Visualizing the PCA transformation

UNSUPERVISED LEARNING IN PYTHON
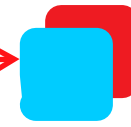
Benjamin Wilson
Director of Research at lateral.io

datacamp

Dimension reduction

Find the pattern in the data then use these pattern to express the data in the more compressed form

- More efficient storage and computation

- Remove less-informative "noise" features

- ... which cause problems for prediction tasks, e.g. classification, regression
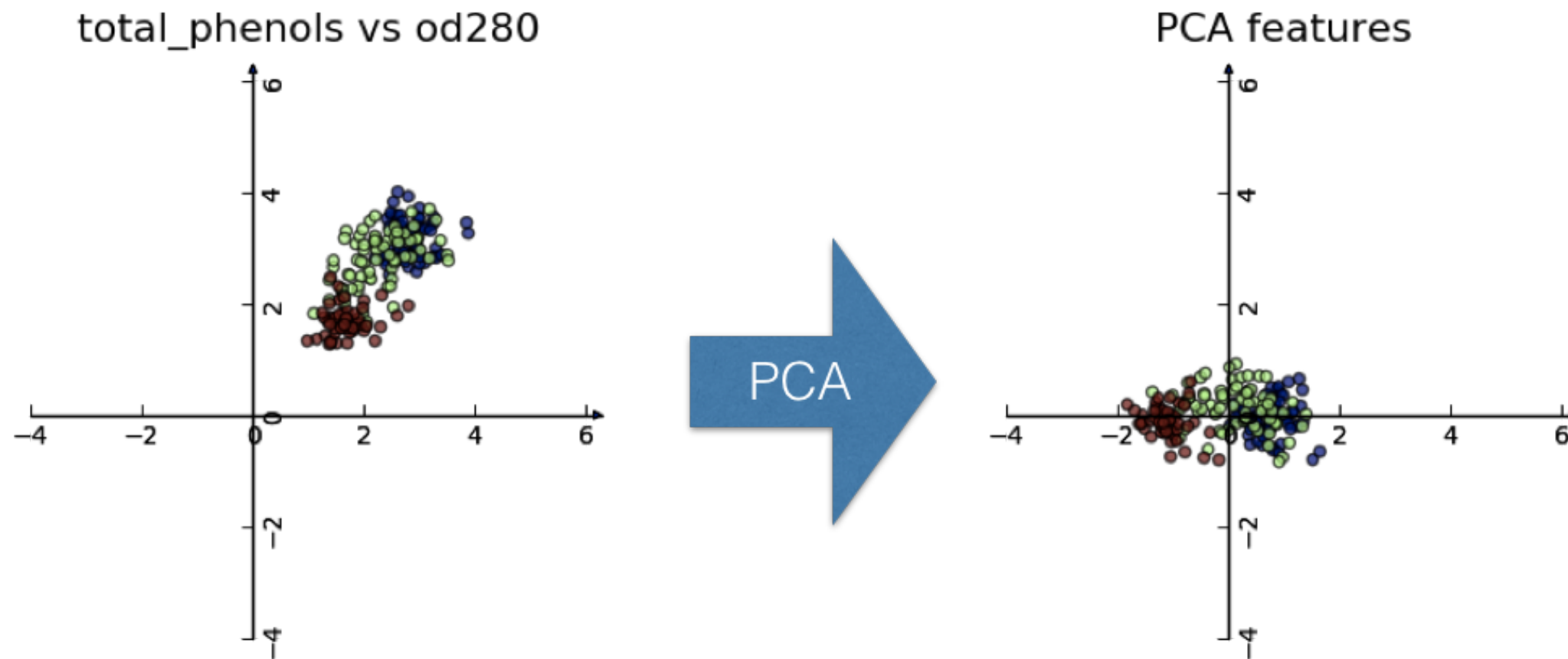
Principal Component Analysis

- PCA = "Principal Component Analysis"

- Fundamental dimension reduction technique

- First step "decorrelation" (considered here)

- Second step reduces dimension (considered later)

