Notebook for the Project

Introduction

Do MNIST-1D, compare CNN, RandomForest with PCA, LinearRegression with PCA

Goal: Compare the relation of accuracy to training and prediction time. Expected outcome: CNN is the most accurate, but will be a lot slower than the others.

Dependencies

In [1]:
```python
# !pip install torch
# !pip install pandas
# !pip install scikit-learn
# !pip install tensorboard
# !pip install seaborn
# !pip install torchvision
```

Imports

In [12]:
```python
import torch
from torch import autograd
from torch import nn
from torch.utils.data import TensorDataset, DataLoader
from torchvision.datasets import MNIST
from torchvision import transforms

from matplotlib import pyplot as plt
import numpy as np
import pandas as pd
import seaborn as sns
import numpy as np
from tqdm import tqdm
from copy import deepcopy

from collections import OrderedDict
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
from torch.utils.tensorboard import SummaryWriter
import sklearn.metrics as metrics
from pandas import Series
from typing import Union
import json
from sklearn.metrics import confusion_matrix, accuracy_score


from sklearn.decomposition import PCA
from sklearn.tree import DecisionTreeClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import RandomizedSearchCV
```

Helper functions

In [2]:
```python
def train(train_loader, model, optimizer, criterion, device, detect_bad_gradients=False, clip_grad_norm=False):
    """
    Trains PyTorch modelfor one epoch in batches.

    Args:
        train_loader: Data loader for training set.
        model: Neural network model.
        optimizer: Optimizer (e.g. SGD).
        criterion: Loss function (e.g. cross-entropy loss).
    """

    avg_loss = 0

    model.train()

    # Iterate through batches
    for i, data in enumerate(train_loader):
        # Get the inputs; data is a list of [inputs, labels]
        inputs, labels = data

        # Move data to target device
        inputs, labels = inputs.to(device), labels.to(device)

        # Zero the parameter gradients
        optimizer.zero_grad()

        # Forward + backward + optimize
        outputs = model(inputs)
        loss = criterion(outputs, labels)  # Compute RMSE from MSE
        if detect_bad_gradients:
            with autograd.detect_anomaly():
                loss.backward()
        else:
            loss.backward()
        if clip_grad_norm:
            grad_norm = torch.nn.utils.clip_grad_norm_(model.parameters(), clip_grad_norm)  # Clip gradients
        optimizer.step()

        # Keep track of loss (MSE) and r2
        avg_loss += torch.sqrt(loss)

    return avg_loss / len(train_loader)


def test(test_loader, model, criterion, device):
    """
    Evaluates network in batches.

    Args:
        test_loader: Data loader for test set.
        model: Neural network model.
        criterion: Loss function (e.g. cross-entropy loss).
    """

    avg_loss = 0

    model.eval()

    # Use torch.no_grad to skip gradient calculation, not needed for evaluation
    with torch.no_grad():

        # Iterate through batches
        all_predictions = []
        all_labels = []

        for data in test_loader:
            # Get the inputs; data is a list of [inputs, labels]
            inputs, labels = data

            # Move data to target device
            inputs, labels = inputs.to(device), labels.to(device)

            # Forward pass
            outputs = model(inputs)
            loss = torch.sqrt(criterion(outputs, labels))  # Compute RMSE from MSE

            all_predictions.extend(outputs.detach().numpy())
            all_labels.extend(labels.detach().numpy())

            # Keep track of loss (MSE) and r2
            avg_loss += loss

    return avg_loss / len(test_loader)
      # Track the average loss and the r2 of the last batch



def run_torch(model, train_set, val_set, test_set, log_comment="", log_hparams=False, writer=None, **config):
    """
    Run a test
    """
    try:
        if writer is None:
            # Create a writer to write to Tensorboard
            writer = SummaryWriter(comment=log_comment)
            writer.add_text("run_params", json.dumps(config, indent=2))

        # Create the dataloaders
        train_loader = DataLoader(
            train_set, batch_size=config["batch_size"], shuffle=False, num_workers=0, persistent_workers=False
        )
        val_loader = DataLoader(
            val_set, batch_size=config["batch_size"], shuffle=False, num_workers=0, persistent_workers=False
        )
        test_loader = DataLoader(
            test_set, batch_size=config["batch_size"], shuffle=False, num_workers=0, persistent_workers=False
        )

        # Create loss function and optimizer
        if config["loss"] == "MSE" or config["loss"] == "RMSE":
            criterion = nn.MSELoss()
        else:
            raise ValueError(f"Loss {config['loss']} not recognized.")

        optimizer = torch.optim.Adam(
            model.parameters(), lr=config["optimizer"]["lr"], weight_decay=config["optimizer"]["weight_decay"]
        )
        if config["lr_scheduler"]:
            scheduler = torch.optim.lr_scheduler.MultiStepLR(optimizer=optimizer, **config["lr_scheduler"])

        # Use GPU if available
        device = "cuda" if torch.cuda.is_available() else "cpu"

        model = model.to(device)

        patience = config.get("early_stopping_patience", torch.inf)
        best_model = None
        best_loss = np.inf
        counter = 0

        print("Starting initial training")
        for epoch in tqdm(range(config["epochs"])):
            # Train on data
            train_loss = train(
                train_loader, model, optimizer, criterion, device, config["detect_bad_gradients"]
            )
            # After training set eval mode on
            model.eval()
            # Test on data
            val_loss = test(val_loader, model, criterion, device)
            test_loss = test(test_loader, model, criterion, device)

            if config["lr_scheduler"]:
                scheduler.step()

            # Write metrics to Tensorboard
            writer.add_scalars("Loss", {"Train_loss": train_loss, "Val_loss": val_loss, "Test_loss": test_loss}

            if log_hparams:

                report_metrics = {
                    "hparam/test_loss": test_loss,
                    "hparam/train_loss": train_loss,
                }
                writer.add_hparams(log_hparams, report_metrics, run_name=log_comment)

            # Early stopping
            if best_loss > val_loss.detach().numpy():
                best_loss = val_loss.detach().numpy()
                counter = 0
                best_model = deepcopy(model)
            else:
                counter += 1
                if counter > patience:
                    print("Initiating early stopping")
                    if best_model is not None:
                        print("Restoring best weights")
                        model = best_model
                    break

        print("\nTraining Finished.")
        writer.flush()
        writer.close()

        # Finally, use the model to predict the train, validation and test sets
    except KeyboardInterrupt:
        print("Interrupted")
    print("Gathering final predictions")

    if not log_hparams:
        results, predictions, model = gather_results(model, train_loader, val_loader, test_loader)

        return results, predictions, model
    else:
        return


def gather_results(model, train_loader, val_loader, test_loader):
    """
    Gather the results for train, val and test sets.
    Returns:
        results, predictions, model
    """
    model.eval()
    with torch.no_grad():

        y_train = []
        y_pred_train = []

        y_val = []
        y_pred_val = []

        y_test = []
        y_pred_test = []

        for data in train_loader:
            inputs, labels = data
            pred = model(inputs)
            y_train.extend(labels.detach().numpy().flatten())
            y_pred_train.extend(pred.detach().numpy().flatten())

        # Iterate through batches
        for data in val_loader:
            inputs, labels = data
            pred = model(inputs)
            y_val.extend(labels.detach().numpy().flatten())
            y_pred_val.extend(pred.detach().numpy().flatten())

        for data in test_loader:
            inputs, labels = data
            pred = model(inputs)
            y_test.extend(labels.detach().numpy().flatten())
            y_pred_test.extend(pred.detach().numpy().flatten())

    y_pred_train = np.array(y_pred_train)
    y_pred_val = np.array(y_pred_val)
    y_pred_test = np.array(y_pred_test)
    y_train = np.array(y_train)
    y_val = np.array(y_val)
    y_test = np.array(y_test)
    train_res = classification_report(y_train, y_pred_train)
    validation_res = classification_report(y_val, y_pred_val)
    test_res = classification_report(y_test, y_pred_test)

    results = pd.DataFrame({"train": train_res, "validate": validation_res, "test": test_res})

    predictions = {
        "train": {"y": y_train, "pred": y_pred_train},
        "validate": {"y": y_val, "pred": y_pred_val},
        "test": {"y": y_test, "pred": y_pred_test},
    }

    return results, predictions, model
```

