Random Forests in Practice

Data Science Lab

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Overview

Random forests are ensemble models that aggregate many decision trees to reduce variance and improve generalization.[1] This document walks through training and interpreting a random forest classifier in Python, with a mix of narrative, math, and visuals.

Mathematical Model

Each tree T_b is trained on a bootstrap sample $\mathcal{D}_b$ and a random subset of features. The forest prediction for a classification task with B trees is the majority vote:

[1] Introduced the random forest algorithm with theoretical justification and empirical benchmarks.

$$\hat{y} = \text{mode}\left(\{T_b(\mathbf{x})\}_{b=1}^{B}\right)$$

For regression, the trees are averaged:

$$\hat{y} = \frac{1}{B}\sum_{b=1}^{B} T_b(\mathbf{x})$$

The randomization across bootstrapped data and feature subsampling drives decorrelation between trees, delivering lower variance than single-tree models.

Environment Setup

```python
import importlib
import subprocess
import sys

def ensure(package):
    try:
        importlib.import_module(package)
    except ImportError:
        subprocess.check_call([sys.executable, "-m", "pip", "install", package])

for pkg in ("numpy", "pandas", "seaborn", "matplotlib", "scikit-learn"):
    ensure(pkg)
```

```
Requirement already satisfied: scikit-learn in /Users/luciusjmorningstar/Desktop/GIT-
REPOSITORY/JJB_Gallery/.venv/lib/python3.13/site-packages (1.7.2)
Requirement already satisfied: numpy>=1.22.0 in /Users/luciusjmorningstar/Desktop/GIT-
REPOSITORY/JJB_Gallery/.venv/lib/python3.13/site-packages (from scikit-
learn) (2.3.5)
Requirement already satisfied: scipy>=1.8.0 in /Users/luciusjmorningstar/Desktop/GIT-
REPOSITORY/JJB_Gallery/.venv/lib/python3.13/site-packages (from scikit-
learn) (1.16.3)
Requirement already satisfied: joblib>=1.2.0 in /Users/luciusjmorningstar/Desktop/GIT-
REPOSITORY/JJB_Gallery/.venv/lib/python3.13/site-packages (from scikit-
learn) (1.5.2)
Requirement already satisfied: threadpoolctl>=3.1.0 in /Users/luciusjmorningstar/Desktop/GIT-
REPOSITORY/JJB_Gallery/.venv/lib/python3.13/site-packages (from scikit-
learn) (3.6.0)
```

```python
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt

from sklearn.datasets import load_breast_cancer, make_classification
from sklearn.model_selection import train_test_split, cross_val_score
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import RocCurveDisplay, ConfusionMatrixDisplay, classification_report
from sklearn.decomposition import PCA
from sklearn.inspection import DecisionBoundaryDisplay

sns.set_theme(style="whitegrid")
```

Data Loading and Preparation

We will use the Breast Cancer Wisconsin dataset bundled with scikit-learn, which contains 30 features computed from digitized fine needle aspirate images.[2]

```python
dataset = load_breast_cancer(as_frame=True)
df = dataset.frame
df.head()
```

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mea
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.300
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.086
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.197
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.241
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.198

Split the data into training and testing sets (stratified to maintain label balance).

```python
X_train, X_test, y_train, y_test = train_test_split(
    df.drop(columns="target"),
    df["target"],
    test_size=0.25,
    random_state=42,
    stratify=df["target"]
```

[2] Official description of the dataset, feature definitions, and usage considerations.

```
)

X_train.shape, X_test.shape
```

```
((426, 30), (143, 30))
```

