

# INTRODUCTION



## TO STATISTICAL LEARNING

# Introduction to Statistical Learning

## Unsupervised Learning - Class 13

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# Intro. to Unsupervised Learning

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# From Supervised to Unsupervised

- Recall: each observation is made of a vector  $x \in \mathcal{X}$  (for example  $x \in \mathbb{R}^p$ ) and a scalar  $y$
- Our goal is to build a model of the relationship between  $x$  and  $y$ :

$$y \approx f(x)$$

- IID assumption: each pair  $(x_i, y_i)$  is drawn independently from some distribution  $P_{x,y}$
- A modeling approach takes  $(X, y)$  as input and outputs a *prediction model*  $\hat{f}(x)$
- In prediction: we get a new value  $x_0$  and predict  $\hat{y}_0 = \hat{f}(x_0)$ .
- How good is our prediction? We typically define a loss function  $L(y, \hat{y})$  and the quality of the model is  $\mathbb{E}_{x_0, y_0}(L(y_0, \hat{y}_0))$

What if there is no  $y$ ?

# Unsupervised Learning

- Now: each observation is made of a vector  $x \in \mathcal{X}$  (for example  $x \in \mathbb{R}^p$ )
- IID assumption: each observation  $x_i$  is drawn independently from some distribution  $P_x$
- Our goal is to *learn* distribution  $P_x$  (or properties of it)
- “without a supervisor”
- Example: **Clustering** = Finding modes of  $P_x$  with high density
  - If we do find them, maybe  $P_x$  can be represented by a mixture of simpler densities?

# K-means Clustering

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# How to evaluate a partition?

- Assume  $K$  clusters are given
- $C(i) = k$  is some function assigning cluster  $k \in \{1, \dots, K\}$  to observation  $i \in \{1, \dots, n\}$
- $d(x_i, x_j)$  is a distance metric for pair  $i, j$ , e.g. Euclidean
- We wish to minimize the extent to which observations assigned to the same cluster tend to be close to one another
- Minimizing “within cluster” scatter/loss:

$$W(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(j)=k} d(x_i, x_j)$$

- Equivalent to maximizing  $B(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(j) \neq k} d(x_i, x_j)$
- Can we go over all possible  $C(i)$  to find the global minimum?

# Road to K-means

- Euclidean distance:  $d(x_i, x_j) = \sum_{m=1}^p (x_{im} - x_{jm})^2 = \|x_i - x_j\|^2$

- Can show that:

$$W(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(j)=k} \|x_i - x_j\|^2 = \sum_{k=1}^K n_k \sum_{C(i)=k} \|x_i - \bar{x}_k\|^2$$

- $\bar{x}_k \in \mathbb{R}^p$  being the mean in cluster  $k$ , and  $n_k$  number of observations in cluster  $k$
- But for any set of observations  $S$ , which  $m$  would minimize  $\sum_{i \in S} \|x_i - m\|^2$ ?
- Thus, the final goal of K-means:

$$\min_{C, m_1, \dots, m_K} \sum_{k=1}^K n_k \sum_{C(i)=k} \|x_i - m_k\|^2$$

# K-means

0. Start with initial guess for  $m_1, \dots, m_K$
1. Assign each observation to the closest cluster mean. That is:

$$C(i) = \arg \min_{k=1, \dots, K} \|x_i - m_k\|^2$$

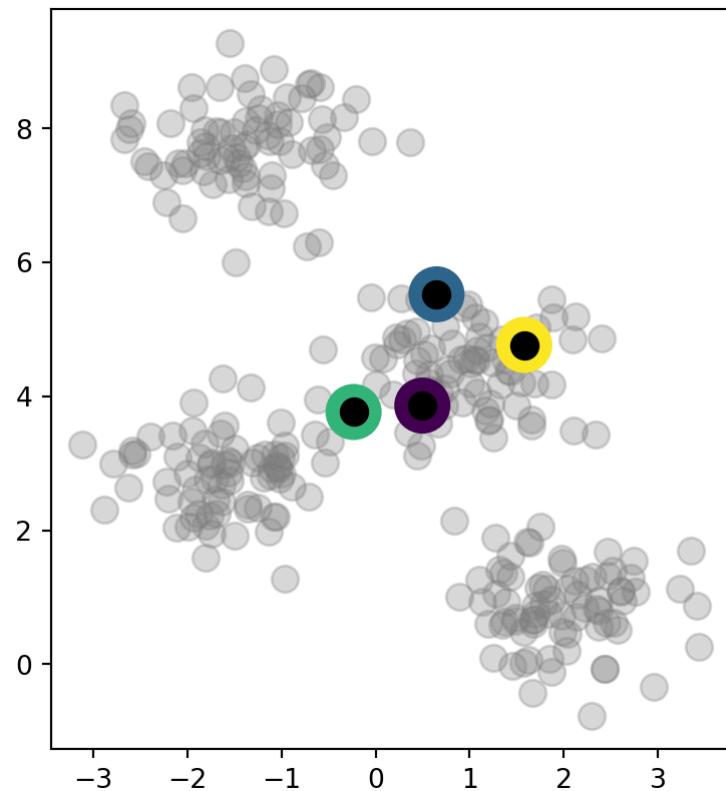
2. Update means  $m_1, \dots, m_K$ . That is the centroids:

$$m_k = \frac{\sum_{C(i)=k} x_i}{n_k}$$

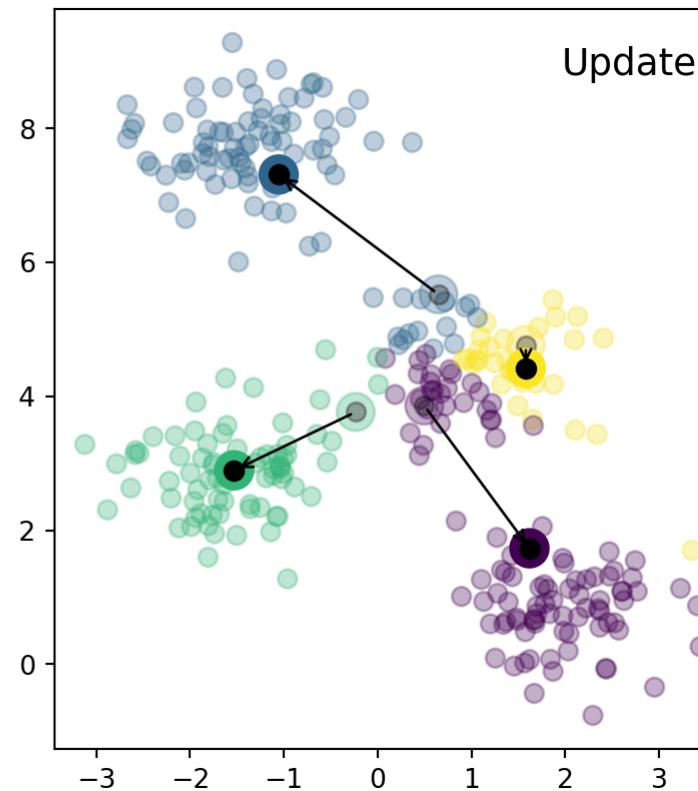
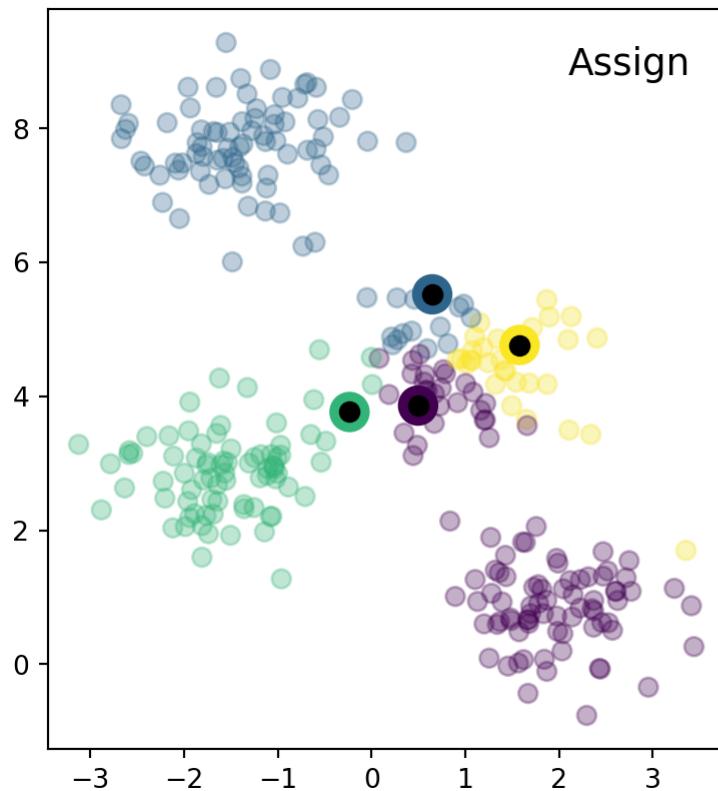
3. Repeat 1 and 2 until  $C(i)$  doesn't change

- Convergence is guaranteed (steps 1 and 2 can only reduce  $W(C)$ )
- Global optimum is NOT guaranteed
- Can try many different initial starting points

