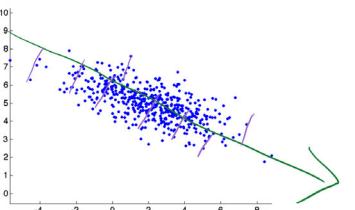


CS 189/289

Today's lecture outline

1. Finish PCA.
2. Non-linear dimensionality reduction (t-SNE)

Recall: PCA



- Goal: find $k < d$ dimensions w most of the “information” in the original data, $X \in \mathbb{R}^{n \times d}$.
- Directions accounting for most variance and yielding lowest $\|X_{recon-k} - X\|_F$.

5K original faces, $x_j \in \mathbb{R}^{1024}$



1024 PCA basis vectors, $u_i \in \mathbb{R}^{1024}$
(from $X^T X = UDU^T$)



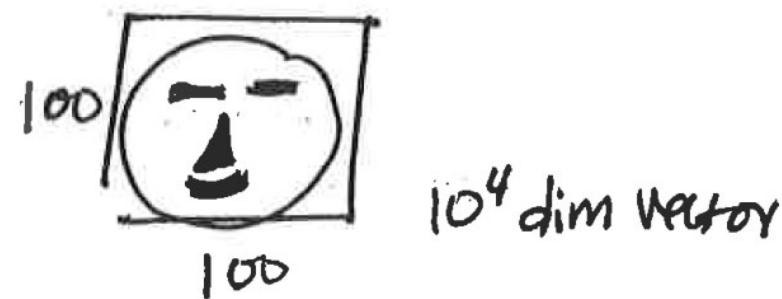
Reconstruction, $X_{recon-k} = XU_kU_k^T$



Linear algebra for PCA

$$\bar{X} \in \mathbb{R}^{n \times d}$$

- Need to compute the principal axes, Q , of $\bar{X}^T \bar{X} = Q D Q^T \in \mathbb{R}^{d \times d}$.
- This is an *eigendecomposition* of the matrix $\bar{X}^T \bar{X}$.
- Computing its eigendecomposition has time complexity $O(d^3)$.
- What if $d \gg n$? e.g., images of $d = 100 \times 100 = 10^4$ pixels, and $n = 1,000$ images.
- Could we do something cheaper?
- Yes. Need to understand the SVD.



Linear algebra for PCA

mean centered data, $\bar{X} \in \mathbb{R}^{n \times d}$

Recall the spectral theorem from MVG lecture, which gives a *spectral (eigen) decomposition*:

When A is symmetric $A = A^T$

$A = Q D Q^T$ with real eigenvalues in D
and orthonormal vectors in $S = Q$

Q is an orthonormal matrix $[q_1 \ q_2 \dots \ q_n]$

\Downarrow
each is
of length 1
any two
are orthogonal
true for col and row

$$A = Q D Q^{-1}$$

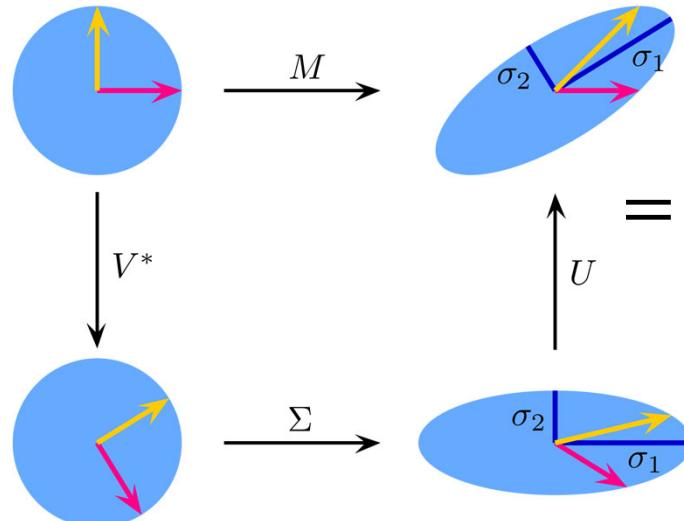
$Q^{-1} = Q^T$
(rotations & reflections)

- The covariance matrix for PCA, $\bar{X}^T \bar{X}$, is **symmetric** (and PSD).
- It turns out, there is a **generalization** of the spectral decomposition, for **non-symmetric** and **non-square** matrices, the **SVD** that will be helpful.

Singular Value Decomposition (SVD)

Can think of M as linear transformation broken down into three steps, by looking at its effect on the unit disc and the two canonical unit vectors e_1 and e_2 :

1. **Left:** V^T rotates the disc and unit vectors.
2. **Bottom:** Σ stretches scales axes by $\sigma_i = \Sigma_{i,i}$ (singular values).
3. **Right:** U performs another rotation.



$$M = U \cdot \Sigma \cdot V^*$$

Can be applied to any matrix M .

$$M_{m \times n} = U_{m \times m} \Sigma_{m \times n} V^*_{n \times n}$$

$$\begin{aligned} Mv_1 &= \Sigma_{1,1}u_1 \\ Mv_2 &= \Sigma_{2,2}u_2 \\ &\dots \\ Mv_r &= \Sigma_{r,r}u_r \end{aligned}$$

$$U_{m \times m} \cdot U^*_{m \times m} = I_m$$

$$r = \text{rank}(M) \leq \min(m, n)$$

$$V_{n \times n} \cdot V^*_{n \times n} = I_n$$

- Has time complexity $O(m^2n + mn^2)$.
- Σ is unique (if in descending order), but V and U are generally not: e.g. sign flips.
- (Eigendecomposition is unique if all eigenvalues are unique)
- If M is square+symmetric, yields the spectral decomposition.

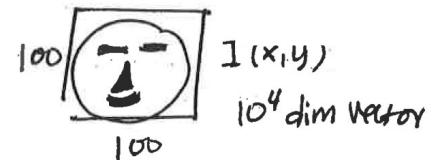
Singular Value Decomposition (SVD)

- Columns in \mathbf{U} are the eigenvectors of $\mathbf{M}\mathbf{M}^T$, called the *left singular vectors* of \mathbf{M} ($\mathbf{M}\mathbf{M}^T = \mathbf{U}\Sigma\mathbf{V}^T\mathbf{V}\Sigma^T\mathbf{U}^T = \mathbf{U}\Sigma^2\mathbf{U}^T$). Can be applied to any matrix \mathbf{M} .
- Columns in \mathbf{V} are the eigenvectors of $\mathbf{M}^T\mathbf{M}$, called the *right singular vectors* of \mathbf{M} ($\mathbf{M}^T\mathbf{M} = \mathbf{V}\Sigma^T\mathbf{U}^T\mathbf{U}\Sigma\mathbf{V}^T = \mathbf{V}\Sigma^2\mathbf{V}^T$).
- Both spectral decompositions at once!
- Eigenvalues are the same, given by $\lambda_i = \Sigma_{i,i}^2$ (Σ_i , i are the *singular values* of \mathbf{M}):
 - Since v_i is an eigenvector for $\mathbf{M}^T\mathbf{M}$, it follows that $\mathbf{M}^T\mathbf{M}v_i = \lambda_i v_i$. It follows that...
 -($\mathbf{M}\mathbf{M}^T\mathbf{M}v_i = \lambda_i(\mathbf{M}v_i)$) thus $\mathbf{M}v_i$ is an eigenvector for $\mathbf{M}\mathbf{M}^T$ with eigenvalue λ_i !

$$\mathbf{M} = \mathbf{U} \Sigma \mathbf{V}^*$$
$$\mathbf{m} \times \mathbf{n} \quad \mathbf{m} \times \mathbf{m} \quad \mathbf{m} \times \mathbf{n} \quad \mathbf{n} \times \mathbf{n}$$
$$\mathbf{U} \quad \mathbf{U}^* = \mathbf{I}_m$$
$$\mathbf{V} \quad \mathbf{V}^* = \mathbf{I}_n$$

$$X \in \mathbb{R}^{n \times d}$$

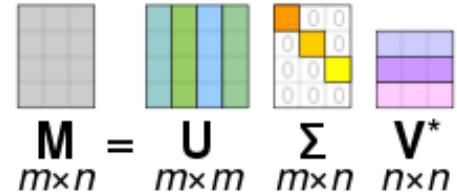
Singular Value Decomposition (SVD)



- Recall this example with $d \gg n$, e.g. $d = 10^4$ pixels, $n = 1000$ images.
- How can we make use of what we just learned to do PCA faster than the eigendecomposition $O(d^3)$?
- Instead of spectral decomposition of $X^T X$...
- ...directly use SVD of the data matrix: $SVD(X) = U\Sigma V^T$
- Because columns in V are the eigenvectors of $X^T X$.
- $\lambda_i = \Sigma_{i,i}^2$ are needed eigenvalues.
- SVD has time complexity $O(dn^2)$.

$$\begin{matrix} M \\ m \times n \end{matrix} = \begin{matrix} U \\ m \times m \end{matrix} \begin{matrix} \Sigma \\ m \times n \end{matrix} \begin{matrix} V^* \\ n \times n \end{matrix}$$

Singular Value Decomposition (SVD)

$$\mathbf{M}_{m \times n} = \mathbf{U}_{m \times m} \mathbf{\Sigma}_{m \times n} \mathbf{V}^*_{n \times n}$$


For PCA we want projections onto top k PCs.

- When we used a spectral decomposition, $\mathbf{X}^T \mathbf{X} = \mathbf{Q} \mathbf{D} \mathbf{Q}^T$, we compute: $\mathbf{X}_k = \mathbf{X} \mathbf{Q}_k \in \mathbb{R}^{n \times k}$ (\mathbf{Q} are eigvecs of $\mathbf{X}^T \mathbf{X}$).
- When using the SVD of \mathbf{X} , we can instead get this from:
- $\mathbf{X}_k = \mathbf{X} \mathbf{V}_{:,1:k} = \mathbf{U}_{:,1:k} \mathbf{\Sigma}_{1:k,1:k} \in \mathbb{R}^{n \times k}$ ("scores" in PCA basis). $Xv_i = \sigma_i u_i$
- We don't need to compute covariance matrix, or do the projections, we just need $SVD(\mathbf{X})$!

