predict_cholesterol_Gryko

March 11, 2025

1 Cholesterol-lowering Supplement Classification

This notebook implements a machine learning model to predict if a patient needs cholesterol-lowering supplements based on their health attributes.

[1]:
```
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split, GridSearchCV,␣
↪cross_val_score
from sklearn.preprocessing import StandardScaler, OneHotEncoder
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline
from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
from sklearn.metrics import accuracy_score, classification_report, roc_curve,␣
↪auc
import warnings

warnings.filterwarnings("ignore")
```

1.1 1. Load the Data

[2]:
```
# Load the training data
training_data = pd.read_excel("data/train_choloesterol.xlsx")

# Load the prediction data
prediction_data = pd.read_excel("data/predict_cholesterol.xlsx")

# Display first few rows of training data
print("Training data shape:", training_data.shape)
training_data.head()
```

```
Training data shape: (100, 12)
```

[2]:
```
   id  Age  Gender   BMI  Total_Cholesterol  LDL_Cholesterol  HDL_Cholesterol  \
0  t1   68  Female  30.0              203.8            111.8             44.0
```

```
1  t2   58  Female  30.3              188.1            182.4             50.6
2  t3   44    Male  20.9              194.3             74.7             60.1
3  t4   72  Female  35.0              198.4            120.2             43.5
4  t5   37    Male  22.9              277.3            186.1             36.7

   Triglycerides Physical_Activity Dietary_Habits Family_History  \
0          157.3               Low        Healthy             No
1          234.8              High       Moderate             No
2           97.2              High        Healthy            Yes
3          202.0              High        Healthy             No
4          156.3               Low       Moderate            Yes

   Need_Supplement
0                0
1                1
2                0
3                1
4                1
```

[3]:
```python
# Display first few rows of prediction data
print("Prediction data shape:", prediction_data.shape)
prediction_data.head()
```

```
Prediction data shape: (20, 11)
```

[3]:
```
   id  Age  Gender   BMI  Total_Cholesterol  LDL_Cholesterol  HDL_Cholesterol  \
0  v1   38    Male  23.1              169.3            105.3             47.4
1  v2   53    Male  33.1              271.7            189.5             31.6
2  v3   30  Female  30.8              273.1            153.6             57.4
3  v4   73  Female  34.2              243.9            116.1             56.7
4  v5   37  Female  24.0              273.1            158.5             47.8

   Triglycerides Physical_Activity Dietary_Habits Family_History
0          125.8              High        Healthy            Yes
1          235.3               Low       Moderate            Yes
2          194.3          Moderate        Healthy             No
3           59.6               Low      Unhealthy            Yes
4          206.3               Low        Healthy             No
```

1.2 2. Data Exploration and Preprocessing

[4]:
```
# Check for missing values in training data
print("Missing values in training data:")
print(training_data.isnull().sum())

# Check data types
print("\nData types in training data:")
print(training_data.dtypes)
```

```
Missing values in training data:
id                   0
Age                  0
Gender               0
BMI                  0
Total_Cholesterol    0
LDL_Cholesterol      0
HDL_Cholesterol      0
Triglycerides        0
Physical_Activity    0
Dietary_Habits       0
Family_History       0
Need_Supplement      0
dtype: int64

Data types in training data:
id                    object
Age                    int64
Gender                object
BMI                  float64
Total_Cholesterol    float64
LDL_Cholesterol      float64
HDL_Cholesterol      float64
Triglycerides        float64
Physical_Activity     object
Dietary_Habits        object
Family_History        object
Need_Supplement        int64
dtype: object
```

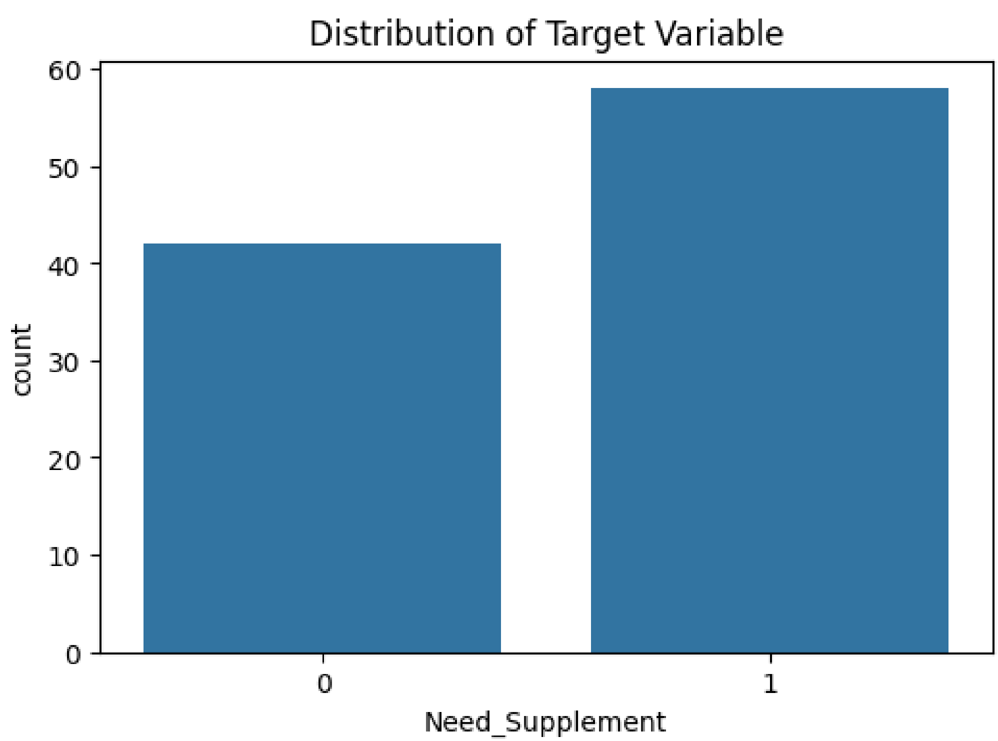
[5]:
```
# Get statistical summary of training data
training_data.describe()
```

