

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
- The “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:

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

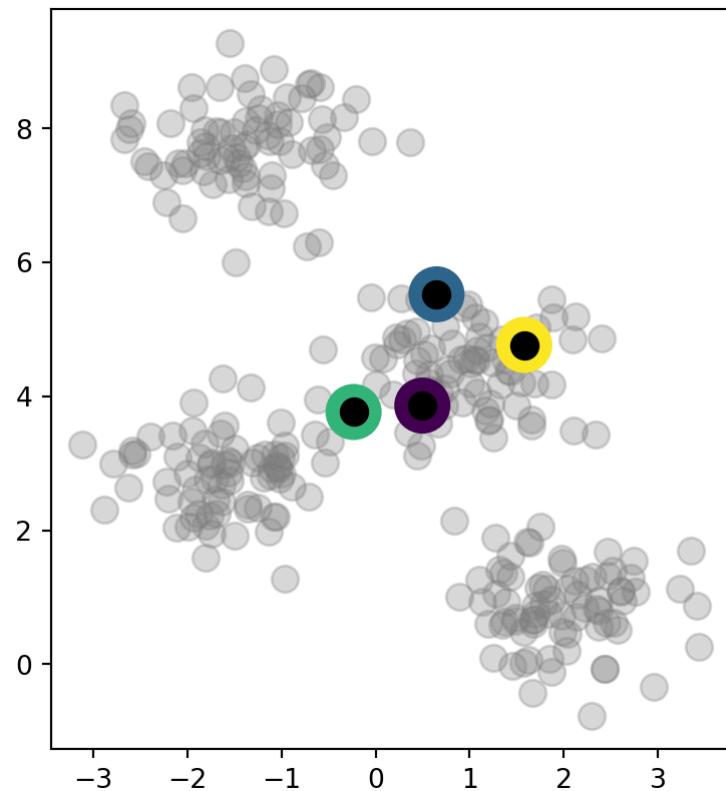
2. Update means m_1, \dots, m_K . That is the centroids:

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

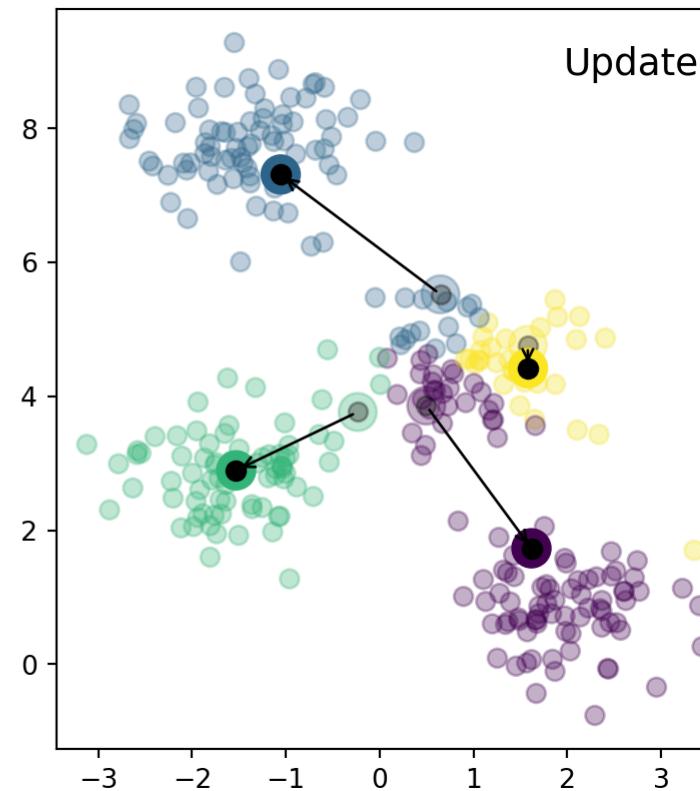
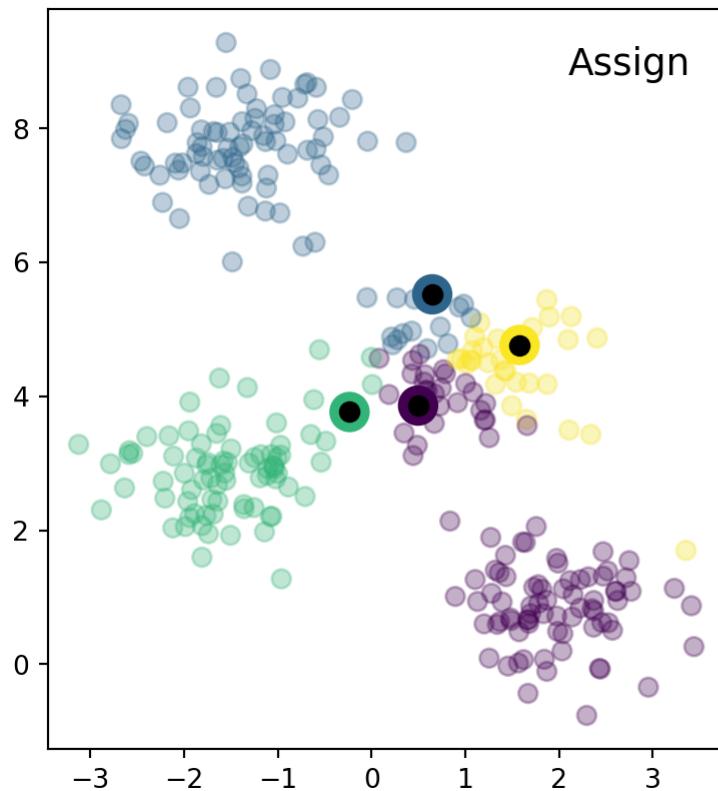
3. Repeat 1 and 2 until $C(i)$ doesn't change

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

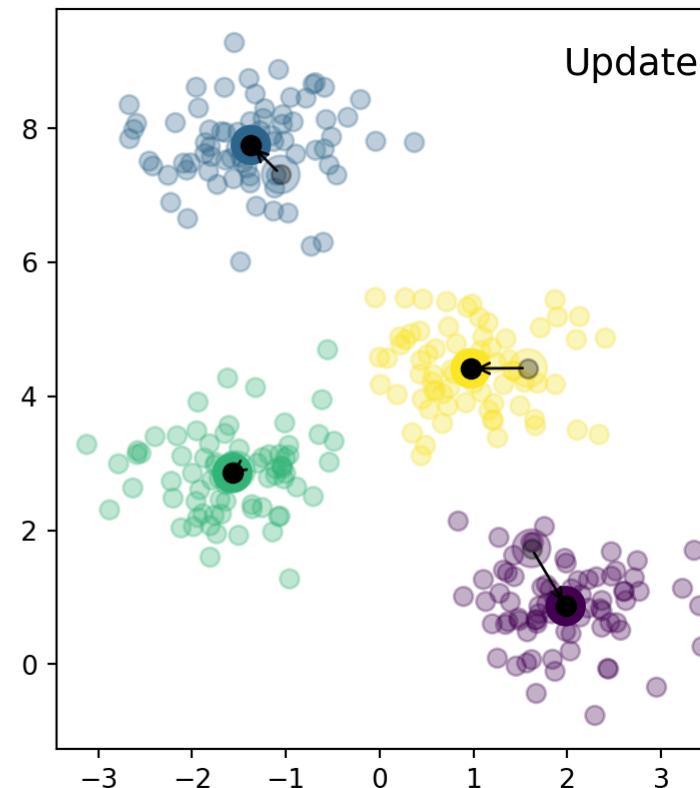
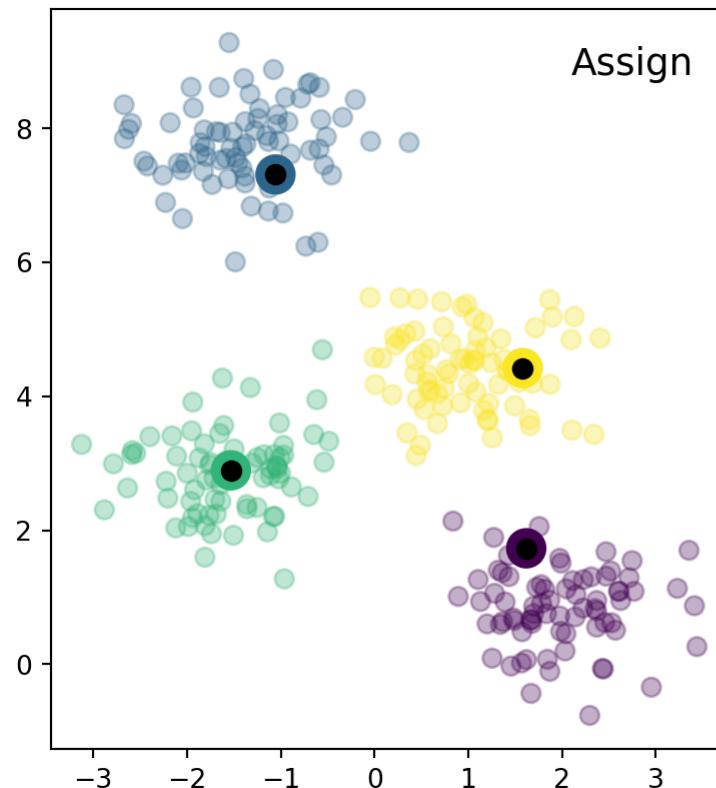
K-means Demo: Initial Guess



