regression_tree_testing

December 14, 2025

1 Testing Notebook - Regression Tree

TODO: - [ ] create random regressions datasets for testing - [ ] run training and prediction on these datasets and collect statistics - [ ] same as 3 but with the scikit regression tree - [ ] try a bunch of different settings, most likely use grid search with cross validation - [ ] visualize the results

[1]:
```
from scripts.regression_tree import RegressionTree
from sklearn.tree import DecisionTreeRegressor
from sklearn.model_selection import train_test_split, cross_validate
from sklearn.datasets import make_regression
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd


RANDOM_STATE = 42
```

1.1 Helper functions

[2]:
```
"""Generate synthetic regression data using scikit-learn's make_regression␣
 ↪function."""
def generate_regression_data(n_samples=100, n_features=1, noise=0.1,␣
 ↪random_state=RANDOM_STATE):
  X, y = make_regression(n_samples=n_samples, n_features=n_features,␣
 ↪noise=noise, random_state=random_state)
  print("Generated regression data with {} samples and {} features.".
 ↪format(n_samples, n_features))
  print("First 5 samples of X:\n", X[:5])
  print("First 5 samples of y:\n", y[:5])
  return X, y

"""Evaluate a regression model using cross-validation and return performance␣
 ↪metrics."""
def evaluate_model(model, X, y, cv=5):
    cv_results = cross_validate(
        model,
        X,
```

```
        y,
        cv=cv,
        scoring=["r2", "neg_mean_squared_error", "neg_mean_absolute_error"],
        return_train_score=False,
    )

    return {
        "r2_mean": np.mean(cv_results["test_r2"]),
        "r2_std":  np.std(cv_results["test_r2"]),
        "mse_mean": -np.mean(cv_results["test_neg_mean_squared_error"]),
        "mae_mean": -np.mean(cv_results["test_neg_mean_absolute_error"]),
    }
```

1.2 Definition of testing configurations

[3]:
```
TESTING_CONFIGS = [
  {
    "description": "Basic regression data with low noise",
    "n_samples": 100,
    "n_features": 1,
    "noise": 0.1
  },
  {
    "description": "Regression data with higher noise",
    "n_samples": 100,
    "n_features": 1,
    "noise": 10.0
  },
  {
    "description": "Regression data with multiple features",
    "n_samples": 200,
    "n_features": 5,
    "noise": 5.0
  },
  {
    "description": "Larger dataset with moderate noise",
    "n_samples": 5000,
    "n_features": 3,
    "noise": 2.0
  },
  {
    "description": "Large dataset with low noise",
    "n_samples": 10000,
    "n_features": 2,
    "noise": 0.5
  },
  {
```

```
    "description": "Large dataset with high noise",
    "n_samples": 10000,
    "n_features": 2,
    "noise": 20.0
  },
  {
    "description": "Moderate dataset with many features",
    "n_samples": 1000,
    "n_features": 50,
    "noise": 5.0
  }
]

HYPERPARAM_CONFIGS = [
    {
        "name": "shallow",
        "max_depth": 2,
        "min_samples_leaf": 1,
        "min_samples_split": 2,
    },
    {
        "name": "medium",
        "max_depth": 4,
        "min_samples_leaf": 1,
        "min_samples_split": 2,
    },
    {
        "name": "deep",
        "max_depth": 8,
        "min_samples_leaf": 1,
        "min_samples_split": 2,
    },
    {
        "name": "unrestricted",
        "max_depth": None,
        "min_samples_leaf": 1,
        "min_samples_split": 2,
    },
    {
        "name": "regularized_leaf",
        "max_depth": None,
        "min_samples_leaf": 5,
        "min_samples_split": 2,
    },
    {
        "name": "strongly_regularized",
        "max_depth": None,
```

```
        "min_samples_leaf": 10,
        "min_samples_split": 10,
    },
]
```

1.3 Runing the tests

For each configuration we will train the scikit-learn's built-in regression tree model as well as our implementation, we collect useful statistics and compare them.

