Unsupervised Learning

- Question: Which of the follow are unsupervised learning methods? (choose all that apply)
  - A. Principal components analysis
  - B. Causal Discovery
  - C. T-tests
  - D. GLMs
  - E. K-means

- All of the previous lectures have been on *supervised learning*
  - Supervised learning is the class of data method for mapping inputs to outputs, like prediction or inference
  - Supervised learning data: $(X_1, Y_1), \ldots, (X_n, Y_n)$
  - Goal: Minimize some loss function: $L(f(X), Y)$
  - Typically, we think of X and Y as a joint distribution, $P(X, Y) = P(Y|X)P(X)$
  - In supervised learning, we are more interested $P(Y|X)$ (or $E(Y|X)$) than $P(X)$

- *Unsupervised learning* is a class of data methods for unlabeled data
  - Here, we are interested in learning properties of $P(X)$ without using labels, Y
  - examples: clustering, anomaly detection, latent variable analysis

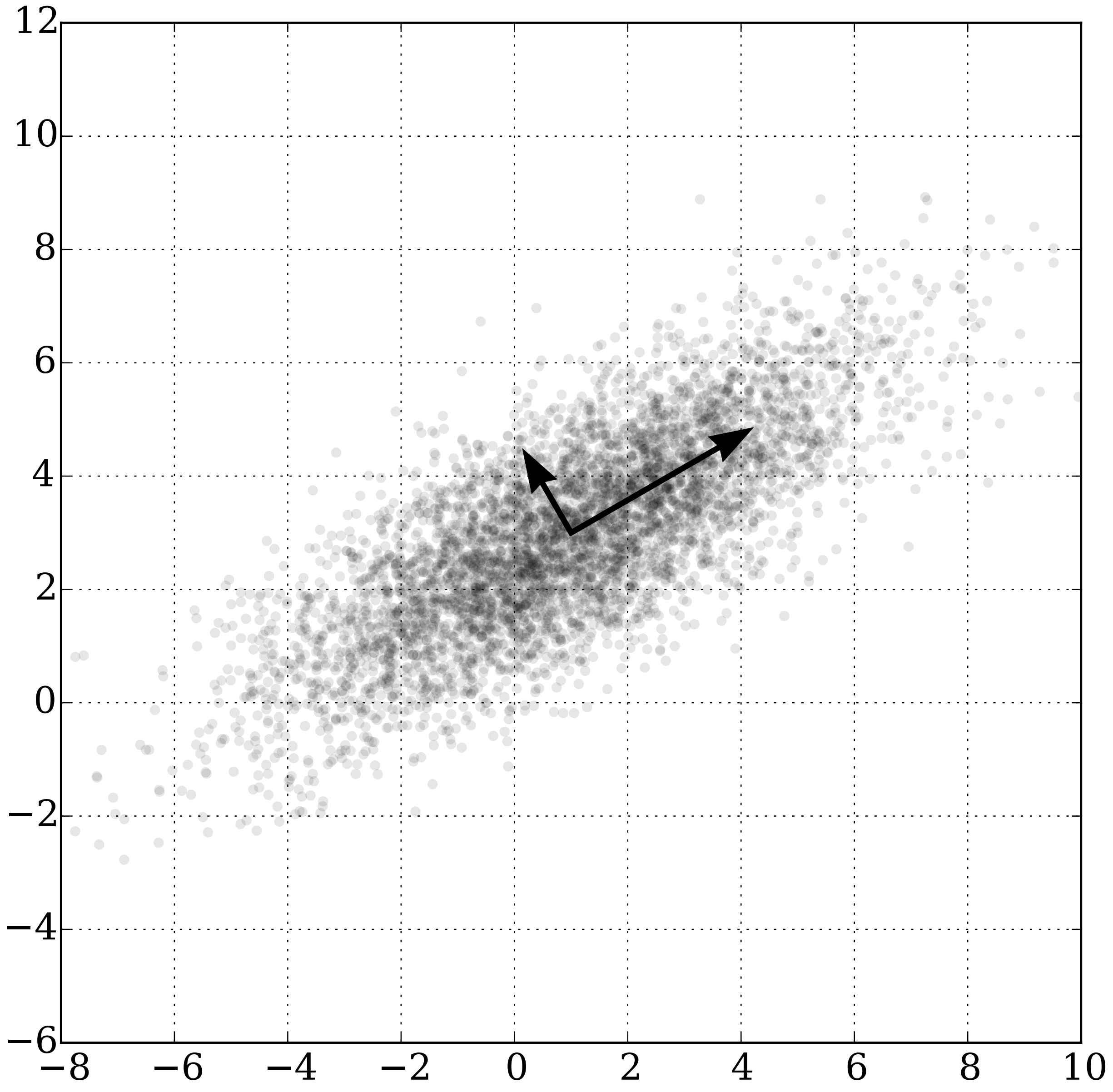
Dimensionality Reduction

- Methods for reducing the number of variables in a dataset

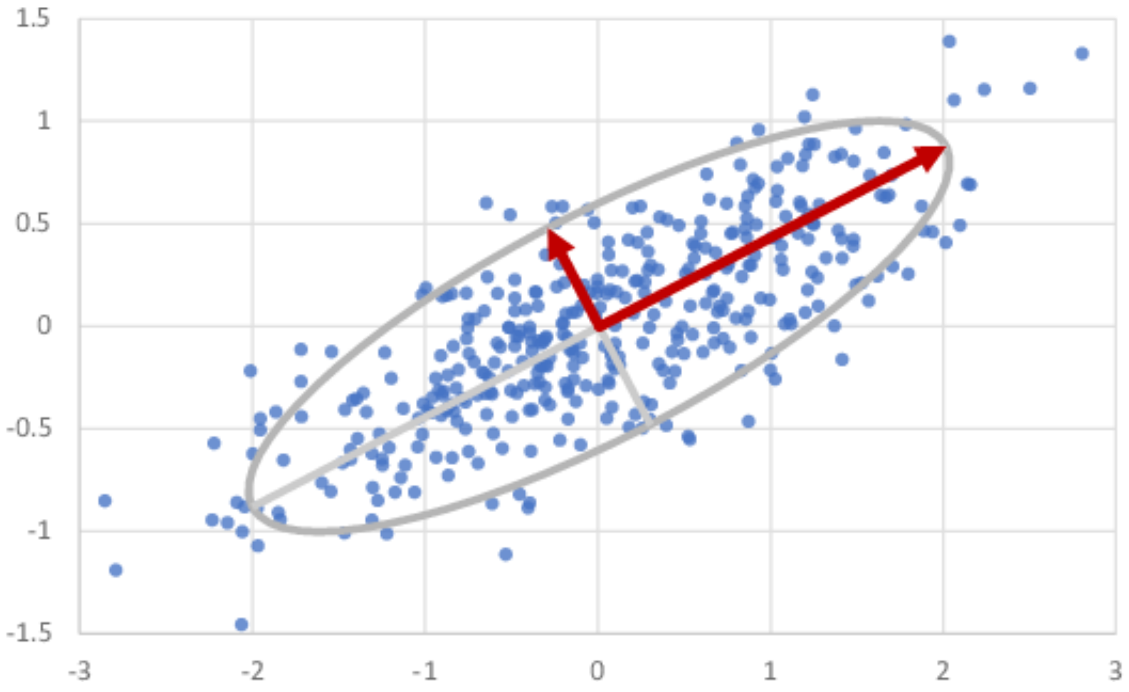
Principle Components Analysis (PCA)

- Question: Have you ever used PCA?
  - A. Yes
  - B. No

- PCA tries to explain variance in the data using linear combinations of the variables



- [Developed in 1901 by Pearson (https://en.wikipedia.org/wiki/Principal_component_analysis)](https://en.wikipedia.org/wiki/Principal_component_analysis)



- PCA can be thought of as fitting a p-dimensional ellipsoid to the data, where each axis of the ellipsoid represents a principal component

- If some axis of the ellipsoid is small, then the variance along that axis is also small

- Assume X is an $n \times p$ *standardized* data matrix
  - standardized data: for each column, X_j of X, replace with $\frac{X_j - \bar{X}_j}{\widehat{\text{var}(X_j)}}$

- First principal component: find unit-vector (direction), w, that best fits the data
  - find the directions within the data with the greatest variance

