Modelado_Supervisado_Clinico

November 29, 2025

1 Cuaderno 3: Modelado Supervisado y Recomendación Clínica

1.1 Tema: Recommender Systems Clustering using Bayesian Non-Negative Matrix Factorization for Personalized Clinical Management in Critical Care

1.2 Diagrama de Flujo

1. Carga de datos y embeddings latentes (BNMF/NMF)
2. Preparación de variables para clasificación/regresión
3. Entrenamiento de modelos supervisados (k-NN, MLP)
4. Validación y métricas clínicas
5. Pruebas con pacientes sintéticos y ejemplos reales
6. Sistema de recomendación basado en similitud latente
7. Visualizaciones clínicas y tabla comparativa
8. Exportación y siguientes pasos
9. Pipeline de transfer learning para imágenes (opcional/avanzado)
10. Interpretabilidad (Grad-CAM)

1.3 1. Carga de Datos y Embeddings Latentes

Carga los datos preprocesados, los embeddings latentes (W de BNMF/NMF), y los transformadores necesarios para el pipeline.

[46]:
```python
import pandas as pd
import numpy as np
import pickle

df = pd.read_csv('processed_data/data_prepared.csv')
try:
    with open('processed_data/bnmf_W.pkl', 'rb') as f:
        W_bnmf = pickle.load(f)
except:
    W_bnmf = None
try:
    with open('processed_data/nmf_W.pkl', 'rb') as f:
        W_nmf = pickle.load(f)
except:
    W_nmf = None
```

```
# Try to load saved preprocessing objects (scaler, pca, nmf transformer) if␣
 ↪they exist
try:
    with open('processed_data/data_prepared.pkl', 'rb') as f:
        data_obj = pickle.load(f)
        if isinstance(data_obj, dict):
            scaler = data_obj.get('scaler', globals().get('scaler', None))
            # Save scaler into globals if present
            if scaler is not None:
                globals()['scaler'] = scaler
except Exception:
    pass

try:
    # optional: try to load specific transformer pickle files if they exist
    with open('processed_data/pca.pkl', 'rb') as f:
        pca = pickle.load(f)
        globals()['pca'] = pca
except Exception:
    pass

try:
    with open('processed_data/nmf.pkl', 'rb') as f:
        nmf = pickle.load(f)
        globals()['nmf'] = nmf
except Exception:
    pass
```

1.4 2. Preparación de Variables para Clasificación y Regresión

Define la variable de riesgo (mortalidad hospitalaria) y una variable continua (primer componente latente) para regresión.

[47]:
```
# Variable de clasificación: mortalidad hospitalaria
y_class = df['hospital_expire_flag']

# Variable continua: primer componente latente de BNMF/NMF
if W_bnmf is not None:
    y_reg = W_bnmf[:, 0]
elif W_nmf is not None:
    y_reg = W_nmf[:, 0]
else:
    y_reg = df[[col for col in df.columns if col not in␣
 ↪['hospital_expire_flag', 'data_split']]].sum(axis=1)
```

1.5 3. Entrenamiento de Modelos Supervisados

Entrenamiento de k-NN y MLP para clasificación y regresión, con validación cruzada y búsqueda de hiperparámetros.