Model Training

```
rf = RandomForestClassifier(
    n_estimators=400,
    max_features="sqrt",
    min_samples_leaf=2,
    random_state=42,
    n_jobs=-1
)
rf.fit(X_train, y_train)
```

n_estimators	400
criterion	'gini'
max_depth	None
min_samples_split	2
min_samples_leaf	2
min_weight_fraction_leaf	0.0
max_features	'sqrt'
max_leaf_nodes	None
min_impurity_decrease	0.0
bootstrap	True
oob_score	False
n_jobs	-1
random_state	42
verbose	0
warm_start	False
class_weight	None
ccp_alpha	0.0
max_samples	None
monotonic_cst	None

Evaluate cross-validated training performance to estimate generalization ability.

```python
cv_scores = cross_val_score(rf, X_train, y_train, cv=5)
cv_scores.mean(), cv_scores.std()
```

```
(np.float64(0.9600547195622434), np.float64(0.020556647327639923))
```

Diagnostics

```python
y_pred = rf.predict(X_test)
print(classification_report(y_test, y_pred, target_names=dataset.target_names))
```

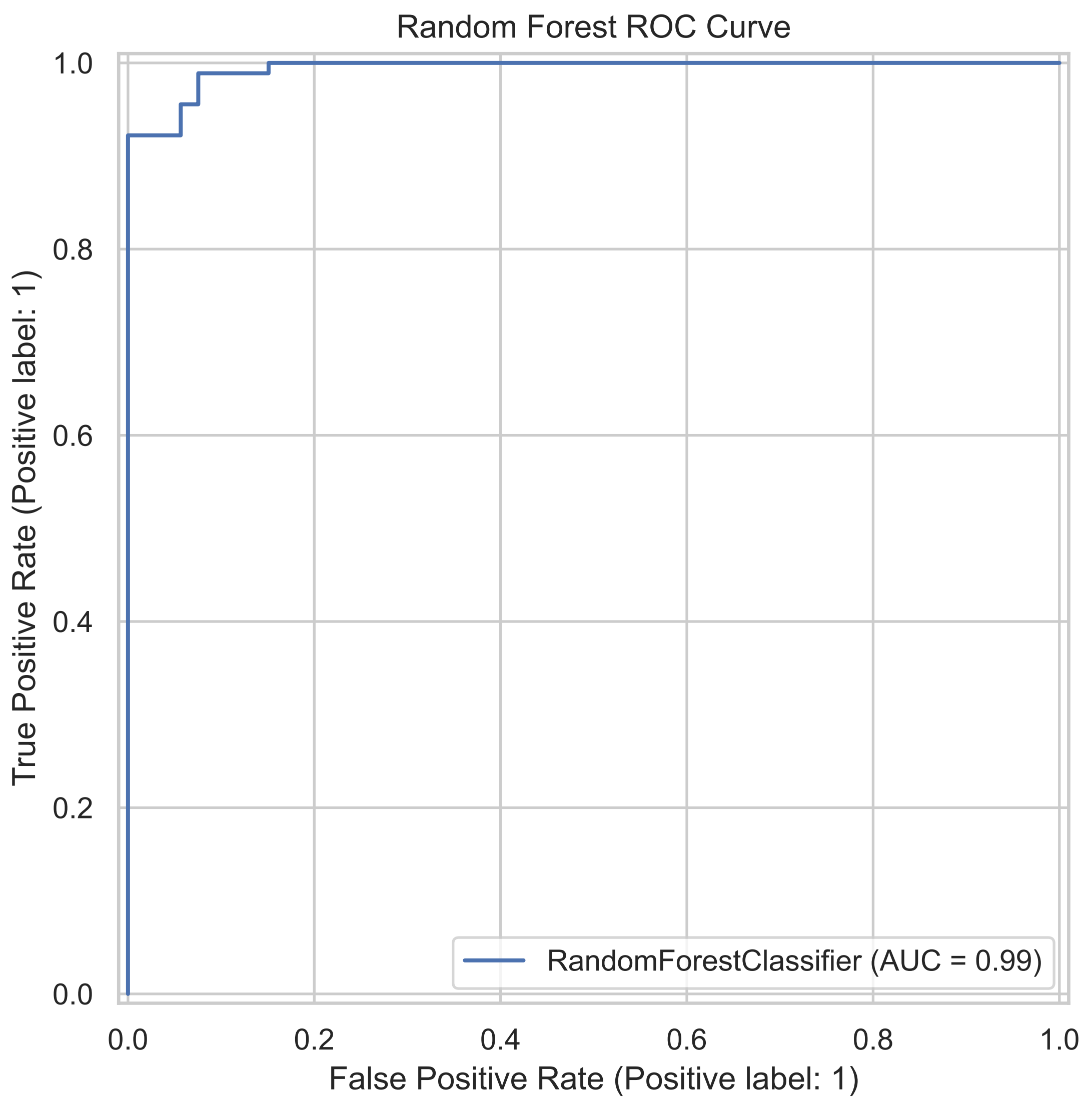
```
              precision    recall  f1-score   support

   malignant       0.96      0.92      0.94        53
      benign       0.96      0.98      0.97        90

    accuracy                           0.96       143
   macro avg       0.96      0.95      0.95       143
weighted avg       0.96      0.96      0.96       143
```

