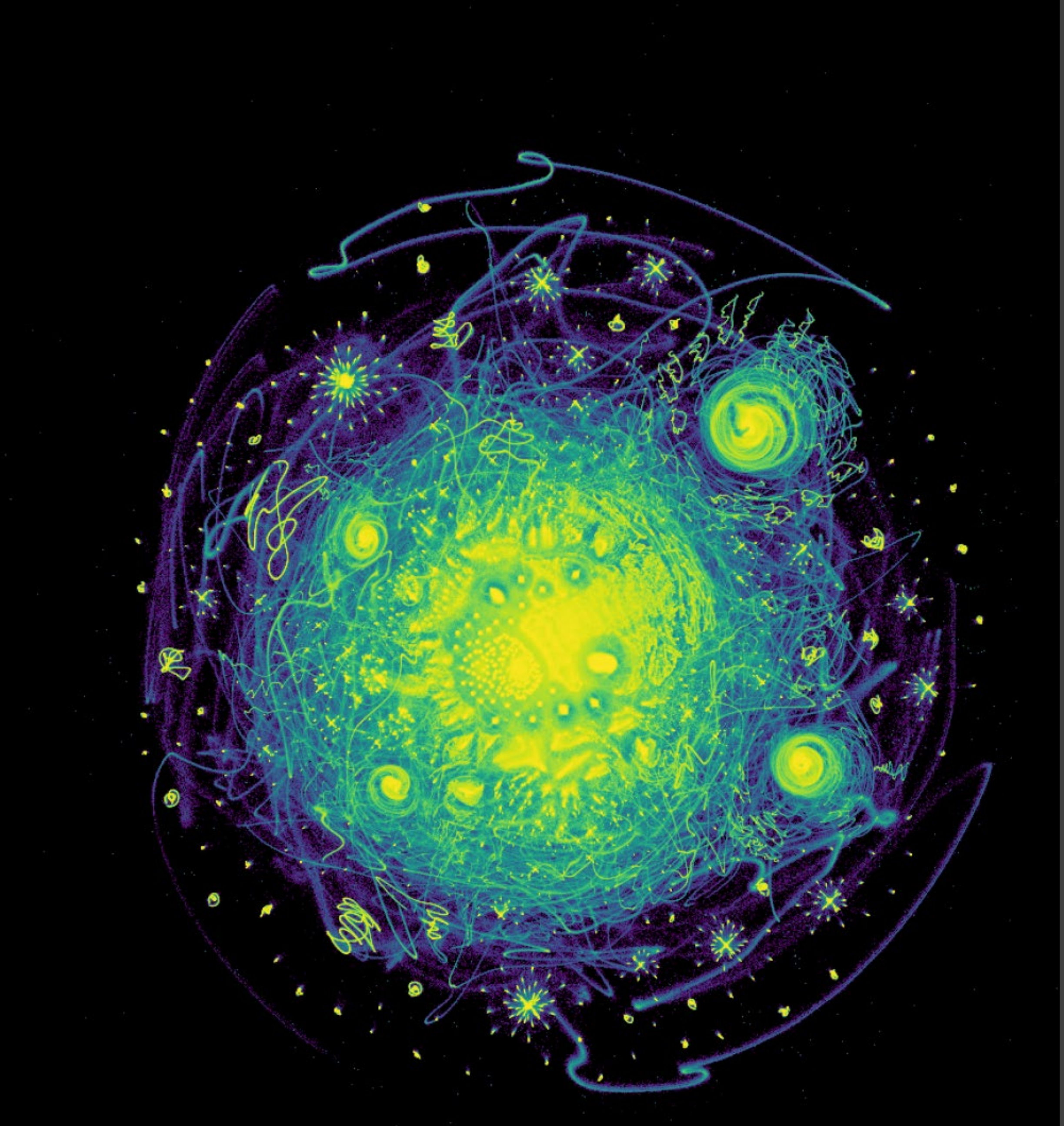


Dimensionality Reduction: PCA and low-D embeddings

Applied Machine Learning
Derek Hoiem

McInnes et al. (UMAP, 2000): Visualization of 30,000,000 integers as represented by binary vectors of prime divisibility, colored by integer value of the point

Last class: PDF Estimation

- Several methods to estimate 1D densities
  - Parametric models (least flexible)
  - Mixture of Gaussian
  - Histograms and kernel density estimation (most flexible)

- Kernel density estimation won the decathlon of 1-D data fits, even performing similarly to Gaussian when the data was Gaussian

- N-D probability estimation can be achieved by
  - Assuming independence or modeling small groups of dependent variables
  - Discretizing using K-means or multi-dimensional binning (for low-D)
  - Projecting into a lower dimension and then estimating, e.g. with PCA, manifold fitting, or autoencoding

This class – dimensionality reduction

- Goal: We want to represent high dimensional data with fewer dimensions, e.g. for:
  - Compression: reduced storage, faster retrieval
  - Visualization: plot in two dimensions

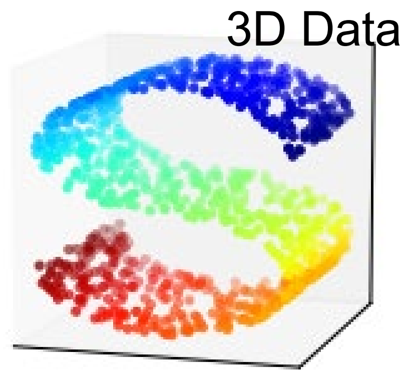
- A good dimensionality reduction can be defined in different ways
  - Be able to reproduce the original data
  - Preserve discriminative features
  - Preserve the neighborhood structure

- One main strategy is linear projection, e.g. a street map projects everything onto the 2D ground dimensions and ignores height

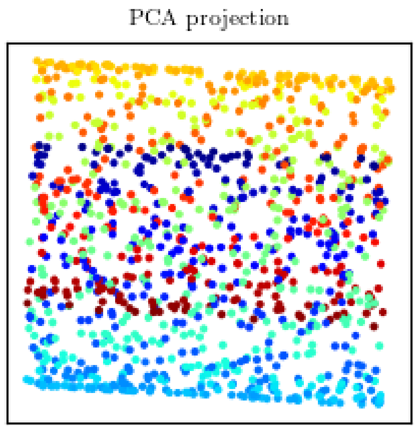
- Another strategy is embedding or manifold fitting, where we try to preserve relationships in the data

PDF = probability density function

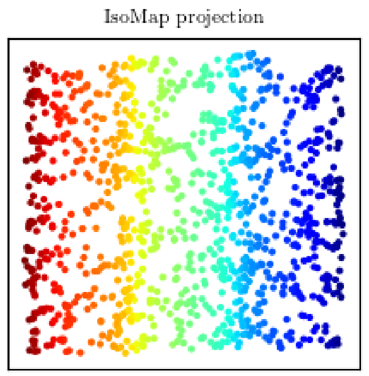
This class – PCA and manifolds



- Linear projection
  - PCA: Principal Components Analysis
  - Reduce dimension while preserving variance of data



- Embedding/manifold learning
  - MDS (multidimensional scaling), IsoMap and t-SNE
  - Preserve point distances and/or local structure



Key terms

- Vectors and matrices
- Translation
- Projection
- Scaling
- Rotation
- Rank
- Eigenvectors/eigenvalues
- SVD

Key terms

Vector can represent a data point $\boldsymbol{x}$ or a **projection** $\boldsymbol{w}$ onto a **coordinate**

- $\boldsymbol{w}^T \boldsymbol{x}$ projects data point $\boldsymbol{x}$ onto the axis defined by $\boldsymbol{w}$
- E.g. suppose $d = 2$
    - $\boldsymbol{w} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ selects the first value of $\boldsymbol{x}$
    - $\boldsymbol{w} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ adds the two values of $\boldsymbol{x}$ together

Matrix can represent a set of data points or a set of projection vectors

Key terms

Translation is a transformation that adds a constant value to each vector

- E.g. centering is $\boldsymbol{x}_c = \boldsymbol{x} - \boldsymbol{\mu}_x$, where $\boldsymbol{\mu}_x$ is the mean of $\boldsymbol{x}$

Scaling is a transformation that multiplies each coordinate by a constant value

- E.g. $\boldsymbol{W} = \begin{bmatrix} 2 & & \\ & 1 & \\ & & 1 \end{bmatrix}$ will double the value of the first coordinate of $\boldsymbol{x}$ when applied as $\boldsymbol{W}\boldsymbol{x}$ (blanks are assumed to be zero)

Key terms

Rotation is a set of projections that preserves the distances between points and distances to the origin

- Each row and column represents a **basis vector**
- The basic vectors must have a unit norm and be orthogonal to each other: $\boldsymbol{r}_i^T \boldsymbol{r}_i = 1, \boldsymbol{r}_i^T \boldsymbol{r}_j = 0,\ \forall (i, j \neq i)$

Key terms

Rank of matrix $\boldsymbol{M}$ is the number of linearly independent vectors in the rows or columns of $\boldsymbol{M}$

- $Rank(\boldsymbol{M})$ is at most the smaller of the number of rows and columns in $\boldsymbol{M}$
- $Rank\left(\begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{bmatrix}\right) = 2$
- $Rank\left(\begin{bmatrix} \mathbf{1} & \mathbf{2} \\ \mathbf{2} & \mathbf{4} \end{bmatrix}\right) = 1$ because one of the rows (or columns) can be composed of a weighted sum of the others

Key terms

Eigenvector $\boldsymbol{v}$ and corresponding **eigenvalue** λ of matrix $\boldsymbol{M}$ are defined by having the special property $\boldsymbol{M}\boldsymbol{v} = \lambda\boldsymbol{v}$

- Eigenvectors characterize matrices, and appear as part of a solution to many linear algebra problems

SVD (singular value decomposition) is a factorization of a matrix $\boldsymbol{A}$ into $\boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$, where:

- Columns of $\boldsymbol{U}$ are eigenvectors of $\boldsymbol{A}\boldsymbol{A}^T$
- Columns of $\boldsymbol{V}$ are eigenvectors of $\boldsymbol{A}^T\boldsymbol{A}$
- $\boldsymbol{\Sigma}$ is a diagonal (scaling) matrix of singular values, which are square roots of the eigenvalues of both $\boldsymbol{A}\boldsymbol{A}^T$ and $\boldsymbol{A}^T\boldsymbol{A}$