“Eckart Young theorem” 1936

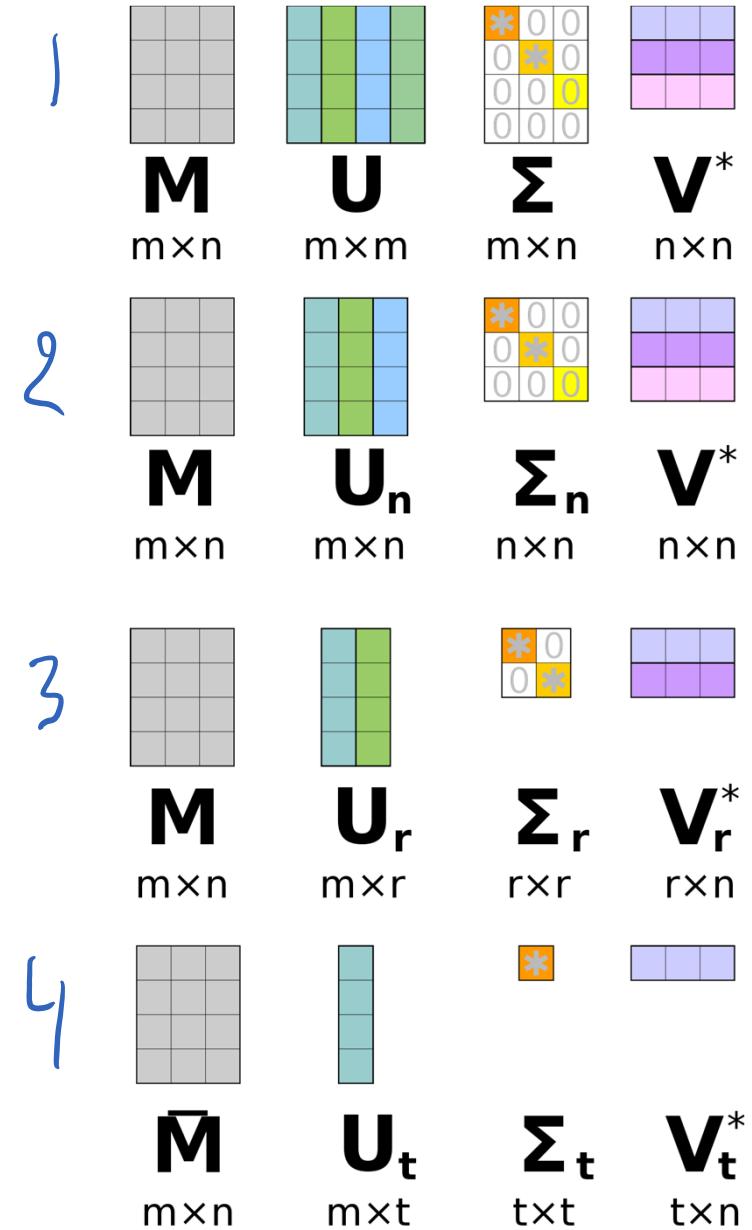
- The SVD “k-reconstruction” produces the best k -rank approximation by the matrix norm, $\|X - X_{recon-k}\|_F$.
- First proven by Schmidt (of Gram-Schmidt fame) in 1907 for Froebenius norm.
- Later rediscovered by Eckart & Young 1936, also generalized to other norms..
- Thus, PCA provides the best low rank approximation to the data matrix.

$$\|\mathbf{A}\|_F \equiv \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2}$$

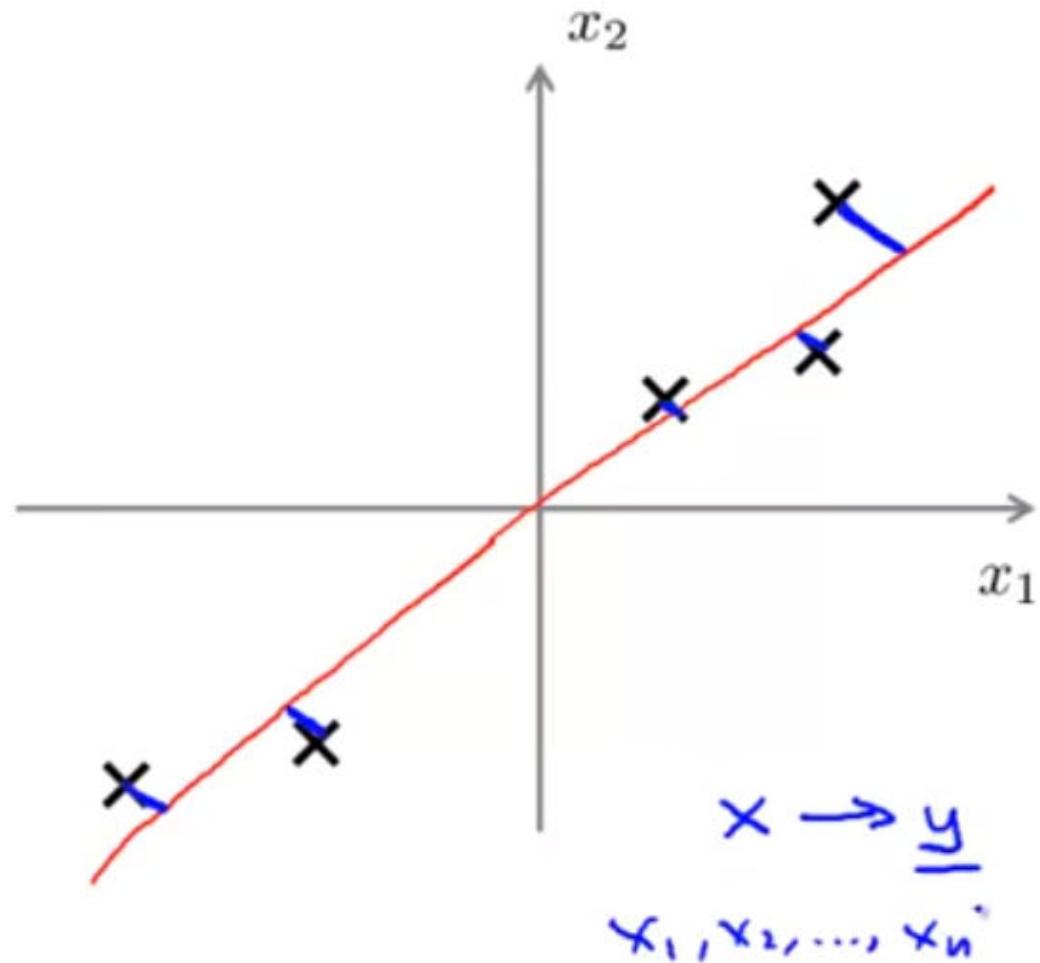
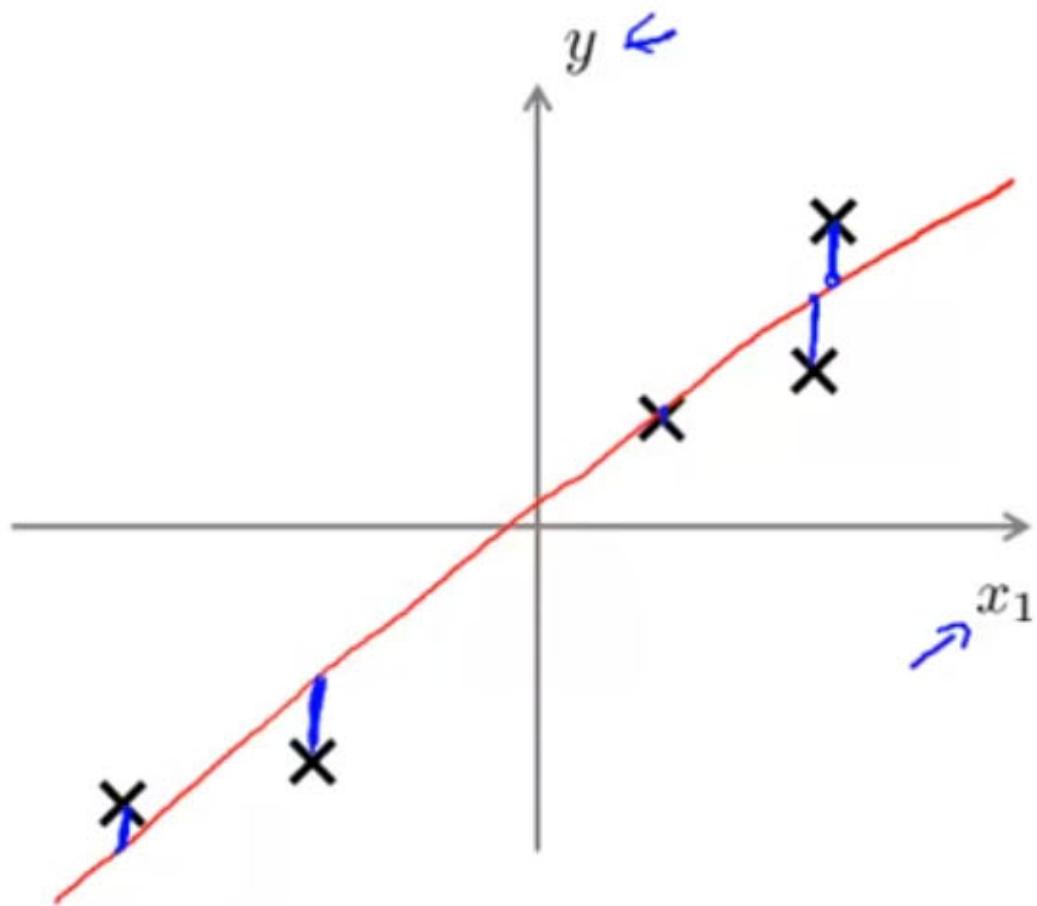
Practicalities: Reduced SVDs

For PCA and other applications, don't need the entire SVD, and can make do with "trimmed down" versions:

1. Full SVD
2. Thin SVD (remove columns of U not corresponding to rows of V^*)
3. Compact SVD (remove vanishing singular values and corresponding columns/rows in U and V^*),
4. Truncated SVD (keep only largest t singular values and corresponding columns/rows in U and V^*)

