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]:
```
# !pip install torch
# !pip install pandas
# !pip install scikit-learn
# !pip install tensorboard
# !pip install seaborn
# !pip install torchvision
```

Imports

In [2]:
```
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
```

```
/Users/veikko/Documents/Kouluhommia/MachineLearning/aalto-machine-learning/.venv/lib/python3.9/site-packages/tqdm/auto.py:22: TqdmWarning: IProgress not found. Please update jupyter and ipywidgets. See https://ipywidgets.readthedocs.io/en/stable/user_install.html
  from .autonotebook import tqdm as notebook_tqdm
```

Helper functions

In [3]:

```python
def train(train_loader, model, optimizer, criterion, device, detect_bad_gradients=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_nor
        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, wr
    """
    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, pe
        )
        val_loader = DataLoader(
            val_set, batch_size=config["batch_size"], shuffle=False, num_workers=0, pers
        )
        test_loader = DataLoader(
            test_set, batch_size=config["batch_size"], shuffle=False, num_workers=0, per
        )

        # 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["optim
        )
        if config["lr_scheduler"]:
            scheduler = torch.optim.lr_scheduler.MultiStepLR(optimizer=optimizer, **conf

        # 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_gr
            )
            # 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,

            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, te

        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

    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 [4]:
```
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

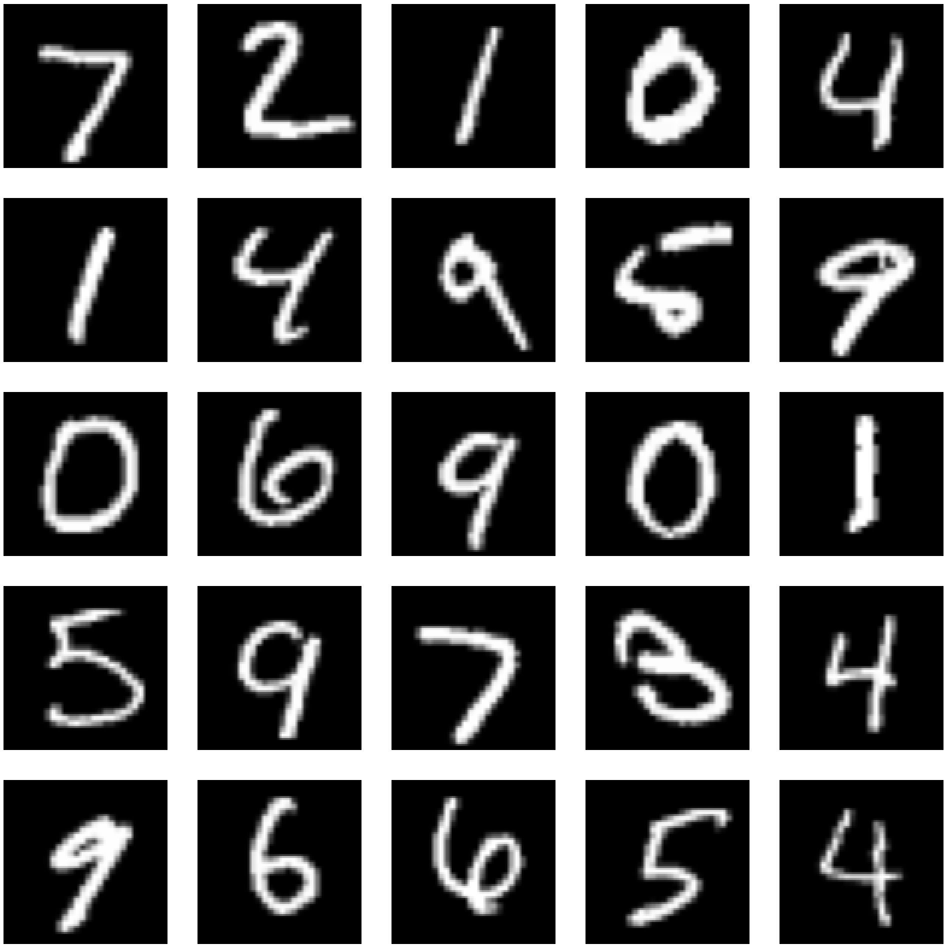
In [5]:
```
print("Lenght of the training set:", len(train_data))
print("Lenght of the test set:", len(test_data))
print()
print("Shape of \"features\", i.e. images: ", train_data[0][0].shape)
```

```
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 [6]:
```
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 [7]:
```
# Distribution of labels in train and test sets

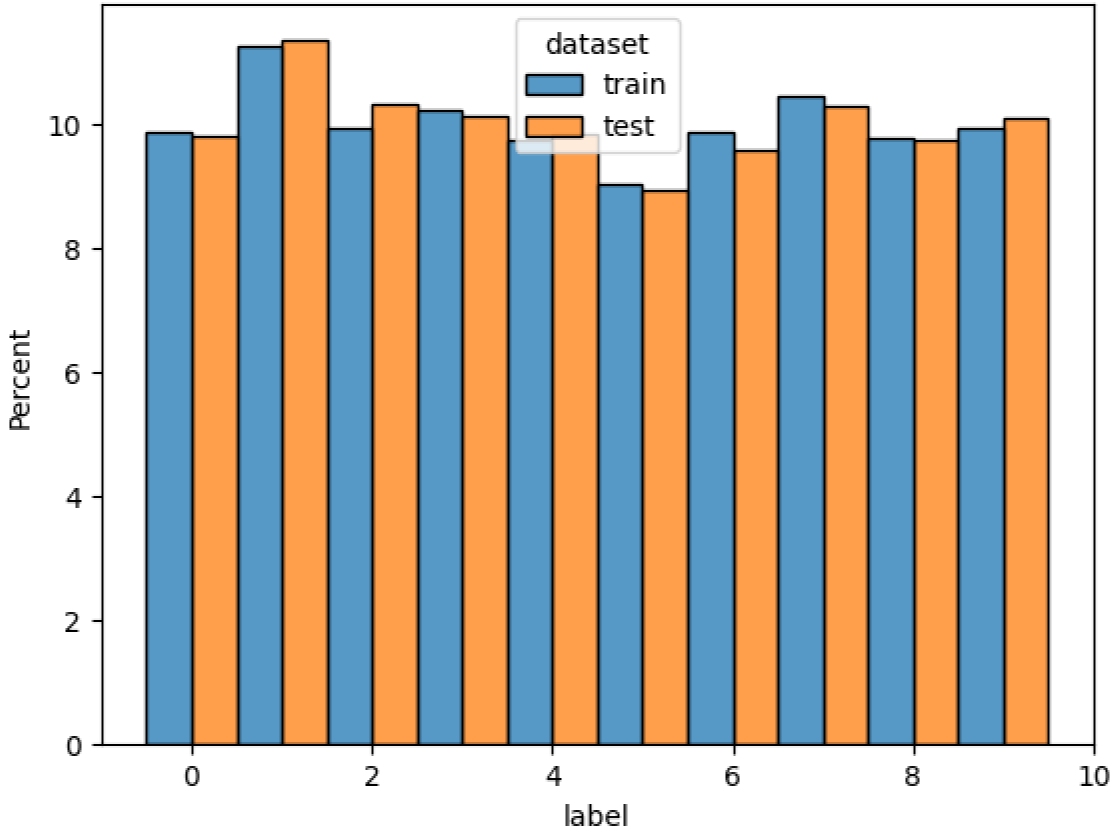
train_labels = [train_data[i][1] for i in range(len(train_data))]
test_labels = [test_data[i][1] for i in range(len(test_data))]

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 [8]:
```
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[8]:
```
<AxesSubplot: xlabel='label', ylabel='Percent'>
```



