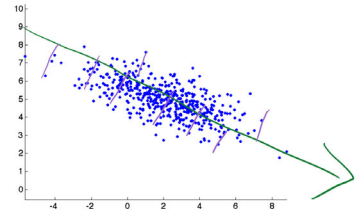
# CS 189/289

Today's lecture outline

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

Assigned reading: none
(t-SNE is not in the book)

# 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 $X^T X = QDQ^T$)

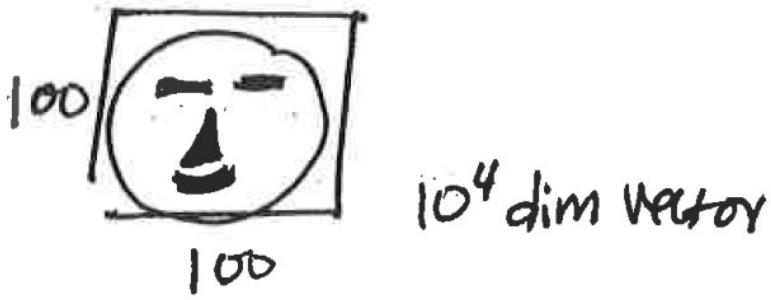
Reconstruction, $X_{recon-k} = XQ_kQ_k^T$

# Linear algebra for PCA

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

- Need to compute the principal axes, $Q$, of $\bar{X}^T \bar{X} = QDQ^T \in \mathbb{R}^{d \times d}$.
- This is an *eigendecomposition* of the matrix $\bar{X}^T \bar{X}$.

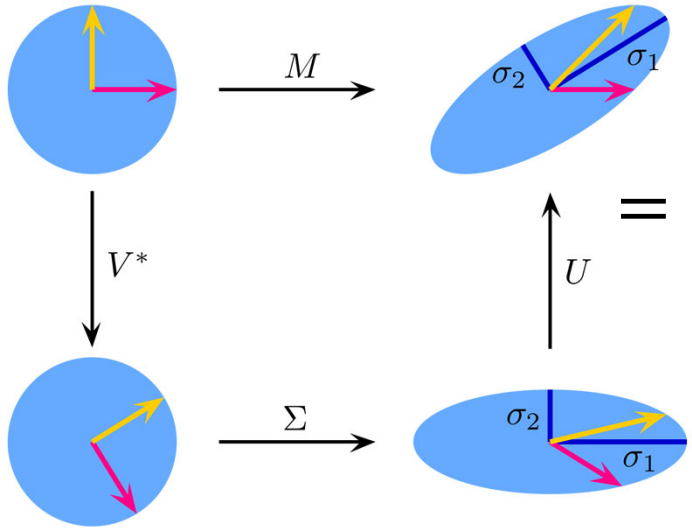
- Computing its eigendecomposition has time complexity $O(d^3)$.
- What if $d \gg n$? *e.g.*, images of $\mathbf{d = 100 \times 100 = 10^4}$ pixels, and $n = \mathbf{1{,}000}$ images.
- Could we do something cheaper?
- Yes. Need to understand the SVD.



# 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 $e_2$:

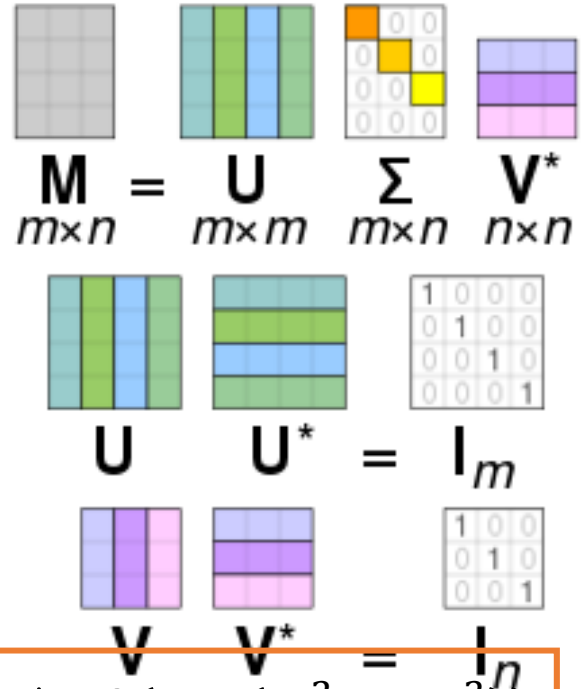
1. **Left: $V^T$** rotates the disc and unit vectors.
2. **Bottom: Σ** stretches scales axes by $\sigma_i = \Sigma_{i,i}$ (singular values).
3. **Right: U** performs another rotation.




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

$$= M \begin{bmatrix} e_2 \\ e_1 \end{bmatrix} = U\Sigma V^* \begin{bmatrix} e_2 \\ e_1 \end{bmatrix}$$

Can be applied to any matrix $M$.




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

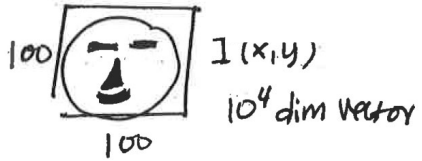
$$r = rank(M) \leq \min(m, n)$$

- *Has time complexity $O(\min(m^2n, mn^2))$.*
- *$\Sigma$ 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.*

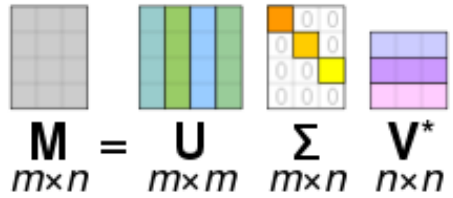
https://en.wikipedia.org/wiki/Singular_value_decomposition

# Singular Value Decomposition (SVD)

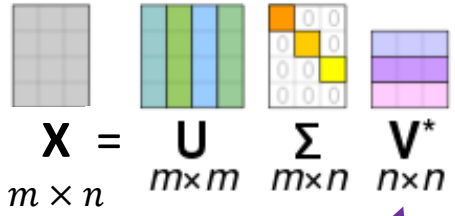
$X \in \mathbb{R}^{n \times d}$




- 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 $O(dn^2)$.



# Singular Value Decomposition (SVD)

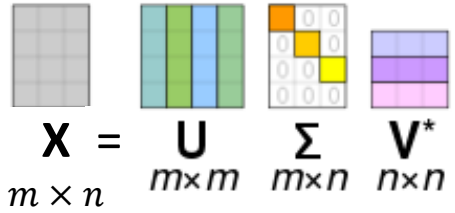



For PCA we want projections onto top $k$ PCs.

- When we used a spectral decomposition, $X^T X = QDQ^T$, we compute: $X_k = XQ_k \in \mathbb{R}^{n \times k}$ ($Q$ are eigvecs of $X^T X$).
- When using the SVD of $X$, we can instead get this from:
- $X_k = XV_{:,1:k}$

*columns $V$ are eigenvectors of $X^T X$*

# Singular Value Decomposition (SVD)




For PCA we want projections onto top $k$ PCs.

- When we used a spectral decomposition, $X^T X = QDQ^T$, we compute: $X_k = XQ_k \in \mathbb{R}^{n \times k}$ ($Q$ are eigvecs of $X^T X$).
- When using the SVD of $X$, we can instead get this from:
- $X_k = XV_{:,1:k} = U_{:,1:k}\Sigma_{1:k,1:k} \in \mathbb{R}^{n \times k}$ ("scores" in PCA basis).
- $X_{k-recon} = XV_{:,1:k}(V_{:,1:k})^T = U_{:,1:k}\Sigma_{1:k,1:k}(V_{:,1:k})^T$
- We don't need to compute covariance matrix, or do the projections, we just need $SVD(X)$!

$$Xv_i = \Sigma_{i,i}u_i$$

# "Eckart Young theorem" 1936

- The SVD "k-reconstruction" produces the best $\boldsymbol{k}$-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.

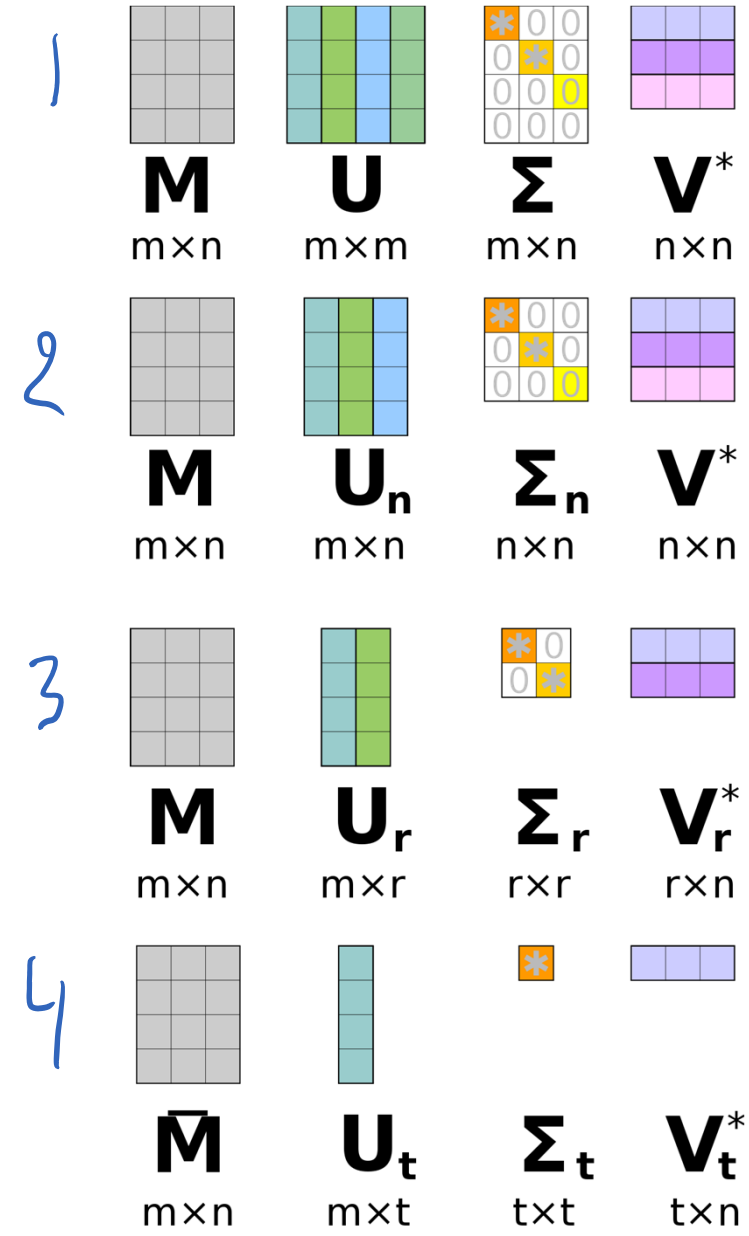
$$\|\mathbf{A}\|_F \equiv \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2}$$