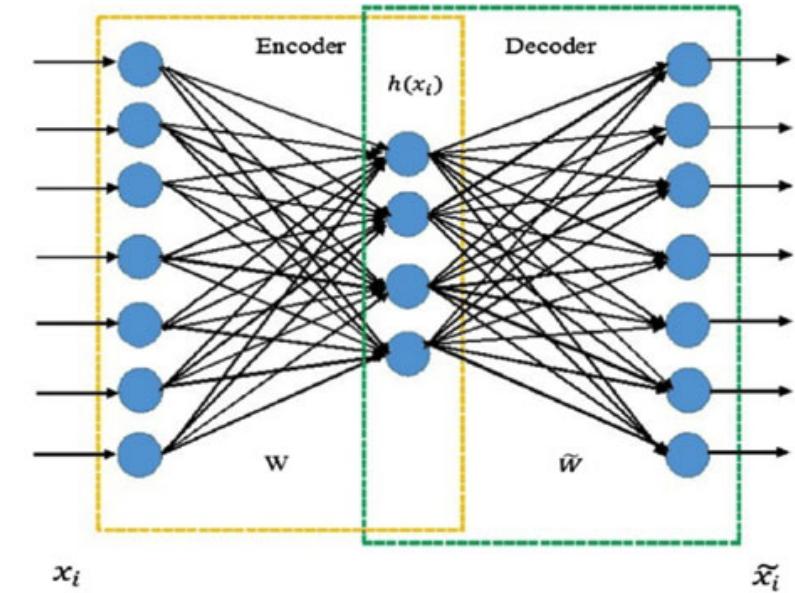


PCA is not linear regression



PCA from neural networks!

- Special kind of neural network: an *autoencoder*.
- Learned parameters with MLE recovers the same subspace as PC-k (one layer, all linear, k nodes).
- Can generalize by making non-linear transfers, and more layers, etc.



Can we do PCA if don't have X explicitly?

- Suppose you're given pairwise distances between n cities, $M \in \mathbb{R}^{n \times n}$, and asked you to find a 2D representation?
- Think of $M = XX^T \in \mathbb{R}^{n \times n}$ for some unobserved X (instead of $X^T X$).
- Now new basis is in U from: $M = USV^T$.
- We just performed *Multidimensional Scaling* (MDS):
- Implicitly assumes some latent space X of unknown dimension for which the distance is an inner product distance, $d(x', x) = x'x^T$.
- Could be non-linear distance function of actual x (e.g., if latent space had a polynomial expansion).

- Example: given pairwise distances between cities

	Atl	Chi	Den	Hou	LA	Mia	NYC	SF	Sea	DC
Atlanta	0									
Chicago	587	0								
Denver	1212	920	0							
Houston	701	940	879	0						
LA	1936	1745	831	1374	0					
Miami	604	1188	1726	968	2339	0				
NYC	748	713	1631	1420	2451	1092	0			
SF	2139	1858	949	1645	347	2594	2571	0		
Seattle	2182	1737	1021	1891	959	2734	2406	678	0	
DC	543	597	1494	1220	2300	923	205	2442	2329	0

– Want to recover locations

[Pellacini et al.]

- Result ($k = 2$):

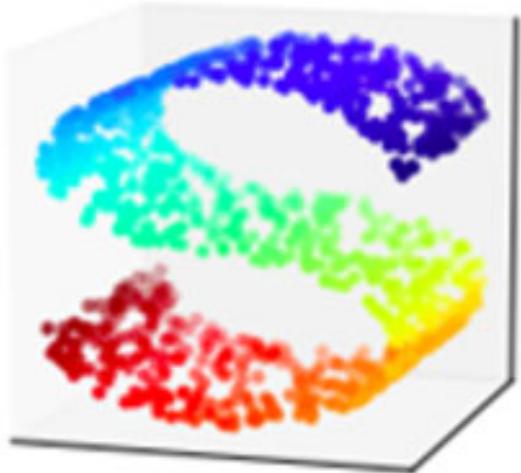


CS 189/289

Today's lecture outline

1. Finish PCA.
2. Non-linear dimensionality reduction (t-SNE)

Recall the “swiss roll” type of data from last class

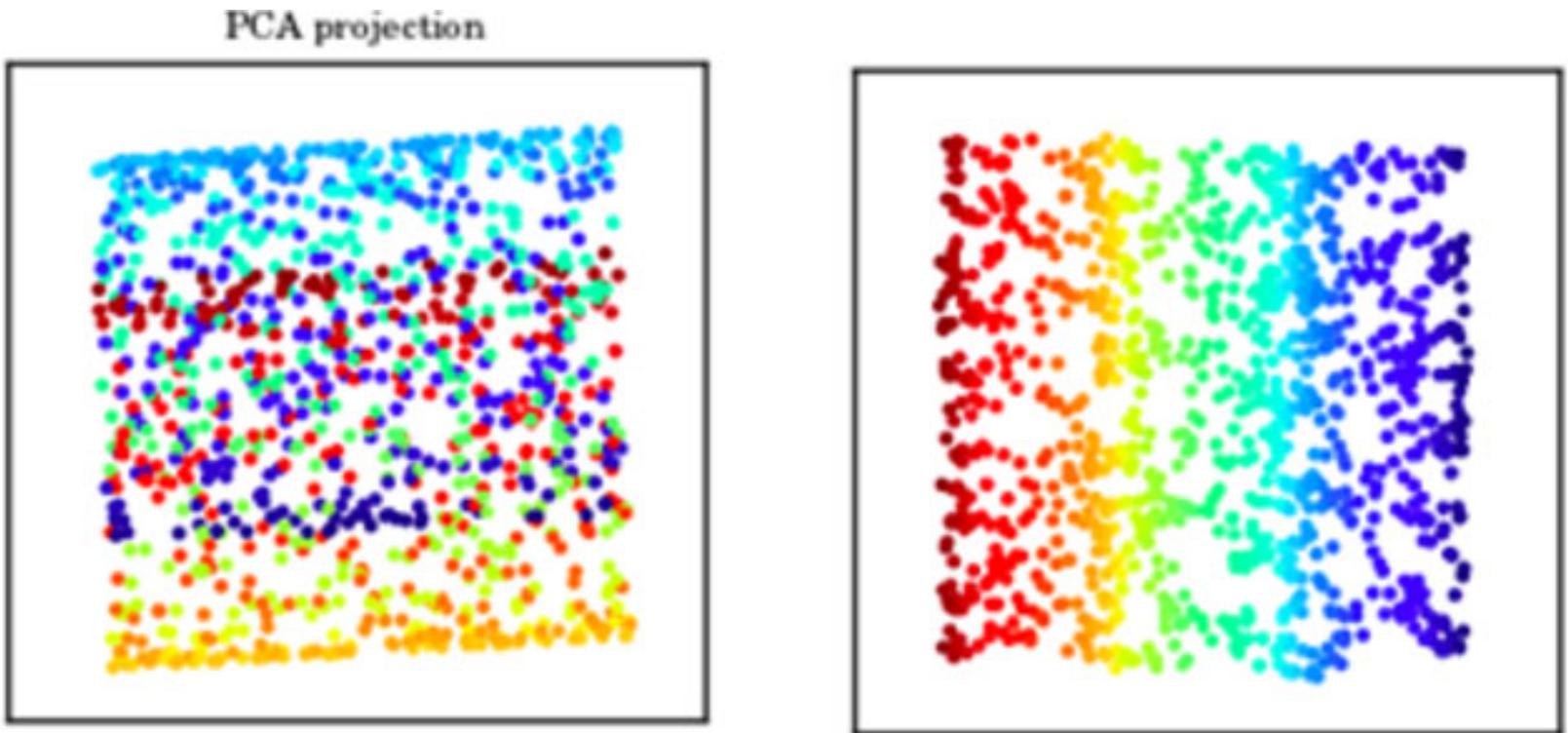
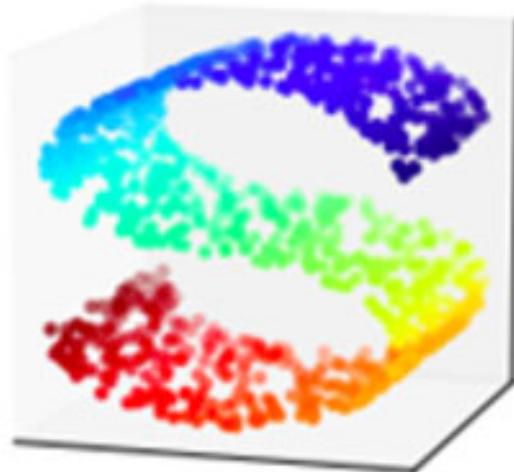


What would happen if we applied PCA with two dimensions to these data?

