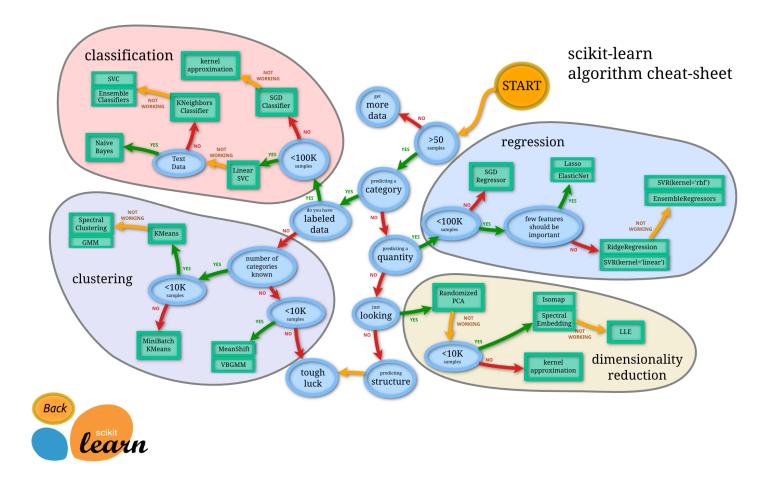
Unsupervised Learning



Supervised Learning

```
• Dataset = X, y
• X = feature matrix (n, p)
• y = targets vector (n, 1)
```

```
Find h_{eta}(X) as close to y as possible
```

Unsupervised Algorithms

```
find patterns in X , without supervision from a target y
```

Unsupervised Learning helps us reduce dimensions

- Feature Engineering/less features (saves time)
- Compress (saves space)

It also allows us to cluster data (= group data points based on similarities)

- Understand data (explore, visualize, etc.)
- Find anomalies/outliers?
- Recommendations
- Semi-supervised classifications

Plan

- 1. Principal Component Analysis (PCA)
- 2. Clustering with K-Means Algorithm

1. Principal Component Analysis (PCA)

- · Squashes our high-dimensional dataset down into a lower dimension
- Aims to find the best linear combination of features (= columns) that best represents the underlying structure of the data

Remember Linear Regression Variants?

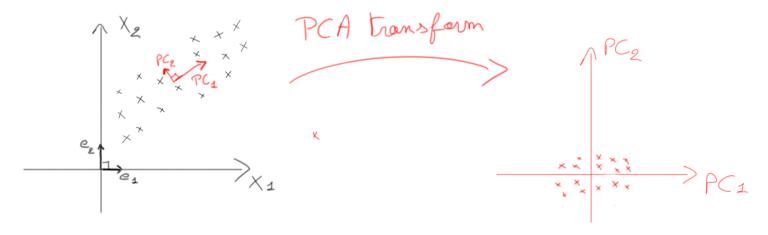
Polynomial \hat{y} Log transformation \hat{y} Linear combination of features (while avoiding multicollinearity) \hat{y}

PCA = finding the best linear combination of features

- Canceling ALL multicollinearity
- Ranking the newly created PCs Z from most to least important

 Z_i

is a so-called Principal Component (PC)



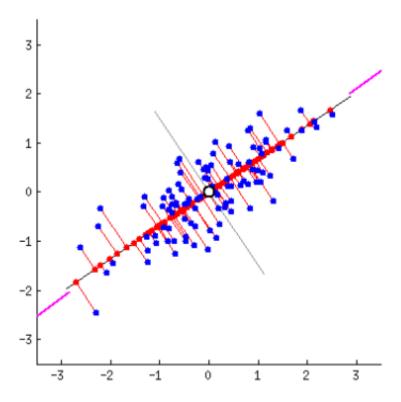
PCA is essentially a projection of the data that is

- oriented towards specific directions, defined by the Principal Components
- orthonormal to each other (0 multicollinearity)
- ranked by decreasing "explaining power" (measured by the variance of our data when projected onto this PC)

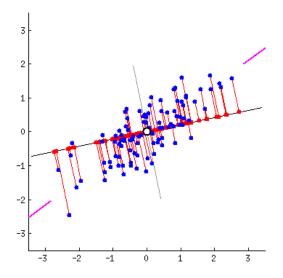
Intuition

If we had to keep only one direction to describe our data, this direction should

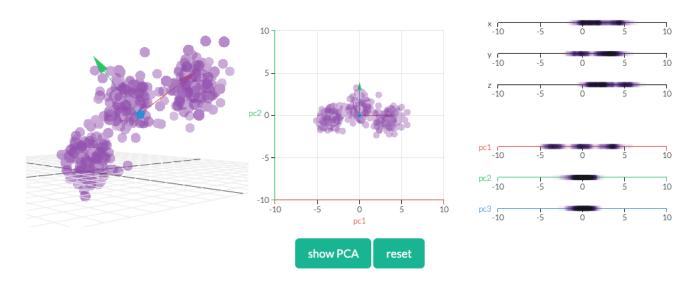
- preserve most of the variance in the data when projected onto it (see spread of red dots)
- minimize "reconstruction errors" (see red lines)