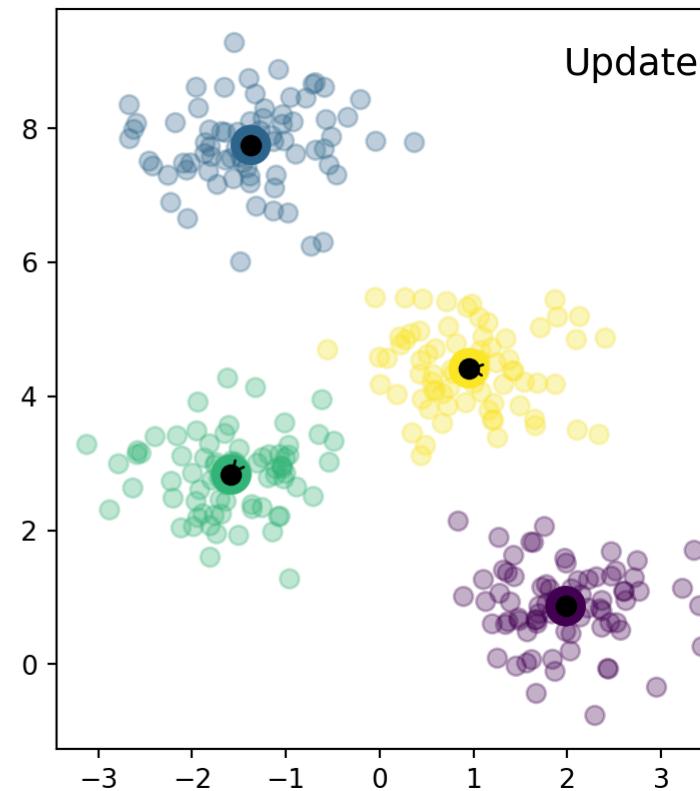
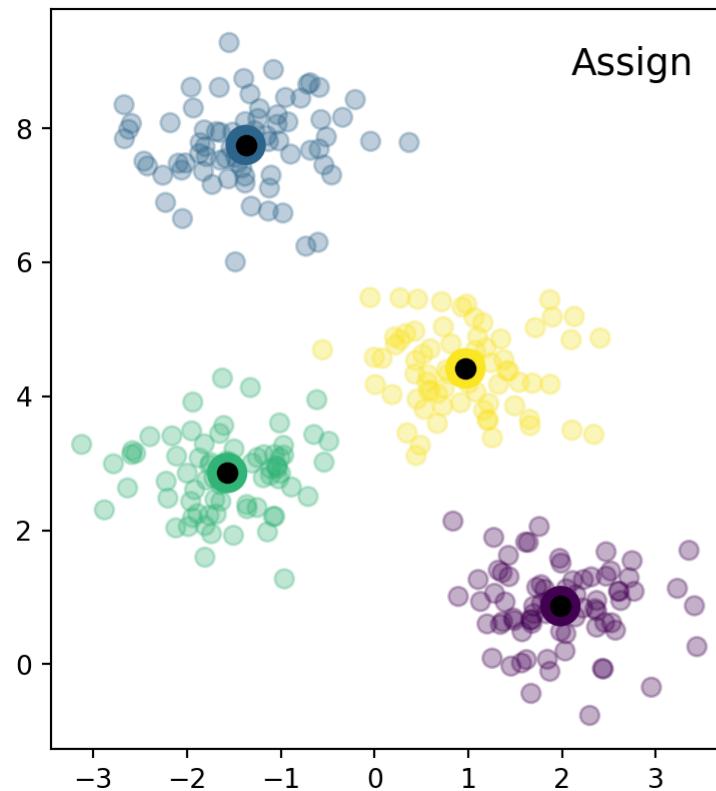
K-means Demo: Iteration 1



