Principle Component Analysis (PCA)

In today's data-driven landscape, many real-world datasets are high-dimensional — meaning they contain a large number of variables or features. While rich in information, these datasets often pose significant challenges for modeling, visualization, and computation. **Principal Component Analysis (PCA)** is a powerful unsupervised machine learning technique designed to tackle this problem by reducing the dimensionality of such data while retaining the most important patterns.

Purpose of This Project

This project demonstrates how PCA can be used to simplify complex datasets by projecting them onto a lower-dimensional space without losing the core structure of the data. The notebook walks through intuitive and technical explanations of PCA, its use cases, and practical implementation using Python. It is well-suited for analysts, data scientists, and machine learning practitioners who want to:

- **Understand** how variance and correlation among features affect modeling.
- **Visualize** high-dimensional data in two or three dimensions.
- **Reduce** noise and redundancy to improve algorithm performance and generalization.
- **Compress** data for storage or faster computation without significant information loss.

Why PCA Matters

Consider a portfolio of 200 stocks. Analyzing relationships between them would require interpreting a 200×200 covariance matrix. PCA simplifies this by identifying the top principal components (example:- 10 out of 200) that explain the majority of the variance, making the problem more interpretable and tractable.

This approach is widely applicable in fields like:

- **Finance** – Risk modeling and portfolio management
- **Computer Vision** – Facial recognition and image compression
- **Bioinformatics** – Gene expression analysis
- **Marketing** – Customer segmentation and behavioral clustering

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What the Project Covers

The notebook includes the following core sections:

1. **Background and Objectives** – Conceptual overview of PCA and its mathematical foundation

2. **Data Setup** – Importing libraries, loading datasets, and preparing data for analysis
3. **PCA Implementation** – Step-by-step walkthrough of applying PCA using `scikit-learn`, visualizing results, and interpreting components
4. **Use Cases** – Real-world scenarios demonstrating the value of PCA in reducing dimensions while preserving data integrity

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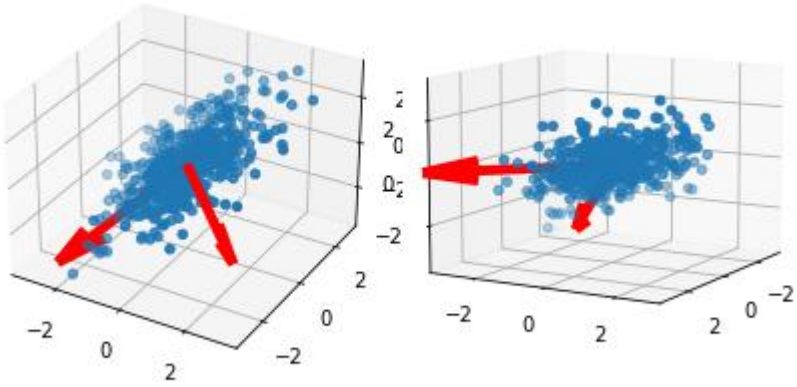
Learning Outcomes

By the end of this project, you should be able to:

- Explain what PCA does and why it is useful
- Apply PCA to real datasets to reduce dimensions
- Visualize the effect of PCA on data distribution
- Interpret principal components in terms of original variables



Use cases of PCA

- Facial Recognition
- Image Compression
- Finding patterns in data of high dimension in the field of quantitative finance.

For instance, suppose you are a fund manager who has 200 stocks in a portfolio. To analyze the potential movements and relationships of the stocks, you would need to at least work with a 200×200 correlation or covariance matrix, which is very complex.

However, instead of looking at 200 stock variances, would it be more efficient to just look at 10 most dominant/principal directions of variances that best represent the original variances of the stocks?

PCA is a methodology to reduce the dimensionality of a complex problem.

In this notebook, we will explore how to simplify and reduce the dimensionality of various data using **principle component analysis** (PCA)

Table of Contents

Objectives

After completing this lab you will be able to:

- **Understand** what PCA is and how (generally) it works.
- **Understand** when PCA is useful.
- **Apply** PCA effectively.

Datasets

Datasets for this lab are gathered from the UCI Machine Learning Repository under the MIT License.

Setup

For this lab, we will be using the following libraries:

- `pandas` for managing the data.
- `numpy` for mathematical operations.
- `sklearn` for machine learning and machine-learning-pipeline related functions.
- `seaborn` for visualizing the data.
- `matplotlib` for additional plotting tools.

Installing Required Libraries

In [ ]:
```
# All Libraries required for this lab are listed below. The libraries pre-instal
# !mamba install -qy pandas==1.3.4 numpy==1.21.4 seaborn==0.9.0 matplotlib==3.5.
# Note: If your environment doesn't support "!mamba install", use "!pip install
```

Importing Required Libraries

In [ ]:
```
# Surpress warnings from using older version of sklearn:
def warn(*args, **kwargs):
    pass
import warnings
warnings.warn = warn

from tqdm import tqdm
import numpy as np
import pandas as pd
from itertools import accumulate

import matplotlib.pyplot as plt
import seaborn as sns
%matplotlib inline

from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.model_selection import train_test_split
from sklearn.model_selection import RandomizedSearchCV
from sklearn.datasets import fetch_lfw_people
from sklearn.metrics import classification_report
from sklearn.metrics import confusion_matrix
from sklearn.svm import SVC
from scipy.stats import loguniform

warnings.filterwarnings('ignore')

sns.set_context('notebook')
sns.set_style('white')
```

Defining Helper Functions

Below, we define helper functions to simplify your code later on:

In [ ]:
```
def plot_explained_variance(pca):
    # This function graphs the accumulated explained variance ratio for a fitted
    acc = [*accumulate(pca.explained_variance_ratio_)]
    fig, ax = plt.subplots(1, figsize=(50, 20))
    ax.stackplot(range(pca.n_components_), acc)
    ax.scatter(range(pca.n_components_), acc, color='black')
    ax.set_ylim(0, 1)
    ax.set_xlim(0, pca.n_components_-1)
    ax.tick_params(axis='both', labelsize=36)
    ax.set_xlabel('N Components', fontsize=48)
    ax.set_ylabel('Accumulated explained variance', fontsize=48)
    plt.tight_layout()
    plt.show()
```

Background

Before we begin using **PCA**, we should first understand:

1. What PCA does
2. How PCA Works

What does PCA do?

- Reduces the dimensionality of data. By reducing data dimensionality, PCA can also help with visualization.
- May reduce noise in the process

-Can be used to pre-process data improving the result of your algorithm

How does PCA work? (optional)

1. Looks at an n -dimensional dataset and breaks it down into "general trends" or **components**

   ```
   - When we say "$n$-dimensional", we mean the data has $n$ features.
   ```

2. The components are then **sorted by how much of the explained variance they account for** (*eigenvalues* provide this information)

   ```
   - This means if a component is highly-uncorrelated with all others, it's a "strong" component and provides useful information that is very hard to infer from all other components.
   ```

3. Then, given some parameter (usually chosen by the data engineer), the new dimension of the data is decided. Let this be k.

   ```
   - Note $k$ is always $k \leq n$ because we're only trying to reduce the dimension of our data.
   ```

4. Finally, the original n dimensional dataset is projected onto the k-dimensional plane chosen by our **top-k components that take care of the most explained variance**.

   ```
   - These top- $k$ components are now used
   ```

Because principle components span an (at most) k-dimensional surface, we have successfully reduced our data to at least $k \leq n$ dimensions!

Visual Example

Let's look at an example that will visually demonstrate PCA in action.

Load the dataset `HeightsWeights.csv` which contains a list of various people's heights (in inches) and weight (in pounds and kg):

In [ ]:
```
hwdf = pd.read_csv('HeightsWeights.csv', index_col=0)
hwdf.head()
```

Out[ ]:

Index	Height(Inches)	Weight(Pounds)	Weight(Kilograms)
1	65.78331	112.9925	51.253062
2	71.51521	136.4873	61.910233
3	69.39874	153.0269	69.412546
4	68.21660	142.3354	64.562914
5	67.78781	144.2971	65.452735

Scaling data

You should (almost) always scale your data before applying PCA

Why?: There are many reasons, here are some:

- Scaling your features make the features have the same standard deviation => same weight.
- If the features have the same weight, PCA is able to best find the most significant components (principal components) without being biased towards features with high variance.
- Computers do not do well in adding large numbers and small numbers, so, if all data is in the same range algorithms usually perform better.