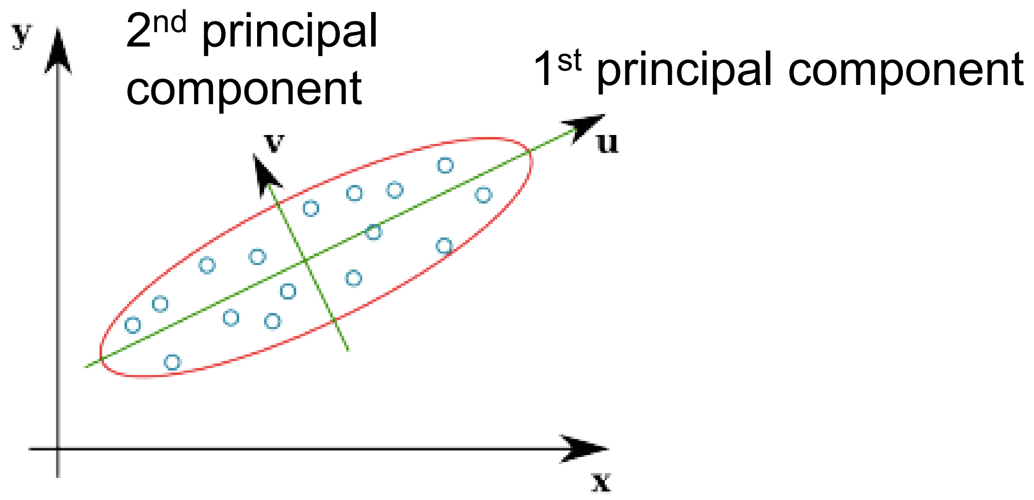
PCA

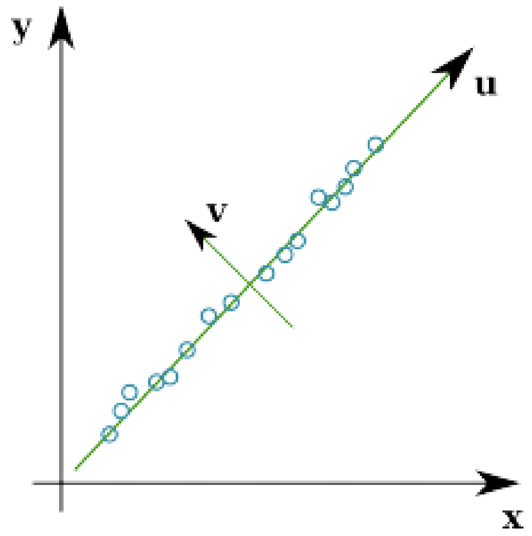
- General dimensionality reduction technique
  - Finds major orthogonal directions of variation

- Preserves most of variance with a much more compact representation
  - – Lower storage requirements
  - – Faster matching/retrieval
  - – Easier to work in low dimensions, e.g. for probability estimation

Principal Component Analysis

- Given a point set $\{\vec{\mathrm{p}}_j\}_{j=1\ldots P}$, in an M-dim space, PCA finds a basis such that
  - The most variation is in the first basis vector
  - The second most, in the second vector that is orthogonal to the first vector
  - The third…





Principal Component Analysis (PCA)

- Given: N data points $\mathbf{x}_1, \ldots, \mathbf{x}_N$ in R^d

- We want to find a new set of features that are linear combinations of original ones:

$$u(\mathbf{x}_i) = \mathbf{u}^T(\mathbf{x}_i - \boldsymbol{\mu})$$

  ($\boldsymbol{\mu}$: mean of data points)

- Choose unit vector **u** in R^d that captures the most data variance

Principal Component Analysis

Direction that maximizes the variance of the projected data:

Maximize $$\frac{1}{N}\sum_{i=1}^{N} \underbrace{\mathbf{u}^{\mathrm{T}}(\mathbf{x}_i-\mu)}_{\text{Projection of data point}}(\mathbf{u}^{\mathrm{T}}(\mathbf{x}_i-\mu))^{\mathrm{T}}$$ subject to ||**u**||=1

$$= \quad \mathbf{u}^{\mathrm{T}}\underbrace{\left[1/N\sum_{i=1}^{N}(\mathbf{x}_i-\mu)(\mathbf{x}_i-\mu)^{\mathrm{T}}\right]}_{\text{Covariance matrix of data}}\mathbf{u}$$

$$= \quad \mathbf{u}^{\mathrm{T}}\Sigma\mathbf{u}$$

The direction that maximizes the variance is the eigenvector associated with the largest eigenvalue of Σ (can be derived using Raleigh's quotient or Lagrange multiplier)

PCA in Python

```python
print(X.shape)
x_mu = np.mean(X, axis=0)
X_cov = np.matmul((X-x_mu).transpose(), X-x_mu)/X.shape[0]
[lam, v] = np.linalg.eig(X_cov)
print(lam[:3])
v = v.transpose()
from sklearn.decomposition import PCA
pca_transform = PCA().fit(X)
print(np.max(np.abs(v[0]-pca_transform.components_[0])))
print(pca_transform.explained_variance_[:3])
```

Compute PCA components as eigenvectors of covariance matrix

Compute PCA using the PCA function

```
(50000, 784)
[5.0695131  3.7301149  3.25871794]
3.981190377366772 3e-16
[5.06961449 3.7301895  3.25878311]
```

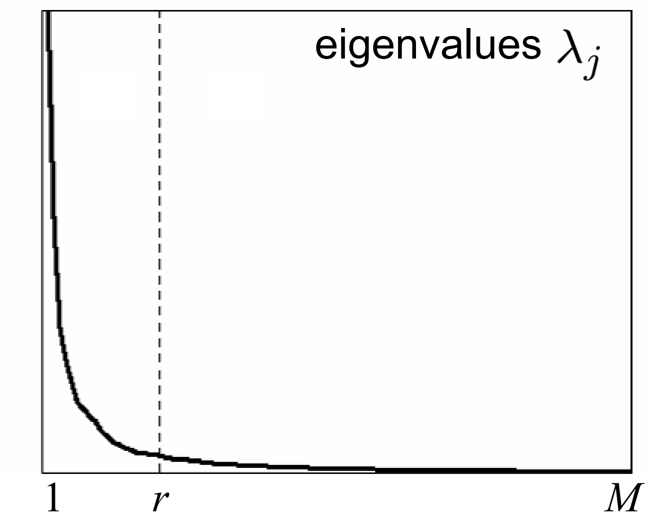
Printout shows that eigenvalues are the same as the explained variance, and the first component is identical (up to numerical precision)

Principal Component Analysis

First $r < M$ principal component vectors provide an approximate basis that minimizes the mean-squared-error (MSE) of reconstructing the original points

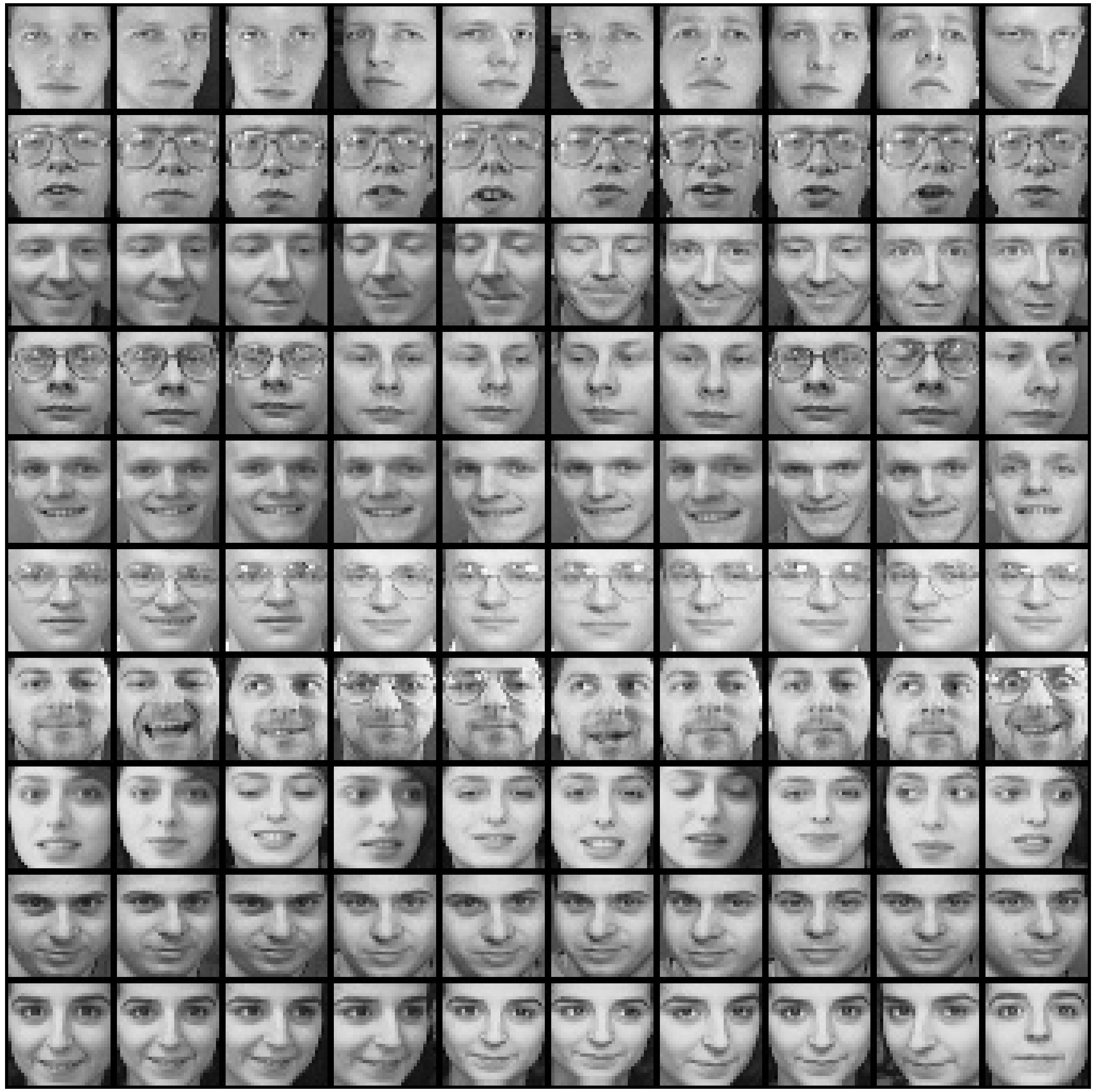
Choosing subspace dimension r:

- look at decay of the eigenvalues as a function of r
- Larger r means lower expected error in the subspace data approximation