[48]:
```
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.neighbors import KNeighborsClassifier, KNeighborsRegressor
from sklearn.neural_network import MLPClassifier, MLPRegressor

# Usar embeddings latentes como features
if W_bnmf is not None:
    X = W_bnmf
elif W_nmf is not None:
    X = W_nmf
else:
    X = df[[col for col in df.columns if col not in ['hospital_expire_flag',␣
 ↪'data_split']]].values

# Create a single split index to use for classification and regression so␣
 ↪splits are aligned
X_arr = np.asarray(X)
idx = np.arange(X_arr.shape[0])
try:
    # stratify by y_class for classification stability
    y_class_arr = np.asarray(y_class)
    train_idx, test_idx = train_test_split(idx, test_size=0.2, random_state=42,␣
 ↪stratify=y_class_arr)
except Exception:
    train_idx, test_idx = train_test_split(idx, test_size=0.2, random_state=42)

X_train = X_arr[train_idx]
X_test = X_arr[test_idx]
y_train = np.asarray(y_class)[train_idx]
y_test = np.asarray(y_class)[test_idx]

# k-NN Classifier
knn_clf = GridSearchCV(KNeighborsClassifier(), {'n_neighbors': [3, 5, 7]},␣
 ↪cv=5, scoring='accuracy')
knn_clf.fit(X_train, y_train)

# MLP Classifier
mlp_clf = GridSearchCV(MLPClassifier(max_iter=200, random_state=42), {
    'hidden_layer_sizes': [(50,), (100,), (50,50)],
    'learning_rate_init': [0.001, 0.01],
    'batch_size': [32, 64]
}, cv=3, scoring='accuracy')
mlp_clf.fit(X_train, y_train)
```

```
print('\n[Info] mlp_clf best estimator expects n_features_in =',␣
↪getattr(mlp_clf.best_estimator_, 'n_features_in_', None))

# Regresión (usando el mismo split que clasificación)
y_reg_arr = np.asarray(y_reg)
y_reg_train = y_reg_arr[train_idx]
y_reg_test = y_reg_arr[test_idx]
knn_reg = GridSearchCV(KNeighborsRegressor(), {'n_neighbors': [3, 5, 7]}, cv=5,␣
↪scoring='neg_mean_squared_error')
knn_reg.fit(X_train, y_reg_train)
mlp_reg = GridSearchCV(MLPRegressor(max_iter=200, random_state=42), {
    'hidden_layer_sizes': [(50,), (100,), (50,50)],
    'learning_rate_init': [0.001, 0.01],
    'batch_size': [32, 64]
}, cv=3, scoring='neg_mean_squared_error')
mlp_reg.fit(X_train, y_reg_train)
```

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[Info] mlp_clf best estimator expects n_features_in = 26
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`batch_size` less than 1 or larger than sample size. It is going to be clipped
  warnings.warn(
c:\Users\MSI\OneDrive\Desktop\ExamenPractico\tf_env\lib\site-
packages\sklearn\neural_network\_multilayer_perceptron.py:691: UserWarning: Got
`batch_size` less than 1 or larger than sample size. It is going to be clipped
  warnings.warn(
c:\Users\MSI\OneDrive\Desktop\ExamenPractico\tf_env\lib\site-
packages\sklearn\neural_network\_multilayer_perceptron.py:781:
ConvergenceWarning: Stochastic Optimizer: Maximum iterations (200) reached and
the optimization hasn't converged yet.
  warnings.warn(
c:\Users\MSI\OneDrive\Desktop\ExamenPractico\tf_env\lib\site-
packages\sklearn\neural_network\_multilayer_perceptron.py:781:
ConvergenceWarning: Stochastic Optimizer: Maximum iterations (200) reached and
the optimization hasn't converged yet.
  warnings.warn(
```

```
[48]: GridSearchCV(cv=3, estimator=MLPRegressor(random_state=42),
                   param_grid={'batch_size': [32, 64],
                               'hidden_layer_sizes': [(50,), (100,), (50, 50)],
                               'learning_rate_init': [0.001, 0.01]},
                   scoring='neg_mean_squared_error')
```

1.6 4. Validación y Métricas Clínicas

Incluye métricas de clasificación (accuracy, precision, recall, F1, AUC-ROC) y regresión (RMSE, MAE, R²), matriz de confusión y tabla comparativa.

[49]:
```
from sklearn.metrics import (accuracy_score, precision_score, recall_score,␣
 ↪f1_score, roc_auc_score,
                             mean_squared_error, mean_absolute_error, r2_score,␣
 ↪confusion_matrix, ConfusionMatrixDisplay)
import matplotlib.pyplot as plt