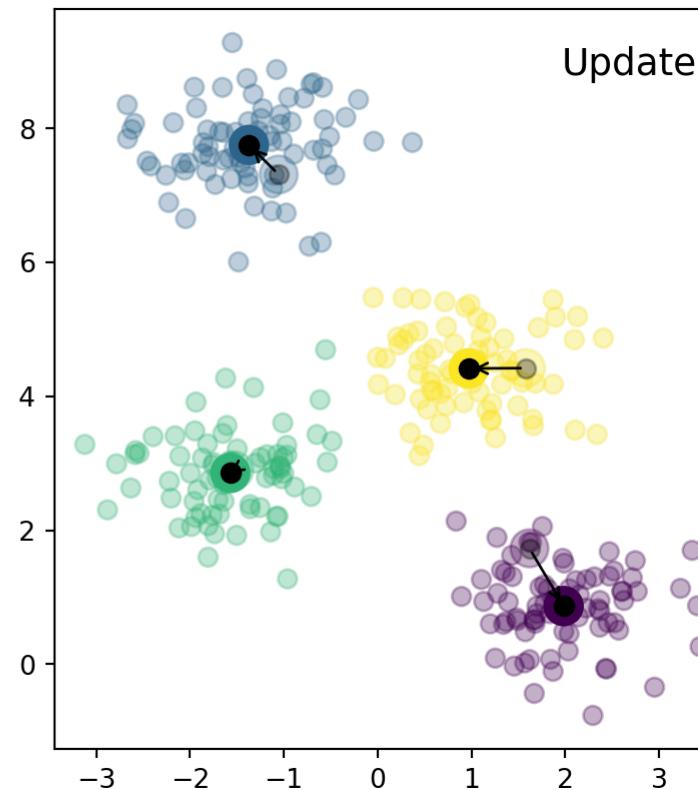
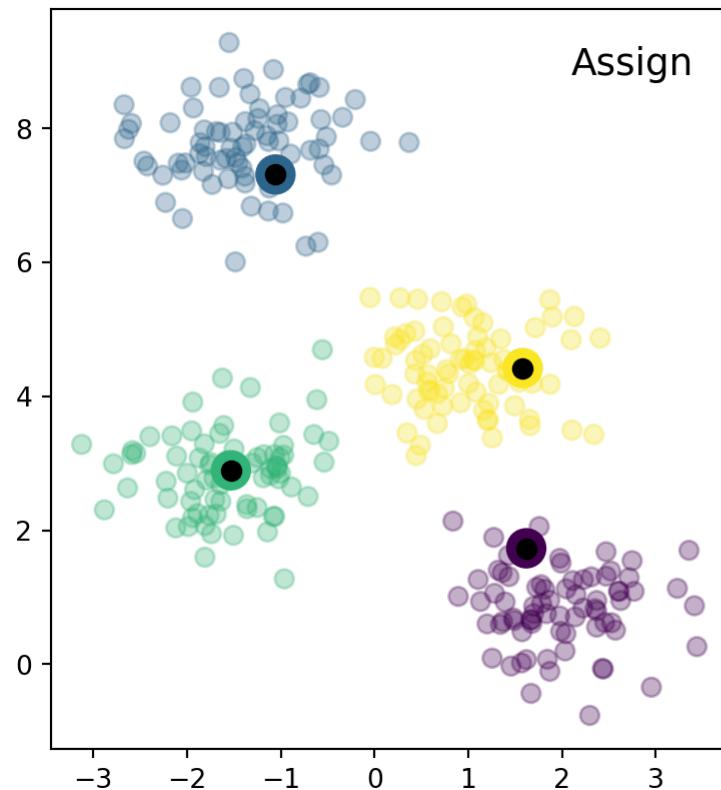
# K-means Demo: Initial Guess



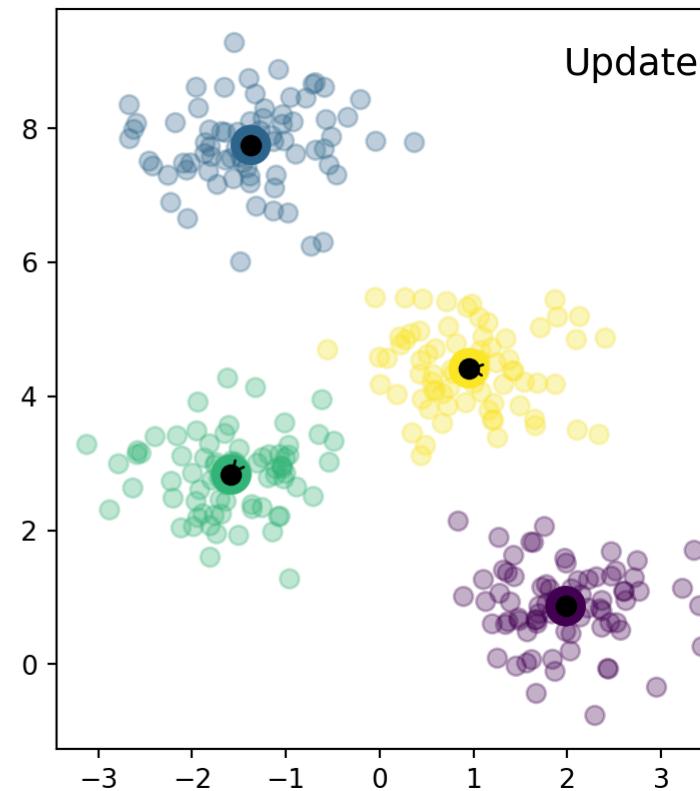
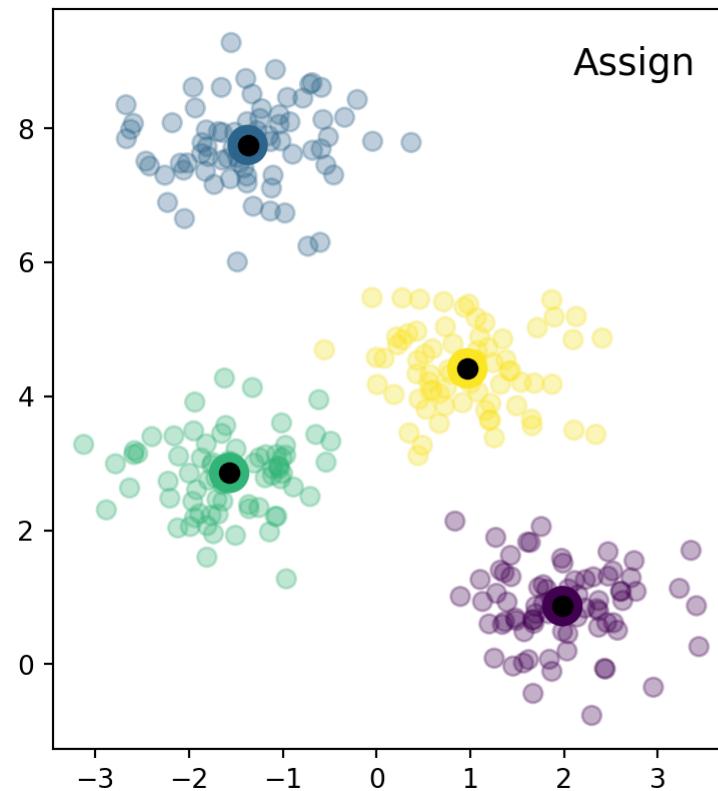
# K-means Demo: Iteration 1