- Optimization:

$$w^* = \arg \max_{\|w\|=1} \widehat{\text{var}}(Xw) = \arg \max_{\|w\|=1} \|Xw\| = \arg \max_{w} \frac{w^T X^T X w}{w^T w}$$

where $\|w\| = \sqrt{\sum_i w_i^2}$ is the Euclidean norm

- Recall that $X^T X$ is the empirical covariance matrix

- Eigenvectors of $X^T X$ solve the problem
  - Lagrangian:
  $$\mathcal{L}(w, \lambda) = w^T X^T X w - \lambda w^T w$$
  - Gradient with respect to w:
  $$\nabla_w \mathcal{L} = 2X^T X w - 2\lambda w = 0$$
  - Then $X^T X w = \lambda w$, so principal components are eigenvectors of $X^T X$
  - The first principal component has largest corresponding eigenvalue, λ
  - The second principal component has second largest, etc

- Notice that there will be p total principal components
  - it is common to use the first k principal components with the that explain the majority of the variance, above some pre-set cutoff

- If $w_1, w_2, \ldots, w_k$ are the first $k < p$ components, we can regress an outcome on $Xw_1, \ldots, Xw_k$ in place of X

- All principal component vectors, $w_1, \ldots, w_p$ are mutually orthogonal (zero dot product or forming right angles)

- PCA is an old method that is still sometimes used but it has inspired many other methods

Iris Data

- 150 rows, 4 features

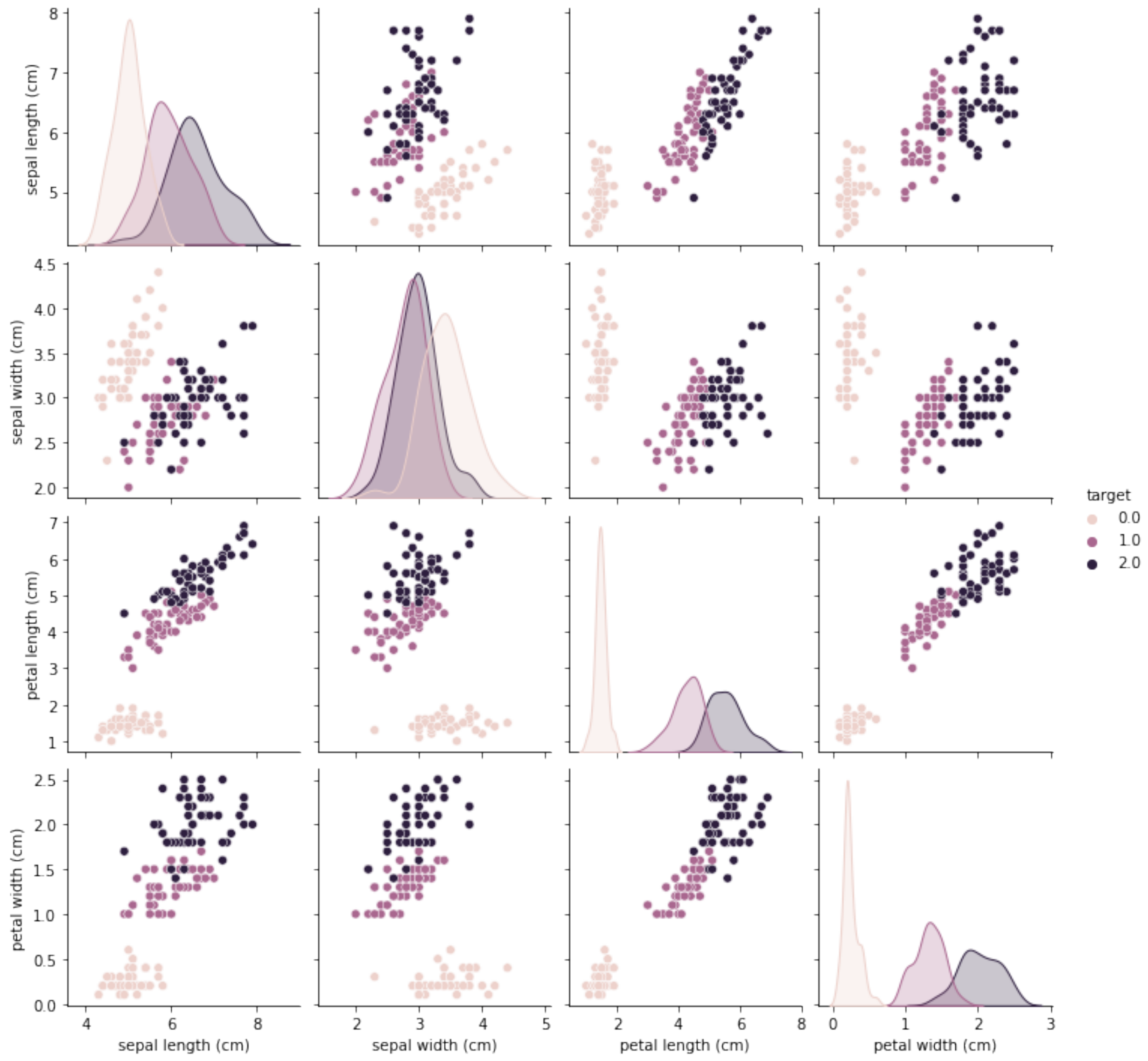
- Label (target): 0,1,2 (flower type)

- We only label for color coding but won't use in analysis

- Below is are scatter and density plots

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
from sklearn.decomposition import PCA

from sklearn.datasets import load_iris
iris = load_iris()
label_data = pd.DataFrame(
    data= np.c_[iris['data'], iris['target']],
    columns= iris['feature_names'] + ['target'])
data = iris['data']

print(f'number of rows, number of columns: {data.shape}')

sns.pairplot(label_data, hue="target");
```

```
number of rows, number of columns: (150, 4)
```



Below: Using PCA to explain variance in data with `sklearn`

In [2]:
```
pca = PCA()
pca.fit(data)
print(f'Variance explained in each component: \
{pca.explained_variance_ratio_}')
print(f'lambda values: {pca.singular_values_}')
print(f'All components: {pca.components_}')
```

