Imports

In [1]:
```
# Data handling
import numpy as np
import pandas as pd

# Visualization
import matplotlib.pyplot as plt

# Scikit-learn: model selection, preprocessing, metrics
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.metrics import mean_squared_error, mean_absolute_error, r2_scor

# Scikit-learn: regressors and decomposition
from sklearn.linear_model import Ridge, Lasso
from sklearn.decomposition import PCA
from sklearn.linear_model import LinearRegression
from sklearn.neighbors import KNeighborsRegressor
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor, AdaBoostRegressor
from sklearn.neural_network import MLPRegressor

# Statsmodels and Scipy
import statsmodels.api as sm
import scipy.stats as stats

# XGBoost
from xgboost import XGBRegressor

# TensorFlow / Keras
import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers
from tensorflow.keras.callbacks import EarlyStopping
```

Data Prep

In [3]:
```
df = pd.read_csv("../data/regression.csv")
```

In [4]:
```
df = df.dropna()
```

In [5]:
```
X = df.drop("Y", axis=1)
y = df["Y"]
```

In [6]:
```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42
)
```

In [7]:
```
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled  = scaler.transform(X_test)
```

In [8]:
```
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled  = scaler.transform(X_test)
```

Linear Regression

In [9]:
```
lr = LinearRegression()
lr.fit(X_train, y_train)
y_pred = lr.predict(X_test)
mse_num = mean_squared_error(y_test, y_pred)
```

In [10]:
```
results_reg = pd.DataFrame([
    {
        'Modelo': 'Linear Regression',
        'MSE': mean_squared_error(y_test, y_pred),
        'RMSE': np.sqrt(mean_squared_error(y_test, y_pred)),
        'MAE': mean_absolute_error(y_test, y_pred),
        'R2': r2_score(y_test, y_pred),
        'N_features': len(X.columns)
    }
])
results_reg
```

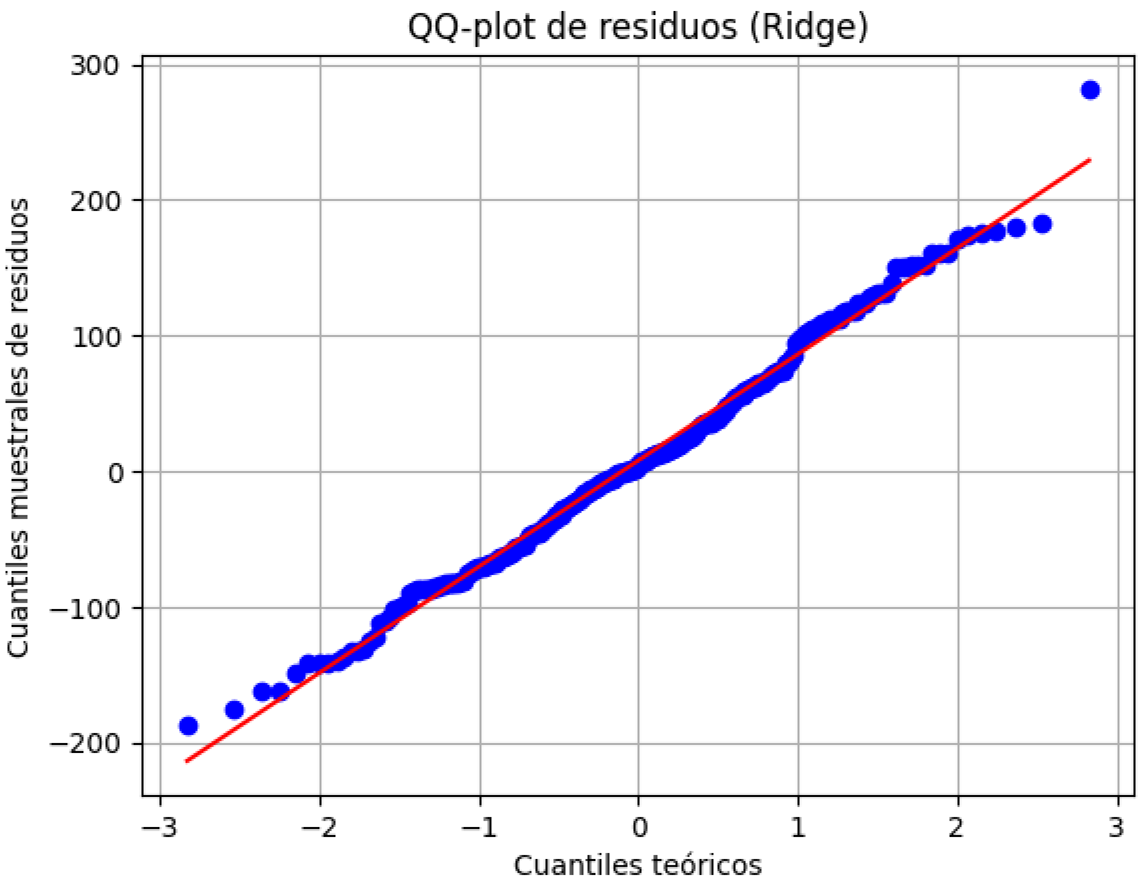
Out[10]:

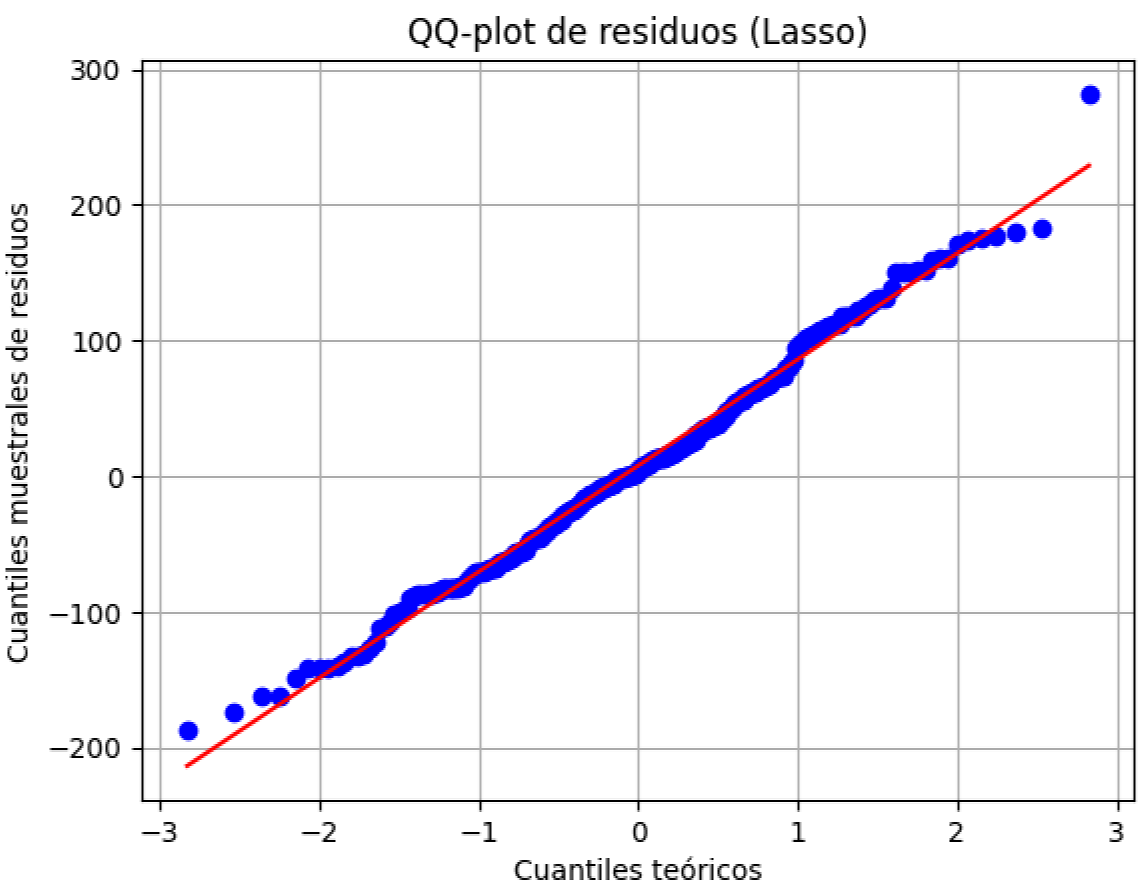
	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.70014	12

In [11]:
```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42
)

ridge = Ridge(alpha=1.0)
ridge.fit(X_train, y_train)
y_pred_ridge = ridge.predict(X_test)

lasso = Lasso(alpha=0.1)
lasso.fit(X_train, y_train)
y_pred_lasso = lasso.predict(X_test)

results = pd.DataFrame({
    'Modelo': ['Ridge', 'Lasso'],
    'MSE': [
        mean_squared_error(y_test, y_pred_ridge),
        mean_squared_error(y_test, y_pred_lasso)
    ],
    'RMSE': [
        np.sqrt(mean_squared_error(y_test, y_pred_ridge)),
        np.sqrt(mean_squared_error(y_test, y_pred_lasso))
```

```
    ],
    'MAE': [
        mean_absolute_error(y_test, y_pred_ridge),
        mean_absolute_error(y_test, y_pred_lasso)
    ],
    'R2': [
        r2_score(y_test, y_pred_ridge),
        r2_score(y_test, y_pred_lasso)
    ]
})
print(results.to_string(index=False))

residuals = y_test - y_pred_ridge
plt.figure()
stats.probplot(residuals, dist="norm", plot=plt)
plt.title("QQ-plot de residuos (Ridge)")
plt.xlabel("Cuantiles teóricos")
plt.ylabel("Cuantiles muestrales de residuos")
plt.grid(True)
plt.show()

res_lasso = y_test - y_pred_lasso
plt.figure()
stats.probplot(res_lasso, dist="norm", plot=plt)
plt.title("QQ-plot de residuos (Lasso)")
plt.xlabel("Cuantiles teóricos")
plt.ylabel("Cuantiles muestrales de residuos")
plt.grid(True)
plt.show()
```

```
Modelo         MSE      RMSE       MAE       R2
 Ridge 6139.201206 78.353055 61.638011 0.700107
 Lasso 6135.228052 78.327697 61.628791 0.700301
```


QQ-plot de residuos (Ridge)
Cuantiles muestrales de residuos
Cuantiles teóricos
300
200
100
0
−100
−200
−3
−2
−1
0
1
2
3


QQ-plot de residuos (Lasso)
Cuantiles muestrales de residuos
Cuantiles teóricos
300
200
100
0
−100
−200
−3
−2
−1
0
1
2
3

KNN

In [12]:
```
knn = KNeighborsRegressor(n_neighbors=5, weights='uniform', metric='euclidea
knn.fit(X_train_scaled, y_train)
y_pred = knn.predict(X_test_scaled)
```

In [13]:
```
mse  = mean_squared_error(y_test, y_pred)
rmse = np.sqrt(mse)
mae  = mean_absolute_error(y_test, y_pred)
r2  = r2_score(y_test, y_pred)
```

In [14]:
```
new_row = {
    'Modelo'     : 'k-NN Regressor (k=5) escaladas',
    'MSE'        : mse,
    'RMSE'       : rmse,
    'MAE'        : mae,
    'R2'         : r2,
    'N_features': len(X.columns)
}

results_reg = pd.concat([results_reg, pd.DataFrame([new_row])], ignore_index
results_reg
```

Out[14]:

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12

KNN + PCA & GridSearch

In [15]:
```
param_grid = {
    'n_neighbors': [3, 7,13, 17, 25],
    'weights'    : ['uniform', 'distance']
}

n_feats    = X_train_scaled.shape[1]
components = [n_feats, int(0.75*n_feats), int(0.50*n_feats), int(0.25*n_feat

best = {'cv_mse': np.inf}

for n_comp in components:
    pca = PCA(n_components=n_comp).fit(X_train_scaled)
    Xtr = pca.transform(X_train_scaled)
    Xte = pca.transform(X_test_scaled)

    knn_cv = GridSearchCV(
        KNeighborsRegressor(metric='euclidean'),
        param_grid,
```

```
        cv=5,
        scoring='neg_mean_squared_error',
        n_jobs=-1,
        verbose=0
    )
    knn_cv.fit(Xtr, y_train)

    cv_mse = -knn_cv.best_score_
    y_pred = knn_cv.predict(Xte)
    test_mse  = mean_squared_error(y_test, y_pred)
    test_rmse = np.sqrt(test_mse)
    test_mae  = mean_absolute_error(y_test, y_pred)
    test_r2   = r2_score(y_test, y_pred)

    if cv_mse < best['cv_mse']:
        best.update({
            'n_comp'    : n_comp,
            'params'    : knn_cv.best_params_,
            'cv_mse'    : cv_mse,
            'test_mse'  : test_mse,
            'test_rmse' : test_rmse,
            'test_mae'  : test_mae,
            'test_r2'   : test_r2
        })

new_row = {
    'Modelo'    : f"k-NN grid (k={best['params']['n_neighbors']}, comp={best
    'MSE'       : best['test_mse'],
    'RMSE'      : best['test_rmse'],
    'MAE'       : best['test_mae'],
    'R2'        : best['test_r2'],
    'N_features': best['n_comp']
}

results_reg = pd.concat([results_reg, pd.DataFrame([new_row])], ignore_index
results_reg
```

Out[15]:

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12

OLS

In [16]:

```
X_train_ols = sm.add_constant(X_train_scaled)
X_test_ols  = sm.add_constant(X_test_scaled)

ols = sm.OLS(y_train, X_train_ols).fit()
y_pred_ols = ols.predict(X_test_ols)
```

```
mse_ols  = mean_squared_error(y_test, y_pred_ols)
rmse_ols = np.sqrt(mse_ols)
mae_ols  = mean_absolute_error(y_test, y_pred_ols)
r2_ols   = r2_score(y_test, y_pred_ols)

new_row = {
    'Modelo'     : 'OLS Regression escaladas',
    'MSE'         : mse_ols,
    'RMSE'        : rmse_ols,
    'MAE'         : mae_ols,
    'R2'          : r2_ols,
    'N_features'  : len(X.columns)
}

results_reg = pd.concat([results_reg, pd.DataFrame([new_row])], ignore_index
display(results_reg)

print(ols.summary())
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12

```
                            OLS Regression Results
==============================================================================
==
Dep. Variable:                      Y   R-squared:                       0.7
25
Model:                            OLS   Adj. R-squared:                  0.7
22
Method:                 Least Squares   F-statistic:                     25
6.1
Date:                Thu, 26 Jun 2025   Prob (F-statistic):          2.28e-3
16
Time:                        20:36:21   Log-Likelihood:                -676
2.1
No. Observations:                1178   AIC:                         1.355e+
04
Df Residuals:                    1165   BIC:                         1.362e+
04
Df Model:                          12
Covariance Type:            nonrobust
==============================================================================
==
                 coef    std err          t      P>|t|      [0.025      0.97
5]
------------------------------------------------------------------------------
--
const         -2.3697      2.206     -1.074      0.283      -6.698       1.9
58
x1            -0.4162      2.217     -0.188      0.851      -4.766       3.9
33
x2             5.2817      2.218      2.381      0.017       0.930       9.6
34
x3            67.1600      2.215     30.327      0.000      62.815      71.5
05
x4             0.9542      2.210      0.432      0.666      -3.381       5.2
90
x5            40.3338      2.220     18.166      0.000      35.978      44.6
90
x6             3.8796      2.219      1.749      0.081      -0.473       8.2
33
x7             8.9022      2.220      4.010      0.000       4.547      13.2
57
x8             7.9245      2.212      3.583      0.000       3.585      12.2
64
x9            29.0109      2.220     13.066      0.000      24.654      33.3
67
x10           20.5627      2.220      9.262      0.000      16.207      24.9
19
x11           71.4295      2.219     32.195      0.000      67.077      75.7
82
x12           46.1045      2.218     20.786      0.000      41.753      50.4
56
==============================================================================
==
Omnibus:                        1.775   Durbin-Watson:                   1.9
24
Prob(Omnibus):                  0.412   Jarque-Bera (JB):                1.6
```

```
51
Skew:                          -0.080   Prob(JB):                        0.4
38
Kurtosis:                       3.088   Cond. No.                         1.
17
=============================================================================
==

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is corre
ctly specified.
```

Decision Tree

In [17]:

```
dt = DecisionTreeRegressor(random_state=42)
dt.fit(X_train_scaled, y_train)
y_pred_dt = dt.predict(X_test_scaled)

mse_dt  = mean_squared_error(y_test, y_pred_dt)
rmse_dt = np.sqrt(mse_dt)
mae_dt  = mean_absolute_error(y_test, y_pred_dt)
r2_dt   = r2_score(y_test, y_pred_dt)

new_row = {
    'Modelo'    : 'Decision Tree escaladas',
    'MSE'        : mse_dt,
    'RMSE'       : rmse_dt,
    'MAE'        : mae_dt,
    'R2'         : r2_dt,
    'N_features' : len(X.columns)
}

results_reg = pd.concat([results_reg, pd.DataFrame([new_row])],
                        ignore_index=True)
display(results_reg)
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12