<u>stats-exchange story (https://stats.stackexchange.com/a/140579/286995)</u>



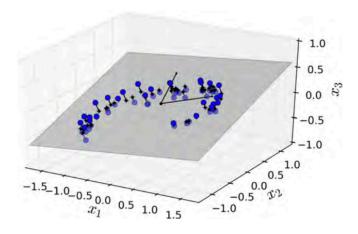
3 components

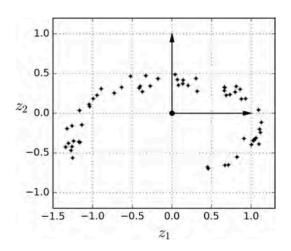


<u>interactive visuals (http://setosa.io/ev/principal-component-analysis/)</u>

PCA helps to reduce dimensions!

$$(X_1,X_2,X_3) \sim (Z_1,Z_2)$$





Earning/9781492032632/)

1.2 Let's Code an Example (with a Wine Dataset)

In []: from sklearn.datasets import load wine

wine = load_wine(as_frame=True) X = wine.datay = wine.target wine features = X.columns

#1 Data must be centered around its mean before applying PCA 1. from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()

scaler.fit(X)

X = pd.DataFrame(scaler.transform(X), columns=wine features)

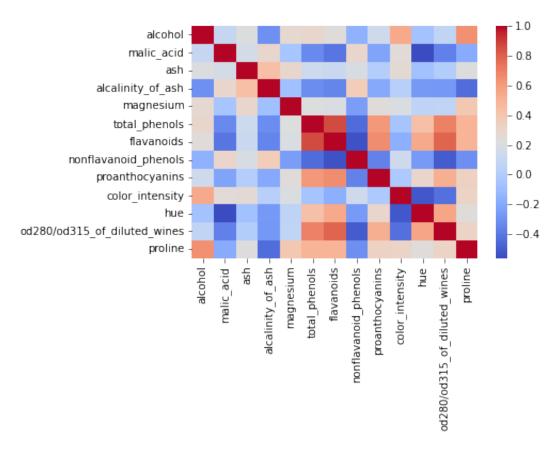
Out[]:

	alcohol	malic_acid	ash	alcalinity_of_ash	magnesium	total_phenols	flavanoids
0	1.518613	-0.562250	0.232053	-1.169593	1.913905	0.808997	1.034819
1	0.246290	-0.499413	-0.827996	-2.490847	0.018145	0.568648	0.733629
2	0.196879	0.021231	1.109334	-0.268738	0.088358	0.808997	1.215533
3	1.691550	-0.346811	0.487926	-0.809251	0.930918	2.491446	1.466525
4	0.295700	0.227694	1.840403	0.451946	1.281985	0.808997	0.663351
173	0.876275	2.974543	0.305159	0.301803	-0.332922	-0.985614	-1.424900
174	0.493343	1.412609	0.414820	1.052516	0.158572	-0.793334	-1.284344
175	0.332758	1.744744	-0.389355	0.151661	1.422412	-1.129824	-1.344582
176	0.209232	0.227694	0.012732	0.151661	1.422412	-1.033684	-1.354622
177	1.395086	1.583165	1.365208	1.502943	-0.262708	-0.392751	-1.274305

178 rows × 13 columns

```
In [ ]: sns.heatmap(pd.DataFrame(X).corr(), cmap='coolwarm')
```

Out[]: <AxesSubplot:>



a) Compute the Principal Components

```
In [ ]: from sklearn.decomposition import PCA
    pca = PCA()
    pca.fit(X)

Out[ ]: PCA()
```

Out[]:

. <u>.</u>	PC1	PC2	PC3	PC4	PC5	PC6
alcohol	0.144329	-0.483652	-0.207383	-0.017856	-0.265664	-0.213539
malic_acid	-0.245188	-0.224931	0.089013	0.536890	0.035214	-0.536814
ash	-0.002051	-0.316069	0.626224	-0.214176	-0.143025	-0.154475
alcalinity_of_ash	-0.239320	0.010591	0.612080	0.060859	0.066103	0.100825
magnesium	0.141992	-0.299634	0.130757	-0.351797	0.727049	-0.038144
total_phenols	0.394661	-0.065040	0.146179	0.198068	-0.149318	0.084122
flavanoids	0.422934	0.003360	0.150682	0.152295	-0.109026	0.018920
nonflavanoid_phenols	-0.298533	-0.028779	0.170368	-0.203301	-0.500703	0.258594
proanthocyanins	0.313429	-0.039302	0.149454	0.399057	0.136860	0.533795
color_intensity	-0.088617	-0.529996	-0.137306	0.065926	-0.076437	0.418644
hue	0.296715	0.279235	0.085222	-0.427771	-0.173615	-0.105983
od280/od315_of_diluted_wines	0.376167	0.164496	0.166005	0.184121	-0.101161	-0.265851
proline	0.286752	-0.364903	-0.126746	-0.232071	-0.157869	-0.119726