In [9]:
```
print("Feature statistics")
print("Min:", train_features.min())
print("Max:", train_features.max())
print("Mean:", train_features.mean())
print("Std:", train_features.std())
```

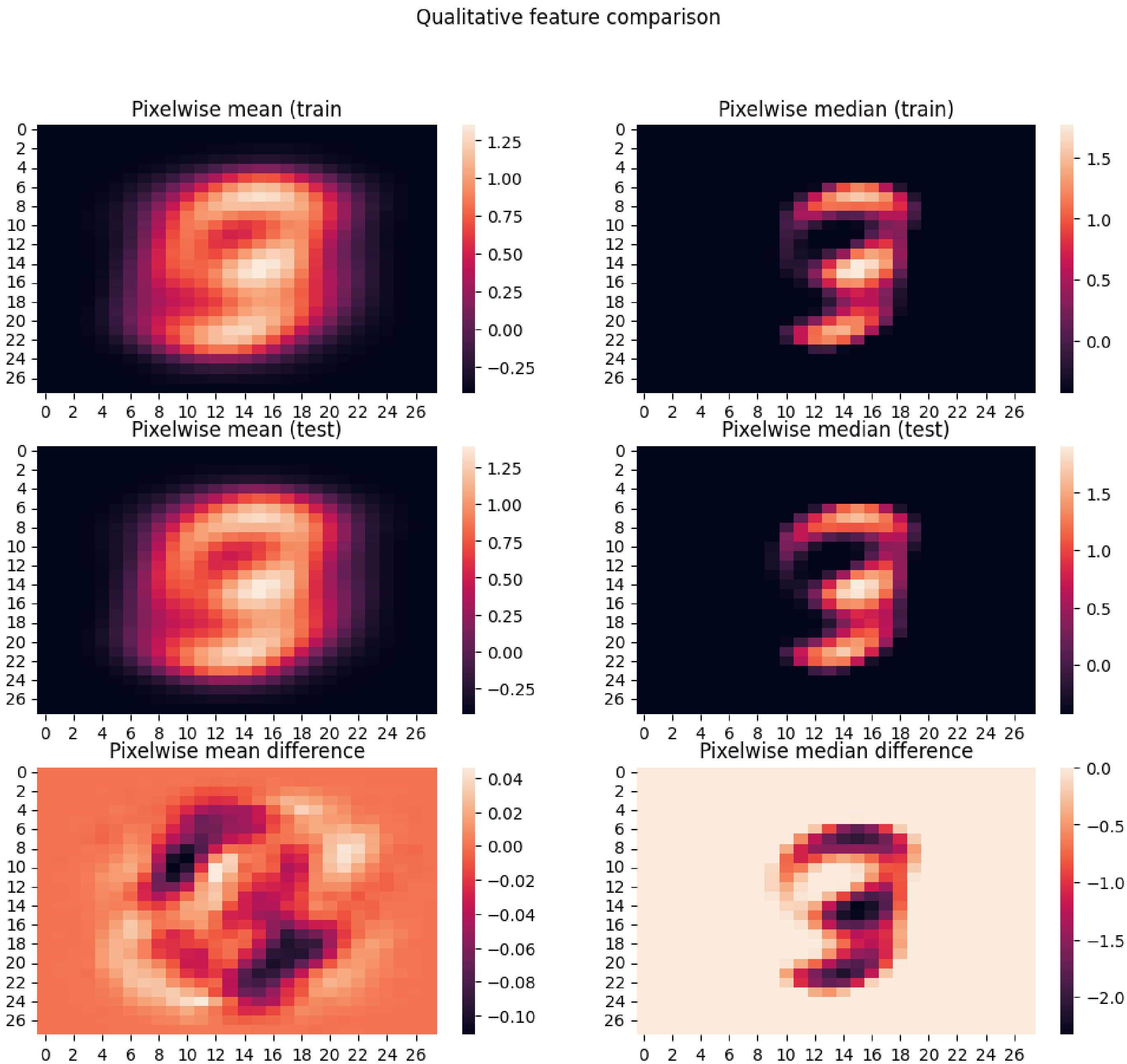
```
Feature statistics
Min: tensor(-0.4242)
Max: tensor(2.8215)
Mean: tensor(-0.0001)
Std: tensor(1.0000)
```

The data is normalized correctly as we see.

Visualize the pixel distributions in training set

In [10]:
```
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).detac
axs[2,1].set_title("Pixelwise median difference")
```

