AUTOMATED HYPERPARAMETER OPTIMISATION

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Introduction:

For this project we will be creating an automated hyperparameter optimization (HPO) system using Bayesian optimisation to optimise hyperparameters of specific machine learning models. To test this we are going to be applying this system to a Random Forest Classifier which is predicting whether a certain video game will have high sales or low sales given a dataset of video game sales greater than 100,000.

Code Explanation:

Data Loading and Processing

First, we load the dataset vgsales.csv using Pandas' read_csv function, any rows containing missing values are removed using dropna. Categorical variables such as Platform, Genre, and Publisher are encoded into numerical values using Scikit-learn's LabelEncoder and the target variable, Global_Sales, undergoes transformation into a binary classification problem by assigning values based on whether they are above or below its median. This step simplifies the prediction task to distinguish between high and low sales scenarios. Finally, the dataset is split into training (X_train, y_train) and testing (X_test, y_test) sets using train_test_split, with 80% of the data allocated for training and 20% for testing.

```python
import numpy as np
import pandas as pd
from scipy.stats import norm
from scipy.optimize import minimize
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import roc_auc_score
from sklearn.preprocessing import LabelEncoder

# Load dataset
data = pd.read_csv('vgsales.csv')

# Drop rows with missing values
data.dropna(inplace=True)

# Encode categorical variables
label_encoders = {}
for col in ['Platform', 'Genre', 'Publisher']:
    label_encoders[col] = LabelEncoder()
    data[col] = label_encoders[col].fit_transform(data[col])

# Convert target to binary classification problem
threshold = data['Global_Sales'].median()
data['Global_Sales_Binary'] = (data['Global_Sales'] > threshold).astype(int)

# Split data into features (X) and target (y)
X = data[['Platform', 'Genre', 'Publisher', 'Year']]
y = data['Global_Sales_Binary']

# Split data into train and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
```

Gaussian Process Definition

The GaussianProcess class is designed to implement a Gaussian Process regression model, a probabilistic approach for modeling relationships in data. When initializing the class (__init__ method), it sets up the model with parameters such as the kernel function (kernel), length scale (length_scale), noise level (noise), and a flag (is_fitted) to indicate if the model has been trained. The rbf_kernel method defines the Radial Basis Function (RBF) kernel, a key component in Gaussian Processes, which computes the covariance matrix between two sets of input data points (X1 and X2). This kernel function captures the similarity between data points, crucial for modeling correlations in the data. The fit method trains the Gaussian Process model on input data (X for features and y for targets) by computing the kernel matrix K, adjusting for noise by adding it to the diagonal, and then computing the inverse (K_inv) of the kernel matrix. This fitting process allows the model to learn from the data and estimate the underlying relationships. The predict method makes predictions on new input data (X) based on the trained model parameters, providing estimates of the mean (mu) and diagonal of the covariance (cov).

```
class GaussianProcess:
    def __init__(self, kernel='RBF', length_scale=1.0, noise=1e-6):
        self.kernel = kernel
        self.length_scale = length_scale
        self.noise = noise
        self.is_fitted = False

    def rbf_kernel(self, X1, X2):
        """Radial Basis Function (RBF) Kernel"""
        sqdist = np.sum(X1**2, 1).reshape(-1, 1) + np.sum(X2**2, 1) - 2 * np.dot(X1, X2.T)
        return np.exp(-0.5 / self.length_scale**2 * sqdist)

    def fit(self, X, y):
        self.X_train = X
        self.y_train = y
        K = self.rbf_kernel(X, X) + self.noise * np.eye(len(X))
        self.K_inv = np.linalg.inv(K)
        self.is_fitted = True

    def predict(self, X):
        if not self.is_fitted:
            raise RuntimeError("You must train the model before making predictions")
        K_s = self.rbf_kernel(self.X_train, X)
        K_ss = self.rbf_kernel(X, X) + self.noise * np.eye(len(X))
        mu = K_s.T.dot(self.K_inv).dot(self.y_train)
        cov = K_ss - K_s.T.dot(self.K_inv).dot(K_s)
        return mu, np.diag(cov)
```