# K-means Demo: Iteration 2



# K-means Demo: Iteration 3



# Some issues with K-means

- Limited to Euclidean distance
- Need to always specify  $K$ !
- How to choose  $K$ ?
- Prefers separable spherical clusters (Gaussian)
  - Bad with unequal densities, unequal cluster sizes
- No concept of outliers
  - See DBSCAN for an alternative

# Dimensionality Reduction

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# Dimensionality Reduction

- We have  $n$  observations in  $p$  dimensions:  $X_{n \times p}$
- Why would we want to reduce the data dimensionality to  $q \ll p$  dimensions?
  - EDA:
    - Visualize the data (2-d or 3-d visualizations)
    - Identify important dimensions which summarize the data well
  - Speed-up/Improve/Enable machine-learning algorithms (PCR)
  - Clustering after dimensionality reduction
  - Generative modeling - see later
- Naive way: select  $q$  out of the original  $p$  dimensions (best subset)
- Less Naive way: Look for interesting “projections”:
  - linear/non-linear combinations of features

# A non-standard motivation (I)

- We are given:
  - An **encoder**  $g(X) = Xw$ , where  $w \in \mathbb{R}^{p \times 1}$  is a vector with  $\|w\| = 1$
  - A **decoder**  $f(u) = uw^T$ , where  $u \in \mathbb{R}^{n \times 1}$
- The reconstructed matrix is therefore:  $\hat{X} = f(g(X)) = (Xw)w^T = Xww^T$
- Goal: find  $w$  that minimizes the **reconstruction error**  $\|X - \hat{X}\|_F^2$ 
  - $\|A\|_F^2 = \sum_{i=1}^m \sum_{j=1}^n a_{ij}^2$  is the squared Frobenius norm, the sum of squared elements of any real matrix  $A$
  - Also:  $\|A\|_F^2 = \text{Tr}(AA^T)$

$$\begin{aligned} w &= \arg \min_{w: \|w\|=1} \|X - \hat{X}\|_F^2 \\ &= \arg \min_{w: \|w\|=1} \text{Tr}((X - Xww^T)(X - Xww^T)^T) \end{aligned}$$

# A non-standard motivation (II)

$$w = \arg \min_{w: \|w\|=1} \text{Tr}((X - Xww^T)(X - Xww^T)^T)$$

$$\begin{aligned} & \text{Tr}((X - Xww^T)(X - Xww^T)^T) \\ &= \text{Tr}((X - Xww^T)(X^T - ww^T X^T)) \\ &= \text{Tr}(XX^T - Xww^T X^T - Xww^T X^T + Xww^T ww^T X^T) \\ &= \text{Tr}(XX^T - Xww^T X^T - Xww^T X^T + Xww^T X^T) \\ &= \text{Tr}(XX^T) - \text{Tr}(Xww^T X^T) \end{aligned}$$

But:  $\text{Tr}(Xww^T X^T) = \text{Tr}(w^T X^T X w) = w^T X^T X w$

$$\Rightarrow w = \arg \max_{w: \|w\|=1} w^T X^T X w$$

# PCA Dimensionality Reduction

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# PCA: the “standard” motivation

- Goal: Find the  $q$  direction(s) with the most dispersion
- Center  $X$ 's columns
- First direction:  $w_1 = \arg \max_{w_1: \|w_1\|=1} \|Xw_1\|^2 = \arg \max_{w_1: \|w_1\|=1} w_1^T X^T X w_1$
- Second direction:  $w_2 = \arg \max_{\|w_2\|=1, w_2^T w_1=0} w_2^T X^T X w_2$
- Can keep going looking for new directions
- Assuming  $p < n$ , up to  $p$  principal directions can be found this way, stack them into a  $p \times q$  “loadings” matrix  $W$
- Data with reduced dimensionality:  $T_{n \times q} = X_{n \times p} W_{p \times q}$  taking only the first  $q$  principal directions

But PCA solution also minimizes the reconstruction error of a linear encoder/decoder system!

# Eigendecomposition: Reminder

A non-zero vector  $\mathbf{v}$  is an eigenvector of a square  $p \times p$  matrix  $\mathbf{A}$  if it satisfies:

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v},$$

for some scalar  $\lambda$ .