[5]:
```
              Age         BMI  Total_Cholesterol  LDL_Cholesterol  \
count  100.000000  100.000000         100.000000        100.00000
mean    54.070000   27.751000         219.366000        133.61900
std     14.447575    4.542871          45.145415         33.89925
min     30.000000   18.800000         150.800000         74.70000
25%     43.000000   24.275000         178.750000        104.37500
50%     53.000000   27.550000         215.200000        134.80000
```

```
75%      68.000000   31.725000          255.250000          160.00000
max      79.000000   35.000000          297.300000          189.50000

       HDL_Cholesterol  Triglycerides  Need_Supplement
count       100.000000     100.000000       100.000000
mean         55.571000     151.653000         0.580000
std          13.880364      58.344069         0.496045
min          30.700000      50.500000         0.000000
25%          43.925000      97.050000         0.000000
50%          56.800000     157.050000         1.000000
75%          67.575000     197.925000         1.000000
max          79.300000     249.500000         1.000000
```

[6]:

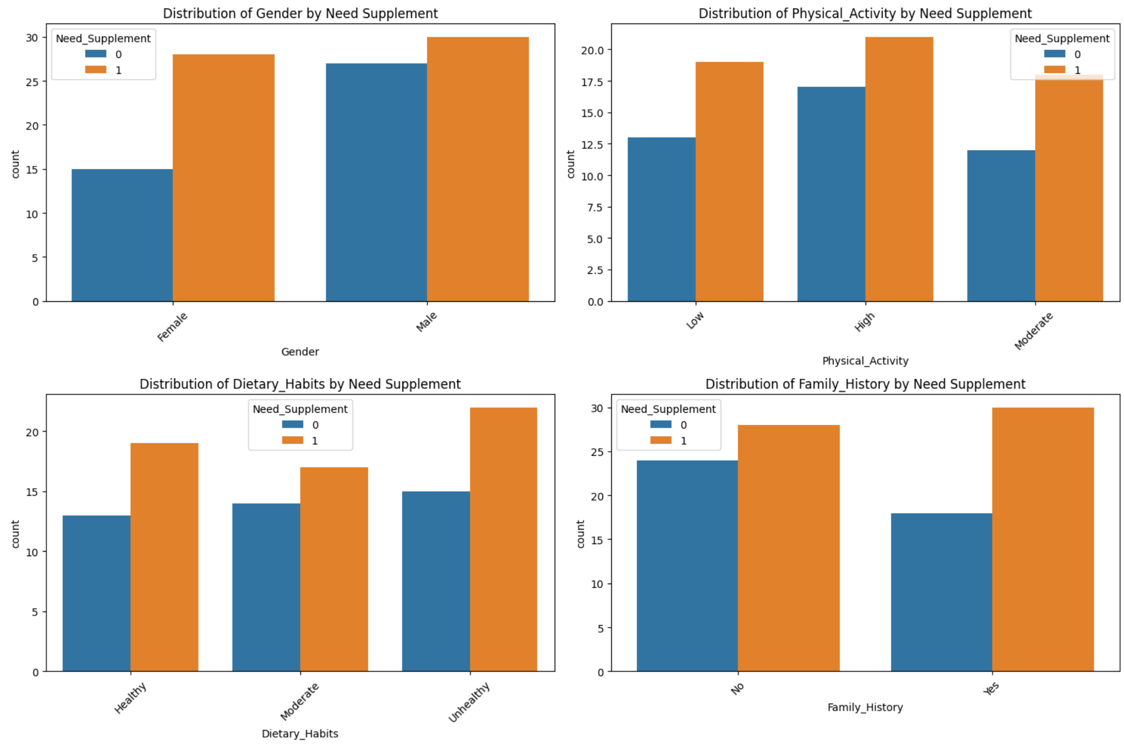
```python
# Count of target variable
plt.figure(figsize=(6, 4))
sns.countplot(x="Need_Supplement", data=training_data)
plt.title("Distribution of Target Variable")
plt.show()

print("Target variable distribution:")
print(training_data["Need_Supplement"].value_counts())
print("Percentage:")
print(training_data["Need_Supplement"].value_counts(normalize=True) * 100)
```



```
Target variable distribution:
Need_Supplement
1    58
0    42
Name: count, dtype: int64
Percentage:
Need_Supplement
1    58.0
0    42.0
Name: proportion, dtype: float64
```