Let's use the `StandardScaler` from `sklearn.preprocessing`:

In [ ]:
```
scaler = StandardScaler()
hwdf[:] = scaler.fit_transform(hwdf)
hwdf.columns = [f'{c} (scaled)' for c in hwdf.columns]
hwdf.head()
```

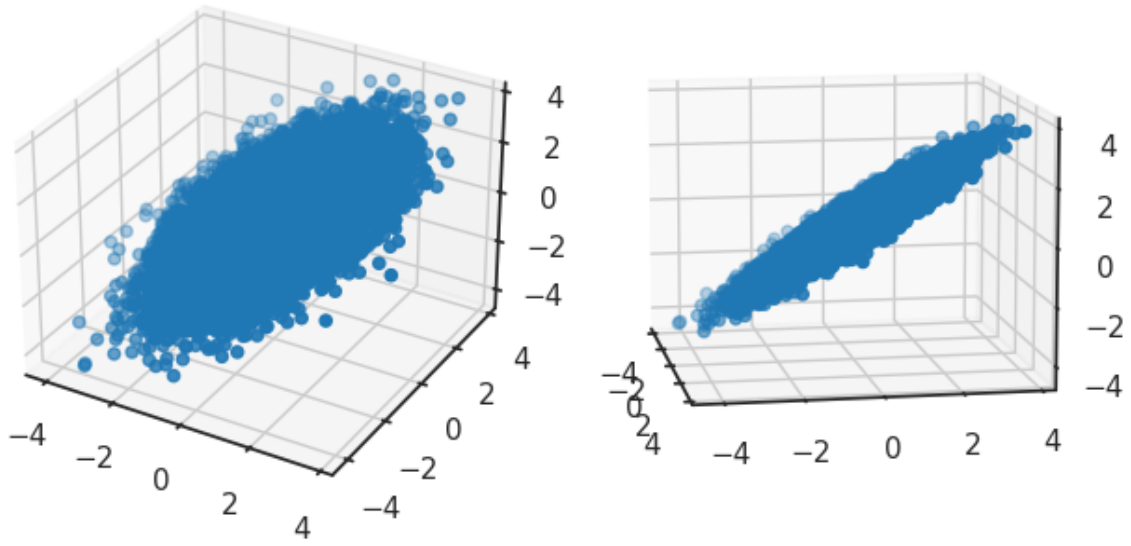
Out[ ]:

Index	Height(Inches) (scaled)	Weight(Pounds) (scaled)	Weight(Kilograms) (scaled)
1	-1.162051	-1.208072	-1.208072
2	1.852136	0.806805	0.806805
3	0.739165	2.225214	2.225214
4	0.117523	1.308328	1.308328
5	-0.107961	1.476561	1.476561

Let's look at 3-D plot of our data (one dimension per feature):

In [ ]:
```
fig = plt.figure()
ax1 = fig.add_subplot(121, projection='3d')
xs, ys, zs = [hwdf[attr] for attr in hwdf.columns]
```

```
ax1.scatter(xs, ys, zs)

ax2 = fig.add_subplot(122, projection='3d')
xs, ys, zs = [hwdf[attr] for attr in hwdf.columns]
ax2.view_init(elev=10, azim=-10)
ax2.scatter(xs, ys, zs)

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

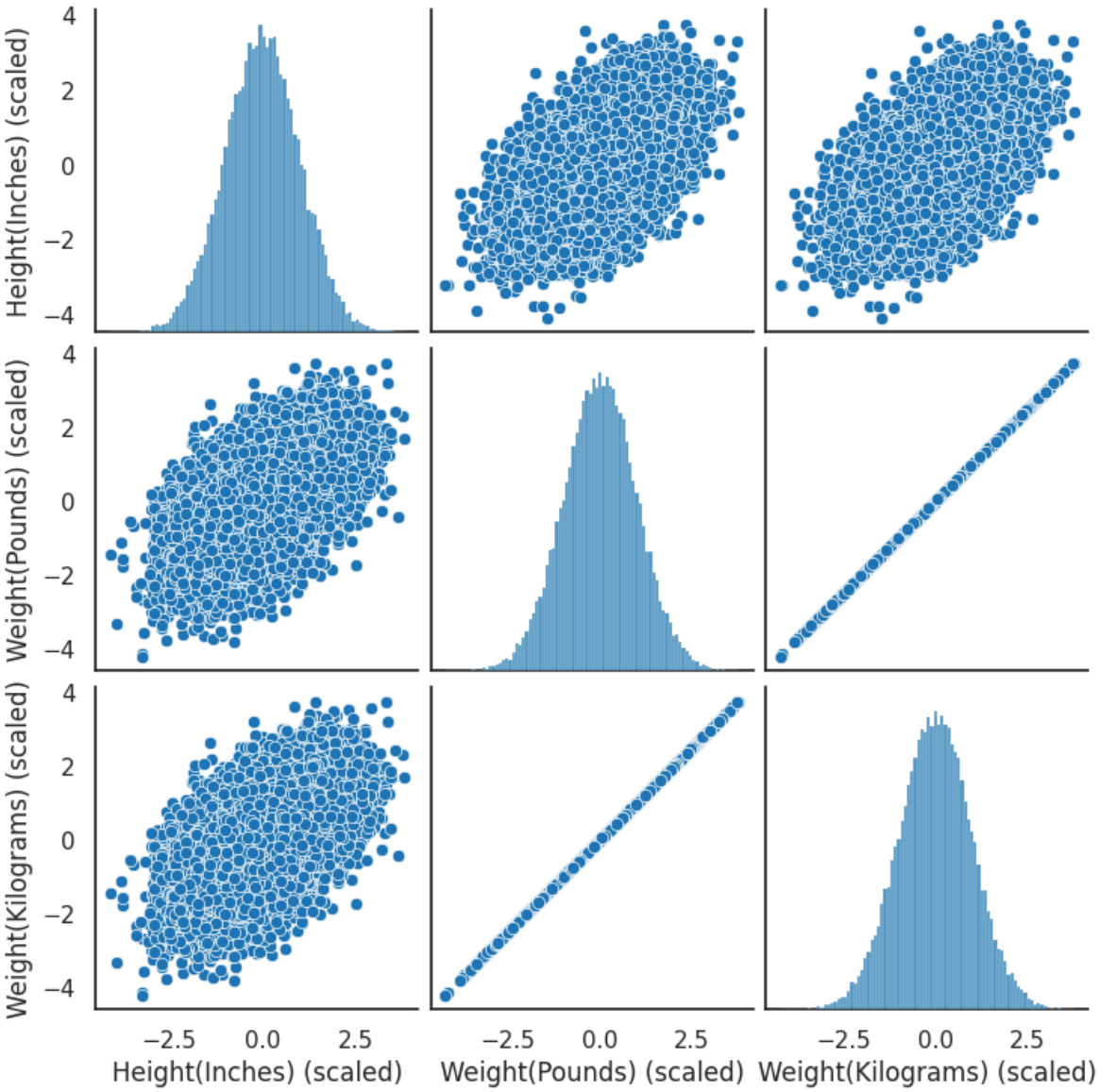


As you can see, our data here forms a plane.

This is because the *weight in kilograms does not provide any more information than weight in pounds* (or vice-versa).

This becomes clear with the following, alternate perspective, showing the 2d relationships between the pairs of data and calculating the correlation :

In [ ]:
```
sns.pairplot(hwdf)
plt.show()
```



In [ ]:
```
hwdf.corr().style.background_gradient(cmap='coolwarm')
```

Out[ ]:

	Height(Inches) (scaled)	Weight(Pounds) (scaled)	Weight(Kilograms) (scaled)
Height(Inches) (scaled)	1.000000	0.502859	0.502859
Weight(Pounds) (scaled)	0.502859	1.000000	1.000000
Weight(Kilograms) (scaled)	0.502859	1.000000	1.000000

We see the weights are perfectly correlated, which means **Weight(Pounds)** tells us everything we need to know about **Weight(Kilograms)** ,thus we have clearly **redundant** data! Although, this example is exaggerated, it'll help demonstrate where PCA shines.

Note Standardizing your data before applying PCA is called *whitening*.

Applying PCA

It's time to apply PCA, let's first apply PCA keeping the same dimension as the original data, i.e.: `n_components=3` .

In [ ]:
```
pca = PCA()
pca.fit(hwdf)
```

Out[ ]:
```
PCA()
```

We can find the projection of the dataset onto the principal components call it `Xhat` , this is our "new" dataset, it is the same shape as the original dataset

In [ ]:
```
Xhat = pca.transform(hwdf)
Xhat.shape
```

Out[ ]:
```
(25000, 3)
```

Let's look at the new dataset as a dataframe.

In [ ]:
```
hwdf_PCA = pd.DataFrame(columns=[f'Projection on Component {i+1}' for i in range
hwdf_PCA.head()
```

Out[ ]:

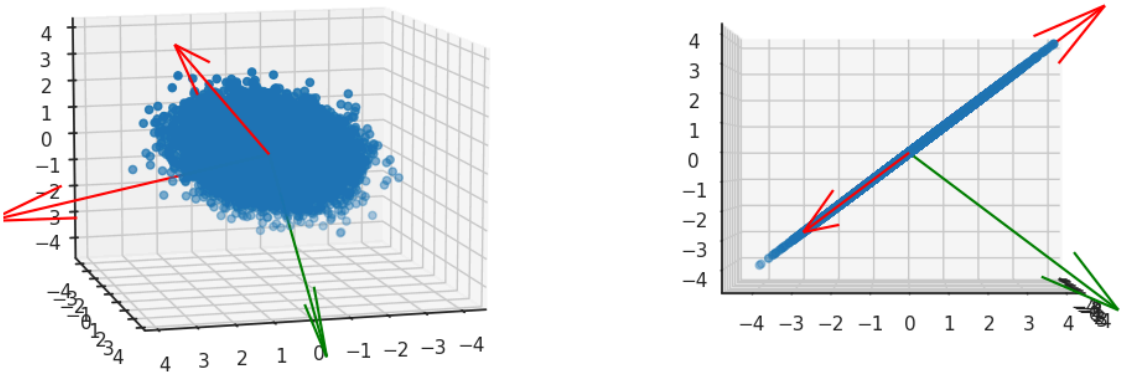
	Projection on Component 1	Projection on Component 2	Projection on Component 3
0	-2.051774	-0.243847	1.094627e-15
1	1.866218	1.117813	3.299626e-16
2	3.133436	-0.794420	3.332217e-16
3	1.696186	-0.748473	-3.318554e-16
4	1.803402	-1.058234	-1.055047e-16

Why are the values in the third column all essentially zero?

Let's look at the principle components:

In [ ]:
```
colors = ['red', 'red', 'green']

fig = plt.figure(figsize=(12,8))
ax1 = fig.add_subplot(121, projection='3d')
xs, ys, zs = [hwdf[attr] for attr in hwdf.columns]
ax1.view_init(elev=10, azim=75)
ax1.scatter(xs, ys, zs)

for component, color in zip(pca.components_, colors):
    ax1.quiver(*[0, 0, 0], *(8 * component), color=color)


ax2 = fig.add_subplot(122, projection='3d')
xs, ys, zs = [hwdf[attr] for attr in hwdf.columns]
ax2.view_init(elev=0, azim=0)
```