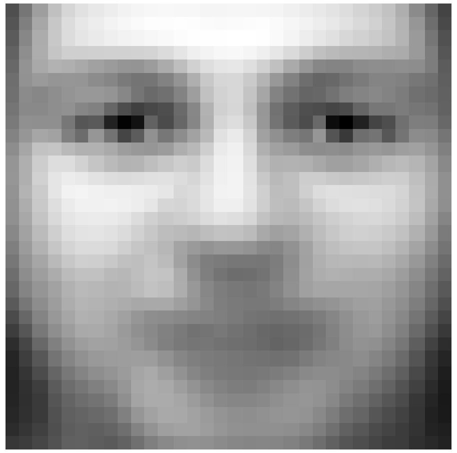
Example on aligned faces

$\mathbf{x}_1,\ldots,\mathbf{x}_N$ are pixel values of each face

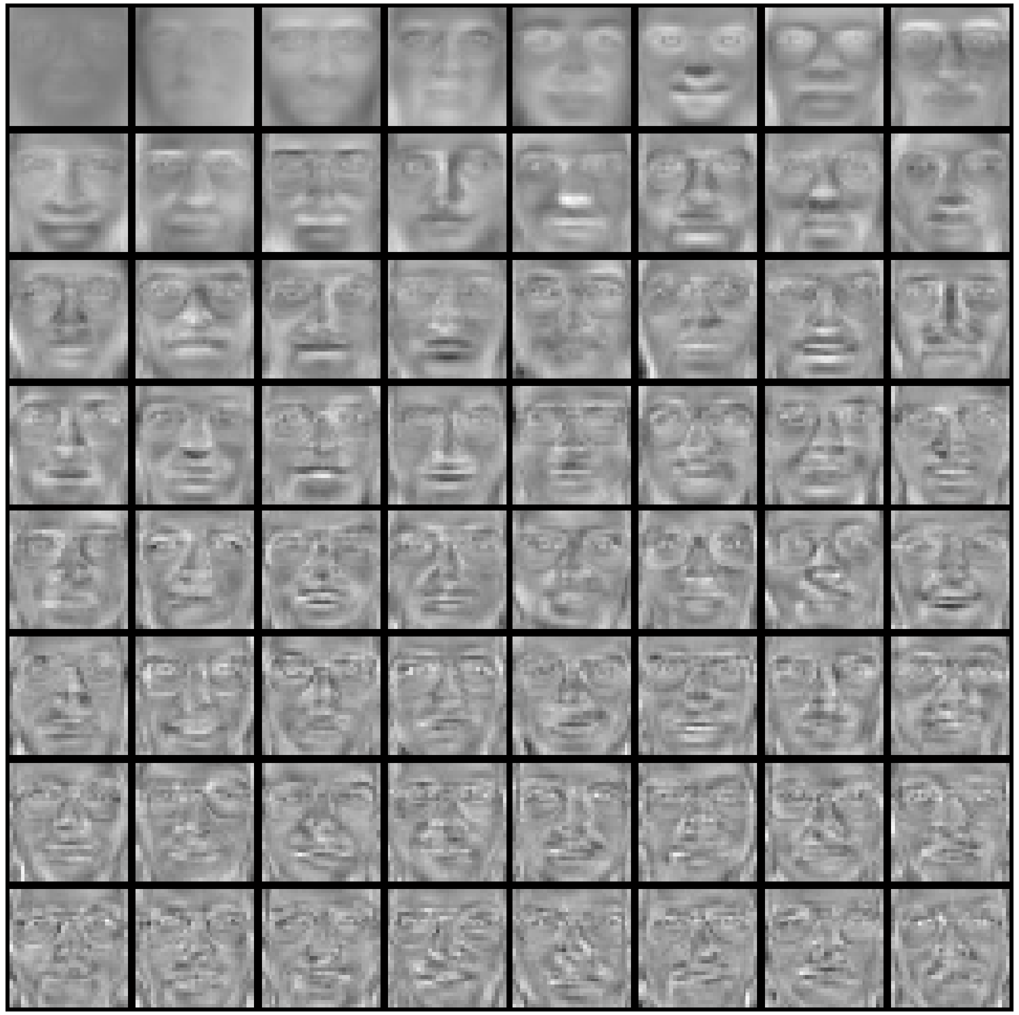


PCA of aligned face images (called “eigenfaces”)

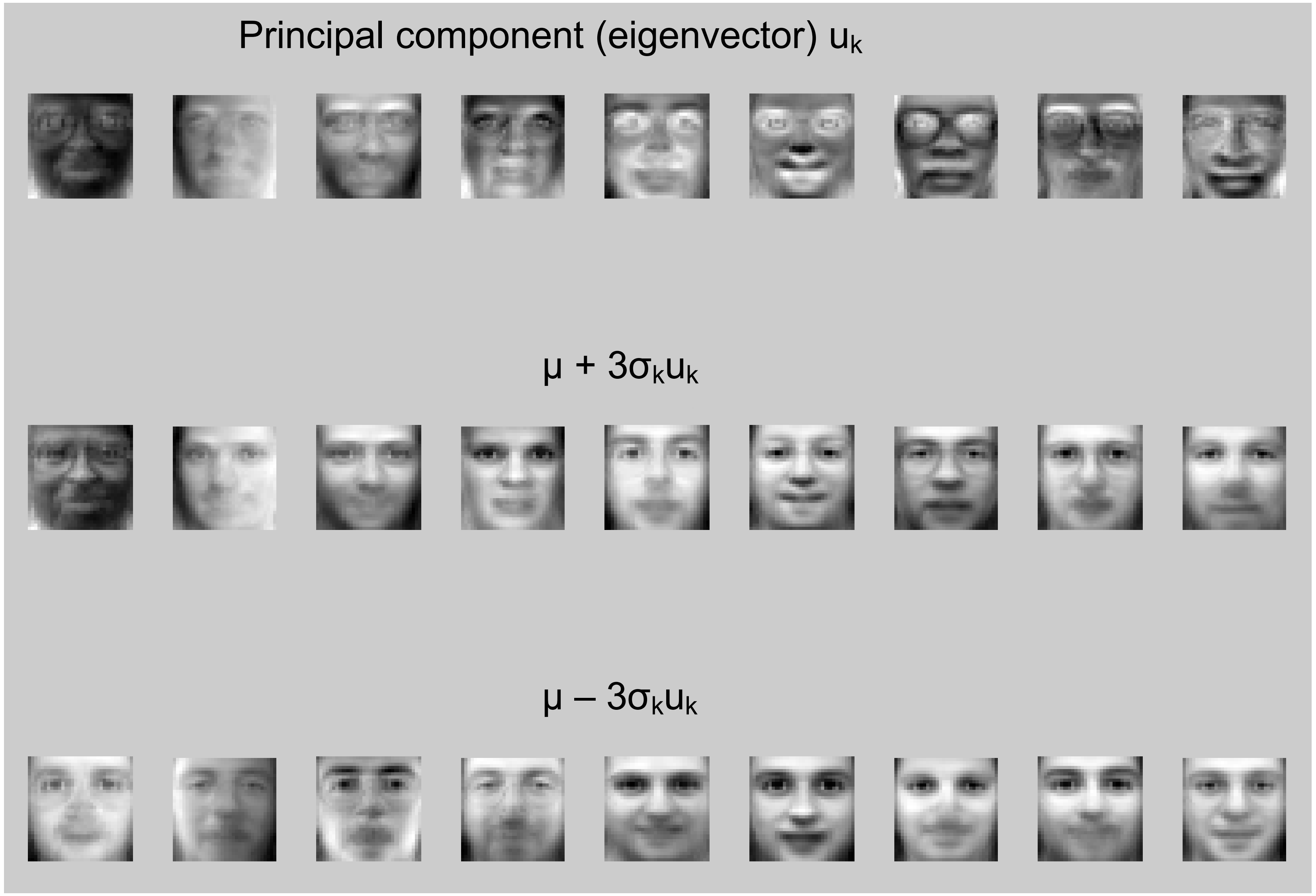
Mean: μ



Top eigenvectors: $u_1, \ldots u_k$



Visualization of eigenfaces (appearance variation)



Representation and reconstruction

- Face **x** in “face space” coordinates:

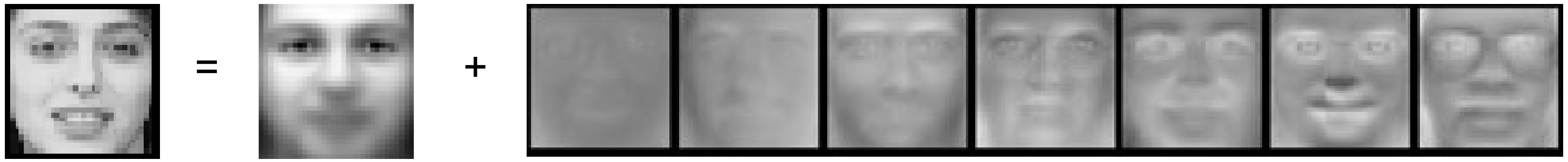
$$\mathbf{x} \rightarrow [\mathbf{u}_1^{\mathrm{T}}(\mathbf{x} - \mu), \ldots, \mathbf{u}_k^{\mathrm{T}}(\mathbf{x} - \mu)]$$
$$= \quad w_1, \ldots, w_k$$

Representation and reconstruction

- Face **x** in "face space" coordinates:

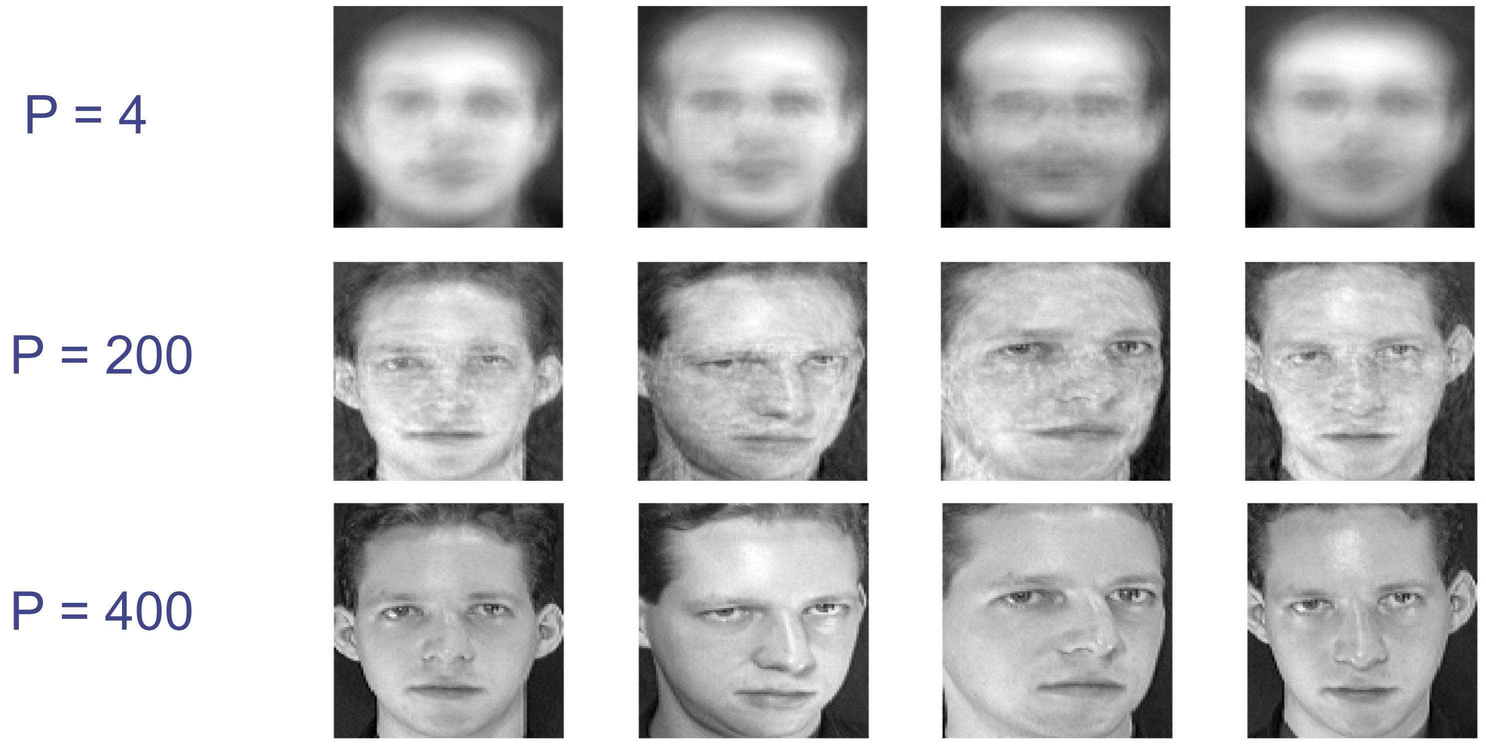
$$\mathbf{x} \rightarrow [\mathbf{u}_1^{\mathrm{T}}(\mathbf{x}-\mu), \ldots, \mathbf{u}_k^{\mathrm{T}}(\mathbf{x}-\mu)]$$
$$= \quad w_1, \ldots, w_k$$

