Visualizing the PCA transformation

UNSUPERVISED LEARNING IN PYTHON

Benjamin Wilson
Director of Research at lateral.io

Dimension reduction

- More efficient storage and computation
- Remove less-informative "noise" features
- ... which cause problems for prediction tasks, e.g. classification, regression

Principal Component Analysis (PCA) is a dimensionality reduction technique used to simplify complex datasets. It transforms a large set of variables (features) into a smaller set of uncorrelated variables called principal components, while retaining as much of the original information as possible.

How is PCA Used?
Data Preprocessing:Before applying machine learning algorithms, PCA can reduce the number of features
.
Visualization:Reduce data to 2D or 3D for easy plotting.

Noise Reduction:By keeping only the most important components, PCA can filter out noise.

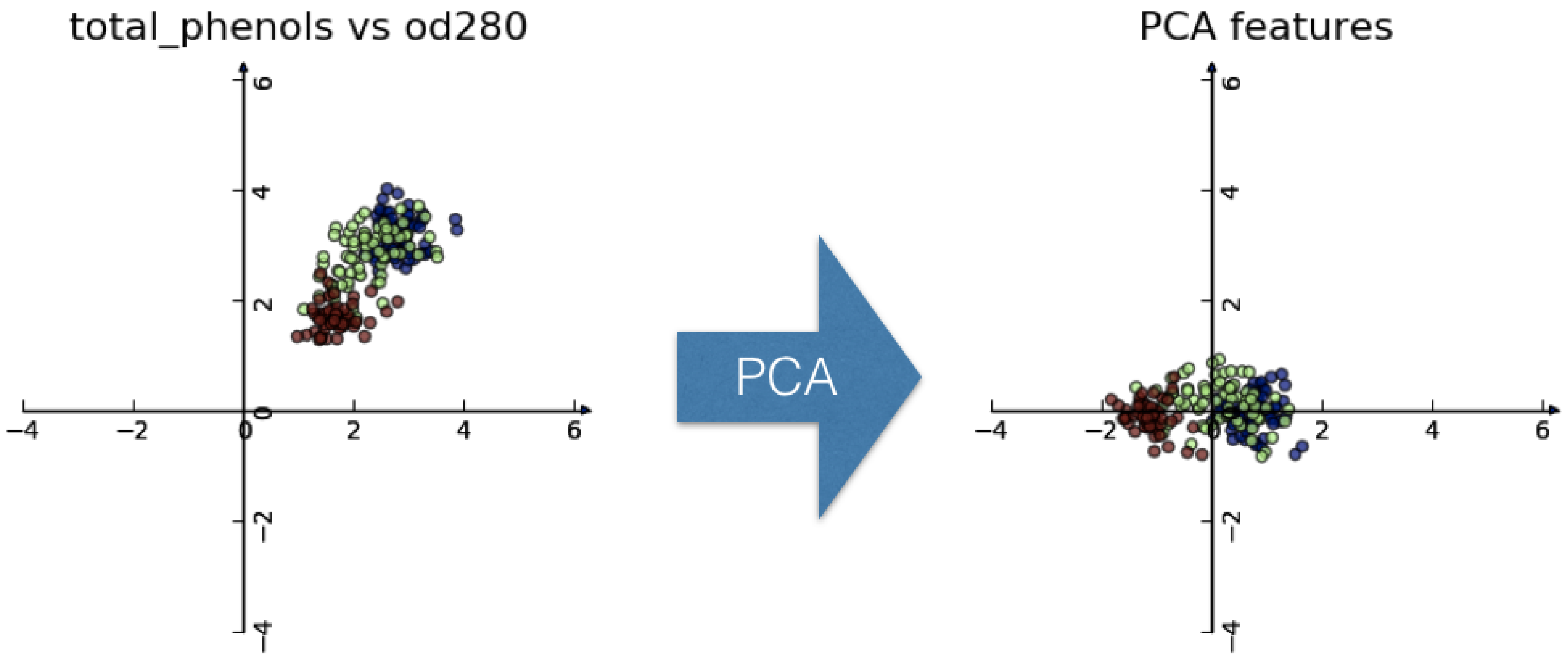
Feature Engineering:PCA creates new, uncorrelated features that can improve model performance