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: $\|A\|_F^2 = \text{Tr}(AA^T)$
 - $w = \arg \min_{w: \|w\|=1} \text{Tr}((X - Xww^T)(X - Xww^T)^T)$

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 λ .

- Then λ 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 Λ 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 λ_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 λ_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 λ_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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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?

Enter **t-Distributed Stochastic Neighbor Embedding (t-SNE)**:

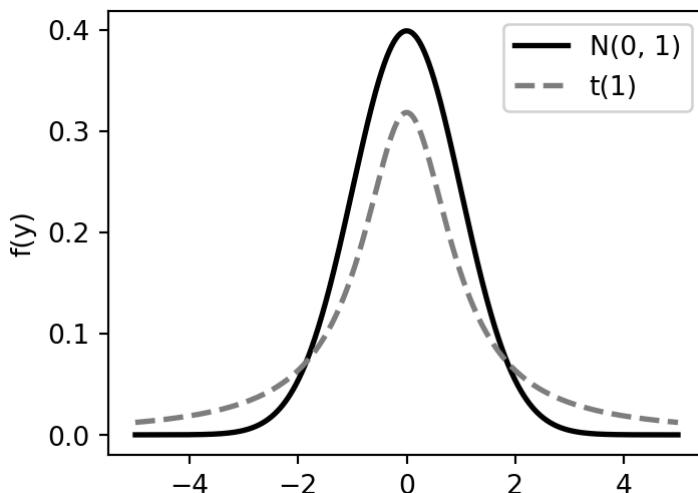
- Non-linear mapping
- Focus on preserving **local** structure through pairwise similarities:
 - close observations in high dimension should likely be close in low dimension
 - distant observations in high dimension should likely be distant in low dimension
- Specifically designed for visualization (2-D, 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 σ_i not shown here, but:
 - for observation i in a dense area, want to be specific \Rightarrow need small σ_i
 - for observation i in a sparse area, need large σ_i