*https://en.wikipedia.org/wiki/Low-rank_approximation#Proof_of_Eckart%E2%80%93Young%E2%80%93Mirsky_theorem_(for_spectral_norm)*

# Practicalities: Reduced SVDs

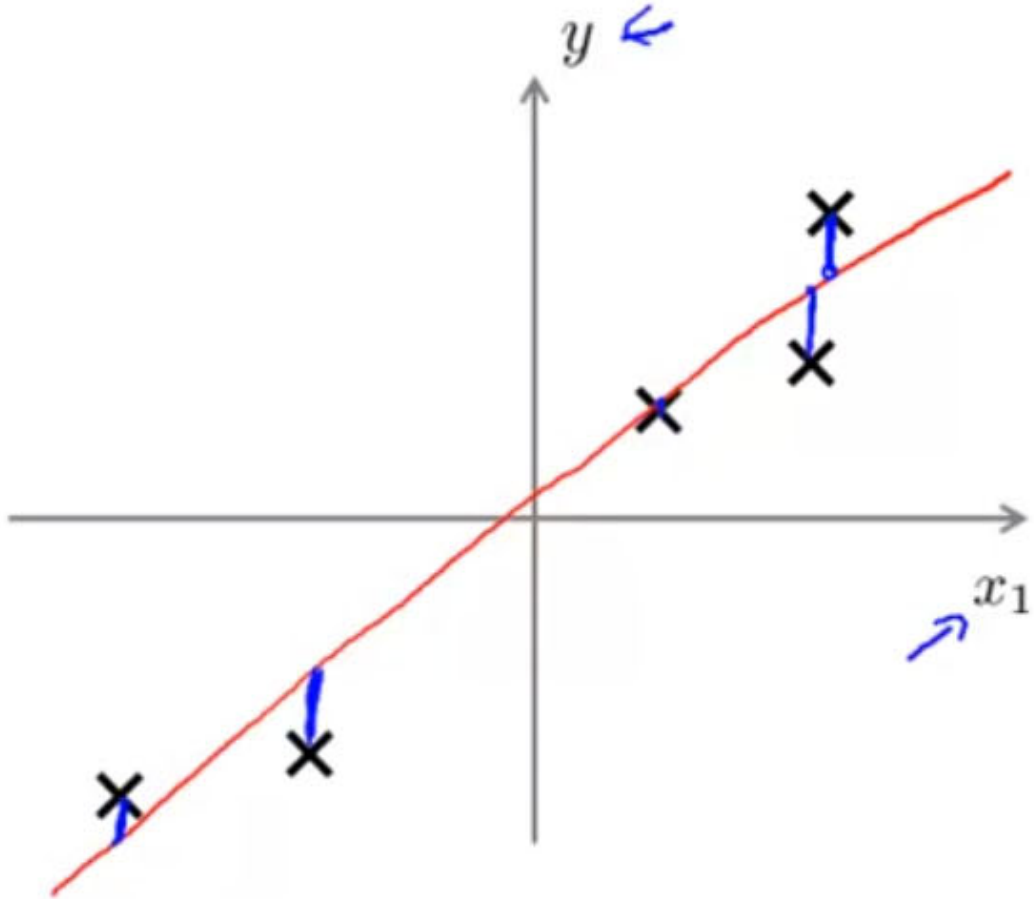
For PCA and other applications, don't need the entire SVD, and can make do with "trimmed down" versions:

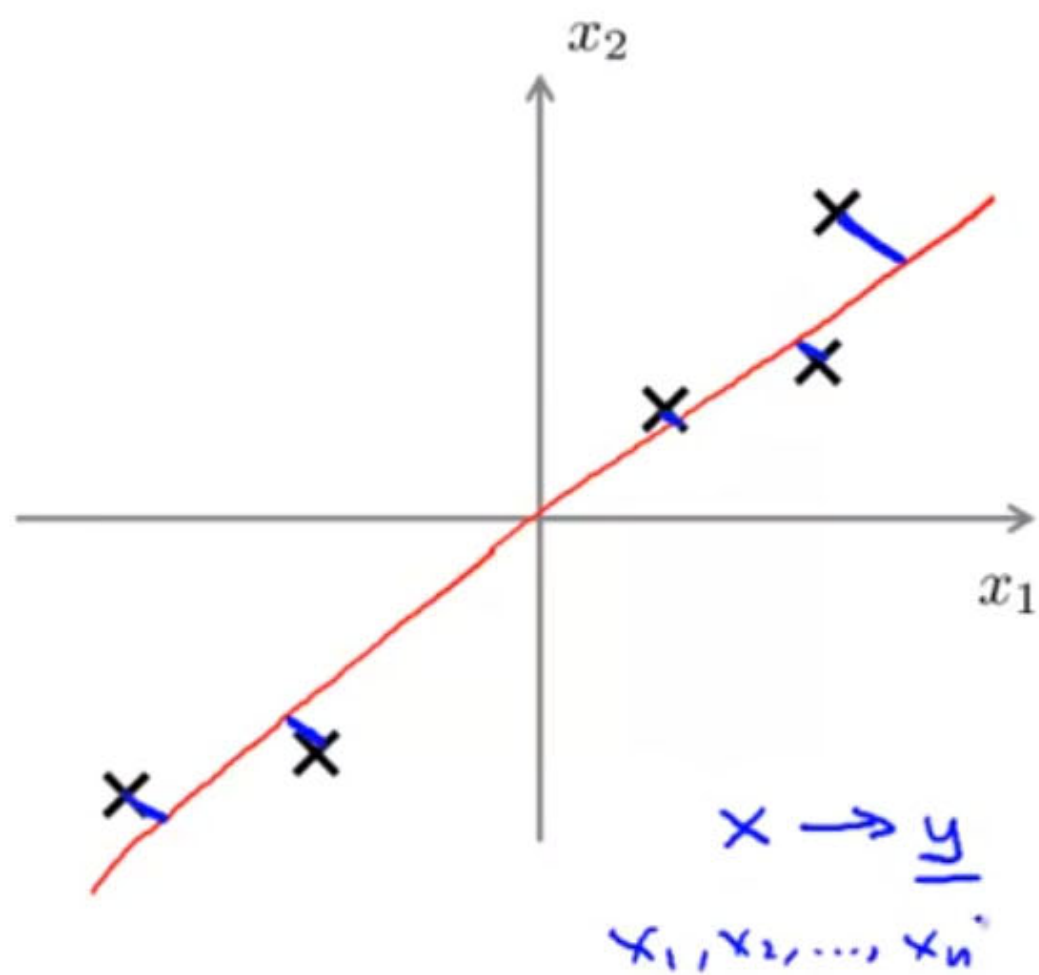
1. Full SVD
2. Thin SVD (remove columns of U not corresponding to rows of V*)
3. Compact SVD (remove vanishing singular values and corresponding columns/rows in U and V*),
4. Truncated SVD (keep only largest t singular values and corresponding columns/rows in U and V*)




https://en.wikipedia.org/wiki/Singular_value_decomposition

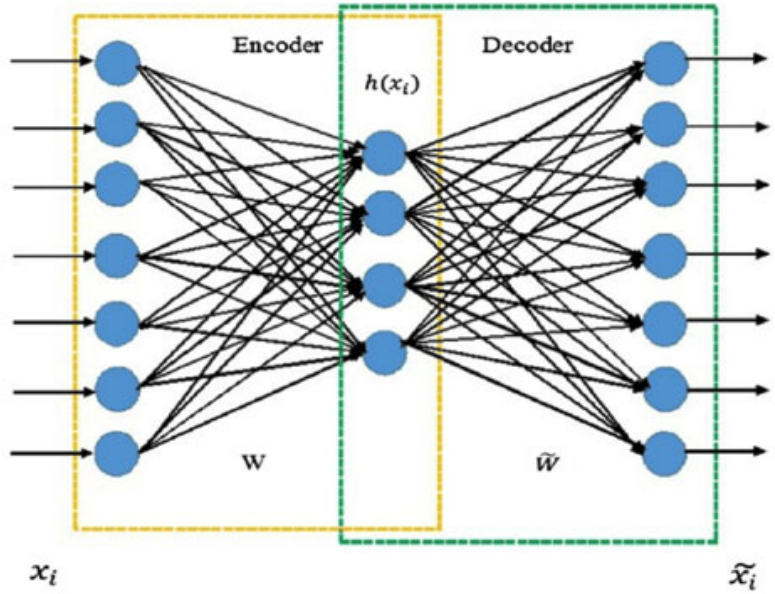
# PCA is not linear regression



# 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 activations, more layers, etc.




https://towardsdatascience.com/understanding-pca-autoencoders-algorithms-everyone-can-understand-28ee89b570e2

# 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 $X^T X$ as with PCA).
- Now new basis is in $U$ from: $M = USV^T$.