```
Variance explained in each component: [0.92461872 0.05306648 0.01710
261 0.00521218]
lambda values: [25.09996044  6.01314738  3.41368064  1.88452351]
All components: [[ 0.36138659 -0.08452251  0.85667061  0.3582892 ]
 [ 0.65658877  0.73016143 -0.17337266 -0.07548102]
 [-0.58202985  0.59791083  0.07623608  0.54583143]
 [-0.31548719  0.3197231   0.47983899 -0.75365743]]
```

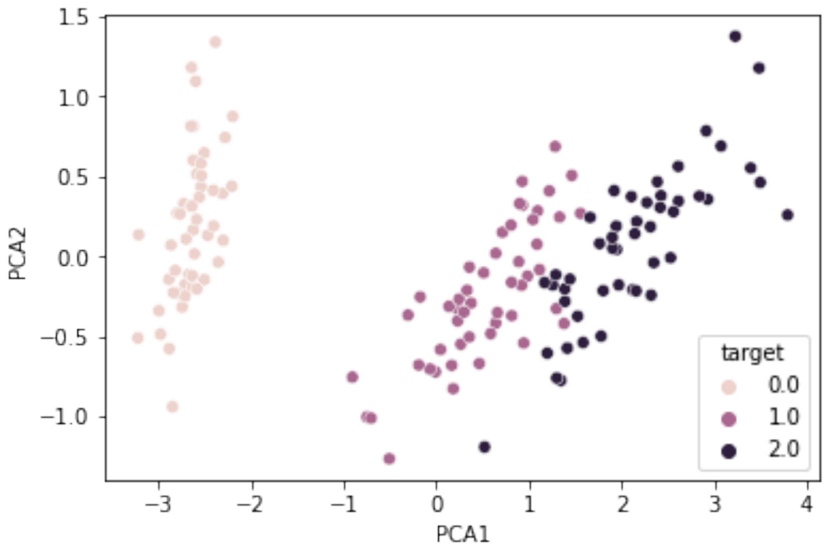
- Choosing the top two components
- Jointly they explain ~98% of the variance in features

In [3]:
```
pca = PCA(n_components=2)
pca.fit(data)
pca_iris = pca.fit_transform(data)
pca_iris[0:5,]
```

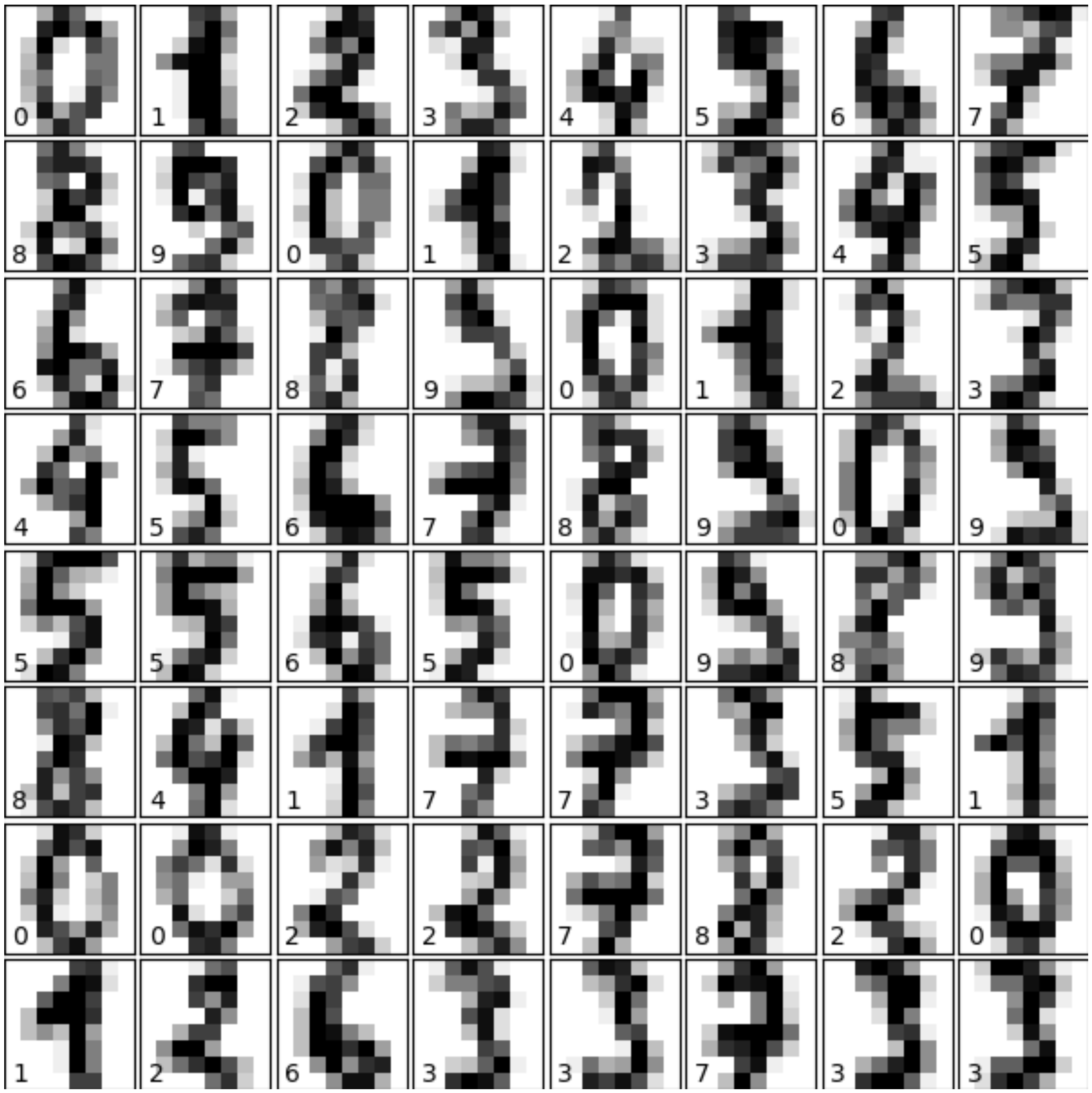
Out[3]:
```
array([[-2.68412563,  0.31939725],
       [-2.71414169, -0.17700123],
       [-2.88899057, -0.14494943],
       [-2.74534286, -0.31829898],
       [-2.72871654,  0.32675451]])
```

Below: Labeled scatter plot of first two principal components

In [4]:
```
pca_label = pd.DataFrame(
    data= np.c_[pca_iris, iris['target']],
    columns= ['PCA1', 'PCA2'] + ['target'])
sns.scatterplot(data=pca_label, x='PCA1', y='PCA2', hue='target');
```



[**Handwritten Digit Data** (https://archive.ics.uci.edu/ml/datasets/Pen-Based+Recognition+of+Handwritten+Digits)](https://archive.ics.uci.edu/ml/datasets/Pen-Based+Recognition+of+Handwritten+Digits)



- 250 samples from 44 writers (according to UCI data repo)
- 1797 8x8 images transformed into feature vectors of length 64
- There is variation in writing style, thickness, and orientation

In [5]:
```
from sklearn.datasets import load_digits
X, y = load_digits(return_X_y=True)
print(f'Dimensions of X: {X.shape}')
print(f'Dimensions of y: {y.shape}')
print('Looking at top left corner of data:')
X[0:5,0:10]
```

```
Dimensions of X: (1797, 64)
Dimensions of y: (1797,)
Looking at top left corner of data:
```

Out[5]:
```
array([[ 0.,  0.,  5., 13.,  9.,  1.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0., 12., 13.,  5.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  4., 15., 12.,  0.,  0.,  0.,  0.],
       [ 0.,  0.,  7., 15., 13.,  1.,  0.,  0.,  0.,  8.],
       [ 0.,  0.,  0.,  1., 11.,  0.,  0.,  0.,  0.,  0.]])
```

In [6]:
```
pca = PCA()
pca.fit(X)
print(f'Variance explained in first 10 components:\n\
{np.round(pca.explained_variance_ratio_[0:10], 4)}')
print(f'Variances of first 10: \n\
{np.round(pca.singular_values_[0:10], 2)}')
```

```
Variance explained in first 10 components:
[0.1489 0.1362 0.1179 0.0841 0.0578 0.0492 0.0432 0.0366 0.0335 0.03
08]
Variances of first 10:
[567.01 542.25 504.63 426.12 353.34 325.82 305.26 281.16 269.07 257.
82]
```

- How well do the first 10 principal components predict the digit compared to the entire data?
- Below we'll use random forest on the full data and on the PCA transformed data
- Rather than using cross (or held out) validation, we will use out of bag sample accuracy

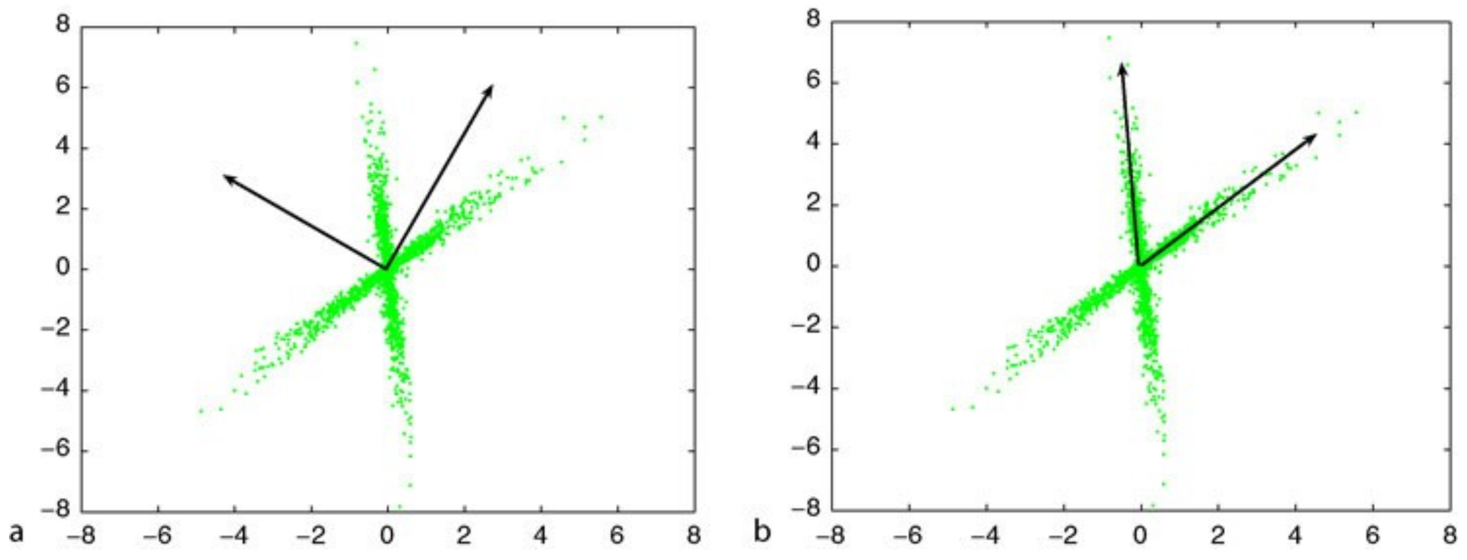
In [7]:
```
pca10 = PCA(n_components=10)
pca10.fit(X)
X_pca10 = pca.fit_transform(X)

from sklearn.ensemble import RandomForestClassifier
rf_full = RandomForestClassifier(max_depth=2, random_state=0,
                                 oob_score=True)
rf_full.fit(X, y)
print(f'Out of bag accuracy for full data: {rf_full.oob_score_}')

rf_pca = RandomForestClassifier(max_depth=2, random_state=0,
                               oob_score=True)
rf_pca.fit(X_pca10, y)
print(f'Out of bag accuracy PCA transformed data: \
{rf_pca.oob_score_}')
```