PCA aligns data with axes

- Rotates data samples to be aligned with axes

- Shifts data samples so they have mean 0

- No information is lost

PCA follows the fit/transform pattern

- `PCA` is a scikit-learn component like `KMeans` or `StandardScaler`

- `fit()` learns the transformation from given data

- `transform()` applies the learned transformation

- `transform()` can also be applied to new data

Using scikit-learn PCA

- `samples` = array of two features (`total_phenols` & `od280`)

```
[[ 2.8   3.92]
 ...
 [ 2.05  1.6 ]]
```

```python
from sklearn.decomposition import PCA
model = PCA()
model.fit(samples)
```

```
PCA(copy=True, ...)
```

```python
transformed = model.transform(samples)
```
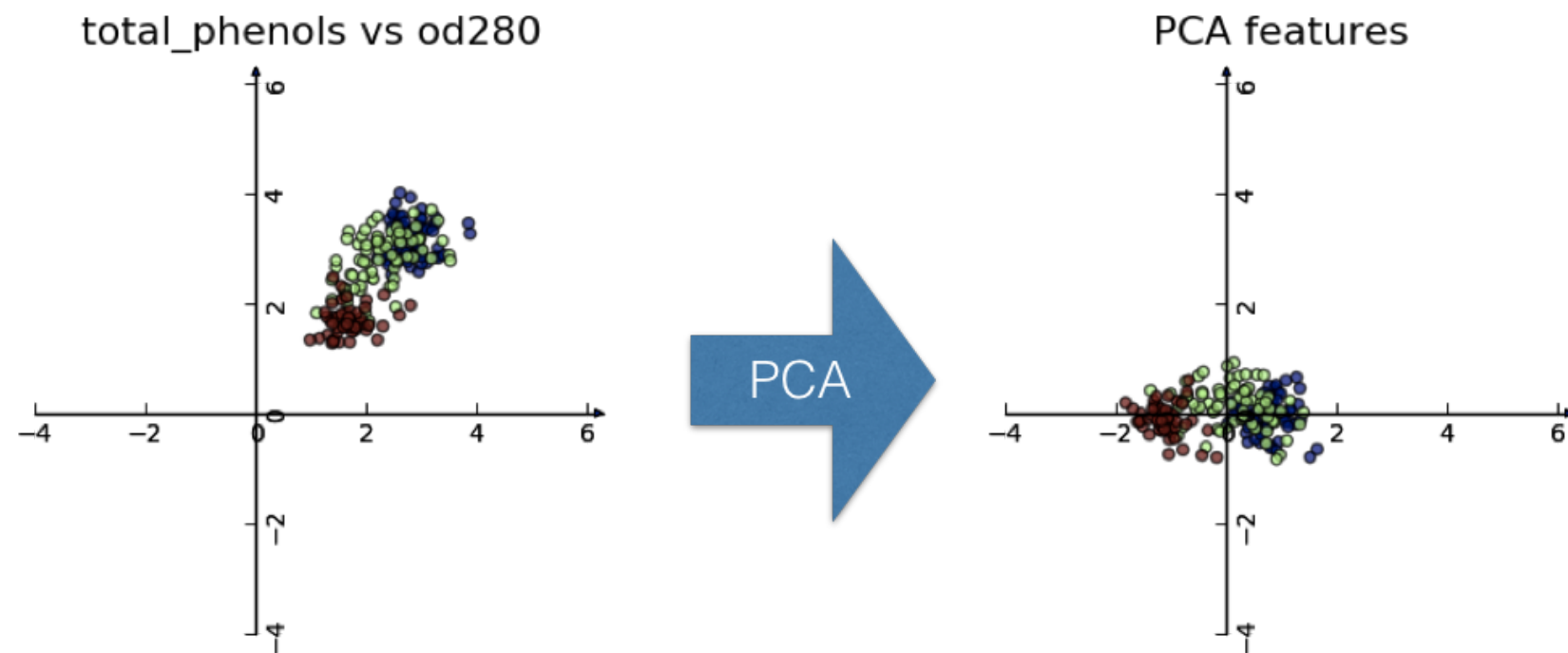
PCA features

- Rows of transformed correspond to samples

- Columns of transformed are the "PCA features"

- Row gives PCA feature values of corresponding sample

```
print(transformed)
```

```
[[  1.32771994e+00   4.51396070e-01]
 [  8.32496068e-01   2.33099664e-01]
 ...
 [ -9.33526935e-01  -4.60559297e-01]]
```
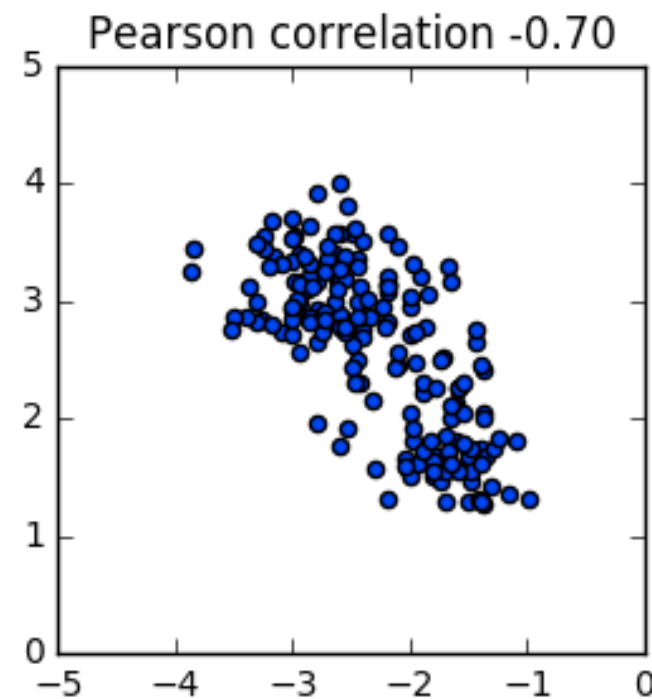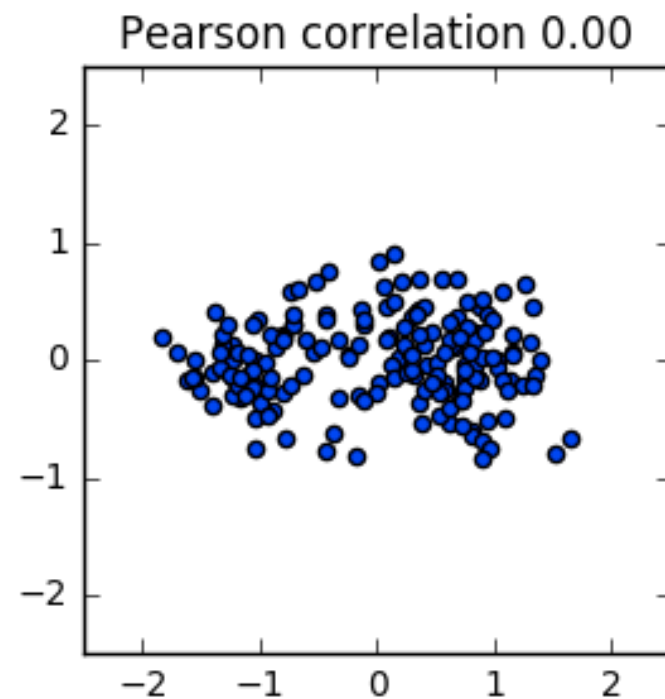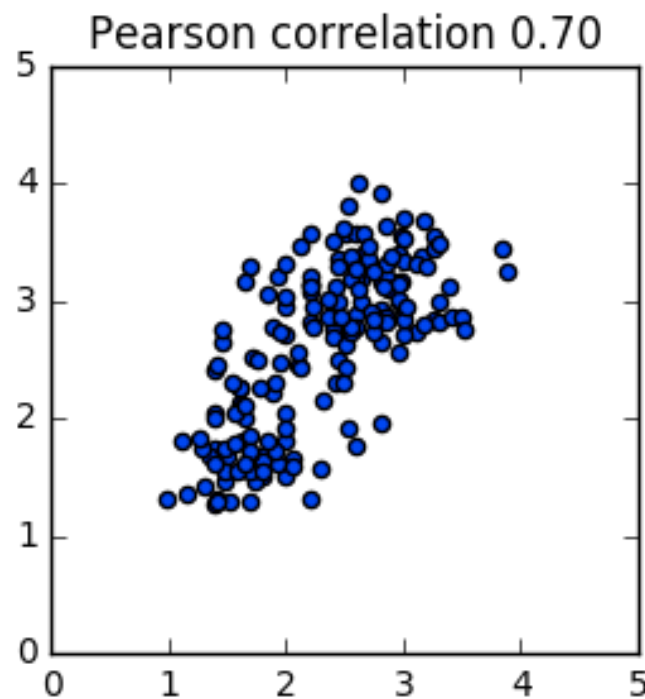
PCA features are not correlated