- Then  $\lambda$  is called the eigenvalue corresponding to  $\mathbf{v}$ .
- Geometrically speaking, the eigenvectors of  $\mathbf{A}$  are the vectors that  $\mathbf{A}$  merely elongates or shrinks, and the amount that they elongate/shrink by is the eigenvalue
- An eigendecomposition of  $\mathbf{A}$  is then:  $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^{-1}$
- where  $\mathbf{V}$  is the square  $p \times p$  matrix whose  $j$ -th column is the eigenvector  $\mathbf{v}_j$  of  $\mathbf{A}$ , and  $\Lambda$  is the diagonal matrix whose diagonal elements are the corresponding eigenvalues,  $\Lambda_{jj} = \lambda_j$
- If  $\mathbf{A}$  is real and symmetric,  $\mathbf{V}$  is orthogonal,  $\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^T$  and  $\lambda_j$  are real scalars
- If  $\mathbf{A}$  is also positive semidefinite (PSD), then  $\lambda_j \geq 0$

# Calculating Principal Components

- Look again at the PCA problem:  $w_1 = \arg \max_{w_1: \|w_1\|=1} \|Xw_1\|^2$
- Using Lagrange multiplier  $\lambda_1$ :  $\max_{w_1} w_1^T X^T X w_1 + \lambda_1(1 - w_1^T w_1)$
- Take derivative with respect to  $w_1$ , compare to 0:

$$2X^T X w_1 - 2\lambda_1 w_1 = \mathbf{0} \Rightarrow X^T X w_1 = \lambda_1 w_1$$

- So  $w_1$  must be an eigenvector of the square, real, symmetric, PSD  $X^T X$  matrix, and  $\lambda_1$  its eigenvalue!
- Which eigenvalue and eigenvector?
- So we're looking for the set of  $W_{p \times q}$  eigenvectors  $\mathbf{V}_q$  of  $X^T X$  with their corresponding eigenvalues  $\lambda_1, \dots, \lambda_q$  ordered from largest to smallest

# t-SNE Dimensionality Reduction

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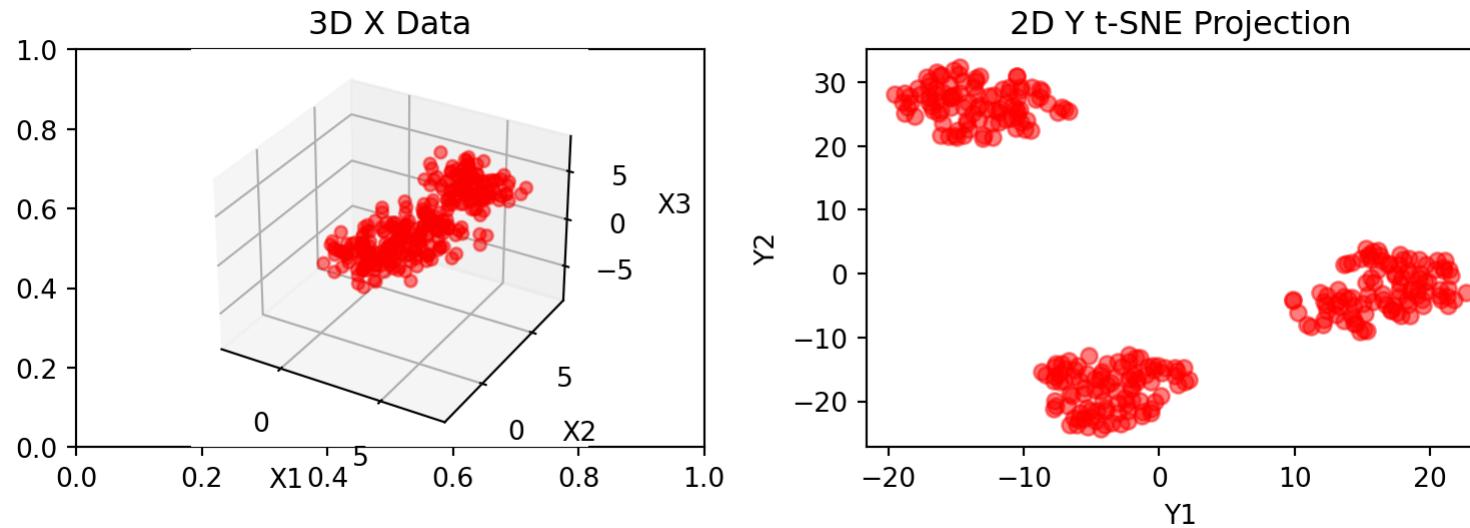


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# PCA Limitations

- Linear mapping (encoder/decoder)
- Squared reconstruction error: “punishes” more large differences in  $\|X - \hat{X}\|_F^2$
- Focus on preserving **global** structure
- No probabilistic meaning?