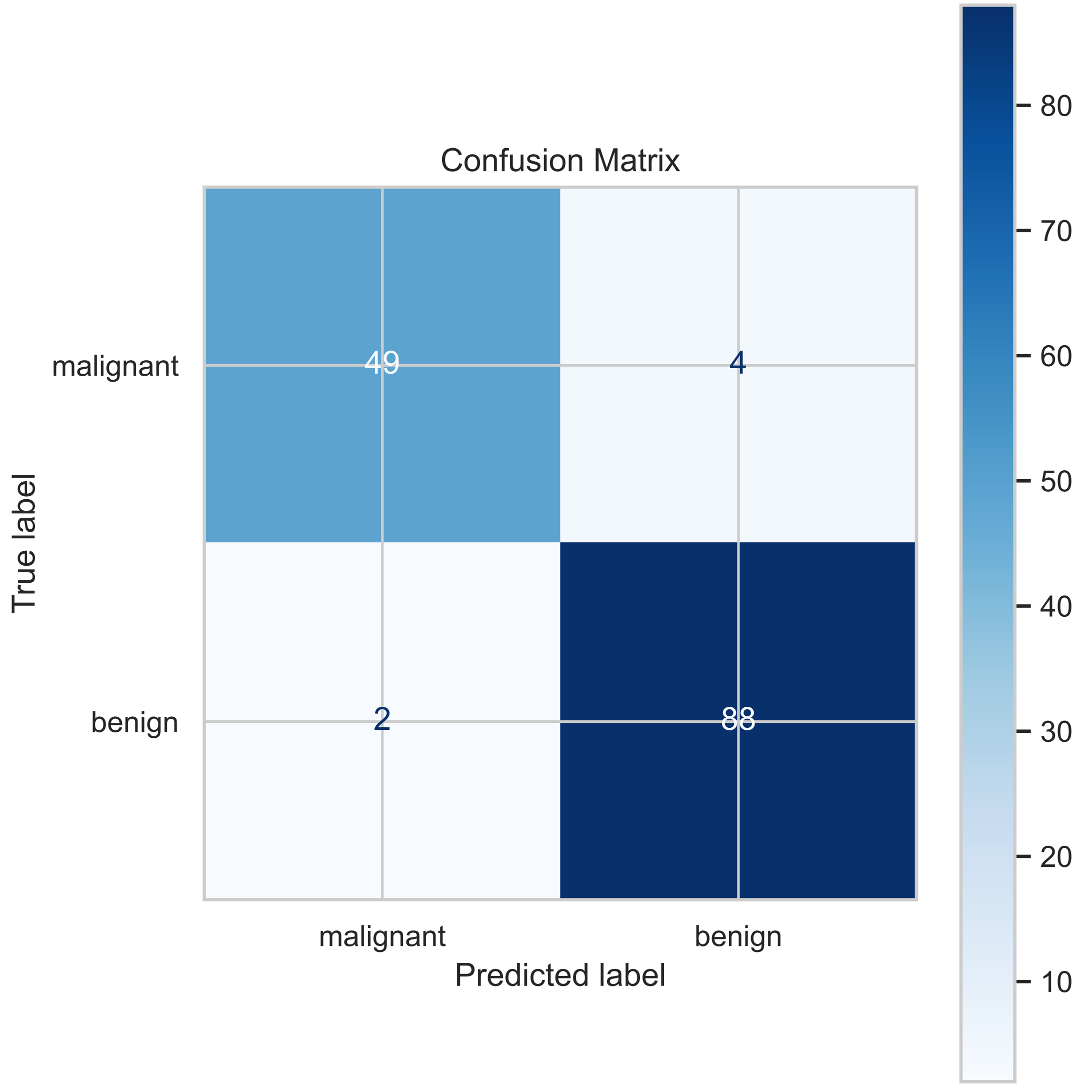
Receiver Operating Characteristic

```python
fig, ax = plt.subplots(figsize=(8, 6))
RocCurveDisplay.from_estimator(rf, X_test, y_test, ax=ax)
ax.set_title("Random Forest ROC Curve")
plt.tight_layout()
plt.show()
```