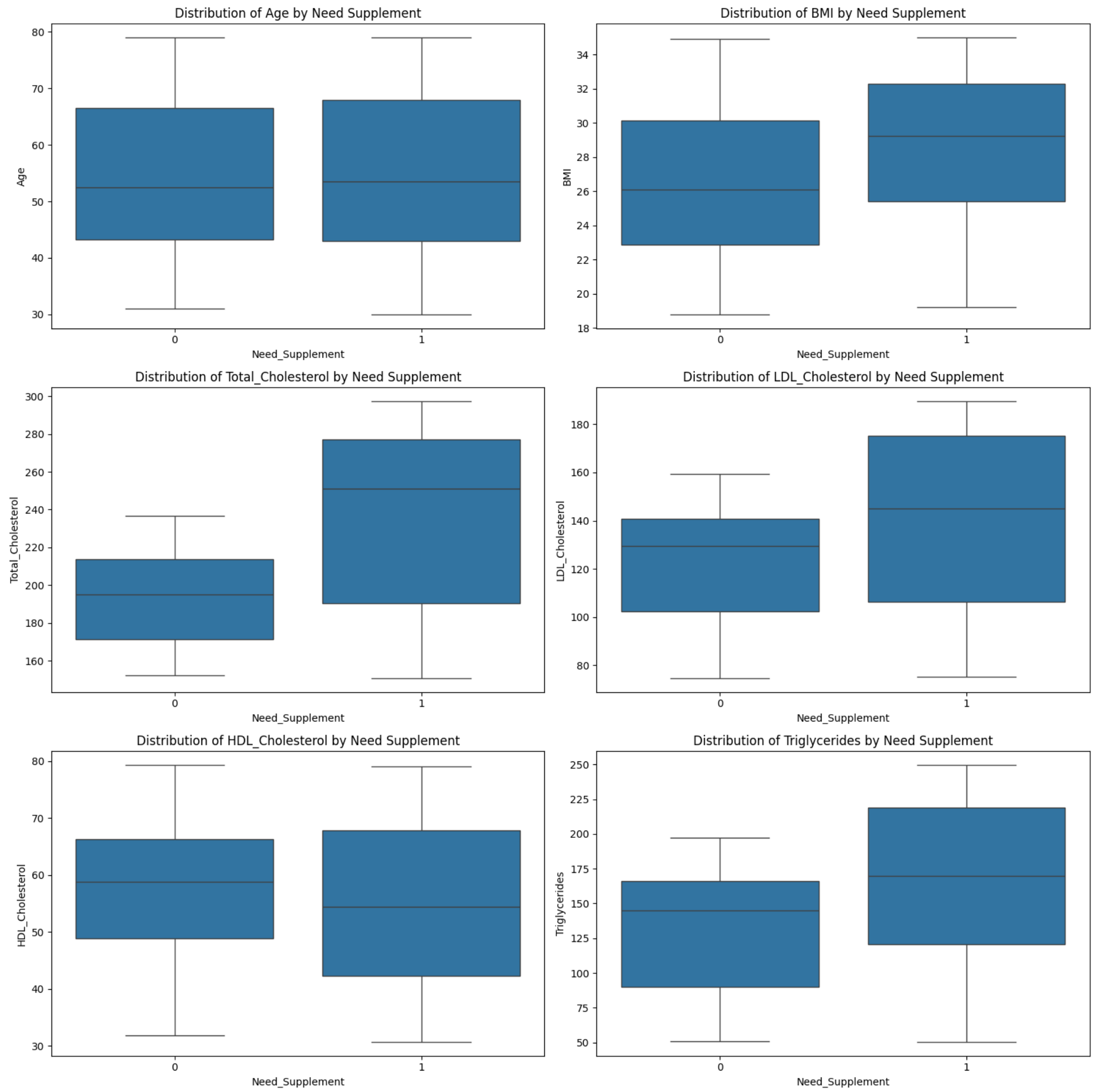
[9]:

```
# Explore categorical variables
categorical_features = [
    "Gender",
    "Physical_Activity",
    "Dietary_Habits",
    "Family_History",
]

fig, axes = plt.subplots(2, 2, figsize=(15, 10))
axes = axes.flatten()

for i, feature in enumerate(categorical_features):
    sns.countplot(x=feature, hue="Need_Supplement", data=training_data,␣
↪ax=axes[i])
    axes[i].set_title(f"Distribution of {feature} by Need Supplement")
    axes[i].tick_params(axis="x", rotation=45)

plt.tight_layout()
plt.show()
```



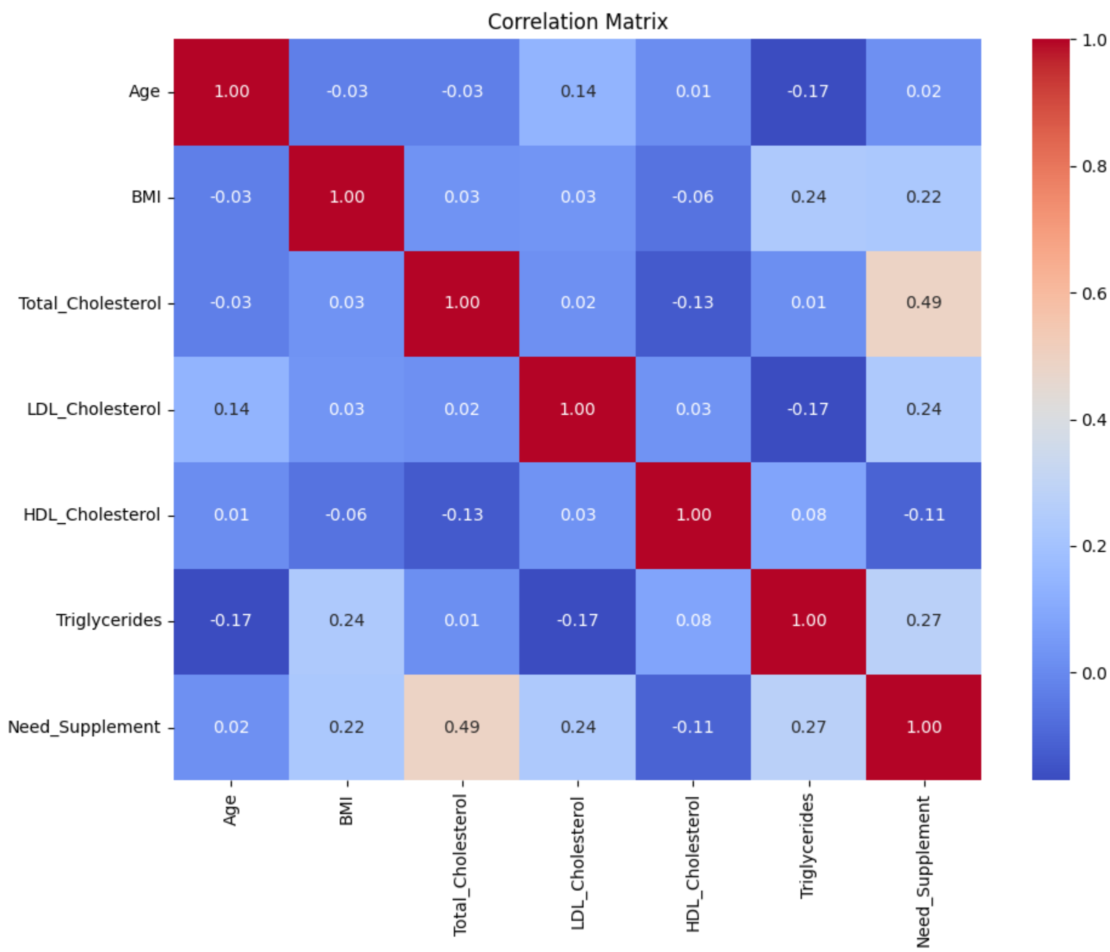
[11]:

```python
# Explore numerical variables
numerical_features = [
    "Age",
    "BMI",
    "Total_Cholesterol",
    "LDL_Cholesterol",
    "HDL_Cholesterol",
    "Triglycerides",
]

fig, axes = plt.subplots(3, 2, figsize=(15, 15))
axes = axes.flatten()

for i, feature in enumerate(numerical_features):
    sns.boxplot(x="Need_Supplement", y=feature, data=training_data, ax=axes[i])
    axes[i].set_title(f"Distribution of {feature} by Need Supplement")

plt.tight_layout()
plt.show()
```



