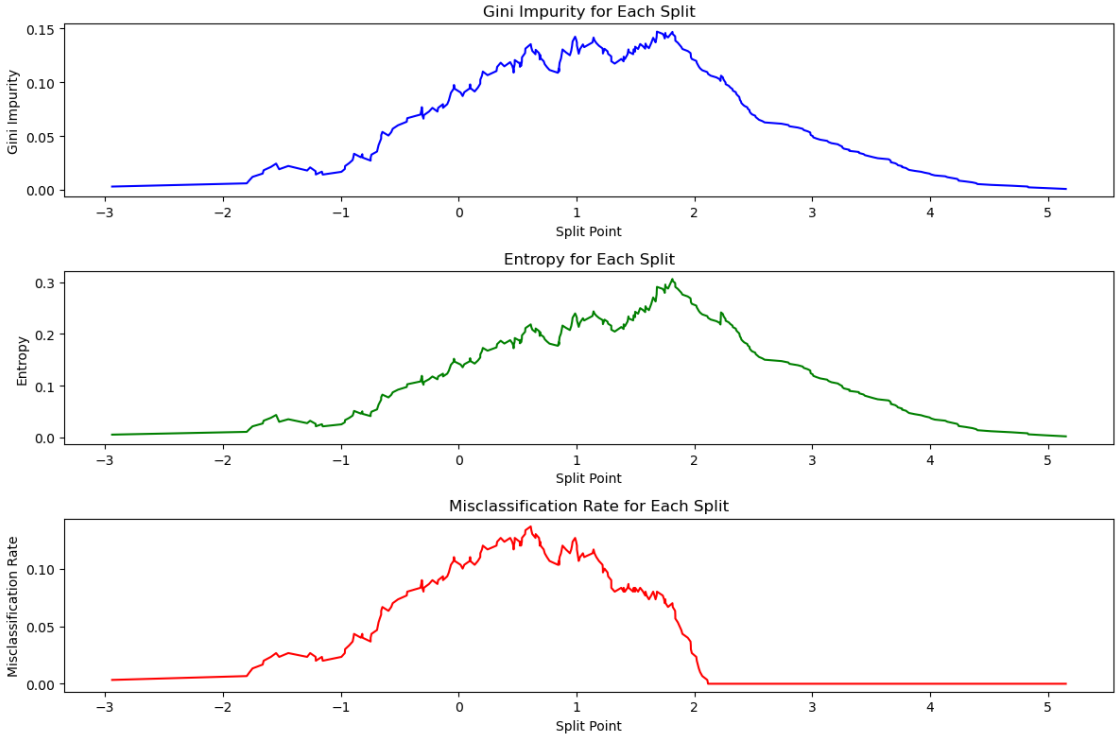
[5]:
```
# load the data
pts = np.load('data/data1d.npy')
labels = np.load('data/labels1d.npy')

# TODO: Sort the points to easily split them

# TODO: Implement or find implementation for Gini impurity, entropy and␣
 ↪misclassifcation rate

def probabilities(partition):
    # divide counts by size of dataset to get cluster probabilites
    return np.unique(partition, return_counts=True)[1] / len(partition)

def compute_split_measure(l, l0, l1, method):
    p0 = probabilities(l0)
    p1 = probabilities(l1)
    p = probabilities(l)
    return method(p) - (len(l0) * method(p0) + len(l1) * method(p1)) / (len(l))

# TODO: Iterate over the possible splits, evaulating and saving the three␣
 ↪criteria for each one
# TODO: Then, Compute the split that each criterion favours and visualize them
#       (e.g. with a histogram for each class and vertical lines to show the␣
 ↪splits)
```