Load the data

In [3]:
```python
transform = transforms.Compose([transforms.ToTensor(),
                                transforms.Normalize((0.1307,), (0.3081,))])

train_data = MNIST('./data', train=True, download=True, transform=transform)
test_data = MNIST('./data', train=False, download=True, transform=transform)
```

Study the MNIST-2D dataset

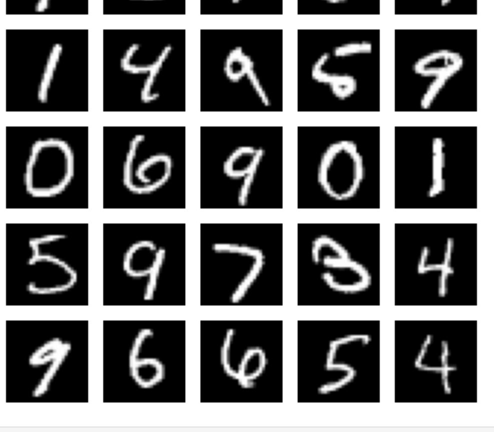
Length of the dataset

In [4]:
```python
print("Lenght of the training set:", len(train_data))
print("Lenght of the test set:", len(test_data))
print()
print("Shape of \"features\", i.e. images: ", train_data[0][0].shape)
```

```
Lenght of the training set: 60000
Lenght of the test set: 10000

Shape of "features", i.e. images:  torch.Size([1, 28, 28])
```

Show some example images

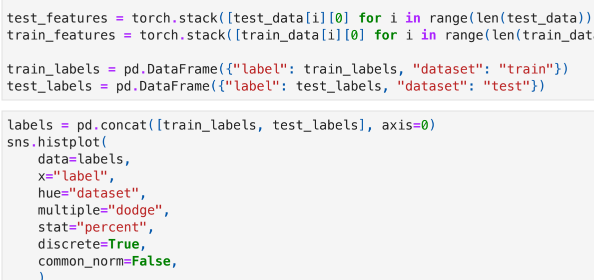
In [5]:
```python
fig, axs = plt.subplots(5, 5, figsize=(5, 5))
for i in range(25):
    x, _ = test_data[i]
    ax = axs[i // 5][i % 5]
    ax.imshow(x.view(28, 28), cmap='gray')
    ax.axis('off')
    ax.axis('off')
plt.tight_layout()
plt.show()
```



In [6]:
```python
# Distribution of labels in train and test sets

train_labels = [train_data[i][1] for i in range(len(train_data))]
test_labels = [test_data[i][1] for i in range(len(test_data))]

test_features = torch.stack([test_data[i][0] for i in range(len(test_data))])
train_features = torch.stack([train_data[i][0] for i in range(len(train_data))])

train_labels = pd.DataFrame({"label": train_labels, "dataset": "train"})
test_labels = pd.DataFrame({"label": test_labels, "dataset": "test"})
```

In [7]:
```python
labels = pd.concat([train_labels, test_labels], axis=0)
sns.histplot(
    data=labels,
    x="label",
    hue="dataset",
    multiple="dodge",
    stat="percent",
    discrete=True,
    common_norm=False,
    )
```