- 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 ($k = 2$):


We just performed *Multidimensional Scaling* (MDS):

- Implicitly assumes some latent space $X$ of unknown dimension for which the distance is an inner product distance, $\mathbf{d}(\mathbf{x}', \mathbf{x}) = x' x^T$.
- Could be non-linear distance function of actual $x$ (*e.g.*, if latent space had a polynomial expansion).

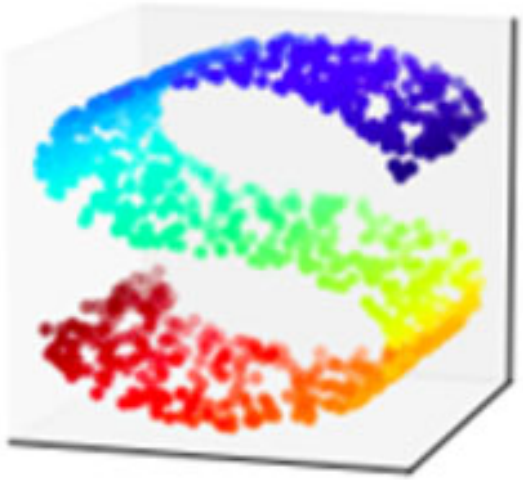
https://www.cs.princeton.edu/courses/archive/fall13/cos323/notes/cos323_f13_lecture11_dim_red.pdf

# 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



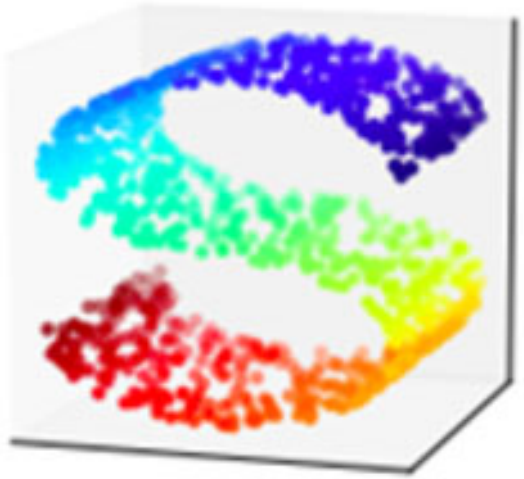
What would happen if we applied PCA with two dimensions to these data?

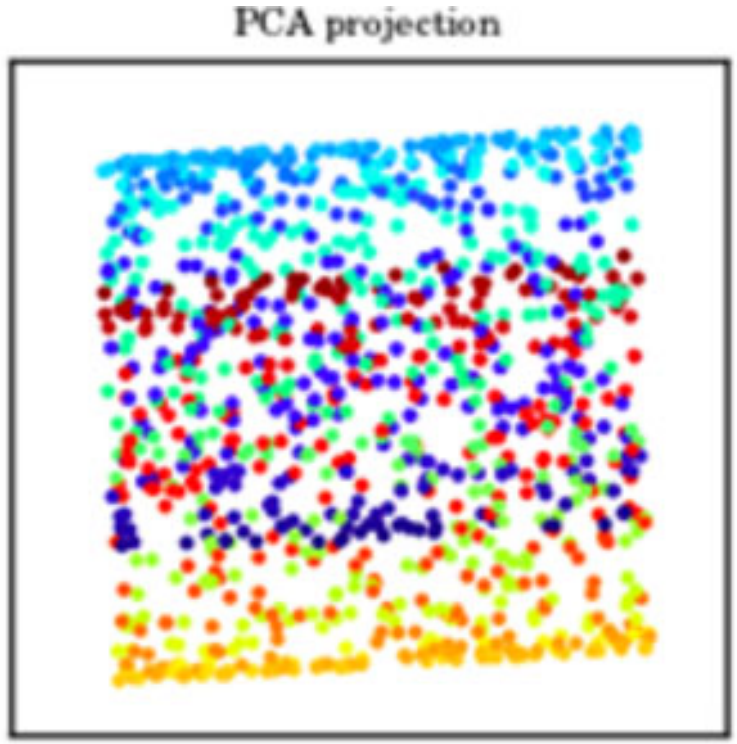
Ambient dimension=3
Manifold dimension=2

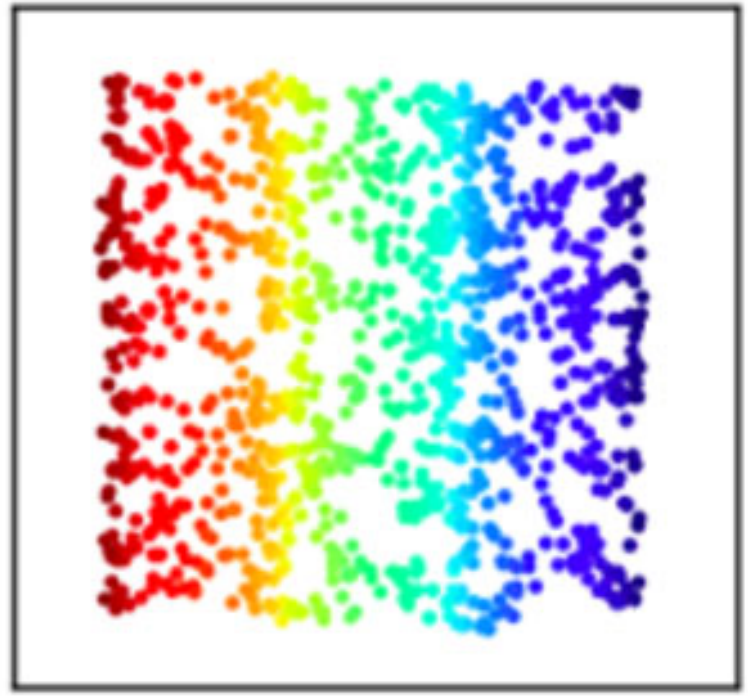
Hint: PCA is a *linear* transformation,
$X_k' = XU_k$

https://jhui.github.io/2017/01/15/Machine-learning-Multi-dimensional-scaling-and-visualization/

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





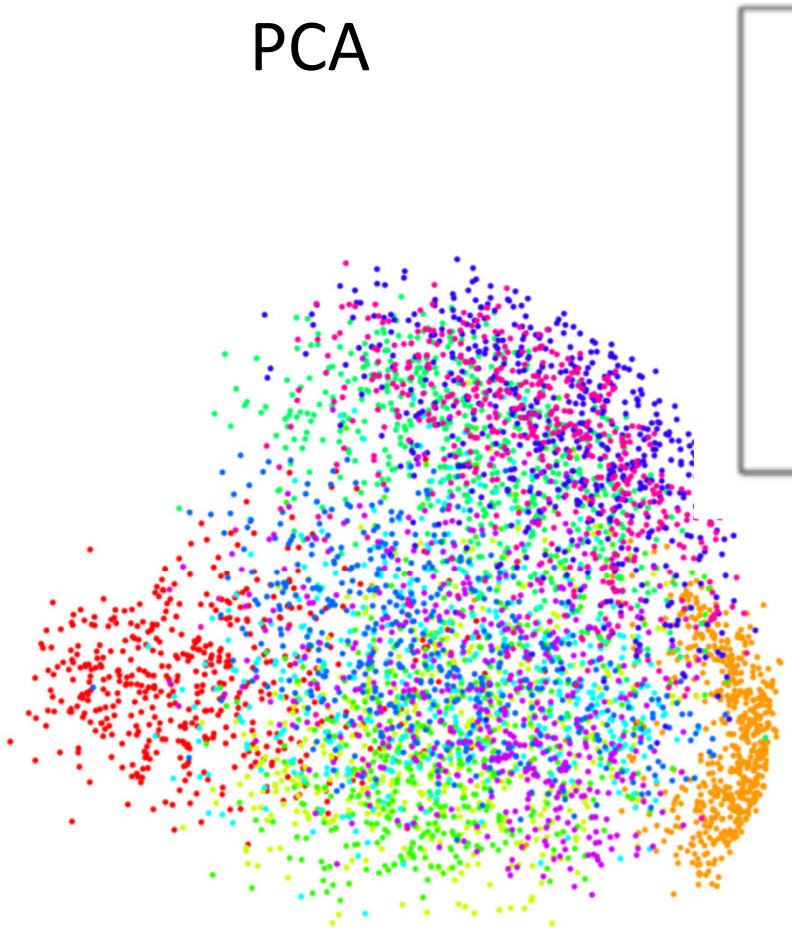



- This is not what we want!
- These data require a non-linear mapping.