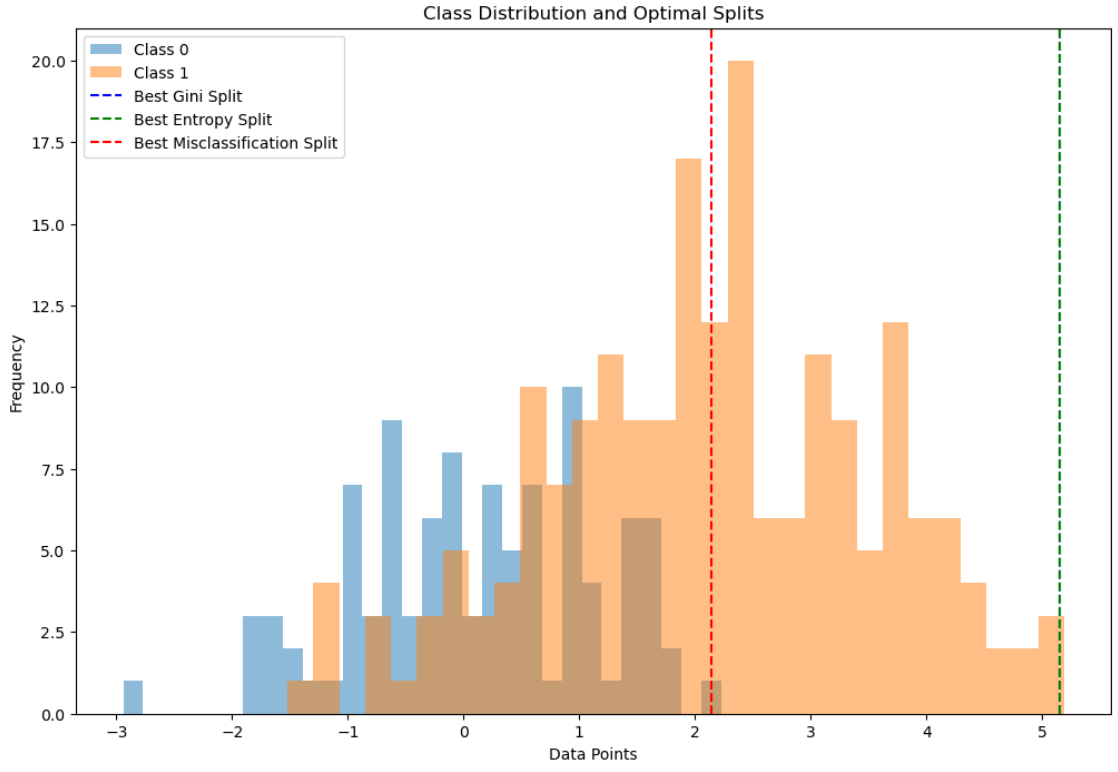
1.4.1 (b)

[6]:
```
# load the data
pts = np.load('data/data1d.npy')
labels = np.load('data/labels1d.npy')

# TODO: Sort the points to easily split them

sorted_indices = np.argsort(pts)
sorted_pts = pts[sorted_indices]
sorted_labels = labels[sorted_indices]


# TODO: Implement or find implementation for Gini impurity, entropy and␣
 ↪misclassifcation rate

def gini_impurity(p):
```

```
    return 1 - np.sum(p**2)

def entropy(p):
    return -np.sum(p * np.log2(p + np.finfo(float).eps))  # Avoid log(0)

def misclassification_rate(p):
    return 1 - np.max(p)

def probabilities(partition):
    # divide counts by size of dataset to get cluster probabilites
    return np.unique(partition, return_counts=True)[1] / len(partition)

def compute_split_measure(l, l0, l1, method):
    p0 = probabilities(l0)
    p1 = probabilities(l1)
    p = probabilities(l)
    return method(p) - (len(l0) * method(p0) + len(l1) * method(p1)) / (len(l))

# TODO: Iterate over the possible splits, evaulating and saving the three␣
 ↪criteria for each one

gini_values = []
entropy_values = []
misclassification_values = []

# Iterate over potential splits (between each pair of consecutive data points)
for i in range(1, len(sorted_pts)):
    # Split the dataset into two parts
    l0 = sorted_labels[:i]
    l1 = sorted_labels[i:]

    # Compute the split measure for each criterion
    gini_values.append(compute_split_measure(sorted_labels, l0, l1,␣
 ↪gini_impurity))
    entropy_values.append(compute_split_measure(sorted_labels, l0, l1, entropy))
    misclassification_values.append(compute_split_measure(sorted_labels, l0,␣
 ↪l1, misclassification_rate))

# TODO: Then, Compute the split that each criterion favours and visualize them
#       (e.g. with a histogram for each class and vertical lines to show the␣
 ↪splits)

# Plot Gini impurity, entropy, and misclassification rate
plt.figure(figsize=(12, 8))

# Gini Impurity Plot
plt.subplot(3, 1, 1)
```

```
plt.plot(sorted_pts[:-1], gini_values, label='Gini Impurity', color='blue')
plt.title('Gini Impurity for Each Split')
plt.xlabel('Split Point')
plt.ylabel('Gini Impurity')

# Entropy Plot
plt.subplot(3, 1, 2)
plt.plot(sorted_pts[:-1], entropy_values, label='Entropy', color='green')
plt.title('Entropy for Each Split')
plt.xlabel('Split Point')
plt.ylabel('Entropy')

# Misclassification Rate Plot
plt.subplot(3, 1, 3)
plt.plot(sorted_pts[:-1], misclassification_values, label='Misclassification␣
 ↪Rate', color='red')
plt.title('Misclassification Rate for Each Split')
plt.xlabel('Split Point')
plt.ylabel('Misclassification Rate')

plt.tight_layout()
plt.show()

# Create histograms of the class distribution with vertical lines showing splits
plt.figure(figsize=(12, 8))
plt.hist(pts[labels == 0], bins=30, alpha=0.5, label='Class 0')
plt.hist(pts[labels == 1], bins=30, alpha=0.5, label='Class 1')
plt.axvline(sorted_pts[np.argmin(gini_values)], color='blue',␣
 ↪linestyle='dashed', label='Best Gini Split')
plt.axvline(sorted_pts[np.argmin(entropy_values)], color='green',␣
 ↪linestyle='dashed', label='Best Entropy Split')
plt.axvline(sorted_pts[np.argmin(misclassification_values)], color='red',␣
 ↪linestyle='dashed', label='Best Misclassification Split')
plt.title('Class Distribution and Optimal Splits')
plt.xlabel('Data Points')
plt.ylabel('Frequency')
plt.legend()
plt.show()
```