Out[10]:
```
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

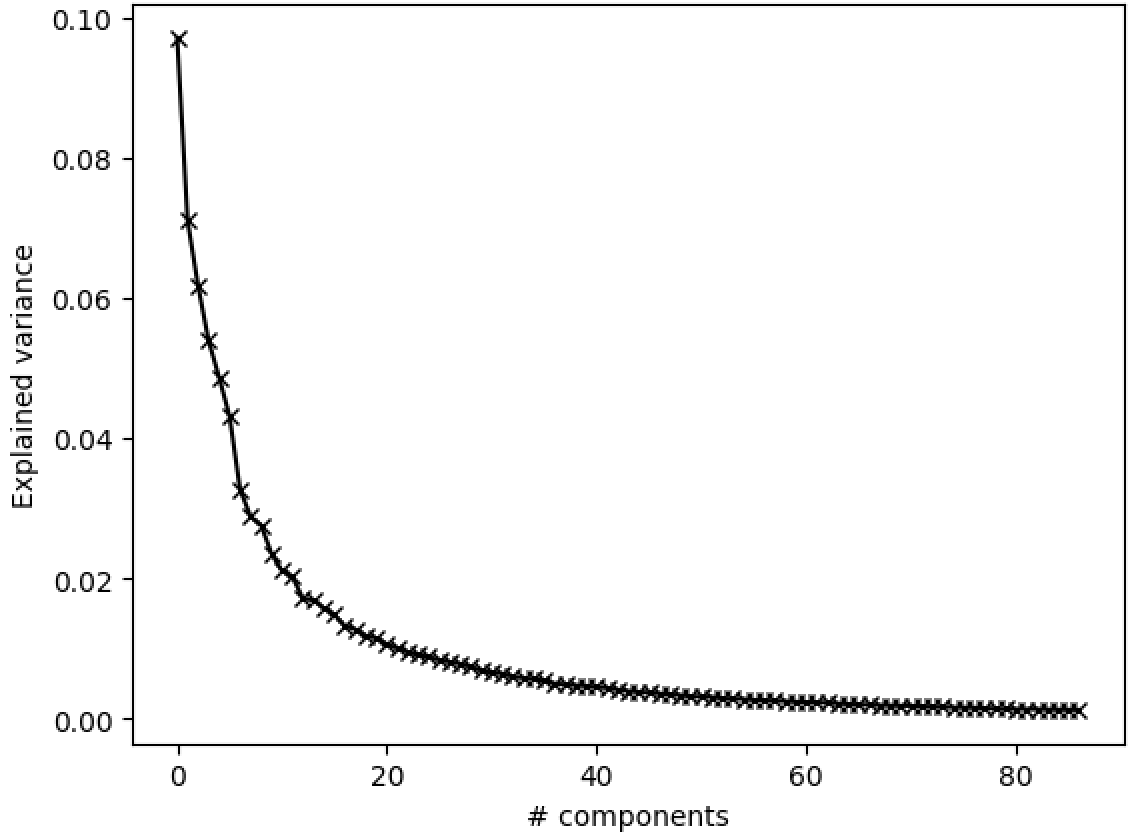
In [11]:
```
train_set_flat = train_features.flatten(start_dim=-2).squeeze()
test_set_flat = test_features.flatten(start_dim=-2).squeeze()
train_set_flat.shape, test_set_flat.shape
```

Out[11]:
```
(torch.Size([60000, 784]), torch.Size([10000, 784]))
```

PCA Elbow Curve

In [12]:
```
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[12]: 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 [13]:
```
model = Pipeline(
    [
    ("pca", PCA(n_components=20)),
    ("reg", LogisticRegression(multi_class='multinomial', fit_intercept=True, max_iter=5
    ]
)
X_train = train_set_flat
y_train = train_labels["label"]

X_test = test_set_flat
y_test = test_labels["label"]

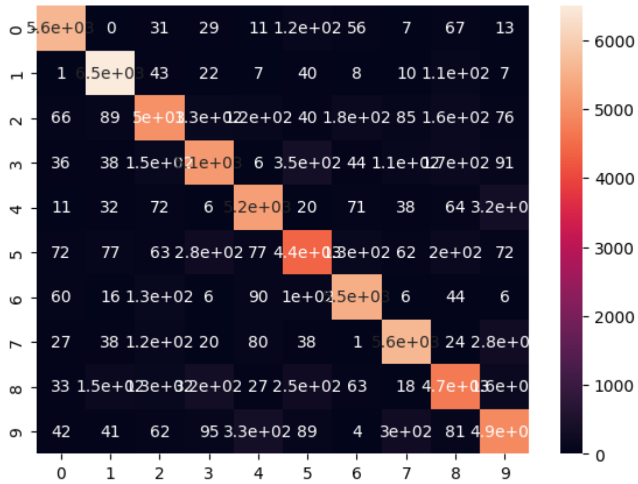
model.fit(X_train, y_train)
y_pred_train = model.predict(X_train)
y_pred_test = model.predict(X_test)

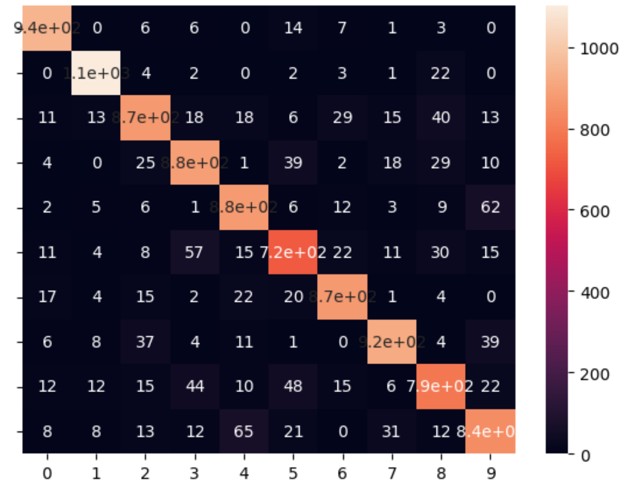
# Additional
print("Train accuracy", accuracy_score(y_train, y_pred_train))
print("Test accuracy", accuracy_score(y_test, y_pred_test))

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 0.8750666666666667
Test accuracy 0.881
```

Out[13]: <AxesSubplot: >





Decision Tree

In [14]:
```
def optimize_randomforest(X_train, y_train, random_grid, hparam_max_evals, metric, kfold
    # Inspiration from https://towardsdatascience.com/hyperparameter-tuning-the-random-f
    # 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_
    # 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 [15]:
```
# 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
}

