HIPERPARAMETER OPTIMIZATION

Optuna

Optuna es un framework de optimización automática de hiperparámetros diseñado para hacer que el proceso de ajuste de modelos de machine learning sea más eficiente y flexible. Aquí te detallo sus aspectos clave:

Conceptos Fundamentales:

Estudios (Studies): Un estudio en Optuna representa un proceso completo de optimización. Contiene todas las pruebas y los resultados asociados. Pruebas (Trials): Una prueba es un intento de evaluar un conjunto específico de hiperparámetros. Optuna explora diferentes combinaciones de hiperparámetros a través de múltiples pruebas. Función Objetivo: Debes definir una función objetivo que Optuna intentará minimizar o maximizar. Esta función generalmente evalúa el rendimiento de tu modelo utilizando un conjunto de validación. Características Distintivas:

Define-by-Run: Optuna permite definir el espacio de búsqueda de hiperparámetros de forma dinámica dentro de la función objetivo. Esto proporciona una gran flexibilidad, especialmente cuando los hiperparámetros dependen unos de otros. Algoritmos de Muestreo Eficientes: Optuna implementa algoritmos de muestreo avanzados que le permiten explorar el espacio de búsqueda de manera eficiente. Esto incluye algoritmos basados en procesos gaussianos y otros métodos bayesianos. Poda (Pruning): Optuna puede podar automáticamente las pruebas que muestran un rendimiento deficiente durante el entrenamiento. Esto ahorra tiempo y recursos al evitar la evaluación completa de combinaciones de hiperparámetros poco prometedoras. Visualizaciones: Optuna proporciona herramientas de visualización que te permiten analizar el proceso de optimización. Puedes ver la importancia de los hiperparámetros, la evolución del rendimiento y otras métricas útiles. Integración: Optuna se integra fácilmente con muchos frameworks de machine learning populares, como scikit-learn, TensorFlow, PyTorch y XGBoost. En resumen:

Optuna se destaca por su flexibilidad, eficiencia y facilidad de uso. Su capacidad "define-by-run" y sus algoritmos de muestreo avanzados lo convierten en una herramienta poderosa para la optimización de hiperparámetros en una amplia gama de aplicaciones de machine learning.

Visualizaciones incluidas:

Importancia de los hiperparámetros (plot_param_importances) Evolución del rendimiento a lo largo de las iteraciones (plot_optimization_history) Relaciones entre hiperparámetros y el rendimiento (plot_slice) Matriz de interacciones entre los hiperparámetros (plot_parallel_coordinate)

```
!pip install optuna
```

```
Collecting optuna
  Downloading optuna-4.2.1-py3-none-any.whl.metadata (17 kB)
Collecting alembic>=1.5.0 (from optuna)
  Downloading alembic-1.14.1-py3-none-any.whl.metadata (7.4 kB)
Collecting colorlog (from optuna)
  Downloading colorlog-6.9.0-py3-none-any.whl.metadata (10 kB)
Requirement already satisfied: numpy in /usr/local/lib/python3.11/dist-packages (from optuna) (1.26.
Requirement already satisfied: packaging>=20.0 in /usr/local/lib/python3.11/dist-packages (from optu
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Requirement already satisfied: tqdm in /usr/local/lib/python3.11/dist-packages (from optuna) (4.67.1
Requirement already satisfied: PyYAML in /usr/local/lib/python3.11/dist-packages (from optuna) (6.0.
Collecting Mako (from alembic>=1.5.0->optuna)
  Downloading Mako-1.3.9-py3-none-any.whl.metadata (2.9 kB)
Requirement already satisfied: typing-extensions>=4 in /usr/local/lib/python3.11/dist-packages (from
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Requirement already satisfied: greenlet!=0.4.17 in /usr/local/lib/python3.11/dist-packages (from sql
Requirement already satisfied: MarkupSafe>=0.9.2 in /usr/local/lib/python3.11/dist-packages (from Ma
Downloading optuna-4.2.1-py3-none-any.whl (383 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 383.6/383.6 kB 17.1 MB/s eta 0:00:00
Downloading alembic-1.14.1-py3-none-any.whl (233 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 233.6/233.6 kB 16.2 MB/s eta 0:00:00
Downloading colorlog-6.9.0-py3-none-any.whl (11 kB)
Downloading Mako-1.3.9-py3-none-any.whl (78 kB)
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Installing collected packages: Mako, colorlog, alembic, optuna
Successfully installed Mako-1.3.9 alembic-1.14.1 colorlog-6.9.0 optuna-4.2.1
```

```python
# Reimportar las bibliotecas necesarias para la optimización con Optuna
# Reimportar las bibliotecas necesarias después del reinicio
import pandas as pd
import numpy as np
import optuna
import joblib
import matplotlib.pyplot as plt
from sklearn.model_selection import KFold, cross_val_score, cross_val_predict
from sklearn.preprocessing import LabelEncoder
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.metrics import mean_absolute_error, mean_squared_error, r2_score

# Cargar los datos nuevamente
file_path = "DatosmodeloRaigrasfinalv10-yield.xlsx"
df = pd.read_excel(file_path)

# Seleccionar las variables predictoras y la variable objetivo
features = ['Localidad', 'Cultivar', 'Tmax(ºC)', 'Tmin(ºC)', 'Precipitación(mm)', 'Radiación(MJ/m2 dia)
target = 'kg MS/ha'

# Codificar las variables categóricas
label_encoders = {}
for col in ['Localidad', 'Cultivar']:
    le = LabelEncoder()
    df[col] = le.fit_transform(df[col])
    label_encoders[col] = le

# Definir X e y
X = df[features]
y = df[target]

# Configurar validación cruzada
kf = KFold(n_splits=5, shuffle=True, random_state=42)

# Definir la función objetivo para la optimización con Optuna
def objective(trial):
    # Definir los hiperparámetros a optimizar
    n_estimators = trial.suggest_int('n_estimators', 50, 300, step=50)
    max_depth = trial.suggest_int('max_depth', 2, 6)
    learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
    subsample = trial.suggest_float('subsample', 0.7, 1.0)

    # Crear el modelo con los hiperparámetros sugeridos
    model = GradientBoostingRegressor(
        n_estimators=n_estimators,
        max_depth=max_depth,
        learning_rate=learning_rate,
        subsample=subsample,
        random_state=42
    )

    # Evaluar el modelo con validación cruzada
```

```
    # Evaluar el modelo con validación cruzada
    score = cross_val_score(model, X, y, cv=kf, scoring='r2').mean()

    return score

# Ejecutar la optimización con Optuna
study = optuna.create_study(direction='maximize')
study.optimize(objective, n_trials=20, n_jobs=-1)

# Obtener los mejores hiperparámetros encontrados
best_params = study.best_params

# Ajustar el mejor modelo con los hiperparámetros óptimos
best_model = GradientBoostingRegressor(
    n_estimators=best_params['n_estimators'],
    max_depth=best_params['max_depth'],
    learning_rate=best_params['learning_rate'],
    subsample=best_params['subsample'],
    random_state=42
)

# Evaluar el mejor modelo con validación cruzada
y_pred_best = cross_val_predict(best_model, X, y, cv=kf)

# Calcular métricas de evaluación para el mejor modelo
mae_best = mean_absolute_error(y, y_pred_best)
mse_best = mean_squared_error(y, y_pred_best)
rmse_best = np.sqrt(mse_best)
r2_best = r2_score(y, y_pred_best)

# Ajustar el modelo final con todos los datos
best_model.fit(X, y)

# Guardar el modelo ajustado con Optuna
model_optuna_path = "gradient_boosting_optuna.pkl"
joblib.dump(best_model, model_optuna_path)

# Obtener importancia de las variables del mejor modelo
importances_best = best_model.feature_importances_
importance_df_best = pd.DataFrame({"Variable": features, "Importancia": importances_best})
importance_df_best = importance_df_best.sort_values(by="Importancia", ascending=False)

# Gráfica de importancia de las variables
plt.figure(figsize=(8, 6))
plt.barh(importance_df_best["Variable"], importance_df_best["Importancia"], color='blue')
plt.xlabel("Importancia")
plt.ylabel("Variable")
plt.title("Importancia de las variables GBR-Optuna")
plt.gca().invert_yaxis()
plt.show()

# Gráfica de valores predichos vs reales
plt.figure(figsize=(8, 6))
plt.scatter(y, y_pred_best, color='blue', alpha=0.6, label="Predicciones")
plt.plot([min(y), max(y)], [min(y), max(y)], 'k--', lw=1, label="Línea de igualdad")
plt.grid(True, linestyle='--', linewidth=0.7, alpha=0.8)
plt.gca().set_axisbelow(False)
plt.xlabel("Valores reales")
plt.ylabel("Valores predichos")
plt.title("Valores predichos vs Valores reales (GBR-Optuna)")
plt.legend()

plt.show()

# Mostrar resultados
```

```
# Mostrar resultados
{
    "Mejores hiperparámetros": best_params,
    "Métricas mejor modelo": {"MAE": mae_best, "MSE": mse_best, "RMSE": rmse_best, "R²": r2_best},
    "Enlace modelo optimizado": model_optuna_path
}

