UNSUPERVISED LEARNING IN PYTHON

Unsupervised learning

Unsupervised learning

- Unsupervised learning finds patterns in data
- E.g. *clustering* customers by their purchases
- Compressing the data using purchase patterns (*dimension reduction*)

Supervised vs unsupervised learning

- *Supervised* learning finds patterns for a prediction task
- E.g. classify tumors as benign or cancerous (*labels*)
- Unsupervised learning finds patterns in data
- ... but *without* a specific prediction task in mind

Iris dataset

- Measurements of many iris plants
- 3 species of iris: setosa, versicolor, virginica
- Petal length, petal width, sepal length, sepal width (the *features* of the dataset)



Source: http://scikit-learn.org/stable/modules/generated/sklearn.datasets.load_iris.html

Arrays, features & samples

- 2D NumPy array
- Columns are measurements (the *features*)
- Rows represent iris plants (the *samples*)

Iris data is 4-dimensional

- Iris samples are points in 4 dimensional space
- Dimension = number of features
- Dimension too high to visualize!
- ... but unsupervised learning gives insight

k-means clustering

- Finds clusters of samples
- Number of clusters must be specified
- Implemented in **sklearn** ("scikit-learn")

k-means clustering with scikit-learn

```
In [1]: print(samples)
[[ 5.   3.3  1.4  0.2]
 [ 5.   3.5  1.3  0.3]
 [ 4.9  2.4  3.3  1. ]
 [ 6.3  2.8  5.1  1.5]
 ...
 [ 7.2  3.2  6.   1.8]]

In [2]: from sklearn.cluster import KMeans

In [3]: model = KMeans(n_clusters=3)

In [4]: model.fit(samples)
Out[4]: KMeans(algorithm='auto', ...)

In [5]: labels = model.predict(samples)

In [6]: print(labels)
[0 0 1 1 0 1 2 1 0 1 ...]
```

Cluster labels for new samples

- New samples can be assigned to existing clusters
- k-means remembers the mean of each cluster (the "centroids")
- Finds the nearest centroid to each new sample

Cluster labels for new samples

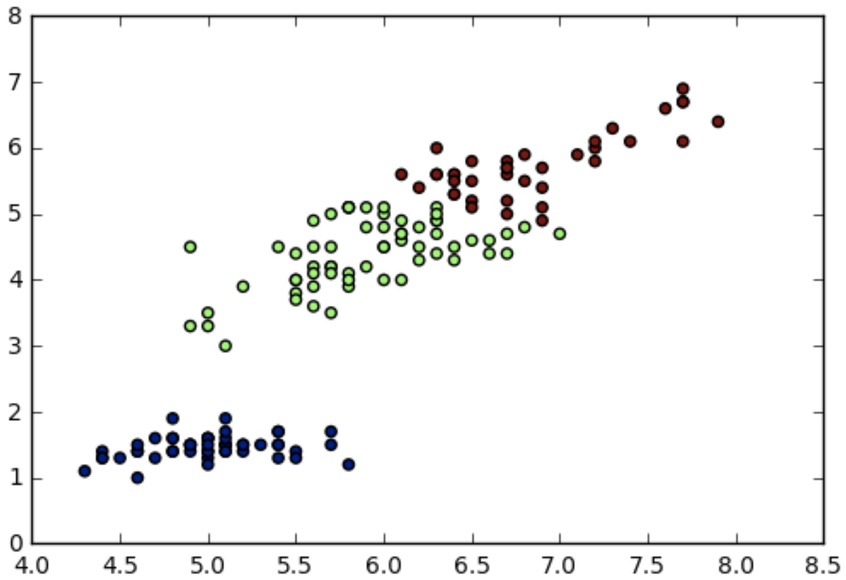
```
In [7]: print(new_samples)
[[ 5.7  4.4  1.5  0.4]
 [ 6.5  3.   5.5  1.8]
 [ 5.8  2.7  5.1  1.9]]

In [8]: new_labels = model.predict(new_samples)

In [9]: print(new_labels)
[0 2 1]
```

Scatter plots

- Scatter plot of sepal length vs petal length
- Each point represents an iris sample
- Color points by cluster labels
- PyPlot (**matplotlib.pyplot**)