```
Out of bag accuracy for full data: 0.7835281023928771
Out of bag accuracy PCA transformed data: 0.7857540345019477
```

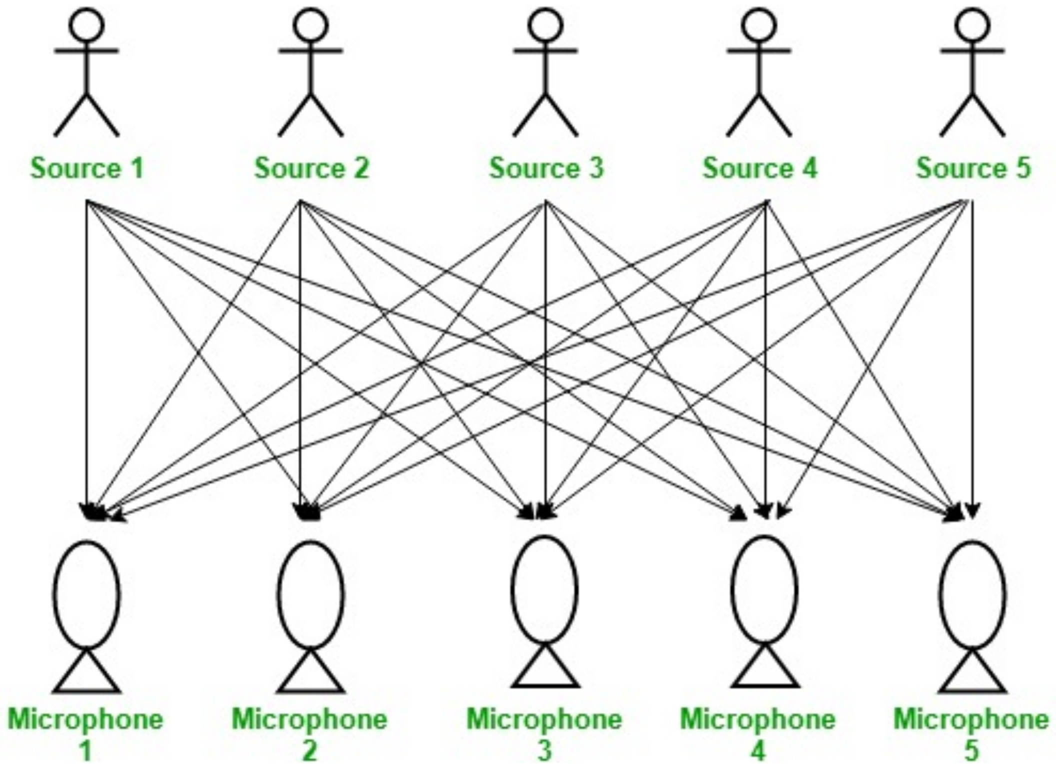
Independent Componenets Analysis (ICA)

- Question: Have you heard of ICA before?
  - A. Yes
  - B. No

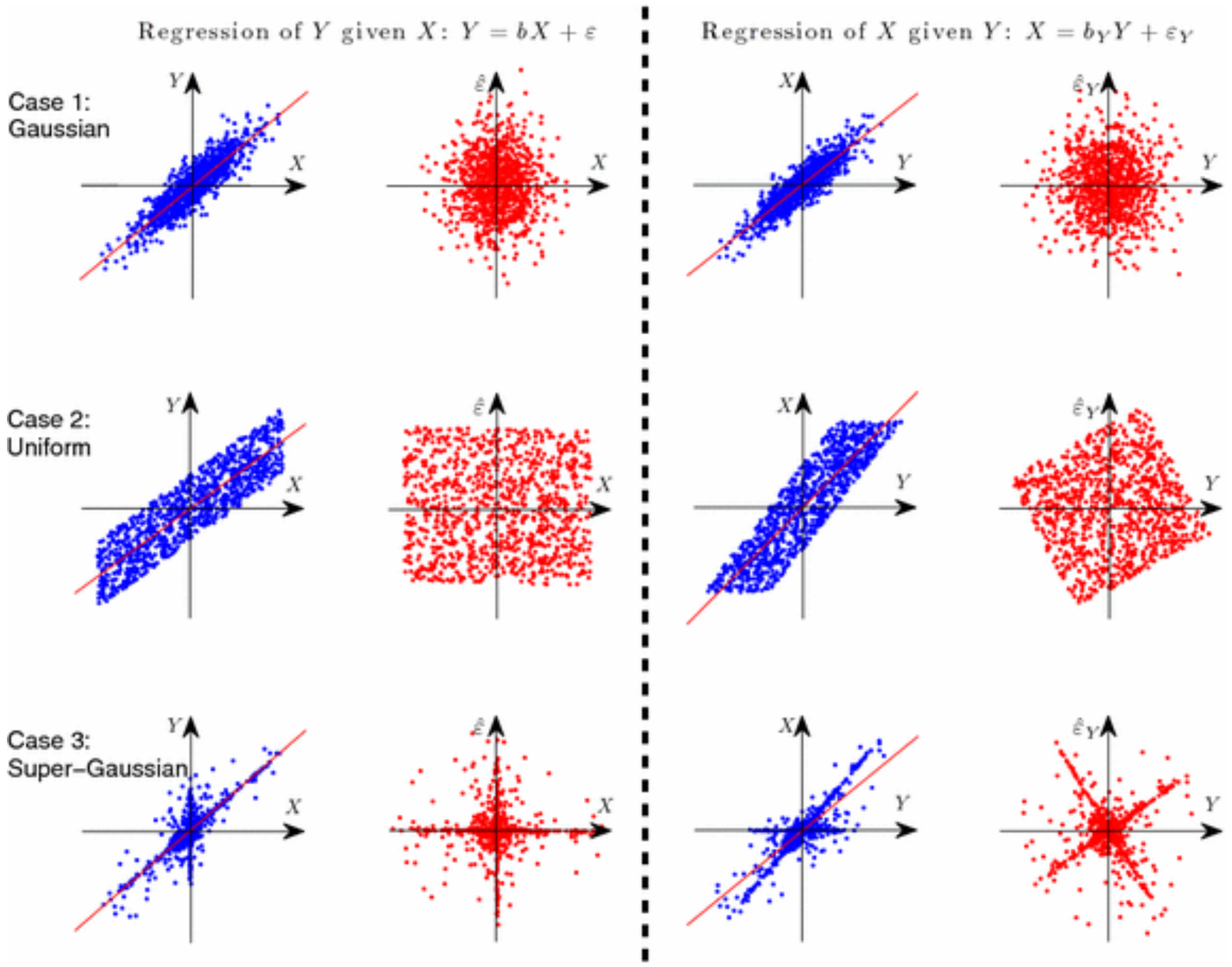
- What if the sources of noise in the data are not orthogonal?
- Image below: left panel is PCA; right panel is ICA



- ICA attempts to factor a random matrix $X = AS$ where X is the $n \times p$ data matrix
- S is an $n \times p$ matrix called the latent source matrix
- A is a $p \times p$ matrix called the mixing matrix
- Goal: Estimate A so that the columns of S are *mutually independent*
- Interestingly, this is only possible for non-Gaussian distributions
- Cocktail Party Example: Assume that there are p mircophones placed around a room with p people speaking at the same time
  - Goal: Use signal from each mircophone to distinguish each speaker



- Without loss of generality, we can assume that $E(S) = 0$ and $\text{Cov}(S) = I_p$ (this covariance assume uncorrelated, not independent!)
- Then
$$\text{Cov}(X) = \text{Cov}(AS) = AA^T$$
- If R is any orthogonal $p \times p$ matrix ($R^{-1} = R^T$), then
$$X = AS = AR^T RS = (AR^T)(RS)$$
- And, $\text{Cov}(RS) = RI_pR^T = I_p$, because correlation is not unique under rotations
- For Gaussian distribution, it is perfectly characterized by its first and second moments
  - For Gaussian distributions uncorrelated implied independent, which is why we assume non-Gaussian
- ICA uses third and higher moments to estimate A
  - In fact, it attempts to maximize divergence from Gaussianity
- ICA can be used for *causal discovery*
  - Causal discovery methods estimate a causal Bayesian network from data
  - Assume $X \to Y$ as $Y = bX + \epsilon$ where X and ϵ are independent random variables, and $E[\epsilon] = 0$ (zero-mean noise)