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()
```

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

PCA features

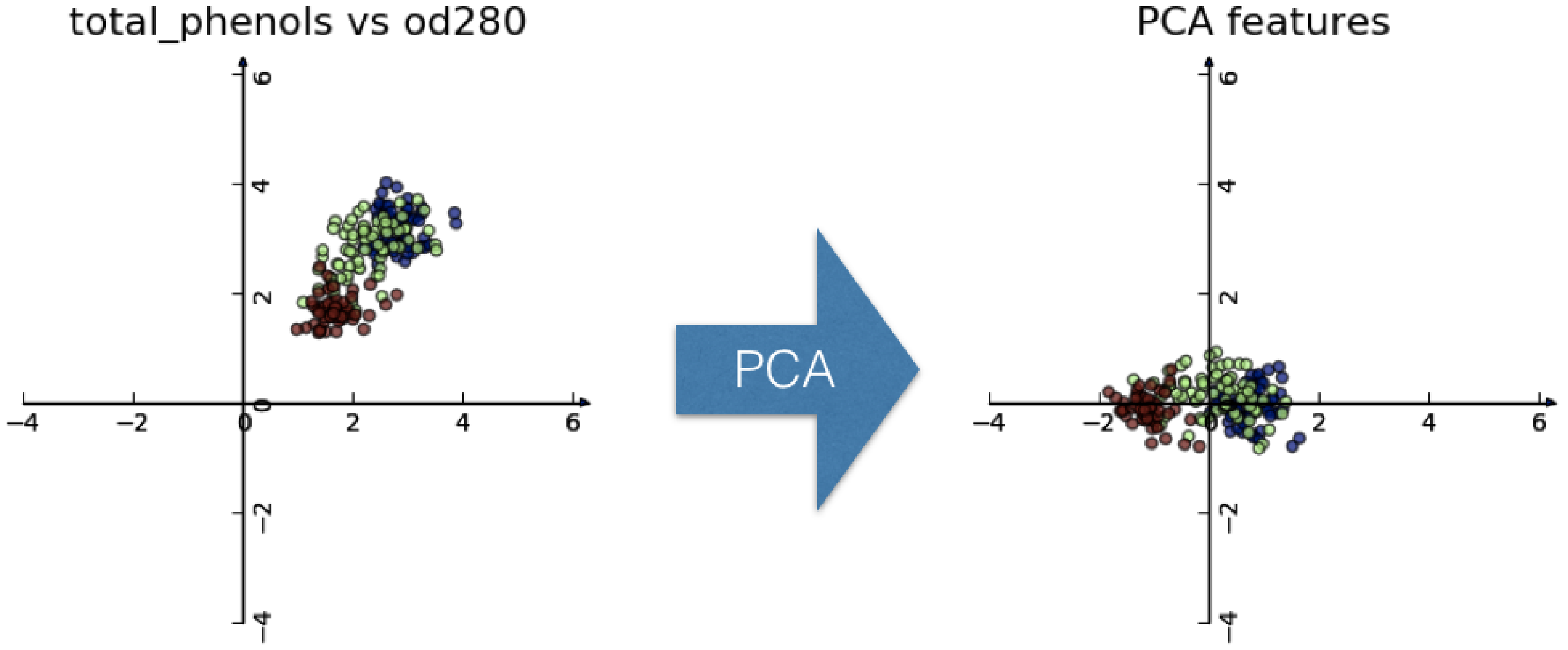
- Rows of transformed correspond to samples
- Columns of transformed are the "PCA features"
- Row gives PCA feature values of corresponding sample