```
ax2.scatter(xs, ys, zs)

for component, color in zip(pca.components_, colors):
    ax2.quiver(*[0, 0, 0], *(8 * component), color=color)

plt.show()

for color, ev in zip(colors, pca.explained_variance_ratio_):
    print(f'{color} component accounts for {ev * 100:.2f}% of explained variance
```



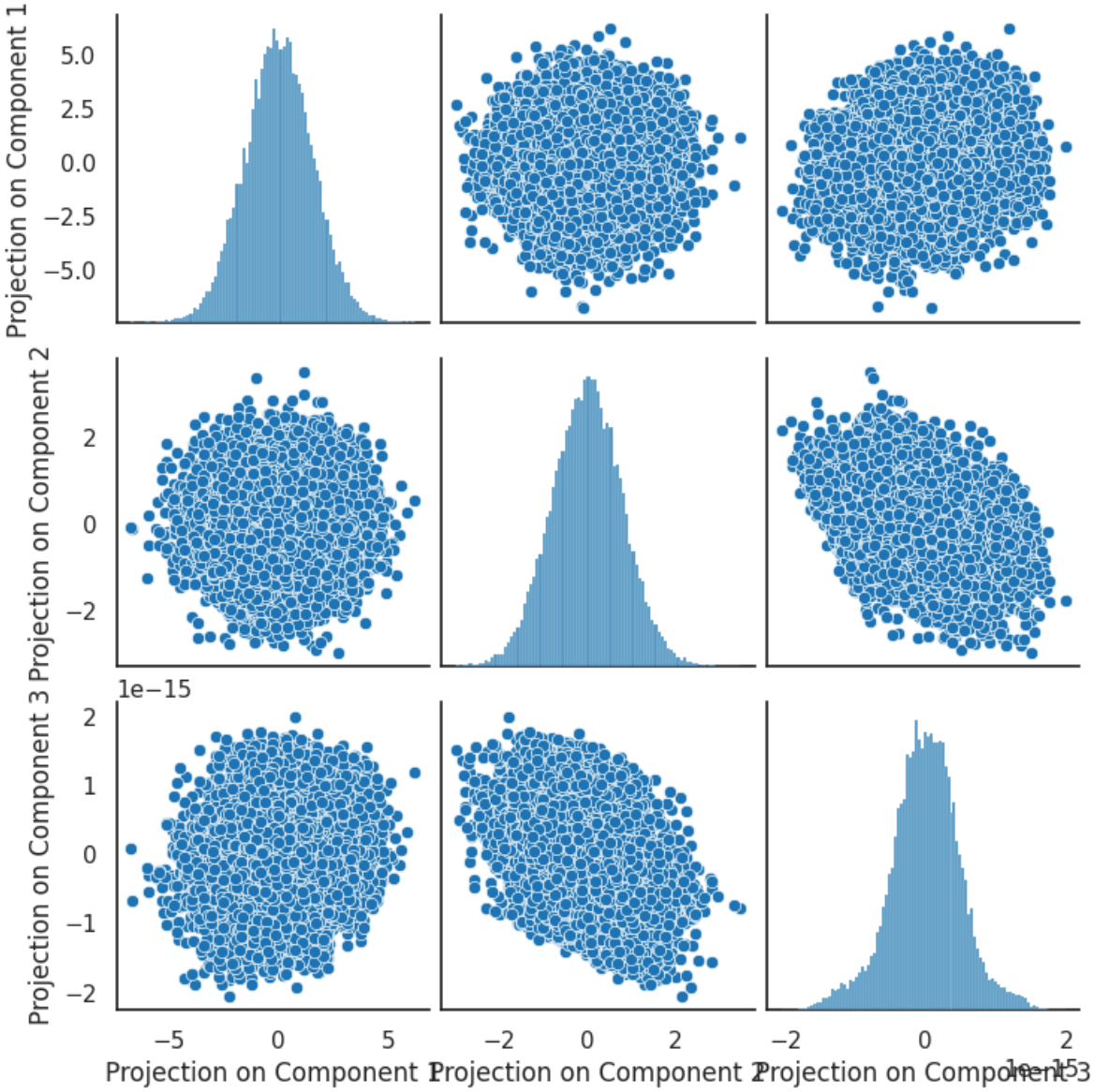
```
red component accounts for 78.98% of explained variance
red component accounts for 21.02% of explained variance
green component accounts for 0.00% of explained variance
```

The 3 colored arrows represent the directions of maximum variance in the original data `hwdf`. The new dataset `Xhat` is the projection of `hwdf` onto each principal component.

Most of the original data seems parallel to the red principle components meaning they are the two most dominant directions of variance of `hwdf`. The green component is perpendicular to the data, as a result the projection is small.

We convert this new data to a Dataframe and see the points appear uncorrelated:

In [ ]:
```
sns.pairplot(hwdf_PCA)
plt.show()
```



In [ ]:
```
hwdf_PCA.corr().style.background_gradient(cmap='coolwarm')
```

Out[ ]:

	Projection on Component 1	Projection on Component 2	Projection on Component 3
Projection on Component 1	1.000000	-0.000000	0.156017
Projection on Component 2	-0.000000	1.000000	-0.412401
Projection on Component 3	0.156017	-0.412401	1.000000

As you can see, the correlations of the 3 principal components are now zero, meaning we have successfully de-correlated `hwdf` and obtained features that are linearly independent of each other.

Each component provides variance/information on a different direction. As we saw before that, the third component had a small projection, which means it doesn't provide much information about our original data `hwdf` in the new feature space.

Thus, we can remove the third dimension, while still keeping the vast majority of our data's information:

In [ ]:
```
hwdf_PCA.drop('Projection on Component 3', axis=1, inplace=True)
hwdf_PCA.head()
```

Out[ ]:

	Projection on Component 1	Projection on Component 2
0	-2.051774	-0.243847
1	1.866218	1.117813
2	3.133436	-0.794420
3	1.696186	-0.748473
4	1.803402	-1.058234

Putting it all Together

Now that you have some intuition behind PCA, let's start from the beginning and understand the PCA-pipeline.

In **sklearn.decomposition.PCA**, there is a parameter called `whiten` which helps standardize your input data if you set `whiten = True`. You could also use `StandardScaler()` as a separate step before using PCA.

In [ ]:
```
scaler = StandardScaler()
X = pd.DataFrame(scaler.fit_transform(hwdf), index=hwdf.index, columns=hwdf.colu
X.head()

pca = PCA()
X_PCA = pd.DataFrame(pca.fit_transform(X), index=X.index, columns=[f'Component {
# (Remember it's technically "Projection onto Component {i}")
X_PCA.head()
```

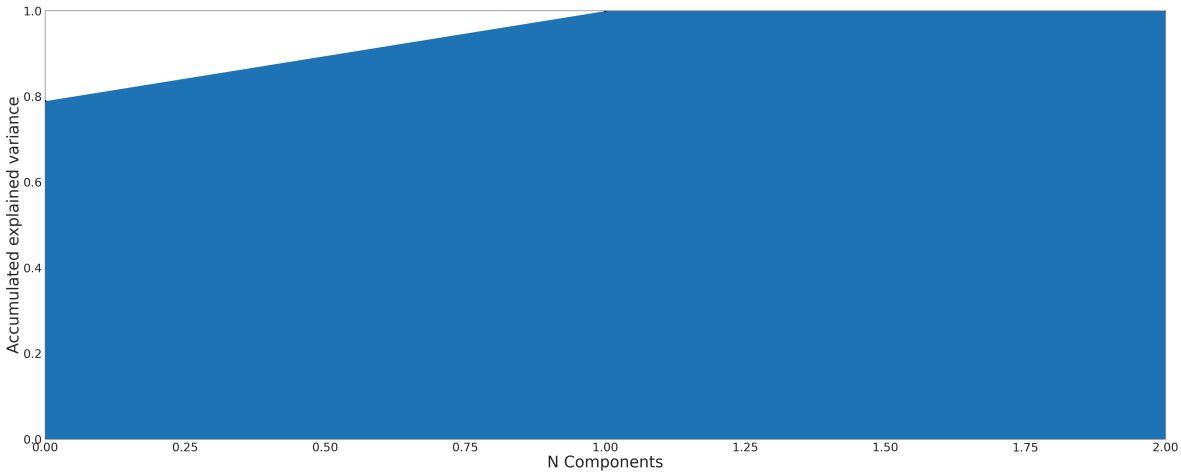
Out[ ]:

Index	Component 0	Component 1	Component 2
1	-2.051774	-0.243847	1.179062e-15
2	1.866218	1.117813	2.899065e-16
3	3.133436	-0.794420	5.765177e-17
4	1.696186	-0.748473	-4.504161e-16
5	1.803402	-1.058234	-2.240654e-16

By default, `sklearn.decomposition.PCA` sorts the components by their explained variance.

Let's analyze the explained variance ratios:

In [ ]:
```
plot_explained_variance(pca)
```



Suppose a 99 threshold is sufficient for our task, let's see how many components (dimensions) we can drop:

In [ ]:
```
threshold = 0.99
num = next(i for i, x in enumerate(accumulate(pca.explained_variance_ratio_), 1)
print(f'We can keep the first {num} components and discard the other {pca.n_comp
print(f'keeping >={100 * threshold}% of the explained variance!')
```