- Reconstruction:



$\hat{x} = \mu + w_1u_1+w_2u_2+w_3u_3+w_4u_4+ \ldots$

Reconstruction

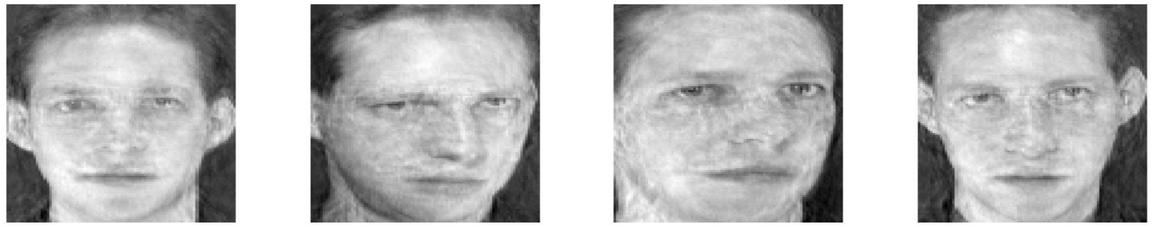


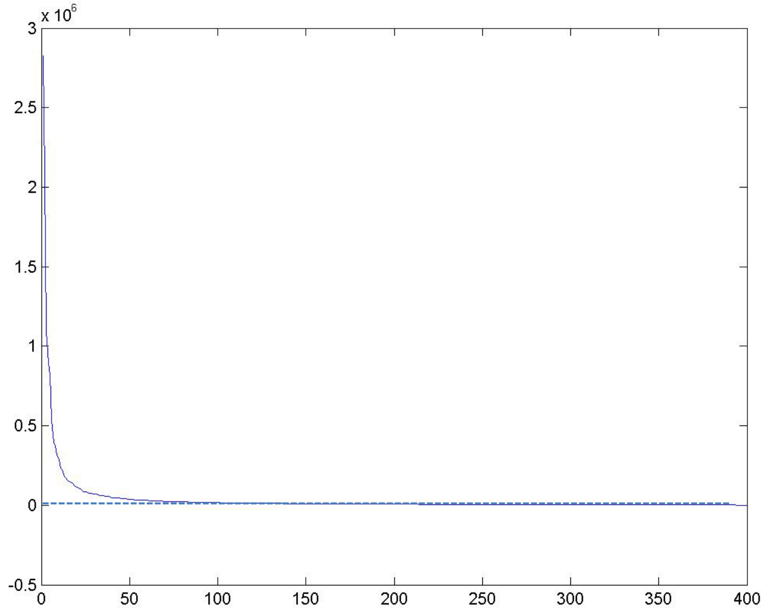
After computing eigenfaces using 400 face images from ORL face database

Note

Preserving variance (minimizing MSE) does not necessarily lead to qualitatively good reconstruction.

P = 200

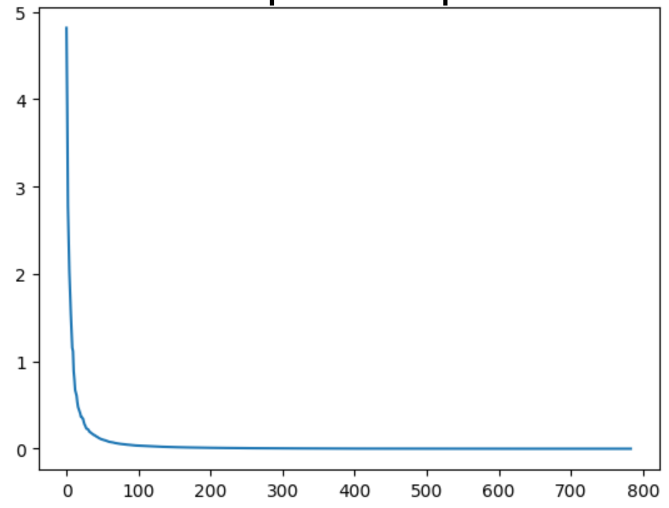




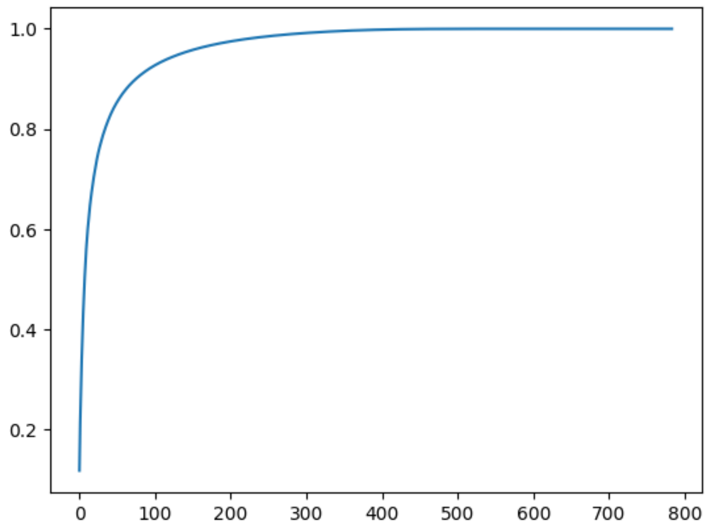
Plot of eigenvalues for each eigenvector of the covariance matrix, equivalent to the variance contained along each principal component