# t-Distributed Stochastic Neighbor Embedding



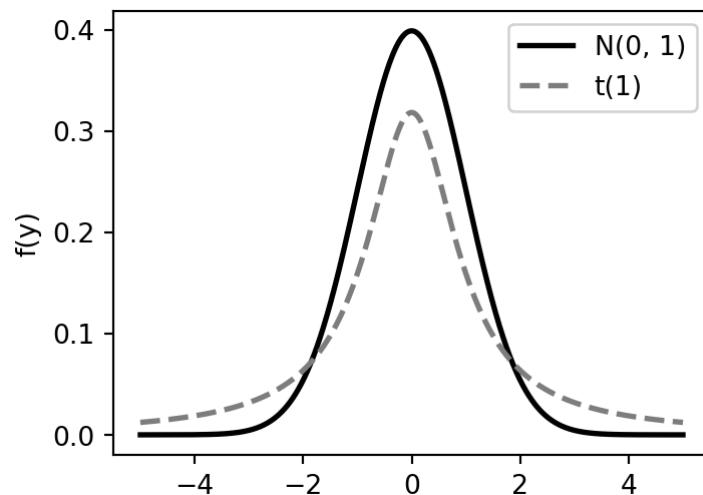
- Non-linear mapping
- Focus on preserving **local** structure through pairwise similarities:
  - close observations in high dimension should likely be close in low dimension
  - distant observations in high dimension should likely be distant in low dimension
- Specifically designed for visualization (2-D, 3-D)
- Probabilistic meaning

# t-SNE: How to define close/distant? (I)

- In high dimension ( $p$ ) with a Gaussian kernel:
  - Let  $\mathbf{x}_1, \dots, \mathbf{x}_n$  be the data rows (each  $\mathbf{x}_i \in \mathbb{R}^p$ )
  - $p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$
  - Notice that  $p_{j|i} \in [0, 1]$  and  $\sum_j p_{j|i} = 1$
  - Set  $p_{i|i} = 0$
  - “Symmetrize”:  $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$  (makes sense if  $p_i = \frac{1}{n} \forall i$ )
  - This  $n \times n$  table is computed once
  - Why not model  $p_{ij}$  directly?
  - How to get  $\sigma_i$  not shown here, but:
    - for observation  $i$  in a dense area, want to be specific  $\Rightarrow$  need small  $\sigma_i$
    - for observation  $i$  in a sparse area, need large  $\sigma_i$

# t-SNE: How to define close/distant? (II)

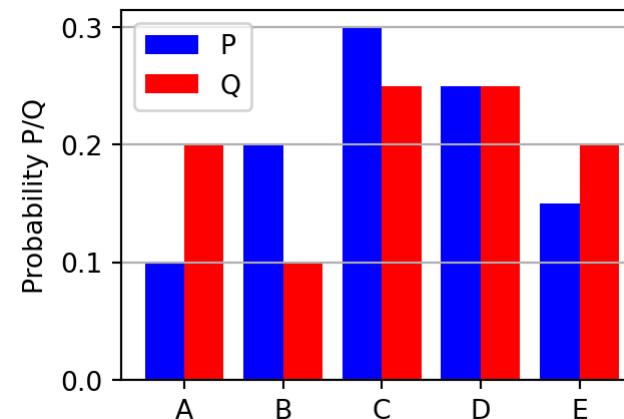
- In low dimension ( $q = 2, 3$ ) with a  $t(1)$ -distribution kernel:
  - Define  $\mathbf{y}_1, \dots, \mathbf{y}_n$  the low-dimensional mappings (each  $\mathbf{y} \in \mathbb{R}^q$ )
  - If  $Z \sim t(1)$ , then:  $f(z) = \frac{1}{\pi(1+z^2)}$  (also called Cauchy)
  - Here, no need to go through conditional probs
  - $q_{ij} = \frac{(1+\|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_k \sum_{k \neq l} (1+\|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$ , and set  $q_{ii} = 0 \forall i$
  - Why  $t(1)$ ? See the “crowding problem”.



# t-SNE: How to compare $p$ and $q$ distributions?

- The Kullback-Leibler (KL) divergence is a distance metric from distribution  $p$  to  $q$ :

$$KL(p||q) = \sum_i \sum_j p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

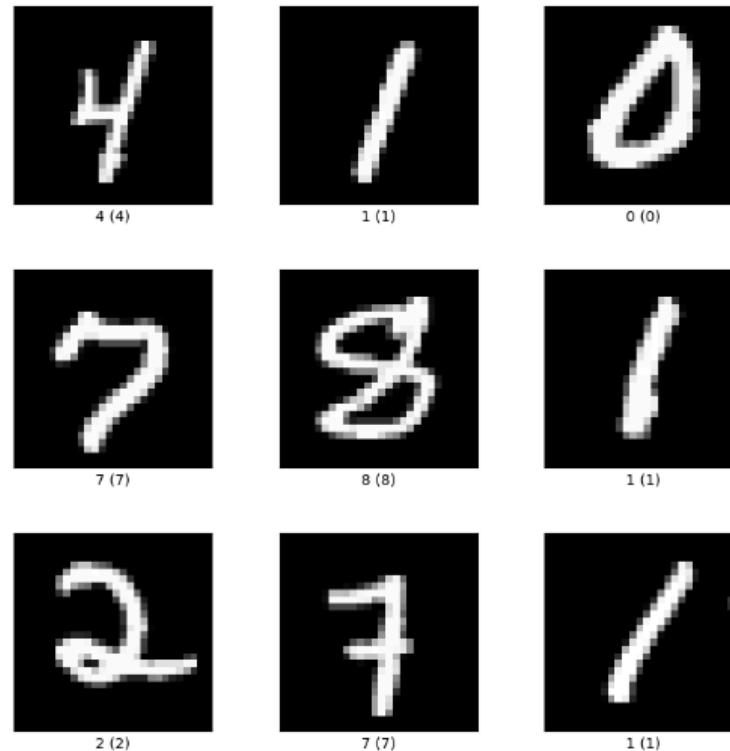


- At each iteration of t-SNE we walk a step down the gradient of  $KL(p||q)$  with respect to every  $\mathbf{y}_i$