Each PC is a linear combination of initial wine features

b) Project our dataset into this new space of PCs

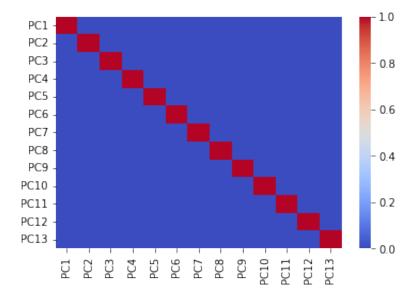
Out[]:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	
0	3.316751	-1.443463	-0.165739	-0.215631	0.693043	-0.223880	0.596427	0.065139	0.
1	2.209465	0.333393	-2.026457	-0.291358	-0.257655	-0.927120	0.053776	1.024416	-0.
2	2.516740	-1.031151	0.982819	0.724902	-0.251033	0.549276	0.424205	-0.344216	-1.
3	3.757066	-2.756372	-0.176192	0.567983	-0.311842	0.114431	-0.383337	0.643593	0.
4	1.008908	-0.869831	2.026688	-0.409766	0.298458	-0.406520	0.444074	0.416700	0.
173	-3.370524	-2.216289	-0.342570	1.058527	-0.574164	-1.108788	0.958416	-0.146097	-0.
174	-2.601956	-1.757229	0.207581	0.349496	0.255063	-0.026465	0.146894	-0.552427	-0.
175	-2.677839	-2.760899	-0.940942	0.312035	1.271355	0.273068	0.679235	0.047024	0.
176	-2.387017	-2.297347	-0.550696	-0.688285	0.813955	1.178783	0.633975	0.390829	0.
177	-3.208758	-2.768920	1.013914	0.596903	-0.895193	0.296092	0.005741	-0.292914	0.

178 rows × 13 columns

- 178 wine bottles, each expressed as a linear combination of 13 Principal Components
- ✓ As expected, the PCA reduces multicollinearity to the absolute minimum (0)!

In []: sns.heatmap(X_proj.corr(), cmap='coolwarm');

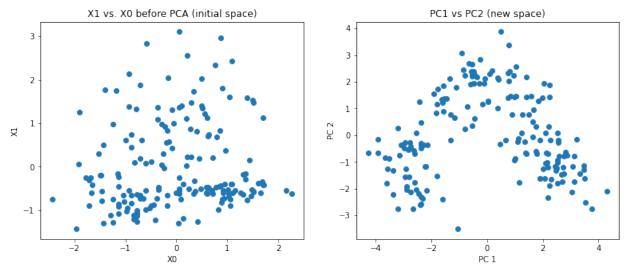


Our wine dataset is also easier to observe in this new space

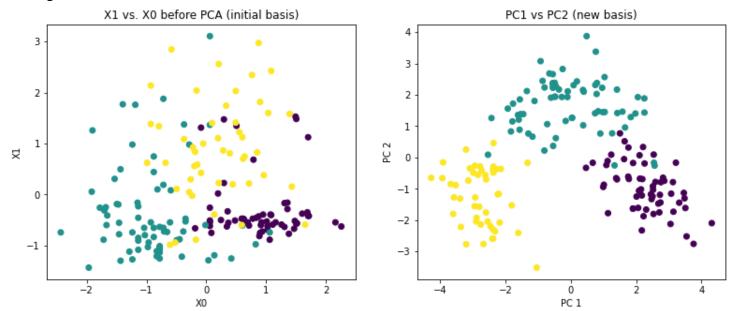
```
In []: # 2D-slice

plt.figure(figsize=(13,5))
plt.subplot(1,2,1)
plt.title('X1 vs. X0 before PCA (initial space)'); plt.xlabel('X0'); p
lt.ylabel('X1')
plt.scatter(X.iloc[:,0], X.iloc[:,1])

plt.subplot(1,2,2)
plt.title('PC1 vs PC2 (new space)'); plt.xlabel('PC 1'); plt.ylabel('PC 2')
plt.scatter(X_proj.iloc[:,0], X_proj.iloc[:,1]);
```