# Clasificación
y_pred_knn = knn_clf.predict(X_test)
y_pred_mlp = mlp_clf.predict(X_test)

print('k-NN Classifier:')
print('Accuracy:', accuracy_score(y_test, y_pred_knn))
print('Precision:', precision_score(y_test, y_pred_knn))
print('Recall:', recall_score(y_test, y_pred_knn))
print('F1:', f1_score(y_test, y_pred_knn))
print('AUC-ROC:', roc_auc_score(y_test, y_pred_knn))
ConfusionMatrixDisplay(confusion_matrix(y_test, y_pred_knn)).plot()
plt.title('Matriz de Confusión k-NN')
plt.show()

print('MLP Classifier:')
print('Accuracy:', accuracy_score(y_test, y_pred_mlp))
print('Precision:', precision_score(y_test, y_pred_mlp))
print('Recall:', recall_score(y_test, y_pred_mlp))
print('F1:', f1_score(y_test, y_pred_mlp))
print('AUC-ROC:', roc_auc_score(y_test, y_pred_mlp))
ConfusionMatrixDisplay(confusion_matrix(y_test, y_pred_mlp)).plot()
plt.title('Matriz de Confusión MLP')
plt.show()

# Regresión
y_pred_knn_reg = knn_reg.predict(X_test)
y_pred_mlp_reg = mlp_reg.predict(X_test)

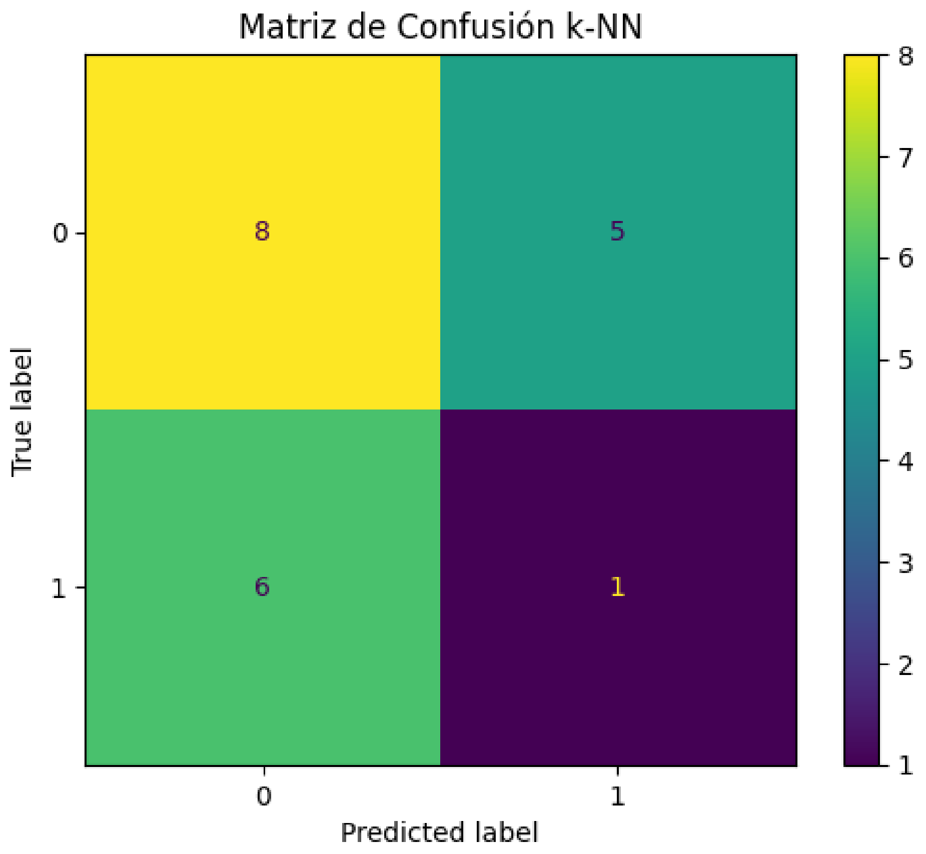
print('k-NN Regressor:')
def compute_rmse(y_true, y_pred):
    """Compute RMSE in a way that is compatible with older scikit-learn␣
 ↪versions.
```