Random Forest

In [18]:
```
rf = RandomForestRegressor(n_estimators=100, random_state=42)
rf.fit(X_train_scaled, y_train)
y_pred_rf = rf.predict(X_test_scaled)

mse_rf  = mean_squared_error(y_test, y_pred_rf)
rmse_rf = np.sqrt(mse_rf)
mae_rf  = mean_absolute_error(y_test, y_pred_rf)
r2_rf   = r2_score(y_test, y_pred_rf)

new_row = {
    'Modelo'    : 'Random Forest escaladas',
    'MSE'        : mse_rf,
    'RMSE'       : rmse_rf,
    'MAE'        : mae_rf,
    'R2'         : r2_rf,
    'N_features' : len(X.columns)
}

results_reg = pd.concat([results_reg, pd.DataFrame([new_row])],
                        ignore_index=True)
display(results_reg)
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12

Ada Boost

In [19]:
```
param_grid_ada = {
    'n_estimators'    : [50, 100, 150],
    'learning_rate'   : [0.01, 0.1, 1.0],
    'loss'            : ['linear', 'square', 'exponential']
}

grid_search_ada = GridSearchCV(
```

```
    estimator=AdaBoostRegressor(random_state=42),
    param_grid=param_grid_ada,
    cv=5,
    scoring='neg_mean_squared_error',
    n_jobs=-1,
    verbose=1
)
grid_search_ada.fit(X_train_scaled, y_train)

best_ada    = grid_search_ada.best_estimator_
y_pred_ada  = best_ada.predict(X_test_scaled)

print("Mejores parámetros AdaBoost:", grid_search_ada.best_params_)

mse_ada  = mean_squared_error(y_test, y_pred_ada)
rmse_ada = np.sqrt(mse_ada)
mae_ada  = mean_absolute_error(y_test, y_pred_ada)
r2_ada   = r2_score(y_test, y_pred_ada)

new_row = {
    'Modelo'     : 'AdaBoostRegressor (grid) escaladas',
    'MSE'        : mse_ada,
    'RMSE'       : rmse_ada,
    'MAE'        : mae_ada,
    'R2'         : r2_ada,
    'N_features' : len(X.columns)
}
results_reg = pd.concat([results_reg, pd.DataFrame([new_row])], ignore_index
display(results_reg)
```

```
Fitting 5 folds for each of 27 candidates, totalling 135 fits
Mejores parámetros AdaBoost: {'learning_rate': 1.0, 'loss': 'square', 'n_est
imators': 150}
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12
6	AdaBoostRegressor (grid) escaladas	7793.258046	88.279432	69.394143	0.619308	12

XGBoost

In [20]:
```
param_grid_xgb = {
    'n_estimators'  : [50, 100, 150],
    'learning_rate' : [0.01, 0.1, 0.2],
    'max_depth'     : [3, 5, 7],
    'subsample'     : [0.8, 1.0]
}

grid_search_xgb = GridSearchCV(
    estimator=XGBRegressor(
        objective='reg:squarederror', random_state=42,
    ),
    param_grid=param_grid_xgb,
    cv=5,
    scoring='neg_mean_squared_error',
    n_jobs=-1,
    verbose=1
)
grid_search_xgb.fit(X_train_scaled, y_train)

best_xgb    = grid_search_xgb.best_estimator_
y_pred_xgb  = best_xgb.predict(X_test_scaled)

print("Mejores parámetros XGBoost:", grid_search_xgb.best_params_)

mse_xgb  = mean_squared_error(y_test, y_pred_xgb)
rmse_xgb = np.sqrt(mse_xgb)
mae_xgb  = mean_absolute_error(y_test, y_pred_xgb)
r2_xgb   = r2_score(y_test, y_pred_xgb)

new_row = {
    'Modelo'     : 'XGBRegressor (grid) escaladas',
    'MSE'        : mse_xgb,
    'RMSE'       : rmse_xgb,
    'MAE'        : mae_xgb,
    'R2'         : r2_xgb,
    'N_features' : len(X.columns)
}
results_reg = pd.concat([results_reg, pd.DataFrame([new_row])], ignore_index
display(results_reg)
```

```
Fitting 5 folds for each of 54 candidates, totalling 270 fits
Mejores parámetros XGBoost: {'learning_rate': 0.1, 'max_depth': 3, 'n_estima
tors': 100, 'subsample': 0.8}
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12
6	AdaBoostRegressor (grid) escaladas	7793.258046	88.279432	69.394143	0.619308	12
7	XGBRegressor (grid) escaladas	6939.093852	83.301224	64.691668	0.661033	12

Redes Neuronales

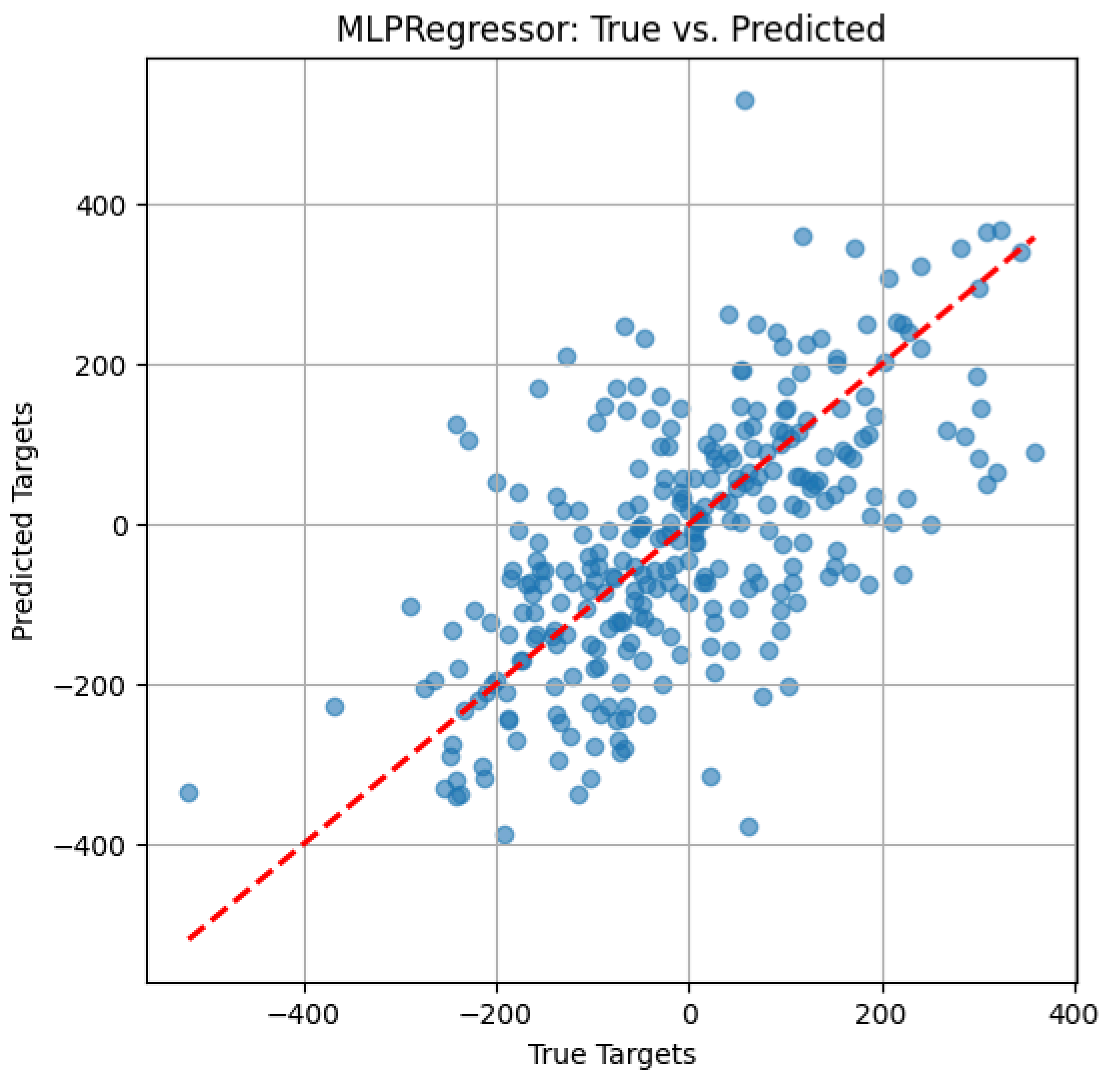
In [21]:

```
reg = MLPRegressor(
    hidden_layer_sizes=(60,),
    solver='lbfgs',
    alpha=1.0,
    random_state=1,
    max_iter=1000
)
reg.fit(X_train_scaled, y_train)
n_features = X_train_scaled.shape[1]

y_pred_reg = reg.predict(X_test_scaled)

mse = mean_squared_error(y_test, y_pred_reg)
r2  = r2_score(y_test, y_pred_reg)
print(f"MLPRegressor MSE: {mse:.4f}")
print(f"MLPRegressor R²:  {r2:.4f}")

plt.figure(figsize=(6,6))
plt.scatter(y_test, y_pred_reg, alpha=0.6)
plt.plot([y_test.min(), y_test.max()],
         [y_test.min(), y_test.max()],
         'r--', lw=2)
plt.xlabel("True Targets")
plt.ylabel("Predicted Targets")
plt.title("MLPRegressor: True vs. Predicted")
plt.grid(True)
plt.show()
```

```
results_reg.loc[len(results_reg)] = {
    'Modelo':    'MLPRegressor',
    'MSE':       mean_squared_error(y_test,   y_pred_reg),
    'RMSE':      np.sqrt(mean_squared_error(y_test,   y_pred_reg)),
    'MAE':       mean_absolute_error(y_test,  y_pred_reg),
    'R2':        r2_score(y_test,            y_pred_reg),
    'N_features': n_features
}

display(results_reg)
```

```
/Users/enriquegomeztagle/anaconda3/envs/ML/lib/python3.11/site-packages/skle
arn/neural_network/_multilayer_perceptron.py:546: ConvergenceWarning: lbfgs
failed to converge (status=1):
STOP: TOTAL NO. OF ITERATIONS REACHED LIMIT.

Increase the number of iterations (max_iter) or scale the data as shown in:
    https://scikit-learn.org/stable/modules/preprocessing.html
  self.n_iter_ = _check_optimize_result("lbfgs", opt_res, self.max_iter)
```