Confusion Matrix

```
fig, ax = plt.subplots(figsize=(6, 6))
ConfusionMatrixDisplay.from_estimator(rf, X_test, y_test, display_labels=dataset.target_names
ax.set_title("Confusion Matrix")
plt.tight_layout()
plt.show()
```

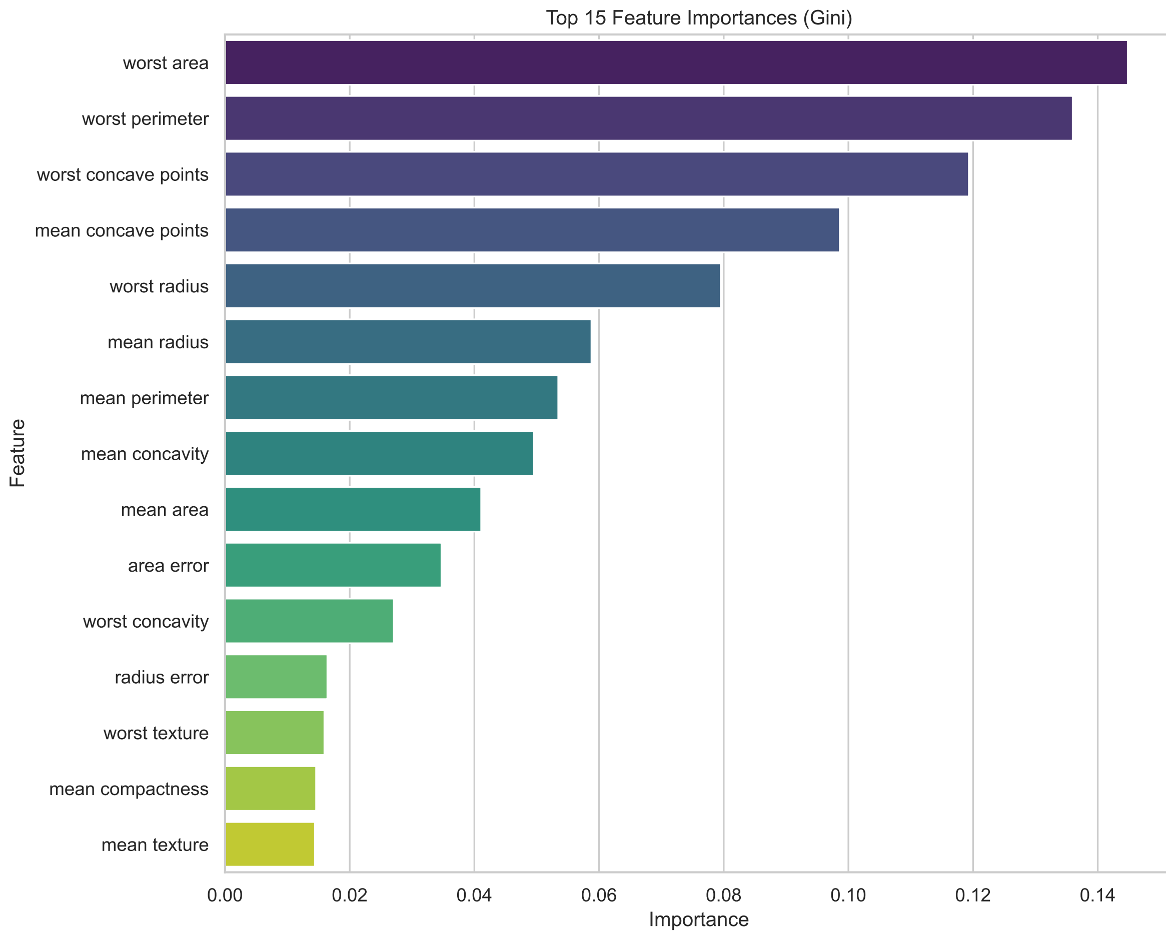


Feature Importance Visualization

```
importances = pd.Series(rf.feature_importances_, index=df.columns[:-1]).sort_values(ascending