Scatter plots

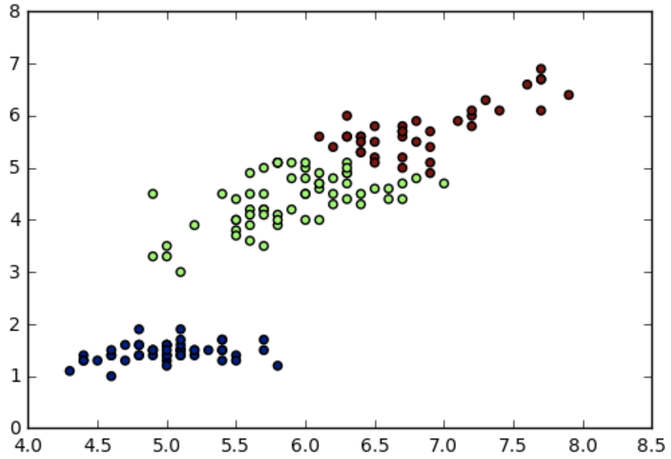
```
In [1]: import matplotlib.pyplot as plt

In [2]: xs = samples[:,0]

In [3]: ys = samples[:,2]

In [4]: plt.scatter(xs, ys, c=labels)

In [5]: plt.show()
```



PYTHON UNSUPERVISED LEARNING

Let’s practice!

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Evaluating a clustering

Evaluating a clustering

- Can check correspondence with e.g. iris species
- ... but what if there are no species to check against?
- Measure quality of a clustering
- Informs choice of how many clusters to look for

Iris: clusters vs species

- k-means found 3 clusters amongst the iris samples
- Do the clusters correspond to the species?

species labels	setosa	versicolor	virginica
0	0	2	36
1	50	0	0
2	0	48	14

Cross tabulation with pandas

- Clusters vs species is a "cross-tabulation"
- Use the **pandas** library
- Given the species of each sample as a list **species**

```
In [1]: print(species)
['setosa', 'setosa', 'versicolor', 'virginica', ... ]
```

Aligning labels and species

```
In [2]: import pandas as pd

In [3]: df = pd.DataFrame({'labels': labels, 'species': species})

In [4]: print(df)
     labels     species
0         1      setosa
1         1      setosa
2         2  versicolor
3         2   virginica
4         1      setosa
...
```

Crosstab of labels and species

```
In [5]: ct = pd.crosstab(df['labels'], df['species'])

In [6]: print(ct)
species  setosa  versicolor  virginica
labels
0             0           2         36
1            50           0          0
2             0          48         14
```

How to evaluate a clustering, if there were no species information?

Measuring clustering quality

- Using only samples and their cluster labels
- A good clustering has tight clusters
- ... and samples in each cluster bunched together

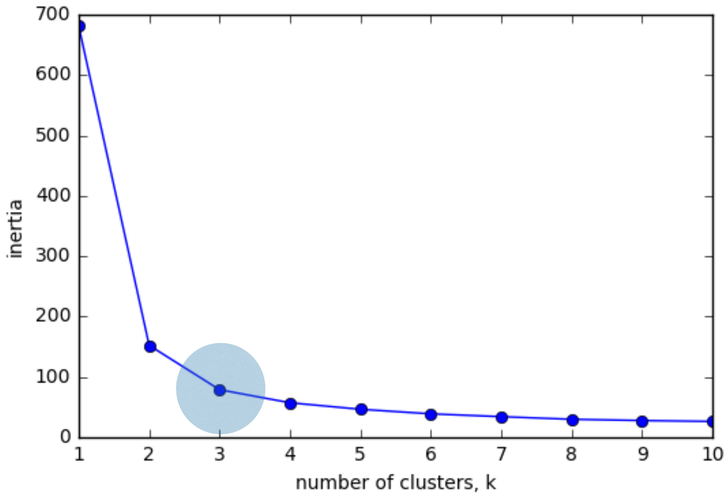
Inertia measures clustering quality

- Measures how spread out the clusters are (*lower* is better)
- Distance from each sample to centroid of its cluster
- After **fit()**, available as attribute **inertia_**
- k-means attempts to minimize the inertia when choosing clusters

```
In [1]: from sklearn.cluster import KMeans

In [2]: model = KMeans(n_clusters=3)

In [3]: model.fit(samples)

In [4]: print(model.inertia_)
78.9408414261
```