```

```
[I 2025-02-26 12:34:11,863] A new study created in memory with name: no-name-82e2704d-af8b-4bba-87
<ipython-input-3-d309168c95c4>:40: FutureWarning: suggest_loguniform has been deprecated in v3.0.0
  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:14,717] Trial 1 finished with value: 0.3780354268462 9293 and parameters: {'n_e
<ipython-input-3-d309168c95c4>:40: FutureWarning: suggest_loguniform has been deprecated in v3.0.0
  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:15,510] Trial 2 finished with value: 0.21828817917384918 and parameters: {'n_e
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[I 2025-02-26 12:34:16,603] Trial 0 finished with value: 0.3709731216736175 and parameters: {'n_es
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[I 2025-02-26 12:34:18,942] Trial 3 finished with value: 0.3287380612155505 and parameters: {'n_es
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:20,716] Trial 5 finished with value: 0.3956715520472781 and parameters: {'n_es
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[I 2025-02-26 12:34:20,838] Trial 4 finished with value: 0.3950359418868644 and parameters: {'n_es
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:23,146] Trial 7 finished with value: 0.4543273795133831 and parameters: {'n_es
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:24,587] Trial 6 finished with value: 0.4698507958041433 and parameters: {'n_es
<ipython-input-3-d309168c95c4>:40: FutureWarning: suggest_loguniform has been deprecated in v3.0.0
  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:27,690] Trial 9 finished with value: 0.49707816040410313 and parameters: {'n_e
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:27,741] Trial 8 finished with value: 0.4891478890179135 and parameters: {'n_es
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:29,160] Trial 11 finished with value: 0.41800917973382334 and parameters: {'n_
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:31,406] Trial 10 finished with value: 0.42170339087326825 and parameters: {'n_
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:34,714] Trial 12 finished with value: 0.5018300071803087 and parameters: {'n_e
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:35,338] Trial 13 finished with value: 0.5196799875590832 and parameters: {'n_e
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:38,687] Trial 14 finished with value: 0.5163953224382815 and parameters: {'n_e
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:39,210] Trial 15 finished with value: 0.5208426342096113 and parameters: {'n_e
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:41,612] Trial 16 finished with value: 0.5052227058167237 and parameters: {'n_e
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:42,713] Trial 17 finished with value: 0.4478105114180676 and parameters: {'n_e
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  learning_rate = trial.suggest_loguniform('learning_rate', 0.01, 0.2)
[I 2025-02-26 12:34:44,195] Trial 18 finished with value: 0.46640645026252747 and parameters: {'n_
[I 2025-02-26 12:34:44,619] Trial 19 finished with value: 0.49389771031118784 and parameters: {'n_
```