[4]:
```
results = []

for config in TESTING_CONFIGS:
    print("=" * 80)
    print(f"Dataset: {config['description']}")
    print("=" * 80)

    X, y = generate_regression_data(
        n_samples=config["n_samples"],
        n_features=config["n_features"],
        noise=config["noise"],
    )

    for hp in HYPERPARAM_CONFIGS:
        print("-" * 80)
        print(f"Hyperparams: {hp['name']}")

        model_specs = [
            (
                "our",
                RegressionTree(
                    max_depth=hp["max_depth"],
                    min_samples_leaf=hp["min_samples_leaf"],
                    min_samples_split=hp["min_samples_split"],
                    random_state=RANDOM_STATE
                ),
            ),
            (
                "sklearn",
                DecisionTreeRegressor(
                    max_depth=hp["max_depth"],
                    min_samples_leaf=hp["min_samples_leaf"],
                    min_samples_split=hp["min_samples_split"],
                    random_state=RANDOM_STATE
                ),
            ),
        ]
```

```python
        for model_name, model in model_specs:
            metrics = evaluate_model(model, X, y)

            print(
                f"{model_name:8s} | "
                f"R²: {metrics['r2_mean']:.3f} ± {metrics['r2_std']:.3f} | "
                f"MSE: {metrics['mse_mean']:.3f} | "
                f"MAE: {metrics['mae_mean']:.3f}"
            )

            results.append({
                "dataset": config["description"],
                "hyperparams": hp["name"],
                "model": model_name,
                **metrics,
            })
```

```
================================================================================
Dataset: Basic regression data with low noise
================================================================================
Generated regression data with 100 samples and 1 features.
First 5 samples of X:
 [[ 0.93128012]
 [ 0.08704707]
 [-1.05771093]
 [ 0.31424733]
 [-0.47917424]]
First 5 samples of y:
 [ 38.9917296    3.4964533  -44.05770173  13.09112657 -19.9786311 ]
--------------------------------------------------------------------------------
Hyperparams: shallow
our      | R²: 0.885 ± 0.029 | MSE: 159.505 | MAE: 10.251
sklearn  | R²: 0.885 ± 0.029 | MSE: 159.505 | MAE: 10.251
--------------------------------------------------------------------------------
Hyperparams: medium
our      | R²: 0.987 ± 0.006 | MSE: 19.322 | MAE: 3.020
sklearn  | R²: 0.987 ± 0.006 | MSE: 19.322 | MAE: 3.020
--------------------------------------------------------------------------------
Hyperparams: deep
our      | R²: 0.994 ± 0.008 | MSE: 10.395 | MAE: 1.420
sklearn  | R²: 0.994 ± 0.008 | MSE: 10.395 | MAE: 1.420
--------------------------------------------------------------------------------
Hyperparams: unrestricted
our      | R²: 0.994 ± 0.008 | MSE: 10.395 | MAE: 1.421
sklearn  | R²: 0.994 ± 0.008 | MSE: 10.395 | MAE: 1.421
--------------------------------------------------------------------------------
Hyperparams: regularized_leaf
```

```
our      | R²: 0.971 ± 0.015 | MSE: 45.195 | MAE: 4.272
sklearn  | R²: 0.971 ± 0.015 | MSE: 45.195 | MAE: 4.272
--------------------------------------------------------------------------------
Hyperparams: strongly_regularized
our      | R²: 0.914 ± 0.032 | MSE: 124.116 | MAE: 8.168
sklearn  | R²: 0.914 ± 0.032 | MSE: 124.116 | MAE: 8.168
================================================================================
Dataset: Regression data with higher noise
================================================================================
Generated regression data with 100 samples and 1 features.
First 5 samples of X:
 [[ 0.93128012]
 [ 0.08704707]
 [-1.05771093]
 [ 0.31424733]
 [-0.47917424]]
First 5 samples of y:
 [ 50.77992943 -10.06527016 -34.91839191  10.52674299 -17.73837724]
--------------------------------------------------------------------------------
Hyperparams: shallow
our      | R²: 0.808 ± 0.073 | MSE: 299.307 | MAE: 13.587
sklearn  | R²: 0.808 ± 0.073 | MSE: 299.307 | MAE: 13.587
--------------------------------------------------------------------------------
Hyperparams: medium
our      | R²: 0.918 ± 0.028 | MSE: 127.604 | MAE: 9.026
sklearn  | R²: 0.918 ± 0.028 | MSE: 127.604 | MAE: 9.026
--------------------------------------------------------------------------------
Hyperparams: deep