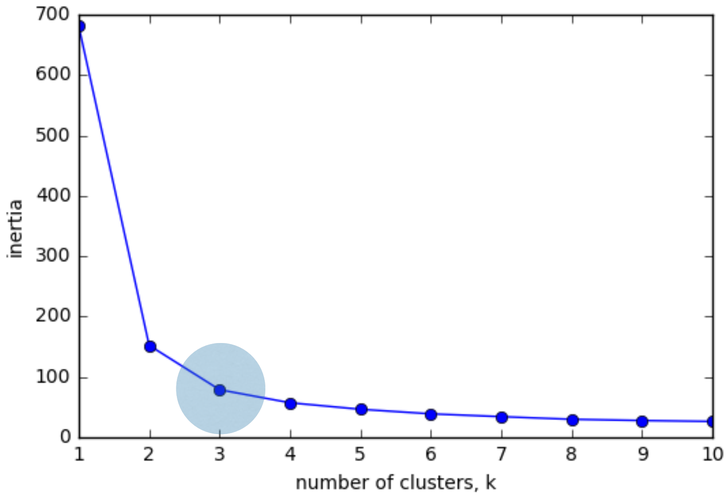
The number of clusters

- Clusterings of the iris dataset with different numbers of clusters
- More clusters means lower inertia
- What is the best number of clusters?



How many clusters to choose?

- A good clustering has tight clusters (so low inertia)
- ... but not too many clusters!
- Choose an "elbow" in the inertia plot
- Where inertia begins to decrease more slowly
- E.g. for iris dataset, 3 is a good choice



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Transforming features for better clusterings

Piedmont wines dataset

- 178 samples from 3 distinct varieties of red wine: *Barolo*, *Grignolino* and *Barbera*
- Features measure chemical composition e.g. alcohol content
- ... also visual properties like “color intensity”

Source: https://archive.ics.uci.edu/ml/datasets/Wine

Clustering the wines

```
In [1]: from sklearn.cluster import KMeans

In [2]: model = KMeans(n_clusters=3)

In [3]: labels = model.fit_predict(samples)
```

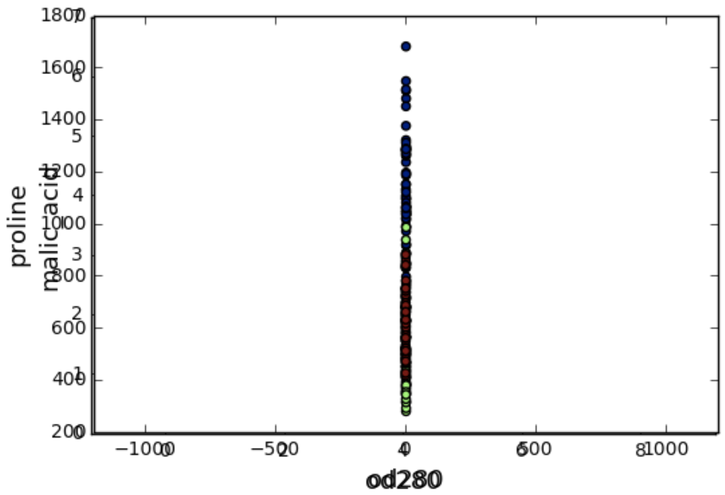
Clusters vs. varieties

```
In [4]: df = pd.DataFrame({'labels': labels,
   ...:                    'varieties': varieties})

In [5]: ct = pd.crosstab(df['labels'], df['varieties'])

In [6]: print(ct)
varieties  Barbera  Barolo  Grignolino
labels
0               29      13          20
1                0      46           1
2               19       0          50
```