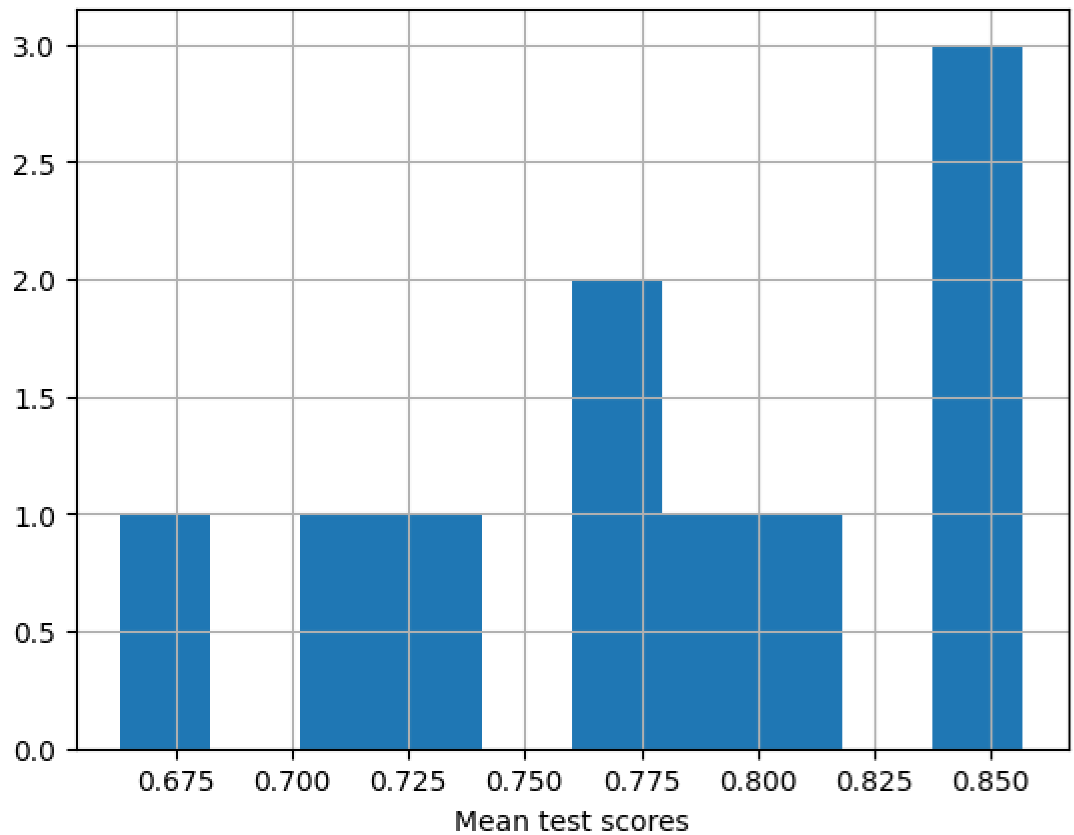
hparam_cv = optimize_randomforest(X_train, y_train,random_grid=random_grid, hparam_max_e
```

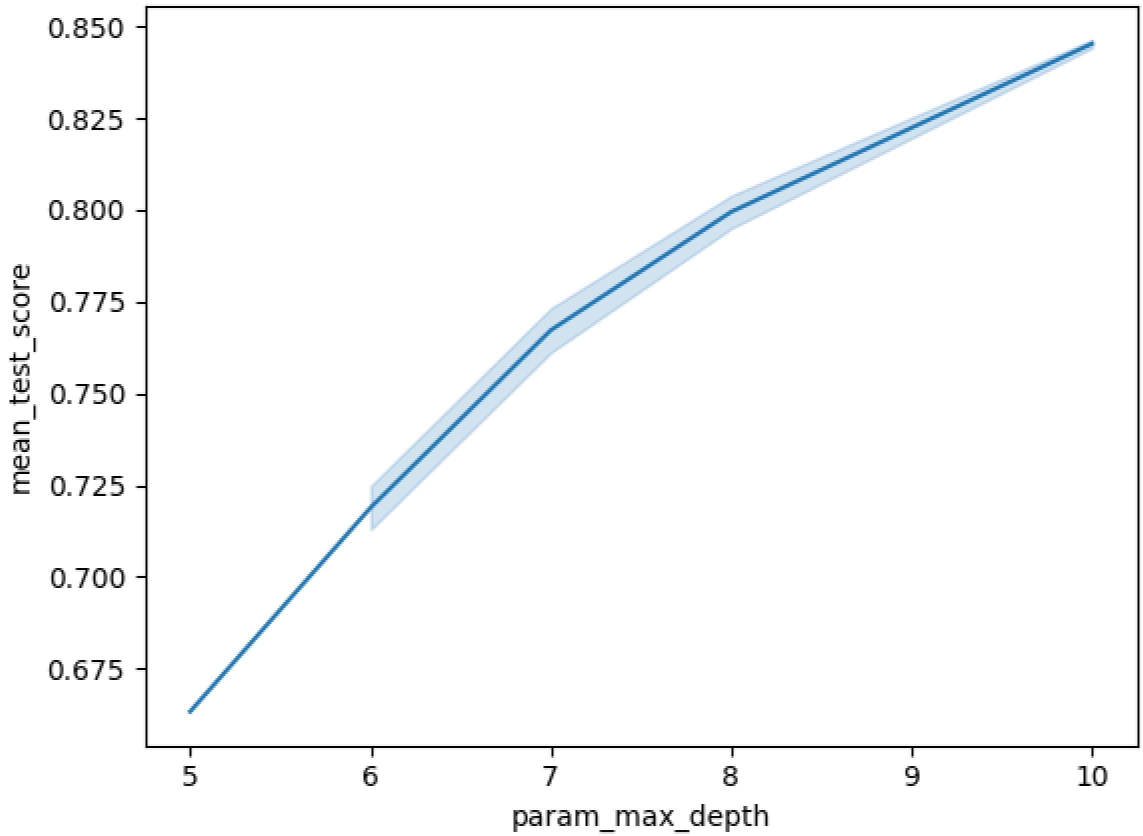
```
Fitting 3 folds for each of 10 candidates, totalling 30 fits
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   5.3s
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   5.2s
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   5.3s
[CV] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tota
l time=   5.8s
[CV] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tota
l time=   5.5s
[CV] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tota
l time=   5.4s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   7.1s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   7.6s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   8.6s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   8.4s
[CV] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=  11.5s
[CV] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=  11.6s
[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
time=   4.3s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   8.1s
[CV] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=  11.2s
[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
time=   3.5s
[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
time=   3.1s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   5.6s
[CV] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   2.2s
[CV] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   2.8s
[CV] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   2.9s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   8.6s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   8.5s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   8.4s
[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
l time=   5.4s
[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
l time=   5.1s
[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
l time=   4.8s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
tal time=   9.3s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
tal time=   9.6s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
tal time=   8.8s
```

In [16]:
```
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	10.000	10.000
mean	0.778	6.543
std	0.064	2.673
min	0.663	2.578
25%	0.734	5.090
50%	0.784	6.315
75%	0.834	8.201
max	0.857	11.278

Out[16]:
```
<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 [17]:
```
pca = PCA(n_components=20)
hparam_cv_pca = optimize_randomforest(pca.fit_transform(X_train), y_train, random_grid=r
```

```
Fitting 5 folds for each of 20 candidates, totalling 100 fits
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   0.7s
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   0.7s
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   0.7s
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   0.7s
[CV] END max_depth=5, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   0.7s
[CV] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tota
l time=   0.8s
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l time=   0.8s
[CV] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tota
l time=   0.8s
[CV] END max_depth=7, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tota
l time=   0.8s
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l time=   0.8s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   0.9s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   0.9s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   0.9s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   0.9s
[CV] END max_depth=6, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tota
l time=   0.9s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   0.7s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   0.7s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   0.7s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   0.7s
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ime=   1.2s
[CV] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=   1.2s
[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
time=   0.4s
[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
time=   0.4s
[CV] END max_depth=7, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
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[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
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[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
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[CV] END max_depth=8, max_features=0.33, min_samples_leaf=1, min_samples_split=10; total
time=   0.4s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   0.7s
[CV] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
```