```
print(transformed)
```

```
[[  1.32771994e+00   4.51396070e-01]
 [  8.32496068e-01   2.33099664e-01]
 ...
 [ -9.33526935e-01  -4.60559297e-01]]
```

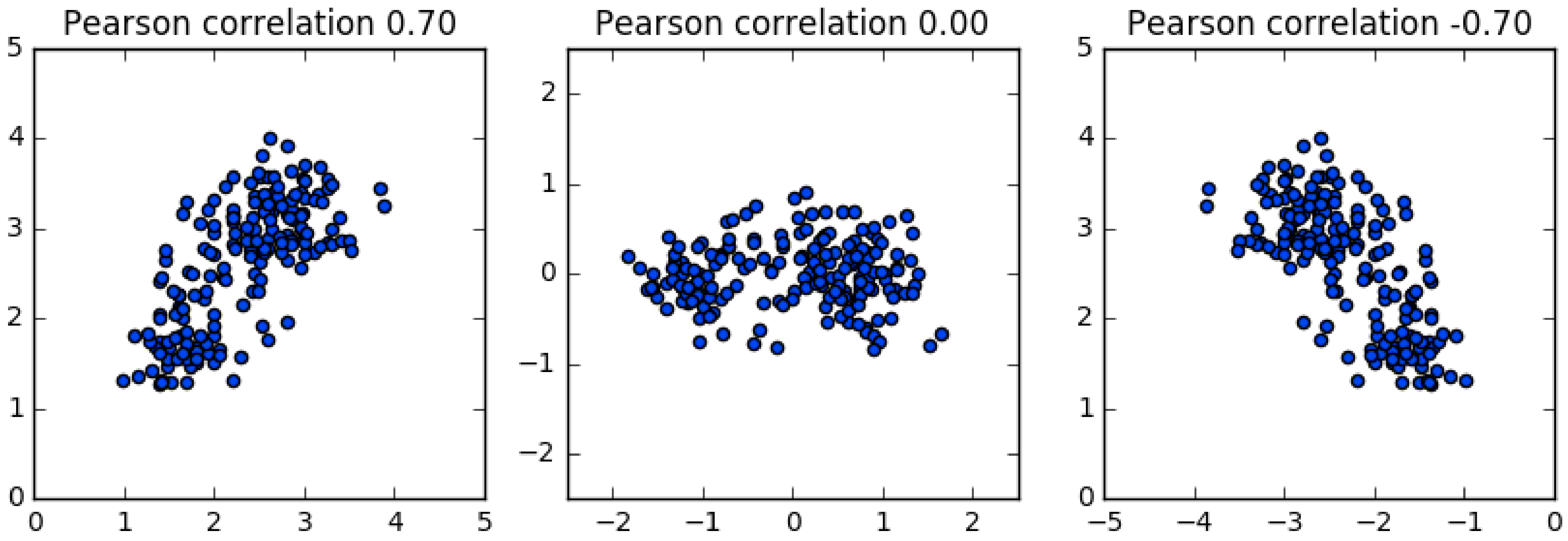
PCA features are not correlated

- Features of dataset are often correlated, e.g. `total_phenols` and `od280`
- PCA aligns the data with axes
- Resulting PCA features are not linearly correlated ("decorrelation")



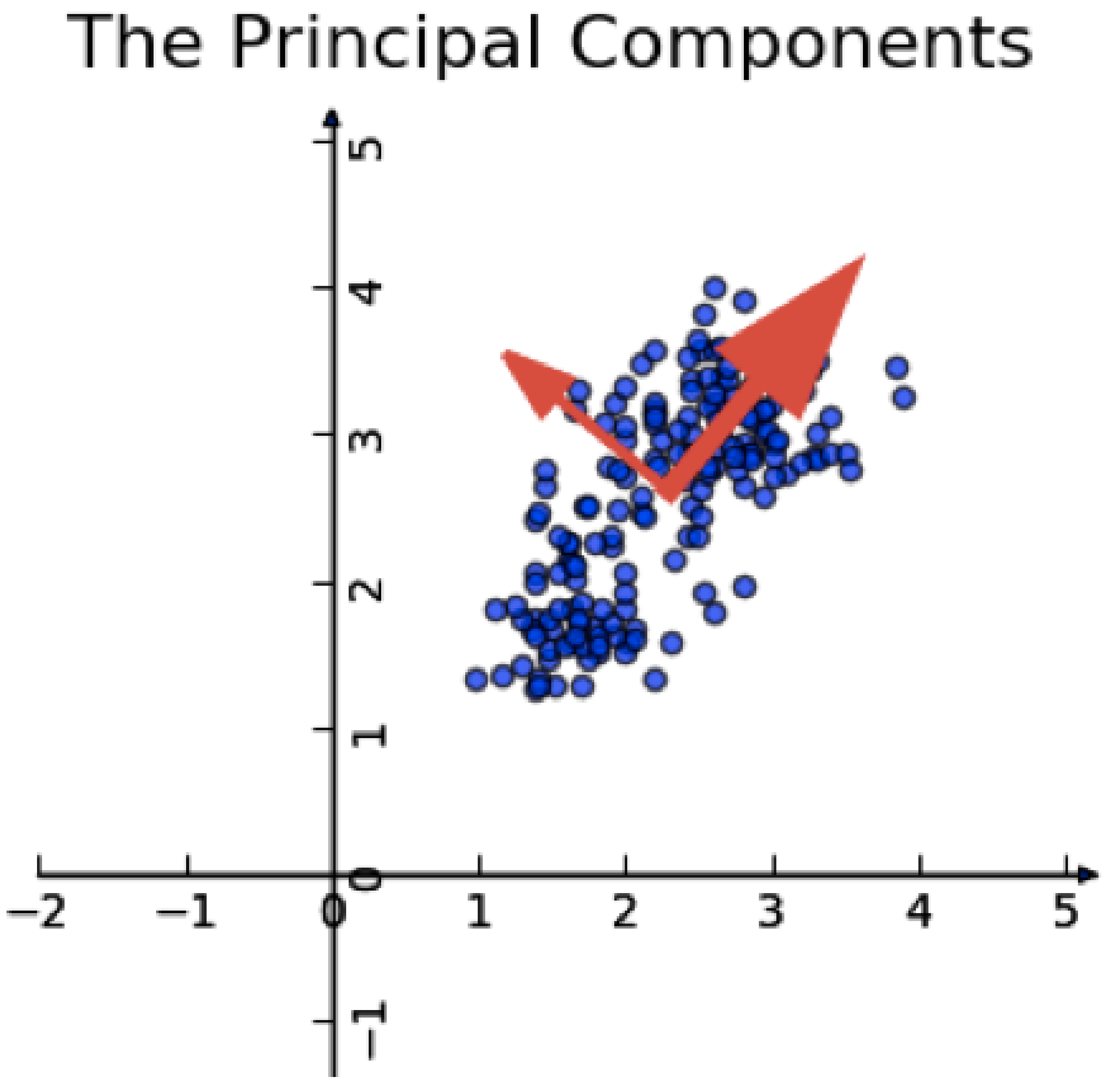
Pearson correlation

- 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



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!

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Intrinsic dimension

