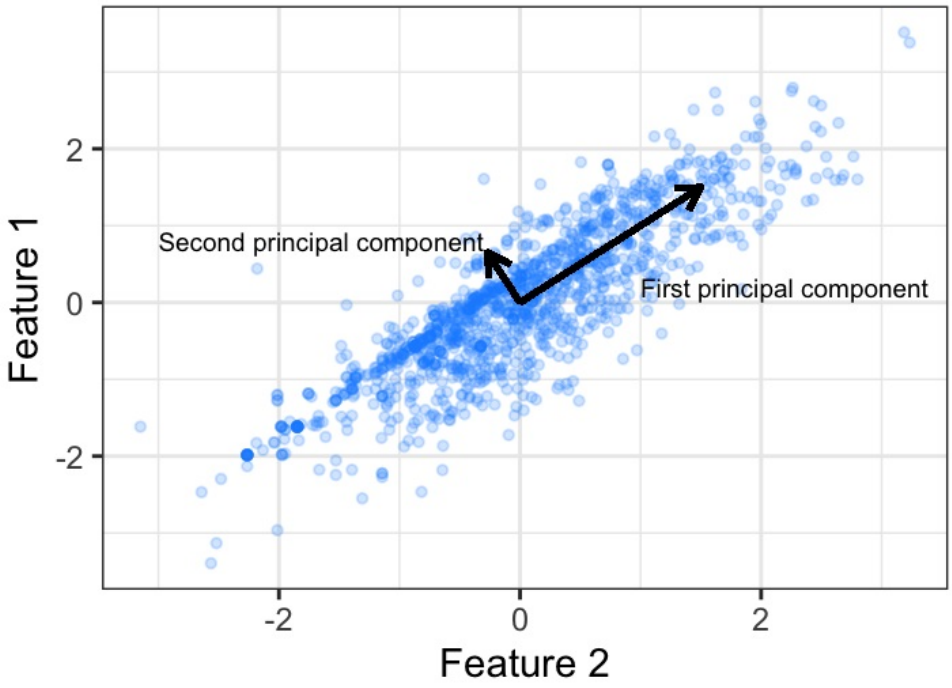
Unsupervised Learning

- x only, no y, learn $P(x)$
- Tasks
  i. **Dimensionality Reduction**: $x \in \mathbb{R}^{10000} \rightarrow x \in \mathbb{R}^{100}$
  ii. **Clustering**: group similar data together
  iii. **Generating Models**: sample new data from $P(x)$

Principal Component Analysis (PAC)



- $x^{(1)}$ and $x^{(2)}$ are highly correlated
  - Principles: find a new basis u_1 and u_2
    s.t. $u_1 \perp u_2$, u_1 keeps the most **information** (**data variance** on u_1 is the largest)
    then throw away u_2. Represent a sample x by $x^T u_1$

PCA derivation

- We have

$$X = \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} \in \mathbb{R}^{n \times d}$$

  then we can calculate the mean and the covariance matrix (it's a *real symmetric* matrix)

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \in \mathbb{R}^d$$

$$\Sigma = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})^T \in \mathbb{R}^{d \times d}$$

- Now compute $u_1 \in \mathbb{R}^d$, we need to project each x_i to u_1 and maximize variance

$$
\begin{aligned}
&\frac{1}{n}\sum_{i=1}^{n}(u_1^T x_i - u_1^T \bar{x})^2 \\
=&\frac{1}{n}\sum_{i=1}^{n} u_1^T (x_i - \bar{x})(x_i - \bar{x})^T u_1 \\
=&u_1^T \Sigma u_1 \\
\Rightarrow \quad &\max_{u_1} u_1^T \Sigma u_1 \quad \text{s.t. } u_1^T u_1 = 1
\end{aligned}
$$

We can use Lagrange function

$$
\begin{aligned}
L(u_1, \lambda_1) &= u_1^T \Sigma u_1 + \lambda_1 (1 - u_1^T u_1) \\
\frac{\partial L}{\partial u_1} &= 2\Sigma u_1 - 2\lambda_1 u_1 = 0 \\
\Rightarrow \quad &\Sigma u_1 = \lambda_1 u_1
\end{aligned}
$$

This means that u_1 is an **eigenvector** of Σ corresponding to eigenvalue λ_1

$$
u_1^T \Sigma u_1 = \lambda_1 u_1^T u_1 = \lambda_1
$$

We need to find **maximum eigenvalue** to maximize $u_1^T \Sigma u_1$

- Next, find u_2, the next direction that preserves the most variance (u_2 should be **orthogonal** to u_1)

$$
\max_{u_2} u_2^T \Sigma u_2 \quad \text{s.t. } u_2^T u_2 = 1, \;\; u_2^T u_1 = 0
$$