# t-SNE: at high level

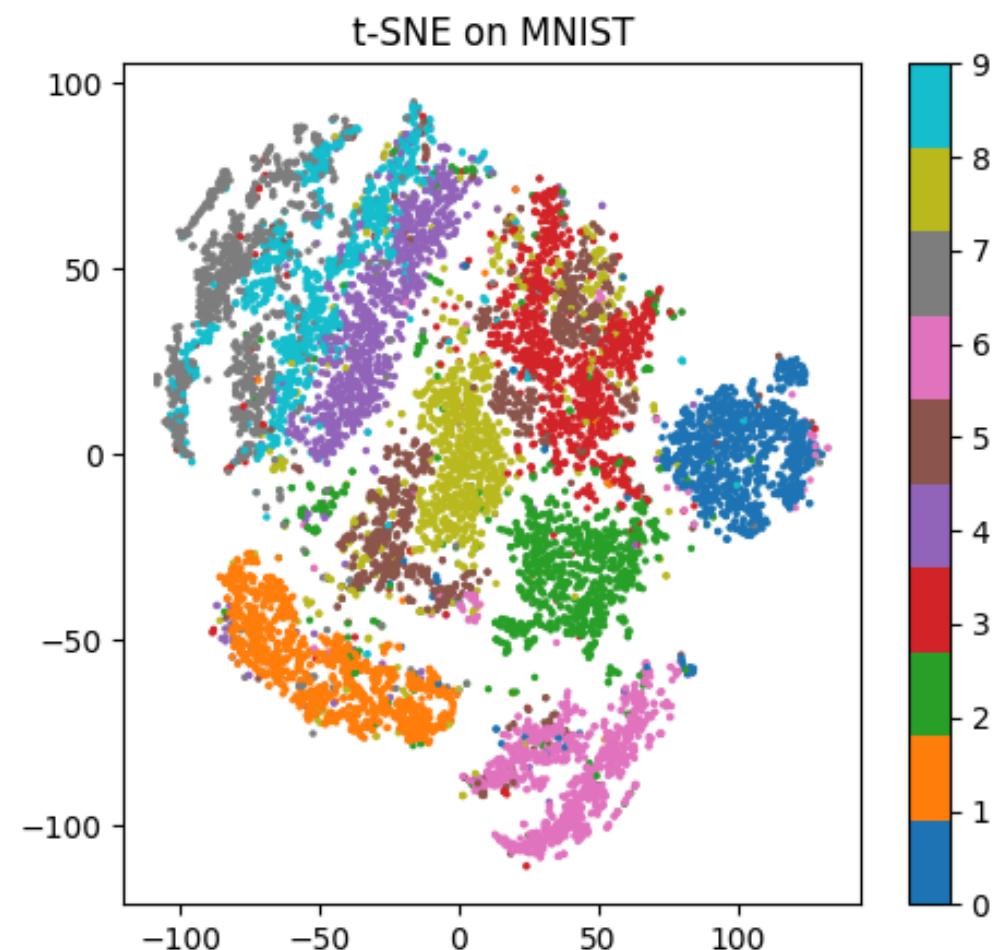
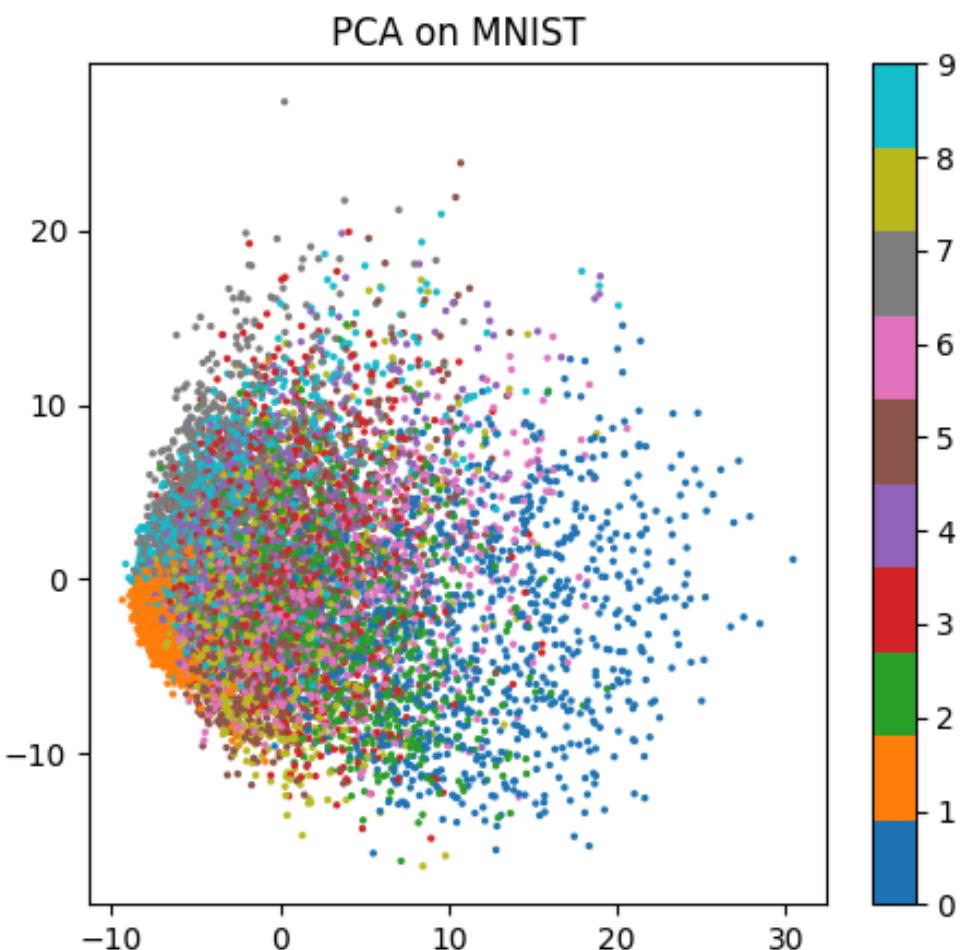
1. Prepare  $p_{ij}$  table with Gaussian kernel and  $\sigma_1, \dots, \sigma_n$
  2. Sample initial low-dimensional mappings  $Y^{(0)} = \mathbf{y}_1^{(0)}, \dots, \mathbf{y}_n^{(0)}$
  3. For  $t = 1$  to  $T$  do:
    - i. Compute  $q_{ij}$  with  $t(1)$  kernel
    - ii. Gradient step:  $\mathbf{y}_i^{(t)} = \mathbf{y}_i^{(t-1)} - \alpha \cdot \frac{\partial KL}{\partial \mathbf{y}_i}$
- $\frac{\partial KL}{\partial \mathbf{y}_i} = 4 \sum_j (p_{ij} - q_{ij})(\mathbf{y}_i - \mathbf{y}_j)(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}$
  - Modifications exist for very large datasets, e.g. consider only local neighborhood for  $i$