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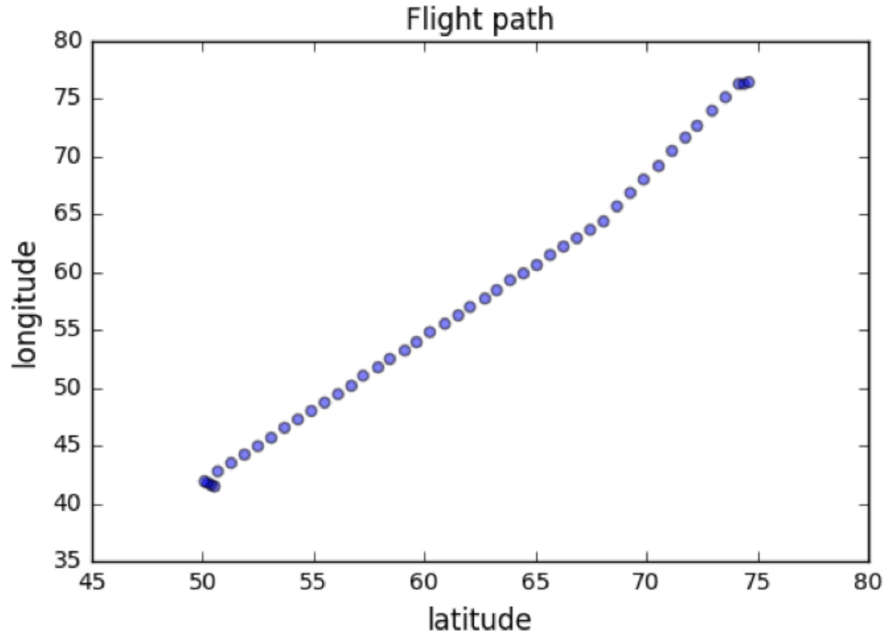
Intrinsic dimension of a flight path

- 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

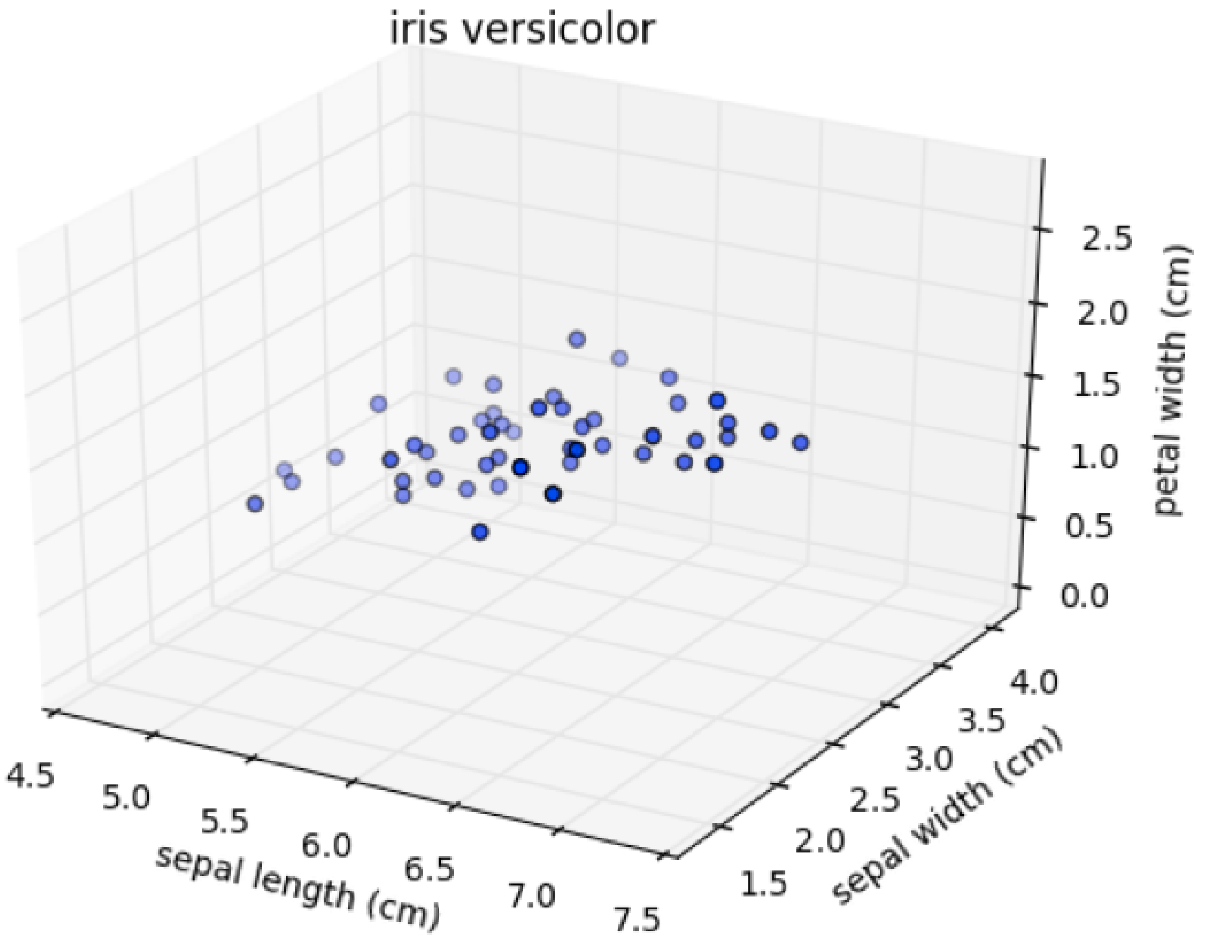
- Intrinsic dimension = number of features needed to approximate the dataset
- Essential idea behind dimension reduction
- What is the most compact representation of the samples?
- Can be detected with PCA

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

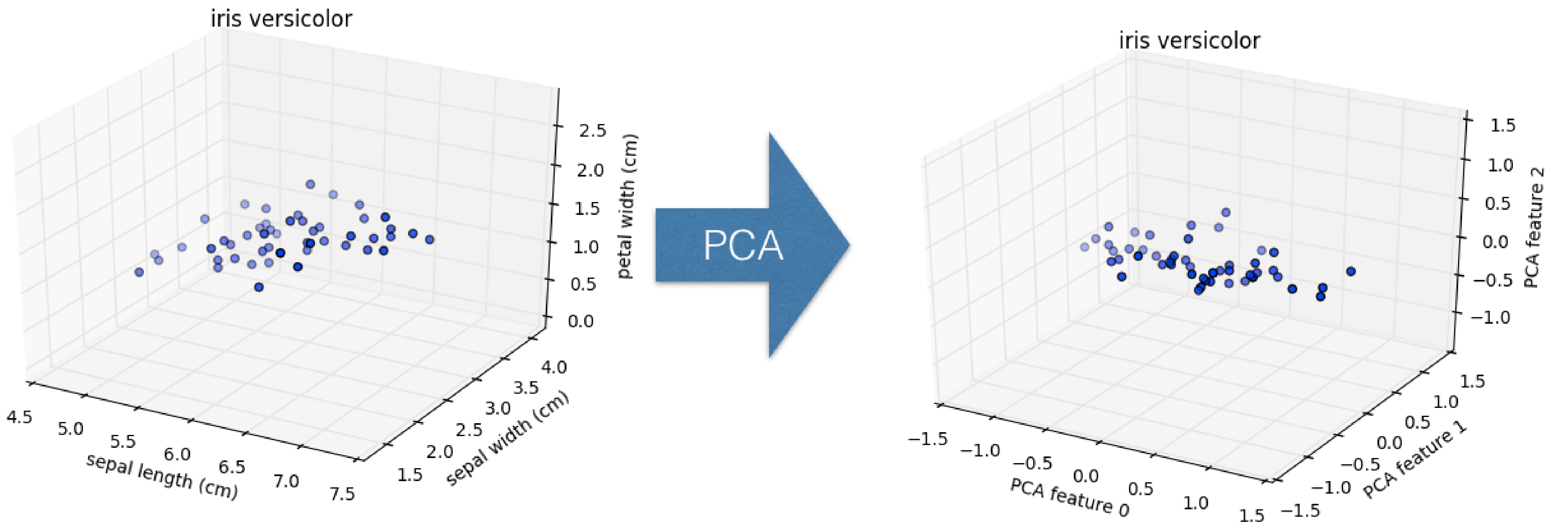
- Samples lie close to a flat 2-dimensional sheet
- So can be approximated using 2 features