our      | R²: 0.885 ± 0.037 | MSE: 177.317 | MAE: 10.900
sklearn  | R²: 0.885 ± 0.037 | MSE: 177.317 | MAE: 10.900
--------------------------------------------------------------------------------
Hyperparams: unrestricted
our      | R²: 0.888 ± 0.035 | MSE: 174.039 | MAE: 10.736
sklearn  | R²: 0.888 ± 0.035 | MSE: 174.039 | MAE: 10.736
--------------------------------------------------------------------------------
Hyperparams: regularized_leaf
our      | R²: 0.909 ± 0.027 | MSE: 148.618 | MAE: 9.392
sklearn  | R²: 0.909 ± 0.027 | MSE: 148.618 | MAE: 9.392
--------------------------------------------------------------------------------
Hyperparams: strongly_regularized
our      | R²: 0.855 ± 0.047 | MSE: 236.005 | MAE: 11.690
sklearn  | R²: 0.855 ± 0.047 | MSE: 236.005 | MAE: 11.690
================================================================================
Dataset: Regression data with multiple features
================================================================================
Generated regression data with 200 samples and 5 features.
First 5 samples of X:
 [[-0.3853136   0.1990597  -0.60021688  0.46210347  0.06980208]
```

```
 [ 0.13074058  1.6324113  -1.43014138 -1.24778318 -0.44004449]
 [-0.77300978  0.22409248  0.0125924  -0.40122047  0.0976761 ]
 [-0.57677133 -0.05023811 -0.23894805  0.27045683 -0.90756366]
 [-0.57581824  0.6141667   0.75750771 -0.2209696  -0.53050115]]
First 5 samples of y:
 [ -23.06825766 -124.34606251    6.99640504  -71.77655611   17.06336023]
--------------------------------------------------------------------------------
Hyperparams: shallow
our      | R²: 0.623 ± 0.079 | MSE: 3325.007 | MAE: 44.673
sklearn  | R²: 0.623 ± 0.079 | MSE: 3325.007 | MAE: 44.673
--------------------------------------------------------------------------------
Hyperparams: medium
our      | R²: 0.766 ± 0.068 | MSE: 2056.622 | MAE: 36.590
sklearn  | R²: 0.759 ± 0.065 | MSE: 2118.765 | MAE: 36.980
--------------------------------------------------------------------------------
Hyperparams: deep
our      | R²: 0.836 ± 0.072 | MSE: 1437.223 | MAE: 29.751
sklearn  | R²: 0.825 ± 0.071 | MSE: 1519.290 | MAE: 29.683
--------------------------------------------------------------------------------
Hyperparams: unrestricted
our      | R²: 0.836 ± 0.066 | MSE: 1435.343 | MAE: 29.745
sklearn  | R²: 0.825 ± 0.063 | MSE: 1545.506 | MAE: 30.016
--------------------------------------------------------------------------------
Hyperparams: regularized_leaf
our      | R²: 0.811 ± 0.043 | MSE: 1709.692 | MAE: 31.868
sklearn  | R²: 0.811 ± 0.043 | MSE: 1709.692 | MAE: 31.868
--------------------------------------------------------------------------------
Hyperparams: strongly_regularized
our      | R²: 0.783 ± 0.014 | MSE: 1974.617 | MAE: 34.900
sklearn  | R²: 0.783 ± 0.014 | MSE: 1974.617 | MAE: 34.900
================================================================================
Dataset: Larger dataset with moderate noise
================================================================================
Generated regression data with 5000 samples and 3 features.
First 5 samples of X:
 [[ 0.67796997 -1.28472777 -0.33102433]
 [ 1.03138053  0.3881858  -0.97027133]
 [-1.21689671  1.36337651 -0.60515624]
 [-0.54429615 -0.50442268 -1.5198928 ]
 [ 0.2074888   0.44567791  0.42350787]]
First 5 samples of y:
 [  -3.90976845  -46.39345674  -98.15873956 -157.1184525    47.56364341]
--------------------------------------------------------------------------------
Hyperparams: shallow
our      | R²: 0.728 ± 0.016 | MSE: 2520.708 | MAE: 39.683
sklearn  | R²: 0.728 ± 0.016 | MSE: 2520.708 | MAE: 39.683
--------------------------------------------------------------------------------
Hyperparams: medium
```

```
our      | R²: 0.904 ± 0.007 | MSE: 890.915 | MAE: 23.495
sklearn  | R²: 0.904 ± 0.007 | MSE: 890.915 | MAE: 23.495
--------------------------------------------------------------------------------
Hyperparams: deep
our      | R²: 0.989 ± 0.001 | MSE: 101.228 | MAE: 7.401
sklearn  | R²: 0.989 ± 0.001 | MSE: 98.149 | MAE: 7.354
--------------------------------------------------------------------------------
Hyperparams: unrestricted
our      | R²: 0.994 ± 0.001 | MSE: 55.475 | MAE: 4.884
sklearn  | R²: 0.994 ± 0.001 | MSE: 53.924 | MAE: 4.859
--------------------------------------------------------------------------------
Hyperparams: regularized_leaf