```
We can keep the first 2 components and discard the other 1,
keeping >=99.0% of the explained variance!
```

In [ ]:
```
X_PCA.drop([f'Component {i}' for i in range(num, pca.n_components_)], axis=1, in
X_PCA.head()
```

Out[ ]:

Index	Component 0	Component 1
1	-2.051774	-0.243847
2	1.866218	1.117813
3	3.133436	-0.794420
4	1.696186	-0.748473
5	1.803402	-1.058234

Using PCA to Improve Facial Recognition

PCA is commonly used for Facial Recognition.

In this example, we will apply a method called "**Eigenfaces**"

The idea of *eigenfaces* is:

1. You have images of faces of dimension $a \times b$ pixels.
2. You "roll" these out into vectors of size $a \cdot n$.
3. You apply PCA to the vectors.

4. You determine how many principal components you want to train under; let's call this C.
5. You train on the original image-vectors of size $a \cdot b$ projected onto your C components, reshaped back to $a \times b$ bitmaps.

Load the Labeled Faces in the Wild (LFW) people datasetclassification

In [ ]:
```
lfw_people = fetch_lfw_people(min_faces_per_person=70, resize=0.4)
```

Introspect the images arrays to find the shapes (for plotting)

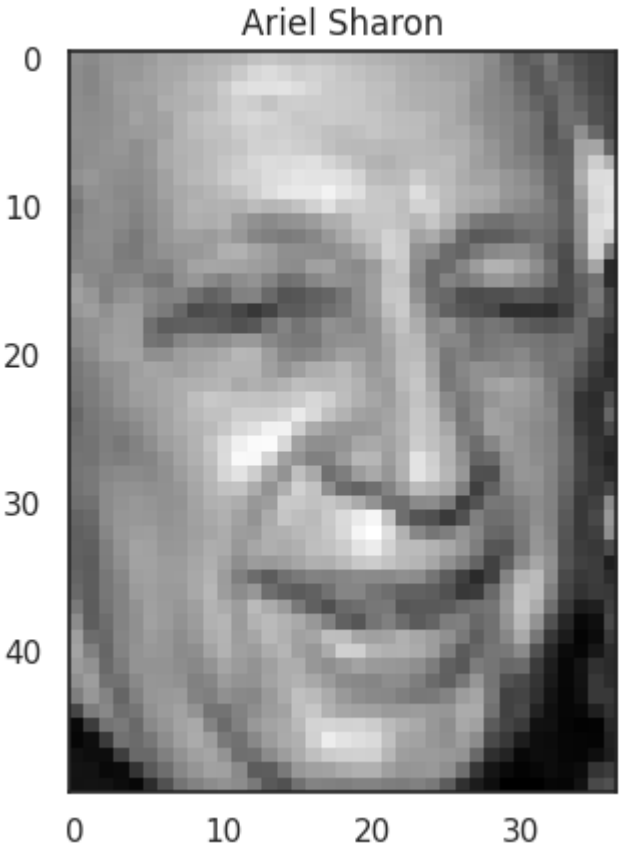
In [ ]:
```
# introspect the images arrays to find the shapes (for plotting)
N, h, w = lfw_people.images.shape
target_names = lfw_people.target_names
```

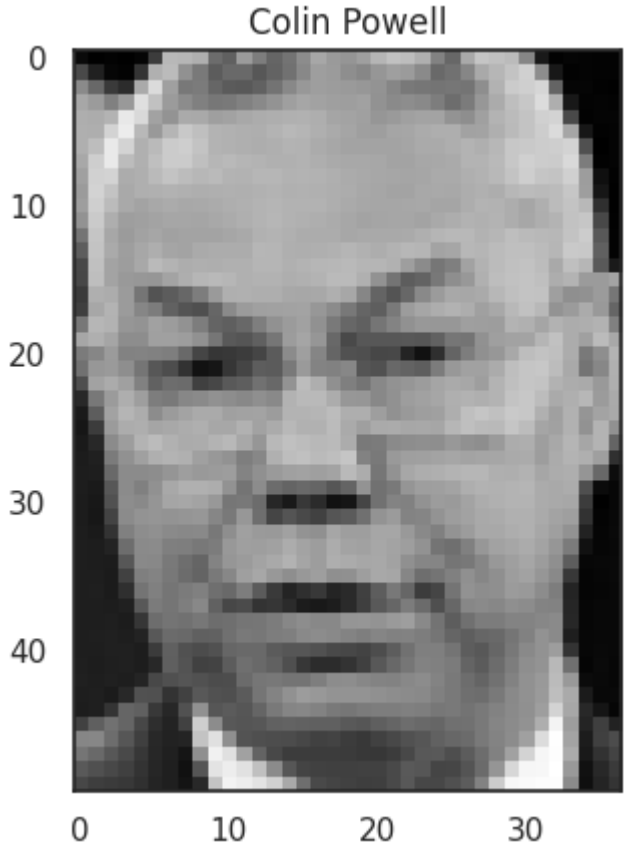
We load our features `X` and labels `y`. The images are flattened such that each one is a row in the NumPy array `X`

In [ ]:
```
y = lfw_people.target
X = lfw_people.data
n_features = X.shape[1]
```

We plot out each class and an image belonging to that class:

In [ ]:
```