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

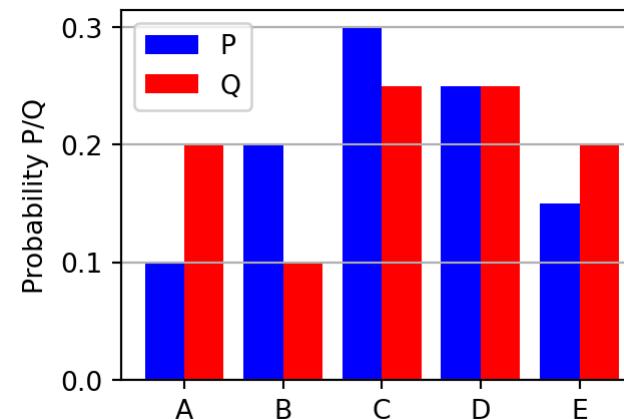
- In low dimension ($q = 2, 3$) with a $t(1)$ -distribution kernel:
 - Define $\mathbf{y}_1, \dots, \mathbf{y}_n$ the low-dimensional mappings (each $\mathbf{y} \in \mathbb{R}^q$)
 - If $Z \sim t(1)$, then: $f(z) = \frac{1}{\pi(1+z^2)}$ (also called Cauchy)
 - Here, no need to go through conditional 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