our      | R²: 0.992 ± 0.001 | MSE: 70.037 | MAE: 5.411
sklearn  | R²: 0.992 ± 0.001 | MSE: 70.044 | MAE: 5.411
--------------------------------------------------------------------------------
Hyperparams: strongly_regularized
our      | R²: 0.989 ± 0.002 | MSE: 99.862 | MAE: 6.621
sklearn  | R²: 0.989 ± 0.002 | MSE: 99.862 | MAE: 6.621
================================================================================
Dataset: Large dataset with low noise
================================================================================
Generated regression data with 10000 samples and 2 features.
First 5 samples of X:
 [[-0.5691482   1.59040357]
 [ 0.73487779  0.49097495]
 [ 0.20069869  1.10623156]
 [-1.07774393 -0.54427443]
 [ 0.10507597 -0.88502863]]
First 5 samples of y:
 [ -47.49496686   75.02051971   25.36349671 -108.87452141    5.49344142]
--------------------------------------------------------------------------------
Hyperparams: shallow
our      | R²: 0.877 ± 0.005 | MSE: 1180.012 | MAE: 27.415
sklearn  | R²: 0.877 ± 0.005 | MSE: 1180.012 | MAE: 27.415
--------------------------------------------------------------------------------
Hyperparams: medium
our      | R²: 0.987 ± 0.001 | MSE: 128.172 | MAE: 8.694
sklearn  | R²: 0.987 ± 0.001 | MSE: 128.172 | MAE: 8.694
--------------------------------------------------------------------------------
Hyperparams: deep
our      | R²: 0.999 ± 0.000 | MSE: 10.967 | MAE: 2.547
sklearn  | R²: 0.999 ± 0.000 | MSE: 10.986 | MAE: 2.547
--------------------------------------------------------------------------------
Hyperparams: unrestricted
our      | R²: 1.000 ± 0.000 | MSE: 2.996 | MAE: 1.118
sklearn  | R²: 1.000 ± 0.000 | MSE: 3.170 | MAE: 1.129
--------------------------------------------------------------------------------
Hyperparams: regularized_leaf
```

```
our      | R²: 0.999 ± 0.000 | MSE: 5.449 | MAE: 1.394
sklearn  | R²: 0.999 ± 0.000 | MSE: 5.448 | MAE: 1.394
--------------------------------------------------------------------------------
Hyperparams: strongly_regularized
our      | R²: 0.999 ± 0.000 | MSE: 10.863 | MAE: 1.810
sklearn  | R²: 0.999 ± 0.000 | MSE: 10.863 | MAE: 1.810
================================================================================
Dataset: Large dataset with high noise
================================================================================
Generated regression data with 10000 samples and 2 features.
First 5 samples of X:
 [[-0.5691482   1.59040357]
 [ 0.73487779  0.49097495]
 [ 0.20069869  1.10623156]
 [-1.07774393 -0.54427443]
 [ 0.10507597 -0.88502863]]
First 5 samples of y:
 [-56.9869474   68.99765941   2.79332014 -93.43973055   7.91252206]
--------------------------------------------------------------------------------
Hyperparams: shallow
our      | R²: 0.841 ± 0.004 | MSE: 1592.545 | MAE: 31.659
sklearn  | R²: 0.841 ± 0.004 | MSE: 1592.545 | MAE: 31.659
--------------------------------------------------------------------------------
Hyperparams: medium
our      | R²: 0.947 ± 0.002 | MSE: 529.733 | MAE: 18.329
sklearn  | R²: 0.947 ± 0.002 | MSE: 529.733 | MAE: 18.329
--------------------------------------------------------------------------------
Hyperparams: deep
our      | R²: 0.955 ± 0.001 | MSE: 446.888 | MAE: 16.879
sklearn  | R²: 0.955 ± 0.001 | MSE: 447.420 | MAE: 16.882
--------------------------------------------------------------------------------
Hyperparams: unrestricted
our      | R²: 0.920 ± 0.001 | MSE: 801.002 | MAE: 22.730
sklearn  | R²: 0.920 ± 0.002 | MSE: 798.026 | MAE: 22.683
--------------------------------------------------------------------------------
Hyperparams: regularized_leaf
our      | R²: 0.945 ± 0.001 | MSE: 552.718 | MAE: 18.864
sklearn  | R²: 0.945 ± 0.001 | MSE: 552.655 | MAE: 18.863
--------------------------------------------------------------------------------
Hyperparams: strongly_regularized
our      | R²: 0.951 ± 0.001 | MSE: 491.906 | MAE: 17.711
sklearn  | R²: 0.951 ± 0.001 | MSE: 491.906 | MAE: 17.711
================================================================================
Dataset: Moderate dataset with many features
================================================================================
Generated regression data with 1000 samples and 50 features.
First 5 samples of X:
 [[ 0.22210537  0.62386678 -0.16605612  0.63463021  0.75376893  1.65859202
```

```
  -0.70189811  0.18361217 -2.08195404  0.60286295  0.14837528 -1.13521912