```
time=   0.3s
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time=   0.3s
[CV] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   0.3s
[CV] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   0.3s
[CV] END max_depth=6, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   0.4s
[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
l time=   0.9s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
l time=   0.8s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
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[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
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[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=8, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tota
l time=   0.9s
[CV] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total
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[CV] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total
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[CV] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total
time=   0.5s
[CV] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total
time=   0.5s
[CV] END max_depth=10, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total
time=   0.6s
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tal time=   1.8s
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tal time=   1.9s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.7s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.8s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
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[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
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tal time=   0.8s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.8s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.7s
[CV] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=   1.0s
[CV] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
```

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ime=   1.0s
[CV] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=   1.0s
[CV] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=   1.0s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   2.8s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   2.8s
[CV] END max_depth=6, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total t
ime=   1.0s
[CV] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   1.0s
[CV] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   1.0s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   2.7s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   2.7s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   2.9s
[CV] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   1.0s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   0.7s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   0.8s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   0.7s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   0.7s
[CV] END max_depth=10, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   0.7s
[CV] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   1.1s
[CV] END max_depth=8, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tota
l time=   1.1s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   0.9s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   0.9s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   0.9s
[CV] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; tot
al time=   0.7s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   0.9s
[CV] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; tot
al time=   0.7s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   0.9s
[CV] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; tot
al time=   0.7s
[CV] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; tot
al time=   0.6s
[CV] END max_depth=8, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; tot
al time=   0.7s
[CV] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; tot
al time=   0.6s
[CV] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; tot
al time=   0.6s
[CV] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; tot
```

```
al time=   0.6s
[CV] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tota
l time=   0.5s
[CV] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tota
l time=   0.5s
[CV] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; tot
al time=   0.5s
[CV] END max_depth=7, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; tot
al time=   0.5s
[CV] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tota
l time=   0.4s
[CV] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tota
l time=   0.4s
[CV] END max_depth=6, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tota
l time=   0.4s
```

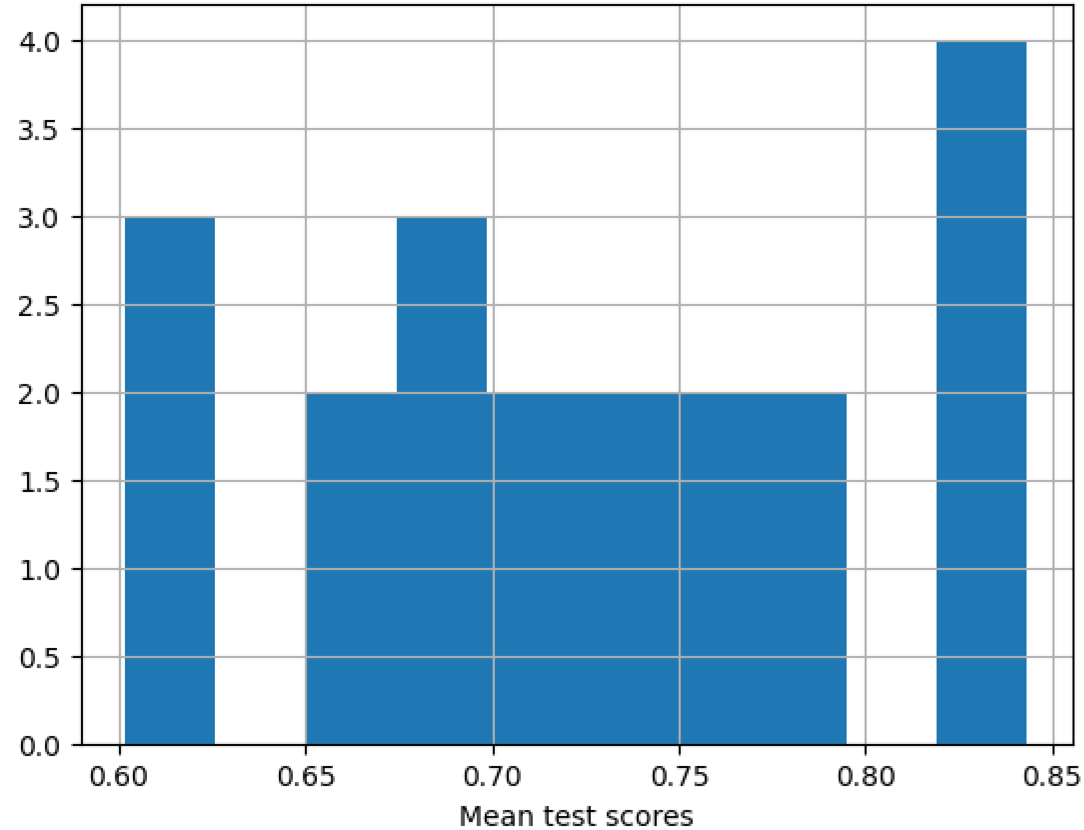
In [18]:

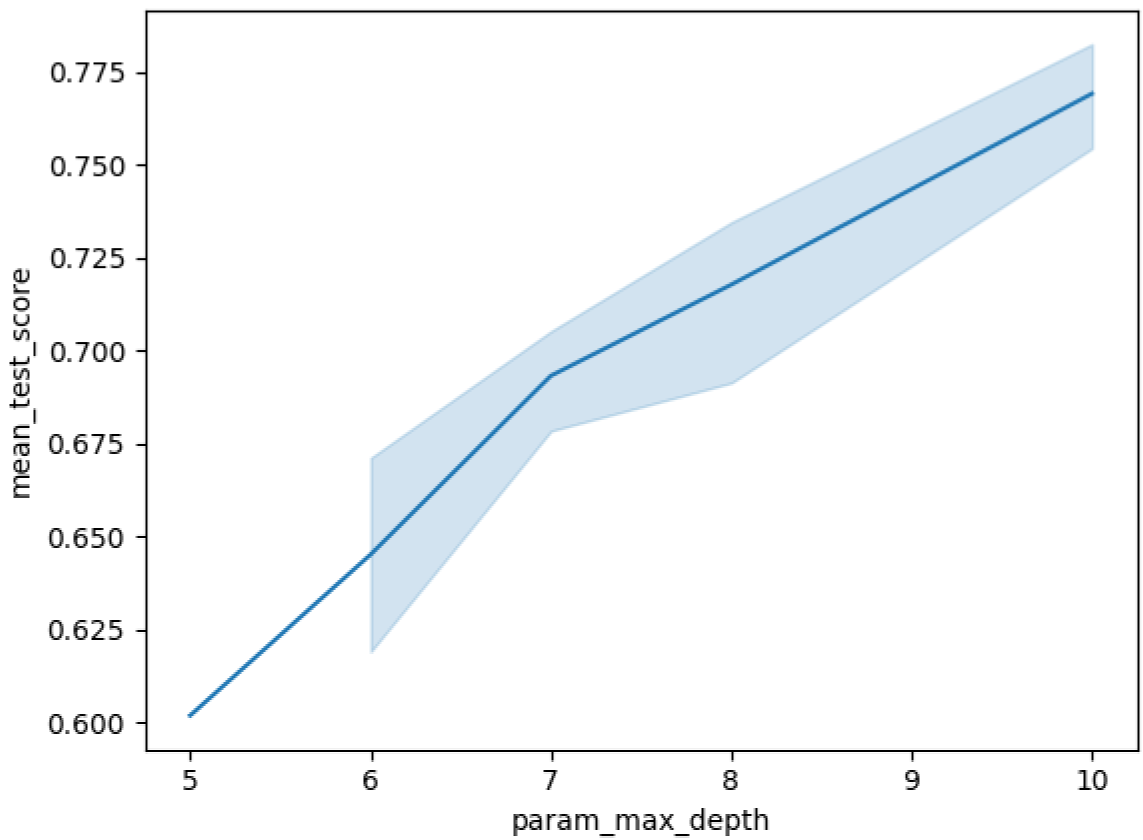
```
hparam_data_pca = pd.DataFrame(hparam_cv_pca.cv_results_)
display(hparam_data_pca[["mean_test_score", "mean_fit_time"]].describe().round(3))
hparam_data_pca["mean_test_score"].hist()
plt.xlabel("Mean test scores")
plt.figure()
sns.lineplot(data=hparam_data_pca, x="param_max_depth", y="mean_test_score",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

	mean_test_score	mean_fit_time
count	20.000	20.000
mean	0.727	0.921
std	0.074	0.553
min	0.602	0.338
25%	0.677	0.634
50%	0.725	0.787
75%	0.778	1.008
max	0.843	2.762

Out[18]:

```
<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 [19]:
```
# 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=r
```

```
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; tot
al time=   1.3s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   1.3s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   1.3s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   1.3s
[CV] END max_depth=10, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   1.3s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tot
al time=   1.5s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tot
al time=   1.5s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tot
al time=   1.5s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tot
al time=   1.6s
[CV] END max_depth=17, max_features=0.665, min_samples_leaf=4, min_samples_split=10; tot
al time=   1.6s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.6s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.6s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.1s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.2s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.2s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.3s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.7s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.7s
[CV] END max_depth=13, max_features=0.8325, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.7s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; tota
l time=   0.8s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; tota
l time=   0.8s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; tota
l time=   0.8s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; tota
l time=   0.8s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.5s
[CV] END max_depth=21, max_features=0.33, min_samples_leaf=1, min_samples_split=10; tota
l time=   0.8s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.5s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=4, min_samples_split=5; tot
al time=   1.2s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.5s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.5s
[CV] END max_depth=17, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.5s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
```

```
time=   0.6s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
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[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   0.6s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   0.7s
[CV] END max_depth=13, max_features=0.33, min_samples_leaf=1, min_samples_split=2; total
time=   0.6s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   2.4s
[CV] END max_depth=21, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tot
al time=   1.7s
[CV] END max_depth=21, max_features=0.665, min_samples_leaf=2, min_samples_split=10; tot
al time=   1.8s
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tal time=   2.3s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   2.4s
[CV] END max_depth=25, max_features=0.8325, min_samples_leaf=1, min_samples_split=10; to
tal time=   2.3s
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tal time=   2.4s
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al time=   1.7s
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al time=   1.7s
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al time=   1.8s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
tal time=   1.9s
[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
tal time=   2.0s
[CV] END max_depth=25, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total
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[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=   0.8s
[CV] END max_depth=25, max_features=0.33, min_samples_leaf=2, min_samples_split=2; total
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[CV] END max_depth=None, max_features=0.665, min_samples_leaf=2, min_samples_split=5; to
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[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.9s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.9s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.9s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=10; to
tal time=   0.9s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   3.3s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
```

```
l time=   3.2s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   3.3s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   3.5s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.3s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.3s
[CV] END max_depth=None, max_features=1.0, min_samples_leaf=4, min_samples_split=5; tota
l time=   3.3s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.3s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.3s
[CV] END max_depth=13, max_features=1.0, min_samples_leaf=1, min_samples_split=5; total
time=   2.3s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   2.4s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   2.5s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   0.9s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   1.0s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.4s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   1.0s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.4s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.4s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.5s
[CV] END max_depth=25, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.4s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   1.0s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   2.4s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   2.5s
[CV] END max_depth=None, max_features=0.33, min_samples_leaf=1, min_samples_split=5; tot
al time=   1.0s
[CV] END max_depth=21, max_features=0.8325, min_samples_leaf=2, min_samples_split=2; tot
al time=   2.4s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.2s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.2s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.3s
[CV] END max_depth=21, max_features=0.4975, min_samples_leaf=1, min_samples_split=10; to
tal time=   1.4s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
```

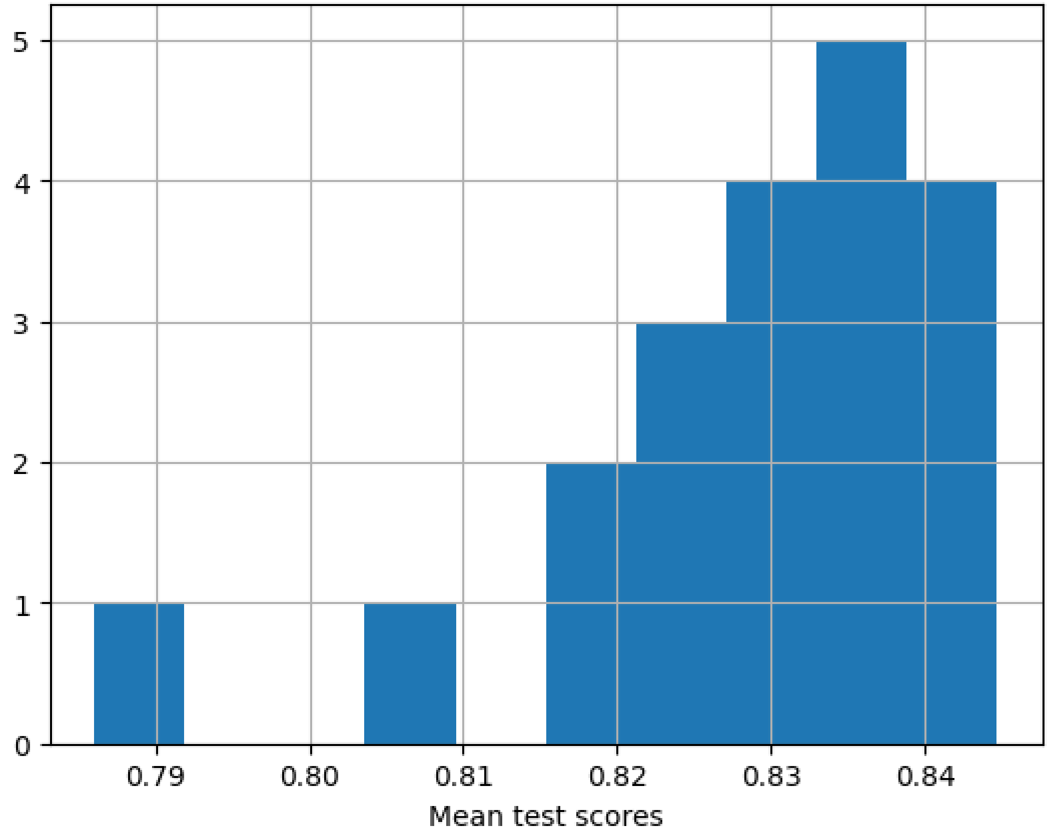
```
tal time=   1.1s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.1s
[CV] END max_depth=17, max_features=0.4975, min_samples_leaf=2, min_samples_split=10; to
tal time=   1.1s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tot
al time=   0.9s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tot
al time=   0.9s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tot
al time=   0.8s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tot
al time=   0.7s
[CV] END max_depth=13, max_features=0.4975, min_samples_leaf=4, min_samples_split=2; tot
al time=   0.7s
```