top_features = importances.head(15)

plt.figure(figsize=(10, 8))
sns.barplot(x=top_features.values, y=top_features.index, palette="viridis")
plt.title("Top 15 Feature Importances (Gini)")
plt.xlabel("Importance")
```

```python
plt.ylabel("Feature")
plt.tight_layout()
plt.show()
```



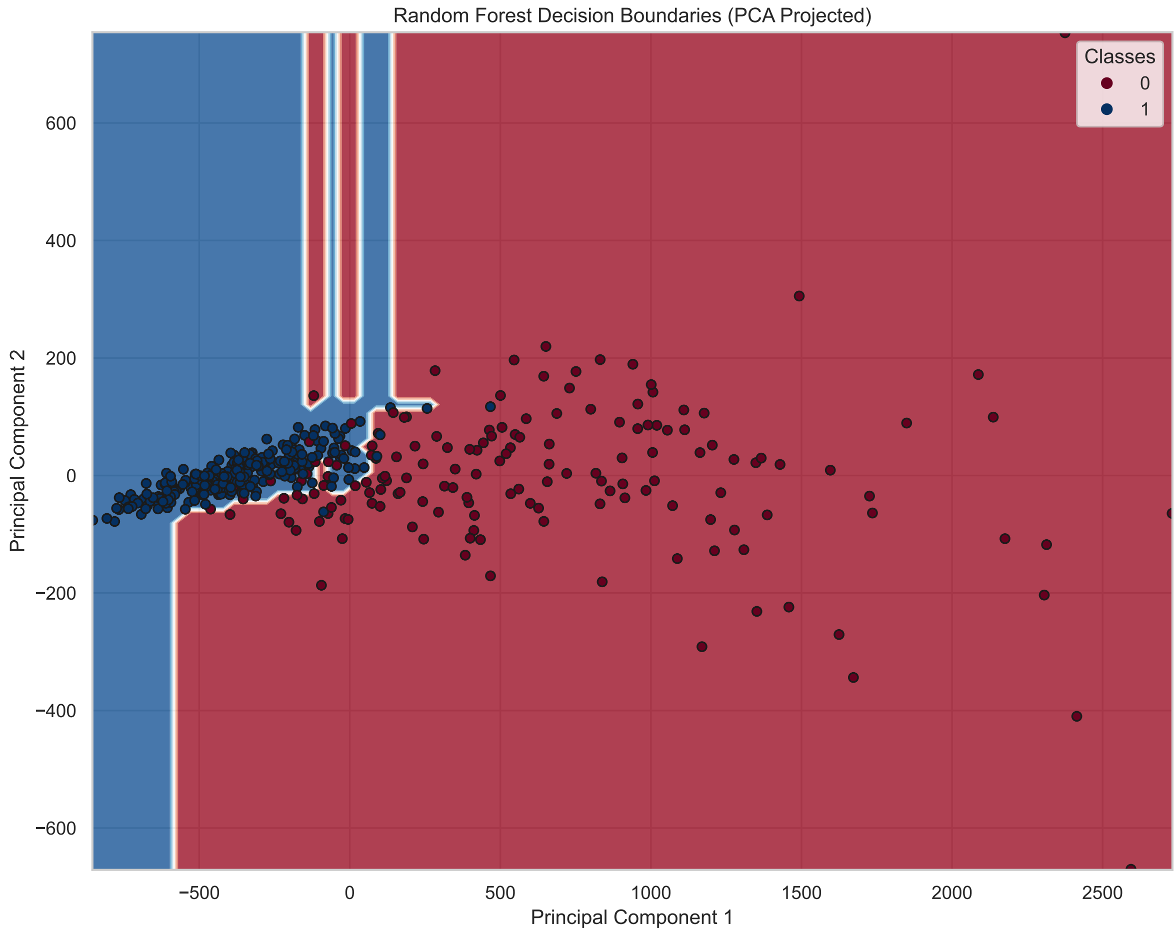
Complex Visualization: Decision Boundaries