for person in np.unique(lfw_people.target):
    idx = np.argmax(lfw_people.target == person)
    plt.imshow(lfw_people.images[idx], cmap='gray')
    plt.title(lfw_people.target_names[person])
    plt.show()
```




Colin Powell
0
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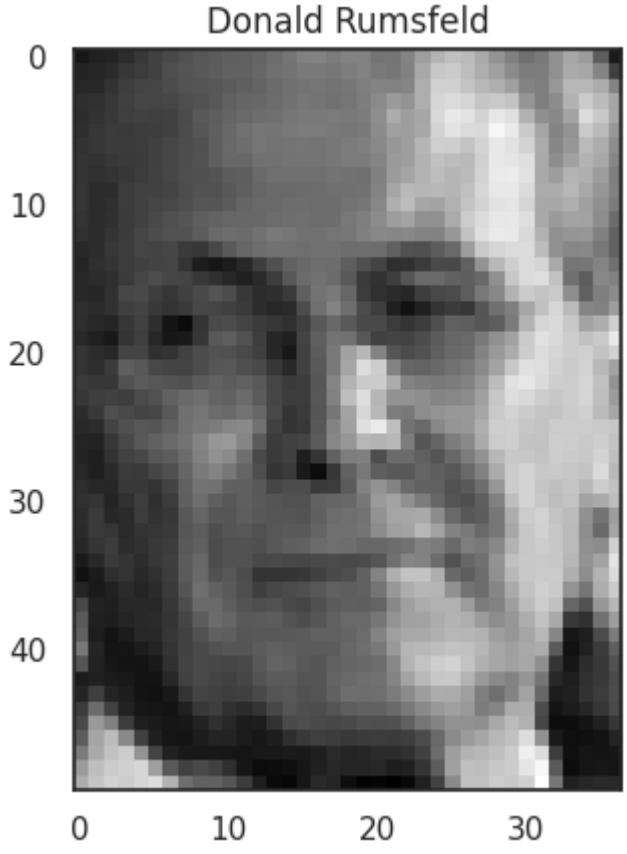
Donald Rumsfeld
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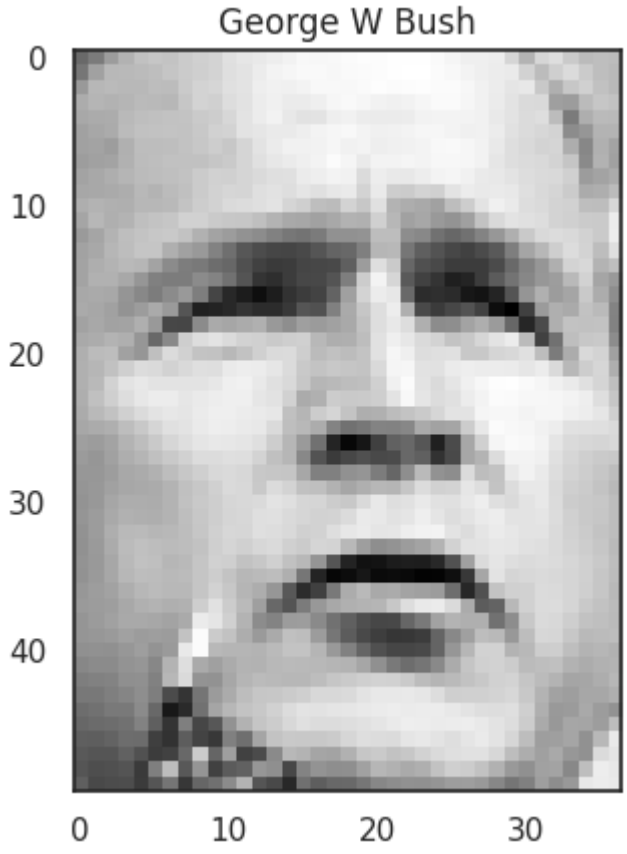
George W Bush
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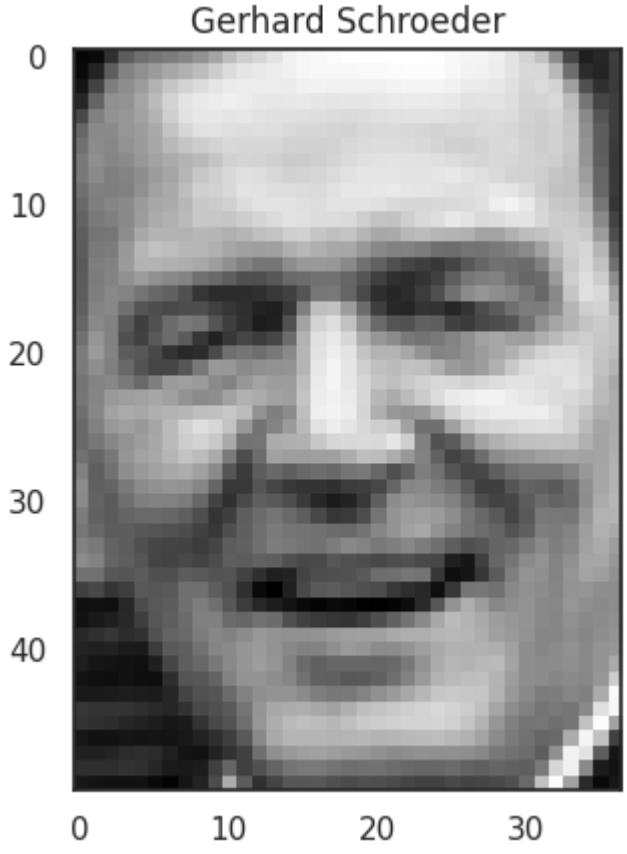
Gerhard Schroeder
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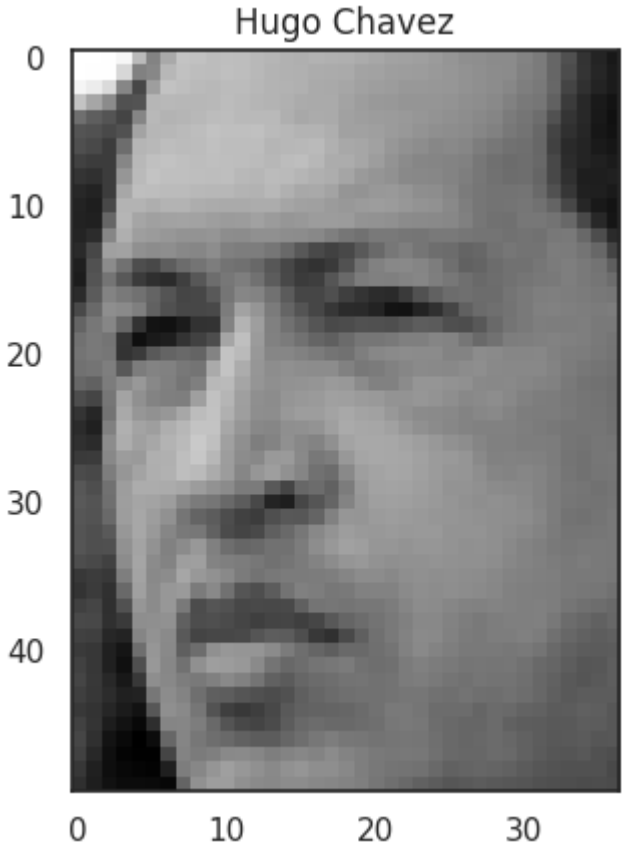
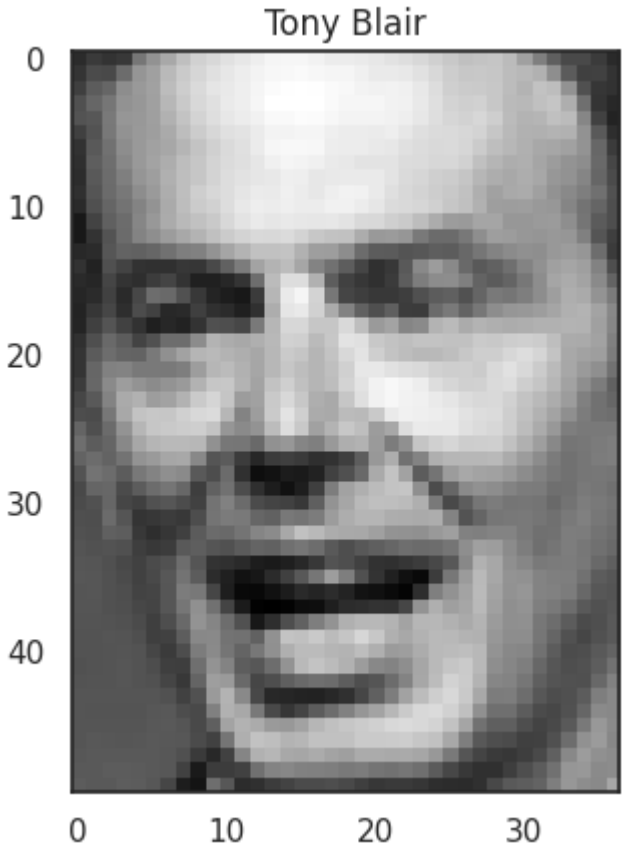
20
30





We split the data into training and testing

In [ ]:
```
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.25, random_state=42
)
```

We train a Support Vector Machines model for classification and use a random search method to find a set of optimal hyperparameters

In [ ]:
```
param_grid = {
    "C": loguniform(1e3, 1e5),
    "gamma": loguniform(1e-4, 1e-1)
}
clf = RandomizedSearchCV(
    SVC(kernel="rbf", class_weight="balanced"), param_grid, n_iter=10
)
clf = clf.fit(X_train, y_train)
```

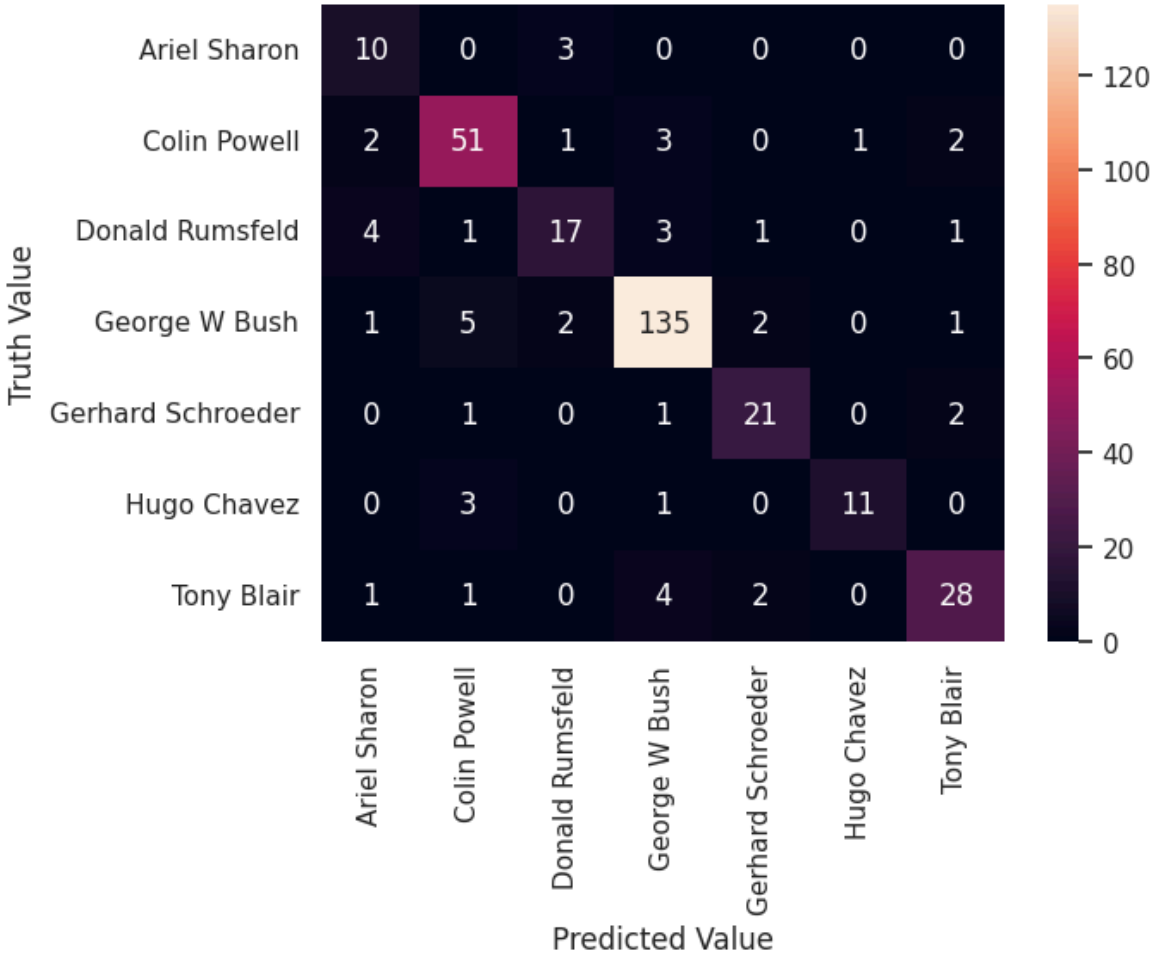
We make a prediction using the test data:

In [ ]:
```
y_pred = clf.predict(X_test)
```

Let's see how well our `SVC` did on the test data:

In [ ]:
```
hmap = sns.heatmap(
    confusion_matrix(y_test, y_pred),
    annot=True,
    xticklabels=lfw_people.target_names,
    yticklabels=lfw_people.target_names,
    fmt='g'
)
hmap.set_xlabel('Predicted Value')
hmap.set_ylabel('Truth Value')
```

Out[ ]:
```