- Features of dataset are often correlated, e.g. `total_phenols` and `od280`

- <mark>PCA aligns the data with axes</mark>

- <mark>Resulting PCA features are not linearly correlated ("decorrelation")</mark>

Pearson correlation

- Measures linear correlation of features

- Value between -1 and 1
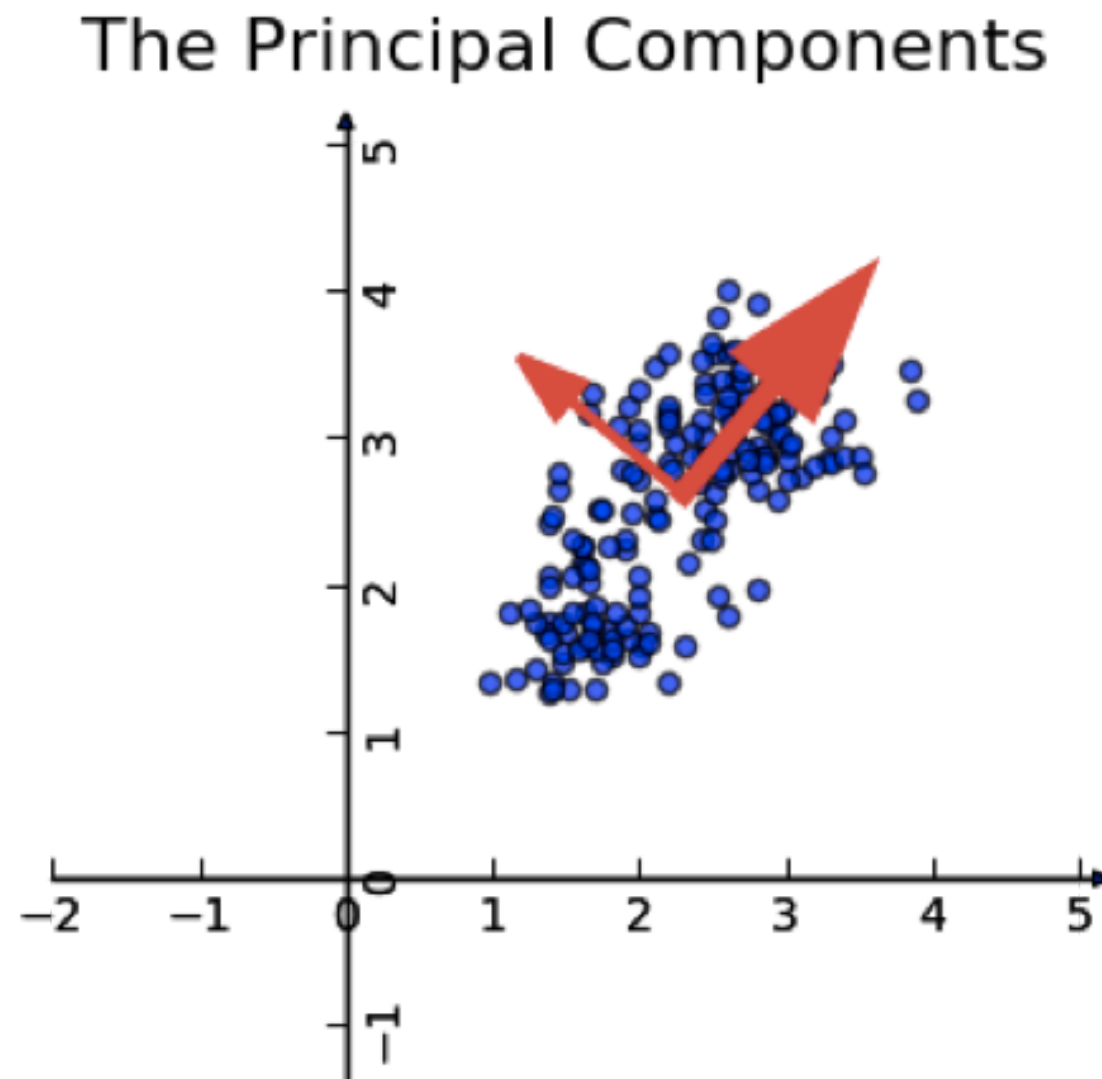
- Value of 0 means no linear correlation

Principal components

- "Principal components" = directions of variance

- PCA aligns principal components with the axes

The Principal Components

Principal components

- Available as `components_` attribute of PCA object

- Each row defines displacement from mean

```
print(model.components_)
```
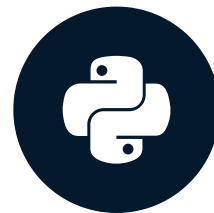
```
[[ 0.64116665  0.76740167]
 [-0.76740167  0.64116665]]
```

Let's practice!