Adding true labels makes it even clearer



Proi

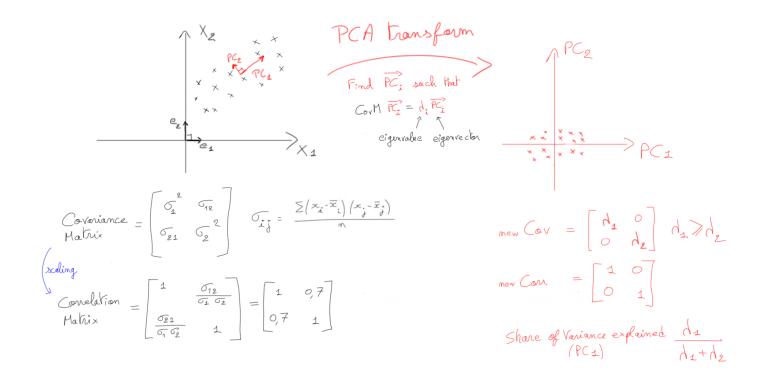
"Projecting" data onto a new space is a simple matrix multiplication

```
(m, k)

Dala projected into PC basis
                       Malrix of PCs in inital basis
    Data expressed in inital bases (e, , , ep)
 In [ ]: # Computational proof
         W = pca.components .T
         print("Shape of W: ", W.shape)
         print("Shape of X", X.shape)
         Shape of W: (13, 13)
         Shape of X (178, 13)
 In [ ]: | np.allclose(
             pca.transform(X),
             np.dot(X,W)
 Out[]: True
```

1.3 How are Principal Components Computed (Mathematically)?

This is the hard part



We can do it with NumPy

- np.linalg.eig(M) computes the eig_vals and eig_vecs of M
- Covariance Matrix =
 X^TX
 of shape (p,p) (if features are centered)
- ! eig() decomposition can take very long
- Eigenvalues and Eigenvectors (https://en.wikipedia.org/wiki/Eigenvalues_and_eigenvectors)

```
In [ ]: # Compute PCs
eig_vals, eig_vecs = np.linalg.eig(np.dot(X.T,X))
```

Out[]:

	PC1	PC2	PC3	PC4	PC5	PC6
alcohol	-0.144329	0.483652	-0.207383	0.017856	-0.265664	0.213539
malic_acid	0.245188	0.224931	0.089013	-0.536890	0.035214	0.536814
ash	0.002051	0.316069	0.626224	0.214176	-0.143025	0.154475
alcalinity_of_ash	0.239320	-0.010591	0.612080	-0.060859	0.066103	-0.100825
magnesium	-0.141992	0.299634	0.130757	0.351797	0.727049	0.038144
total_phenols	-0.394661	0.065040	0.146179	-0.198068	-0.149318	-0.084122
flavanoids	-0.422934	-0.003360	0.150682	-0.152295	-0.109026	-0.018920
nonflavanoid_phenols	0.298533	0.028779	0.170368	0.203301	-0.500703	-0.258594
proanthocyanins	-0.313429	0.039302	0.149454	-0.399057	0.136860	-0.533795
color_intensity	0.088617	0.529996	-0.137306	-0.065926	-0.076437	-0.418644
hue	-0.296715	-0.279235	0.085222	0.427771	-0.173615	0.105983
od280/od315_of_diluted_wines	-0.376167	-0.164496	0.166005	-0.184121	-0.101161	0.265851
proline	-0.286752	0.364903	-0.126746	0.232071	-0.157869	0.119726

1.4 PCs are ranked by order of importance

PCs are ranked by share of **explained variance** $rac{Var(PC_i)}{Var(X)}$

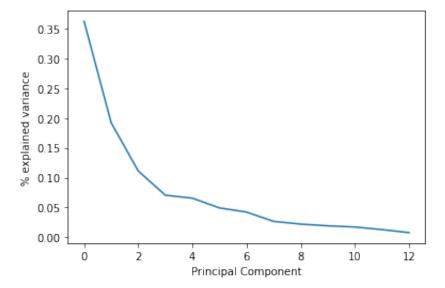
- Remember: information comes in the form of variation
- PC with most variance is the most important one

```
In [ ]: # Let's compute it
        X_proj.std()**2 / ((X.std()**2).sum())
Out[]: PC1
                 0.361988
                 0.192075
        PC2
        PC3
                 0.111236
        PC4
                 0.070690
        PC5
                 0.065633
                 0.049358
        PC6
        PC7
                 0.042387
        PC8
                 0.026807
        PC9
                 0.022222
                 0.019300
        PC10
        PC11
                 0.017368
        PC12
                 0.012982
        PC13
                 0.007952
        dtype: float64
```

🤞 scikit-learn PCA has indeed already ranked them

36% of the dataset's variance lies along the first axis

```
In [ ]: plt.plot(pca.explained_variance_ratio_)
   plt.xlabel('Principal Component'); plt.ylabel('% explained variance');
```



PCA redistributes the ratio among the new features in the most unequal way

1.5 PCA for Dimensionality Reduction

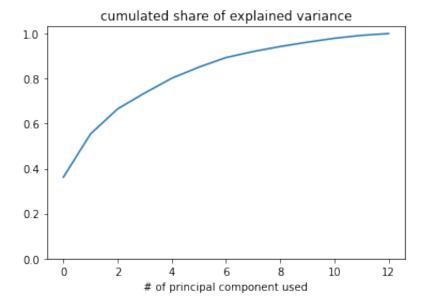
Having computed all PCs, we can now keep only the k most important ones!