  - We only observe X and Y in the data but X and ϵ are the independent components
  - If X and ϵ are non-Gaussian, we can use ICA to determine causal ordering



Optimization

- There is a [lot of literature (https://www.wiley.com/en-us/Independent+Component+Analysis-p-9780471405405)](https://www.wiley.com/en-us/Independent+Component+Analysis-p-9780471405405) on ways to optimize ICA

- Using entropy and mutual information:
  - Recall entropy $H(Y) = -\int p(y) \log p(y) dy$ where $Y \sim p$
  - If $Y = (Y_1, \dots, Y_p)$, then the multivariate mutual information between all variables is
$$I(Y) = \sum_{j=1}^{p} H(Y_j) - H(Y)$$
  - Recall that if $I(Y) = 0$ then all Y_j are mutually independent
  - If $\mathrm{Cov}(X) = I_p$ and W is a $p \times p$ orthogonal matrix, we can minimize
$$W^* = \arg\min_W I(WX) = \arg\min_W \sum_{j=1}^{p} H(w_j^T X) - H(X)$$
where w_j is the jth row of W
  - Then use $A^* = (W^*)^{-1}$
  - Unfortunately, estimating entropy can be challenging and sometimes computationally expensive

- FastICA:

- Interestingly, minimizing $I(WX)$ is equivalent to maximizing the departure of each $w_j^T X$ from Gaussianity
- *Negentropy* $J(Y_j) = H(Y_j) - H(Z_j)$ where Z_j is a Gaussian random variable with the same variance as Y_j (measure departure from Gaussianity)
- FastICA approximates negentropy with
$$J(w_j^T) \approx \left(E[G(w_j^T X)] - E[G(w_j^T Z)]\right)$$
where $G(y) = \frac{1}{a} \log \cosh y$ for $a \in (1, 2)$

ICA notes based on these slides (http://statweb.stanford.edu/~tibs/sta306bfiles/ica.pdf)

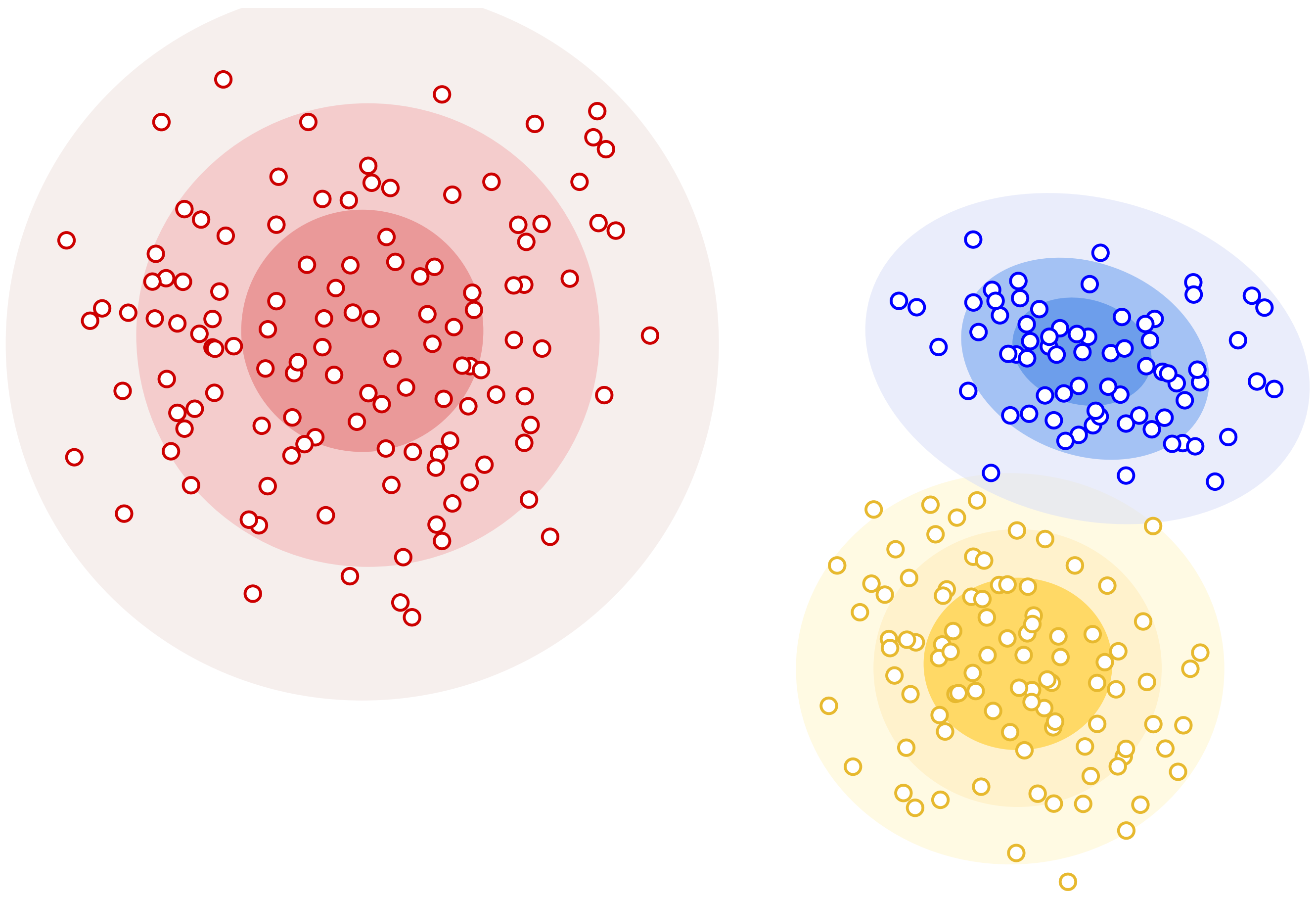
- The code below uses `FastICA` to transform the the data
- Again, we use random forest to see how well the transformed data predicts the label
- Note: it can be difficult to optimize ICA

In [8]:
```
from sklearn.decomposition import FastICA
transformer10 = FastICA(n_components=10, random_state=0)
X_ica10 = transformer10.fit_transform(X)