UNSUPERVISED LEARNING IN PYTHON

datacamp

Intrinsic dimension

UNSUPERVISED LEARNING IN PYTHON

Benjamin Wilson
Director of Research at lateral.io

Intrinsic dimension of a flight path

- 2 features: longitude and latitude at points along a flight path

- Dataset *appears* to be 2-dimensional

- But can approximate using one feature: displacement along flight path

- Is intrinsically 1-dimensional

```
latitude   longitude
50.529      41.513
50.360      41.672
50.196      41.835
...
```
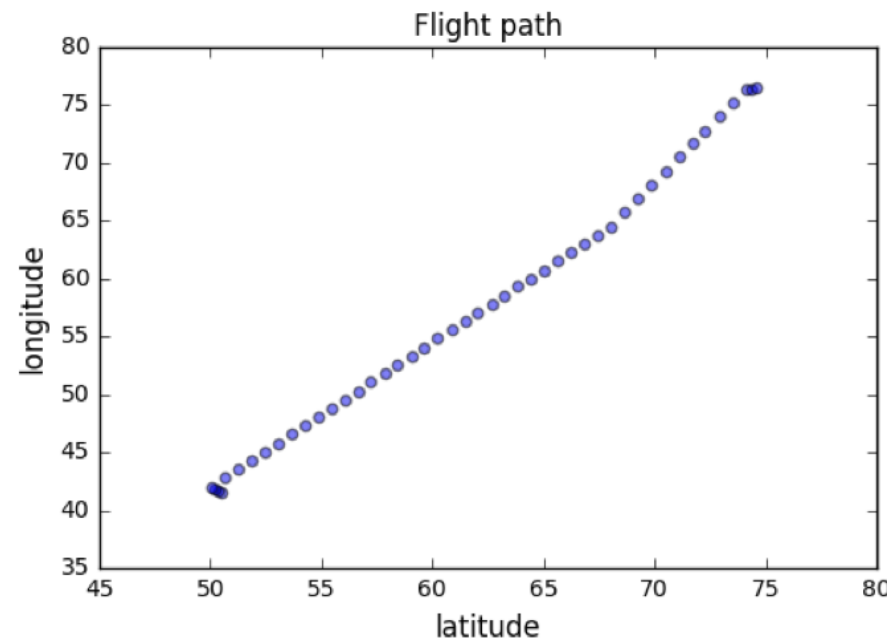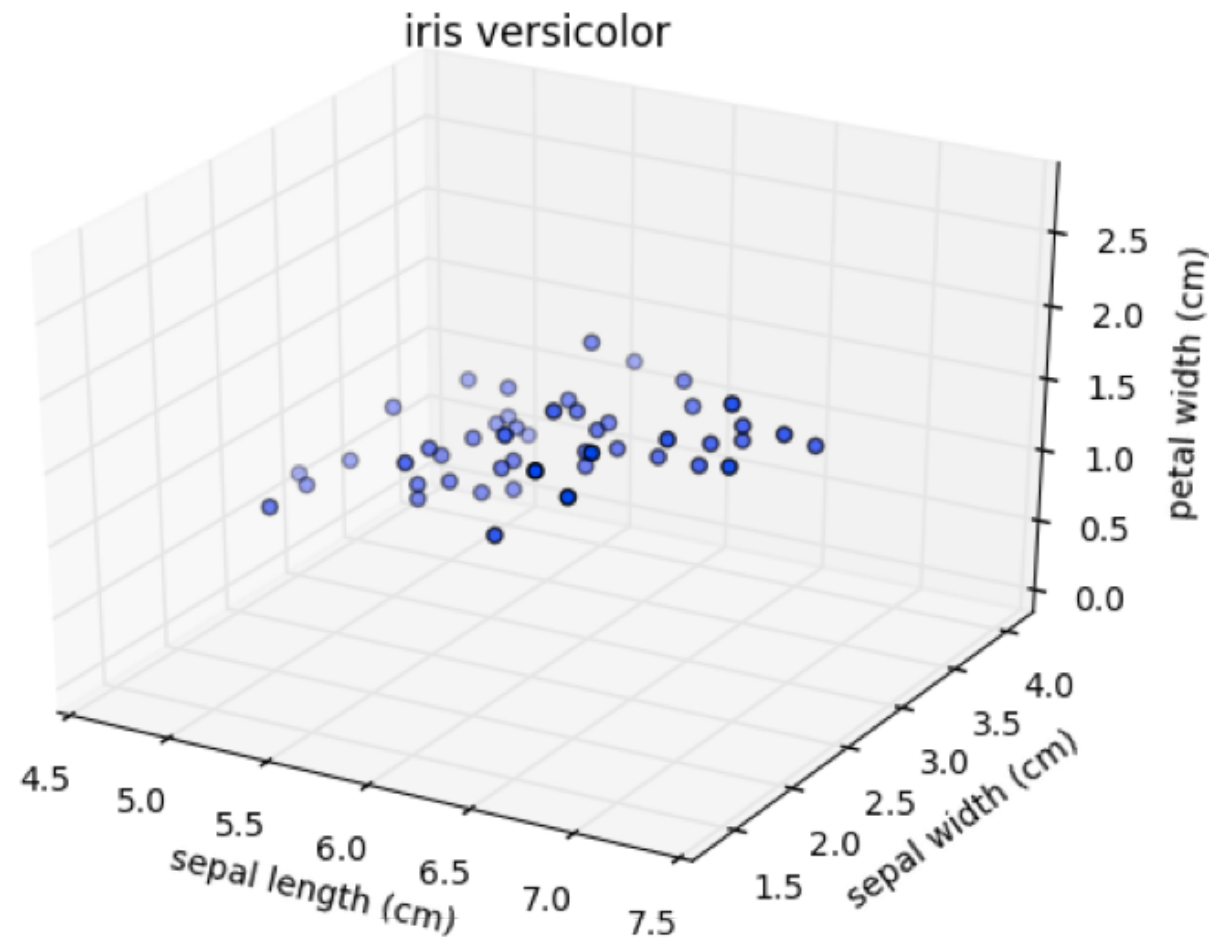
Intrinsic dimension