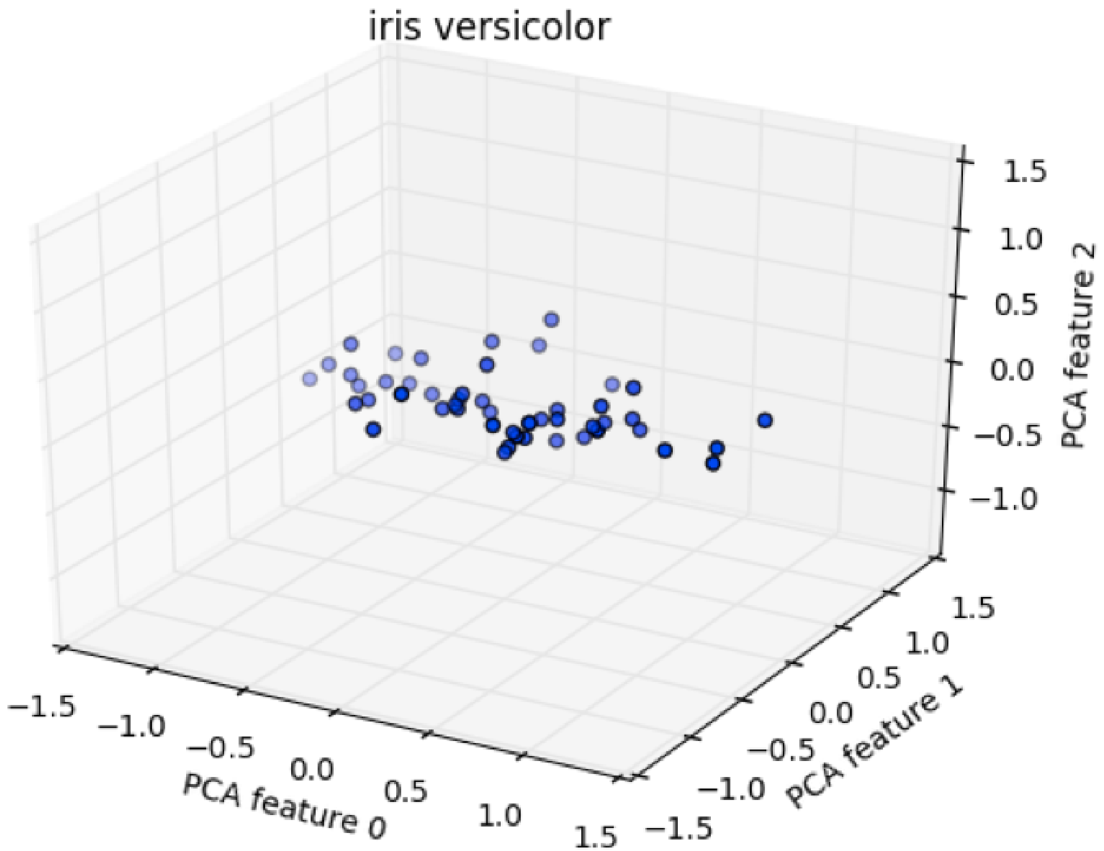
PCA identifies intrinsic dimension

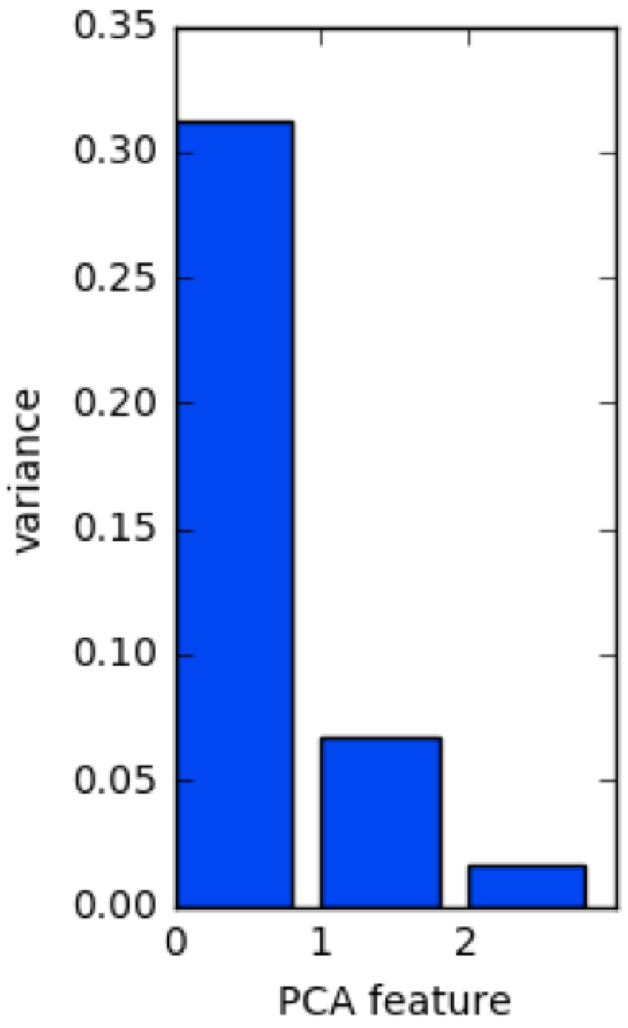
- Scatter plots work only if samples have 2 or 3 features
- PCA identifies intrinsic dimension when samples have any number of features
- Intrinsic dimension = number of PCA features with significant variance

PCA of the versicolor samples



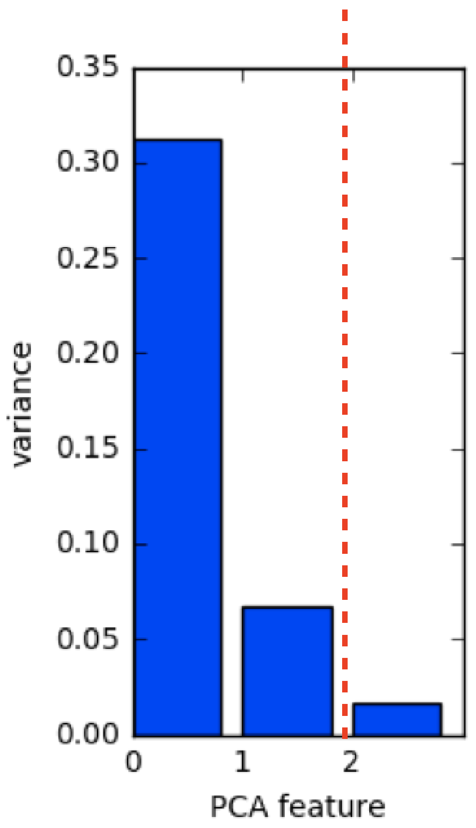
PCA features are ordered by variance descending





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

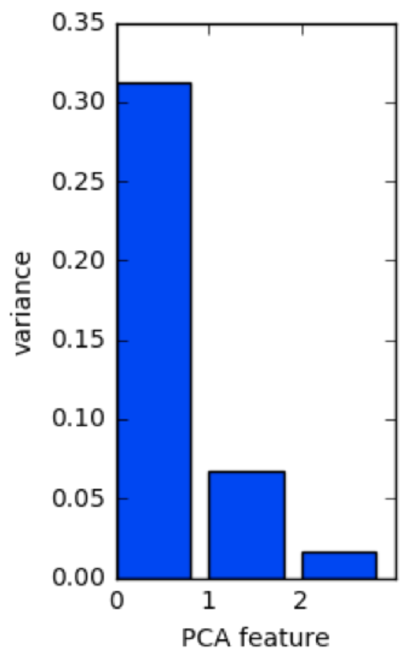
```
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
pca = PCA()
pca.fit(samples)
```