   0.9986041  -0.49461035 -0.51024062  0.93668094 -0.399035   -0.38356556
   1.1898542  -0.5212666  -1.16138215  1.72223231  0.36539182  1.33601969
   0.78801999 -0.83774995  0.56658811  0.92829461 -0.38674766  0.6208172
   0.19797213  1.33836855  0.02365751 -2.52871576  1.75988802 -1.207332
  -0.82470391 -0.68112696  0.6151632   0.35782542 -0.7864838   0.10673978
   0.69987124 -0.03436237 -0.11283199 -0.36389558  0.10516231 -0.53678647
  -0.0572436  -0.30034055]
 [ 0.83057101 -1.71669373 -0.15501343  1.11435578 -0.82530382  0.60915961
  -0.06801749 -0.71940537 -0.05022968 -1.14378475  0.78259513 -0.10643051
   1.68403763 -0.58623557 -0.40156696 -0.59052457  0.96258821  0.79276514
  -0.16365711  0.99107132 -1.08776862 -0.43419762 -1.11047912 -1.56341347
  -0.20934306  0.19477547  1.77209275 -0.18015897  1.54042895  1.66236667
   0.17283733  0.34237509  1.7280638  -0.85290707 -1.17369964  0.55164771
  -1.65811325  0.11898642  0.20540077 -0.43031452  2.22904372 -1.44808321
  -1.14136697 -0.10875609 -0.51455358 -0.14546159  0.740684    0.85154814
  -0.72018801 -0.39993873]
 [-0.96335321  0.5437933  -1.11313988  1.21235947  0.55206656 -0.91026463
  -0.85609014  0.53390779  0.38681169  0.25747809  0.40567447 -1.38173128
  -1.34554208  2.22468763  0.15646961 -1.15238917 -0.11994209 -0.0888014
  -1.33626712 -2.46829003  0.73874622 -0.74254137  0.21518837  2.30103361
   0.6396049  -1.00437615  0.009012    1.53905609  0.68941732 -0.81846411
  -0.33594849  1.13719016 -0.84854273 -0.92413914 -0.1971291  -1.59092134
  -0.20260583  1.09189461 -1.43450227 -1.83909427  0.63691302  1.81273542
  -0.4661267   0.98463866 -0.82158042 -0.80044475 -1.55415405 -0.79595511
   0.85645506 -0.13711049]
 [ 2.1498434  -0.10467932 -0.43722006 -0.33944537  1.17827468  0.60539814
   0.62604166  0.02681872 -0.59611361 -0.325793   -0.26361207  1.89754169
  -0.40314991 -0.14655815  1.29817434  0.3420916  -0.23200561  1.83926104
  -1.72979741  2.16414981  1.01110931 -0.68284508  0.84036538  1.90220597
   2.31782164  0.93558607 -0.64628821 -0.42569971 -0.40269403 -1.27318569
   1.76253455  1.41378331 -0.04727162  1.15564512 -1.09488559  0.69360613
  -0.94454315  0.02231656  0.04946641 -2.29909535 -0.15431771  0.0542324
   0.31923321  0.39123279  0.5049892  -0.00548364 -0.58436466  0.76151403
  -0.75676622 -1.26037829]
 [-0.5372907   0.06883836 -0.49145363 -2.14575896 -0.98773148 -0.43352192
   0.31588178  0.46436161 -0.79141506 -0.20844714 -0.74615901 -0.11587905
   0.32387858  0.28785406 -0.58537497  1.2066765  -0.70211482  0.95639433
  -0.69194153 -0.20713186  0.54609752  0.32999556 -0.36007058  0.95665943
   0.22027397  1.11085552  0.40401589  0.95472592 -0.27240938 -1.51210178
   0.50589761 -0.90487118 -0.41419898 -0.42887986 -2.38069159 -1.0825947
  -0.5624822   0.92588024 -0.8635109   0.42003858 -1.82769117  0.95275321
  -1.41406661 -0.36089524  1.41201599  1.56501888  1.34935979 -0.75915137
  -0.91560975  0.18396914]]
First 5 samples of y:
 [137.83775667  -3.71055967 145.69973099  -9.68172968 -83.67934132]
--------------------------------------------------------------------------------
Hyperparams: shallow
```

```
our      | R²: 0.380 ± 0.039 | MSE: 17106.506 | MAE: 104.267
sklearn  | R²: 0.380 ± 0.039 | MSE: 17106.506 | MAE: 104.267
--------------------------------------------------------------------------------
Hyperparams: medium
our      | R²: 0.670 ± 0.027 | MSE: 9083.463 | MAE: 76.403
sklearn  | R²: 0.668 ± 0.028 | MSE: 9145.507 | MAE: 76.560
--------------------------------------------------------------------------------
Hyperparams: deep
our      | R²: 0.727 ± 0.026 | MSE: 7523.640 | MAE: 67.167
sklearn  | R²: 0.727 ± 0.037 | MSE: 7488.662 | MAE: 66.500
--------------------------------------------------------------------------------
Hyperparams: unrestricted
our      | R²: 0.705 ± 0.032 | MSE: 8120.275 | MAE: 69.466
sklearn  | R²: 0.701 ± 0.039 | MSE: 8223.028 | MAE: 69.967
--------------------------------------------------------------------------------
Hyperparams: regularized_leaf
our      | R²: 0.756 ± 0.026 | MSE: 6707.463 | MAE: 64.719
sklearn  | R²: 0.756 ± 0.027 | MSE: 6696.210 | MAE: 64.661
--------------------------------------------------------------------------------
Hyperparams: strongly_regularized
our      | R²: 0.758 ± 0.028 | MSE: 6653.061 | MAE: 64.376
sklearn  | R²: 0.758 ± 0.028 | MSE: 6653.061 | MAE: 64.376
```