Out[7]:
```
<AxesSubplot: xlabel='label', ylabel='Percent'>
```



In [8]:
```python
print("Feature statistics")
print("Min:", train_features.min())
print("Max:", train_features.max())
print("Mean:", train_features.mean())
print("Std:", train_features.std())
```

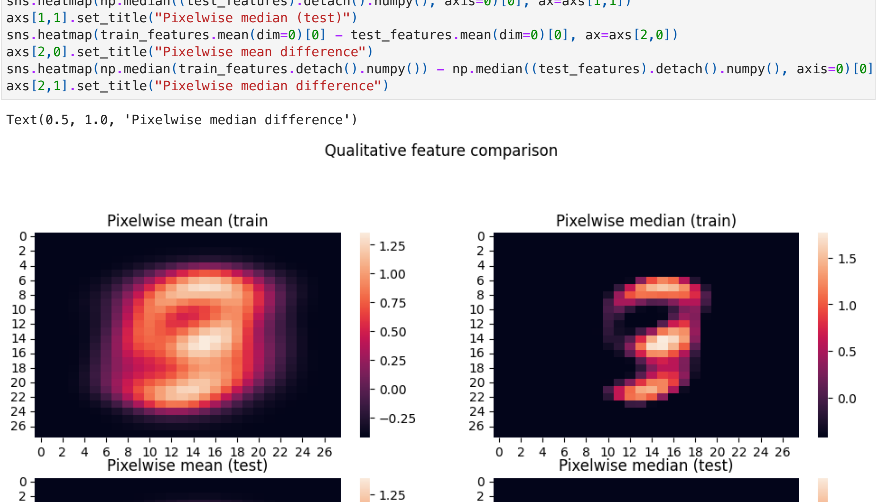
```
Feature statistics
Min: tensor(-0.4242)
Max: tensor(2.8215)
Mean: tensor(-0.0001)
Std: tensor(1.0000)
```

The data is normalized correctly as we see.

Visualize the pixel distributions in training set

In [9]:
```python
fig,axs = plt.subplots(3,2, figsize=(12,10))
plt.suptitle("Qualitative feature comparison")
sns.heatmap(train_features.mean(dim=0)[0], ax=axs[0,0])
axs[0, 0].set_title("Pixelwise mean (train")
sns.heatmap(np.median(train_features.detach().numpy(), axis=0)[0], ax=axs[0,1])
axs[0, 1].set_title("Pixelwise median (train)")
sns.heatmap(test_features.mean(dim=0)[0], ax=axs[1,0])
axs[1,0].set_title("Pixelwise mean (test)")
sns.heatmap(np.median((test_features).detach().numpy(), axis=0)[0], ax=axs[1,1])
axs[1,1].set_title("Pixelwise median (test)")
sns.heatmap(train_features.mean(dim=0)[0] - test_features.mean(dim=0)[0], ax=axs[2,0])
axs[2,0].set_title("Pixelwise mean difference")
sns.heatmap(np.median(train_features.detach().numpy()) - np.median((test_features).detach().numpy(), axis=0)[0]
axs[2,1].set_title("Pixelwise median difference")
```

Out[9]:
```
Text(0.5, 1.0, 'Pixelwise median difference')
```



Feature engineering

For the more traditional models in comparison, the total number of input features 28x28 = 784 is significantly high, and PCA is used to reduce the features

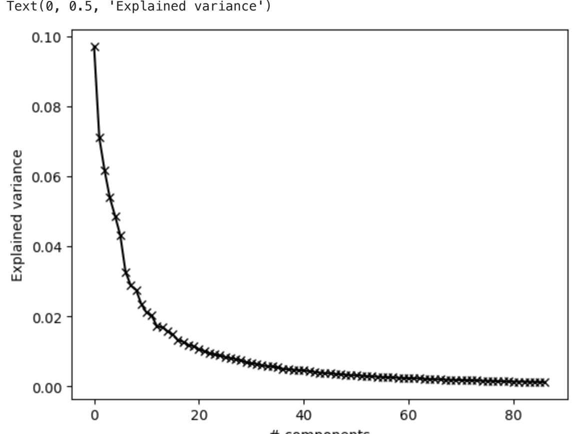
In [10]:
```python
train_set_flat = train_features.flatten(start_dim=-2).squeeze()
test_set_flat = test_features.flatten(start_dim=-2).squeeze()
train_set_flat.shape, test_set_flat.shape
```

Out[10]:
```
(torch.Size([60000, 784]), torch.Size([10000, 784]))
```

PCA Elbow Curve

In [13]:
```python
pca = PCA(0.9)
pca.fit(train_set_flat)
plt.plot(pca.explained_variance_ratio_, 'k-x')
plt.xlabel("# components")
plt.ylabel("Explained variance")
```

Out[13]:
```
Text(0, 0.5, 'Explained variance')
```



We can see that the curve begins to flatten out after 20 components, let's use that.

Logistic Regression Model

In [14]:
```python
model = Pipeline(
    [
    ("pca", PCA(n_components=20)),
    ("reg", LogisticRegression(multi_class='multinomial', fit_intercept=True, max_iter=500)) # Cross-entropy lo
    ]
)
X_train = train_set_flat
y_train = train_labels["label"]

X_test = test_set_flat
y_test = test_labels["label"]

model.fit(X_train, y_train)
y_pred_train = model.predict(X_train)
y_pred_test = model.predict(X_test)

# Additional
print("Train accuracy", accuracy_score(y_train, y_pred_train))
print("Test accuracy", accuracy_score(y_test, y_pred_test))

fig, axs = plt.subplots(1,2, figsize=(15, 5), sharex=True, sharey=True)
sns.heatmap(confusion_matrix(y_train, y_pred_train), annot=True, ax=axs[0])
sns.heatmap(confusion_matrix(y_test, y_pred_test), annot=True, ax=axs[1])
```

```
Train accuracy 0.8752833333333333
Test accuracy 0.881
```