Text(46.24999999999999, 0.5, 'Truth Value')
```



We see all the images are being classifed as George Bush. Clearly it's having trouble differentiating between the faces.

Now, let's try using PCA, we fit a PCA model :

In [ ]:
```
pca = PCA(svd_solver='full',  whiten=True).fit(X_train)
```

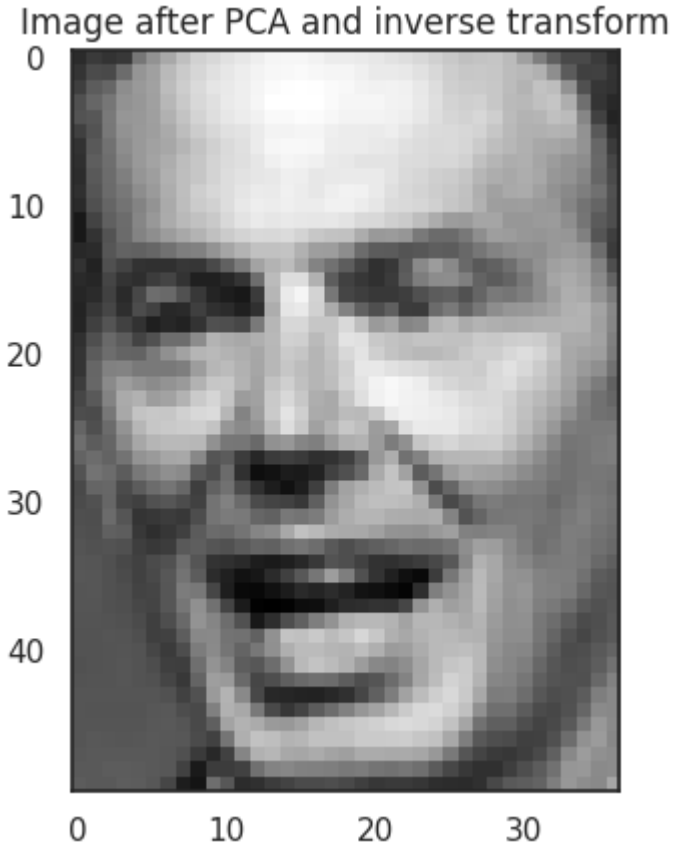
We find the projections on to each principle component for a person int the dataset, we select the sample `person_index` :

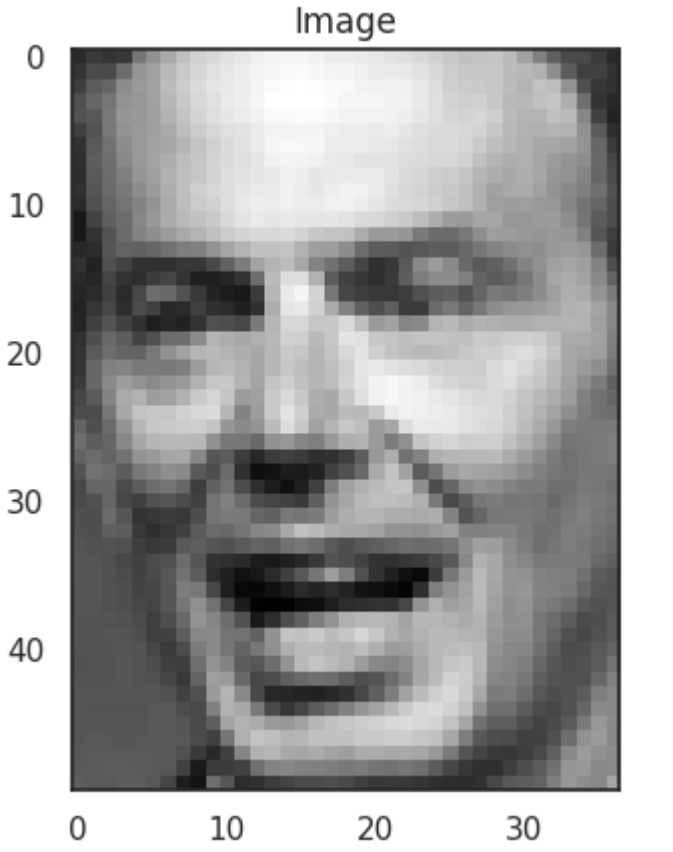
In [ ]:
```
person_index=1
```

In [ ]:
```
Xhat=pca.transform(X[person_index,:].reshape(1, -1))
```

We can find the projections back to each component, i.e the inverse transform;as we use all the non-zero components the images are identical.

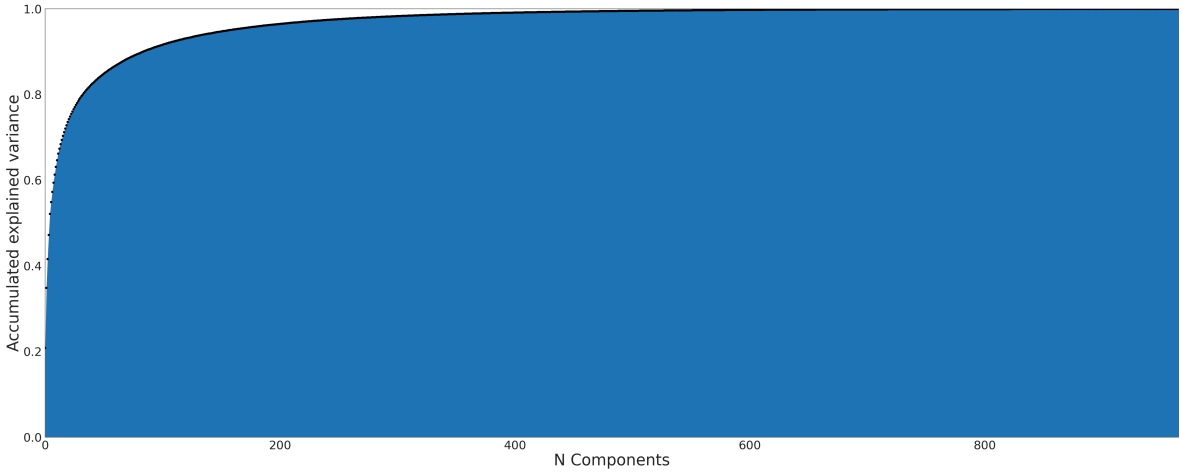
In [ ]:
```
plt.imshow(pca.inverse_transform(Xhat).reshape(h, w), cmap='gray')
plt.title("Image after PCA and inverse transform"  )
plt.show()
plt.imshow(lfw_people.images[person_index],cmap='gray')
plt.title("Image")
plt.show()
```





We can use the Explained variance-ratio to determine the number of components to keep, we can plot it as Cumulative distribution.

In [ ]:
```
plot_explained_variance(pca)
plt.show()
```



It looks like 150 components explain over 95% of the variance, usually 80% will do, let's try and visualize some components.

Note: you can use Cross-validation to select the number of components

Let's select the components that explain over 60% of the variance

In [ ]:
```
threshold = 0.60
```

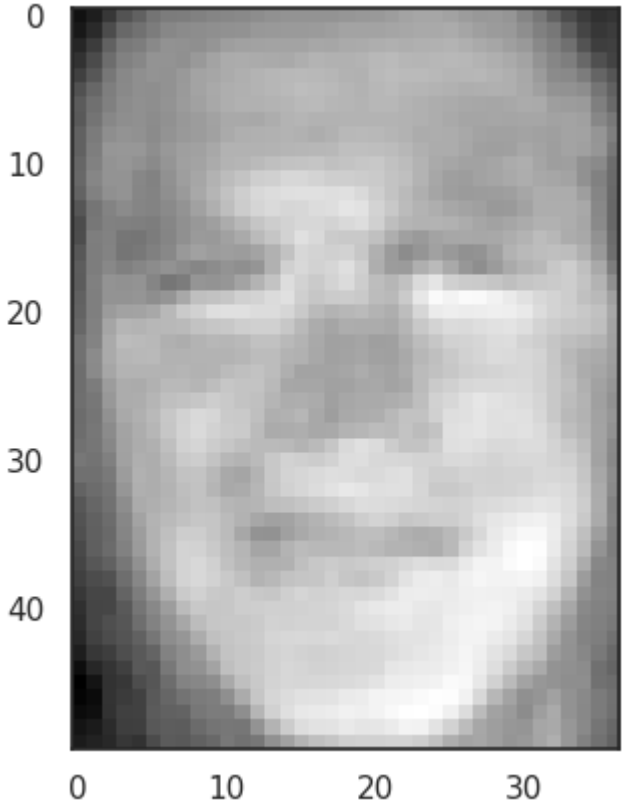
This corresponds to 7 principle components

In [ ]:
```
components = np.cumsum(pca.explained_variance_ratio_) < threshold