rf_ica = RandomForestClassifier(max_depth=2, random_state=0,
                                oob_score=True)
rf_ica.fit(X_ica10, y)
print(f'Out of bag accuracy for ICA transformed data: \
{rf_full.oob_score_}')
```

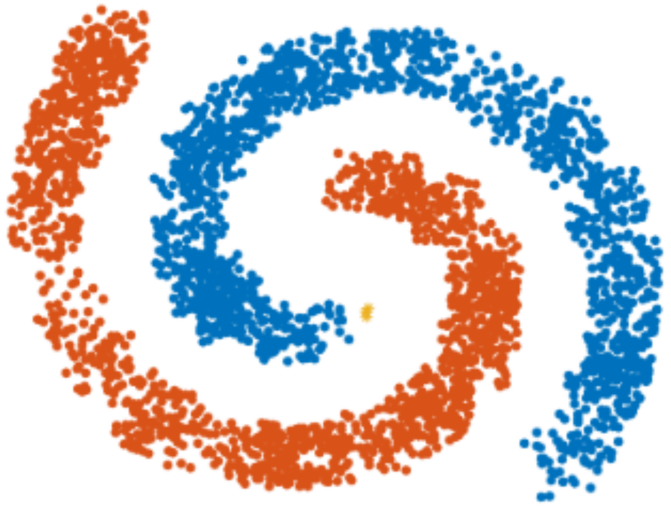
```
Out of bag accuracy for ICA transformed data: 0.7835281023928771
```

Cluster Analysis (clustering)

- Clustering attempts to group together observations that are close to each other
- This can take different forms
- It might be that data points are grouped around central points



- In other cases, groups are formed by proximity to other points in the group, like a chain



K-*means*

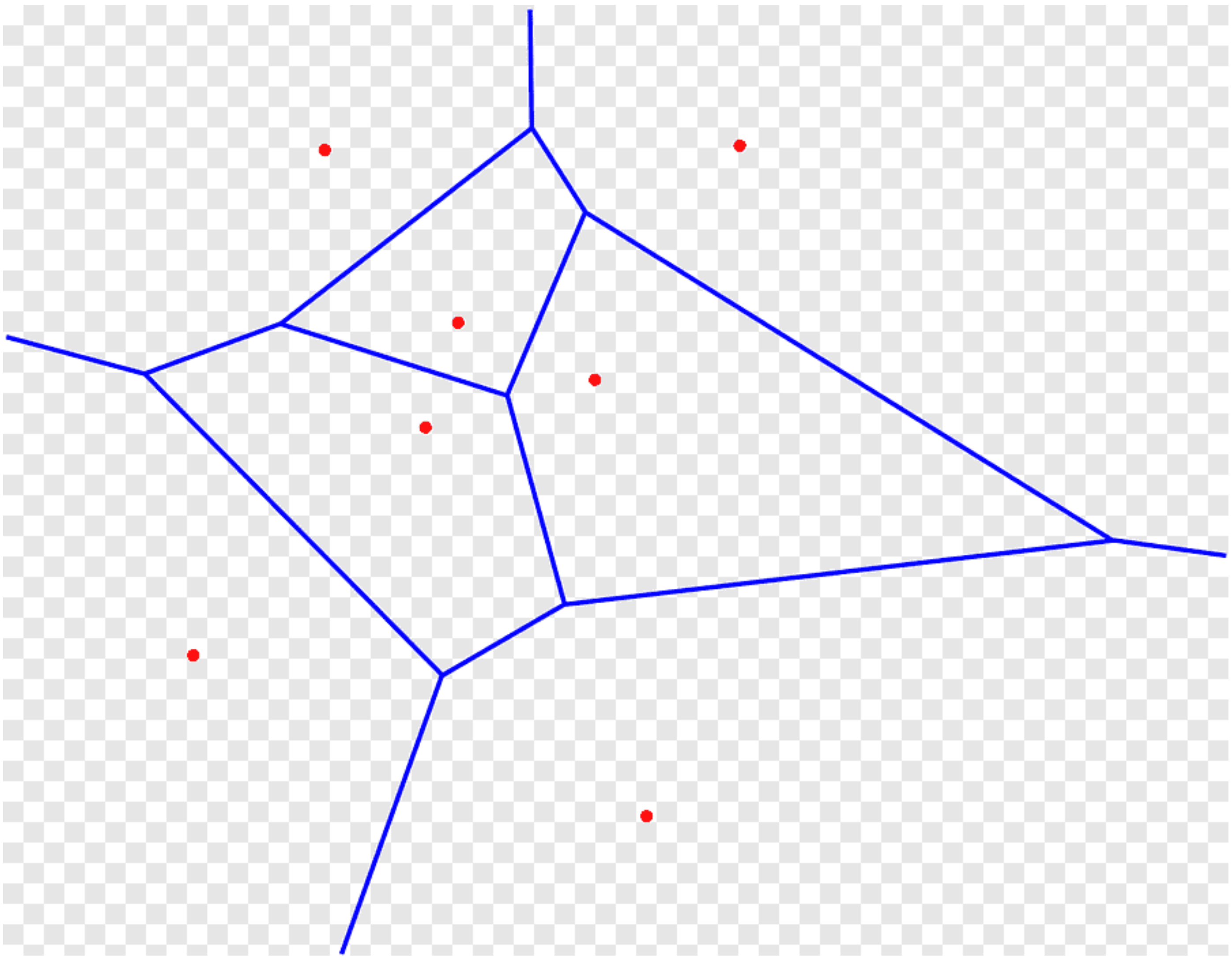
- Goal: group points using proximity to K unknown cluster centers
- This approach would work better for data in the top image, but not the bottom image
- Assume $X_1, \dots, X_n$ is a sample where $X_i \in \mathbb{R}^d$ for $i = 1, \dots, n$
- Let $C = \{c_1, \dots, c_K\}, c_k \in \mathbb{R}^d$, be variable point that we will use to find cluster centers

- [Lloyd's algorithm (https://en.wikipedia.org/wiki/Lloyd%27s_algorithm)](https://en.wikipedia.org/wiki/Lloyd%27s_algorithm) has two steps:

  1. Assign a cluster: for each point, $i = 1, \ldots, n$, find the closest $c_k \in C$,
  $$z_i = \arg \min_{1 \le k \le K} \|X_i - c_k\|$$
  2. Recenter cluster: update each c_k with the new group,
  $$c_k \leftarrow \frac{1}{n_k} \sum_{i:z_i=k} X_i$$
  $n_k = \#\{i : z_i = k\}$
  - We can initialize this algorithm with K random points in $\mathbb{R}^d$
  - These two steps are repeated until C, the cluster center points, converge (until they stop moving between steps)

- Optimization:
$$\frac{1}{n} \sum_{i=1}^{n} \min_{1 \le k \le K} \|X_i - c_{z_i}\|^2$$

- Once the cluster centers are set, they create a *Voronoi Tessellation*:

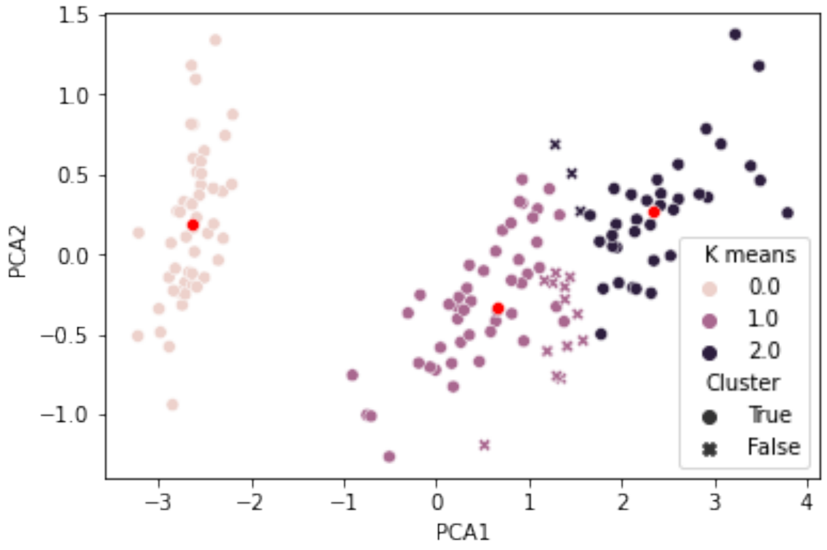


- Below: we run this algorithm on Iris PCA-transformed data

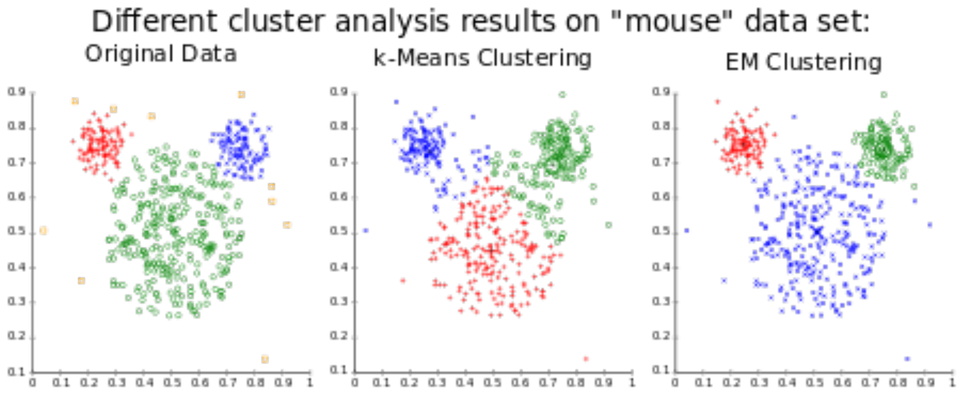
In [9]:
```
from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=3, random_state=0).fit(pca_iris)