- ? Why would we want less features? Because it means we can
 - compress data
 - · reduce model complexity & fit time
 - reduce overfitting

How to choose k?

It's a trade-off between compression and performance

```
In [ ]: plt.plot(np.cumsum(pca.explained_variance_ratio_))
    plt.ylim(ymin=0)
    plt.title('cumulated share of explained variance')
    plt.xlabel('# of principal component used');
```

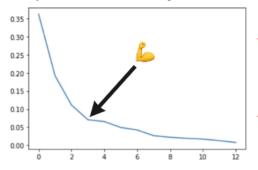


The Elbow Method

Look for the inflection point in the explained variance chart

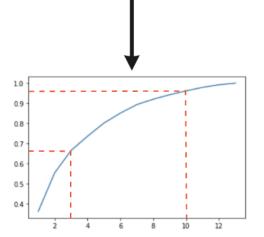
Here, k=3 looks promising

Explained variance by dimension



Explained variance cumulative sum

Number of principal components 1, amount of explained variance held- 0.36
Number of principal components 2, amount of explained variance held- 0.55
Number of principal components 3, amount of explained variance held- 0.67
Number of principal components 4, amount of explained variance held- 0.74
Number of principal components 5, amount of explained variance held- 0.8
Number of principal components 6, amount of explained variance held- 0.85
Number of principal components 7, amount of explained variance held- 0.89
Number of principal components 8, amount of explained variance held- 0.92
Number of principal components 10, amount of explained variance held- 0.94
Number of principal components 10, amount of explained variance held- 0.98
Number of principal components 11, amount of explained variance held- 0.98
Number of principal components 12, amount of explained variance held- 0.99
Number of principal components 12, amount of explained variance held- 0.99
Number of principal components 13, amount of explained variance held- 0.99



Test Model Performance (with k=3 Dimensions)

```
In []: # Fit a PCA with only 3 components
    pca3 = PCA(n_components=3).fit(X)

# Project your data into 3 dimensions
    X_proj3 = pd.DataFrame(pca3.fit_transform(X), columns=['PC1', 'PC2', 'PC3'])

# We have "compressed" our dataset in 3D
    X_proj3
```

Out[]:

	PC1	PC2	PC3
0	3.316751	-1.443463	-0.165739
1	2.209465	0.333393	-2.026457
2	2.516740	-1.031151	0.982819
3	3.757066	-2.756372	-0.176192
4	1.008908	-0.869831	2.026688
173	-3.370524	-2.216289	-0.342570
174	-2.601956	-1.757229	0.207581
175	-2.677839	-2.760899	-0.940942
176	-2.387017	-2.297347	-0.550696
177	-3.208758	-2.768920	1.013914

178 rows × 3 columns

```
In [ ]: from sklearn.linear_model import LogisticRegression
    from sklearn.model_selection import cross_val_score

    print("accuracy 3 PCs")
    print(cross_val_score(LogisticRegression(), X_proj3, y, cv=5).mean())

    print("\naccuracy all 13 initial features")
    print(cross_val_score(LogisticRegression(), X, y, cv=5).mean())
```

accuracy 3 PCs
0.9609523809523809
accuracy all 13 initial features
0.9888888888888888

Decompress

- ? Can you perfectly reconstruct X from X proj3?
- Not if you kept k < 13 dimensions; information has been lost
- We can approximate x by reconstructing it with inverse_transform()

```
In [ ]: X_reconstructed = pca3.inverse_transform(X_proj3)
                X reconstructed.shape
Out[]: (178, 13)
In [ ]: plt.figure(figsize=(15,4))
                plt.subplot(1,2,1)
                sns.heatmap(X)
                plt.title("original data")
                plt.subplot(1,2,2)
                plt.title("reconstructed data")
                sns.heatmap(X reconstructed);
                                      original data
                                                                                                         reconstructed data
                0
9
18
27
36
45
54
63
72
81
90
99
108
117
126
135
144
153
162
171
                                                                                       0
9
18
27
36
45
54
63
72
81
90
99
108
117
126
135
144
153
162
171
                                alcalinity of ash
                                               nonflavanoid_phenols
                                                      color_intensity
                                                             od280/od315 of diluted wines
                                    magnesium
                                       total_phenols
                                                  proanthocyanins
```

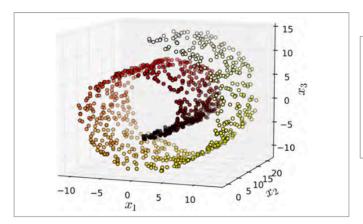
1.6 Limitations of PCA

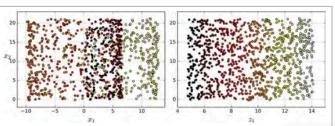
Watch out for manifolds **N**

A manifold is an N-dimensional shape that can be bent and twisted into a higher dimensional shape (9)



Below we can see our data distribution before and after PCA has been applied





Kands-On Machine Learning (https://www.oreilly.com/library/view/hands-on-machinelearning/9781492032632/)