Ambient dimension=3
Manifold dimensions=2

Hint: PCA is a *linear* transformation,
 $X_k' = XU_k$

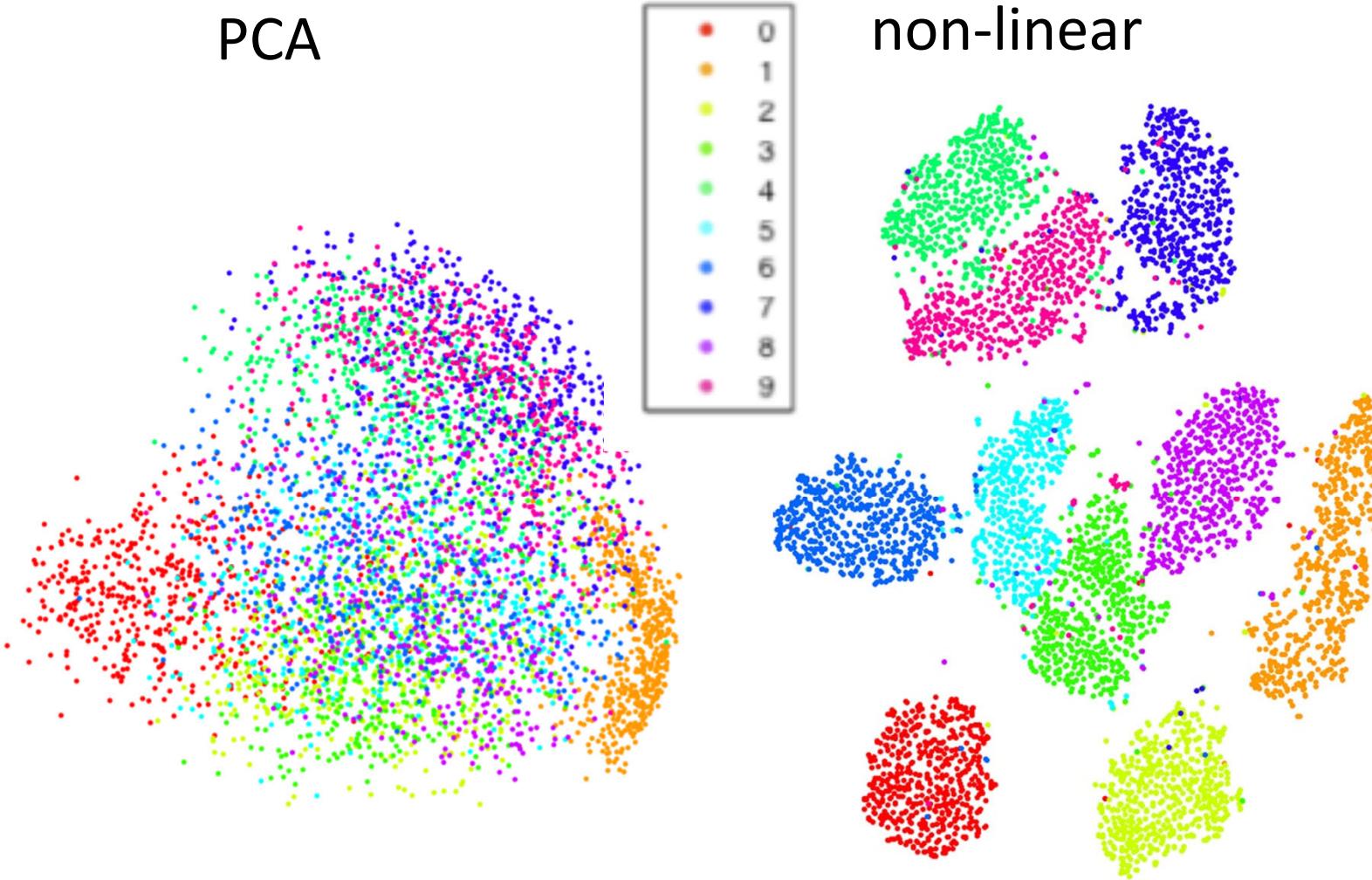
Recall the “swiss roll” type of data from last class



- This is not what we want!
- These data require a non-linear mapping.

PCA vs non-linear embedding on MNIST

PCA



non-linear

Neighborhood embeddings

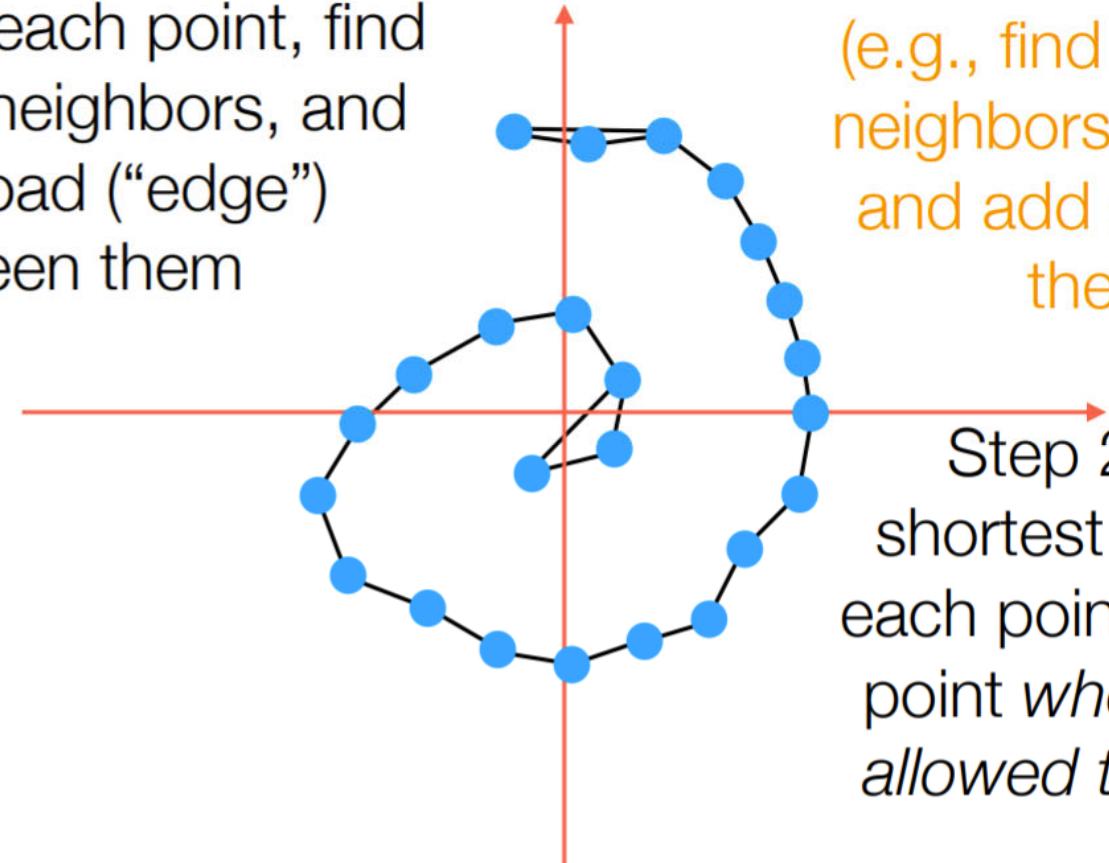
Explicitly try to find a low dimensional embedding that is good at preserving neighborhoods of original points in ambient space.

1. NE: *neighbor embedding* (e.g. *IsoMap* Tenenbaum *et al* 2000)
2. SNE: *stochastic NE* (Hinton & Roweis 2002)
3. t-SNE: *t-distributed SNE* (Van der Maaten & Hinton 2008)

Neighborhood Embedding (NE) aka *Isomap*

Step 1: For each point, find its nearest neighbors, and build a road (“edge”) between them

(e.g., find closest 2 neighbors per point and add edges to them)

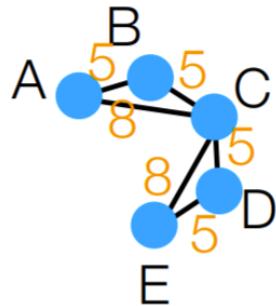


Step 2: Compute shortest distance from each point to every other point *where you're only allowed to travel on the roads*

Step 3: Given this set of pairwise distances, put them in a matrix, M , and perform MDS.

Example of Isomap

In orange: road lengths



- 2 nearest neighbors of A: B, C
- 2 nearest neighbors of B: A, C
- 2 nearest neighbors of C: B, D
- 2 nearest neighbors of D: C, E
- 2 nearest neighbors of E: C, D

Build "symmetric 2-NN" graph

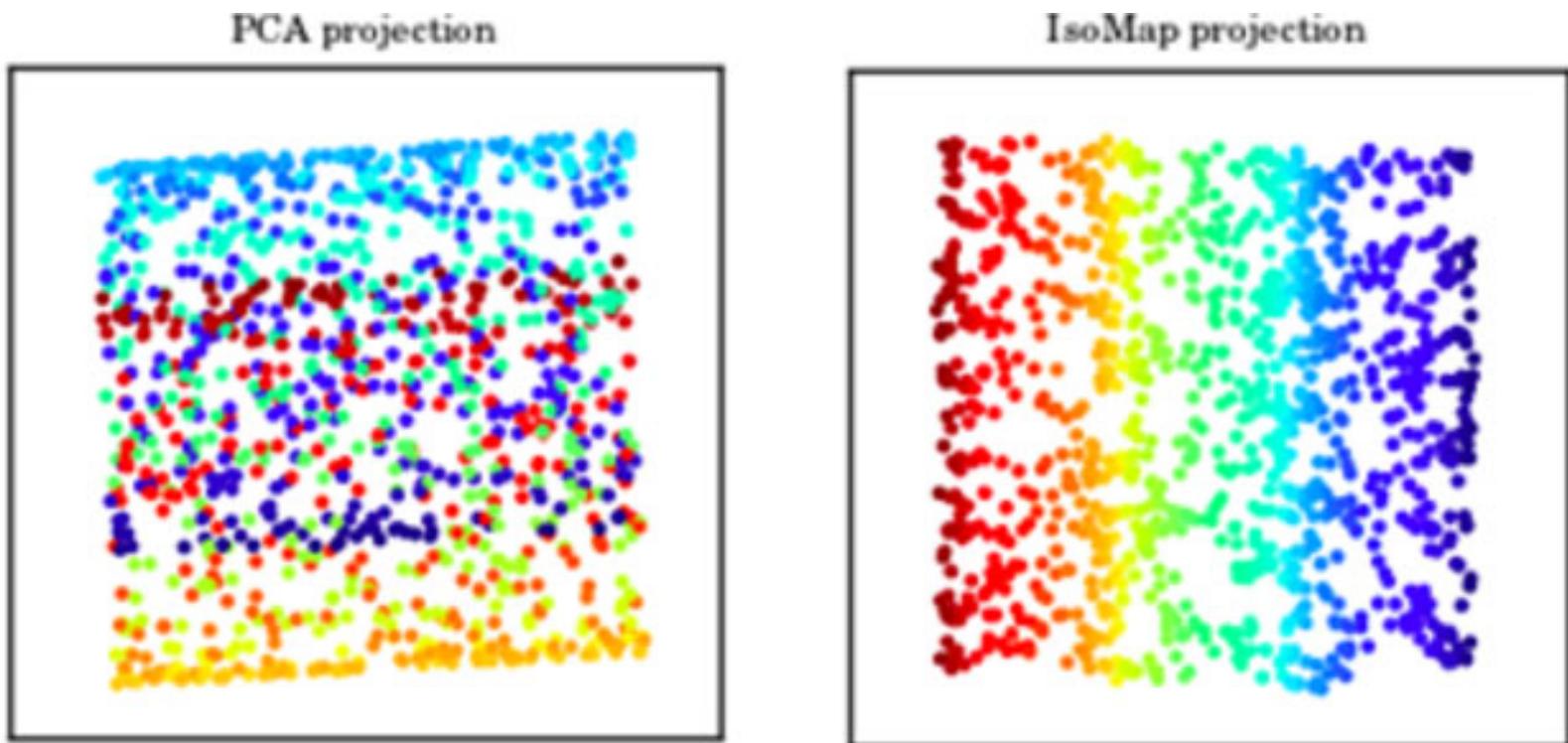
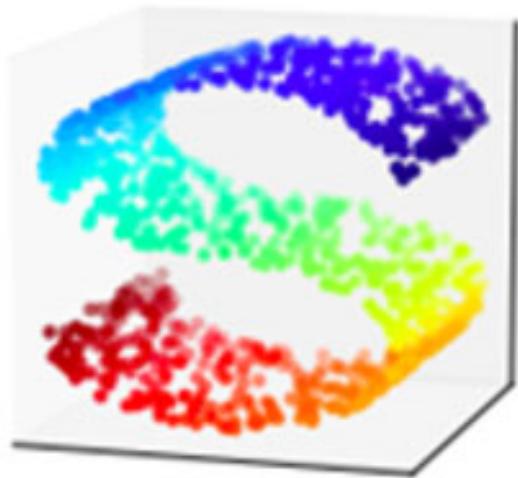
(add edges for each point to
its 2 nearest neighbors)