Gini Impurity for Each Split
Gini Impurity
Split Point
Entropy for Each Split
Entropy
Split Point
Misclassification Rate for Each Split
Misclassification Rate
Split Point


Class Distribution and Optimal Splits
Class 0
Class 1
Best Gini Split
Best Entropy Split
Best Misclassification Split
Frequency
Data Points

[7]:
```
# load the dijet data
features = np.load('data/dijet_features_normalized.npy').T
labels = np.load('data/dijet_labels.npy')

# TODO: define train, val and test splits as specified (make sure to shuffle␣
 ↪the data before splitting it!)

from sklearn.model_selection import train_test_split


# Splitting the data into train, validation, and test sets
X_temp, X_test, y_temp, y_test = train_test_split(features, labels,␣
 ↪test_size=200, random_state=42)
X_train, X_val, y_train, y_val = train_test_split(X_temp, y_temp,␣
 ↪test_size=200, random_state=42)
```

[8]:
```
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score

# TODO: train a random forest classifier for each combination of specified␣
 ↪hyperparameters
#       and evaluate the performances on the validation set.

# Example hyperparameter grid (you can modify this as needed)
hyperparameter_grid = {
    'n_estimators': [50, 100, 200],  # Number of trees
    'max_depth': [None, 10, 20],     # Max depth of each tree
    'min_samples_split': [2, 5, 10]  # Minimum samples to split a node
}

# Placeholder to track best performance
best_score = 0
best_params = None

# Iterate over all combinations of hyperparameters
for n_estimators in hyperparameter_grid['n_estimators']:
    for max_depth in hyperparameter_grid['max_depth']:
        for min_samples_split in hyperparameter_grid['min_samples_split']:

            # Initialize the RandomForestClassifier with the current␣
 ↪hyperparameters
            clf = RandomForestClassifier(
                n_estimators=n_estimators,
                max_depth=max_depth,
                min_samples_split=min_samples_split,
                random_state=42
            )
```

```
            # Train the model on the training set
            clf.fit(X_train, y_train)

            # Evaluate on the validation set
            y_val_pred = clf.predict(X_val)
            val_accuracy = accuracy_score(y_val, y_val_pred)

            # Print the performance for the current hyperparameter combination
            print(f"n_estimators={n_estimators}, max_depth={max_depth},␣
 ↪min_samples_split={min_samples_split} => Validation Accuracy: {val_accuracy:.
 ↪4f}")

            # Update best score and parameters if current model is better
            if val_accuracy > best_score:
                best_score = val_accuracy
                best_params = {
                    'n_estimators': n_estimators,
                    'max_depth': max_depth,
                    'min_samples_split': min_samples_split
                }

# Print the best hyperparameters and their performance
print(f"\nBest Validation Accuracy: {best_score:.4f}")
print("Best Hyperparameters:", best_params)
```

```
n_estimators=50, max_depth=None, min_samples_split=2 => Validation Accuracy:
0.8000
n_estimators=50, max_depth=None, min_samples_split=5 => Validation Accuracy:
0.7850
n_estimators=50, max_depth=None, min_samples_split=10 => Validation Accuracy:
0.7650
n_estimators=50, max_depth=10, min_samples_split=2 => Validation Accuracy:
0.7650
n_estimators=50, max_depth=10, min_samples_split=5 => Validation Accuracy:
0.7500
n_estimators=50, max_depth=10, min_samples_split=10 => Validation Accuracy:
0.7800
n_estimators=50, max_depth=20, min_samples_split=2 => Validation Accuracy:
0.8100
n_estimators=50, max_depth=20, min_samples_split=5 => Validation Accuracy:
0.7850
n_estimators=50, max_depth=20, min_samples_split=10 => Validation Accuracy:
0.7650
n_estimators=100, max_depth=None, min_samples_split=2 => Validation Accuracy:
0.8000
n_estimators=100, max_depth=None, min_samples_split=5 => Validation Accuracy:
```

```
0.7800
n_estimators=100, max_depth=None, min_samples_split=10 => Validation Accuracy:
0.7700
n_estimators=100, max_depth=10, min_samples_split=2 => Validation Accuracy:
0.7850
n_estimators=100, max_depth=10, min_samples_split=5 => Validation Accuracy:
0.7800
n_estimators=100, max_depth=10, min_samples_split=10 => Validation Accuracy:
0.7800
n_estimators=100, max_depth=20, min_samples_split=2 => Validation Accuracy:
0.8050
n_estimators=100, max_depth=20, min_samples_split=5 => Validation Accuracy:
0.7750
n_estimators=100, max_depth=20, min_samples_split=10 => Validation Accuracy:
0.7650
n_estimators=200, max_depth=None, min_samples_split=2 => Validation Accuracy:
0.7850
n_estimators=200, max_depth=None, min_samples_split=5 => Validation Accuracy:
0.7950
n_estimators=200, max_depth=None, min_samples_split=10 => Validation Accuracy:
0.7850
n_estimators=200, max_depth=10, min_samples_split=2 => Validation Accuracy:
0.7950
n_estimators=200, max_depth=10, min_samples_split=5 => Validation Accuracy:
0.7650
n_estimators=200, max_depth=10, min_samples_split=10 => Validation Accuracy:
0.7700
n_estimators=200, max_depth=20, min_samples_split=2 => Validation Accuracy:
0.7950
n_estimators=200, max_depth=20, min_samples_split=5 => Validation Accuracy:
0.7900
n_estimators=200, max_depth=20, min_samples_split=10 => Validation Accuracy:
0.7800

Best Validation Accuracy: 0.8100
Best Hyperparameters: {'n_estimators': 50, 'max_depth': 20, 'min_samples_split':
2}
```