Feature variances

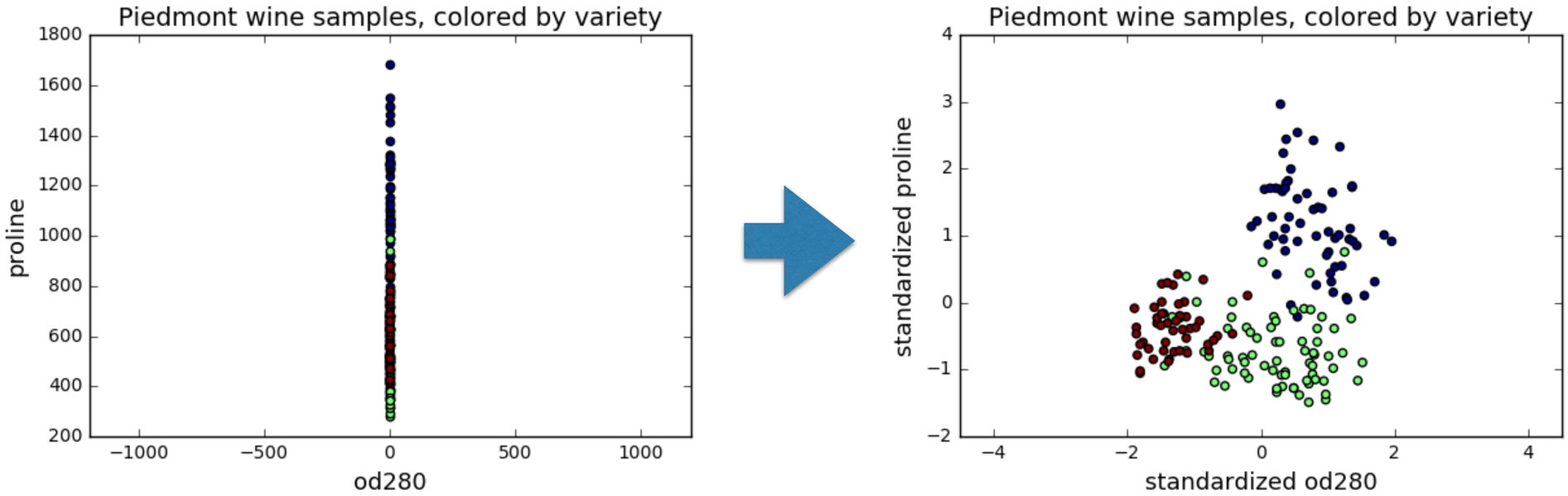
- The wine features have very different variances!
- Variance of a feature measures spread of its values

```
feature      variance
alcohol          0.65
malic_acid       1.24
...
od280            0.50
proline      99166.71
```



StandardScaler

- In kmeans: feature variance = feature influence
- **`StandardScaler`** transforms each feature to have mean 0 and variance 1
- Features are said to be "standardized"



sklearn StandardScaler

```
In [1]: from sklearn.preprocessing import StandardScaler

In [2]: scaler = StandardScaler()

In [3]: scaler.fit(samples)
Out[3]: StandardScaler(copy=True, with_mean=True, with_std=True)

In [4]: samples_scaled = scaler.transform(samples)
```

Similar methods

- **StandardScaler** and **KMeans** have similar methods
- Use **fit()** / **transform()** with **StandardScaler**
- Use **fit()** / **predict()** with **KMeans**

StandardScaler, then KMeans

- Need to perform two steps: **StandardScaler**, then **KMeans**
- Use sklearn pipeline to combine multiple steps
- Data flows from one step into the next

Pipelines combine multiple steps

```
In [1]: from sklearn.preprocessing import StandardScaler

In [2]: from sklearn.cluster import KMeans

In [3]: scaler = StandardScaler()

In [4]: kmeans = KMeans(n_clusters=3)

In [5]: from sklearn.pipeline import make_pipeline

In [6]: pipeline = make_pipeline(scaler, kmeans)

In [7]: pipeline.fit(samples)
Out[7]: Pipeline(steps=...)

In [8]: labels = pipeline.predict(samples)
```

Feature standardization improves clustering

```
In [9]: df = pd.DataFrame({'labels': labels, 'varieties': varieties})

In [10]: ct = pd.crosstab(df['labels'], df['varieties'])

In [11]: print(ct)
varieties  Barbera  Barolo  Grignolino
labels
0                0      59           3
1               48       0           3
2                0       0          65
```

Without **feature standardization was very bad:**

```
varieties  Barbera  Barolo  Grignolino
labels
0               29      13          20
1                0      46           1
2               19       0          50
```

sklearn preprocessing steps

- **StandardScaler** is a "preprocessing" step
- **MaxAbsScaler** and **Normalizer** are other examples

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