components.sum()
```

Out[ ]:
```
np.int64(8)
```

We can reshape the principle components to a rectangle and plot them, remember the images are linear combinations of these components

In [ ]:
```
for component in pca.components_[components,:]:
    plt.imshow(component.reshape(h, w),cmap='gray')
    plt.show()
```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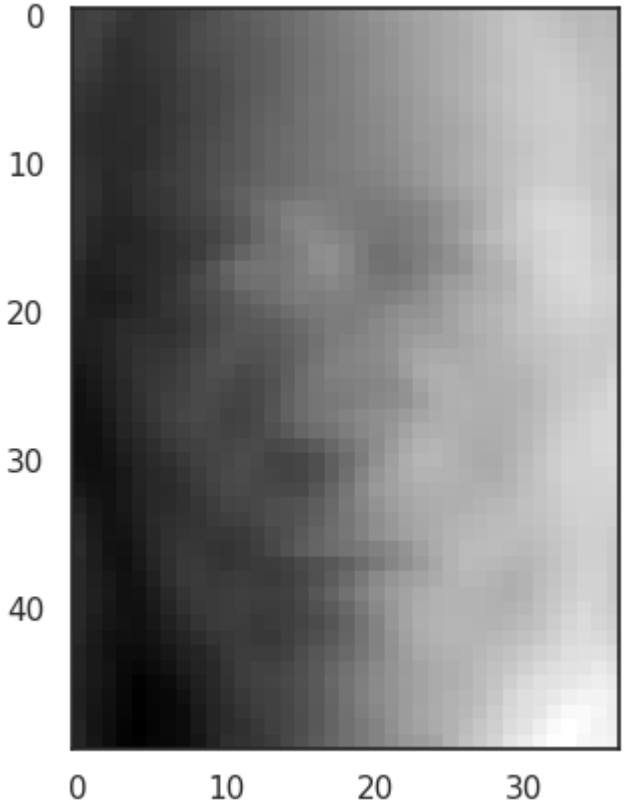
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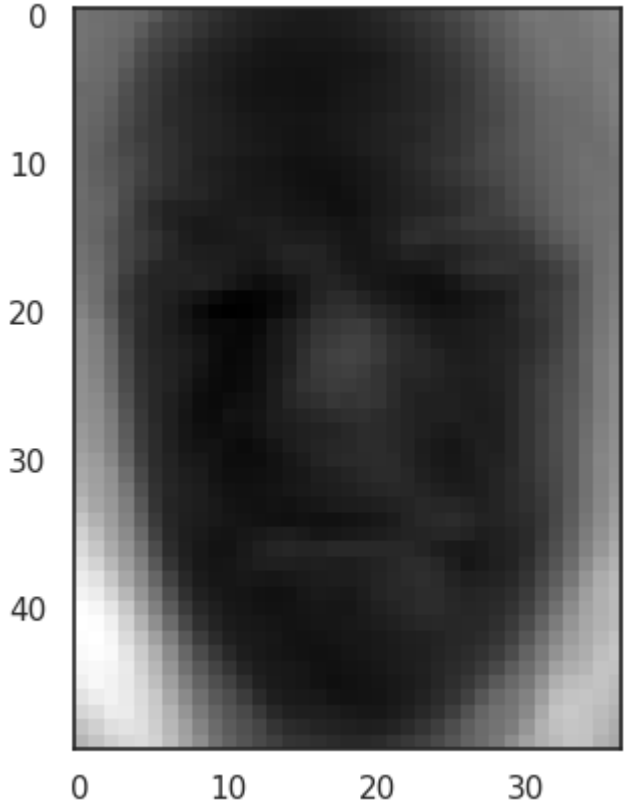
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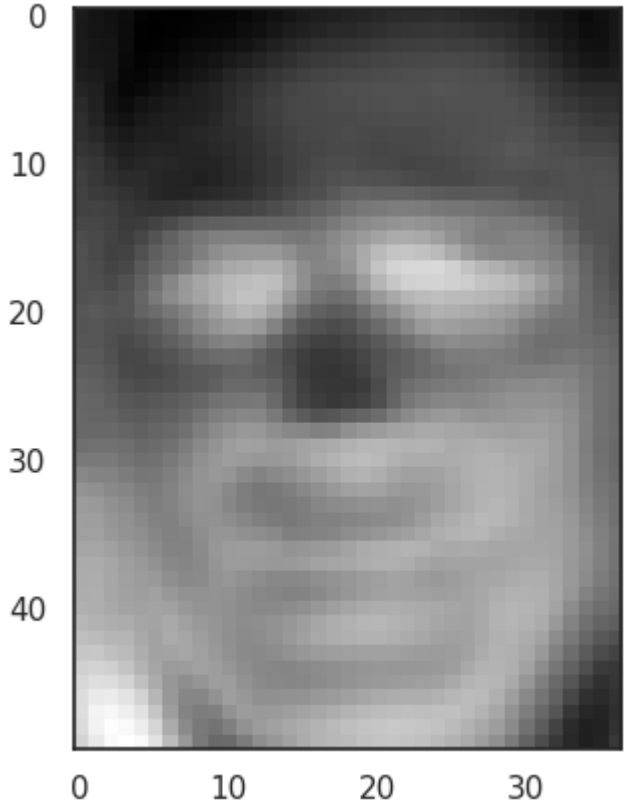
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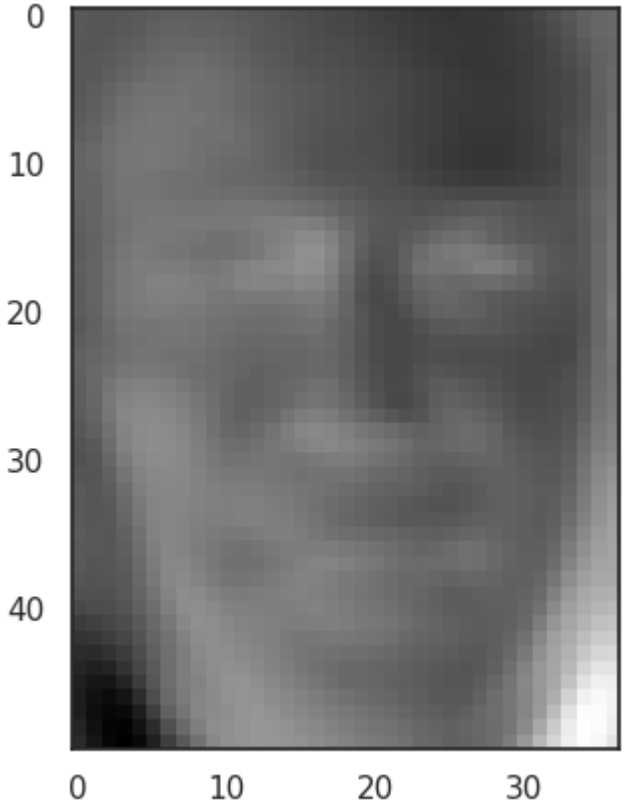
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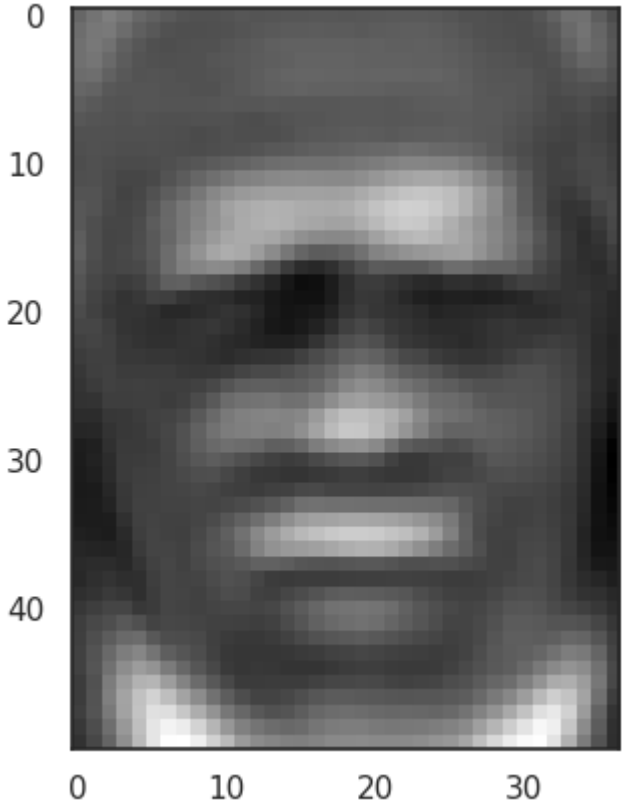
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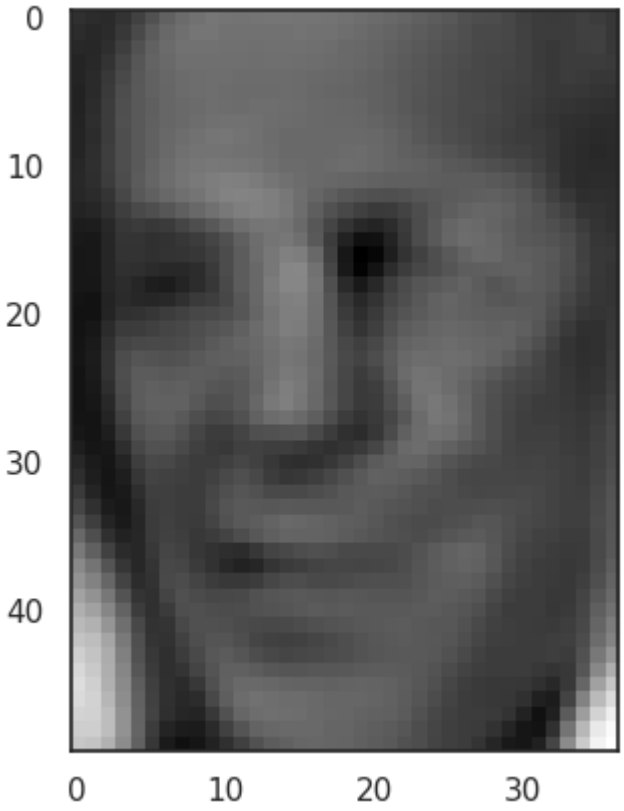
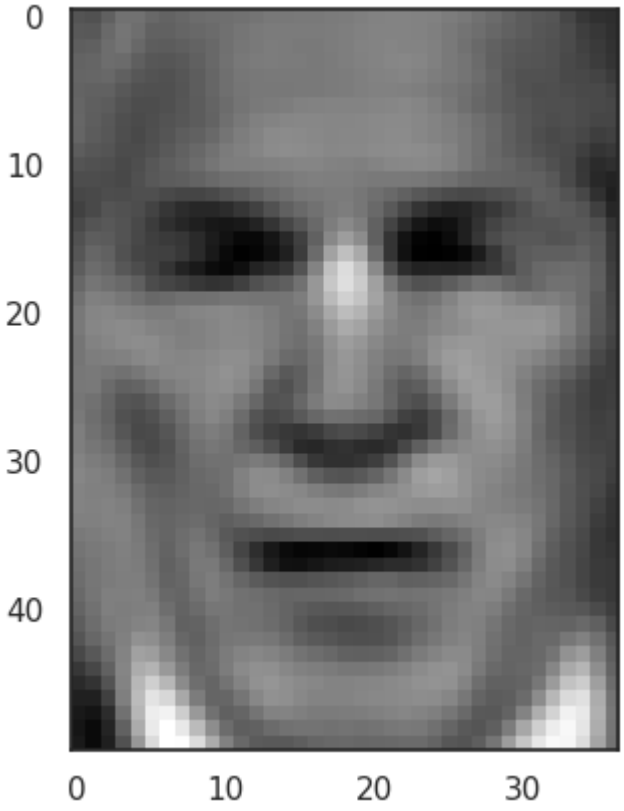




Let's now use PCA with `n_components = 150` :

In [ ]:
```
pca = PCA(n_components=150, svd_solver="randomized", whiten=True).fit(X_train)
```

We apply the PCA transform on the training and testing data

In [ ]:
```
X_train_pca = pca.transform(X_train)
X_test_pca = pca.transform(X_test)
```

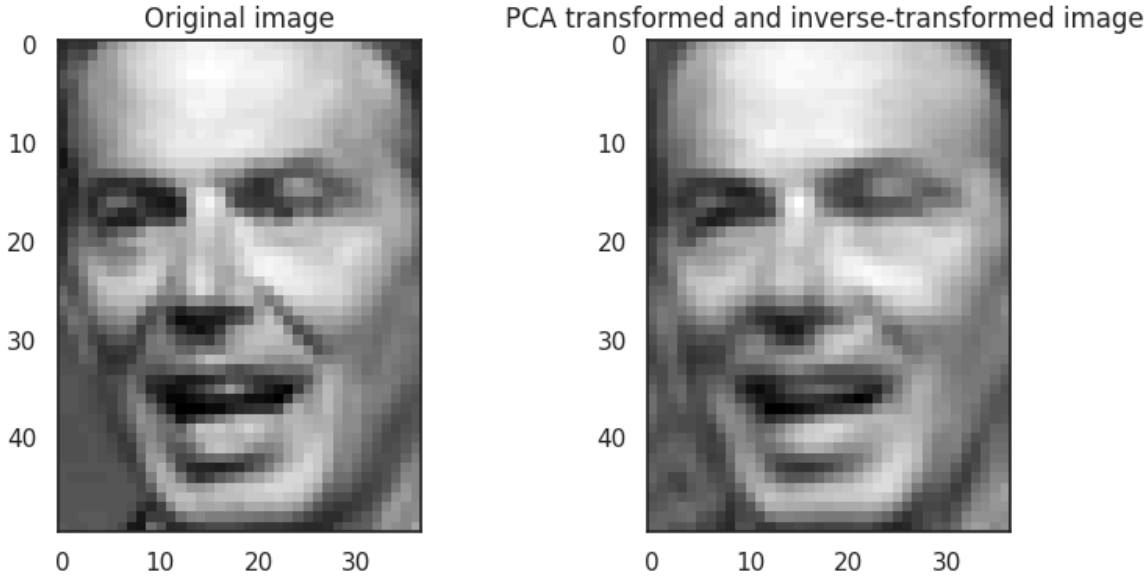
NOTE: We can also transform the data back ("inverse_transform") to its original space, with the rest of the components to zero, then convert it to an image. For instance, let's look at one of the images using `person_index = 1`

In [ ]:
```
person_index = 1
```

In [ ]:
```
plt.figure(figsize=(8, 4))
plt.subplot(1,2,1)
plt.imshow(lfw_people.images[person_index,:,:],cmap='gray')
plt.title("Original image")