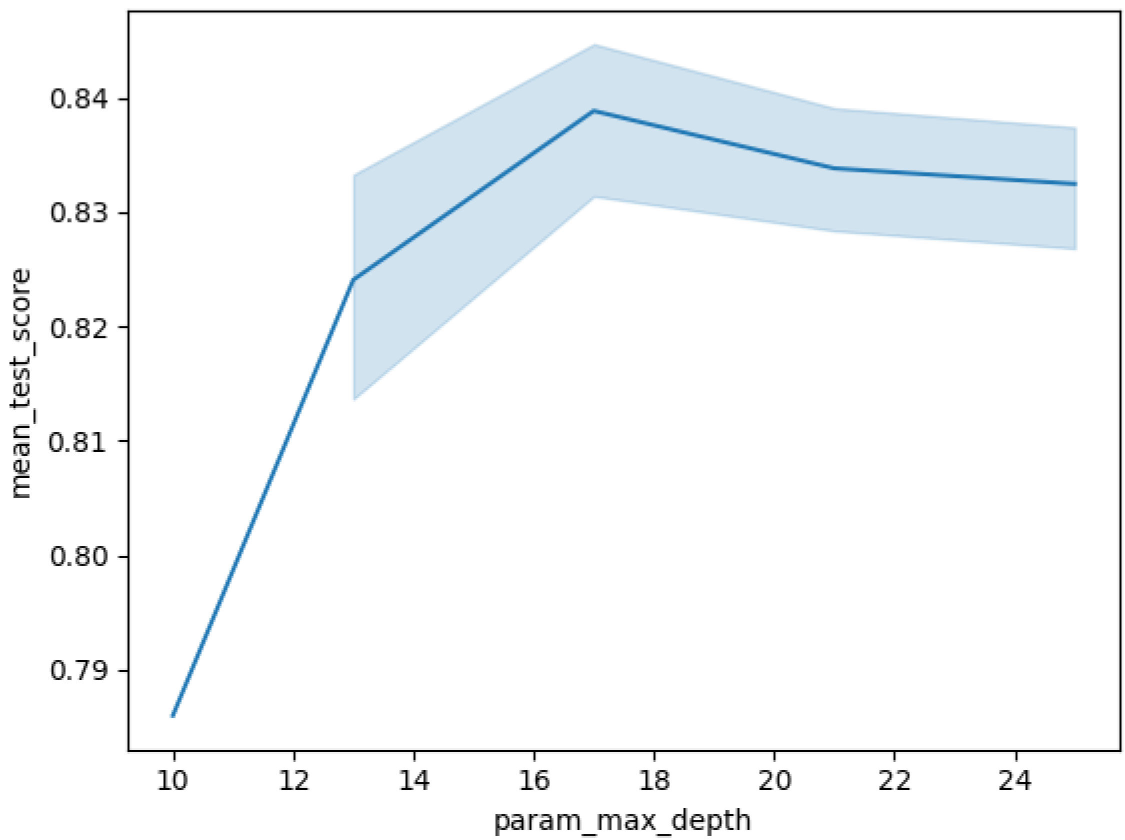
In [20]:

```
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_test_score	mean_fit_time
count	20.000	20.000
mean	0.829	1.554
std	0.014	0.722
min	0.786	0.624
25%	0.823	0.951
50%	0.832	1.361
75%	0.838	2.080
max	0.845	3.304

Out[20]: <AxesSubplot: xlabel='param_max_depth', ylabel='mean_test_score'>





Decision Tree Full Training Set test

In [21]:
```
model_dt = Pipeline(
    [
    ("pca", PCA(n_components=20)),
    ("clf", DecisionTreeClassifier(**hparam_cv.best_params_))
    ]
)
```

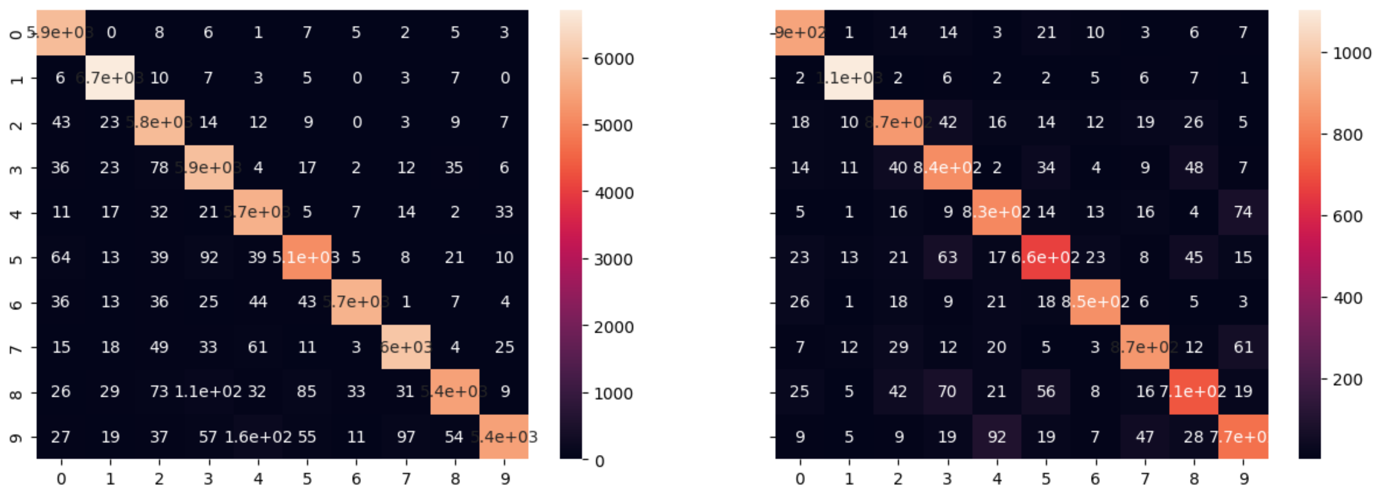
```
model_dt.fit(X_train, y_train)
y_pred_train = model_dt.predict(X_train)
y_pred_test = model_dt.predict(X_test)