```
PCA()
```

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

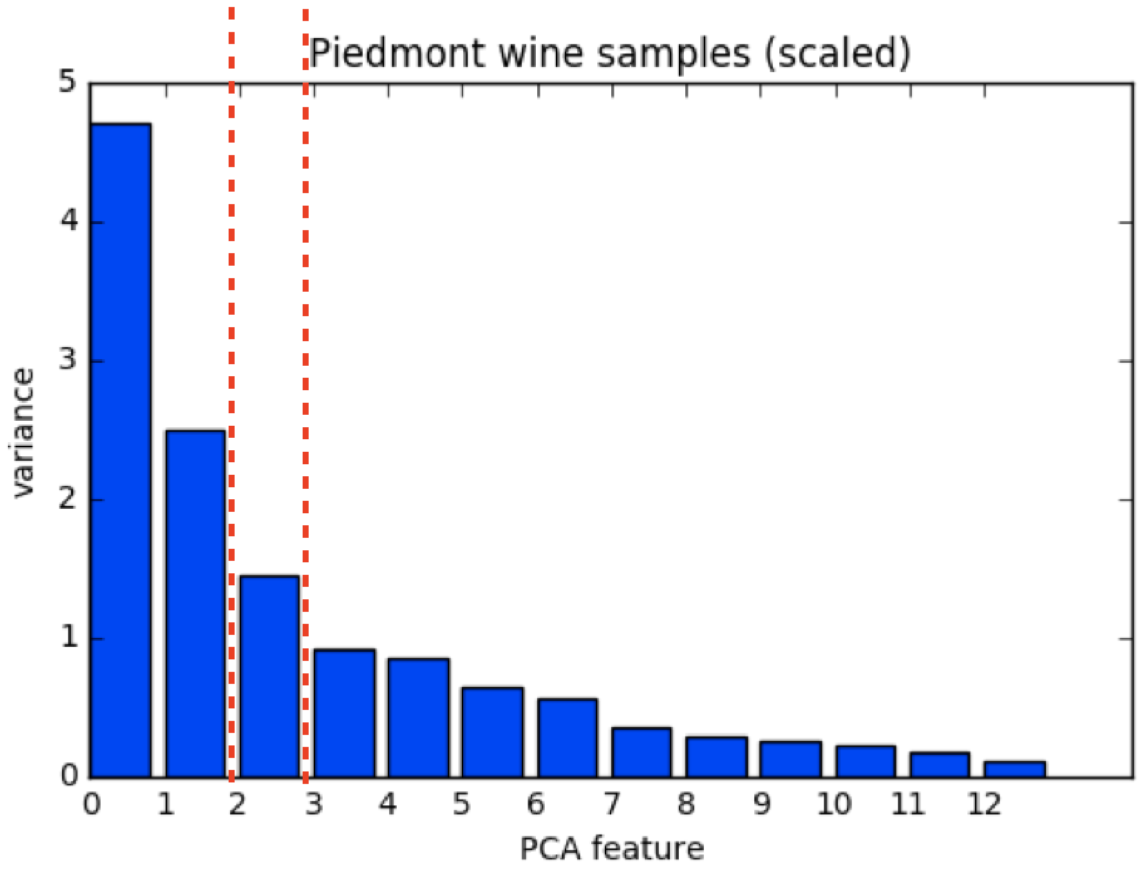
Plotting the variances of PCA features