# Example: MNIST dataset



7000 X 10 digits ( $n = 70000$ ), hand-written, in 28 X 28 pixels ( $p = 784$ )

# PCA vs. t-SNE



# PCA as a Generative Model

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# Probabilistic PCA (I)

- It is not true that there is nothing “probabilistic” about PCA!
- Suppose every data row  $\mathbf{x}_i$  was generated by:

$$\mathbf{x}_i = W\mathbf{u}_i + \mu + \varepsilon_i$$

- $\mathbf{u}_i \in \mathbb{R}^q$  is a **latent** vector from  $\mathcal{N}(\mathbf{0}, I_q)$
- $W$  is a  $p \times q$  matrix
- $\mu \in \mathbb{R}^p$  is a mean vector for  $p$  features
- $\varepsilon_i \in \mathbb{R}^p$  is random noise from  $\mathcal{N}(\mathbf{0}, \sigma^2 I_p)$

$$\Rightarrow \mathbf{x}_i \sim \mathcal{N}(\mu, \Sigma), \text{ where: } \Sigma = WW^T + \sigma^2 I_p$$

It's likelihood:  $f(\mathbf{x}_i) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}_i - \mu)^T \Sigma^{-1} (\mathbf{x}_i - \mu)\right)$

# Probabilistic PCA (II)

- After some algebra, the log-likelihood of our entire data  $X = \mathbf{x}_1, \dots, \mathbf{x}_n$ :

$$\ell(\mu, W, \sigma^2 | X) = -\frac{n}{2} [p \ln(2\pi) + \ln(|\Sigma|) + \text{Tr}(\Sigma^{-1} S)]$$

- where  $S = \frac{1}{n} \sum_i (\mathbf{x}_i - \mu)(\mathbf{x}_i - \mu)^T$  is the covariance matrix of  $X$
- The maximum likelihood estimate (MLE) for  $W$ :
 
$$\hat{W}_{MLE} = \mathbf{V}_q (\boldsymbol{\Lambda}_q - \sigma^2 I_q)^{1/2} \mathbf{R}$$
  - where the columns of  $\mathbf{V}_q$  are eigenvectors of  $S$ , with corresponding  $q$  largest eigenvalues in the diagonal matrix  $\boldsymbol{\Lambda}_q$ , and  $\mathbf{R}$  is a  $q \times q$  arbitrary rotation matrix
  - In the limit  $\sigma^2 \rightarrow 0$  this solution is equivalent to PCA!
- PCA as a generative model:  $\mathbf{x}_* = \hat{W}\mathbf{u}_* + \hat{\mu}$

# The many faces of PCA

Why is this so important?

- PCA as an eigenvalue problem to maximize dispersion of projection
- PCA as an SVD problem
- PCA as an encoder/decoder problem to minimize reconstruction error
- PCA as a generative model to maximize likelihood



- Unsupervised learning can be used to generate new data:
- PCA is the ancestor of many generative models