Out[14]:
```
<AxesSubplot: >
```

Decision Tree

In [15]:
```python
def optimize_randomforest(X_train, y_train, random_grid, hparam_max_evals, metric, kfolds=5):
    # Inspiration from https://towardsdatascience.com/hyperparameter-tuning-the-random-forest-in-python-using-s
    # First create the base model to tune
    rf = DecisionTreeClassifier()
    # Random search of parameters, using k-fold cross validation,
    # search across 100 different combinations, and use all available cores
    rf_random = RandomizedSearchCV(estimator = rf, param_distributions = random_grid, n_iter = hparam_max_evals
    # Fit the random search model
    rf_random.fit(X_train, y_train)
    return rf_random
```

Note: As only the training data is used in the randomized hyperparameter search cross validation, it can be considered as using a separate train-val-test split, in which the train and validation sets are used to optimize the model and the test set is used only for testing to avoid overfitting by hyperparameter optimization.

In [201…
```python
# Number of features to consider at every split
max_features = np.linspace(0.33, 1.0, 5)
# Maximum number of levels in tree
max_depth = [int(x) for x in np.linspace(5, 10, num = 5)]
max_depth.append(None)
# Minimum number of samples required to split a node
min_samples_split = [2, 5, 10]
# Minimum number of samples required at each leaf node
min_samples_leaf = [1, 2, 4]
# Create the random grid
random_grid = {
    'max_features': max_features,
    'max_depth': max_depth,
    'min_samples_split': min_samples_split,
    'min_samples_leaf': min_samples_leaf
}

hparam_cv = optimize_randomforest(X_train, y_train,random_grid=random_grid, hparam_max_evals=10, metric="neg_ac
```

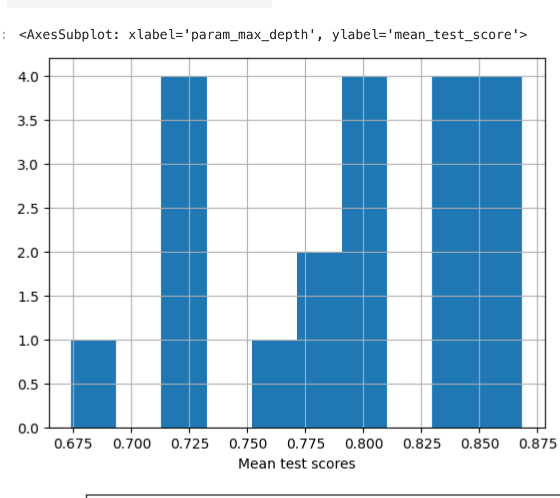
```
Fitting 5 folds for each of 20 candidates, totalling 100 fits
[CV 1/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.675 total time=   4.6s
[CV 2/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.679 total time=   4.9s
[CV 3/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.675 total time=   5.2s
[CV 4/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.649 total time=   5.4s
[CV 5/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.692 total time=   5.6s
[CV 1/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.771 total time=   6.0s
[CV 2/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.768 total time=   6.0s
[CV 3/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.771 total time=   6.0s
[CV 4/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.777 total time=   5.9s
[CV 5/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.789 total time=   5.9s
[CV 1/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.742 total time=   6.5s
[CV 2/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.717 total time=   6.5s
[CV 3/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.731 total time=   6.7s
[CV 4/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.710 total time=   6.7s
[CV 5/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.740 total time=   6.7s
[CV 1/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.778 total time=   9.5s
[CV 2/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.767 total time=   9.8s
[CV 3/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.773 total time=  10.5s
[CV 1/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.846 total time=   7.2s
[CV 4/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.761 total time=  10.0s
[CV 2/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.836 total time=   7.2s
[CV 5/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.794 total time=   9.8s
[CV 3/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.850 total time=   6.7s
[CV 1/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.793 total time=   3.3s
[CV 4/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.827 total time=   6.2s
[CV 2/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.789 total time=   3.1s
[CV 5/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.858 total time=   5.8s
[CV 3/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.789 total time=   2.9s
[CV 4/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.788 total time=   2.8s
[CV 5/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.815 total time=   2.7s
[CV 1/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.724 total time=   2.9s
[CV 2/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.708 total time=   2.9s
[CV 1/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.855 total time=   9.2s
[CV 3/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.701 total time=   2.8s
[CV 2/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.841 total time=   9.3s
[CV 4/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.711 total time=   2.7s
[CV 3/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.844 total time=   9.8s
[CV 5/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.728 total time=   2.6s
[CV 4/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.841 total time=   9.6s
[CV 5/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.861 total time=   9.6s
[CV 1/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.811 total time=   6.0s
[CV 2/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.791 total time=   6.1s
[CV 3/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.809 total time=   6.2s
[CV 4/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.795 total time=   6.5s
[CV 5/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.823 total time=   6.6s
[CV 1/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.859 total time=   4.6s
[CV 2/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.835 total time=   5.2s
[CV 3/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.836 total time=   5.2s
[CV 4/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.843 total time=   5.4s
[CV 5/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.856 total time=   5.2s
[CV 1/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.861 total time=  16.9s
[CV 2/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.857 total time=  17.1s
[CV 4/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.858 total time=  17.0s
[CV 3/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.859 total time=  18.7s
[CV 5/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.872 total time=  16.9s
[CV 1/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.860 total time=  10.2s
[CV 2/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.857 total time=  10.1s
[CV 3/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.851 total time=  10.3s
[CV 4/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.855 total time=  11.3s
[CV 5/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.875 total time=  11.4s
[CV 1/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.738 total time=  12.2s
[CV 1/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.877 total time=  28.0s
[CV 2/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.718 total time=  12.0s
[CV 2/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.861 total time=  29.4s
[CV 3/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.731 total time=  12.3s
[CV 3/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.862 total time=  29.0s
[CV 4/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.716 total time=  12.4s
[CV 4/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.862 total time=  29.1s
[CV 5/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.757 total time=  12.2s
[CV 5/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.880 total time=  29.9s
[CV 1/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.810 total time=  11.9s
[CV 2/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.804 total time=  11.1s
[CV 3/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.797 total time=  10.8s
[CV 1/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.844 total time=   7.4s
[CV 4/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.789 total time=  10.4s
[CV 5/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.818 total time=   9.9s
[CV 2/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.833 total time=   7.1s
[CV 3/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.844 total time=   7.1s
[CV 4/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.845 total time=   7.1s
[CV 5/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.862 total time=   7.3s
[CV 1/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.860 total time=   9.0s
[CV 2/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.854 total time=   9.1s
[CV 3/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.858 total time=   8.7s
[CV 1/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.789 total time=   5.6s
[CV 4/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.859 total time=   8.7s
[CV 2/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.806 total time=   5.6s
[CV 5/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.870 total time=   8.5s
[CV 3/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.811 total time=   5.5s
[CV 4/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.781 total time=   5.3s
[CV 5/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.829 total time=   5.2s
[CV 1/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.771 total time=   4.8s
[CV 2/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.762 total time=   4.4s
[CV 3/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.777 total time=   4.5s
[CV 4/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.749 total time=   4.6s
[CV 5/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.782 total time=   4.6s
[CV 1/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.728 total time=   4.1s
[CV 2/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.714 total time=   3.9s
[CV 3/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.717 total time=   3.6s
[CV 4/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.720 total time=   3.3s
[CV 5/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.740 total time=   3.1s
```