```
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



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Dimension reduction with PCA

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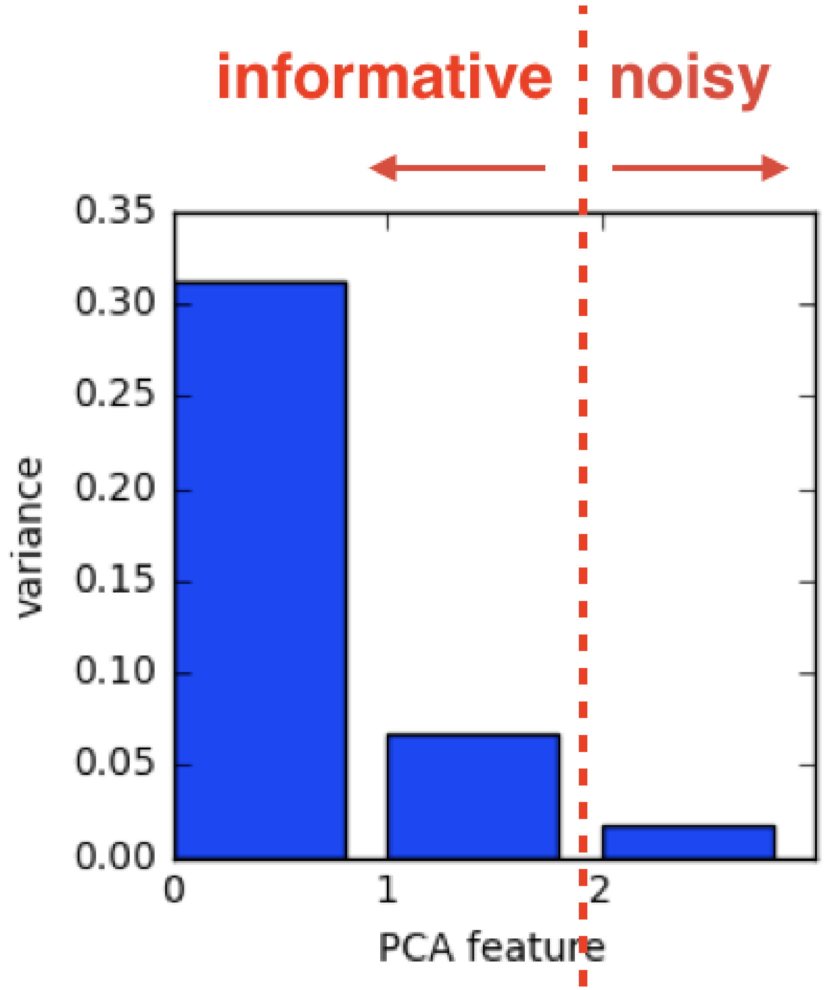
Dimension reduction

- 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

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

```
PCA(n_components=2)
```

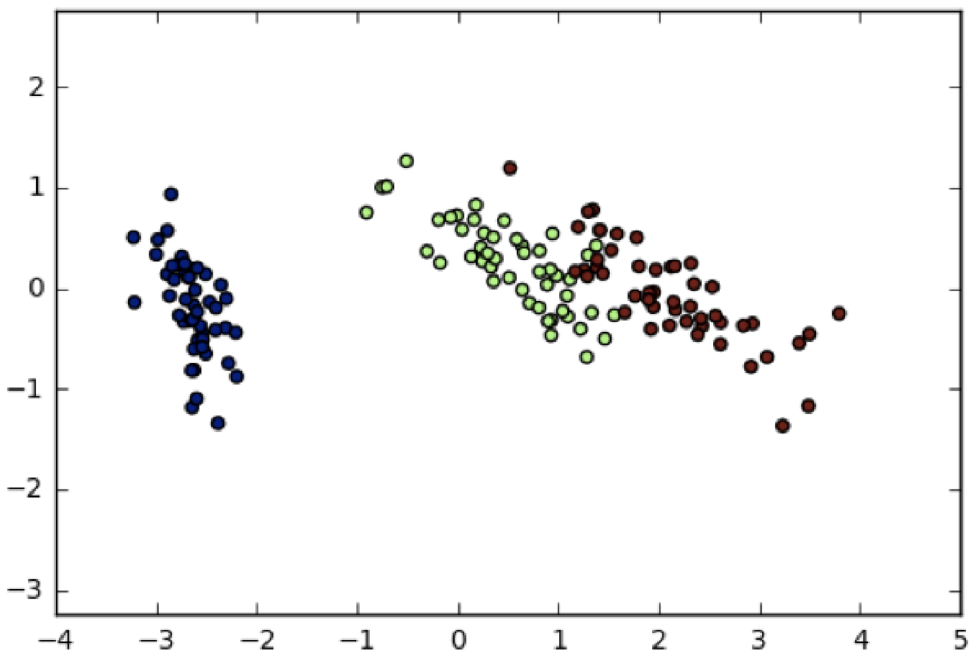
```
transformed = pca.transform(samples)
print(transformed.shape)
```

```
(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()
```