plt.subplot(1,2,2)
plt.imshow(pca.inverse_transform(pca.transform(X[person_index ,:].reshape(1, -1)
plt.title("PCA transformed and inverse-transformed image ")

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



We train the model and find the best Hyperparameters using the transformed data:

In [ ]:
```
param_grid = {
    "C": loguniform(1e3, 1e5),
    "gamma": loguniform(1e-4, 1e-1),
}
clf = RandomizedSearchCV(
    SVC(kernel="rbf", class_weight="balanced"), param_grid, n_iter=10
)

clf = clf.fit(X_train_pca, y_train)
```

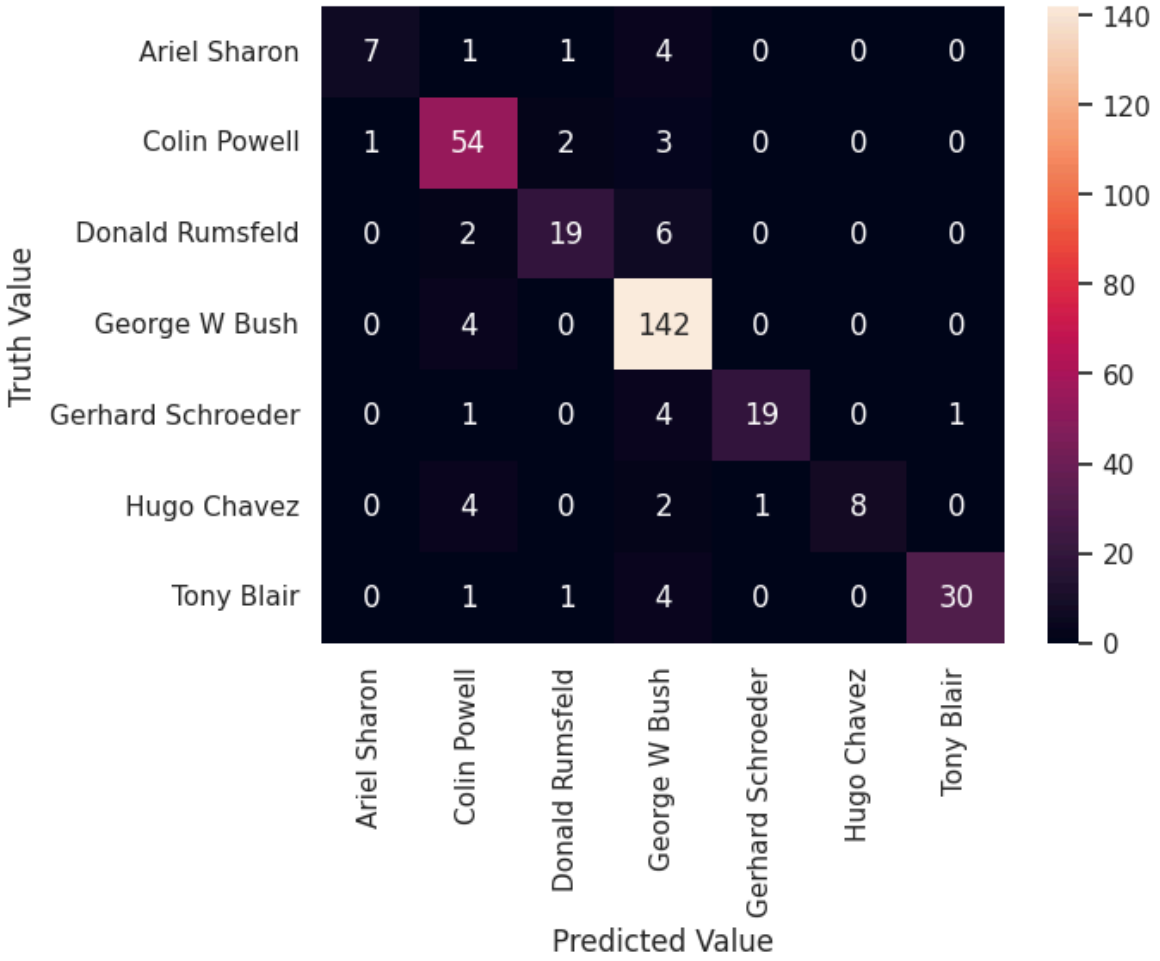
We see the model using PCA performs much better!

In [ ]:
```
y_pred = clf.predict(X_test_pca)
```

In [ ]:
```
hmap = sns.heatmap(
    confusion_matrix(y_test, y_pred),
    annot=True,
    xticklabels=lfw_people.target_names,
```

```
    yticklabels=lfw_people.target_names,
    fmt='g'
)
hmap.set_xlabel('Predicted Value')
hmap.set_ylabel('Truth Value')
```

Out[ ]: Text(46.24999999999999, 0.5, 'Truth Value')



Conclusion: Principal Component Analysis (PCA)

Through this project, we explored the fundamentals and practical applications of **Principal Component Analysis (PCA)**, a widely used dimensionality reduction technique in data science and machine learning. We began by understanding the challenges of working with high-dimensional datasets including computational inefficiency, noise, redundancy, and difficulty in interpretation and showed how PCA offers an elegant solution by projecting data onto a set of orthogonal principal components.

Key Takeaways

- **Dimensionality Reduction with Minimal Information Loss:**
  PCA successfully reduced the number of features while preserving most of the data's

variability. This reduction is not only computationally efficient but also helps reveal underlying data structure more clearly.

- **Variance as a Guiding Metric:**
  The project demonstrated that principal components are ranked based on the amount of variance they explain. This helps in identifying how many components are sufficient to capture the essence of the dataset (example:- retaining 95% of total variance).

- **Orthogonal Transformation:**
  One of PCA's strengths is its ability to transform correlated features into a new set of uncorrelated variables, which is particularly useful in modeling scenarios where multicollinearity is a concern.

- **Visualization of Complex Data:**
  By projecting the high-dimensional data onto the first two or three principal components, we were able to visualize patterns, clusters, and potential outliers that might not have been obvious in the original feature space.

- **Versatile Applications:**
  Whether in finance (example:- portfolio risk modeling), computer vision (example:- facial recognition), bioinformatics, or marketing, PCA proves valuable for data simplification, noise reduction, and feature engineering.

Impact on Future Work

This project provides a solid foundation for using PCA as a preprocessing step for downstream tasks such as clustering (example:- K-Means), classification (example:- logistic regression or SVM), or anomaly detection. PCA can also be paired with other techniques such as t-SNE or UMAP for deeper exploratory data analysis.

Moreover, understanding PCA gives deeper insight into other linear transformation-based methods such as Linear Discriminant Analysis (LDA), Factor Analysis, and Singular Value Decomposition (SVD), which share mathematical roots but differ in purpose.

Final Thoughts

While PCA is a powerful tool, it's essential to remember:

- It is **unsupervised** and does not account for target variables.
- It assumes **linear relationships** among features.
- Principal components can be **difficult to interpret** directly in terms of original variables.

Despite these limitations, PCA remains one of the most reliable first steps in any exploratory data analysis or feature reduction pipeline. When applied thoughtfully, it enhances both the **efficiency** and **effectiveness** of machine learning models by removing noise and emphasizing structure.

With this understanding, you're now equipped to confidently apply PCA to a wide range of real-world problems and integrate it into more advanced analytical pipelines.