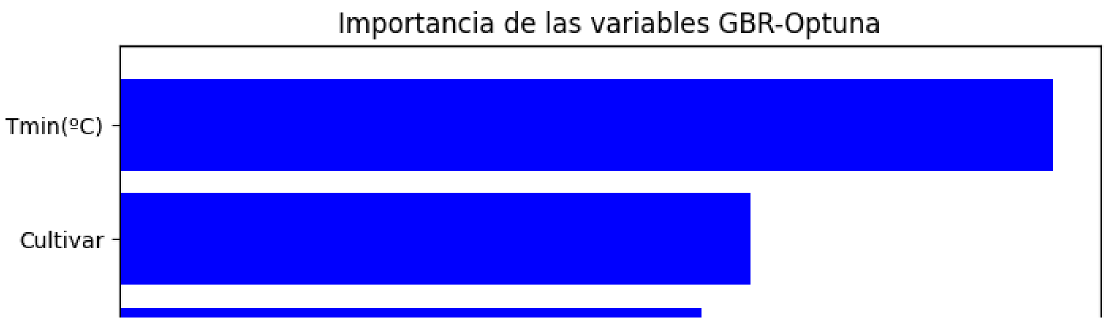

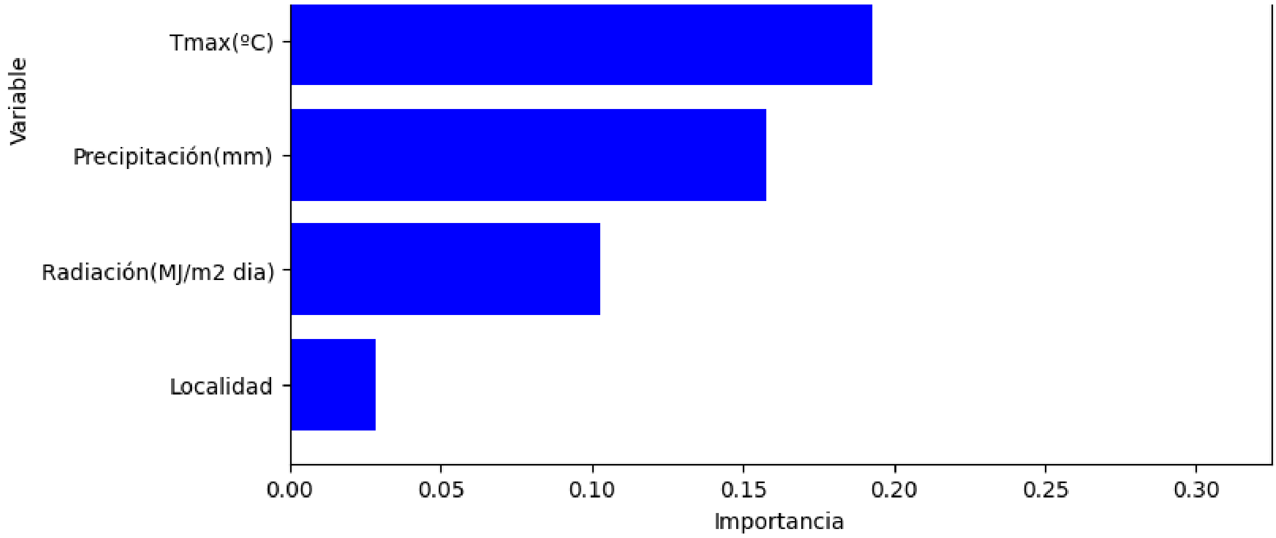

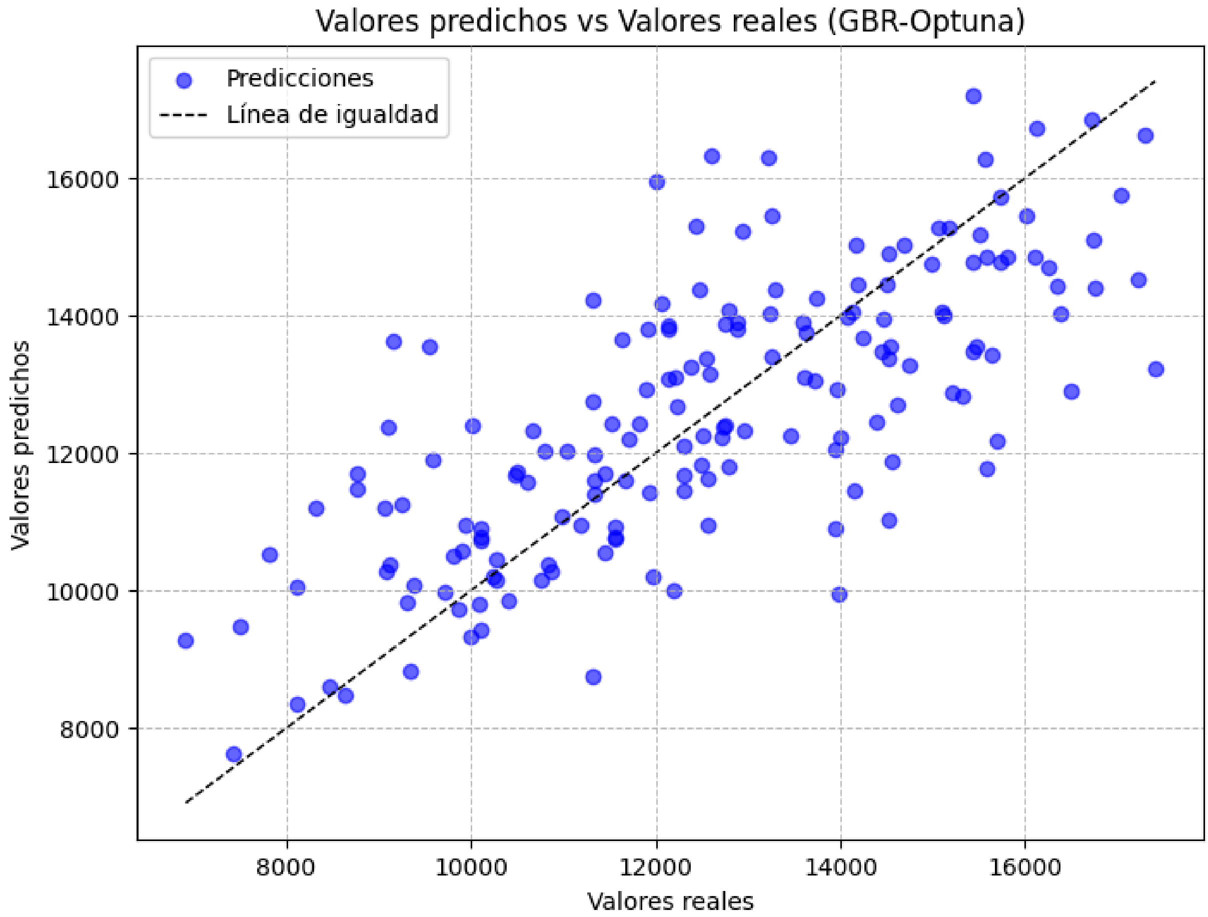


```
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  'R²': 0.5363647102030626},
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```