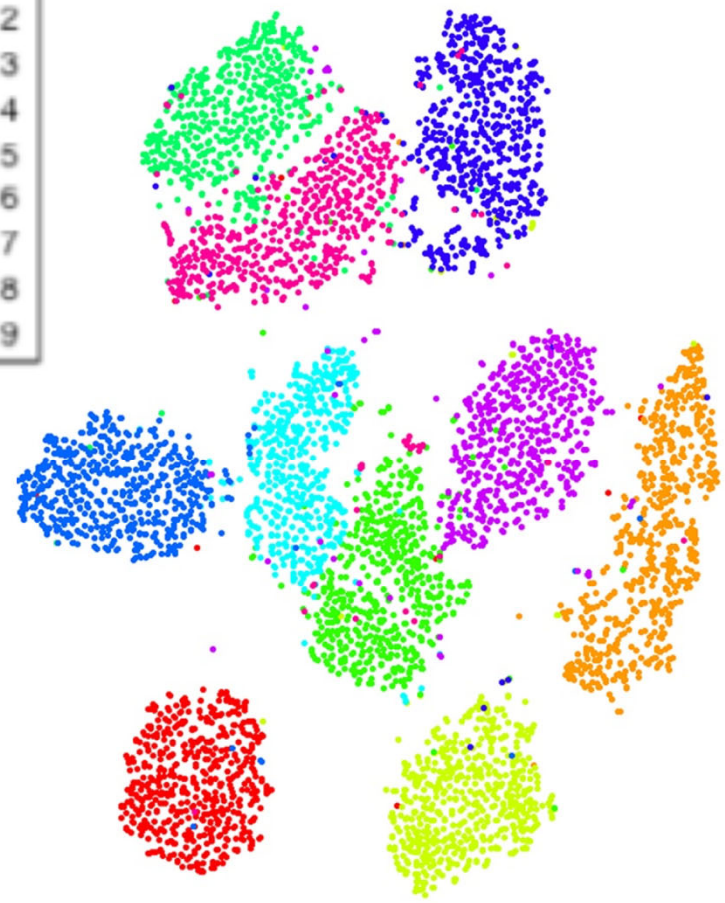
*https://jhui.github.io/2017/01/15/Machine-learning-Multi-dimensional-scaling-and-visualization/*

# PCA vs non-linear embedding on MNIST

PCA




non-linear



# Neighborhood embeddings

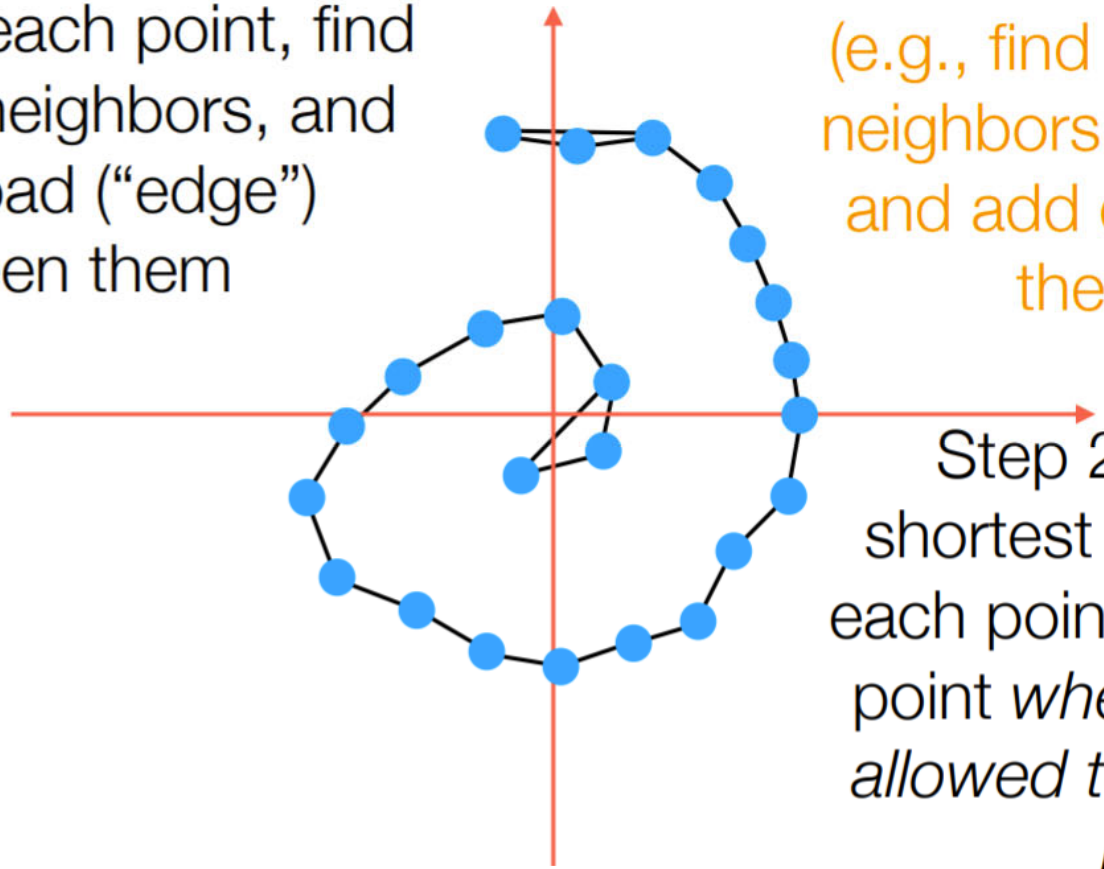
Explicitly try to find a low dimensional embedding that is good at preserving neighborhoods of original points in ambient space.

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)



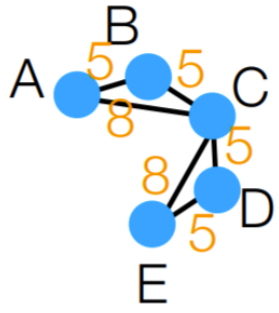
Step 2: Compute shortest distance from each point to every other point *where you're only allowed to travel on the roads*

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

https://www.andrew.cmu.edu/user/georgech/95-865/Lectures/Lecture%20-%2003_essence.pdf

# 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)

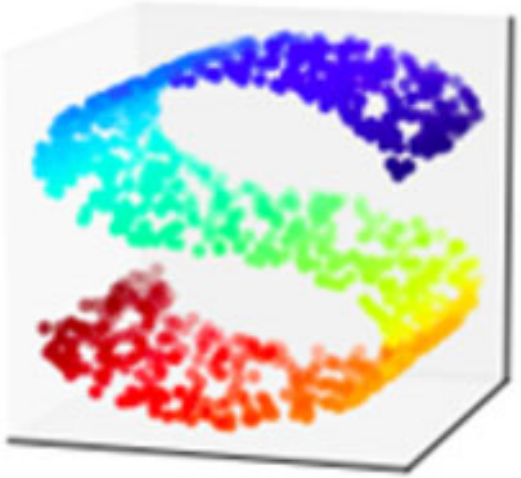
Shortest distances between every point to every other point *where we are only allowed to travel along the roads*

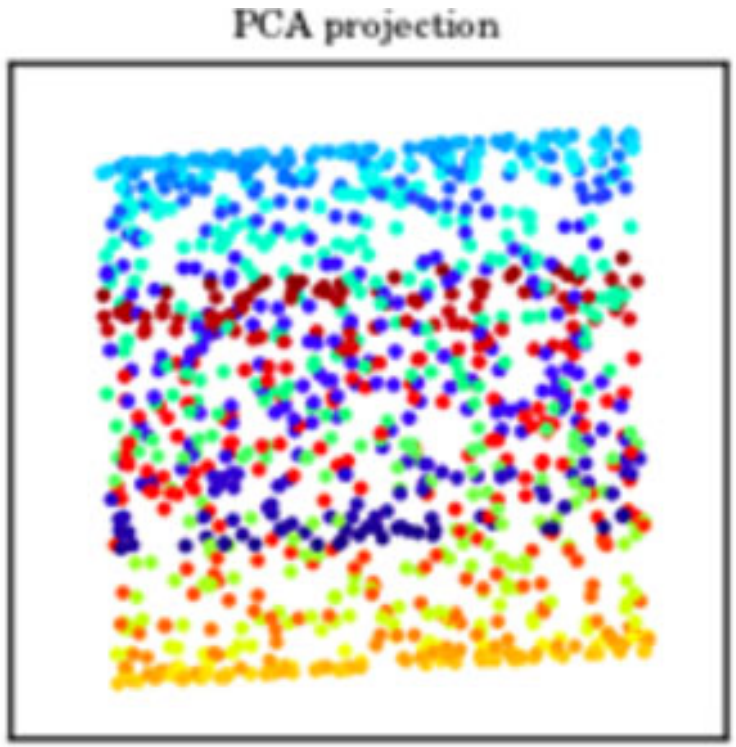
| | A | B | C | D | E |
|---|---|---|---|---|---|
| A | 0 | 5 | 8 | 13 | 16 |
| B | 5 | 0 | 5 | 10 | 13 |
| C | 8 | 5 | 0 | 5 | 8 |
| D | 13 | 10 | 5 | 0 | 5 |
| E | 16 | 13 | 8 | 5 | 0 |