- Intrinsic dimension = number of features needed to approximate the dataset

- Essential idea behind dimension reduction

- What is the most compact representation of the samples?

- Can be detected with PCA

Versicolor dataset

- "versicolor", one of the iris species

- Only 3 features: sepal length, sepal width, and petal width

- Samples are points in 3D space

# Versicolor dataset has intrinsic dimension 2

- Samples lie close to a flat 2-dimensional sheet

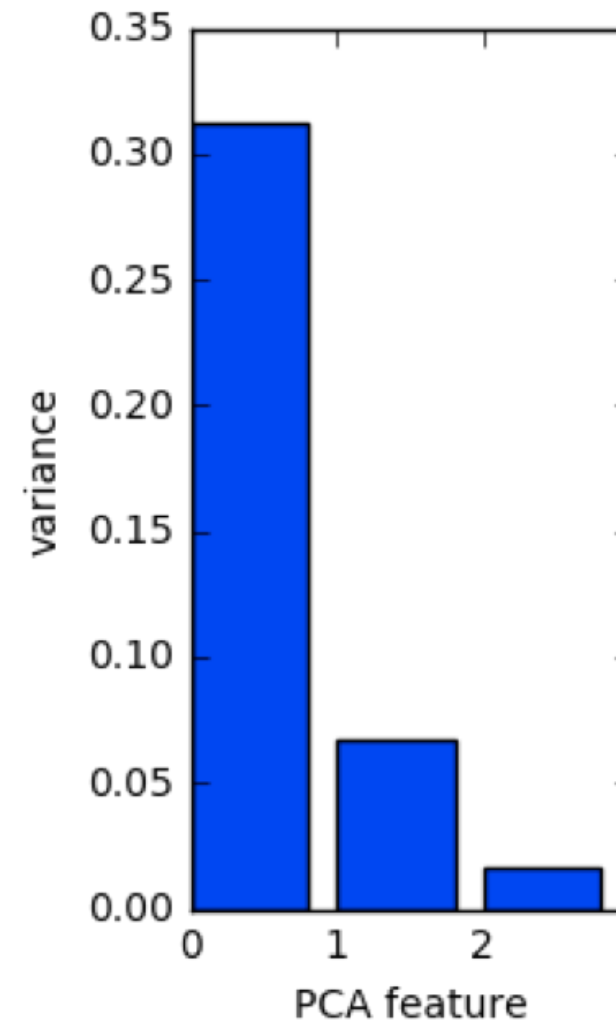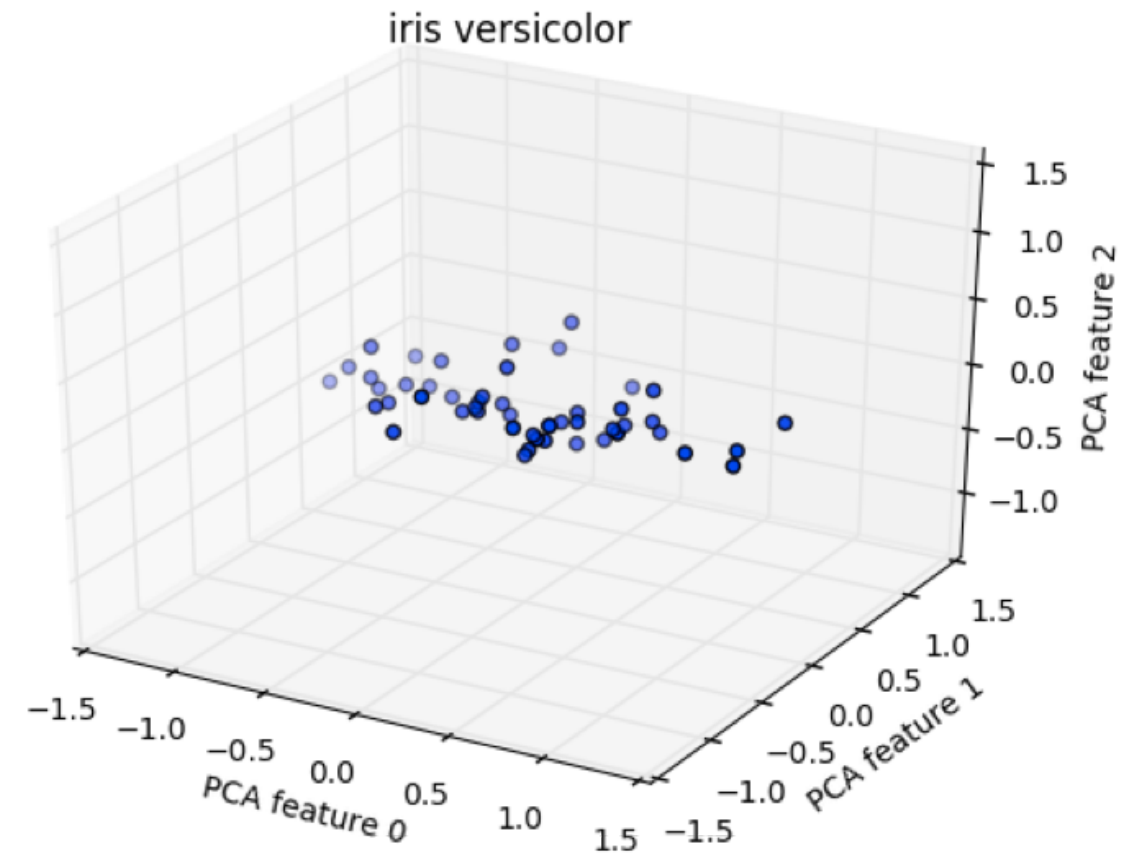- So can be approximated using 2 features