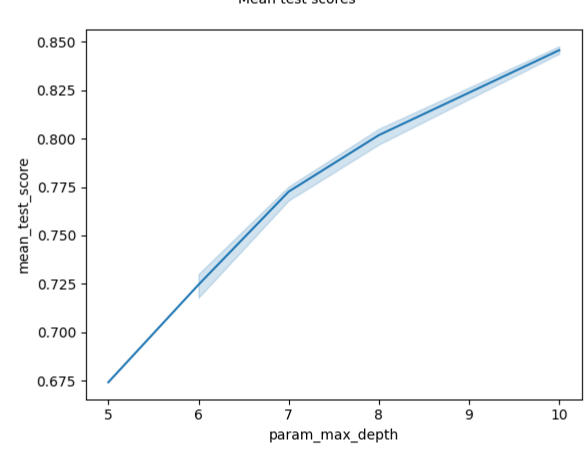
In [230…

```python
hparam_data = pd.DataFrame(hparam_cv.cv_results_)
display(hparam_data[["mean_test_score", "mean_fit_time"]].describe().round(3))
hparam_data["mean_test_score"].hist()
plt.xlabel("Mean test scores")
plt.figure()
sns.lineplot(data=hparam_data, x="param_max_depth", y="mean_test_score", estimator="mean")
```

	mean_test_score	mean_fit_time
count	20.000	20.000
mean	0.797	8.481
std	0.058	5.967
min	0.674	2.769
25%	0.759	5.113
50%	0.803	6.584
75%	0.846	9.968
max	0.868	28.951

Out[230]: <AxesSubplot: xlabel='param_max_depth', ylabel='mean_test_score'>





We can see that the maximum value of max depth is limiting our performance. However as the parameter also increases fitting time, let us first apply the PCA.

In [214…

```python
pca = PCA(n_components=20)
hparam_cv_pca = optimize_randomforest(pca.fit_transform(X_train), y_train, random_grid=random_grid,hparam_max_e
```