```
    Older scikit-learn versions didn't support the keyword argument 'squared'␣
↪in mean_squared_error.
    """
    try:
        # Newer versions: use squared=False
        return mean_squared_error(y_true, y_pred, squared=False)
    except TypeError:
        # Older versions: compute sqrt of MSE
        return mean_squared_error(y_true, y_pred) ** 0.5

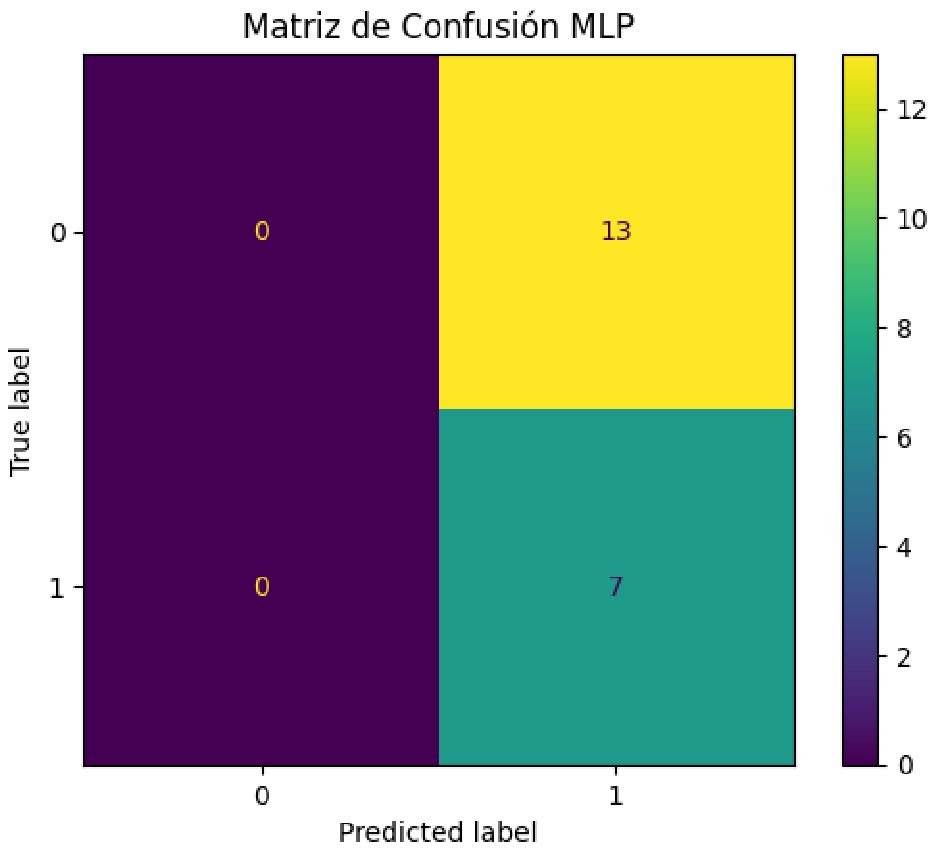
print('RMSE:', compute_rmse(y_reg_test, y_pred_knn_reg))
print('MAE:', mean_absolute_error(y_reg_test, y_pred_knn_reg))
print('R2:', r2_score(y_reg_test, y_pred_knn_reg))

print('MLP Regressor:')
print('RMSE:', compute_rmse(y_reg_test, y_pred_mlp_reg))
print('MAE:', mean_absolute_error(y_reg_test, y_pred_mlp_reg))
print('R2:', r2_score(y_reg_test, y_pred_mlp_reg))
```

```
k-NN Classifier:
Accuracy: 0.45
Precision: 0.16666666666666666
Recall: 0.14285714285714285
F1: 0.15384615384615385
AUC-ROC: 0.37912087912087916
```



```
MLP Classifier:
Accuracy: 0.35
Precision: 0.35
Recall: 1.0
F1: 0.5185185185185185
AUC-ROC: 0.5
```