```
MLPRegressor MSE: 17228.6159
MLPRegressor R²:  0.1584
```



	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12
6	AdaBoostRegressor (grid) escaladas	7793.258046	88.279432	69.394143	0.619308	12
7	XGBRegressor (grid) escaladas	6939.093852	83.301224	64.691668	0.661033	12
8	MLPRegressor	17228.615924	131.257822	100.251268	0.158401	12

In [22]:

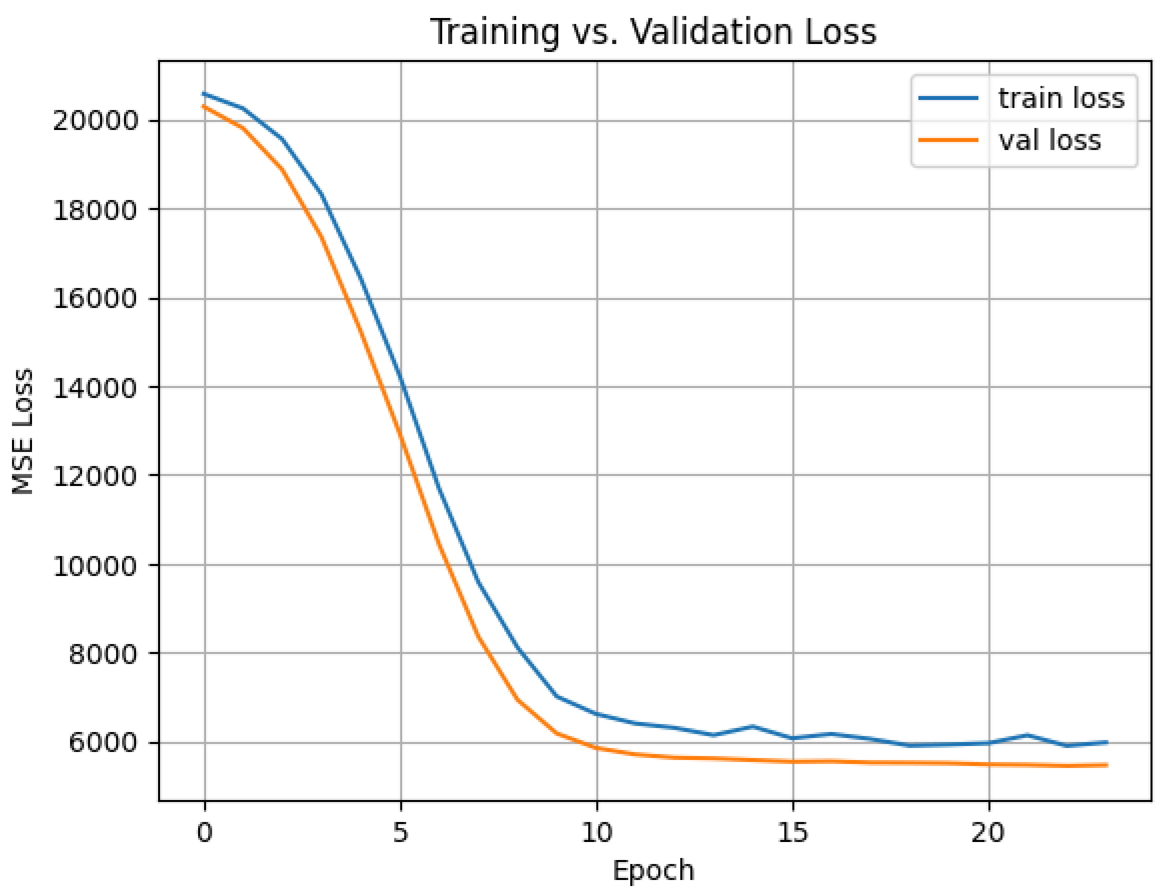
```
def build_regression_model(input_dim):
    model = keras.Sequential([
        layers.Dense(64, activation='relu', input_shape=(input_dim,)),
        layers.Dropout(0.3),
        layers.Dense(32, activation='relu'),
        layers.Dense(1)
    ])
    model.compile(
        optimizer=keras.optimizers.RMSprop(learning_rate=0.001),
        loss='mean_squared_error',
        metrics=['mean_absolute_error']
    )
    return model

model_reg = build_regression_model(X_train_scaled.shape[1])

early_stop = EarlyStopping(
    monitor='mean_absolute_error',
    patience=5,
    restore_best_weights=True,
    verbose=1
)

history = model_reg.fit(
    X_train_scaled, y_train,
    validation_split=0.2,
    epochs=100,
    batch_size=16,
    callbacks=[early_stop],
    verbose=1
)
```

```
mse_nn, mae_nn = model_reg.evaluate(X_test_scaled, y_test, verbose=0)
print(f"Neural Net Regression MSE: {mse_nn:.4f}")
print(f"Neural Net Regression MAE: {mae_nn:.4f}")
print(f"Neural Net Regression R²: {r2_score(y_test, model_reg.predict(X_test

plt.figure()
plt.plot(history.history['loss'], label='train loss')
plt.plot(history.history['val_loss'], label='val loss')
plt.xlabel('Epoch')
plt.ylabel('MSE Loss')
plt.title('Training vs. Validation Loss')
plt.legend()
plt.grid(True)
plt.show()

y_pred_nn = model_reg.predict(X_test_scaled).flatten()
plt.figure(figsize=(6,6))
plt.scatter(y_test, y_pred_nn, alpha=0.6)
plt.plot([y_test.min(), y_test.max()],
         [y_test.min(), y_test.max()],
         'r--', lw=2)
plt.xlabel("True Targets")
plt.ylabel("Predicted Targets")
plt.title("Keras NN: True vs. Predicted")
plt.grid(True)
plt.show()

results_reg.loc[len(results_reg)] = {
    'Modelo':    'KerasNN',
    'MSE':       mean_squared_error(y_test,   y_pred_nn),
    'RMSE':      np.sqrt(mean_squared_error(y_test,   y_pred_nn)),
    'MAE':       mean_absolute_error(y_test,  y_pred_nn),
    'R2':        r2_score(y_test,            y_pred_nn),
    'N_features': n_features
}