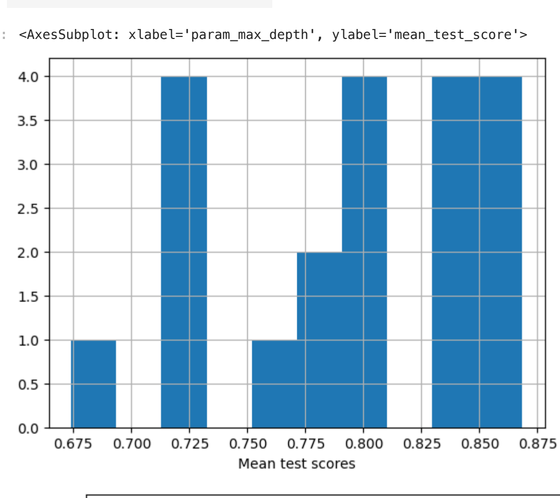
```
Fitting 5 folds for each of 20 candidates, totalling 100 fits
[CV 3/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.632 total time=   0.9s
[CV 1/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.598 total time=   0.9s
[CV 4/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.630 total time=   0.9s
[CV 5/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.623 total time=   0.9s
[CV 2/5] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.561 total time=   0.9s
[CV 1/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.687 total time=   1.0s
[CV 2/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.680 total time=   1.0s
[CV 4/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.710 total time=   1.0s
[CV 3/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.683 total time=   1.0s
[CV 5/5] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10;, score=0.714 total time=   1.0s
[CV 1/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.664 total time=   1.1s
[CV 2/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.618 total time=   1.1s
[CV 4/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.648 total time=   1.1s
[CV 3/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.672 total time=   1.2s
[CV 5/5] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5;, score=0.683 total time=   1.2s
[CV 1/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.777 total time=   1.0s
[CV 2/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.776 total time=   1.0s
[CV 3/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.752 total time=   1.0s
[CV 4/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.767 total time=   1.0s
[CV 2/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.696 total time=   1.5s
[CV 1/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.712 total time=   1.6s
[CV 1/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.719 total time=   0.4s
[CV 2/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.731 total time=   0.4s
[CV 4/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.699 total time=   1.5s
[CV 3/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.691 total time=   1.6s
[CV 5/5] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.725 total time=   1.5s
[CV 3/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.679 total time=   0.5s
[CV 4/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.690 total time=   0.4s
[CV 5/5] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.726 total time=   0.5s
[CV 5/5] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5;, score=0.770 total time=   0.9s
[CV 1/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.630 total time=   0.4s
[CV 2/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.517 total time=   0.5s
[CV 4/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.649 total time=   0.4s
[CV 3/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.582 total time=   0.4s
[CV 5/5] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2;, score=0.668 total time=   0.4s
[CV 1/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.788 total time=   1.5s
[CV 1/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.755 total time=   1.0s
[CV 2/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.735 total time=   1.0s
[CV 2/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.794 total time=   1.5s
[CV 3/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.711 total time=   0.9s
[CV 4/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.805 total time=   1.5s
[CV 4/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.706 total time=   0.9s
[CV 5/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.811 total time=   1.5s
[CV 3/5] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10;, score=0.780 total time=   1.5s
[CV 5/5] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10;, score=0.746 total time=   0.9s
[CV 1/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.762 total time=   0.6s
[CV 2/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.733 total time=   0.6s
[CV 3/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.755 total time=   0.6s
[CV 5/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.778 total time=   0.6s
[CV 4/5] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2;, score=0.689 total time=   0.6s
[CV 1/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.843 total time=   2.1s
[CV 2/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.833 total time=   2.1s
[CV 2/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.820 total time=   0.8s
[CV 1/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.827 total time=   0.9s
[CV 4/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.834 total time=   1.9s
[CV 3/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.829 total time=   2.1s
[CV 5/5] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5;, score=0.845 total time=   2.0s
[CV 3/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.822 total time=   0.8s
[CV 4/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.808 total time=   0.9s
[CV 5/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10;, score=0.825 total time=   0.7s
[CV 1/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.678 total time=   1.0s
[CV 2/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.660 total time=   1.0s
[CV 3/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.659 total time=   1.1s
[CV 4/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.664 total time=   1.1s
[CV 5/5] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5;, score=0.698 total time=   1.1s
[CV 2/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.842 total time=   3.0s
[CV 1/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.845 total time=   3.1s
[CV 1/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.752 total time=   1.1s
[CV 2/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.728 total time=   1.1s
[CV 4/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.840 total time=   2.9s
[CV 5/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.849 total time=   3.0s
[CV 3/5] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5;, score=0.834 total time=   3.2s
[CV 3/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.726 total time=   1.2s
[CV 1/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.782 total time=   0.9s
[CV 2/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.770 total time=   0.8s
[CV 3/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.754 total time=   0.9s
[CV 4/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.745 total time=   0.9s
[CV 4/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.722 total time=   1.2s
[CV 5/5] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.776 total time=   1.0s
[CV 5/5] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2;, score=0.722 total time=   1.3s
[CV 1/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.820 total time=   1.0s
[CV 2/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.822 total time=   1.0s
[CV 1/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.714 total time=   0.7s
[CV 3/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.814 total time=   1.0s
[CV 2/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.718 total time=   0.7s
[CV 3/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.718 total time=   0.7s
[CV 4/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.713 total time=   0.8s
[CV 5/5] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10;, score=0.716 total time=   0.8s
[CV 4/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.821 total time=   1.1s
[CV 5/5] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5;, score=0.823 total time=   1.0s
[CV 1/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.679 total time=   0.7s
[CV 2/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.645 total time=   0.7s
[CV 3/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.615 total time=   0.7s
[CV 4/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.650 total time=   0.7s
[CV 1/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.627 total time=   0.6s
[CV 2/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.626 total time=   0.6s
[CV 3/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.617 total time=   0.6s
[CV 5/5] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10;, score=0.638 total time=   0.6s
[CV 4/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.623 total time=   0.5s
[CV 5/5] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2;, score=0.647 total time=   0.5s
```

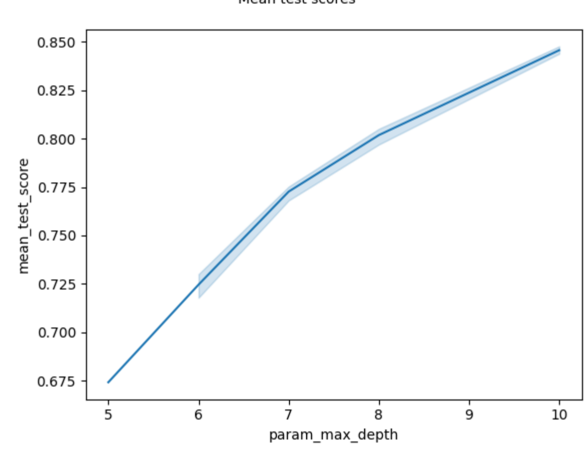
In [231…

```python
hparam_data_pca = pd.DataFrame(hparam_cv_pca.cv_results_)
display(hparam_data_pca[["mean_test_score", "mean_fit_time"]].describe().round(3))
hparam_data_pca["mean_test_score"].hist()
plt.xlabel("Mean test scores")
plt.figure()
sns.lineplot(data=hparam_data_pca, x="param_max_depth", y="mean_test_score", estimator="mean")
```

	mean_test_score	mean_fit_time
count	20.000	20.000
mean	0.797	8.481
std	0.058	5.967
min	0.674	2.769
25%	0.759	5.113
50%	0.803	6.584
75%	0.846	9.968
max	0.868	28.951

Out[231]: <AxesSubplot: xlabel='param_max_depth', ylabel='mean_test_score'>





As we can see the performance didn't decrease even though the number of features is lower after the PCA. Let us increase the depth, since the training is significantly faster with the PCA.