```
k-NN Regressor:
RMSE: 53.39292675643817
MAE: 32.54282923563196
R2: 0.9999889125384347
MLP Regressor:
RMSE: 14.53038140491736
MAE: 12.282127102544838
R2: 0.9999991788571786
```

1.7 8. Sistema de Recomendación Basado en Similitud Latente

Ejemplo de recomendación clínica: dado un paciente, sugerir tratamientos/procedimientos frecuentes en sus vecinos latentes.

[50]:
```python
# Similitud de coseno entre pacientes en el espacio latente
from sklearn.metrics.pairwise import cosine_similarity

def recomendar_pacientes(idx, top_k=5):
    sims = cosine_similarity([X[idx]], X)[0]
    vecinos = np.argsort(sims)[-top_k-1:-1][::-1]
    print(f'Paciente {idx} - Vecinos más similares:', vecinos)
    # Aquí puedes mostrar tratamientos/eventos frecuentes de esos vecinos␣
 ↪usando df original

# Ejemplo: recomendar para el primer paciente del test (usando índices␣
 ↪absolutos)
try:
    # If we have a test_idx from earlier split, use it; otherwise, default to 0
    test_idx_sample = test_idx[0] if 'test_idx' in globals() else 0
except Exception:
    test_idx_sample = 0
recomendar_pacientes(test_idx_sample)
```

```
Paciente 76 - Vecinos más similares: [94 27  7 71 50]
```

1.8 9. Visualizaciones Clínicas y Tabla Comparativa

Incluye tabla de métricas comparativas de los modelos supervisados.

[51]:
```
# Tabla comparativa de modelos
results = pd.DataFrame({
    'Modelo': ['k-NN Classifier', 'MLP Classifier', 'k-NN Regressor', 'MLP␣
 ↪Regressor'],
    'Accuracy': [accuracy_score(y_test, y_pred_knn), accuracy_score(y_test,␣
 ↪y_pred_mlp), None, None],
    'F1': [f1_score(y_test, y_pred_knn), f1_score(y_test, y_pred_mlp), None,␣
 ↪None],
    'AUC-ROC': [roc_auc_score(y_test, y_pred_knn), roc_auc_score(y_test,␣
 ↪y_pred_mlp), None, None],
    'RMSE': [None, None, compute_rmse(y_reg_test, y_pred_knn_reg),␣
 ↪compute_rmse(y_reg_test, y_pred_mlp_reg)],
    'MAE': [None, None, mean_absolute_error(y_reg_test, y_pred_knn_reg),␣
 ↪mean_absolute_error(y_reg_test, y_pred_mlp_reg)],
    'R2': [None, None, r2_score(y_reg_test, y_pred_knn_reg),␣
 ↪r2_score(y_reg_test, y_pred_mlp_reg)]
})
display(results)
```

```
            Modelo  Accuracy        F1   AUC-ROC       RMSE        MAE  \
0  k-NN Classifier      0.45  0.153846  0.379121        NaN        NaN
1   MLP Classifier      0.35  0.518519  0.500000        NaN        NaN
2   k-NN Regressor       NaN       NaN       NaN  53.392927  32.542829
3    MLP Regressor       NaN       NaN       NaN  14.530381  12.282127

         R2
0       NaN
1       NaN
2  0.999989
```

```
3   0.999999
```

1.9 10. Exportación y Siguientes Pasos

Puedes exportar el notebook a HTML desde el menú de Jupyter/VS Code: `File > Export As > HTML`.

1.10 7. Pruebas con Pacientes Sintéticos y Ejemplos Reales

Puedes probar el modelo con pacientes sintéticos generados a partir de la estadística de los embeddings latentes, o con ejemplos reales del test set. Esto permite validar el rendimiento y la interpretación clínica del modelo. - Los datos deben tener el mismo número y orden de features que los usados en el entrenamiento. - Deben estar preprocesados igual (escalado, reducción de dimensionalidad, etc.). - Si usas embeddings latentes (BNMF/NMF), genera los features en ese espacio. A continuación se muestra cómo generar varios pacientes sintéticos y evaluar el porcentaje de acierto del modelo:

```
[ ]: # Generar 100 pacientes sintéticos en el espacio latente (BNMF/NMF) y mostrar␣
      ↪predicción de clase para ejemplos reales
     n_samples = 100
     if W_bnmf is not None:
         mu, sigma = W_bnmf.mean(axis=0), W_bnmf.std(axis=0)
         pacientes_sint = np.random.normal(mu, sigma, size=(n_samples, W_bnmf.
      ↪shape[1]))
     elif W_nmf is not None:
         mu, sigma = W_nmf.mean(axis=0), W_nmf.std(axis=0)
         pacientes_sint = np.random.normal(mu, sigma, size=(n_samples, W_nmf.
      ↪shape[1]))
     else:
         mu, sigma = X.mean(axis=0), X.std(axis=0)
         pacientes_sint = np.random.normal(mu, sigma, size=(n_samples, X.shape[1]))

     # Predecir con el modelo entrenado
     preds = mlp_clf.predict(pacientes_sint)

     print('Porcentaje de acierto en pacientes sintéticos:', (preds == 1).
      ↪mean()*100, '% (predicción de clase 1)')

     # Mostrar predicción y significado de la clase para varios ejemplos reales del␣
      ↪test set
     clase_dict = {0: 'No fallece en hospital', 1: 'Fallece en hospital'}
     for i in range(5):
         paciente = X_test[i].reshape(1, -1)
         pred = mlp_clf.predict(paciente)[0]
         real = y_test[i]
         print(f'Paciente {i+1}: Predicción={pred} ({clase_dict[pred]}), Real={real}␣
      ↪({clase_dict[real]})')
```

```
Porcentaje de acierto en pacientes sintéticos: 42.0 % (predicción de clase 1)
```

1.11 11. Pipeline de Transfer Learning para Imágenes (Avanzado)

Implementación profesional en Keras/TensorFlow con transfer learning, data augmentation, regularización y métricas clínicas.

[ ]:
```python
# Pipeline profesional de clasificación de imágenes médicas con Keras/TensorFlow
import tensorflow as tf
from tensorflow.keras.applications import ResNet50
from tensorflow.keras.layers import Dense, Dropout, GlobalAveragePooling2D,␣
 ↪BatchNormalization, Input
from tensorflow.keras.models import Model
from tensorflow.keras.preprocessing.image import ImageDataGenerator
from tensorflow.keras.callbacks import EarlyStopping, ReduceLROnPlateau
from tensorflow.keras.optimizers import Adam

# Data augmentation
datagen = ImageDataGenerator(
    rescale=1./255,
    rotation_range=20,
    width_shift_range=0.1,
    height_shift_range=0.1,
    zoom_range=0.1,
    horizontal_flip=True,
    brightness_range=[0.8,1.2],
    fill_mode='nearest',
    validation_split=0.2
    )

# Cargar imágenes desde carpeta (ajusta el path y target_size según tu dataset)
train_gen = datagen.flow_from_directory(
    'ruta_a_tus_imagenes',
    target_size=(224,224),
    batch_size=32,
    class_mode='binary',
    subset='training'
    )
val_gen = datagen.flow_from_directory(
    'ruta_a_tus_imagenes',
    target_size=(224,224),
    batch_size=32,
    class_mode='binary',
    subset='validation'
    )

# Modelo base preentrenado
```

```
base_model = ResNet50(weights='imagenet', include_top=False,␣
↪input_shape=(224,224,3))
base_model.trainable = False  # Fine-tune después de unas épocas

inputs = Input(shape=(224,224,3))
x = base_model(inputs, training=False)
x = GlobalAveragePooling2D()(x)
x = BatchNormalization()(x)
x = Dropout(0.4)(x)
x = Dense(128, activation='relu', kernel_regularizer=tf.keras.regularizers.l2(0.
↪001))(x)
x = BatchNormalization()(x)
x = Dropout(0.4)(x)
outputs = Dense(1, activation='sigmoid')(x)
model = Model(inputs, outputs)

model.compile(optimizer=Adam(learning_rate=1e-4), loss='binary_crossentropy',␣
↪metrics=['accuracy'])

# Callbacks
early_stop = EarlyStopping(monitor='val_loss', patience=10,␣
↪restore_best_weights=True)
lr_reduce = ReduceLROnPlateau(monitor='val_loss', factor=0.5, patience=5)