To visualize the decision boundaries of the high-dimensional Random Forest model, we project the data onto its first two Principal Components (PCA). This allows us to see how the model separates classes in a 2D latent space.

```python
# PCA Projection
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_train)
```

```python
# Train a new RF on PCA components for visualization
rf_pca = RandomForestClassifier(n_estimators=100, random_state=42)
rf_pca.fit(X_pca, y_train)

# Plot Decision Boundary
fig, ax = plt.subplots(figsize=(10, 8))
DecisionBoundaryDisplay.from_estimator(
    rf_pca,
    X_pca,
    response_method="predict",
    cmap="RdBu",
    alpha=0.8,
    ax=ax,
    xlabel="Principal Component 1",
    ylabel="Principal Component 2",
)
scatter = ax.scatter(X_pca[:, 0], X_pca[:, 1], c=y_train, cmap="RdBu", edgecolors="k", s=30)
ax.set_title("Random Forest Decision Boundaries (PCA Projected)")
plt.legend(*scatter.legend_elements(), title="Classes")
plt.tight_layout()
plt.show()
```



Error Rate vs. Number of Trees

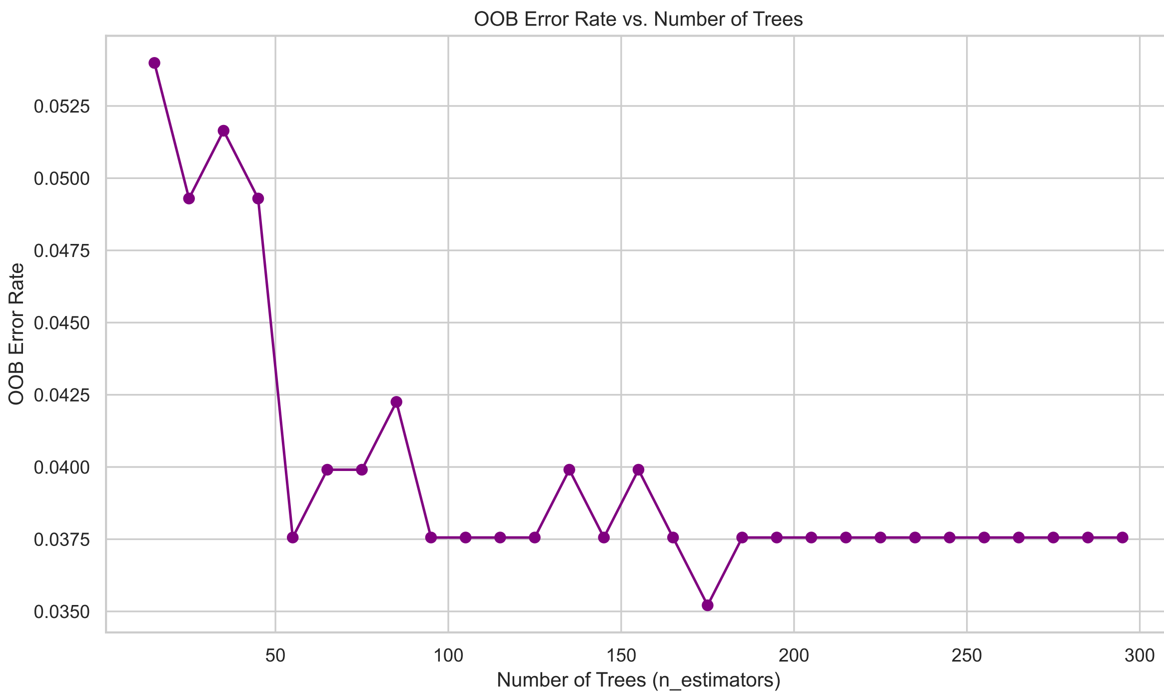
This graph illustrates how the model's Out-of-Bag (OOB) error rate stabilizes as the number of trees in the forest increases, demonstrating the ensemble effect.

```
n_estimators_range = range(15, 300, 10)
oob_errors = []

for n in n_estimators_range:
    rf_oob = RandomForestClassifier(n_estimators=n, warm_start=True, oob_score=True, random_s
    rf_oob.fit(X_train, y_train)
    oob_errors.append(1 - rf_oob.oob_score_)

plt.figure(figsize=(10, 6))
```

```
plt.plot(n_estimators_range, oob_errors, marker='o', linestyle='-', color='purple')