PCA identifies intrinsic dimension

- Scatter plots work only if samples have 2 or 3 features

- PCA identifies intrinsic dimension when samples have any number of features

- Intrinsic dimension = number of PCA features with significant variance
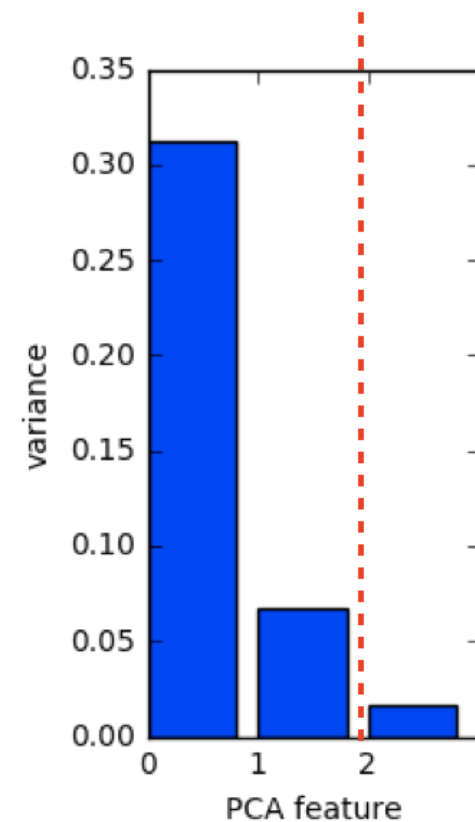
PCA of the versicolor samples
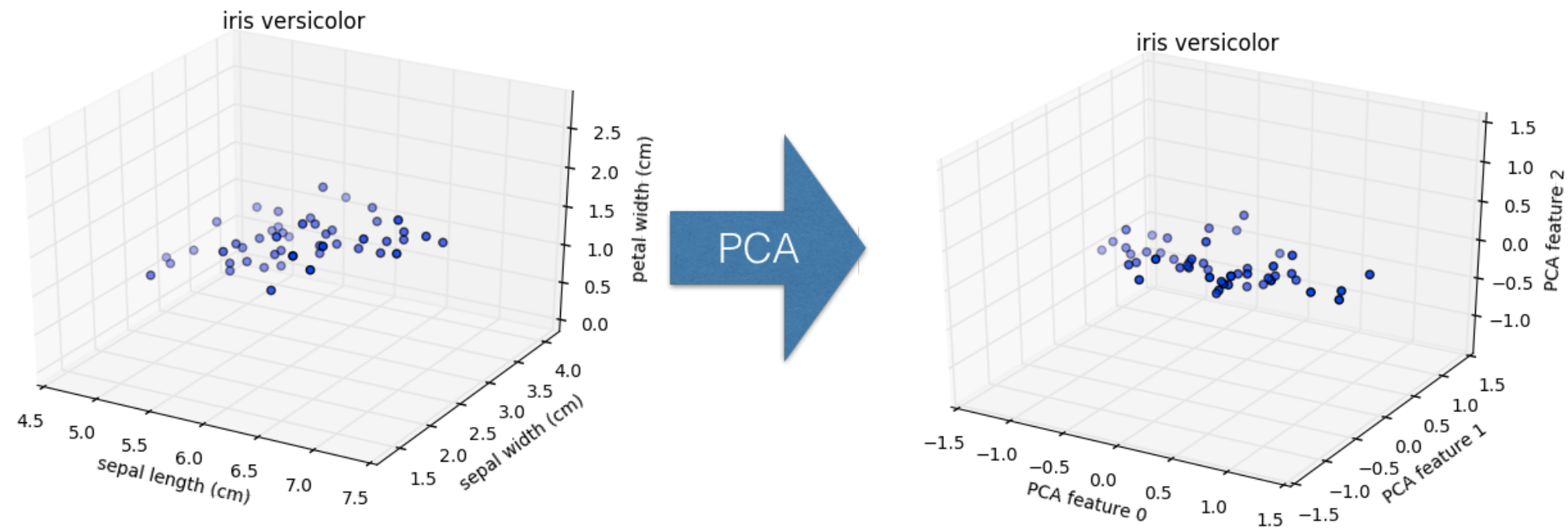
PCA features are ordered by variance descending

Variance and intrinsic dimension

- Intrinsic dimension is number of PCA features with significant variance

- In our example: the first two PCA features

- So intrinsic dimension is 2

Plotting the variances of PCA features

- `samples` = array of versicolor samples

```python
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
pca = PCA()
pca.fit(samples)
```
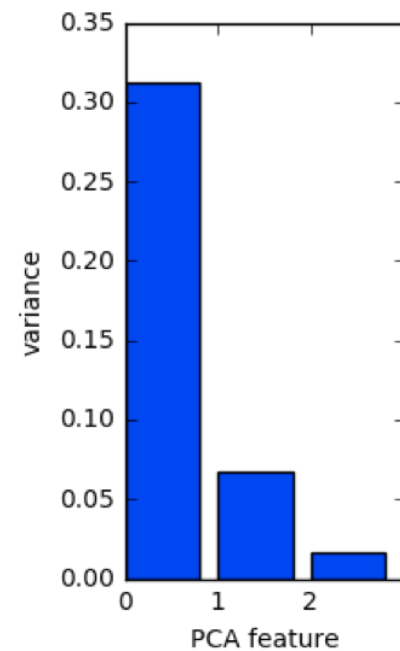
```python
PCA(copy=True, ... )
```

```python
features = range(pca.n_components_)
```