Other dimensionality reduction techniques:

- t-Distributed Stochastic Neighbor Embedding (t-SNE) Aims to reduce dimensionality while keeping similar observations close together and dissimilar ones apart. This is a great technique for visualizing clusters of higher dimensions
- **Kernel PCA** Captures non-linear patterns (similar principle to SVM kernels)

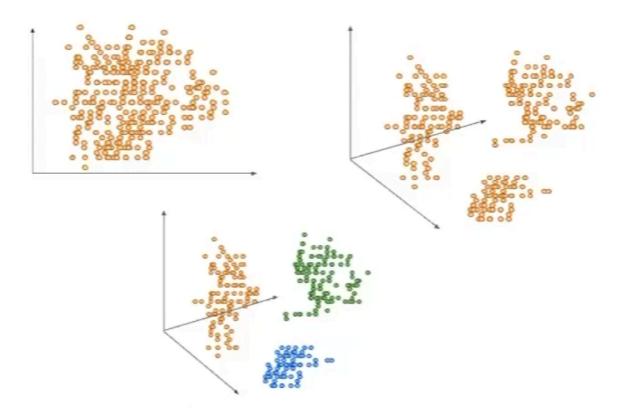
Summary

- We use PCA to deal with high-dimensional datasets; some pros are:
 - Better visualization of the data
 - Reduction of the effects of the curse of dimensionality
 - Reduction of file size
- PCA compresses the datasets into a lower-dimensional state by projecting observations onto a new space
- · More variation, more information, easier to distinguish between observations
- When we use PCA we lose data interpretability

2. Clustering (Intro Through K-Means)

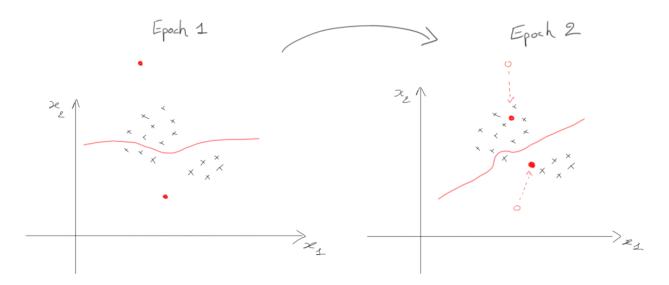
The process of organizing data points into groups whose members are similar in some way

Find categories (classes, segments) of unlabelled data rather than just trying to reduce dimensionality



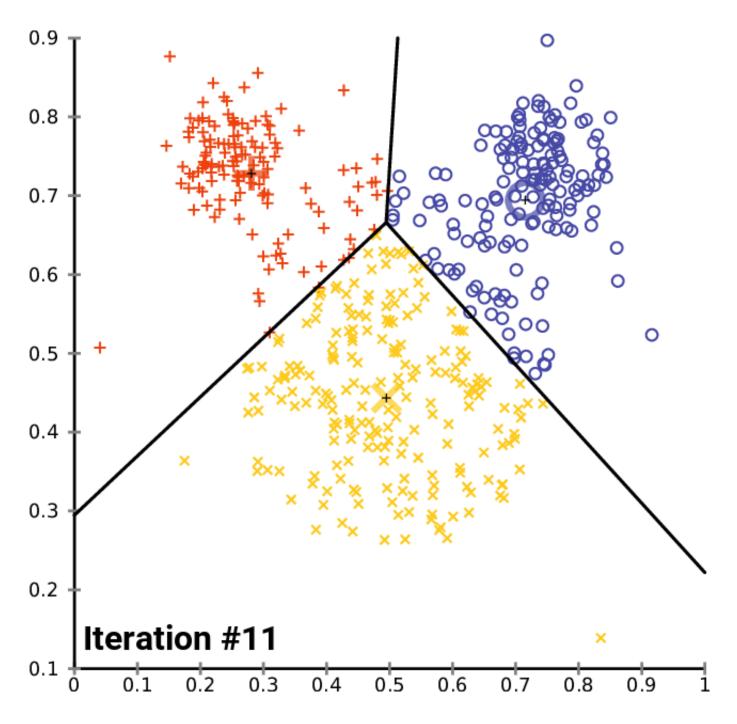
- Works better on data that is already clustered, geometrically speaking
- Use PCA for dimensionality reduction beforehand Euclidean distances work better in lower dimensions)!

2.1 K-Means Explained



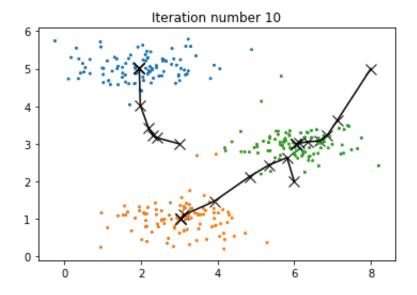
- 1. Choose the number of clusters K to look for
- 2. Initialize K centroids at random
- 3. Compute the mean square distance between each data point and each centroid
- 4. Assign each data point to the closest centroid (a cluster is formed)
- 5. Compute the mean μ_j of each cluster, the result of which becomes your new centroid

One epoch is done, repeat from step 3!