Another example, representing MNIST 4’s

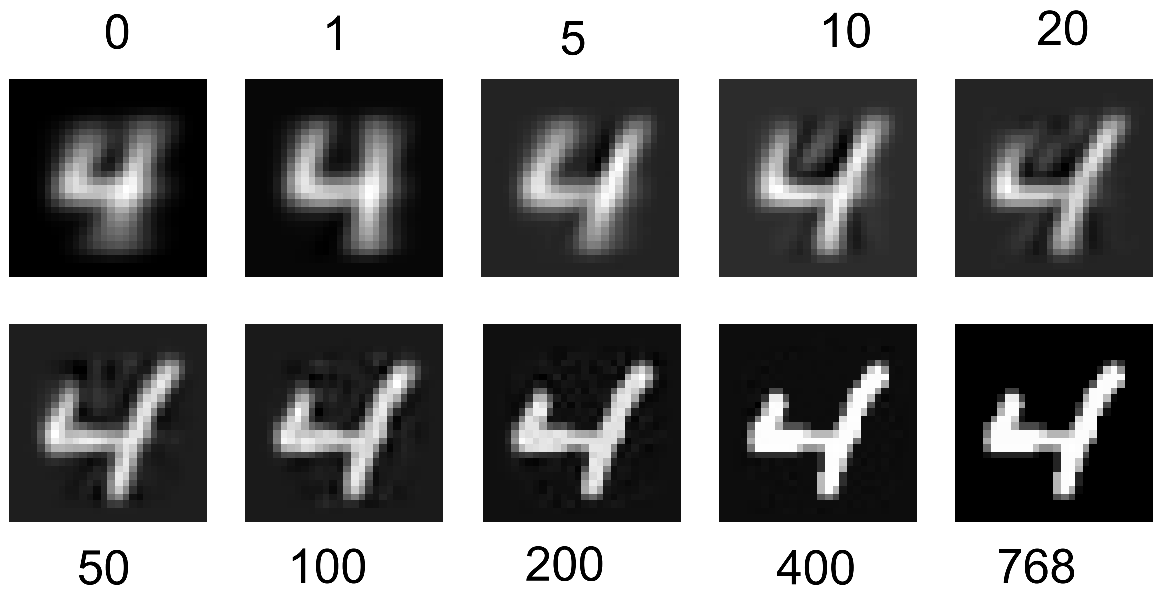
Variance per component

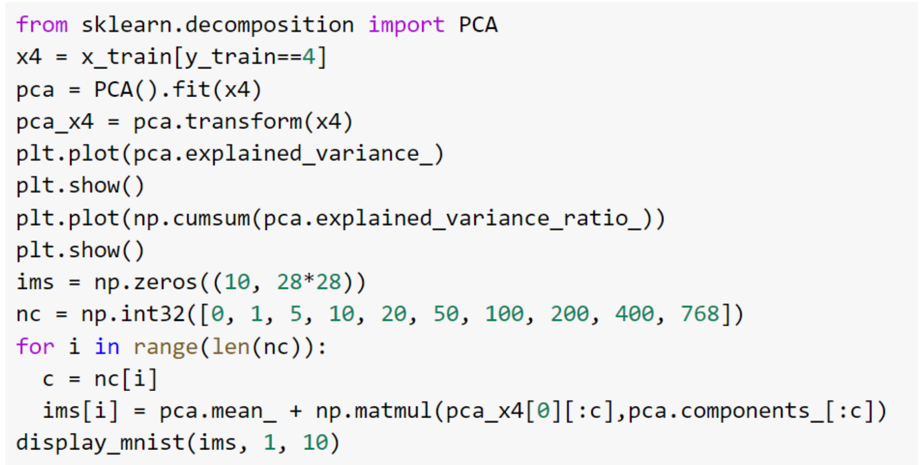


Cumulative % variance explained



Reconstructions with varying # PCs

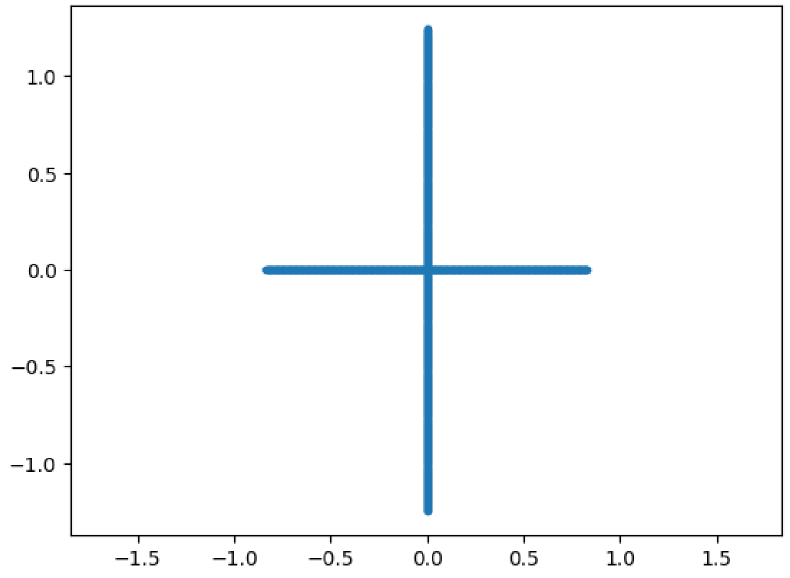
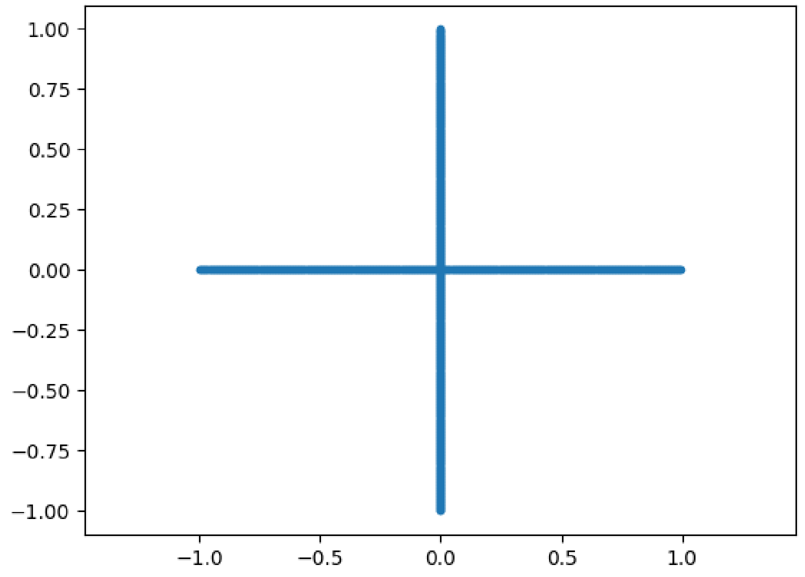
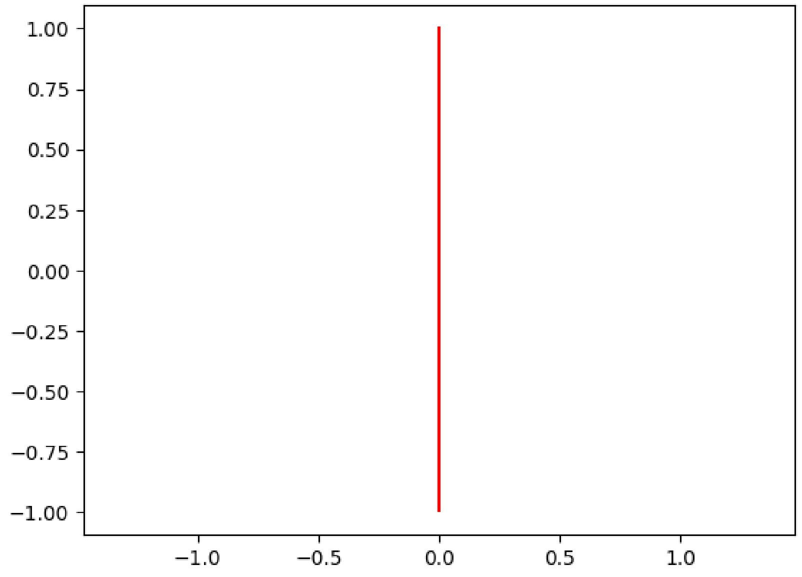
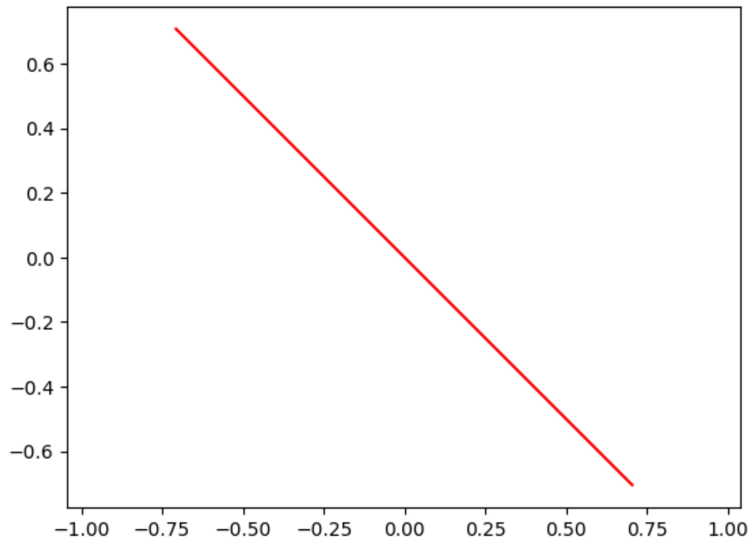




```
from sklearn.decomposition import PCA
x4 = x_train[y_train==4]
pca = PCA().fit(x4)
pca_x4 = pca.transform(x4)
plt.plot(pca.explained_variance_)
plt.show()
plt.plot(np.cumsum(pca.explained_variance_ratio_))
plt.show()
ims = np.zeros((10, 28*28))
nc = np.int32([0, 1, 5, 10, 20, 50, 100, 200, 400, 768])
for i in range(len(nc)):
  c = nc[i]
  ims[i] = pca.mean_ + np.matmul(pca_x4[0][:c],pca.components_[:c])
display_mnist(ims, 1, 10)
```

Two minute break (3 questions)

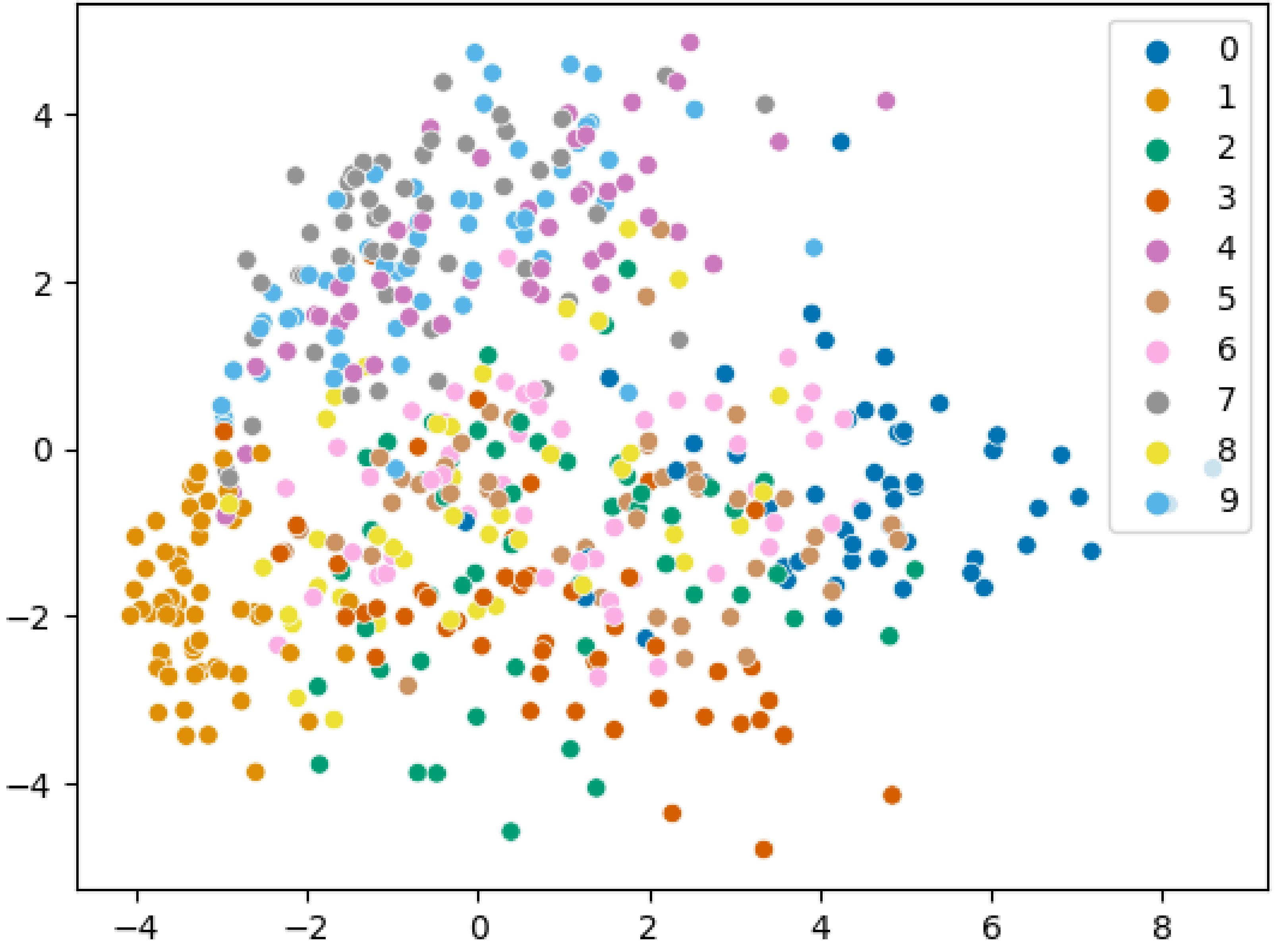
For each plot of data, what is the direction of the first principal component?

If X consists of N data points of d dimensions, what is the maximum number of PCA components that would be needed to perfectly reconstruct the data?

Rank(X) <= min(N, d)

PCA: MNIST at 2 dimensions



Note: I’m only plotting the ‘s’ data in this lecture (500 points)

Non-Linear Scaling and Manifold Estimation

We may care less about being able to reconstruct each data point than representing the relationships between data points

- MDS: Preserve Euclidean pairwise distances

- Non-metric MDS: Preserve distance orderings

- ISOMAP: Define distances in terms of “geodesic” (graph-based) similarity

MultiDimensional Scaling (MDS)

- For all data points, solve for new coordinate positions that preserve some input set of pairwise distances
- Classic case (equations on right) uses Euclidean distance and has closed form solution
- More generally, distance can be defined arbitrarily (e.g. from user surveys)
- Major drawback is that the solution is most influenced by points that are far from each other

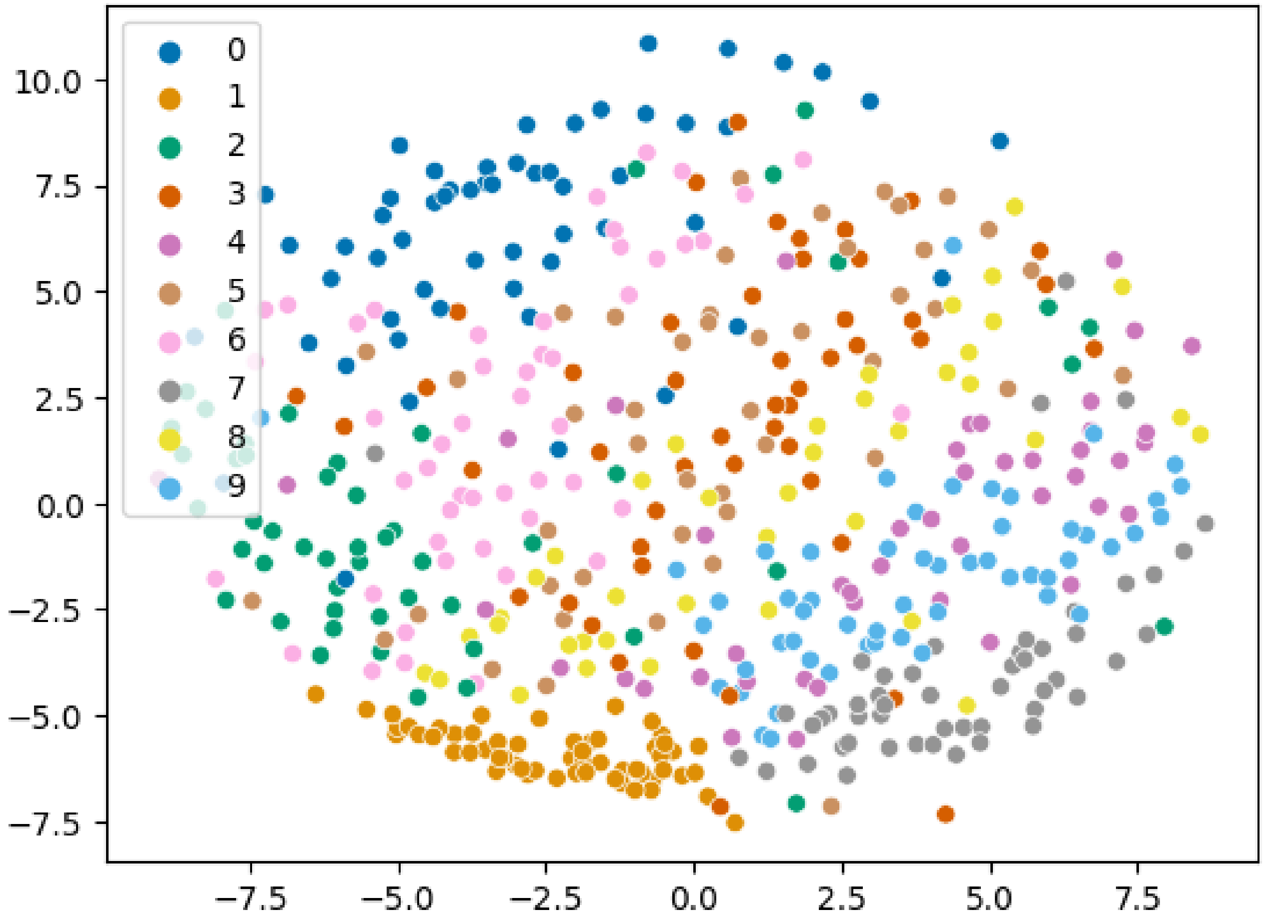
Solve for y that minimizes $$\sum_{ij}\left(D_{ij}^{(2)}(\mathbf{x}) - D_{ij}^{(2)}(\mathbf{y})\right)^2$$