Shortest distances between
every point to every other
point where we are only
allowed to travel along the
roads

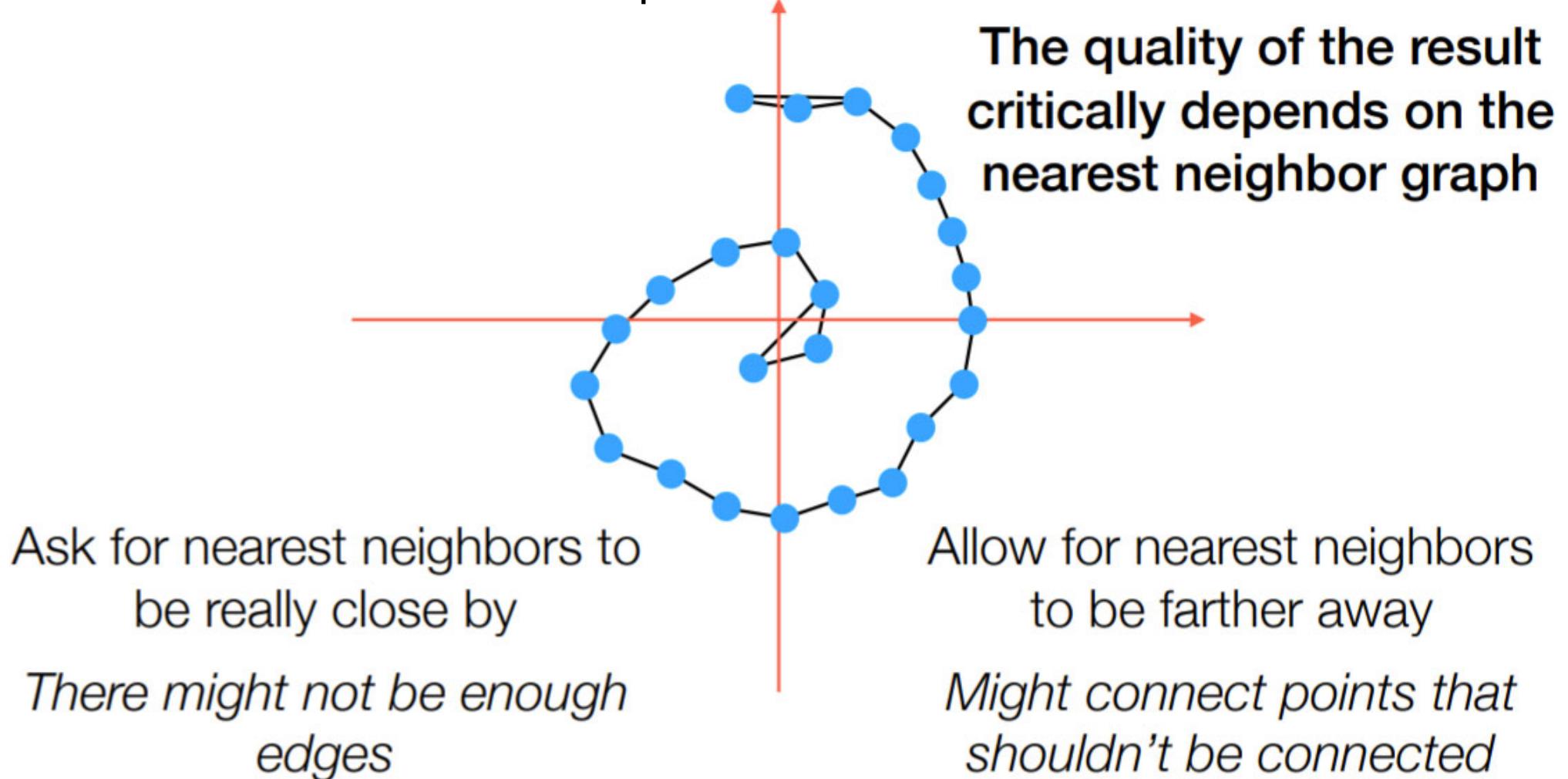
M matrix in MDS

	A	B	C	D	E
A	0	5	8	13	16
B	5	0	5	10	13
C	8	5	0	5	8
D	13	10	5	0	5
E	16	13	8	5	0

IsoMap on Swiss Roll type example

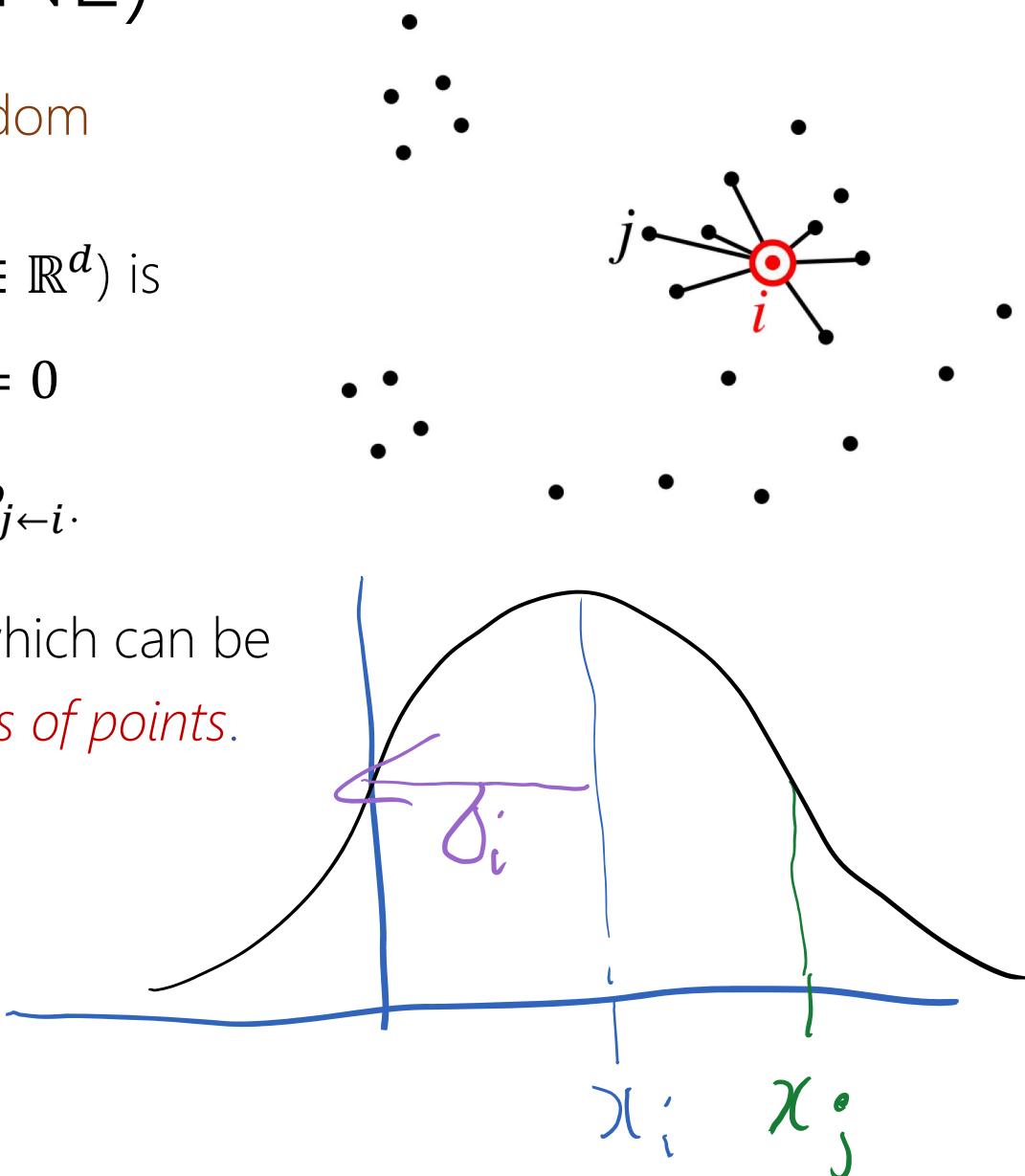


Comments on Isomap



From NE to stochastic NE (SNE)

- Make the event of two samples being neighbors a random variable:
- The probability that x_i “chooses” x_j as its neighbor ($x \in \mathbb{R}^d$) is given by $P_{j \leftarrow i} = \frac{\exp(-\|x_i - x_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|x_i - x_k\|^2 / 2\sigma_i^2)}$, and $P_{j \leftarrow j} = 0$
- Smells like a Gaussian, but normalized so that $1 = \sum_j P_{j \leftarrow i}$.
- Symmetrize & normalize, $P_{ij} = P_{ji} = \frac{1}{2n} (P_{j \leftarrow i} + P_{i \leftarrow j})$ which can be interpreted *as probability to pick this pair out of all pairs of points.*
- Set σ_i^2 adaptively such that entropy of $P_{\cdot \leftarrow i}$ is constant, $\sum_{j \neq i} P_{j \leftarrow i} \log P_{j \leftarrow i}$.