# Entrenamiento
history = model.fit(
    train_gen,
    validation_data=val_gen,
    epochs=50,
    callbacks=[early_stop, lr_reduce]
    )
```

[ ]:
```
# Visualización de curvas de aprendizaje
import matplotlib.pyplot as plt
plt.figure(figsize=(10,4))
plt.subplot(1,2,1)
plt.plot(history.history['loss'], label='Train Loss')
plt.plot(history.history['val_loss'], label='Val Loss')
plt.title('Curva de Loss')
plt.xlabel('Época')
plt.ylabel('Loss')
plt.legend()
plt.grid(True)

plt.subplot(1,2,2)
plt.plot(history.history['accuracy'], label='Train Acc')
plt.plot(history.history['val_accuracy'], label='Val Acc')
plt.title('Curva de Accuracy')
plt.xlabel('Época')
plt.ylabel('Accuracy')
plt.legend()
plt.grid(True)
plt.tight_layout()
plt.show()
```

[ ]:
```
# Métricas clínicas y matriz de confusión
from sklearn.metrics import classification_report, confusion_matrix,␣
 ↪roc_auc_score
import numpy as np

# Obtener predicciones en el set de validación
val_gen.reset()
y_true = val_gen.classes
y_pred_prob = model.predict(val_gen)
y_pred = (y_pred_prob > 0.5).astype(int).flatten()

print(classification_report(y_true, y_pred, target_names=['No fallece',␣
 ↪'Fallece']))
print('AUC-ROC:', roc_auc_score(y_true, y_pred_prob))
cm = confusion_matrix(y_true, y_pred)
plt.figure(figsize=(4,4))
plt.imshow(cm, cmap='Blues')
plt.title('Matriz de Confusión')
plt.xlabel('Predicho')
plt.ylabel('Real')
plt.colorbar()
plt.xticks([0,1], ['No fallece', 'Fallece'])
plt.yticks([0,1], ['No fallece', 'Fallece'])
for i in range(2):
    for j in range(2):
        plt.text(j, i, cm[i, j], ha='center', va='center', color='black',␣
 ↪fontsize=14)
plt.tight_layout()
plt.show()
```

1.12 12. Interpretabilidad: Grad-CAM para Imágenes

Visualiza qué zonas de la imagen utiliza el modelo para tomar decisiones clínicas.

[ ]:
```
# Ejemplo básico de Grad-CAM para ResNet50 en Keras
import tensorflow as tf
import numpy as np
import matplotlib.pyplot as plt
```

```
def make_gradcam_heatmap(img_array, model, last_conv_layer_name,␣
 ↪pred_index=None):
    grad_model = tf.keras.models.Model([model.inputs], [model.
 ↪get_layer(last_conv_layer_name).output, model.output])
    with tf.GradientTape() as tape:
        conv_outputs, predictions = grad_model(img_array)
        if pred_index is None:
            pred_index = tf.argmax(predictions[0])
        class_channel = predictions[:, pred_index]
    grads = tape.gradient(class_channel, conv_outputs)
    pooled_grads = tf.reduce_mean(grads, axis=(0, 1, 2))
    conv_outputs = conv_outputs[0]
    heatmap = conv_outputs @ pooled_grads[..., tf.newaxis]
    heatmap = tf.squeeze(heatmap)
    heatmap = tf.maximum(heatmap, 0) / tf.math.reduce_max(heatmap)
    return heatmap.numpy()

# Selecciona una imagen de validación
img, label = val_gen[0][0][0], val_gen[0][1][0]
img_array = np.expand_dims(img, axis=0)

# Genera el heatmap Grad-CAM
heatmap = make_gradcam_heatmap(img_array, model,␣
 ↪last_conv_layer_name='conv5_block3_out')

# Superpone el heatmap sobre la imagen original
plt.imshow(img)
plt.imshow(heatmap, cmap='jet', alpha=0.5)
plt.title('Grad-CAM: Zonas relevantes para la predicción')
plt.axis('off')
plt.show()
```