# switching labels to match
def switch_1_2(x):
    if x==0.0:
        return 0.0
    if x==1.0:
        return 2.0
    if x==2.0:
        return 1.0
kmeans_labs = np.vectorize(switch_1_2)(kmeans.labels_)

pca_label = pd.DataFrame(
    data= np.c_[pca_iris, iris['target'], kmeans_labs],
    columns= ['PCA1', 'PCA2', 'True Label', 'K means'])
def class_error(row):
    return row['True Label'] == row['K means']
pca_label['Cluster'] = pca_label.apply(class_error, axis=1)

sns.scatterplot(data=pca_label, x='PCA1', y='PCA2', hue='K means',
               style='Cluster', style_order=[True,False]);
centers = pd.DataFrame(
    kmeans.cluster_centers_, columns=['PCA1', 'PCA2'])
sns.scatterplot(data=centers, x='PCA1', y='PCA2', color='red');
print(f'Number of misclassifications:')
pca_label.Cluster.value_counts()
```

```
Number of misclassifications:
```

Out[9]:
```
True     133
False     17
Name: Cluster, dtype: int64
```

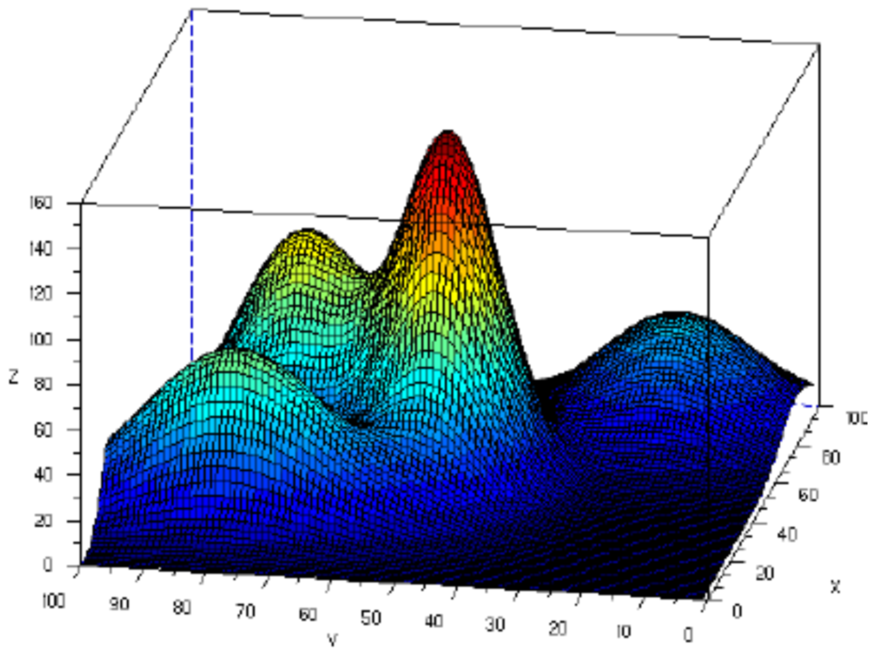


- Above: Showing K means groups with error as 'x' point markers
- The red points show the cluster centers
- This model does not account for different sized cluster



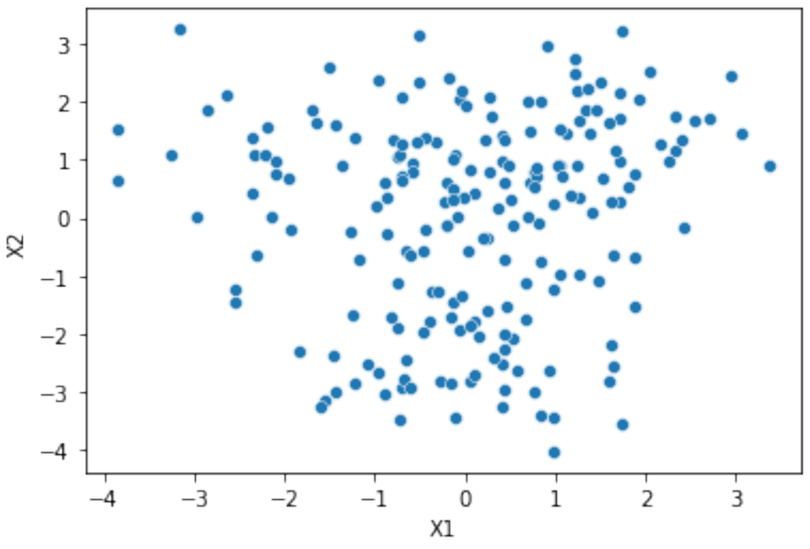
Gaussian Mixture Model and EM Clustering

- Another way to think about clustering is with a *Gaussian* [mixture model (https://en.wikipedia.org/wiki/Mixture_model)](https://en.wikipedia.org/wiki/Mixture_model) (GMM)



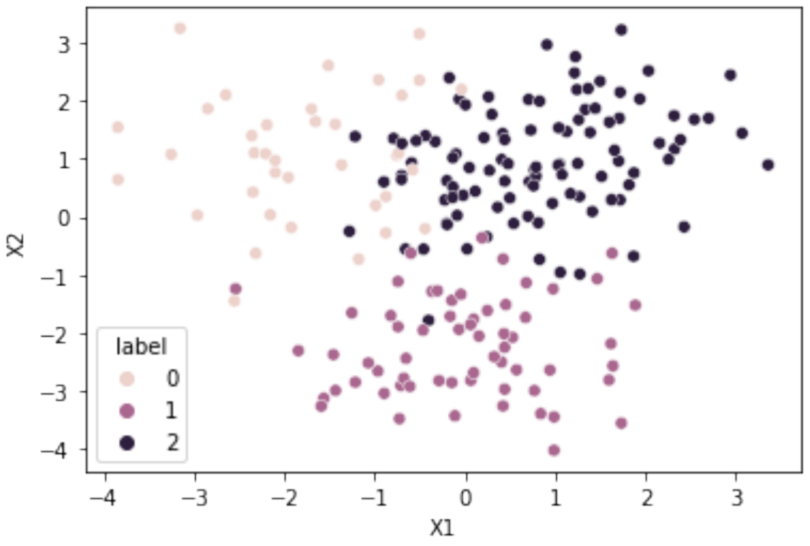
- Assume that our data points are each generated from different Gaussian distributions
- All we see is the location, not the *latent* variable which determines which distribution each sample was generated from
- $x_1, \dots, x_n$ is a random sample
- Each x_i is associated with a latent random variable, z_i, that indicates the cluster/distribution of x_i
- Density of z is multinomial with probabilities, $\pi_1, \dots, \pi_K$
- Let (μ_k, Σ_k) for $j = 1, \dots, K$ be the mean vector and covariance matrix for K multivariate Gaussian distributions
- In a Gaussian mixture model, each data point is generated from one of the K multivariate Gaussian distribution,
$$x_i \sim \text{Gaussian}(\mu_k, \Sigma_k)$$
with probability π_k
- For $i = 1, \dots, n$, if $z_i = k$ then
$$x_i \sim \text{Gaussian}(\mu_k, \Sigma_k) := p(x_i | z_i = k)$$
- Joint distribution of x and z
$$p(x, z) = \prod_{k=1}^{K} \pi_k^{I(z=k)} \cdot [\text{Gaussian}(x; \mu_k; \Sigma_k)]^{I(z=k)}$$
- Marginal distribution x (summing over the values of z)
$$p(x) = \sum_{k=1}^{K} \pi_k \cdot \text{Gaussian}(x; \mu_k, \Sigma_k)$$
- Each point is generated from one of these Gaussian distributions but we won't know which

In [10]:
```python
dist_probs = [0.2, 0.3, 0.5]
data = []
samp_size = 200