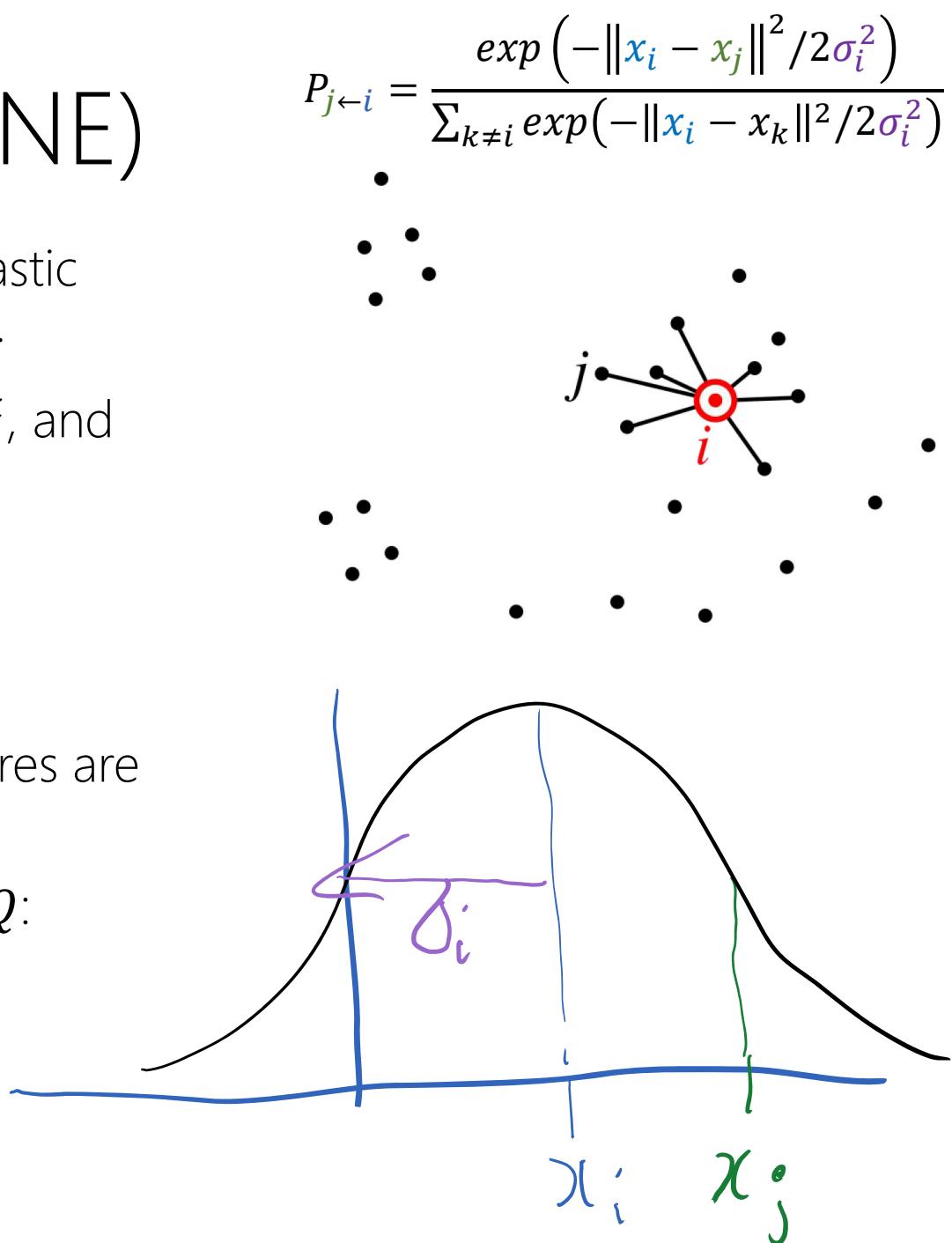
From NE to stochastic NE (SNE)

- From original data, $X \in \mathbb{R}^{n \times d}$, we have defined stochastic neighborhoods with probability distribution, $P = \{P_{ij}\}$.
- Now posit low-dimensional representations, $Y \in \mathbb{R}^{n \times k}$, and define stochastic neighborhoods for them, $Q = \{Q_{ij}\}$,

$$Q_{ji} = \frac{\exp(-\|y_i - y_j\|^2)}{\sum_{l \neq k} \exp(-\|y_l - y_k\|^2)} \quad (\text{setting } \sigma^2 = \frac{1}{2})$$

- Goal: find Y such that stochastic neighborhood structures are preserved ($Q \approx P$).
- Solution: minimize the KL-divergence between P and Q :

$$\hat{Y} = \underset{Y}{\operatorname{argmin}} \text{KL}(P||Q) = \sum_{i,j} P_{ij} \log \frac{P_{ij}}{Q_{ij}}$$



Aside: Kullback-Leibler (KL) Divergence

- Also called *Relative Entropy*.
- Measures how much one distribution diverges from another.
- For discrete probability distributions, P and Q , it is defined as:

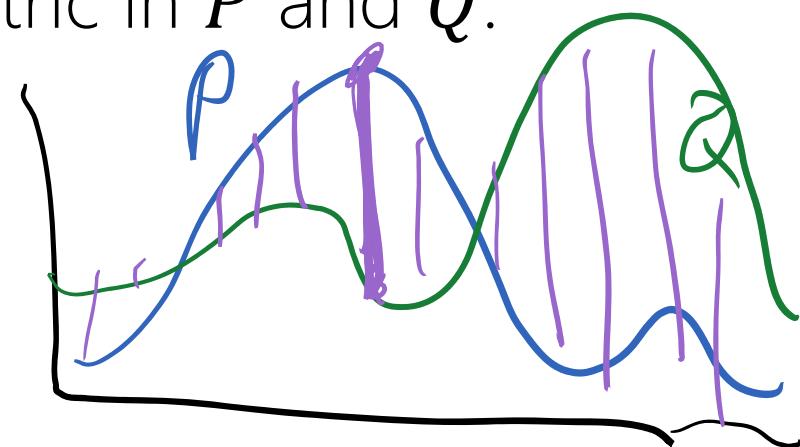
$$D_{KL}(P||Q) = \sum_x P(x) \ln \frac{P(x)}{Q(x)}$$

- Not a true distance metric because not symmetric in P and Q :

$$D_{KL}(P||Q) \neq D_{KL}(Q||P)$$

Properties of KL Divergence

- ▶ $\text{KL}(p\|q) \geq 0$
- ▶ $\text{KL}(p\|q) = 0$ if and only if $p = q$



Aside: Kullback-Leibler (KL) Divergence

$$\begin{aligned} D_{KL}(P||Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\ &= E_{P(x)} \left[\log \frac{1}{Q(X)} \right] - E_{P(x)} \left[\log \frac{1}{P(X)} \right] \end{aligned}$$

Aside: Kullback-Leibler (KL) Divergence

$$\begin{aligned} D_{KL}(P||Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\ &= E_{P(x)} \left[\log \frac{1}{Q(X)} \right] - E_{P(x)} \left[\log \frac{1}{P(X)} \right] \\ &= \underbrace{H(P, Q)}_{\text{cross-entropy}} - \underbrace{H(P)}_{\text{entropy}} \end{aligned}$$

- Consider data, D where $x_i \sim \hat{p}_{data}$ and a model with params θ , $p(x|\theta)$.
- If minimizing the KL divergence (instead of MLE),
 $\arg\min_{\theta} D_{KL}(\hat{p}_{data} || p(x|\theta)) =) =$

Aside: Kullback-Leibler (KL) Divergence

$$\begin{aligned} D_{KL}(P||Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\ &= E_{P(x)} \left[\log \frac{1}{Q(X)} \right] - E_{P(x)} \left[\log \frac{1}{P(X)} \right] \\ &= H(P, Q) - H(P) \end{aligned}$$

cross-entropy *entropy*

no dependence
on θ

- Consider data, D where $x_i \sim \hat{p}_{data}$ and a model with params θ , $p(x|\theta)$.
- If minimizing the KL divergence (instead of likelihood for MLE),

$$\arg\min_{\theta} D_{KL}(\hat{p}_{data} || p(x|\theta)) = \arg\min_{\theta} H(\hat{p}_{data}, p(x|\theta)) + H(\hat{p}_{data})$$

$$= \arg\max_{\theta} E_{\hat{p}_{data}} [\log p(x|\theta)]$$

negative cross-entropy

Aside: Kullback-Leibler (KL) Divergence

$$\begin{aligned} D_{KL}(P||Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\ &= E_{P(x)} \left[\log \frac{1}{Q(X)} \right] - E_{P(x)} \left[\log \frac{1}{P(X)} \right] \\ &= H(P, Q) - H(P) \end{aligned}$$