display(results_reg)
```

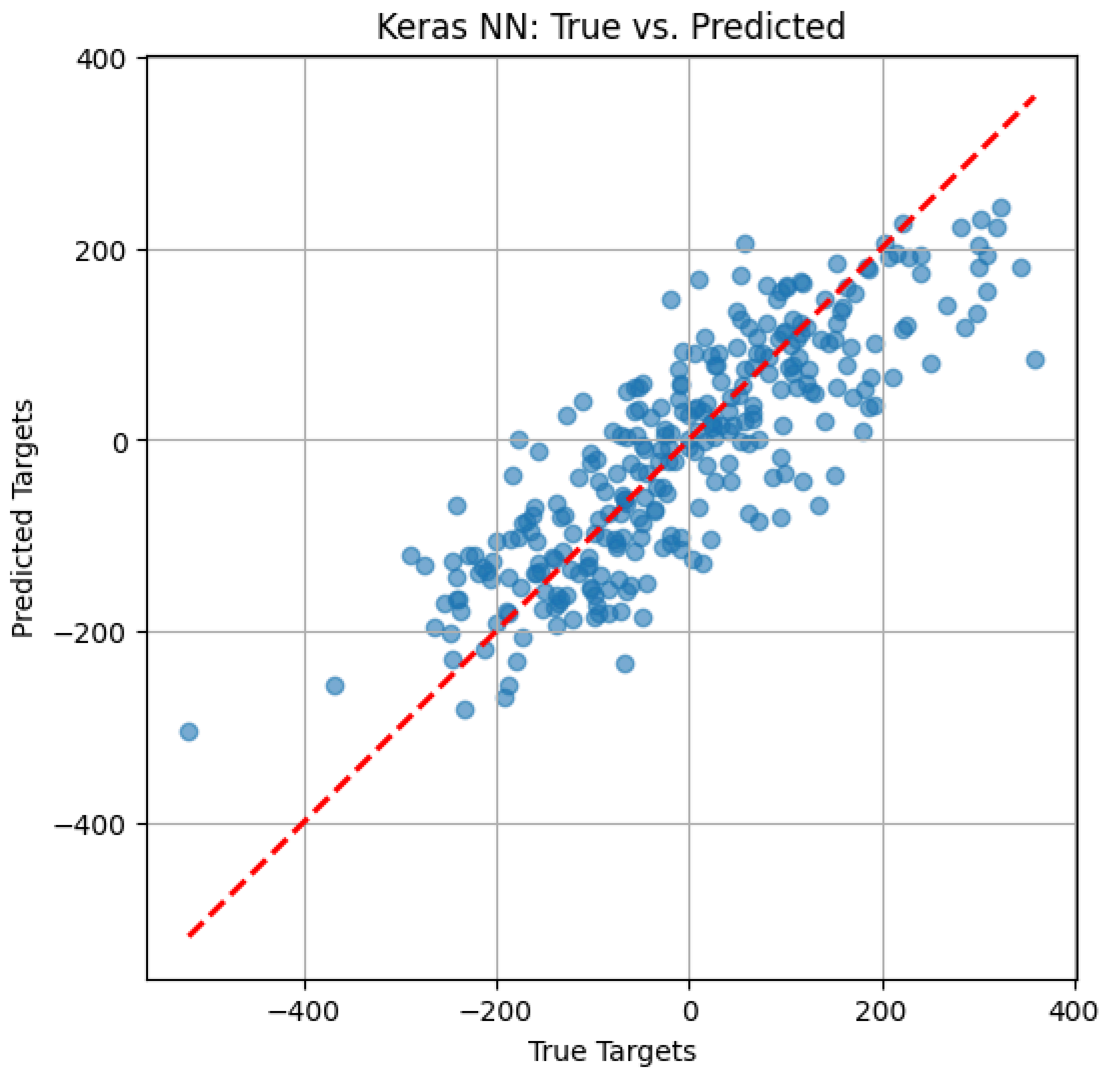
```
/Users/enriquegomeztagle/anaconda3/envs/ML/lib/python3.11/site-packages/kera
s/src/layers/core/dense.py:93: UserWarning: Do not pass an `input_shape`/`in
put_dim` argument to a layer. When using Sequential models, prefer using an
`Input(shape)` object as the first layer in the model instead.
  super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

```
Epoch 1/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 1s 3ms/step - loss: 19429.8848 - mean_absolute_er
ror: 111.0767 - val_loss: 20289.2207 - val_mean_absolute_error: 112.5766
Epoch 2/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 19286.1309 - mean_absolute_er
ror: 108.2360 - val_loss: 19806.6426 - val_mean_absolute_error: 111.2844
Epoch 3/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 20579.1172 - mean_absolute_er
ror: 113.0644 - val_loss: 18874.8184 - val_mean_absolute_error: 108.6872
Epoch 4/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 19047.1914 - mean_absolute_er
ror: 108.3297 - val_loss: 17357.2871 - val_mean_absolute_error: 104.2612
Epoch 5/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 3ms/step - loss: 17270.4004 - mean_absolute_er
ror: 104.6618 - val_loss: 15237.5488 - val_mean_absolute_error: 97.4573
Epoch 6/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 3ms/step - loss: 14672.7129 - mean_absolute_er
ror: 95.8562 - val_loss: 12923.5508 - val_mean_absolute_error: 89.2519
Epoch 7/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 3ms/step - loss: 11723.9609 - mean_absolute_er
ror: 84.3580 - val_loss: 10436.2910 - val_mean_absolute_error: 79.9274
Epoch 8/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 10261.5508 - mean_absolute_er
ror: 78.3146 - val_loss: 8359.9541 - val_mean_absolute_error: 71.3009
Epoch 9/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 8480.8906 - mean_absolute_err
or: 72.8031 - val_loss: 6936.4512 - val_mean_absolute_error: 64.0104
Epoch 10/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 6904.8154 - mean_absolute_err
or: 66.9279 - val_loss: 6178.8081 - val_mean_absolute_error: 60.0091
Epoch 11/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 6624.9761 - mean_absolute_err
or: 65.6615 - val_loss: 5852.2461 - val_mean_absolute_error: 58.5222
Epoch 12/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 6431.1616 - mean_absolute_err
or: 64.0445 - val_loss: 5706.0527 - val_mean_absolute_error: 58.0441
Epoch 13/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 5953.6270 - mean_absolute_err
or: 61.9539 - val_loss: 5634.2690 - val_mean_absolute_error: 57.9979
Epoch 14/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 5988.6016 - mean_absolute_err
or: 62.4010 - val_loss: 5616.0620 - val_mean_absolute_error: 58.1801
Epoch 15/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 6346.8838 - mean_absolute_err
or: 63.0376 - val_loss: 5578.9072 - val_mean_absolute_error: 57.9864
Epoch 16/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 6456.8193 - mean_absolute_err
or: 65.2667 - val_loss: 5543.4775 - val_mean_absolute_error: 57.7983
Epoch 17/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 6334.5015 - mean_absolute_err
or: 63.7222 - val_loss: 5552.5562 - val_mean_absolute_error: 57.7570
Epoch 18/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 1ms/step - loss: 6387.6592 - mean_absolute_err
or: 63.6772 - val_loss: 5521.9326 - val_mean_absolute_error: 57.4786
Epoch 19/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 5518.4829 - mean_absolute_err
```

```
or: 58.5842 - val_loss: 5517.7173 - val_mean_absolute_error: 57.4570
Epoch 20/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 5ms/step - loss: 5862.9019 - mean_absolute_err
or: 61.4726 - val_loss: 5509.1123 - val_mean_absolute_error: 57.4692
Epoch 21/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 1s 8ms/step - loss: 6215.4385 - mean_absolute_err
or: 64.0857 - val_loss: 5480.2207 - val_mean_absolute_error: 57.2351
Epoch 22/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 4ms/step - loss: 6072.4941 - mean_absolute_err
or: 62.8933 - val_loss: 5470.9751 - val_mean_absolute_error: 57.2685
Epoch 23/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 3ms/step - loss: 5592.7959 - mean_absolute_err
or: 60.1789 - val_loss: 5448.9961 - val_mean_absolute_error: 57.1208
Epoch 24/100
59/59 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step - loss: 6053.5244 - mean_absolute_err
or: 62.8069 - val_loss: 5465.5322 - val_mean_absolute_error: 57.3513
Epoch 24: early stopping
Restoring model weights from the end of the best epoch: 19.
Neural Net Regression MSE: 6364.3892
Neural Net Regression MAE: 62.8619
10/10 ━━━━━━━━━━━━━━━━━━━━ 0s 10ms/step
Neural Net Regression R²: 0.6891
```




```
10/10 ━━━━━━━━━━━━━━━━━━━━ 0s 2ms/step
```