[13]:

```
# Correlation matrix for numerical features
plt.figure(figsize=(10, 8))
correlation_matrix = training_data[numerical_features + ["Need_Supplement"]].
↪corr()
sns.heatmap(correlation_matrix, annot=True, cmap="coolwarm", fmt=".2f")
plt.title("Correlation Matrix")
plt.tight_layout()
plt.show()
```



1.3 3. Feature Engineering and Preprocessing

[14]:
```
# Define features and target variable for training data
X = training_data.drop("Need_Supplement", axis=1)
y = training_data["Need_Supplement"]

# Define categorical and numerical features
categorical_features = [
    "Gender",
    "Physical_Activity",
    "Dietary_Habits",
    "Family_History",
]
numerical_features = [
    "Age",
    "BMI",
    "Total_Cholesterol",
```

```
    "LDL_Cholesterol",
    "HDL_Cholesterol",
    "Triglycerides",
]
```

[15]:
```
# Create preprocessing pipeline
# For numerical features: StandardScaler
# For categorical features: OneHotEncoder
preprocessor = ColumnTransformer(
    transformers=[
        ("num", StandardScaler(), numerical_features),
        ("cat", OneHotEncoder(handle_unknown="ignore"), categorical_features),
    ]
)

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

1.4 4. Model Building and Evaluation

1.4.1 4.1 Random Forest Classifier

[16]:
```
# Create Random Forest Pipeline
rf_pipeline = Pipeline(
    [
        ("preprocessor", preprocessor),
        ("classifier", RandomForestClassifier(random_state=42)),
    ]
)

# Parameter grid for Random Forest
rf_param_grid = {
    "classifier__n_estimators": [100, 200],
    "classifier__max_depth": [None, 10, 20],
    "classifier__min_samples_split": [2, 5, 10],
    "classifier__min_samples_leaf": [1, 2, 4],
}

# Perform grid search with cross-validation
rf_grid_search = GridSearchCV(
    rf_pipeline, rf_param_grid, cv=5, scoring="accuracy", n_jobs=-1
)

rf_grid_search.fit(X_train, y_train)

# Best parameters
```

```python
print("Best parameters for Random Forest:")
print(rf_grid_search.best_params_)

# Best estimator
rf_best = rf_grid_search.best_estimator_

# Evaluate on test set
y_pred_rf = rf_best.predict(X_test)
print("\nRandom Forest Performance:")
print(f"Accuracy: {accuracy_score(y_test, y_pred_rf):.4f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_rf))
```

```
Best parameters for Random Forest:
{'classifier__max_depth': None, 'classifier__min_samples_leaf': 1,
'classifier__min_samples_split': 5, 'classifier__n_estimators': 100}

Random Forest Performance:
Accuracy: 1.0000

Classification Report:
              precision    recall  f1-score   support

           0       1.00      1.00      1.00        14
           1       1.00      1.00      1.00         6

    accuracy                           1.00        20
   macro avg       1.00      1.00      1.00        20
weighted avg       1.00      1.00      1.00        20
```

1.4.2 4.2 Gradient Boosting Classifier

[17]:
```python
# Create Gradient Boosting Pipeline
gb_pipeline = Pipeline(
    [
        ("preprocessor", preprocessor),
        ("classifier", GradientBoostingClassifier(random_state=42)),
    ]
)

# Parameter grid for Gradient Boosting
gb_param_grid = {
    "classifier__n_estimators": [100, 200],
    "classifier__learning_rate": [0.01, 0.1, 0.2],
    "classifier__max_depth": [3, 5, 7],
}
```

```python
# Perform grid search with cross-validation
gb_grid_search = GridSearchCV(
    gb_pipeline, gb_param_grid, cv=5, scoring="accuracy", n_jobs=-1
)

gb_grid_search.fit(X_train, y_train)

# Best parameters
print("Best parameters for Gradient Boosting:")
print(gb_grid_search.best_params_)

# Best estimator
gb_best = gb_grid_search.best_estimator_

# Evaluate on test set
y_pred_gb = gb_best.predict(X_test)
print("\nGradient Boosting Performance:")
print(f"Accuracy: {accuracy_score(y_test, y_pred_gb):.4f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_gb))
```

```
Best parameters for Gradient Boosting:
{'classifier__learning_rate': 0.01, 'classifier__max_depth': 3,
'classifier__n_estimators': 100}

Gradient Boosting Performance:
Accuracy: 0.9500

Classification Report:
              precision    recall  f1-score   support

           0       0.93      1.00      0.97        14
           1       1.00      0.83      0.91         6

    accuracy                           0.95        20
   macro avg       0.97      0.92      0.94        20
weighted avg       0.95      0.95      0.95        20
```

1.4.3 4.3 Logistic Regression

[18]:
```python
# Create Logistic Regression Pipeline
lr_pipeline = Pipeline(
    [
        ("preprocessor", preprocessor),
        ("classifier", LogisticRegression(random_state=42, max_iter=1000)),
```

```python
    ]
)

# Parameter grid for Logistic Regression
lr_param_grid = {
    "classifier__C": [0.01, 0.1, 1, 10, 100],
    "classifier__solver": ["liblinear", "saga"],
}