MLE problem

cross-entropy *entropy*

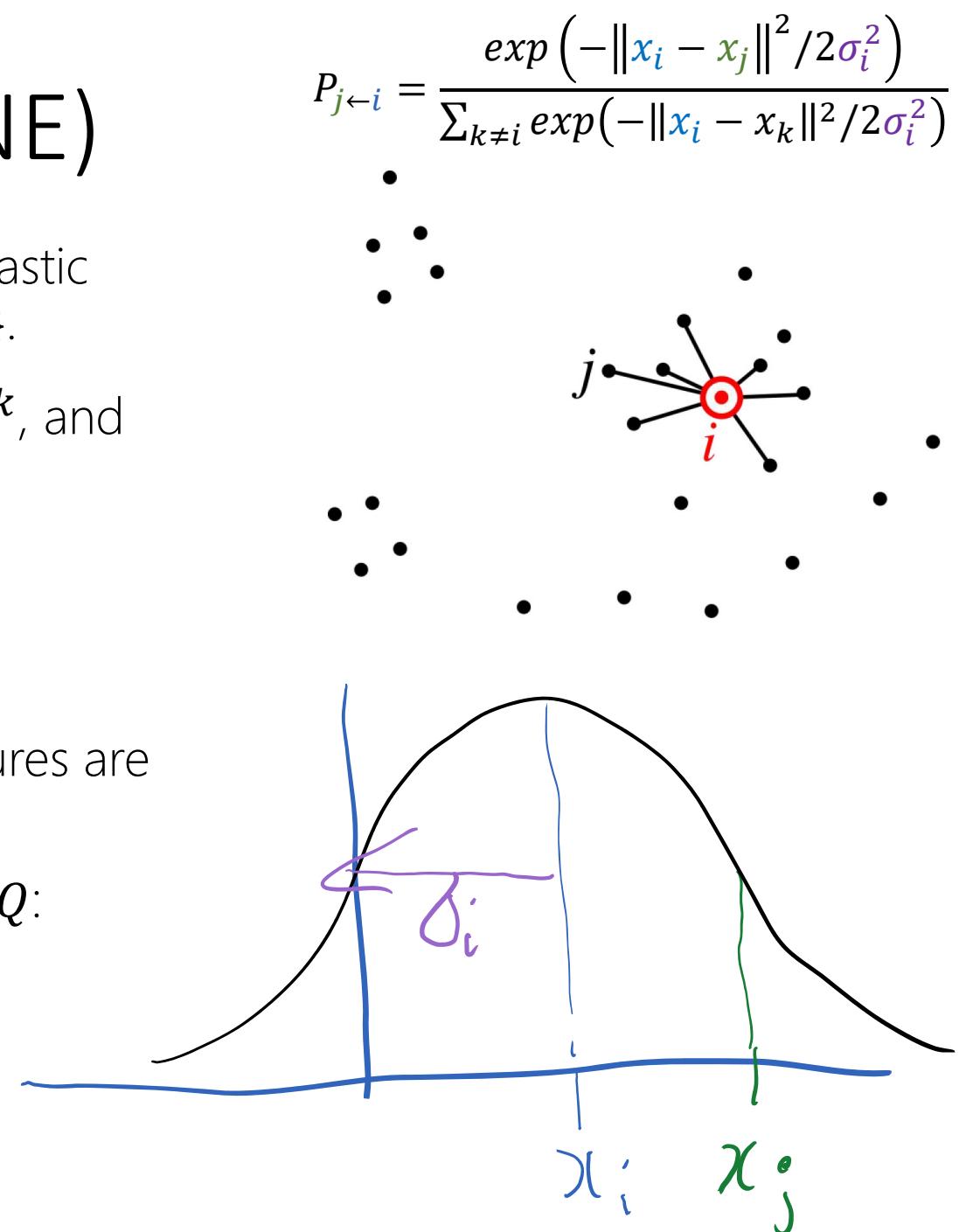
- Consider data, D where $x_i \sim \hat{p}_{data}$ and a model with params θ , $p(x|\theta)$.
- If minimizing the KL divergence (instead of MLE),
$$\arg\min_{\theta} D_{KL}(\hat{p}_{data} || p(x|\theta)) = \arg\min_{\theta} H(\hat{p}_{data}, p(x|\theta)) + H(\hat{p}_{data})$$
$$= \arg\max_{\theta} E_{\hat{p}_{data}} [\log p(x|\theta)] = \arg\max_{\theta} \sum_i^N \log p(x_i|\theta).$$

From NE to stochastic NE (SNE)

- From original data, $X \in \mathbb{R}^{n \times d}$, we have defined stochastic neighborhoods with probability distribution, $P = \{P_{ij}\}$.
- Now posit low-dimensional representations, $Y \in \mathbb{R}^{n \times k}$, and define stochastic neighborhoods for them, $Q = \{Q_{ij}\}$,

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SNE: miminizing the loss function

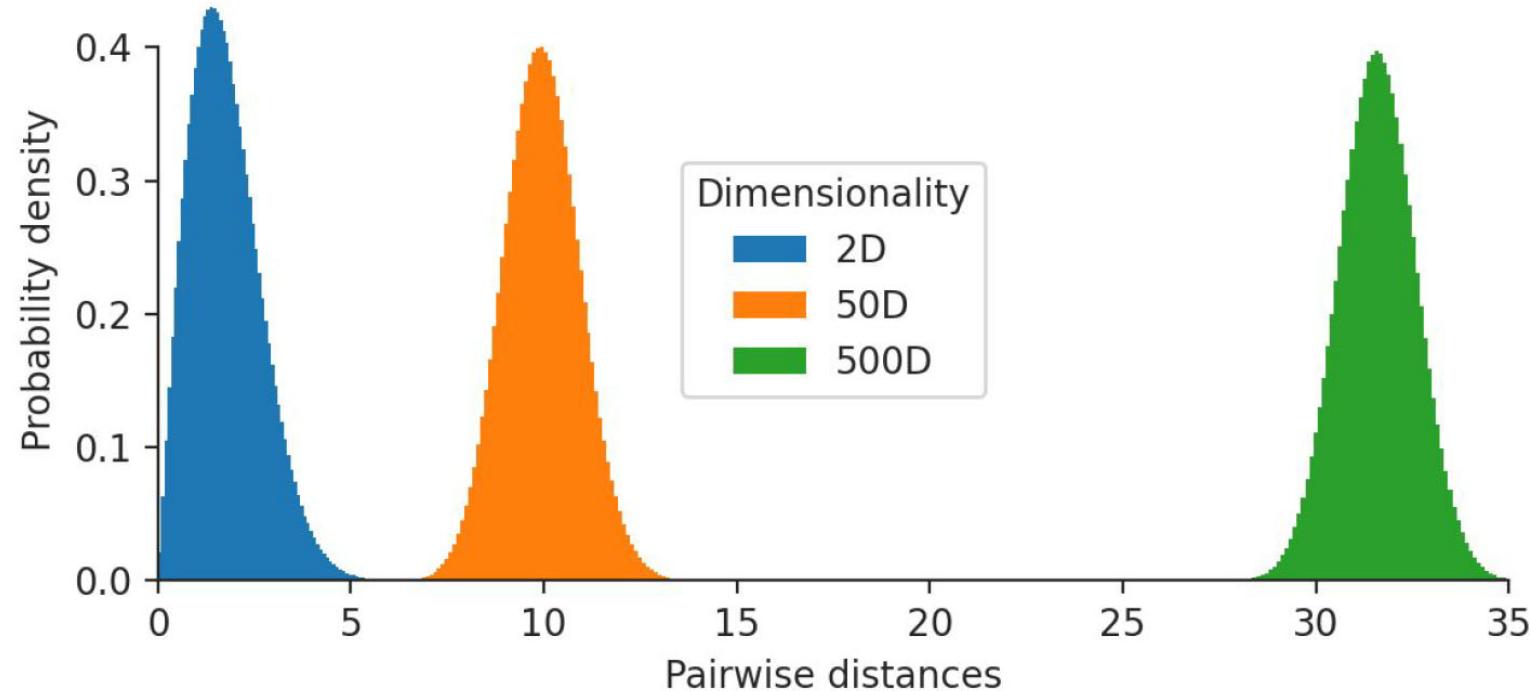
$$\hat{Y} = \underset{Y}{\operatorname{argmin}} KL(P||Q) = \sum_{i,j} P_{ij} \log \frac{P_{ij}}{Q_{ij}}.$$

- Use gradient descent to find embedded points, $\{y_i\}$
- Can show that $\frac{\partial Loss}{\partial y_i} = \sum_j (P_{ij} - Q_{ij})(y_i - y_j)$.
- Not a convex optimization problem, so there are many local minima.

Problem with SNE

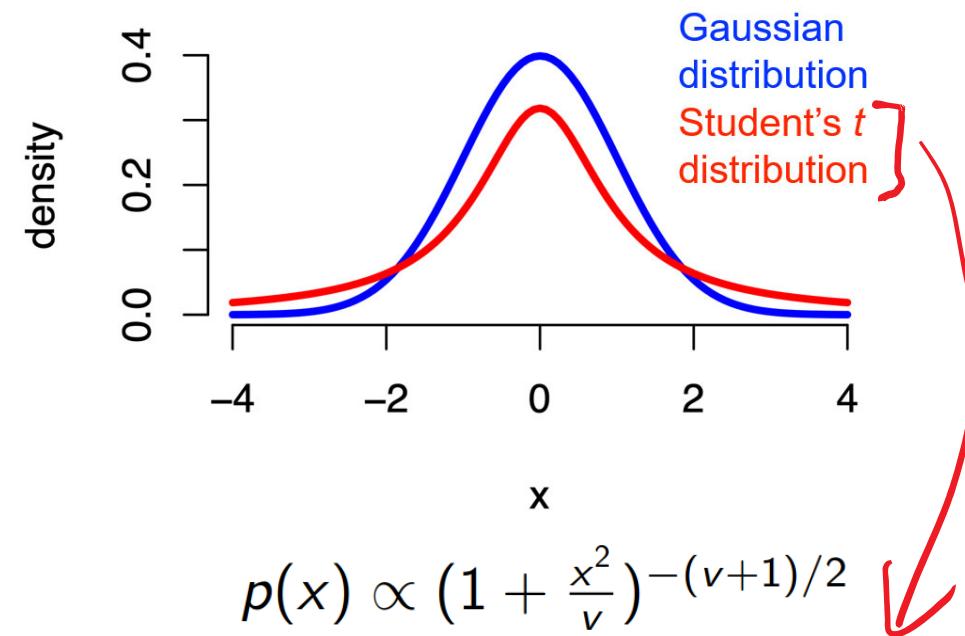
When we try to maintain the same neighborhood probabilities between the low and high dimensional spaces, we end up “crowding” the points in the lower dimensional space.