1.5 5 Bivariate Normal

We consider the bivariate normal $\mathcal{N}(x|\mu,\Sigma) = \mathcal{N}(x|\mu,\Lambda^{-1})$ with $x = (x_1, x_2)^T$ and covariance matrix Σ to show that its conditional and marginal probability densities $p(x_1|x_2 = c)$ and $p(x_1) = \int \mathrm{d}x_2 p(x)$ are again normal with certain parameters.

(a) Conditional

$$\log p(x) \propto \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{21} & \Lambda_{22} \end{bmatrix} \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{bmatrix}$$

$$
\begin{aligned}
&= \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{21} & \Lambda_{22} \end{bmatrix} \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix} \\
&= \bar{x}_1^2 \Lambda_{11} + \bar{x}_1 \bar{x}_2 (\Lambda_{12} + \Lambda_{21}) + \bar{x}_2^2 \Lambda_{22} \\
&= (x_1^2 + \mu_1^2 - 2x_1\mu_1)\Lambda_{11} + (x_1 x_2 + \mu_1\mu_2 - x_1\mu_2 - x_2\mu_1)(\Lambda_{12} + \Lambda_{21}) + c \\
&= x_1(x_1 - 2\mu_1)\Lambda_{11} + x_1(x_2 - \mu_2)(\Lambda_{12} + \Lambda_{21}) + c \\
&\simeq x_1^2 \Lambda_{11} + x_1((\Lambda_{12} + \Lambda_{21})(x_2 - \mu_2) - 2\mu_1\Lambda_{11}) \stackrel{!}{=} \Sigma_{1|2}(x_1^2 - 2\mu_{1|2}x_1) \\
&\implies \Sigma_{1|2} = \Lambda_{11}^{-1} = \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}
\end{aligned}
$$

$$
\mu_{1|2} = -\frac{\Lambda_{12} + \Lambda_{21}}{2\Lambda_{11}}(x_2 - \mu_2) + \mu_1 = -\frac{\Lambda_{12}}{\Lambda_{11}}(x_2 - \mu_2) + \mu_1 = \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) + \mu_1
$$

where we used that the accuracy matrix and precision matrix are symmetric in the calculation of $\mu_{1|2}$.