Plotting the variances of PCA features
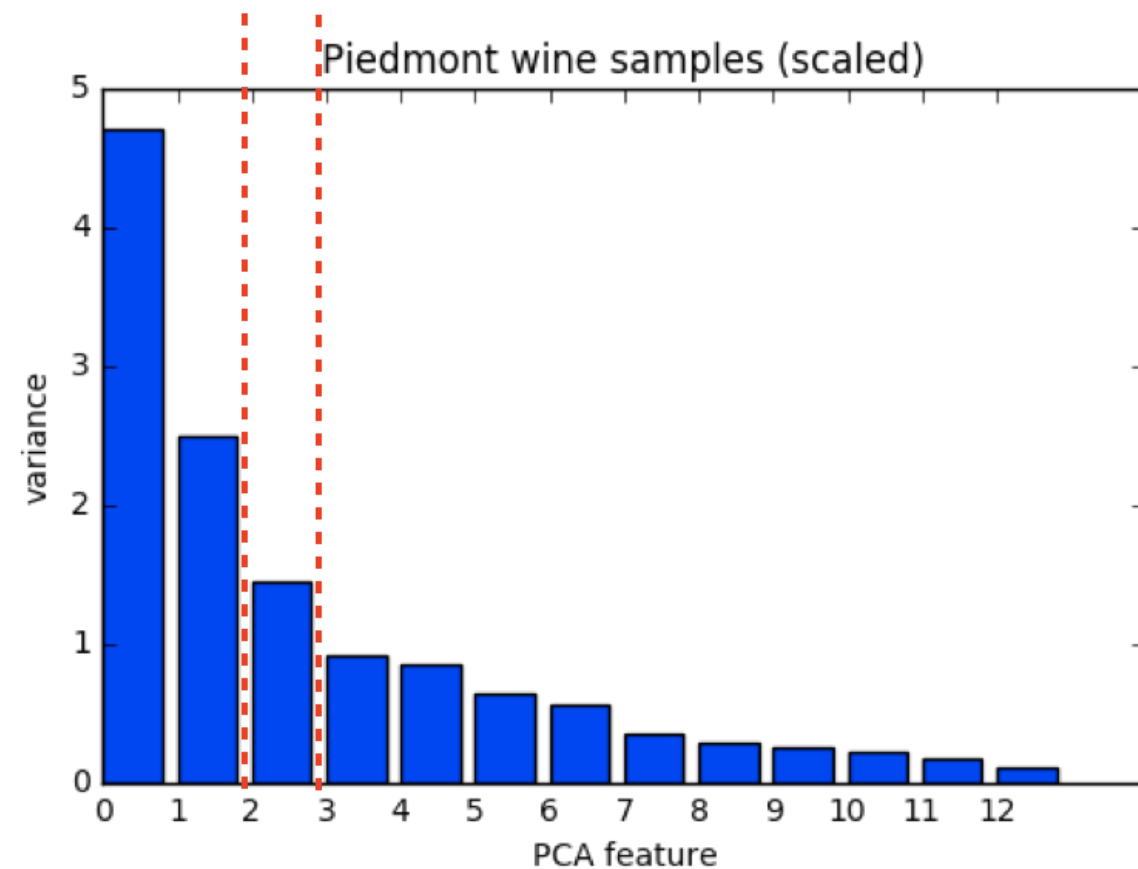
```python
plt.bar(features, pca.explained_variance_)
plt.xticks(features)
plt.ylabel('variance')
plt.xlabel('PCA feature')
plt.show()
```

Intrinsic dimension can be ambiguous

- Intrinsic dimension is an idealization

- ... there is not always one correct answer!

- Piedmont wines: could argue for 2, or for 3, or more

Let's practice!

UNSUPERVISED LEARNING IN PYTHON

Dimension reduction with PCA

UNSUPERVISED LEARNING IN PYTHON

Benjamin Wilson
Director of Research at lateral.io

datacamp

Dimension reduction

- Represents same data, using less features

- Important part of machine-learning pipelines

- Can be performed using PCA

Dimension reduction with PCA

- PCA features are in decreasing order of variance

- Assumes the low variance features are "noise"