1.4 Results

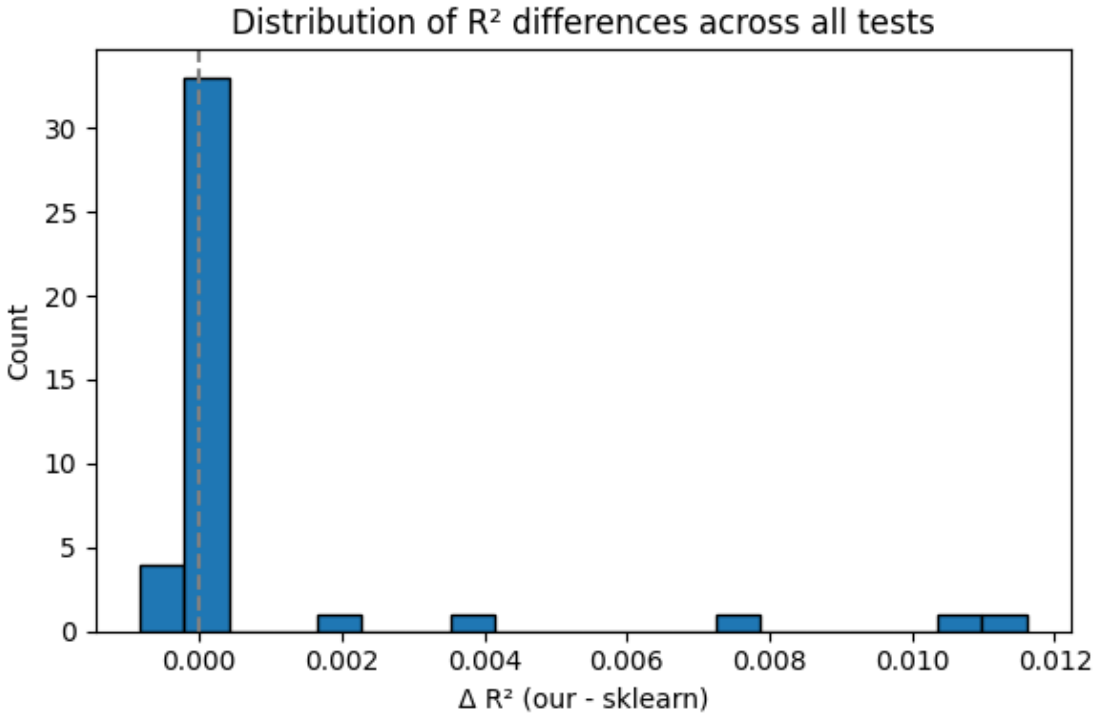
[5]:
```python
df = pd.DataFrame(results)
paired = (
    df.pivot_table(
        index=["dataset", "hyperparams"],
        columns="model",
        values=["r2_mean", "mse_mean", "mae_mean"]
    )
)

paired.columns = ["_".join(col) for col in paired.columns]
paired = paired.reset_index()

paired["r2_diff"]  = paired["r2_mean_our"]  - paired["r2_mean_sklearn"]
paired["mse_diff"] = paired["mse_mean_our"] - paired["mse_mean_sklearn"]
paired["mae_diff"] = paired["mae_mean_our"] - paired["mae_mean_sklearn"]

paired.head()
```

[5]:

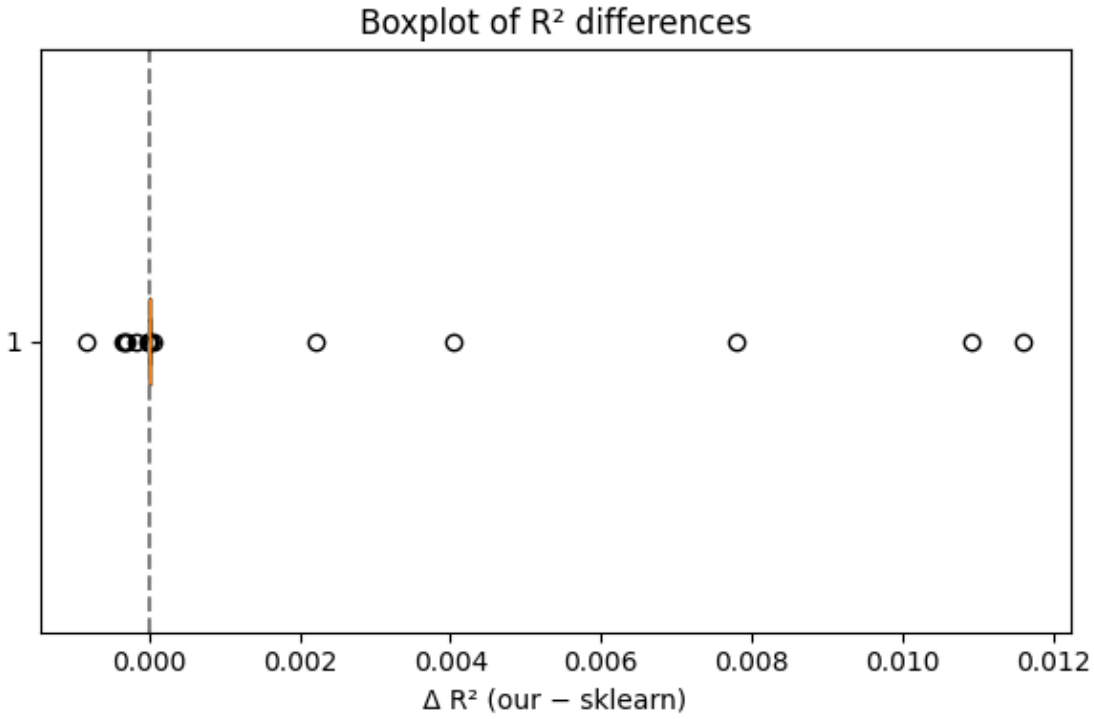
	dataset	hyperparams	mae_mean_our	\
0	Basic regression data with low noise	deep	1.420082	
1	Basic regression data with low noise	medium	3.019620	
2	Basic regression data with low noise	regularized_leaf	4.271927	

```
3  Basic regression data with low noise              shallow     10.251087
4  Basic regression data with low noise  strongly_regularized      8.168215

   mae_mean_sklearn  mse_mean_our  mse_mean_sklearn  r2_mean_our  \
0          1.420082     10.395394         10.395394     0.993668
1          3.019620     19.322168         19.322168     0.986635
2          4.271927     45.194549         45.194549     0.971219
3         10.251087    159.505327        159.505327     0.884677
4          8.168215    124.116470        124.116470     0.913597

   r2_mean_sklearn  r2_diff      mse_diff      mae_diff
0         0.993668      0.0  0.000000e+00  0.000000e+00
1         0.986635      0.0  0.000000e+00  0.000000e+00
2         0.971219      0.0  2.131628e-14  1.776357e-15
3         0.884677      0.0 -5.684342e-14  1.776357e-15
4         0.913597      0.0  0.000000e+00  0.000000e+00
```

[6]:
```
plt.figure(figsize=(6, 4))
plt.hist(paired["r2_diff"], bins=20, edgecolor="black")
plt.axvline(0, linestyle="--", color="gray")
plt.xlabel("Δ R² (our - sklearn)")
plt.ylabel("Count")
plt.title("Distribution of R² differences across all tests")
plt.tight_layout()
plt.show()
```