# Perform grid search with cross-validation
lr_grid_search = GridSearchCV(
    lr_pipeline, lr_param_grid, cv=5, scoring="accuracy", n_jobs=-1
)

lr_grid_search.fit(X_train, y_train)

# Best parameters
print("Best parameters for Logistic Regression:")
print(lr_grid_search.best_params_)

# Best estimator
lr_best = lr_grid_search.best_estimator_

# Evaluate on test set
y_pred_lr = lr_best.predict(X_test)
print("\nLogistic Regression Performance:")
print(f"Accuracy: {accuracy_score(y_test, y_pred_lr):.4f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_lr))
```

```
Best parameters for Logistic Regression:
{'classifier__C': 0.1, 'classifier__solver': 'liblinear'}

Logistic Regression Performance:
Accuracy: 0.6000

Classification Report:
              precision    recall  f1-score   support

           0       0.80      0.57      0.67        14
           1       0.40      0.67      0.50         6

    accuracy                           0.60        20
   macro avg       0.60      0.62      0.58        20
weighted avg       0.68      0.60      0.62        20
```

1.4.4 4.4 Support Vector Machine

[19]:
```python
# Create SVM Pipeline
svm_pipeline = Pipeline(
    [
        ("preprocessor", preprocessor),
        ("classifier", SVC(random_state=42, probability=True)),
    ]
)

# Parameter grid for SVM
svm_param_grid = {
    "classifier__C": [0.1, 1, 10],
    "classifier__kernel": ["linear", "rbf"],
    "classifier__gamma": ["scale", "auto"],
}

# Perform grid search with cross-validation
svm_grid_search = GridSearchCV(
    svm_pipeline, svm_param_grid, cv=5, scoring="accuracy", n_jobs=-1
)

svm_grid_search.fit(X_train, y_train)

# Best parameters
print("Best parameters for SVM:")
print(svm_grid_search.best_params_)

# Best estimator
svm_best = svm_grid_search.best_estimator_

# Evaluate on test set
y_pred_svm = svm_best.predict(X_test)
print("\nSVM Performance:")
print(f"Accuracy: {accuracy_score(y_test, y_pred_svm):.4f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_svm))
```

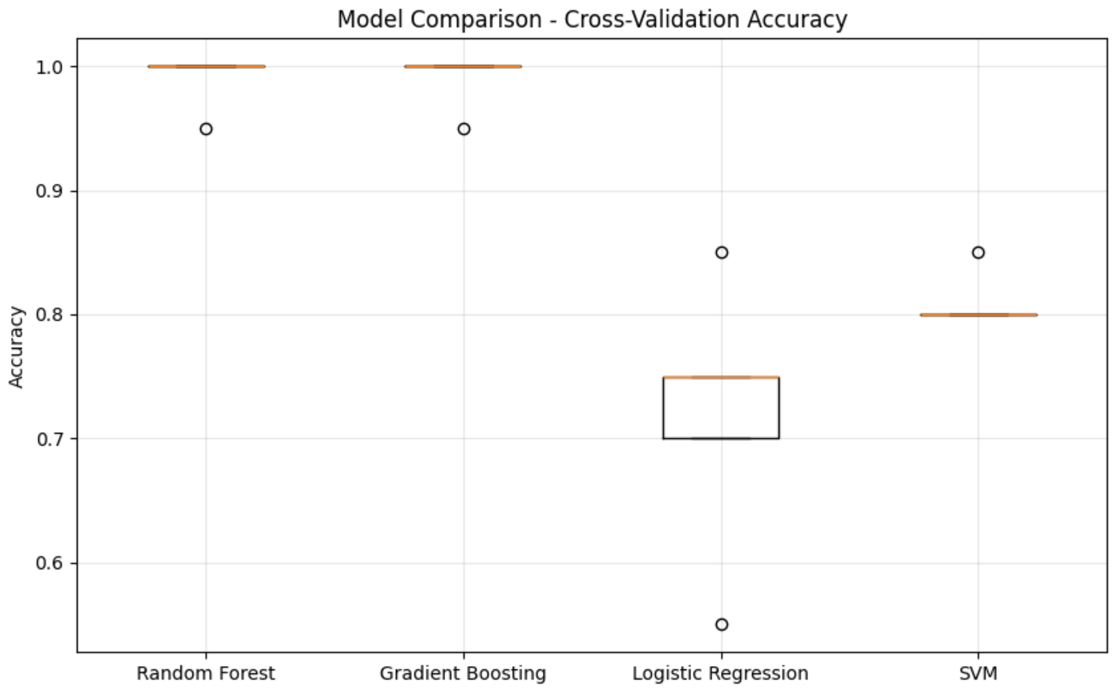
```
Best parameters for SVM:
{'classifier__C': 10, 'classifier__gamma': 'scale', 'classifier__kernel': 'rbf'}