- ... and high variance features are informative
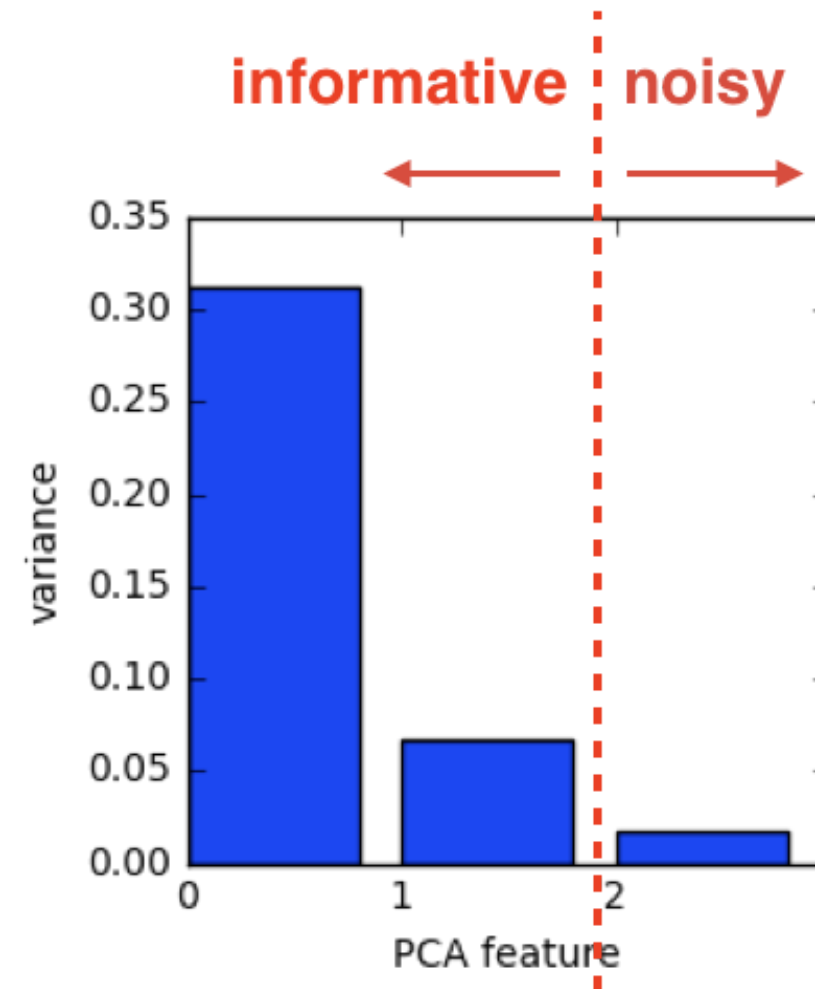
Dimension reduction with PCA

- Specify how many features to keep

- E.g. `PCA(n_components=2)`

- Keeps the first 2 PCA features

- Intrinsic dimension is a good choice

Dimension reduction of iris dataset

- `samples` = array of iris measurements (4 features)

- `species` = list of iris species numbers

```python
from sklearn.decomposition import PCA
pca = PCA(n_components=2)
pca.fit(samples)
```

```
PCA(copy=True, ... )
```

```python
transformed = pca.transform(samples)
print(transformed.shape)
```

```
(150, 2)
```

Iris dataset in 2 dimensions

- PCA has reduced the dimension to 2

- Retained the 2 PCA features with highest variance

- Important information preserved: species remain distinct

```python
import matplotlib.pyplot as plt
xs = transformed[:,0]
ys = transformed[:,1]
plt.scatter(xs, ys, c=species)
plt.show()
```
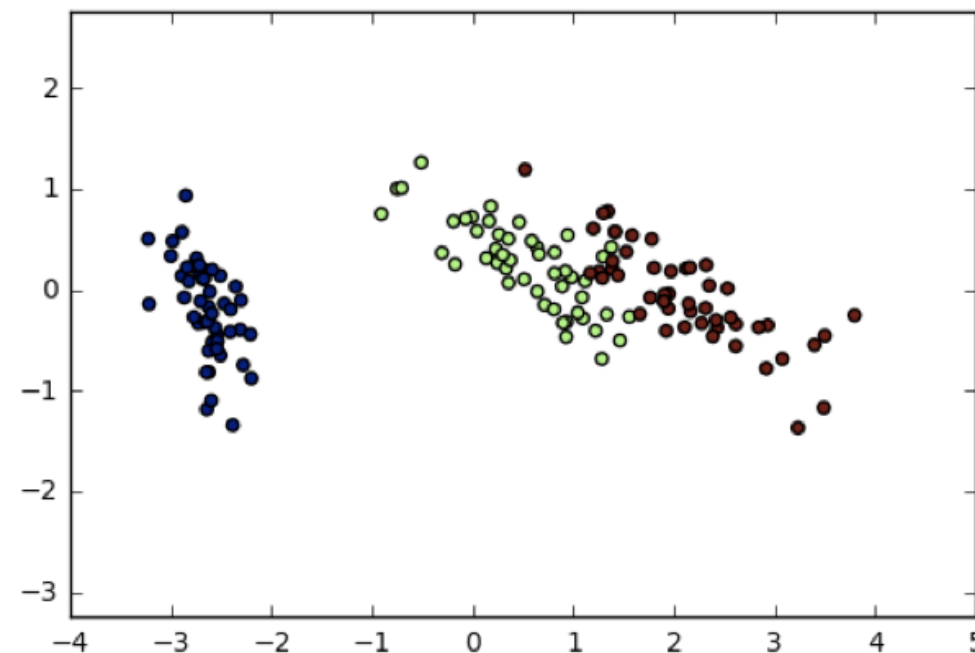
Dimension reduction with PCA

- Discards low variance PCA features

- Assumes the high variance features are informative

- Assumption typically holds in practice (e.g. for iris)

Word frequency arrays

- Rows represent documents, columns represent words

- Entries measure presence of each word in each document

- ... measure using "tf-idf" (more later)

Sparse arrays and csr_matrix

- "Sparse": most entries are zero

- Can use `scipy.sparse.csr_matrix` instead of NumPy array

- `csr_matrix` remembers only the non-zero entries (saves space!)

TruncatedSVD and csr_matrix

- scikit-learn `PCA` doesn't support `csr_matrix`

- Use scikit-learn `TruncatedSVD` instead

- Performs same transformation

```python
from sklearn.decomposition import TruncatedSVD
model = TruncatedSVD(n_components=3)
model.fit(documents)  # documents is csr_matrix
TruncatedSVD(algorithm='randomized', ... )
transformed = model.transform(documents)
```

Let's practice!

UNSUPERVISED LEARNING IN PYTHON