where $$D_{ij}^{(2)}(\mathbf{x}) = \left(\mathbf{x}_i - \mathbf{x}_j\right)^T\left(\mathbf{x}_i - \mathbf{x}_j\right)$$

See Forsyth AML 6.2 for details

MDS on MNIST

- 30 PCA components
- MDS to 2 dimensions



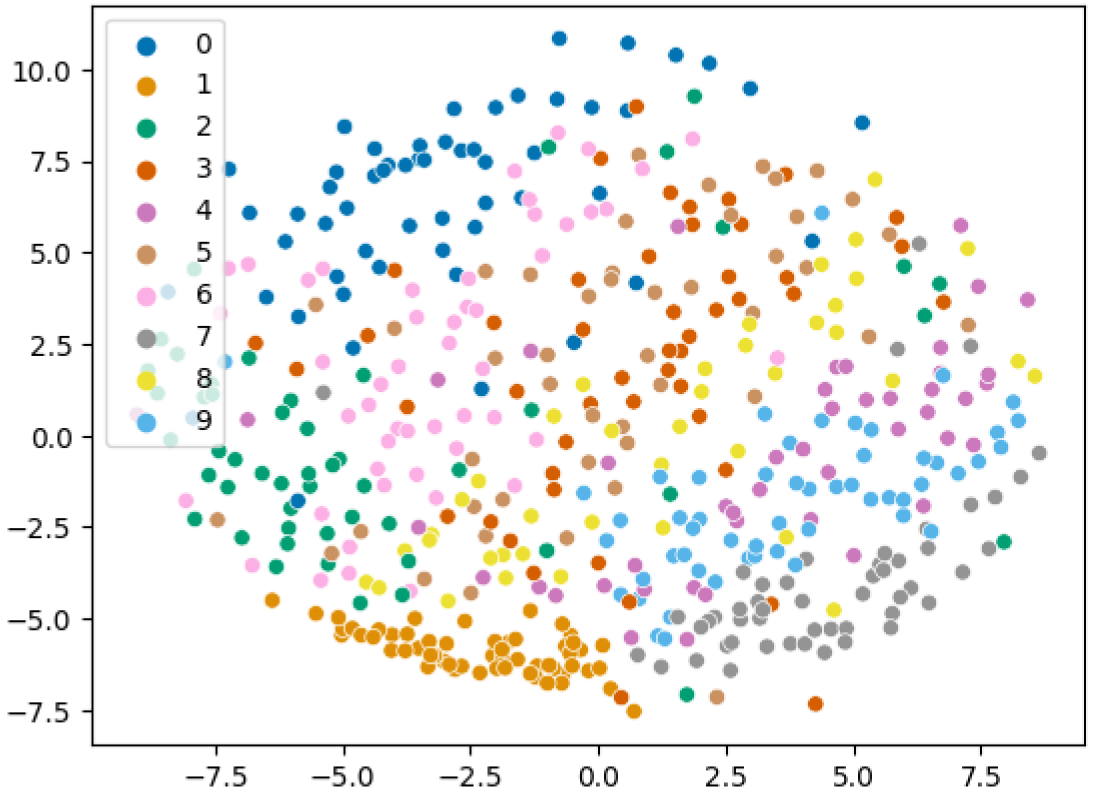
```
from sklearn.manifold import MDS

pca = PCA()
pca.fit(x_train)
x_pca = pca.transform(x_train)
```

```
ind = train_indices['s']
x_mds = MDS(n_components=2, normalized_stress='auto').fit_transform(x_pca[ind, :30])
sns.scatterplot(x=x_mds[ind,0],y=x_mds[ind,1], hue=y_train[ind], palette="colorblind")
```

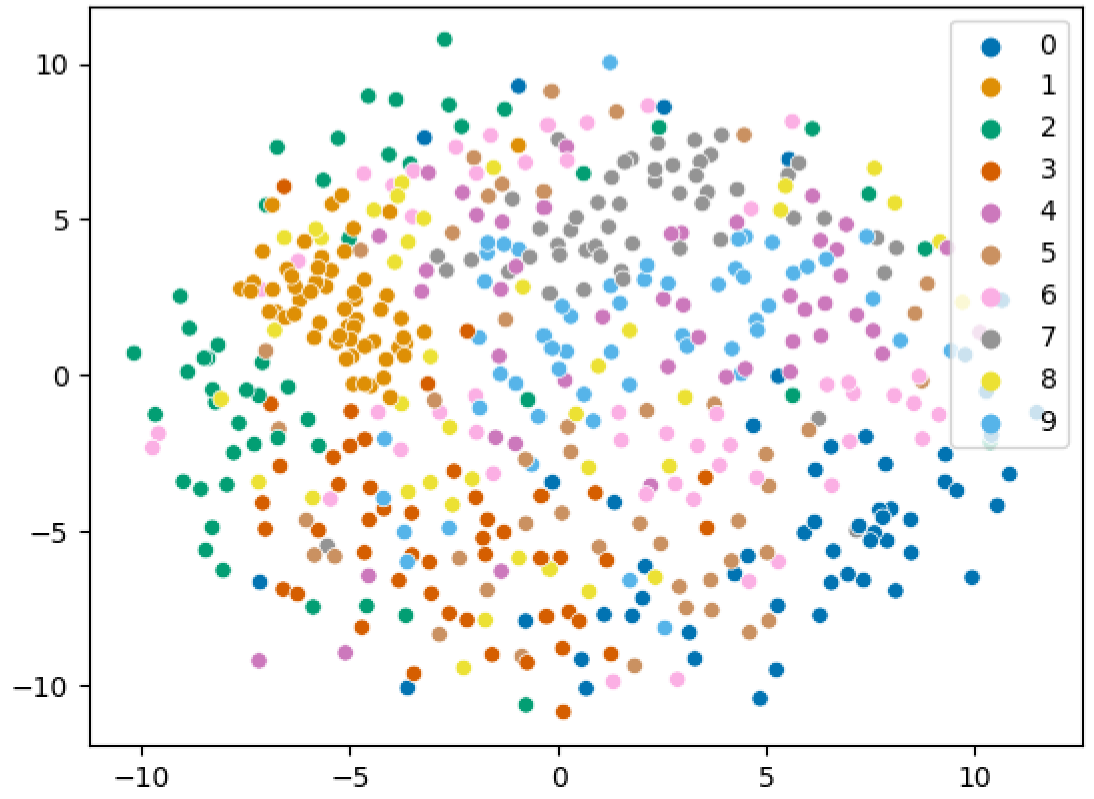
Note: For MDS and others, manifolds are fit on only ‘x’ data for speed (500 pts)

MDS on MNIST

Pre-process with PCA to 30 dim



No PCA



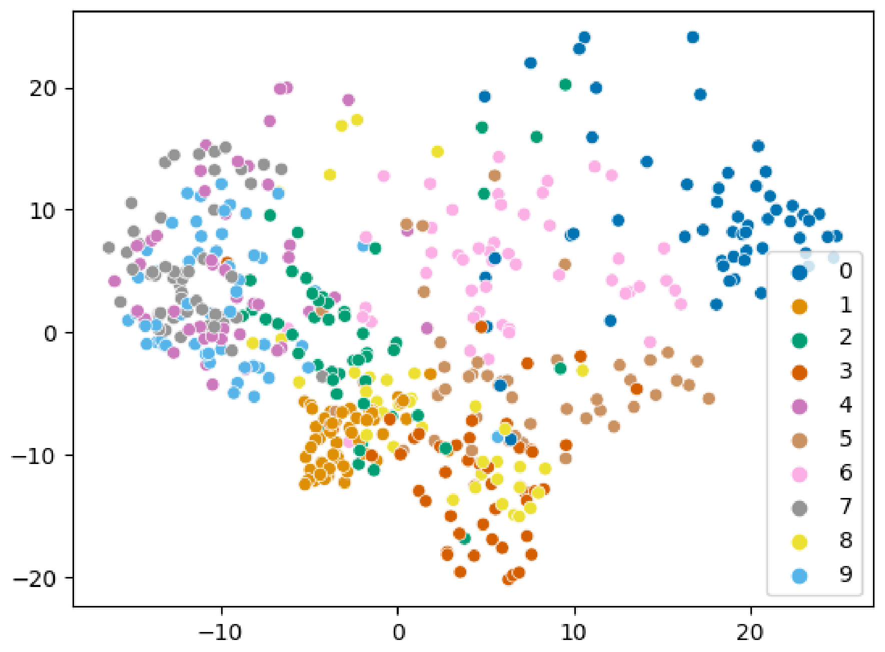
Non-metric MDS

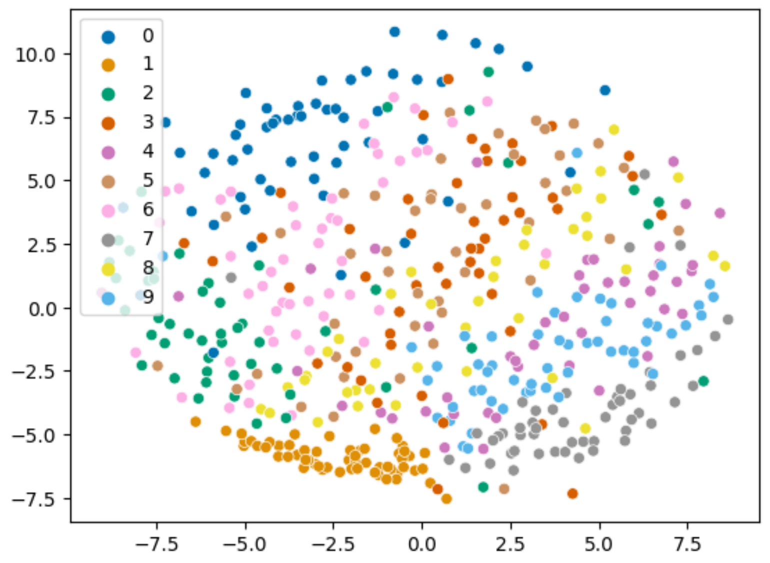
- Optimize position of data points so that Euclidean distance preserves the ordering of input pairwise distances
- Requires only an order of dissimilarities
- Slow because this is a complicated optimization