In practice

- K-means is usually run a few times with different random initializations
- We can use a random mini-batch at each epoch instead of the full dataset
- The algorithm is quite fast



2.2 Implementation

In Scikit-learn

https://scikit-learn.org/stable/modules/clustering.html (https://scikit-learn.org/stable/modules/clustering.html)

Use

- scikit.clustering.KMeans
- scikit.clustering.MiniBatchKMeans same but uses batch samples instead of the whole dataset, in order to go faster



(suppose we don't know the true labels)

Pirst, let's place ourselves in the Principal Component space we had already computed

Although not mandatory, applying PCA first helps to separate data more easily!

```
In [ ]: X_proj
```

Out[]:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	
0	3.316751	-1.443463	-0.165739	-0.215631	0.693043	-0.223880	0.596427	0.065139	0.
1	2.209465	0.333393	-2.026457	-0.291358	-0.257655	-0.927120	0.053776	1.024416	-0.
2	2.516740	-1.031151	0.982819	0.724902	-0.251033	0.549276	0.424205	-0.344216	-1.
3	3.757066	-2.756372	-0.176192	0.567983	-0.311842	0.114431	-0.383337	0.643593	0.
4	1.008908	-0.869831	2.026688	-0.409766	0.298458	-0.406520	0.444074	0.416700	0.
•••									
173	-3.370524	-2.216289	-0.342570	1.058527	-0.574164	-1.108788	0.958416	-0.146097	-0.
174	-2.601956	-1.757229	0.207581	0.349496	0.255063	-0.026465	0.146894	-0.552427	-0.
175	-2.677839	-2.760899	-0.940942	0.312035	1.271355	0.273068	0.679235	0.047024	0.
176	-2.387017	-2.297347	-0.550696	-0.688285	0.813955	1.178783	0.633975	0.390829	0.
177	-3.208758	-2.768920	1.013914	0.596903	-0.895193	0.296092	0.005741	-0.292914	0.

178 rows × 13 columns

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

# Fit K-means
km = KMeans(n_clusters=3)
km.fit(X_proj)

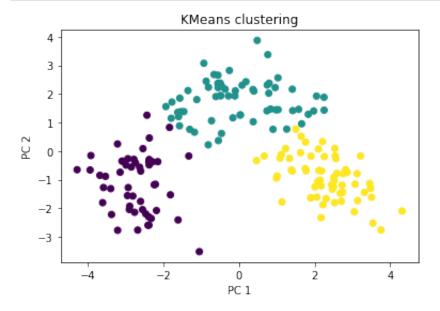
Out[ ]: KMeans(n_clusters=3)
```

```
In [ ]: # The 3 centroids' coordinates (expressed in the space of PCs)
km.cluster_centers_.shape
```

Out[]: (3, 13)

```
In [ ]:
    # The 177 observations are classified automatically
    km.labels
2, 2,
       2, 2,
       1, 1,
       1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1,
    1, 1,
       1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
    1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1,
    0, 0,
       0, 0,
       0, 0,
       0, 0], dtype=int32)
```

In []: plt.scatter(X_proj.iloc[:,0], X_proj.iloc[:,1], c=km.labels_)
 plt.title('KMeans clustering'); plt.xlabel('PC 1'); plt.ylabel('PC 2');



P In our case, we know the true labels; let's measure performance

```
In [ ]:
        # Visualization
         plt.figure(figsize=(13,5))
         plt.subplot(1,2,1)
         plt.scatter(X_proj.iloc[:,0], X_proj.iloc[:,1], c=km.labels_)
         plt.title('KMeans clustering'); plt.xlabel('PC 1'); plt.ylabel('PC 2')
         plt.subplot(1,2,2)
         plt.scatter(X_proj.iloc[:,0], X_proj.iloc[:,1], c=y)
         plt.title('True wine labels'); plt.xlabel('PC 1'); plt.ylabel('PC 2');
                                                               True wine labels
                        KMeans clustering
            3
            2
                                                   2
            1
                                                  1
           0
                                                  0
           -1
                                                  -1
           -3
                                                  -3
                                                                    Ó
                            PC 1
                                                                   PC 1
In [ ]:
        # Accuracy
```

```
In [ ]: # Accuracy
    from sklearn.metrics import accuracy_score

y_pred = pd.Series(km.labels_).map({0:0, 1:2, 2:1}) # WARNING: change
    this manually!
    accuracy_score(y_pred, y)
```

Out[]: 0.9662921348314607

Predict?

We can use the unsupervised K-means algorithm to **predict** (classify) a new X