In [21]:

```python
# Number of features to consider at every split
max_features = np.linspace(0.33, 1.0, 5)
# Maximum number of levels in tree
max_depth = [int(x) for x in np.linspace(10, 25, num = 5)]
max_depth.append(None)
# Minimum number of samples required to split a node
min_samples_split = [2, 5, 10]
# Minimum number of samples required at each leaf node
min_samples_leaf = [1, 2, 4]
# Create the random grid
random_grid = {
    'max_features': max_features,
    'max_depth': max_depth,
    'min_samples_split': min_samples_split,
    'min_samples_leaf': min_samples_leaf
}

pca = PCA(n_components=20)
hparam_cv_pca = optimize_randomforest(pca.fit_transform(X_train), y_train, random_grid=random_grid,hparam_max_e
```

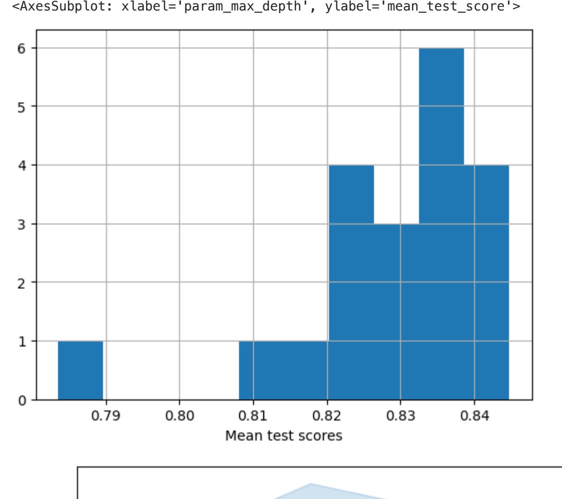
```
Fitting 5 folds for each of 20 candidates, totalling 100 fits
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   1.5s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   1.5s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   1.4s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   1.4s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   1.5s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; total time=   1.6s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; total time=   1.7s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; total time=   1.7s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; total time=   1.7s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; total time=   1.7s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; total time=   1.8s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; total time=   1.8s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; total time=   1.9s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; total time=   1.9s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; total time=   1.4s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; total time=   1.6s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; total time=   1.4s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; total time=   2.0s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; total time=   1.5s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   0.9s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   1.0s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   0.9s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   0.9s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.8s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   0.9s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.9s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.9s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; total time=   1.4s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.9s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.9s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total time=   0.9s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total time=   0.9s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total time=   0.8s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total time=   0.8s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total time=   0.8s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; total time=   2.7s
[CV] END max_depth=21, max_features=0.665, min_samples_leaf=2, min_samples_split=10; total time=   2.0s
[CV] END max_depth=21, max_features=0.665, min_samples_leaf=2, min_samples_split=10; total time=   2.0s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; total time=   2.6s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; total time=   2.7s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; total time=   2.8s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; total time=   2.7s
[CV] END max_depth=21, max_features=0.665, min_samples_leaf=2, min_samples_split=10; total time=   1.8s
[CV] END max_depth=21, max_features=0.665, min_samples_leaf=2, min_samples_split=10; total time=   1.9s
[CV] END max_depth=21, max_features=0.665, min_samples_leaf=2, min_samples_split=10; total time=   1.9s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; total time=   2.0s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; total time=   2.0s
[CV] END max_depth=25, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total time=   0.8s
[CV] END max_depth=25, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total time=   0.8s
[CV] END max_depth=25, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total time=   0.9s
[CV] END max_depth=25, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total time=   0.9s
[CV] END max_depth=25, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total time=   0.8s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; total time=   2.1s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   1.0s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   1.0s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   1.0s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; total time=   2.2s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; total time=   2.3s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   1.1s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total time=   1.1s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; total time=   3.5s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; total time=   3.6s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; total time=   3.6s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; total time=   3.9s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; total time=   3.5s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.6s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.6s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.6s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.6s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total time=   2.6s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   2.7s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   2.7s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; total time=   1.0s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; total time=   1.1s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.6s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.6s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.5s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; total time=   1.1s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.5s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.5s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; total time=   1.0s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   2.5s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   2.7s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; total time=   1.0s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; total time=   2.6s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; total time=   1.4s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.3s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.3s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; total time=   1.4s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; total time=   1.4s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; total time=   1.3s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; total time=   1.3s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.2s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.2s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; total time=   0.9s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; total time=   1.1s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; total time=   0.9s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; total time=   0.8s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; total time=   0.7s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; total time=   0.7s
```

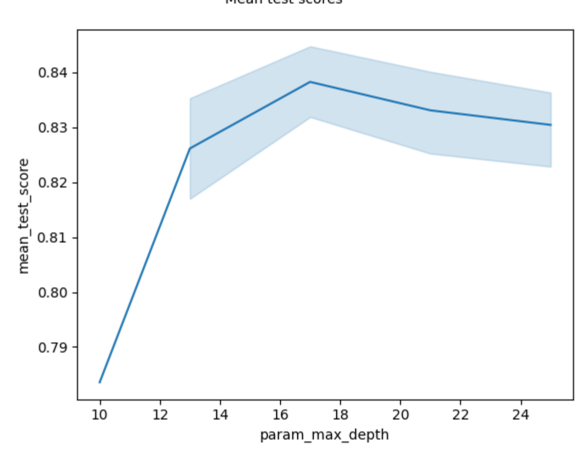
In [23]:

```python
hparam_data_pca = pd.DataFrame(hparam_cv_pca.cv_results_)
display(hparam_data_pca[["mean_test_score", "mean_fit_time"]].describe().round(3))
hparam_data_pca["mean_test_score"].hist()
plt.xlabel("Mean test scores")
plt.figure()
sns.lineplot(data=hparam_data_pca, x="param_max_depth", y="mean_test_score", estimator="mean")
```

	mean_test_score	mean_fit_time
count	20.000	20.000
mean	0.829	1.722
std	0.014	0.804
min	0.784	0.806
25%	0.822	1.032
50%	0.833	1.502
75%	0.838	2.226
max	0.845	3.617