ISOMAP

- Same as MDS but define distance in a graph
  - Compute adjacency graph (e.g. 5 nearest neighbors)
  - Distance is shortest path in graph between two points

MNIST Iso (PCA: 30)





MNIST MDS (PCA: 30)

t-SNE

Map to 2 or 3 dimensions while preserving similarities of nearby points

1. Assign probability p_{ij} that pairs of points are similar, e.g. with Gaussian weighted distance
2. Define similarity q_{ij} in new coordinates
3. Minimize KL divergence between p and q (i.e. they should have similar distributions) using gradient descent

For $i \neq j$, define

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma_i^2)}$$

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

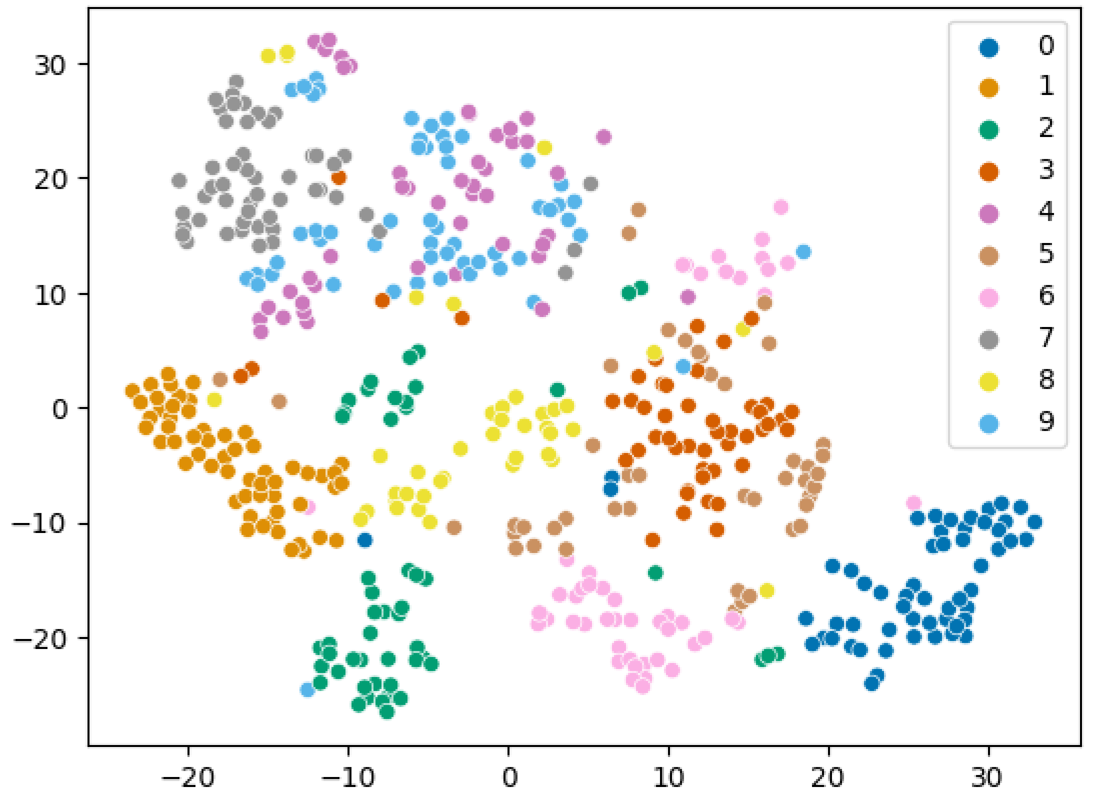
$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$$

$$\mathrm{KL}\left(P \parallel Q\right) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

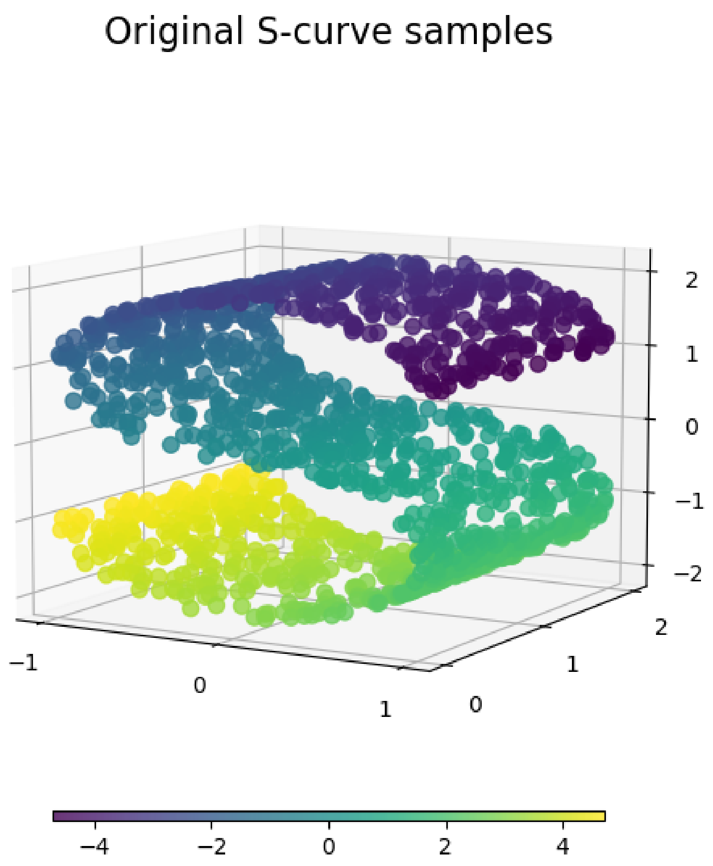
t-SNE

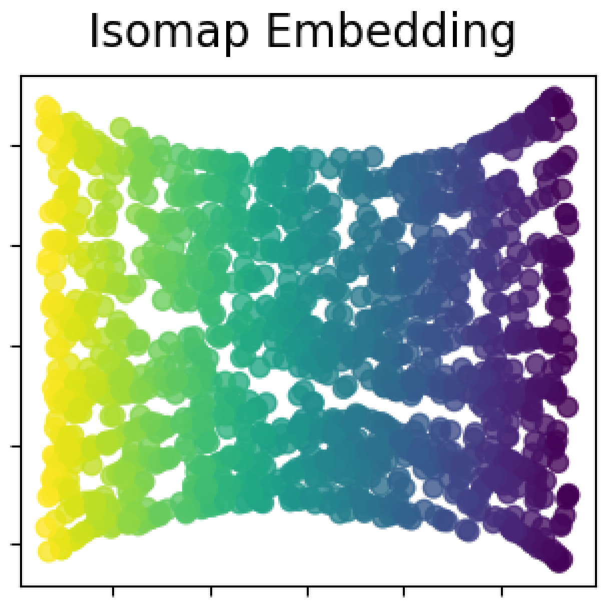
- In high dimensions, each point tends to be similarly distant to many points, so we often use PCA before applying t-SNE

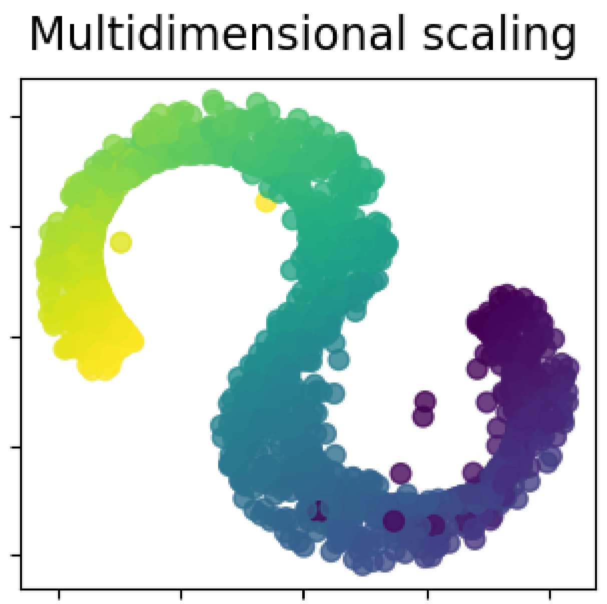
t-SNE on 30 PCA dimensions of MNIST

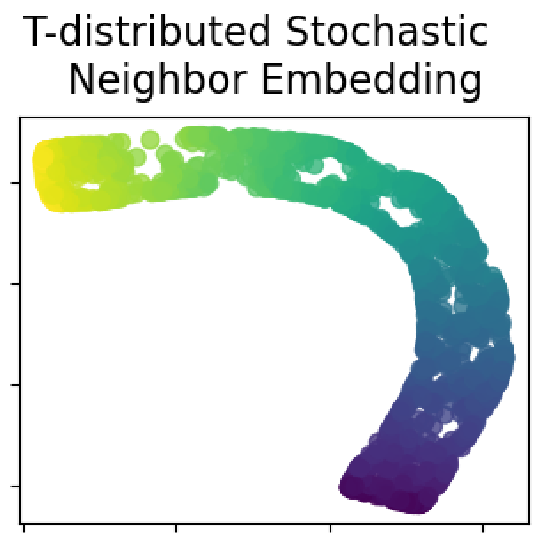


Comparison





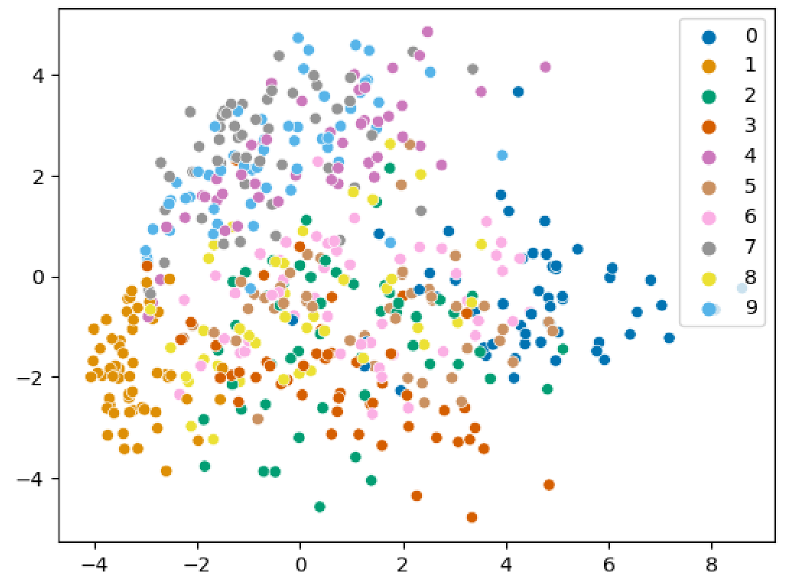




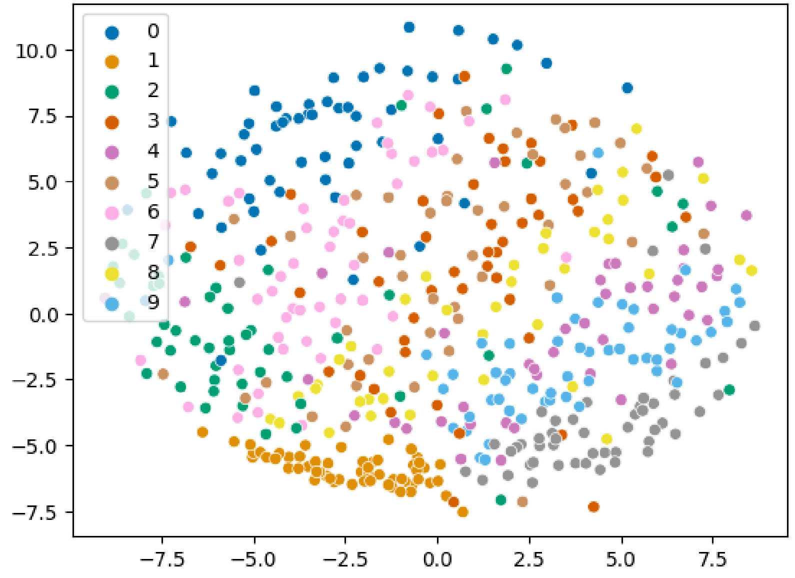
https://scikit-learn.org/stable/auto_examples/manifold/plot_compare_methods.html