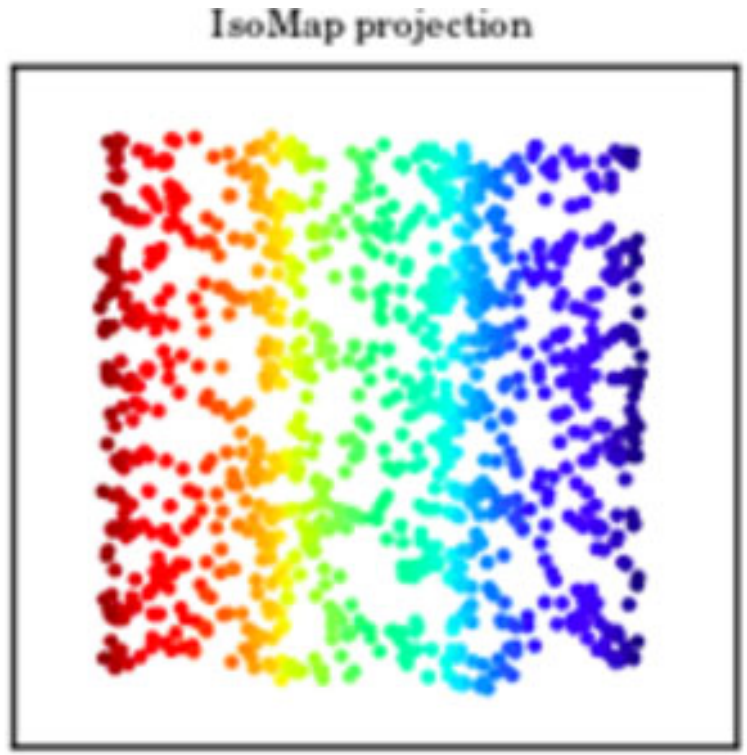
M matrix in MDS

https://www.andrew.cmu.edu/user/georgech/95-865/Lectures/Lecture%20-%2003_essence.pdf

# IsoMap on Swiss Roll type example

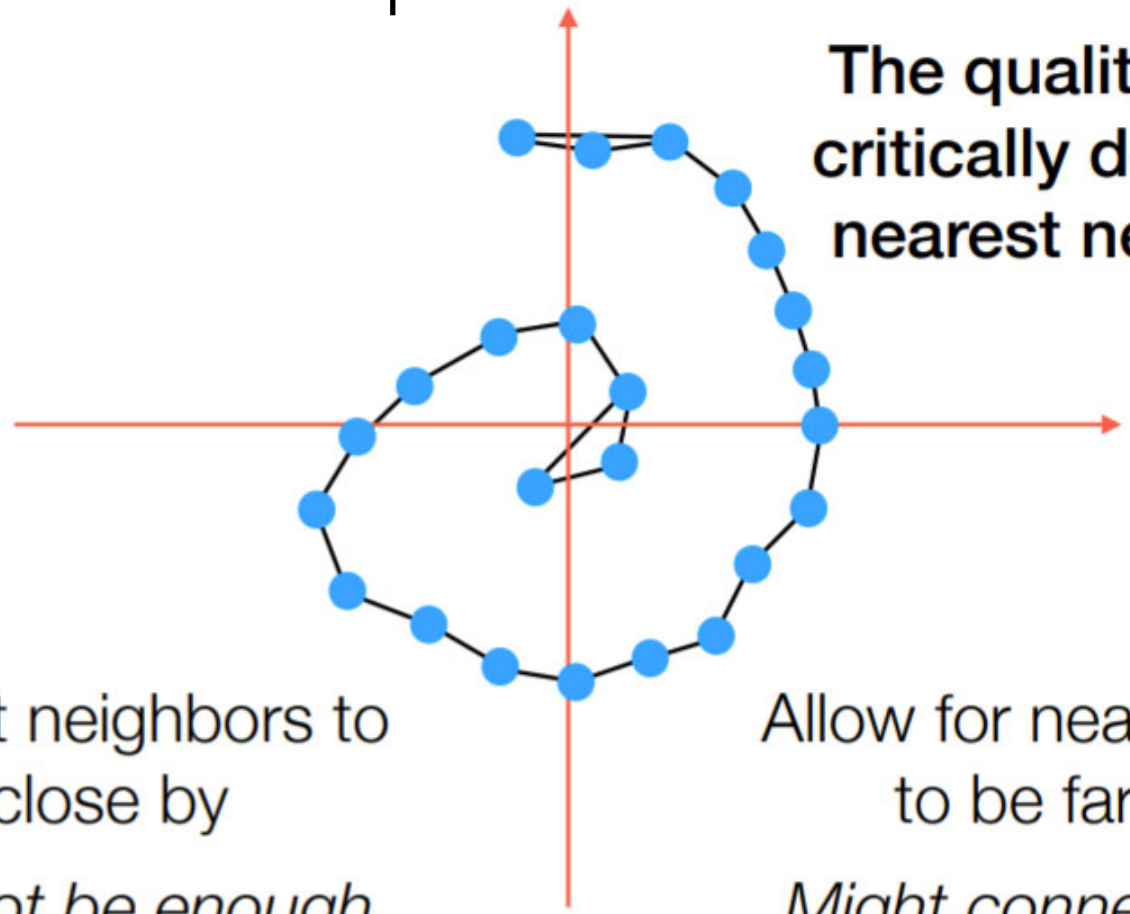





*https://jhui.github.io/2017/01/15/Machine-learning-Multi-dimensional-scaling-and-visualization/*

# Comments on Isomap



**The quality of the result critically depends on the nearest neighbor graph**

Ask for nearest neighbors to be really close by

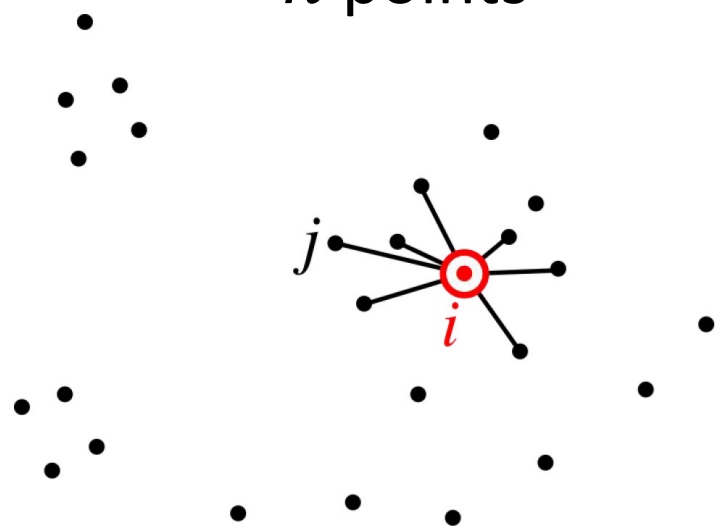
*There might not be enough edges*

Allow for nearest neighbors to be farther away

*Might connect points that shouldn't be connected*

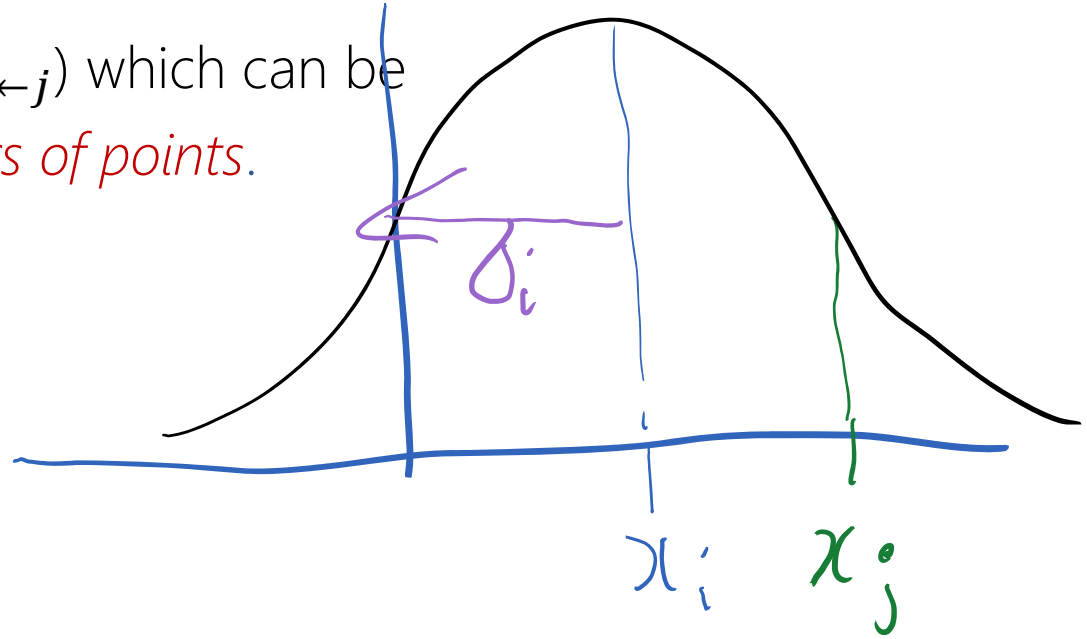
*https://www.andrew.cmu.edu/user/georgech/95-865/Lectures/Lecture%20-%2003_essence.pdf*

# 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 $P_{j\leftarrow i} = \frac{exp\left(-\|x_i - x_j\|^2 / 2\sigma_i^2\right)}{\sum_{k\neq i} exp(-\|x_i - x_k\|^2 / 2\sigma_i^2)}$, and $P_{j\leftarrow j} = 0$
- (Smells like a Gaussian, but normalized so that $1 = \sum_j P_{j\leftarrow i}$).