Pairwise distances between points in a standard Gaussian:



Fixing SNE with t-SNE

- Change the distribution in the embedding space, Q_{ij} to have a heavier-tailed distribution, a t-distribution.
- SNE used $Q_{j \leftarrow i} = \frac{\exp(-\|y_i - y_j\|^2)}{\sum_{i \neq k} \exp(-\|y_i - y_k\|^2)}$
- t-SNE uses $Q_{j \leftarrow i} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{i \neq k} (1 + \|y_i - y_k\|^2)^{-1}}$
- Everything else remains the same as in SNE.



for $v = 1$ we get $p(x) \propto \frac{1}{1+x^2}$

Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

Data: data set $X = \{x_1, x_2, \dots, x_n\}$,

cost function parameters: entropy constant, C to set σ_{ij}

optimization parameters: number of iterations T , learning rate η

Result: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \dots, y_n\}$.

begin

 compute pairwise affinities $p_{j|i}$ with entropy constant, C to set σ_{ij}

 set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$

 sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \dots, y_n\}$ from $\mathcal{N}(0, 10^{-4}I)$

for $t=1$ **to** T **do**

 compute low-dimensional affinities q_{ij} (using Equation 4)

 compute gradient $\frac{\delta C}{\delta \mathcal{Y}}$ (using Equation 5)

 set $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}}$

end

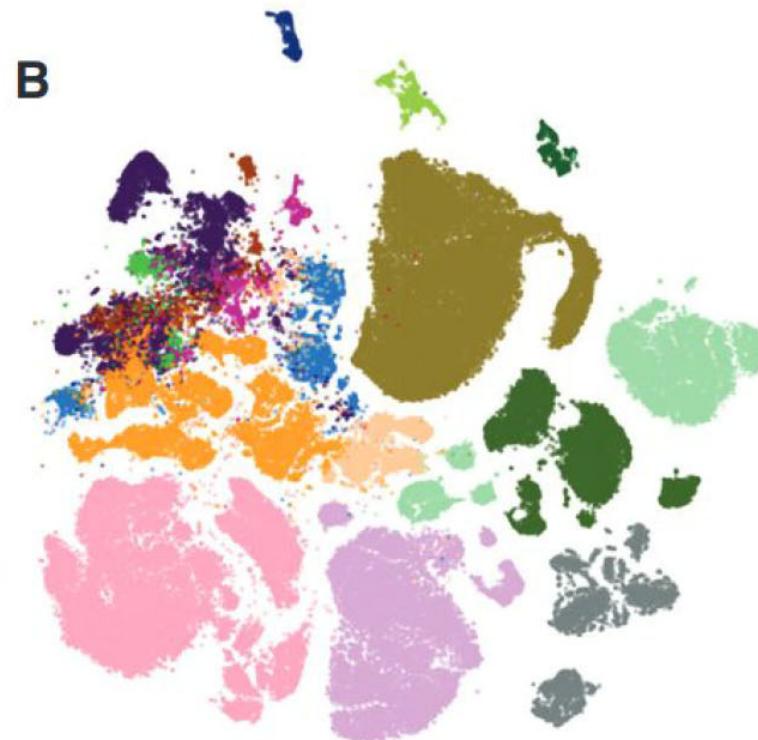
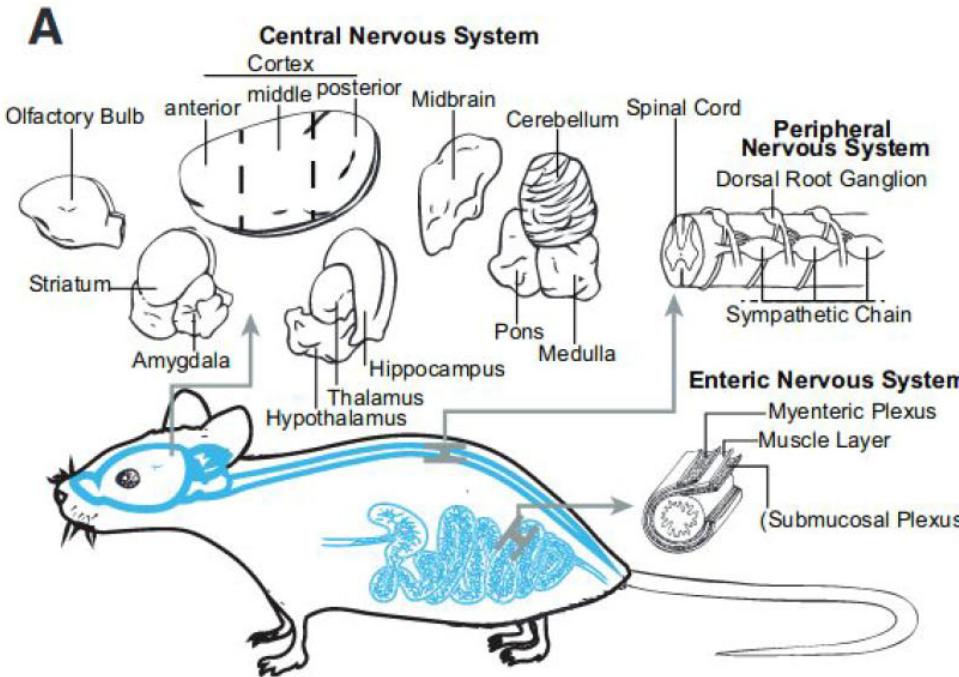
end

t-SNE on MNIST

(each color labels
one of the 10 digits)



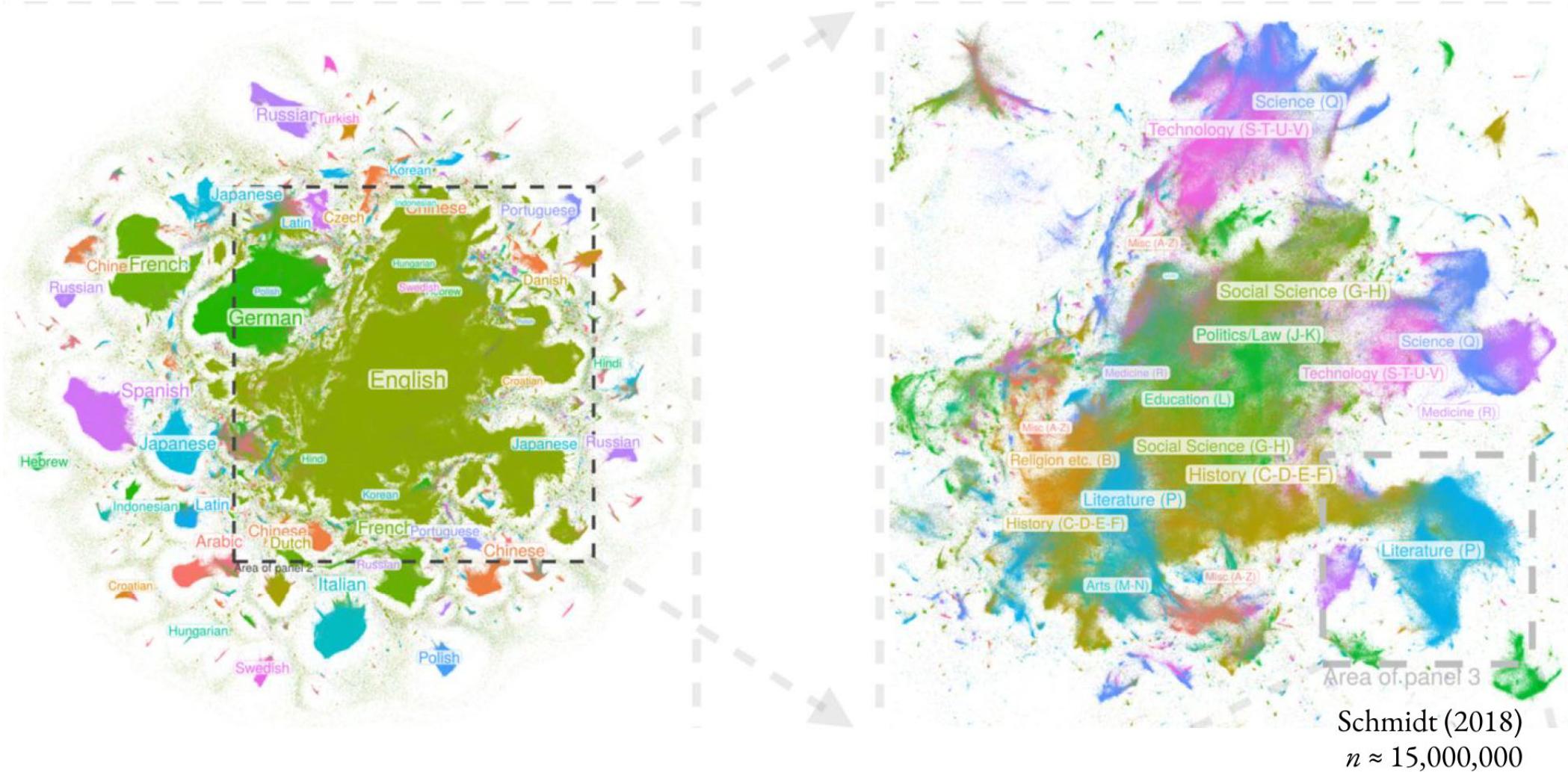
Single-cell transcriptomics (single-cell RNA sequencing): samples are cells, features are genes.



- Astroependymal cells
- Cerebellum neurons
- Cholinergic, monoaminergic, peptidergic
- Di- and mesencephalon neurons
- Enteric neurons
- Hindbrain neurons
- Immature neural
- Immune cells
- Neural crest-like glia
- Oligodendrocytes
- Peripheral sensory neurons
- Spinal cord neurons
- Sympathetic neurons
- Telencephalon interneurons
- Telencephalon projecting neurons
- Vascular cells

Zeisel et al. (2018)
 $n \approx 500,000$

Digital humanities: samples are books, features are words.



Schmidt (2018)
 $n \approx 15,000,000$



Some pros and cons: PCA vs t-SNE

PCA—captures global structure via shared PC axes.

- No issues with local minima / sub-optimal solutions---SVD gives minimal.
- Projection axes can be examined for interpretability.
- Can be computed efficiently (SVD)
- Can embed new points without updating the embedding space.
- Limited to capturing linear structures (but can be generalized using augmented feature space/kernels).

t-SNE—captures local structure by preserving neighborhoods

- Can model non-linear manifolds.
- Thus can preserve richer local structures (e.g. think swiss roll).
- Expensive to compute, but there are tricks to speed it up.
- Subject to local minima during optimization.
- No explicit projection mapping, so:
 - less potential for interpretability
 - cannot be applied to new points (no explicit mapping given).---must re-run it.