Again, use Lagrange function

$$
\begin{aligned}
L(u_2, \lambda_2, \alpha) &= u_2^T \Sigma u_2 + \lambda_2 (1 - u_2^T u_2) + \alpha u_2^T u_2 \\
\frac{\partial L}{\partial u_2} &= 2\Sigma u_2 - 2\lambda_2 u_2 + \alpha u_1 = 0 \\
\Rightarrow \quad &2u_1^T \Sigma u_2 - 2\lambda_2 u_1^T u_2 + \alpha u_1^T u_1 \\
=&2u_2^T \Sigma u_1 + \alpha \\
=&2\lambda_1 u_2^T u_1 + \alpha = 0 \\
\Rightarrow \quad &\alpha = 0 \\
\Rightarrow \quad &\Sigma u_2 = \lambda_2 u_2 \\
&u_2^T \Sigma u_2 = \lambda_2 u_2^T u_2 = \lambda_2
\end{aligned}
$$

This means that u_2 is the second largest **eigenvector** of Σ corresponding to eigenvalue λ_2

- By induction, when we need K principle components, just compute K **largest eigenvalues and eigenvectors**
  $U_k = (u_1, \ldots, u_k) \in \mathbb{R}^{d \times k}$, project X by $XU_k \in \mathbb{R}^{n \times k}$ (k << d)

$$
\begin{aligned}
\Sigma &= U^T \Lambda U \\
&= \begin{pmatrix} u_1 & \ldots & u_d \end{pmatrix} \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_d \end{pmatrix} \begin{pmatrix} u_1^T \\ \vdots \\ u_d^T \end{pmatrix}
\end{aligned}
$$

  - Λ is diagonal and U is orthogonal

- Another representation of Σ

$$
\hat{X} = \begin{pmatrix} x_1^T - \bar{x}^T \\ \vdots \\ x_n^T - \bar{x}^T \end{pmatrix} \in \mathbb{R}^{n \times d}
$$

then

$$
\Sigma = \frac{1}{n} \hat{X}^T \hat{X}
$$

We can directly do eigen-decomposition for $\hat{X}^T \hat{X}$, then U will be the same, λ_i only scales by a factor

- Alternatively, we can perform **Singular Value Decomposition (SVD)** for $\hat{X}^T = U \hat{\Sigma} V^T$, $U \in \mathbb{R}^{d \times d}$, $V \in \mathbb{R}^{n \times n}$, U and V are orthogonal

$$
\begin{aligned}
\hat{X}^T\hat{X} &= U\hat{\Sigma}V^TV\hat{\Sigma}^TU^T \\
&= U(\hat{\Sigma}\hat{\Sigma}^T)U^T \\
\hat{\Sigma} &= \begin{pmatrix} \sigma_1 & & & \\ & \ddots & & 0 \\ & & \sigma_d & \end{pmatrix} \\
\hat{\Sigma}\hat{\Sigma}^T &= \begin{pmatrix} \sigma_1^2 & & \\ & \ddots & \\ & & \sigma_d^2 \end{pmatrix} = \Lambda
\end{aligned}
$$

which means that $\sigma_i^2 = \lambda_i$

Clustering

- Given $D = \{x_1, \dots, x_n\} \in \mathbb{R}^d$, we want to **partition** D into K clusters
  - K is a hyperparameter
  - $\mu_k \in \mathbb{R}^d$ is the center of cluster k
  - $r_{ik} \in \{0, 1\}$ denotes that x_i is closet to μ_k
    - r_{ik} is called **assignment**
    - $\sum_{k=1}^K r_{ik} = 1 \quad \forall i$

K-means Clustering Algorithm

- Find $\{\mu_k | k = 1, \dots, K\}$ and $\{r_{ik}\}$
  s.t. the sum of squared distances of each x_i to its assigned cluster center μ_k is minimized
  Objective:

$$
\underset{r,\mu}{min} \sum_{i=1}^n \sum_{k=1}^K r_{ik} \|x_i - \mu_k\|^2
$$

- Steps: Alternately optimize μ and r
  i. Randomly initialize μ_k
  ii. Given μ fixed, r_{ik} can be updated

$$
r_{ik} = \begin{cases} 1 & \text{if } k = \underset{j=1,\dots,K}{argmin} \|x_i - \mu_j\|^2 \\ 0 & \text{otherwise} \end{cases}
$$

    - assign x_i to the closet cluster center

  iii. Given r fixed, μ can be optimized easily

$$
\begin{aligned}
\frac{\partial L}{\partial \mu_k} &= -\sum_{i=1}^n r_{ik}(x_i - \mu_k) = 0 \\
\Rightarrow \quad \mu_k &= \frac{\sum_{i=1}^n r_{ik} x_i}{\sum_{i=1}^n r_{ik}}
\end{aligned}
$$

    - calculate the mean of all x_i assigned to μ_k

  iv. iterate ii and iii until convergence
    - ii and iii both reduce the *objective* (must convergence)
- K-means only find local minimum of the *objective*
- In practice, we often run K-means **for multiple times**, each with a different initialization, finally use the one with minimum objective

Gaussian Mixture Models (GMM)