- Symmetrize & re-normalize it: $P_{ij} = P_{ji} = \frac{1}{2n}\left(P_{j\leftarrow i} + P_{i\leftarrow j}\right)$ which can be interpreted as *probability to pick this pair out of all pairs of points*.
- Adaptively set each $\sigma_i^2$ such that entropy of $P_{:\leftarrow i}$ is constant, $\mathbf{C_{ent}} = \sum_{j\neq i} P_{j\leftarrow i} \log P_{j\leftarrow i}$.



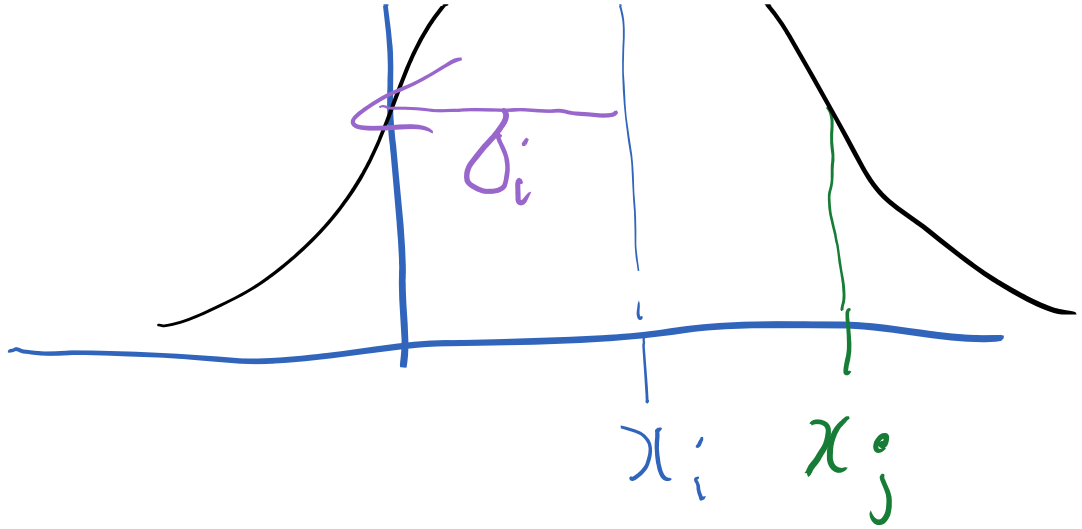
# From NE to *stochastic NE* (SNE)

$n$ points

$Perplexity(p) \equiv 2^{Entropy(p)}$

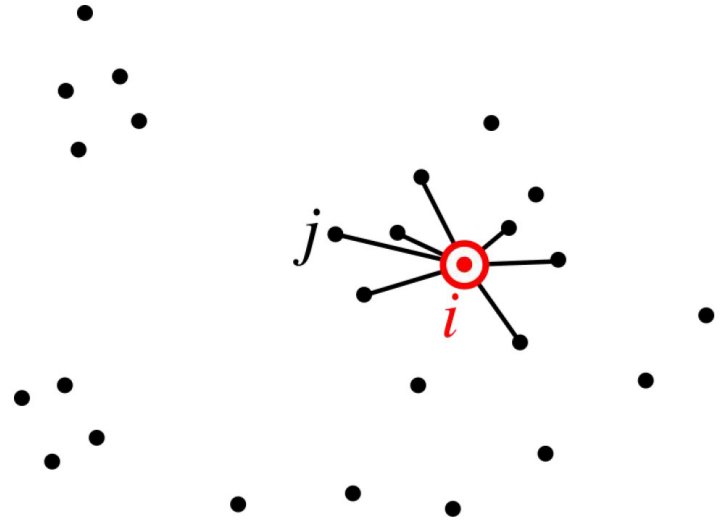

Adaptively set each $\sigma_i^2$ such that entropy of $P_{:\leftarrow i}$ is constant, $\mathbf{C_{ent}} = \sum_{j \neq i} P_{j\leftarrow i} \log P_{j\leftarrow i}$.

$$P_{j\leftarrow i} = \frac{exp\left(-\|x_i - x_j\|^2 / 2\sigma_i^2\right)}{\sum_{k\neq i} exp\left(-\|x_i - x_k\|^2 / 2\sigma_i^2\right)}$$



# From NE to *stochastic NE* (SNE)

$$P_{j\leftarrow i} = \frac{exp\left(-\|x_i - x_j\|^2/2\sigma_i^2\right)}{\sum_{k\neq i} exp(-\|x_i - x_k\|^2/2\sigma_i^2)}$$

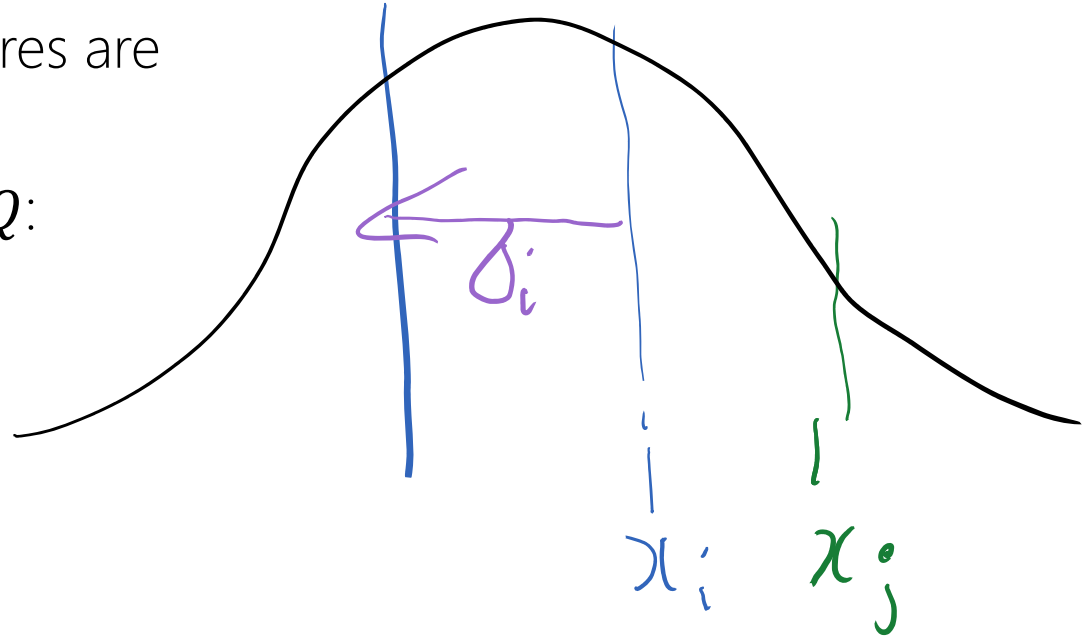



- From original data, $X \in \mathbb{R}^{n\times d}$, we have defined stochastic neighborhoods with probability distribution, $P = \{P_{ij}\}$.
- Now posit low-dimensional representations, $Y \in \mathbb{R}^{n\times k}$, and define stochastic neighborhoods for them, $Q = \{Q_{ij}\}$,

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

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

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



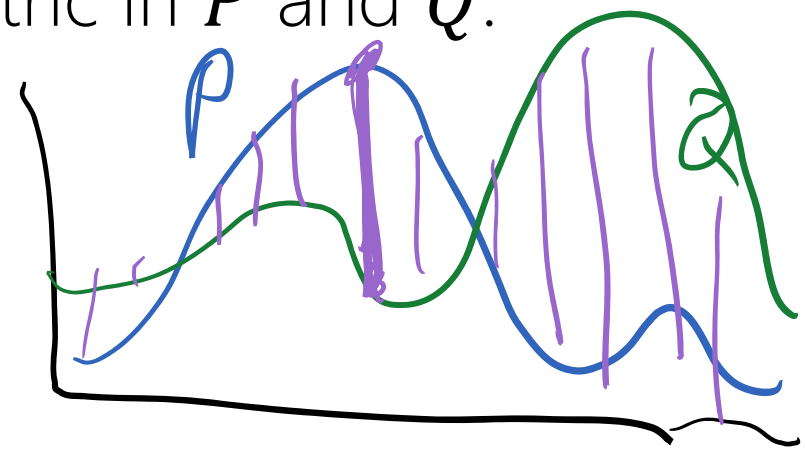
# Aside: Kullback-Leibler (KL) Divergence

- 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**

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

https://www.cs.ox.ac.uk/people/varun.kanade/teaching/ML-MT2016/slides/slides03.pdf