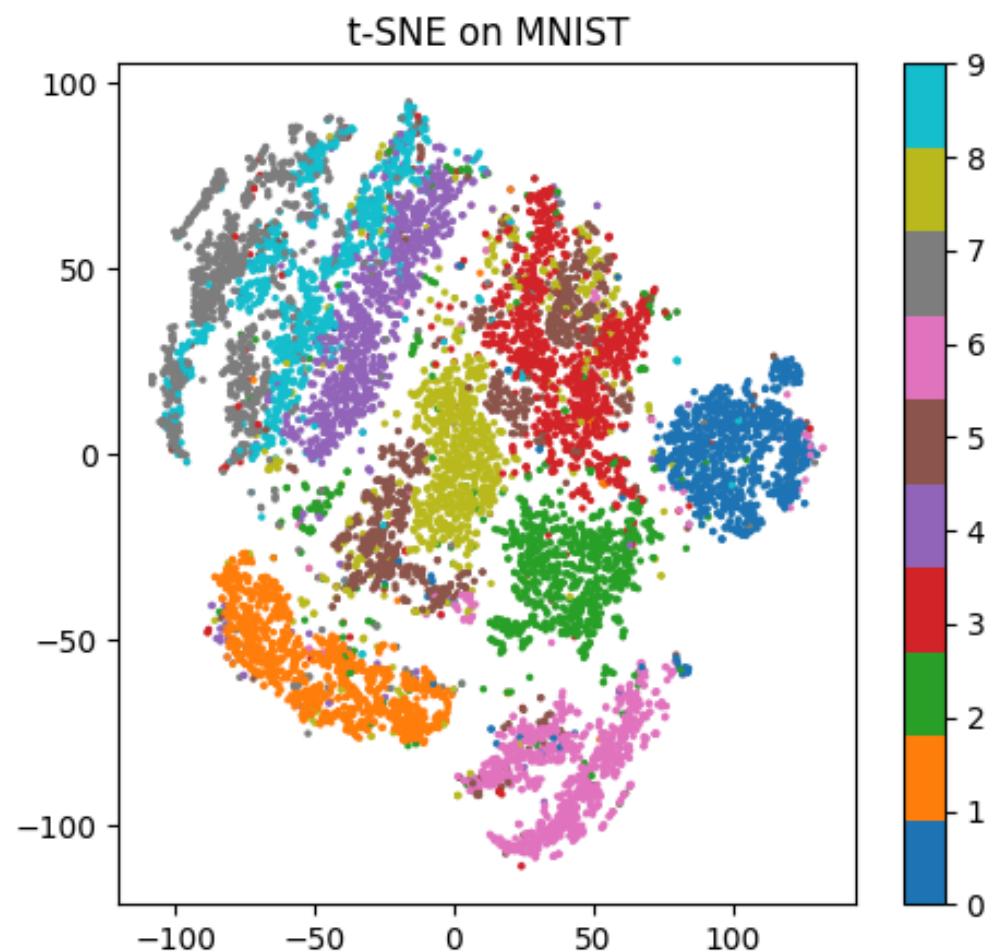
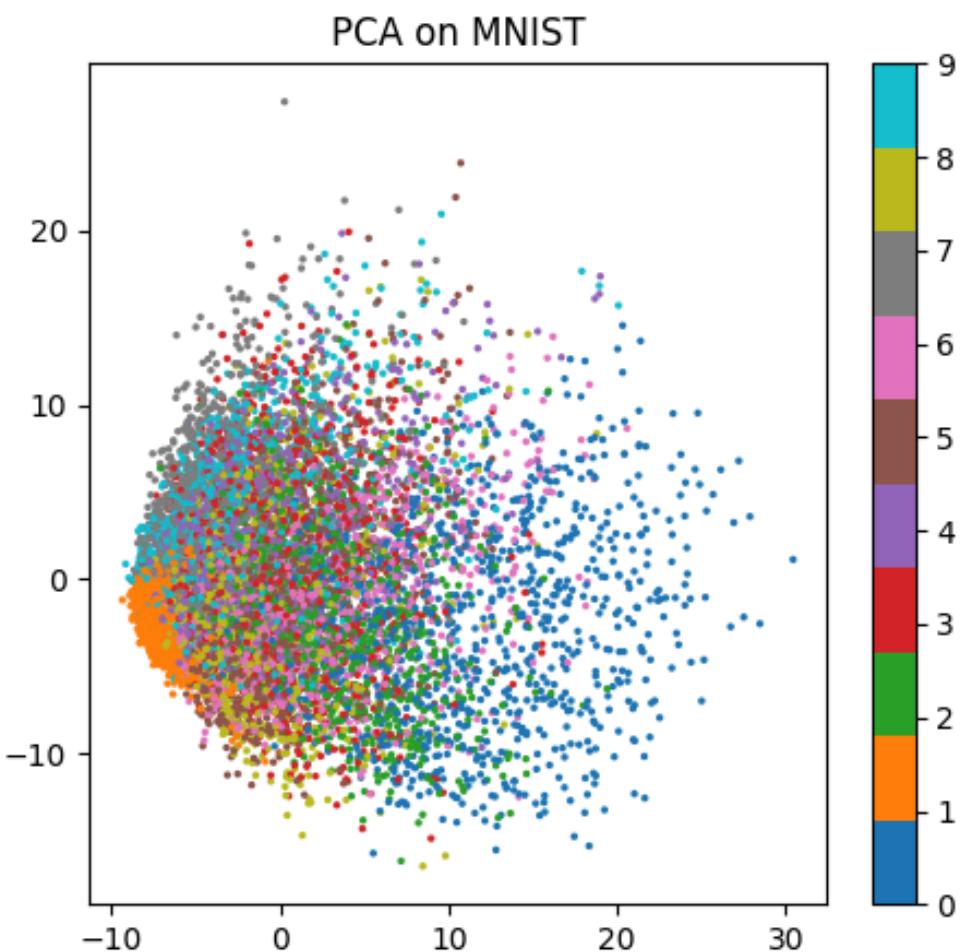
1. Prepare p_{ij} table with Gaussian kernel and $\sigma_1, \dots, \sigma_n$
 2. Sample initial low-dimensional mappings $Y^{(0)} = \mathbf{y}_1^{(0)}, \dots, \mathbf{y}_n^{(0)}$
 3. For $t = 1$ to T do:
 - i. Compute q_{ij} with $t(1)$ kernel
 - ii. Gradient step: $\mathbf{y}_i^{(t)} = \mathbf{y}_i^{(t-1)}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

$$W_{MLE} = \mathbf{V}_q (\boldsymbol{\Lambda}_q - \sigma^2 I_q)^{1/2} \mathbf{R}$$

- 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!

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