- Assume points belonging to cluster k follow a Gaussian distribution $N(\mu_k, \Sigma_k)$
- **A generating model**: $P(x) = \sum_z P(x|z)P(z)$
- For a random variable x, let $z_k \in \{0, 1\}$ be another random variable
  - $z_k = 1$ means x generated from cluster k
  - $\sum_{k=1}^K z_k = 1$

$$P(x|z_k = 1) = N(x|\mu_k, \Sigma_k)$$

$$P(z_k = 1) = \pi_k \in [0, 1], \quad \sum_{k=1}^{K} \pi_k = 1$$

- Steps:
  i. Randomly initialize $r_{ik} \in [0, 1]$
    - $\sum_{k=1}^{K} r_{ik} = 1$
    - r_{ik} is called **soft assignment(responsibility)** of x_i to k
  ii. Compute weighted sample mean and covariance according to r_{ik}

$$\mu_k = \frac{\sum_{i=1}^{n} r_{ik} x_i}{\sum_{i=1}^{n} r_{ik}}$$

$$\Sigma_k = \frac{\sum_{i=1}^{n} r_{ik} (x_i - \mu_k)(x_i - \mu_k)^T}{\sum_{i=1}^{n} r_{ik}}$$

  and update π

$$\pi_k = \frac{\sum_{i=1}^{n} r_{ik}}{n}$$

  iii. Update r_{ik}

$$r_{ik} = \frac{\pi_k \, N(x_i|\mu_k, \Sigma_k)}{\sum_{j=1}^{K} \pi_j \, N(x_i|\mu_k, \Sigma_k)}$$

  iv. Iterate i to iii until convergence
- $\Sigma_k = \sigma^2 I, \;\; \sigma \to 0 \quad \Rightarrow \quad \text{GMM} \to \text{K-means}$

Gaussian Mixture Model vs. KMeans

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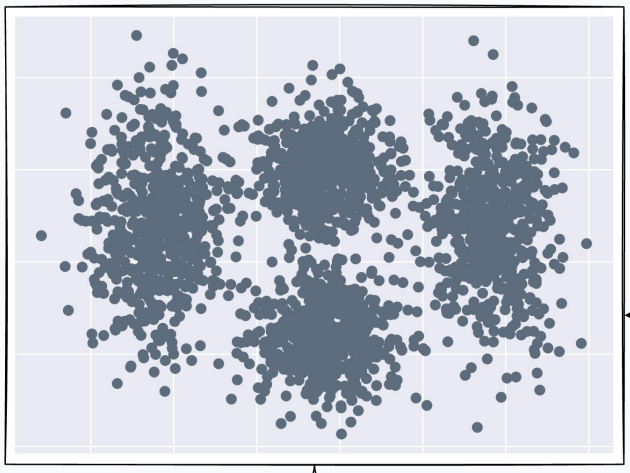
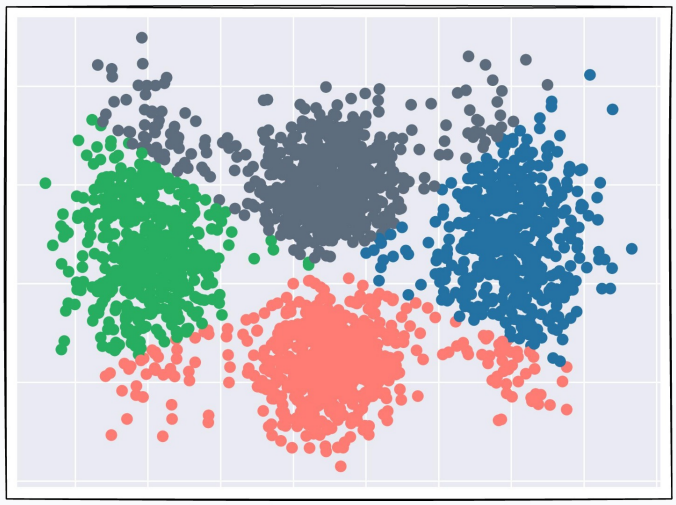


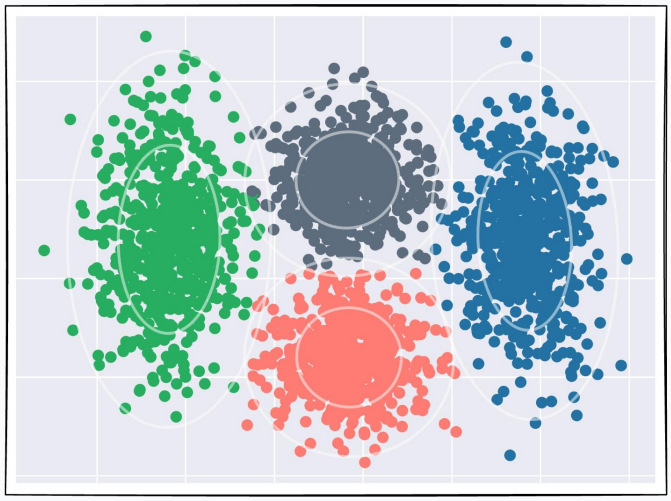
Clusters with different variances

KMeans



❌ Incorrect clustering

Gaussian Mixture Model



✅ Correct clustering