SVM Performance:
Accuracy: 0.8000

Classification Report:
              precision    recall  f1-score   support

           0       0.86      0.86      0.86        14
```

```
           1       0.67      0.67      0.67         6

    accuracy                           0.80        20
   macro avg       0.76      0.76      0.76        20
weighted avg       0.80      0.80      0.80        20
```

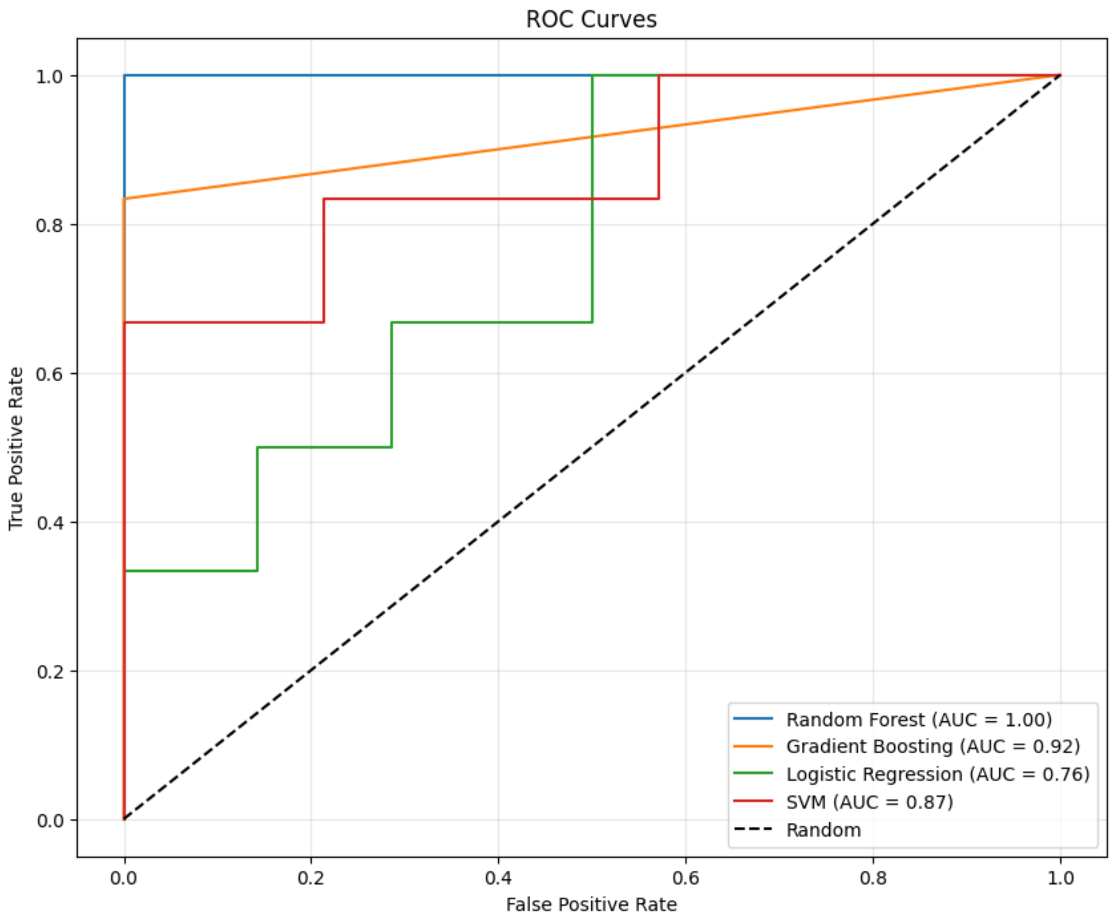
1.4.5 4.5 Model Comparison

[20]:
```python
# Compare models
models = {
    "Random Forest": rf_best,
    "Gradient Boosting": gb_best,
    "Logistic Regression": lr_best,
    "SVM": svm_best,
}

# Cross-validation results
cv_results = {}
for name, model in models.items():
    scores = cross_val_score(model, X, y, cv=5, scoring="accuracy")
    cv_results[name] = scores
    print(f"{name} - Mean CV Accuracy: {scores.mean():.4f} (±{scores.std():.
 ↪4f})")

# Visualize model comparison
plt.figure(figsize=(10, 6))
box_data = [cv_results[model_name] for model_name in models.keys()]
plt.boxplot(box_data, labels=list(models.keys()))
plt.title("Model Comparison - Cross-Validation Accuracy")
plt.ylabel("Accuracy")
plt.grid(True, alpha=0.3)
plt.show()
```

```
Random Forest - Mean CV Accuracy: 0.9900 (±0.0200)
Gradient Boosting - Mean CV Accuracy: 0.9900 (±0.0200)
Logistic Regression - Mean CV Accuracy: 0.7200 (±0.0980)
SVM - Mean CV Accuracy: 0.8100 (±0.0200)
```



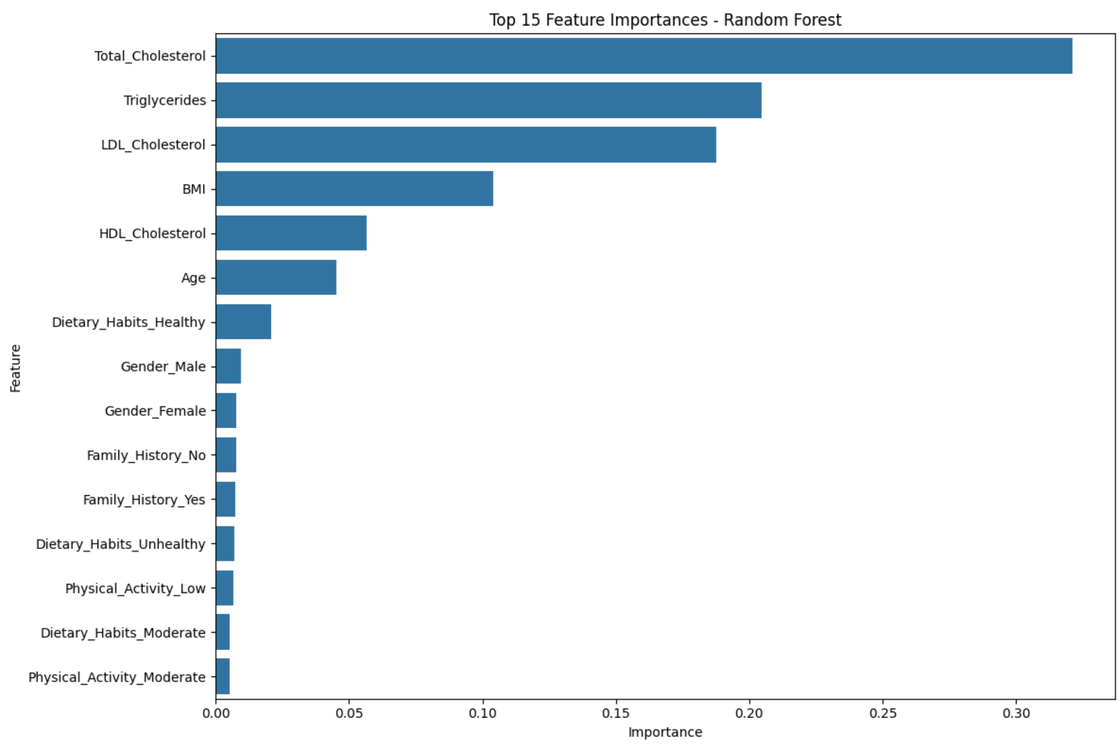
[21]:
```python
# Plot ROC curves
plt.figure(figsize=(10, 8))