# 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 0.9629333333333333
Test accuracy 0.8412
```

Out[21]: <AxesSubplot: >



KMeans

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

In [22]:

```
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)

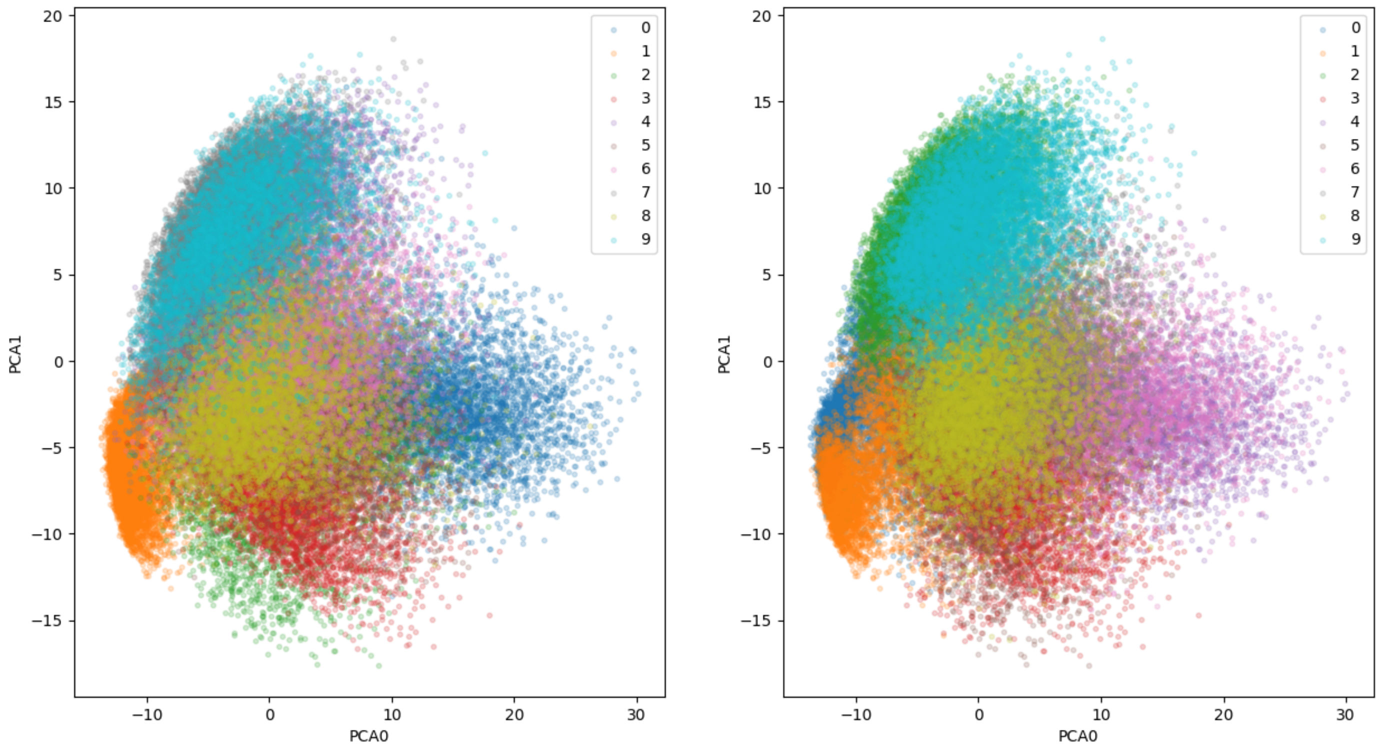
pca_X = pca.fit_transform(X_train)
```

In [23]:

```
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
```

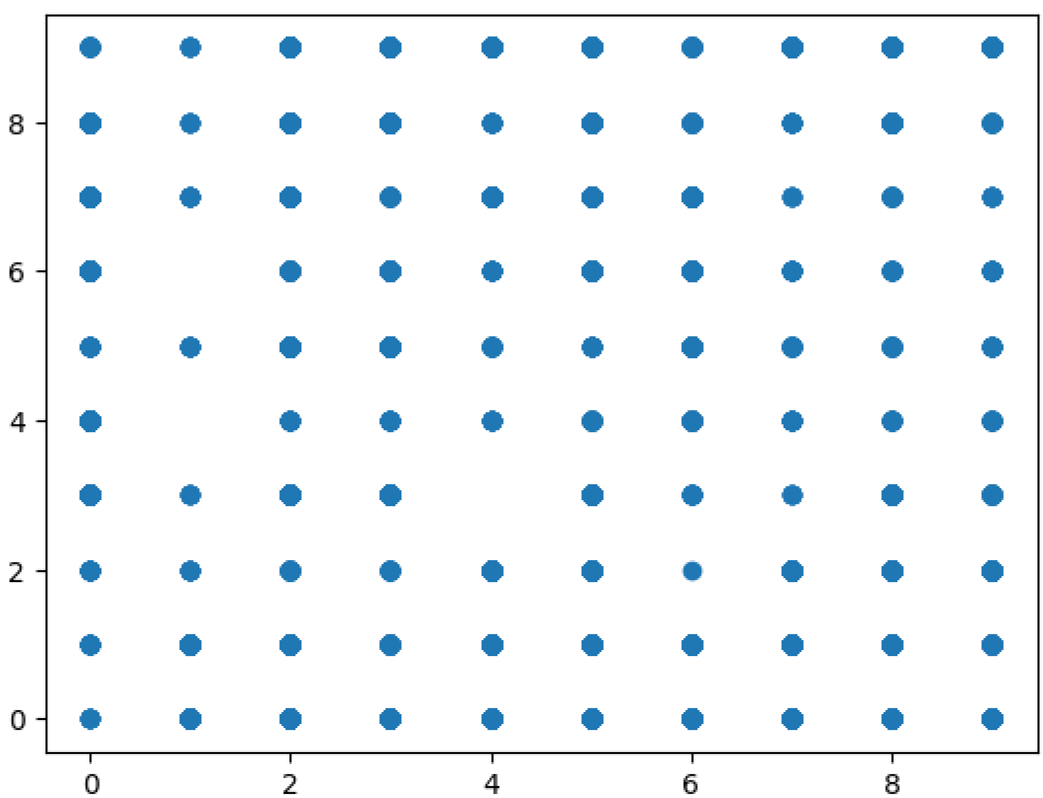
```
    axs[1].scatter(pca_X[mask, 0], pca_X[mask,1], label=i, marker=".", alpha=.2)
    axs[1].legend()

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



In [24]:
```
plt.scatter(y_train, cluster_labels)
```

Out[24]: <matplotlib.collections.PathCollection at 0x7f7bf8dab880>



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