# SNE: miminizing the loss function

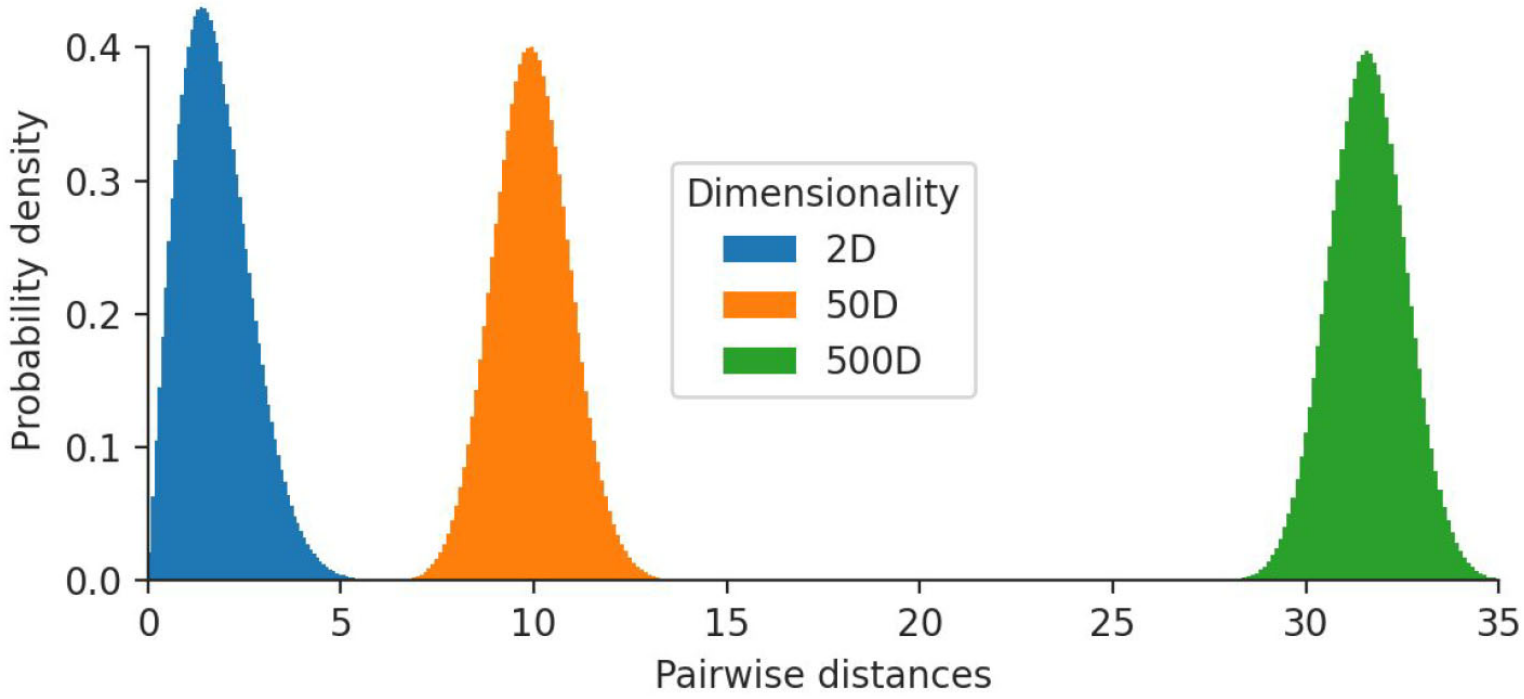
$$\hat{Y} = \underset{Y}{\mathbf{argmin}}\, KL(P||Q) = \sum_{i,j} P_{ij}\, log\, \frac{P_{ij}}{Q_{ij}}.$$

- Use gradient descent to find embedded points, $\{y_i\}$
- 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:



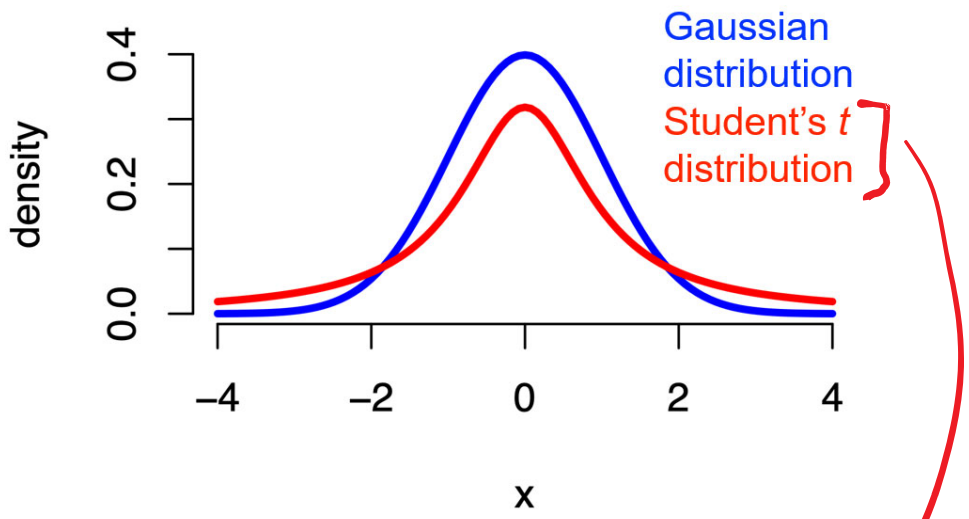
# Fixing SNE with t-SNE

- Change the distribution in the embedding space, $Q_{ij}$ to have a heavier-tailed distribution, a t-distribution.

- SNE used $Q_{j\leftarrow i} = \frac{exp\left(-\|y_i - y_j\|^2\right)}{\sum_{i\neq k} exp(-\|y_i - y_k\|^2)}$

- t-SNE uses $Q_{j\leftarrow i} = \frac{\left(1+\|y_i - y_j\|^2\right)^{-1}}{\sum_{i\neq k}(1+\|y_i - y_k\|^2)^{-1}}$

- Everything else remains the same as in SNE.




$$p(x) \propto (1 + \frac{x^2}{v})^{-(v+1)/2}$$

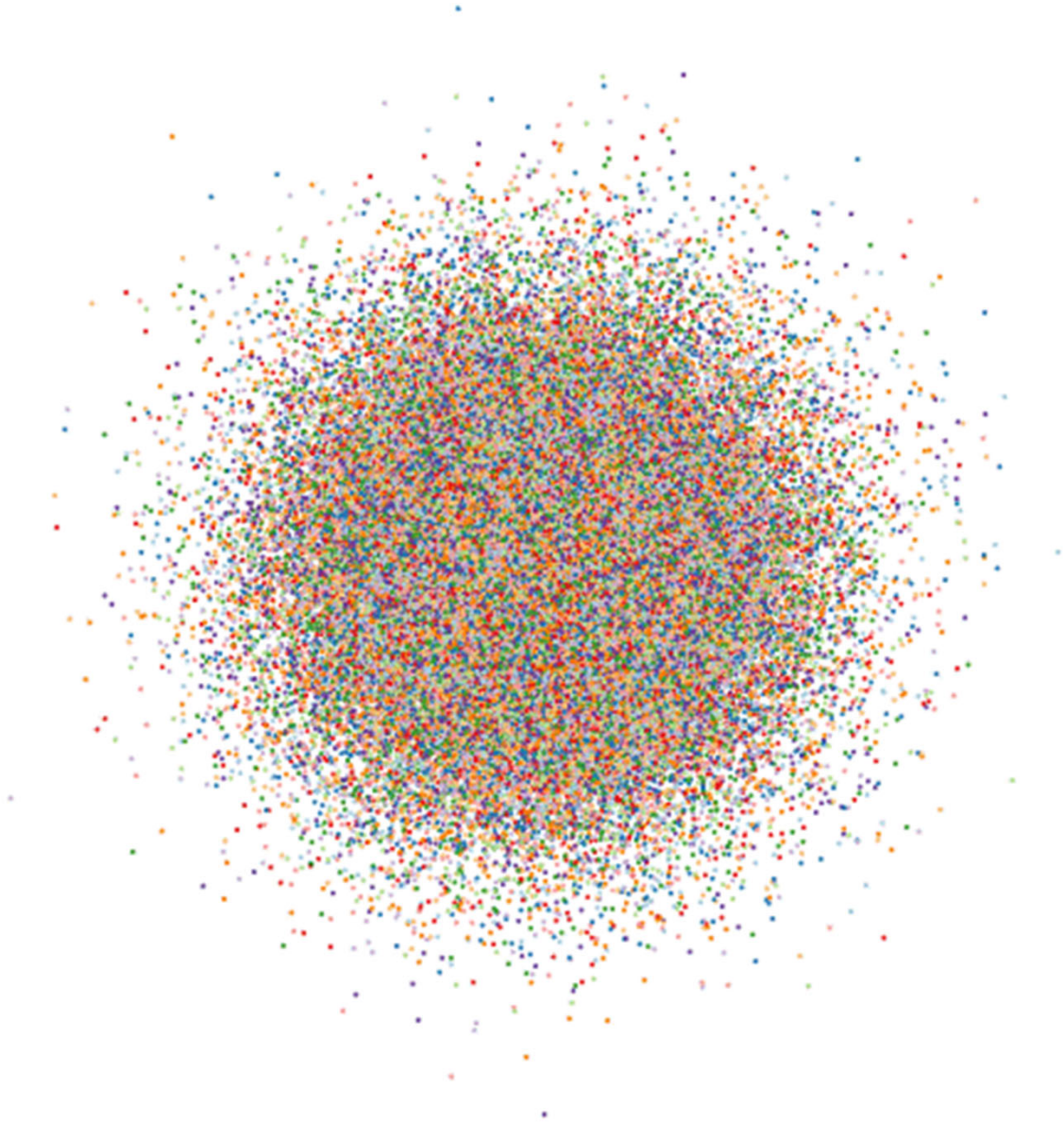
for $v = 1$ we get $p(x) \propto \frac{1}{1+x^2}$