plt.title("OOB Error Rate vs. Number of Trees")
plt.xlabel("Number of Trees (n_estimators)")
plt.ylabel("OOB Error Rate")
plt.grid(True)
plt.tight_layout()
plt.show()
```



Hyperparameter Considerations

- `n_estimators`: Increasing trees generally improves stability until diminishing returns set in.
- `max_depth` or `min_samples_leaf`: Control tree complexity, mitigating overfitting.
- `max_features`: Governs the degree of feature randomness; `sqrt` is typical for classification.
- `class_weight`: Useful for imbalanced datasets to penalize misclassification of minority classes.

Grid search or Bayesian optimization can systematically explore these settings.[3]

[3] Demonstrated the efficiency gains of random search over grid search for hyperparameter tuning.

Practical Tips

- **Feature scaling**: Not required because trees are invariant to monotonic transformations.
- **Missing values**: scikit-learn's implementation does not handle NaNs; impute beforehand.
- **Interpretability**: Use SHAP values or permutation importance for richer explanations.
- **Out-of-bag (OOB) estimates**: Enable `oob_score=True` to get a built-in validation metric without a separate hold-out set.

References

- Breiman, L. (2001). Random forests. *Machine Learning*, 45(1), 5–32. https://doi.org/10.1023/A:1010933404324[4]
- scikit-learn Breast Cancer Dataset docs. https://scikit-learn.org/stable/datasets/toy_dataset.html[5]
- Bergstra, J., & Bengio, Y. (2012). Random search for hyper-parameter optimization. *Journal of Machine Learning Research*, 13, 281–305. https://jmlr.org/papers/v13/bergstra12a.html[6]

[4] b̆reiman2001
[5] ŝklearn_breast
[6] b̆ergstra2012