Expected Improvement Function

The Expected Improvement (EI) function is used to determine the next best sample point in the optimization process. It takes into account the predictions made by a Gaussian Process regression model trained on existing data (X_sample and Y_sample). The function begins by predicting the mean (mu) and standard deviation (sigma) of potential new samples (X) using the trained model. It then identifies the maximum observed value from the existing samples (mu_sample_opt). The improvement (imp) over this maximum value is calculated, and normalized to derive a Z-score (Z). Using the cumulative distribution function (cdf) and probability density function (pdf) of the normal distribution, the Expected Improvement (ei) is computed. This metric balances exploration (seeking areas of the parameter space where uncertainty is high) and exploitation (exploiting areas where the mean predicted value is high), aiding in the selection of the next optimal sample point for evaluation in Bayesian optimization.

```python
def expected_improvement(X, X_sample, Y_sample, model, xi=0.01):
    mu, sigma = model.predict(X)
    mu_sample = model.predict(X_sample)[0]

    sigma = sigma.reshape(-1, 1)
    mu_sample_opt = np.max(mu_sample)

    with np.errstate(divide='warn'):
        imp = mu - mu_sample_opt - xi
        Z = imp / sigma
        ei = imp * norm.cdf(Z) + sigma * norm.pdf(Z)
        ei[sigma == 0.0] = 0.0

    return ei
```

Proposal Function

The Proposal Function suggests the next optimal sample point to evaluate based on an acquisition function such as Expected Improvement (EI). It begins by initializing variables to track the minimum value (min_val) and corresponding location (min_x) in the parameter space. A helper function (min_obj) is defined to minimize the negative of the acquisition function using a gradient-based optimization method. Through multiple iterations, random starting points (x0) within predefined bounds are generated, and the acquisition function is minimized using the minimize function. If a new minimum value is found that improves upon the current best, min_val and min_x are updated accordingly. Finally, the best proposed location (min_x) is returned, reshaped to ensure it conforms to the expected format of a column vector for further evaluation in the Bayesian optimization process.

```python
def propose_location(acquisition, X_sample, Y_sample, model, bounds, n_restarts=25):
    dim = X_sample.shape[1]
    min_val = 1
    min_x = None

    def min_obj(X):
        return -acquisition(X.reshape(-1, dim), X_sample, Y_sample, model)

    for x0 in np.random.uniform(bounds[:, 0], bounds[:, 1], size=(n_restarts, dim)):
        res = minimize(min_obj, x0=x0, bounds=bounds, method='L-BFGS-B')
        if res.fun < min_val:
            min_val = res.fun
            min_x = res.x

    return min_x.reshape(-1, 1)
```

Bayesian Optimization Function

The Bayesian Optimization Function is designed to automate the process of hyperparameter tuning by iteratively selecting and evaluating sample points in a parameter space, aiming to maximize or minimize an objective function. It begins by initializing X_sample and y_sample with initial random samples and their respective objective function values. A GaussianProcess model is instantiated to capture the underlying trend in the sampled data points. Across a specified number of iterations (n_iter), the function fits the GaussianProcess model to the existing data, proposes the next optimal sample point (X_next) using the propose_location function based on an acquisition function like Expected Improvement, evaluates it (y_next) using the objective_function, and then updates X_sample and y_sample with the new sample and its evaluation result. This iterative process

continues until the specified number of iterations is reached. At the end of the function execution, X_sample and y_sample contain a series of sampled points and their corresponding objective function values.

```
def bayesian_optimization(n_iter, initial_samples, bounds):
    X_sample = []
    y_sample = []

    for params in initial_samples:
        X_sample.append([params['max_depth'], params['n_estimators'], params['min_samples_split']])
        y_sample.append(objective_function(params))

    X_sample = np.array(X_sample)
    y_sample = np.array(y_sample)

    model = GaussianProcess()

    for i in range(n_iter):
        model.fit(X_sample, y_sample)

        X_next = propose_location(expected_improvement, X_sample, y_sample, model, bounds)
        y_next = objective_function({'max_depth': X_next[0][0], 'n_estimators': X_next[1][0], 'min_samples_split': X_next[2][0]})

        X_sample = np.vstack((X_sample, X_next.T))
        y_sample = np.append(y_sample, y_next)

    return X_sample, y_sample
```

Now we define bounds for hyperparameters (max_depth, n_estimators, min_samples_split) and initialize 5 random samples for Bayesian Optimization.

```
# Define search space (hyperparameter bounds)
bounds = np.array([
    [1, 20],  # max_depth
    [50, 200],  # n_estimators
    [2, 20]  # min_samples_split
])

# Initial random samples
np.random.seed(42)
initial_samples = [
    {'max_depth': np.random.uniform(1, 20),
     'n_estimators': np.random.uniform(50, 200),
     'min_samples_split': np.random.uniform(2, 20)}
    for _ in range(5)
]
```