Keras NN: True vs. Predicted
400
200
0
−200
−400
Predicted Targets
−400
−200
0
200
400
True Targets

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12
6	AdaBoostRegressor (grid) escaladas	7793.258046	88.279432	69.394143	0.619308	12
7	XGBRegressor (grid) escaladas	6939.093852	83.301224	64.691668	0.661033	12
8	MLPRegressor	17228.615924	131.257822	100.251268	0.158401	12
9	KerasNN	6364.388966	79.777121	62.861893	0.689107	12

In [23]:
```
results_reg = results_reg.sort_values(by='MSE', ascending=True)
display(results_reg)
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
9	KerasNN	6364.388966	79.777121	62.861893	0.689107	12
7	XGBRegressor (grid) escaladas	6939.093852	83.301224	64.691668	0.661033	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12
6	AdaBoostRegressor (grid) escaladas	7793.258046	88.279432	69.394143	0.619308	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
8	MLPRegressor	17228.615924	131.257822	100.251268	0.158401	12

In [24]:
```
results_reg = results_reg.sort_values(by='R2', ascending=False)
display(results_reg)
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
9	KerasNN	6364.388966	79.777121	62.861893	0.689107	12
7	XGBRegressor (grid) escaladas	6939.093852	83.301224	64.691668	0.661033	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12
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2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
8	MLPRegressor	17228.615924	131.257822	100.251268	0.158401	12

In [25]:
```
results_reg = results_reg.sort_values(by=['MSE', 'R2'], ascending=[True, Fal
display(results_reg)
```

	Modelo	MSE	RMSE	MAE	R2	N_features
0	Linear Regression	6138.514703	78.348674	61.638441	0.700140	12
3	OLS Regression escaladas	6138.514703	78.348674	61.638441	0.700140	12
9	KerasNN	6364.388966	79.777121	62.861893	0.689107	12
7	XGBRegressor (grid) escaladas	6939.093852	83.301224	64.691668	0.661033	12
5	Random Forest escaladas	7293.616879	85.402675	67.020350	0.643715	12
6	AdaBoostRegressor (grid) escaladas	7793.258046	88.279432	69.394143	0.619308	12
2	k-NN grid (k=17, comp=12)	9812.593252	99.058534	77.475050	0.520666	12
1	k-NN Regressor (k=5) escaladas	10640.480296	103.152704	80.952047	0.480224	12
4	Decision Tree escaladas	16578.446162	128.757315	103.574863	0.190161	12
8	MLPRegressor	17228.615924	131.257822	100.251268	0.158401	12

Comentarios

- Se entrenaron y compararon 9 modelos de regresión: Regresión Lineal, OLS, K-NN, Árbol de Decisión, Random Forest, AdaBoost, XGBoost, un MLP de *scikit-learn* y una red neuronal densa en Keras, todos con la misma partición 80 / 20 y variables escaladas cuando era necesario.

- Las métricas de referencia muestran que la Regresión Lineal simple lidera con MSE ≈ 6 139, RMSE ≈ 78 y $R^2 \approx 0.70$; el modelo OLS alcanza las mismas métricas.

- Se aplicó regularización con Ridge (α=1.0) y Lasso (α=0.1):

  - Ridge obtuvo MSE ≈ 6 139, RMSE ≈ 78.35, MAE ≈ 61.64 y $R^2 \approx 0.7001$.
  - Lasso obtuvo MSE ≈ 6 135, RMSE ≈ 78.33, MAE ≈ 61.63 y $R^2 \approx 0.7003$.

  Los QQ-plots de residuos de ambos modelos (Ridge y Lasso) muestran una excelente aproximación a la normalidad, pero la regularización no mejoró el R^2 ni redujo de forma significativa el error respecto al modelo lineal sin penalización.

- Aún con ensambles no mejoró el desempeño:

  - Random Forest (100 árboles) alcanza R^2 0.64.
  - AdaBoost óptimo con 150 stumps y learning_rate 1.0 se queda en R^2 0.62.

    - XGBoost con 100 árboles (profundidad 3, eta 0.1) llega a R^2 0.66.

  El grid search confirma que aumentar la complejidad no aporta una ganancia real.
- K-NN, aún tras probar distintos valores de k y aplicar reducción de dimensión con PCA, no se logró un buen desempeño: obtiene RMSE ≈ 99 y $R^2 \approx 0.52$. Esto se debe a que, aunque las variables están escaladas, ninguna de ellas tiene relación significativa con la varlable objetivo.

- El Árbol de Decisión y el MLP muestran error de entrenamiento casi nulo pero caen a $R^2 \leq 0.19$ y 0.18 en prueba, lo que podría indicar un sobreajuste.

- Sugerimos elegir entre Regresión Lineal/OLS por su transparencia, costo computacional mínimo y desempeño destacado.

```
In [ ]:
```