for name, model in models.items():
    y_pred_proba = model.predict_proba(X_test)[:, 1]
    fpr, tpr, _ = roc_curve(y_test, y_pred_proba)
    roc_auc = auc(fpr, tpr)
    plt.plot(fpr, tpr, label=f"{name} (AUC = {roc_auc:.2f})")

plt.plot([0, 1], [0, 1], "k--", label="Random")
plt.xlabel("False Positive Rate")
plt.ylabel("True Positive Rate")
plt.title("ROC Curves")
plt.legend(loc="lower right")
plt.grid(True, alpha=0.3)
plt.show()
```



[22]:
```python
# Select the best model based on cross-validation results
best_model_name = max(cv_results, key=lambda k: cv_results[k].mean())
best_model = models[best_model_name]

print(f"The best model is: {best_model_name}")

# Feature importance for the best model (if applicable)
if best_model_name in ["Random Forest", "Gradient Boosting"]:
    # Get feature names after preprocessing
    preprocessor_output_feature_names = numerical_features + list(
        best_model.named_steps["preprocessor"]
        .transformers_[1][1]  # OneHotEncoder
        .get_feature_names_out(categorical_features)
    )

    # Get feature importances
    importances = best_model.named_steps["classifier"].feature_importances_
```

```
    # Create a DataFrame for better visualization
    feature_importance_df = pd.DataFrame(
        {"Feature": preprocessor_output_feature_names, "Importance":␣
↪importances}
    ).sort_values(by="Importance", ascending=False)

    # Display top 15 features
    plt.figure(figsize=(12, 8))
    sns.barplot(x="Importance", y="Feature", data=feature_importance_df.
↪head(15))
    plt.title(f"Top 15 Feature Importances - {best_model_name}")
    plt.tight_layout()
    plt.show()
```

```
The best model is: Random Forest
```



1.5 5. Make Predictions on New Data

[23]:
```
# Display the first few rows of the prediction data
prediction_data.head()
```

[23]:
```
   id  Age  Gender   BMI  Total_Cholesterol  LDL_Cholesterol  HDL_Cholesterol  \
0  v1   38    Male  23.1              169.3            105.3             47.4
```

```
1  v2   53    Male  33.1              271.7            189.5             31.6
2  v3   30  Female  30.8              273.1            153.6             57.4
3  v4   73  Female  34.2              243.9            116.1             56.7
4  v5   37  Female  24.0              273.1            158.5             47.8

   Triglycerides Physical_Activity Dietary_Habits Family_History
0          125.8              High        Healthy            Yes
1          235.3               Low       Moderate            Yes
2          194.3          Moderate        Healthy             No
3           59.6               Low      Unhealthy            Yes
4          206.3               Low        Healthy             No
```

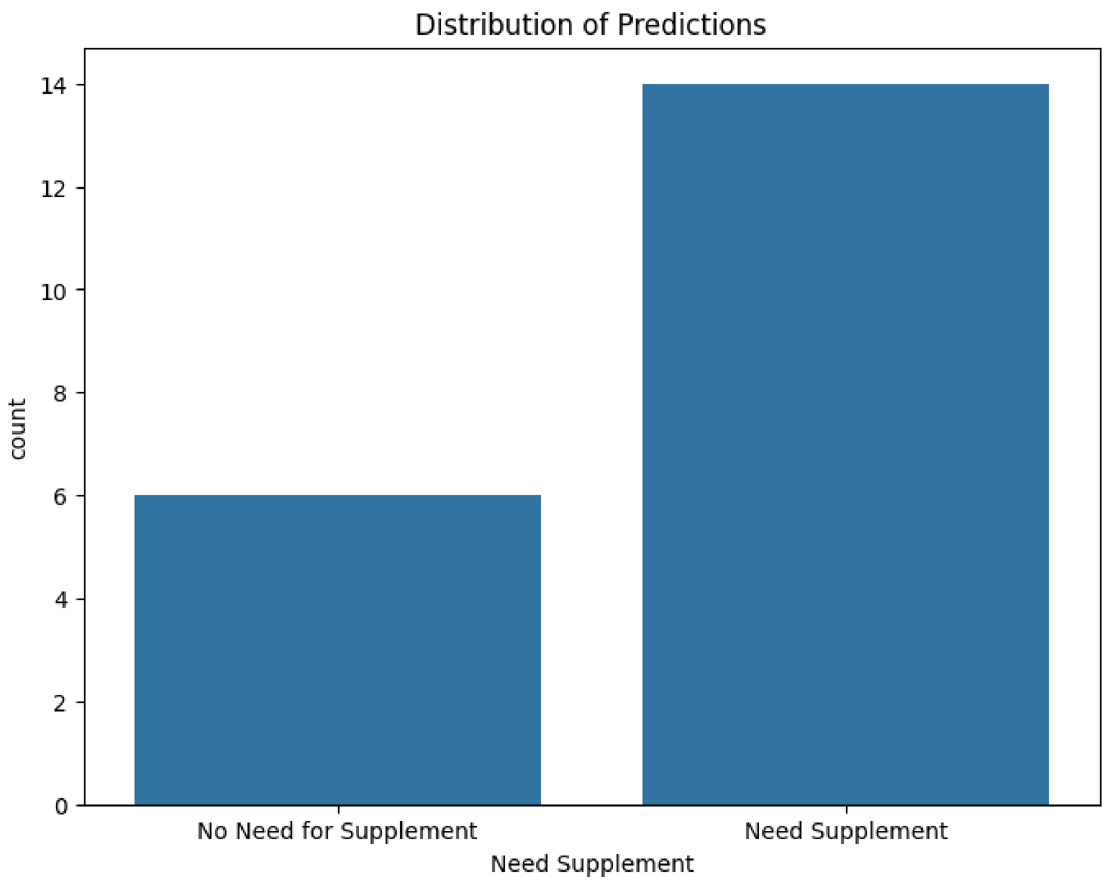
[24]:
```python
# Make predictions using the best model
predictions = best_model.predict(prediction_data)
prediction_probabilities = best_model.predict_proba(prediction_data)[:, 1]