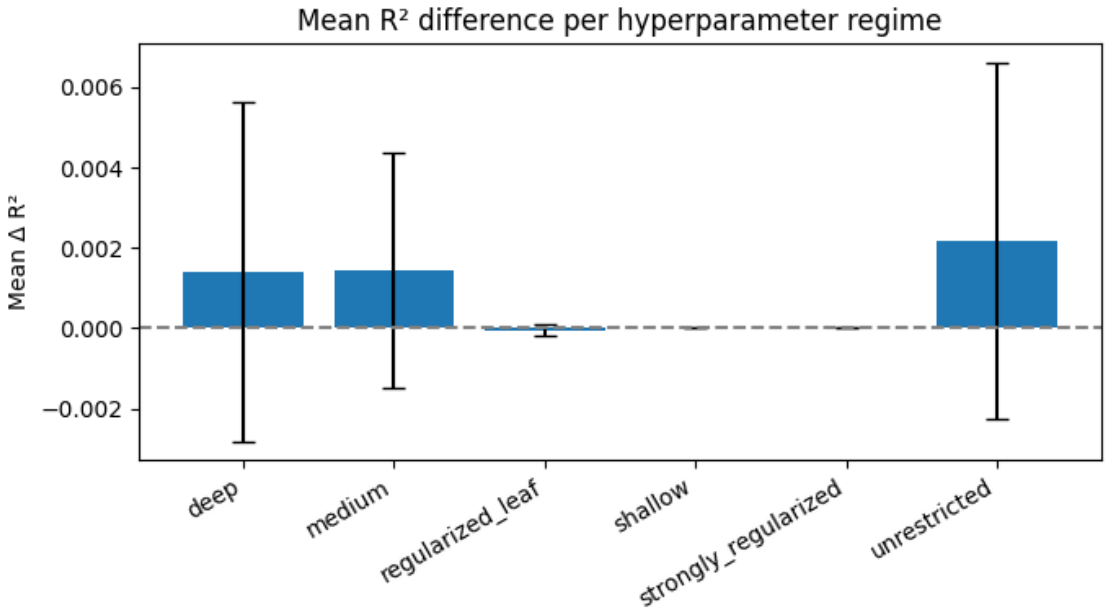


[7]:
```
plt.figure(figsize=(6, 4))
plt.boxplot(
    paired["r2_diff"],
    vert=False,
    showfliers=True
)
plt.axvline(0, linestyle="--", color="gray")
plt.xlabel("Δ R² (our - sklearn)")
plt.title("Boxplot of R² differences")
plt.tight_layout()
plt.show()
```

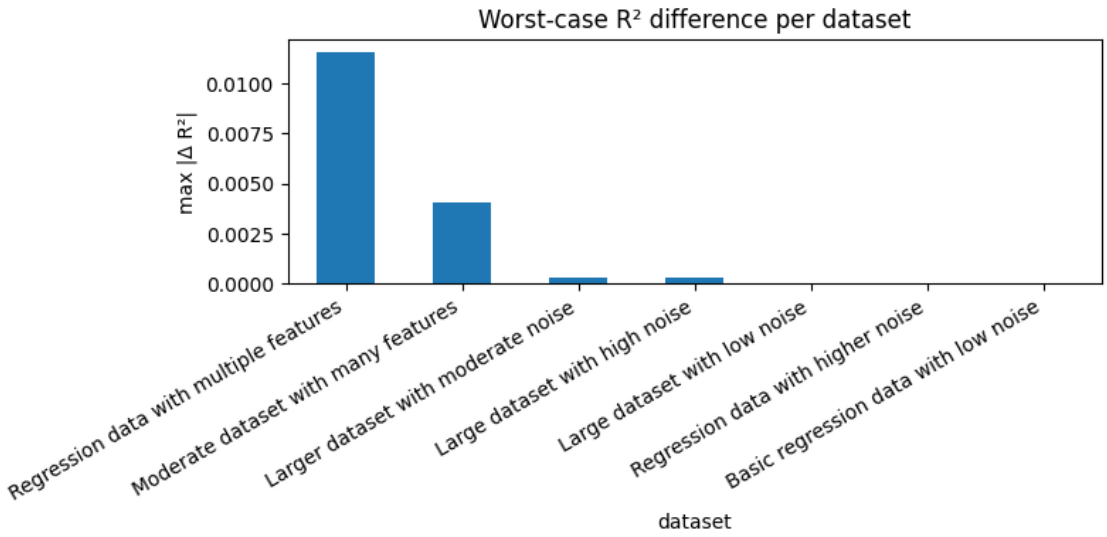


[8]:
```
by_hp = (
    paired.groupby("hyperparams")["r2_diff"]
    .agg(["mean", "std"])
    .reset_index()
)

plt.figure(figsize=(7, 4))
plt.bar(
```

```
    by_hp["hyperparams"],
    by_hp["mean"],
    yerr=by_hp["std"],
    capsize=5
)
plt.axhline(0, linestyle="--", color="gray")
plt.ylabel("Mean Δ R²")
plt.title("Mean R² difference per hyperparameter regime")
plt.xticks(rotation=30, ha="right")
plt.tight_layout()
plt.show()
```



[9]:
```
worst_by_dataset = (
    paired.groupby("dataset")["r2_diff"]
    .apply(lambda x: x.abs().max())
    .sort_values(ascending=False)
)

plt.figure(figsize=(8, 4))
worst_by_dataset.plot(kind="bar")
plt.ylabel("max |Δ R²|")
plt.title("Worst-case R² difference per dataset")
plt.xticks(rotation=30, ha="right")
plt.tight_layout()
plt.show()
```



[10]:
```
fig, axes = plt.subplots(1, 2, figsize=(10, 4))

axes[0].hist(paired["mse_diff"], bins=20, edgecolor="black")
axes[0].axvline(0, linestyle="--", color="gray")
axes[0].set_title("Δ MSE distribution")

axes[1].hist(paired["mae_diff"], bins=20, edgecolor="black")
axes[1].axvline(0, linestyle="--", color="gray")
axes[1].set_title("Δ MAE distribution")

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