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

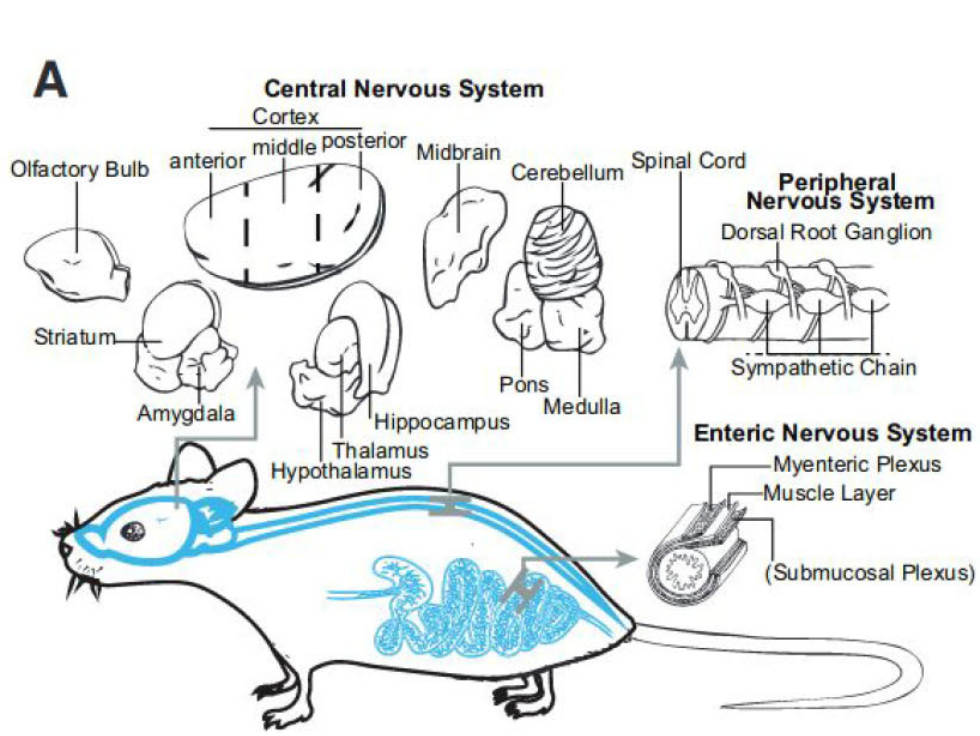
**Data**: data set $\mathcal{X} = \{x_1, x_2, \ldots, x_n\}$,
cost function parameters: entropy constant, C to set $\sigma_{ij}$
optimization parameters: number of iterations $T$, learning rate $\eta$
**Result**: low-dimensional data representation $\mathcal{Y}^{(T)} = \{y_1, y_2, \ldots, y_n\}$.
**begin**
    compute pairwise affinities $p_{j|i}$ with entropy constant, C to set $\sigma_{ij}$
    set $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$
    sample initial solution $\mathcal{Y}^{(0)} = \{y_1, y_2, \ldots, y_n\}$ 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**

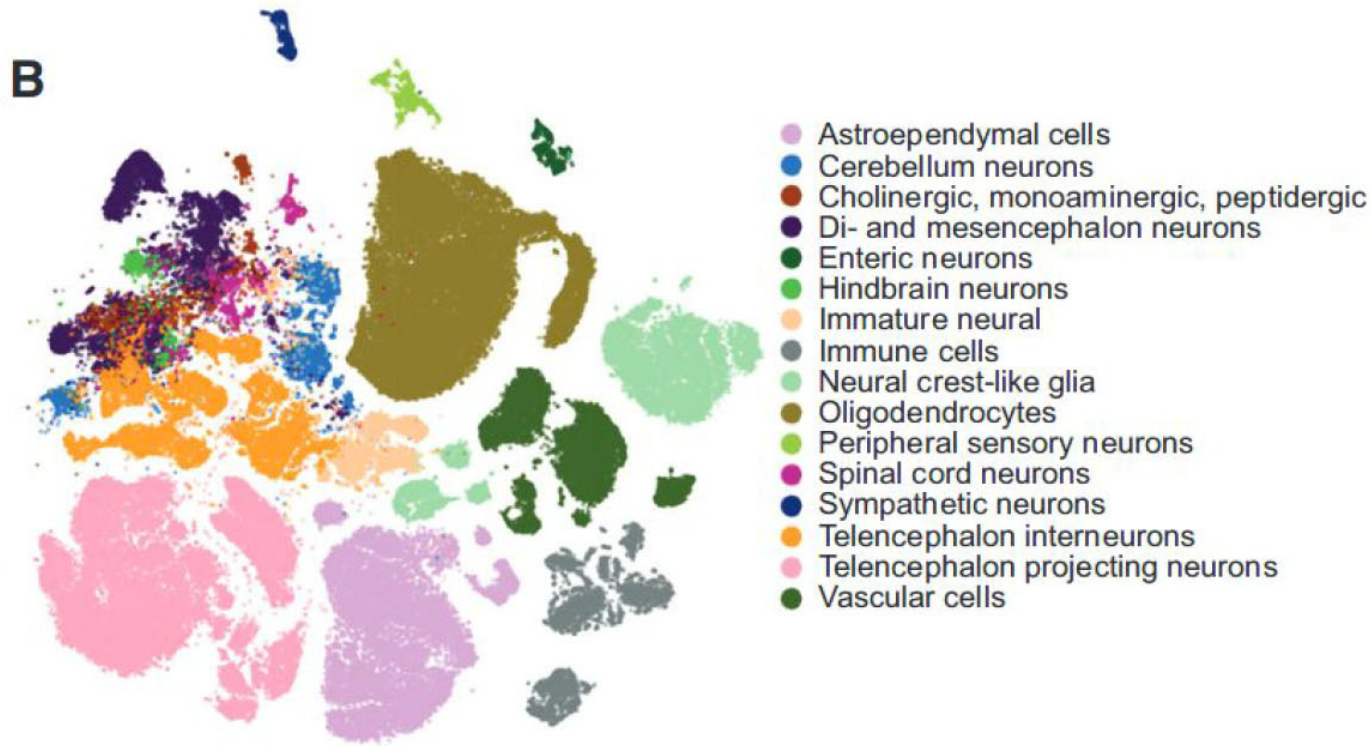
t-SNE on MNIST

(each color labels
one of the 10 digits)



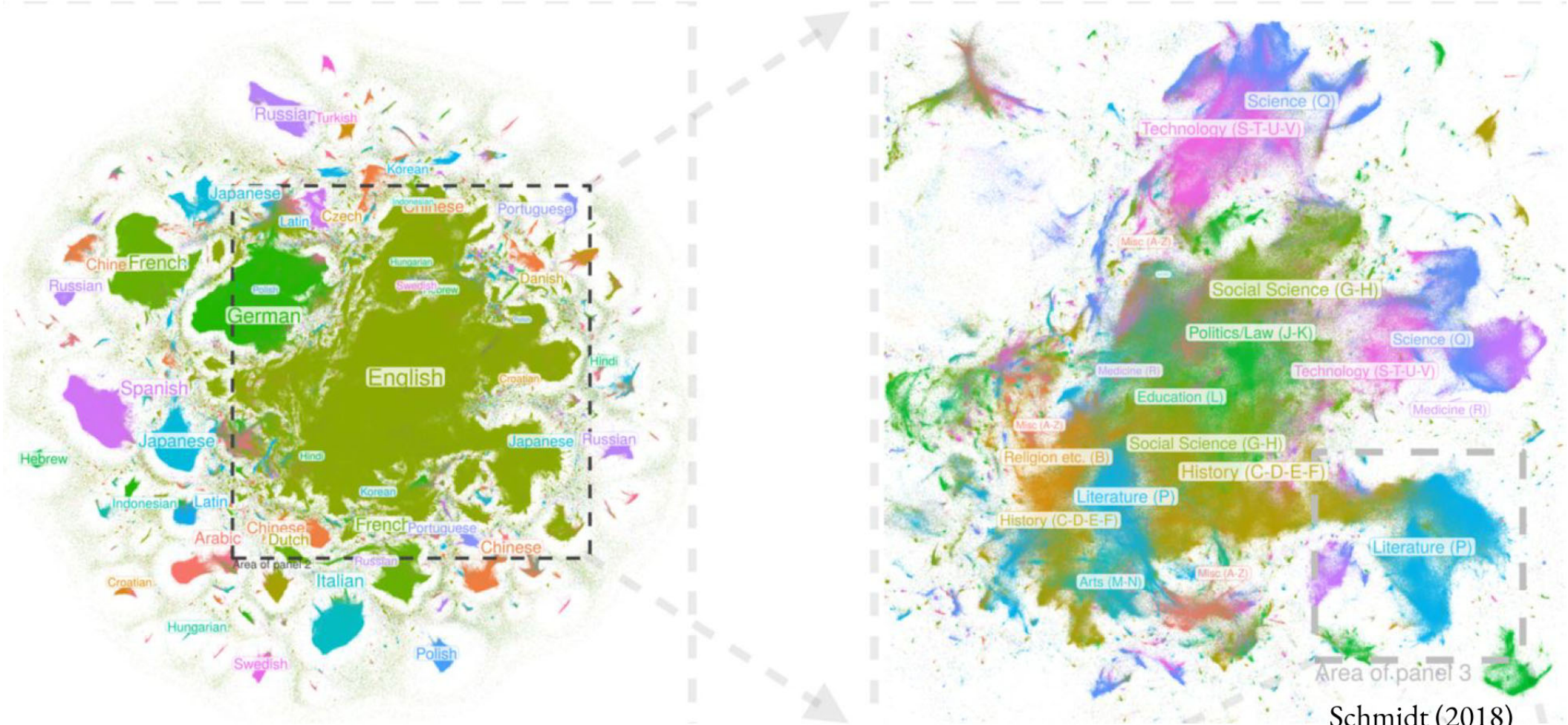
Single-cell transcriptomics (single-cell RNA sequencing): samples are cells, features are genes.




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 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.