for _ in range(samp_size):
    k = np.random.choice(np.arange(0, 3), p=dist_probs)
    if k==0:
        obs = np.random.multivariate_normal(
            [-2,1], [[1,0.2], [0.2,1]]).tolist()
    elif k==1:
        obs = np.random.multivariate_normal(
            [0,-2], [[1,0], [0,1]]).tolist()
    else:
        obs = np.random.multivariate_normal(
            [1,1], [[1,0.3], [0.3,1]]).tolist()
    obs.append(k)
    data.append(tuple(obs))
df = pd.DataFrame(data, columns=['X1', 'X2', 'label'])
sns.scatterplot(x='X1', y='X2', data=df);
```



Below: color by label

In [11]:
```
sns.scatterplot(x='X1', y='X2', data=df, hue='label');
```



EM Algorithm

- EM stands for Expectation Maximization
- We assume that the sample is generated from a Gaussian mixture model
- Using the Gaussian mixture likelihood, cycle between
  - Imputing the expected cluster (probability) of each point, $i = 1, \ldots, n$
  - Recalculate GMM parameters, π_k, μ_k, Σ_k for $k = 1, \ldots, K$, to maximize the likelihood
- Cosma Shalizi: "one man's vicious circle is another man's successive approximation procedure"
- Sample marginal likelihood of x:
$$L(\pi, \mu, \Sigma) = \prod_{i=1}^{n} \sum_{k=1}^{K} \pi_k \cdot \text{Gaussian}(x_i; \mu_k, \Sigma_k)$$
where $\pi = (\pi_1, \ldots, \pi_K), \mu = (\mu_1, \ldots, \mu_K), \Sigma = (\Sigma_1, \ldots, \Sigma_K)$
- **E step**: Calculate expected value of cluster assignments for each point, x_i, using the values of π, μ, Σ from last step,
$$p^{\text{new}}(z_i = k) \leftarrow E[z_i = k | \pi, \mu, \Sigma]$$
  - This expected value is really $P(z_i = k)$ (expected value of an indicator function is a probability)
  - Calculate these probabilities as
$$p^{\text{new}}(z_i = k) \leftarrow \frac{\pi_k^{\text{old}} \cdot \text{Gaussian}(x_i; \mu_k^{\text{old}}, \Sigma_k^{\text{old}})}{\sum_{j=1}^{K} \pi_k^{\text{old}} \cdot \text{Gaussian}(x_i; \mu_j^{\text{old}}, \Sigma_j^{\text{old}})}$$
  - To make the notation in the next step clearer, let
$$r_i(k) \leftarrow p^{\text{new}}(z_i = k)$$
  - For each point, we have a vector of assignment probabilities

$$[r_i(1), \ldots, r_i(K)]$$

- We can think about this vector as the *responsibility* that the GMM takes for explaining observation i

- **M step**: Calculate maximum likelihood estimates for all parameters, π, μ, Σ using the expected cluster assignments, $[r_i(1), \ldots, r_i(K)]$
  - Goal: optimize likelihood of joint distribution $p(x, z)$

$$\pi^{\text{new}}, \mu^{\text{new}}, \Sigma^{\text{new}} \leftarrow \arg\max_{\pi,\mu,\Sigma} E\left[\log\left(\prod_{i=1}^{n} p(x_i, z_i)\right)\right]$$

  - This can be hard because L is not convex with respect to π, μ, Σ
  - Conditional density of x_i given z_i:

$$p(x_i|z_i) = \prod_{k=1}^{K} [\text{Gaussian}(x_i; \mu_k, \Sigma_k)]^{I(z_i=k)}$$

  - Density of z_i:

$$p(z_i) = \prod_{k=1}^{K} \pi_k^{I(z_i=k)}$$

  - Likelihood:

$$\begin{aligned} & E\left[\log\left(\prod_{i=1}^{n} p(x_i, z_i)\right)\right] \\ &= E\left[\log\left(\prod_{i=1}^{n} p(z_i)p(x_i|z_i)\right)\right] \\ &= E\left[\log\left(\prod_{i=1}^{n}\prod_{k=1}^{K} \pi_k^{I(z_i=k)} \cdot [\text{Gaussian}(x_i; \mu_k, \Sigma_k)]^{I(z_i=k)}\right)\right] \\ &= E\left[\sum_{i=1}^{n}\sum_{k=1}^{K} I(z_i = k)\log \pi_k + I(z_i = k)\log[\text{Gaussian}(x_i; \mu_k, \Sigma_k)]\right] \\ &= \sum_{i=1}^{n}\sum_{k=1}^{K} r_i(k)\log \pi_k + r_i(k)\log[\text{Gaussian}(x_i; \mu_k, \Sigma_k)] \end{aligned}$$

  - This can be solved using Lagrange multiplier with the constraint that $\sum_{k=1}^{K} \pi_k = 1$

$$\mathcal{L} = \sum_{i=1}^{n}\sum_{k=1}^{K} r_i(k)\log \pi_k + r_i(k)\log[\text{Gaussian}(x_i; \mu_k, \Sigma_k)] - \lambda\left(\sum_{k=1}^{K} \pi_k - 1\right)$$

  - Differentiate with respect to parameters, π, μ, Σ and λ then set equal to zero
  - Solutions:

$$n_k^{\text{new}} \leftarrow \sum_{i=1}^{n} r_i(k)$$

$$\pi_k^{\text{new}} \leftarrow \frac{n_k^{\text{new}}}{n}$$

$$\mu_k^{\text{new}} \leftarrow \frac{1}{n_k^{\text{new}}} \sum_{i=1}^{n} r_i(k)x_i$$

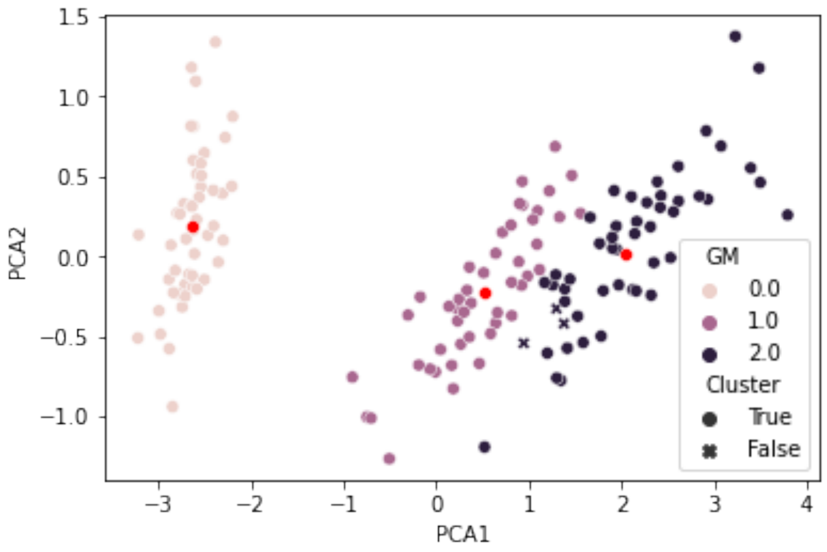
$$\Sigma_k^{\text{new}} \leftarrow \frac{1}{n_k} \sum_{i=1}^{n} r_i(k)(x_i - \mu_k^{\text{new}})(x_i - \mu_k^{\text{new}})^T$$

- The algorithm must begin initialized with parameters, π, μ, Σ
- The algorithm cycles through these steps until the parameters converge

In [12]:
```
from sklearn.mixture import GaussianMixture

# n_components here is number of clusters
gm = GaussianMixture(n_components=3, random_state=0).fit(pca_iris)

# switching cluster labels
gm_labs = np.vectorize(switch_1_2)(gm.fit_predict(pca_iris))

pca_label_gm = pd.DataFrame(
    data= np.c_[pca_iris, iris['target'], gm_labs],
    columns= ['PCA1', 'PCA2', 'True Label', 'GM'])
def class_error(row):
    return row['True Label'] == row['GM']
pca_label_gm['Cluster'] = pca_label_gm.apply(class_error, axis=1)

sns.scatterplot(data=pca_label_gm, x='PCA1', y='PCA2', hue='GM',
               style='Cluster', style_order=[True,False]);
centers = pd.DataFrame(
    gm.means_, columns=['PCA1', 'PCA2'])
sns.scatterplot(data=centers, x='PCA1', y='PCA2', color='red');
print(f'Number of misclassifications:')
pca_label_gm.Cluster.value_counts()
```

```
Number of misclassifications:
```

Out[12]:
```
True      147
False       3
Name: Cluster, dtype: int64
```


PCA2
PCA1
GM
Cluster
True
False