Then we define objective_function, which takes hyperparameters max_depth, n_estimators, and min_samples_split, initializes a Random Forest Classifier, trains it on X_train and y_train, predicts probabilities on X_test, computes ROC AUC, and returns 1 - roc_auc to maximize ROC AUC.

```
# Define objective function (to maximize ROC AUC)
def objective_function(params):
    max_depth = int(params['max_depth'])
    n_estimators = int(params['n_estimators'])
    min_samples_split = int(params['min_samples_split'])

    # Initialize model with current hyperparameters
    model = RandomForestClassifier(max_depth=max_depth,
                                   n_estimators=n_estimators,
                                   min_samples_split=min_samples_split,
                                   random_state=42)

    # Train model
    model.fit(X_train, y_train)

    # Predict on test set
    y_pred_proba = model.predict_proba(X_test)[:, 1]

    # Calculate ROC AUC
    roc_auc = roc_auc_score(y_test, y_pred_proba)

    # Since we want to maximize ROC AUC, return 1 - roc_auc (for minimization)
    return 1 - roc_auc
```

Now we apply the system on our dataset

```
# Perform Bayesian Optimization to find best hyperparameters
X_sample, y_sample = bayesian_optimization(n_iter=50, initial_samples=initial_samples, bounds=bounds)

# Extract best parameters
best_index = np.argmin(y_sample)
best_params = X_sample[best_index]

best_params_dict = {
    'max_depth': best_params[0],
    'n_estimators': best_params[1],
    'min_samples_split': best_params[2]
}

print("Best Hyperparameters found:")
print(best_params_dict)

# Train final model with best hyperparameters
best_model = RandomForestClassifier(max_depth=int(best_params_dict['max_depth']),
                                    n_estimators=int(best_params_dict['n_estimators']),
                                    min_samples_split=int(best_params_dict['min_samples_split']),
                                    random_state=42)

best_model.fit(X_train, y_train)

# Evaluate final model on test set
y_pred_final_proba = best_model.predict_proba(X_test)[:, 1]
roc_auc_final = roc_auc_score(y_test, y_pred_final_proba)
print(f"Final ROC AUC on Test Set: {roc_auc_final}")
```

```
Best Hyperparameters found:
{'max_depth': 16.4987649876311, 'n_estimators': 52.41881217867296, 'min_samples_split': 20.0}
Final ROC AUC on Test Set: 0.7941585959836815
```

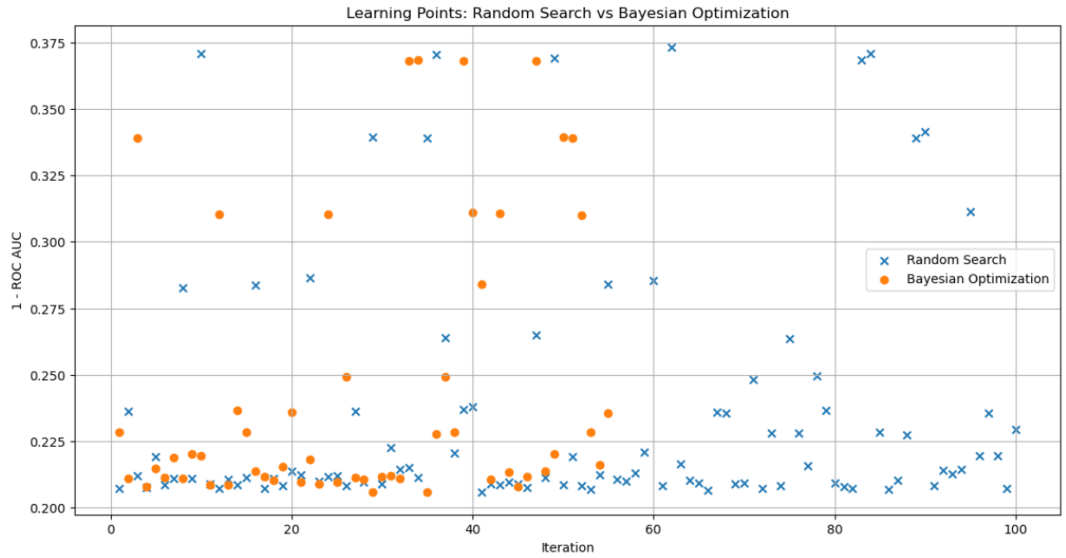
Random Search Vs Bayesian Optimisation:

To compare we perform random search on our dataset

```
# Random Search for Hyperparameter Optimization
random_params_list = []
random_scores = []
for _ in range(100):
    params = {
        'max_depth': np.random.uniform(1, 20),
        'n_estimators': np.random.uniform(50, 200),
        'min_samples_split': np.random.uniform(2, 20)
    }
    score = objective_function(params)
    random_params_list.append(params)
    random_scores.append(score)

# Convert scores to a numpy array
random_scores = np.array(random_scores)
```

Plotting the points

```
# Plot Learning points
plt.figure(figsize=(14, 7))
plt.scatter(range(1, len(random_scores) + 1), random_scores, label='Random Search', marker='x')
plt.scatter(range(1, len(y_sample) + 1), y_sample, label='Bayesian Optimization', marker='o')
plt.xlabel('Iteration')
plt.ylabel('1 - ROC AUC')
plt.legend()
plt.title('Learning Points: Random Search vs Bayesian Optimization')
plt.grid(True)
plt.show()
```

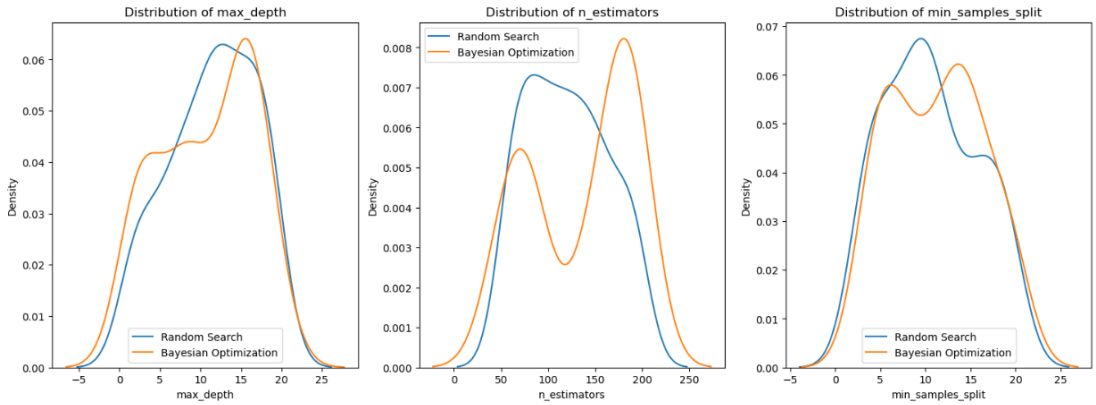


From the above plot we can observe that the hyperparameter scores improves with iterations for Bayesian optimisation. 1 – ROC AUC is marginally decreasing (not that clear due to lesser number of iterations) increasing iterations which means ROC AUC is increasing with further iterations

Now we make charts for all hyperparameters

```
# Plot different graphs for each hyperparameter
fig, axs = plt.subplots(1, 3, figsize=(18, 6))


# Plot for max_depth
sns.kdeplot([params['max_depth'] for params in random_params_list], label='Random Search', ax=axs[0])
sns.kdeplot(X_sample[:, 0], label='Bayesian Optimization', ax=axs[0])
axs[0].set_xlabel('max_depth')
axs[0].set_ylabel('Density')
axs[0].legend()
axs[0].set_title('Distribution of max_depth')

# Plot for n_estimators
sns.kdeplot([params['n_estimators'] for params in random_params_list], label='Random Search', ax=axs[1])
sns.kdeplot(X_sample[:, 1], label='Bayesian Optimization', ax=axs[1])
axs[1].set_xlabel('n_estimators')
axs[1].set_ylabel('Density')
axs[1].legend()
axs[1].set_title('Distribution of n_estimators')

# Plot for min_samples_split
sns.kdeplot([params['min_samples_split'] for params in random_params_list], label='Random Search', ax=axs[2])
sns.kdeplot(X_sample[:, 2], label='Bayesian Optimization', ax=axs[2])
axs[2].set_xlabel('min_samples_split')
axs[2].set_ylabel('Density')
axs[2].legend()
axs[2].set_title('Distribution of min_samples_split')

plt.tight_layout
```

The above code gives:



As we can see that hyperparameter values for Bayesian optimisation align towards more promising values than random search.

Summary:

In this project I implemented automatic hyperparameter tuning using Bayesian optimisation techniques. The system was tested on a sample dataset and gave 2 outcomes:

- Generalisation performance was better for Bayesian optimisation than random search
- Fewer iterations were required to reach to a suitable value for Bayesian optimisation.

Few limitations were also present in the project:

- Due to hardware issues on my side, model was run on fewer iterations which may not have produced the best data.
- Sometimes my overfit training data
- Incorrect hyperparameter bounds may effect efficiency.