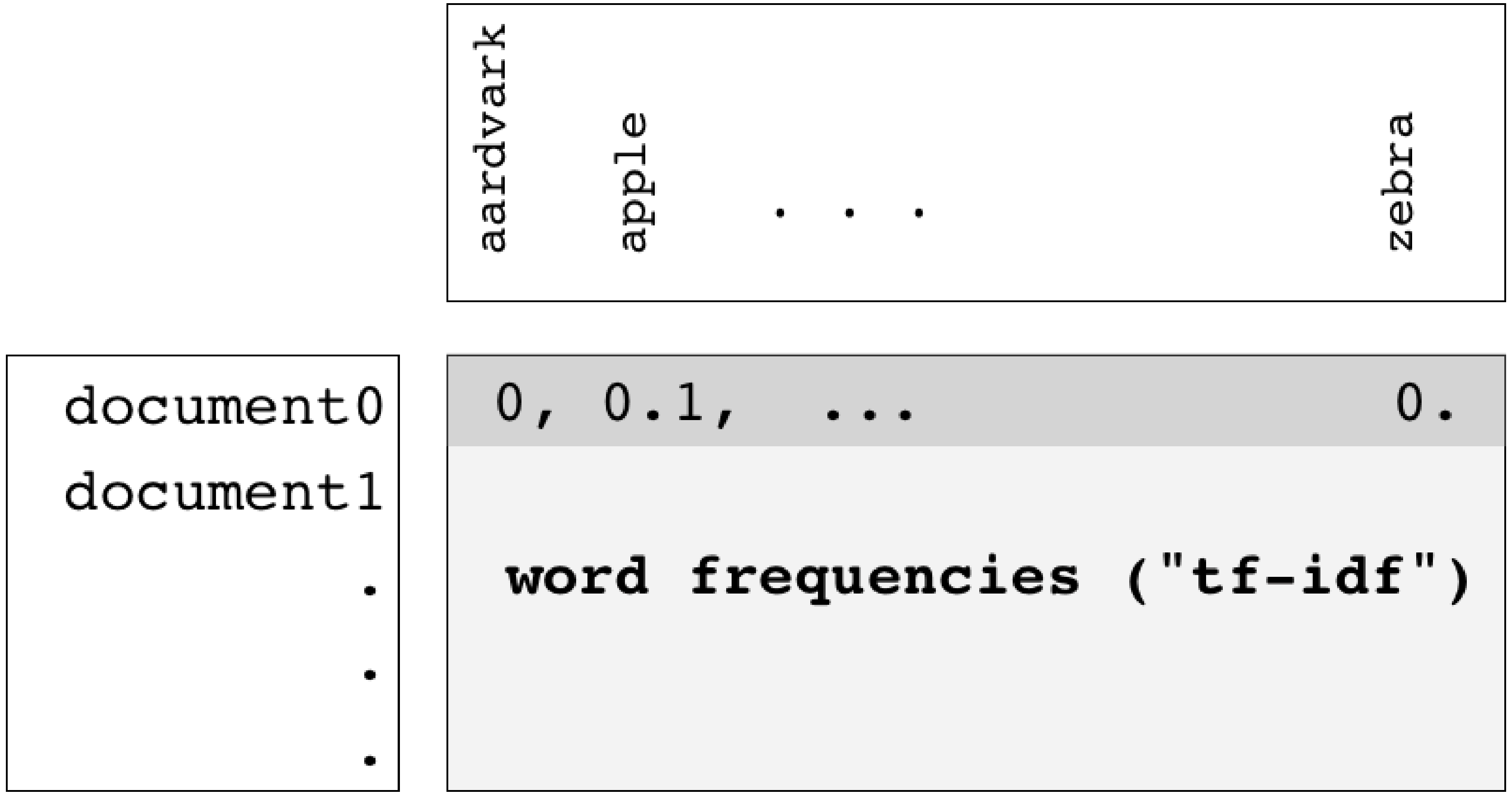


Dimension reduction with PCA

- Discards low variance PCA features
- Assumes the high variance features are informative
- Assumption typically holds in practice (e.g. for iris)

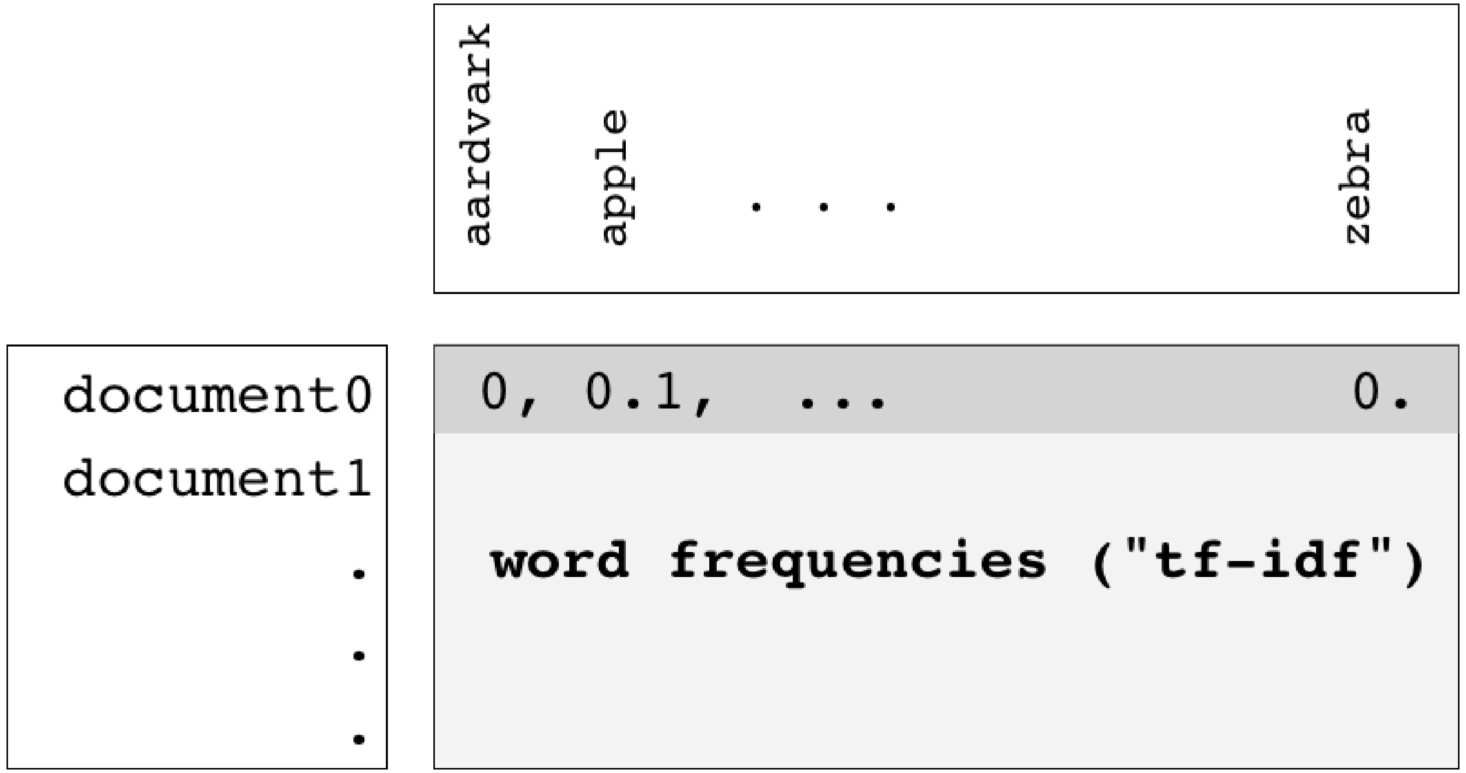
Word frequency arrays

- 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

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

Let's practice!

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