Out[23]: <AxesSubplot: xlabel='param_max_depth', ylabel='mean_test_score'>





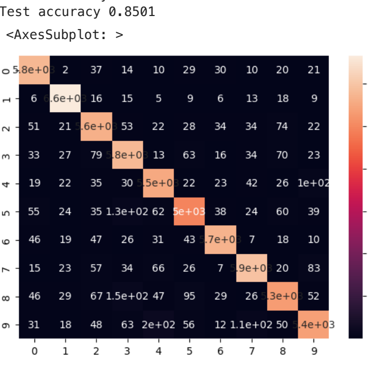
Decision Tree Full Training Set test

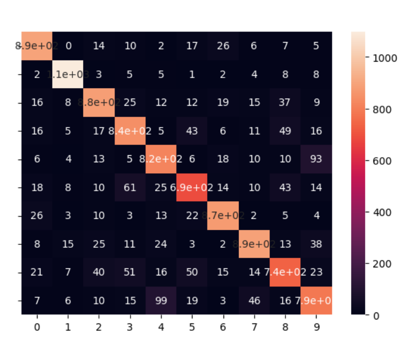
In [234…

```python
model_dt = Pipeline(
    [
    ("pca", PCA(n_components=20)),
    ("clf", DecisionTreeClassifier(**hparam_cv.best_params_))
    ]
)
model_dt.fit(X_train, y_train)
y_pred_train = model_dt.predict(X_train)
y_pred_test = model_dt.predict(X_test)

# Additional
print("Train accuracy", accuracy_score(y_train, y_pred_train))
print("Test accuracy", accuracy_score(y_test, y_pred_test))

fig, axs = plt.subplots(1,2, figsize=(15, 5), sharex=True, sharey=True)
sns.heatmap(confusion_matrix(y_train, y_pred_train), annot=True, ax=axs[0])
sns.heatmap(confusion_matrix(y_test, y_pred_test), annot=True, ax=axs[1])
```

```
Train accuracy 0.9422833333333334
Test accuracy 0.8501
```

Out[234]: <AxesSubplot: >





KMeans

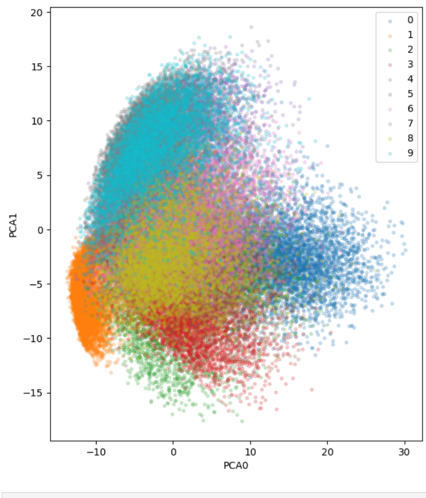
Let us see if the classes are separable in the latent space

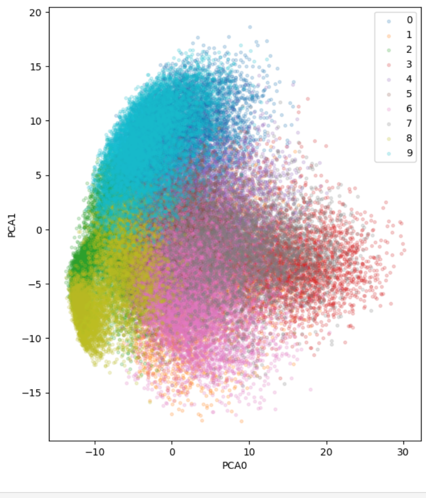
In [42]:

```python
from sklearn.cluster import KMeans
from sklearn.decomposition import PCA

pca = PCA(n_components=20)
kmeans = KMeans(n_clusters=10) # 1 for each label

pipeline = Pipeline(
    [
    ("pca", pca),
    ("kmeans", kmeans)
    ]
    )

cluster_labels = pipeline.fit_predict(X_train)

pca_X = pca.fit_transform(X_train)
```

In [46]:

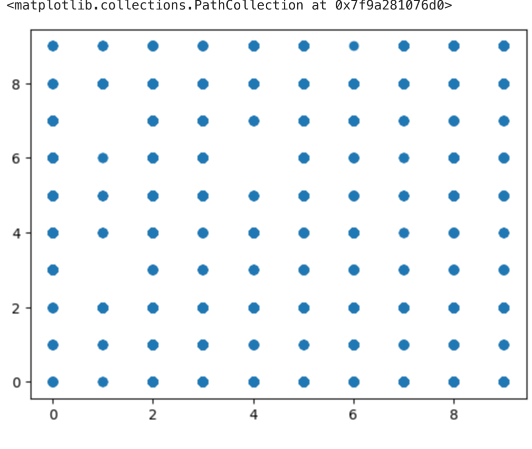
```python
fig, axs = plt.subplots(1,2, figsize=(15,8))
for i in range(10):
    mask = y_train == i
    axs[0].scatter(pca_X[mask, 0], pca_X[mask,1], label=i, marker=".", alpha=.2)
    axs[0].legend()
for i in range(10):
    mask = cluster_labels == i
    axs[1].scatter(pca_X[mask, 0], pca_X[mask,1], label=i, marker=".", alpha=.2)
    axs[1].legend()

for ax in axs:
    ax.set_xlabel("PCA0")
    ax.set_ylabel("PCA1")
```





In [47]:
```
plt.scatter(y_train, cluster_labels)
```

Out[47]: <matplotlib.collections.PathCollection at 0x7f9a281076d0>



...while similar clusters can be seen, no inference can be made directly on the cluster assignment