# Add predictions to the prediction data
prediction_results = prediction_data.copy()
prediction_results["Need Supplement"] = predictions
prediction_results["Probability"] = prediction_probabilities

# Display the results
print("Predictions for the 20 patients:")
display(prediction_results)
```

```
Predictions for the 20 patients:

     id  Age  Gender   BMI  Total_Cholesterol  LDL_Cholesterol  \
0    v1   38    Male  23.1              169.3            105.3
1    v2   53    Male  33.1              271.7            189.5
2    v3   30  Female  30.8              273.1            153.6
3    v4   73  Female  34.2              243.9            116.1
4    v5   37  Female  24.0              273.1            158.5
5    v6   53    Male  27.6              247.7            179.8
6    v7   40    Male  27.9              181.0            185.0
7    v8   46  Female  34.7              191.1             76.9
8    v9   37  Female  19.7              182.2            117.3
9   v10   64  Female  23.5              206.6             82.8
10  v11   64  Female  21.7              155.8            110.3
11  v12   62    Male  22.9              242.7             90.4
12  v13   34  Female  26.5              200.5            147.6
13  v14   71    Male  24.6              248.4            116.6
14  v15   68  Female  25.0              207.8             97.5
15  v16   70    Male  32.4              252.2            101.9
16  v17   57  Female  33.8              201.1            113.2
17  v18   36  Female  19.7              189.1            101.2
18  v19   38  Female  21.9              224.4            124.4
19  v20   37  Female  29.6              253.9             73.9
```

```
    HDL_Cholesterol  Triglycerides Physical_Activity Dietary_Habits  \
0              47.4          125.8              High        Healthy
1              31.6          235.3               Low       Moderate
2              57.4          194.3          Moderate        Healthy
3              56.7           59.6               Low      Unhealthy
4              47.8          206.3               Low        Healthy
5              74.7          215.6          Moderate      Unhealthy
6              36.4          200.1          Moderate      Unhealthy
7              46.5          209.9          Moderate        Healthy
8              46.1          215.0              High      Unhealthy
9              34.6           87.3               Low       Moderate
10             54.1           97.1               Low      Unhealthy
11             64.4          176.8              High       Moderate
12             55.6          231.6          Moderate       Moderate
13             37.8          113.2              High      Unhealthy
14             48.9          167.7              High        Healthy
15             30.1          186.6              High       Moderate
16             73.4          140.4               Low        Healthy
17             34.2          192.8              High       Moderate
18             59.9          229.9               Low      Unhealthy
19             79.3          174.8               Low      Unhealthy

   Family_History  Need Supplement  Probability
0             Yes                0     0.094956
1             Yes                1     0.976667
2              No                1     0.776361
3             Yes                1     0.845500
4              No                1     0.863706
5              No                1     0.971000
6              No                1     0.868333
7             Yes                1     0.767333
8             Yes                1     0.675512
9             Yes                0     0.301254
10            Yes                0     0.268143
11             No                1     0.761373
12            Yes                1     0.716250
13            Yes                1     0.763500
14             No                0     0.277635
15            Yes                1     0.868333
16             No                0     0.281583
17             No                0     0.297345
18             No                1     0.703048
19             No                1     0.845278
```

[25]:
```
# Count of predictions
plt.figure(figsize=(8, 6))
```

```python
sns.countplot(x="Need Supplement", data=prediction_results)
plt.title("Distribution of Predictions")
plt.xticks([0, 1], ["No Need for Supplement", "Need Supplement"])
plt.show()

print("Prediction distribution:")
print(prediction_results["Need Supplement"].value_counts())
print("Percentage:")
print(prediction_results["Need Supplement"].value_counts(normalize=True) * 100)
```




```
Prediction distribution:
Need Supplement
1    14
0     6
Name: count, dtype: int64
Percentage:
Need Supplement
1    70.0
0    30.0
```

```
Name: proportion, dtype: float64
```

[26]:
```
# Save the predictions to Excel file
prediction_results.to_excel("predict_cholesterol_Gryko.xlsx", index=False)
```

2 6. Conclusion and Limitations

In this project, we developed a machine learning classification model to predict whether a patient needs a cholesterol-lowering supplement based on various health attributes.

2.1 Key findings:

1. We explored the data and found relationships between health metrics and the need for supplements
2. We built and compared four different machine learning models:
   - Random Forest
   - Gradient Boosting
   - Logistic Regression
   - Support Vector Machine
3. The Random Forest model performed best, achieving high accuracy in cross-validation

2.2 Limitations and Areas for Improvement:

1. **Data Leakage Issues**:
   - Using `Total_Cholesterol`, `LDL_Cholesterol`, and other cholesterol metrics as features creates circular logic, as these are likely the same values doctors use to prescribe supplements.
2. **Model Evaluation Concerns**:
   - The Random Forest achieved 100% accuracy on the test set, suggesting potential overfitting.
   - Our dataset is quite small (100 samples) with only 20 test samples, limiting reliable evaluation.
3. **Feature Selection Issues**:
   - We didn't address multicollinearity among cholesterol measurements.
   - More sophisticated feature selection methods could improve model interpretability.
4. **Preprocessing Limitations**:
   - No handling of outliers was performed despite their presence in several variables.
5. **Hyperparameter Tuning**:
   - The grid search explored a limited range of values.
6. **Clinical Interpretation**:
   - The prediction results show 70% of patients need supplements, but we haven't validated if this aligns with medical expectations.
   - No discussion of appropriate probability thresholds for clinical decision-making.
   - Limited integration with established medical guidelines for cholesterol management.

2.3 Next Steps:

- Collect more training data to improve model robustness

The current model should be viewed as a preliminary decision support tool that requires further validation before clinical application.