```
In [ ]: # Build DF with column names from X_proj and some random data
    new_X = pd.DataFrame(data = np.random.random((1,13)), columns = X_pro
    j.columns)
    km.predict(new_X)
```

Out[]: array([1], dtype=int32)

2.3 K-Means' Loss Function?

km.fit(X) finds parameters β

that minimize a loss

- Each eta_j parameter is the **centroid** μ_j of its respective cluster C_i
- The loss function is called **inertia** $L(\mu)$
- = sum of squared distance between each observation and their closest centroid
- sum of within-cluster sum of squares (WCSS)
- = variance

$$ext{inertia} = L(\mu) = \sum_{j=1}^K \sum_{x_i \in C_j} (|$$

Choosing Hyperparameter K

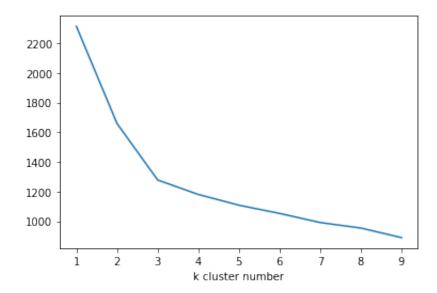
- Choose K such that the inertia (Kmeans().inertia_) is minimized
- Use the elbow method here as well

```
In [ ]: inertias = []
    ks = range(1,10)

for k in ks:
        km_test = KMeans(n_clusters=k).fit(X)
        inertias.append(km_test.inertia_)

plt.plot(ks, inertias)
    plt.xlabel('k cluster number')
```

Out[]: Text(0.5, 0, 'k cluster number')



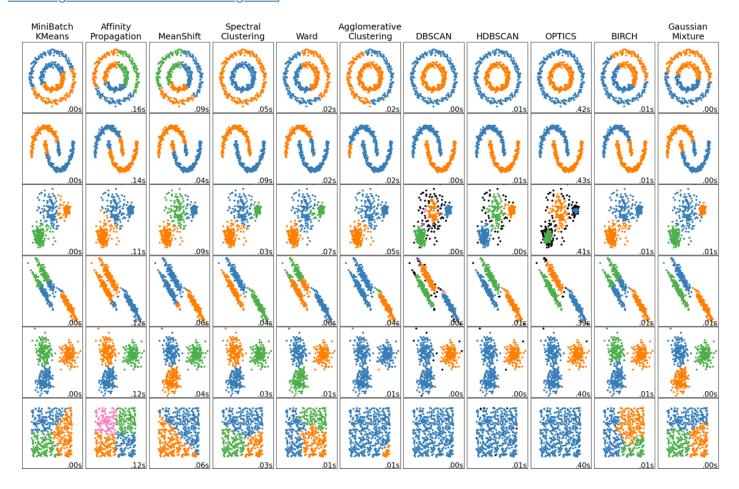
What can we use it for?

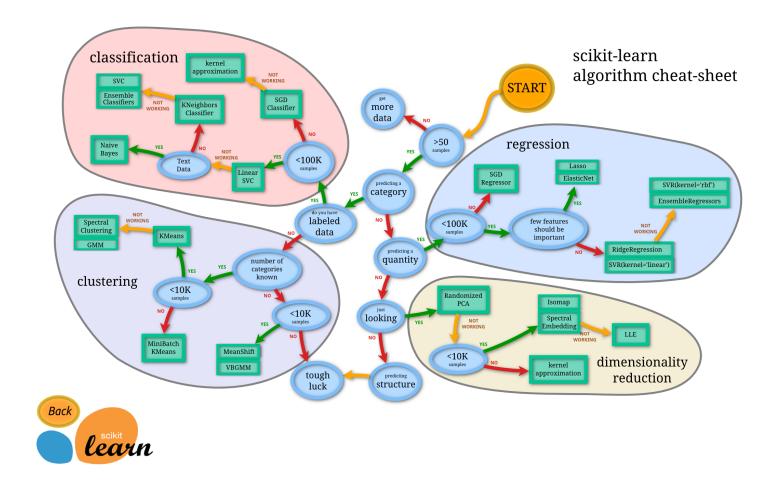
- Document classification (finding unlabeled categories or topics)
- Delivery store optimization (find the optimal number of launch locations)
- Customer segmentation (classify different types of customer based on their behavior)

https://dzone.com/articles/10-interesting-use-cases-for-the-k-means-algorithm (https://dzone.com/articles/10-interesting-use-cases-for-the-k-means-algorithm)

2.4 There are many other clustering approaches

https://scikit-learn.org/stable/modules/clustering.html (https://scikit-learn.org/stable/modules/clustering.html)





Bibliography

- PCA explained to your grandmother (https://stats.stackexchange.com/questions/2691/making-senseof-principal-component-analysis-eigenvectors-eigenvalues) 1700 upvotes on StackExchange
- PCA for ML (https://towardsdatascience.com/using-principal-component-analysis-pca-for-machine-learning-b6e803f5bf1e)
- <u>KMeans explained (https://towardsdatascience.com/k-means-clustering-explain-it-to-me-like-im-10-e0badf10734a)</u>