Comparison on MNIST

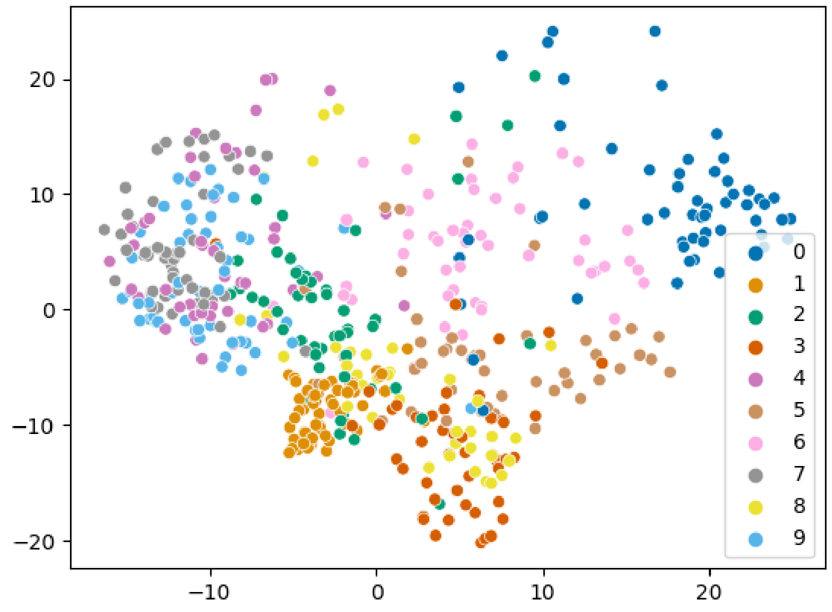
PCA



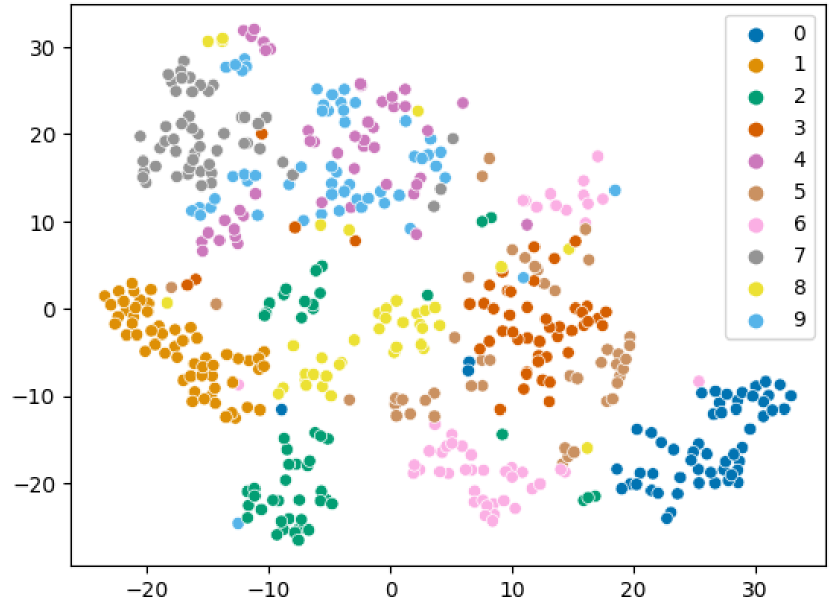
MDS



IsoMap



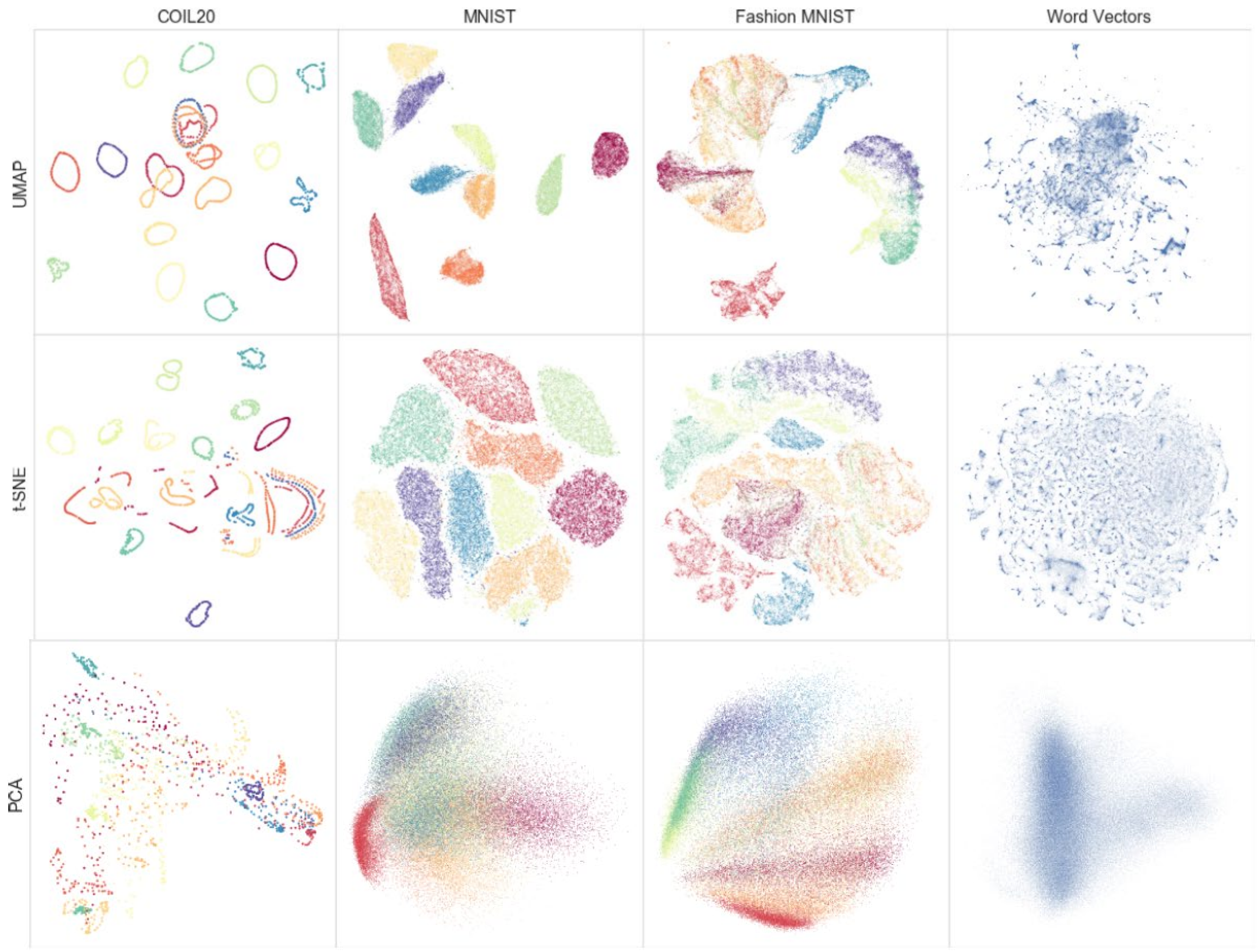
tSNE



UMAP (McInnes, 2020)

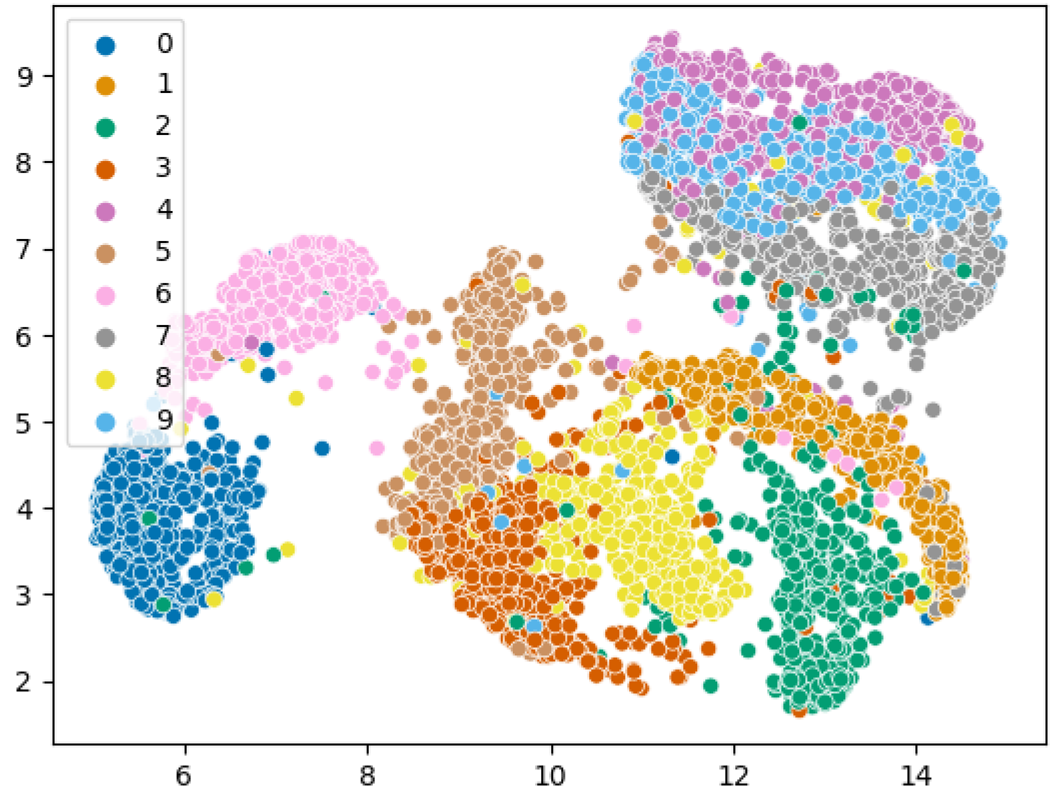
- Assumes data is uniformly distributed on an underlying manifold that is locally connected. Goal is to preserve that local structure.
- Algorithm: relatively complicated, incorporates many ideas from other methods, has strong mathematical foundations
- Hyperparameters:
  - number of neighbors to consider
  - dimension of target embedding
  - desired separation between close points
  - number of training epochs

https://arxiv.org/abs/1802.03426

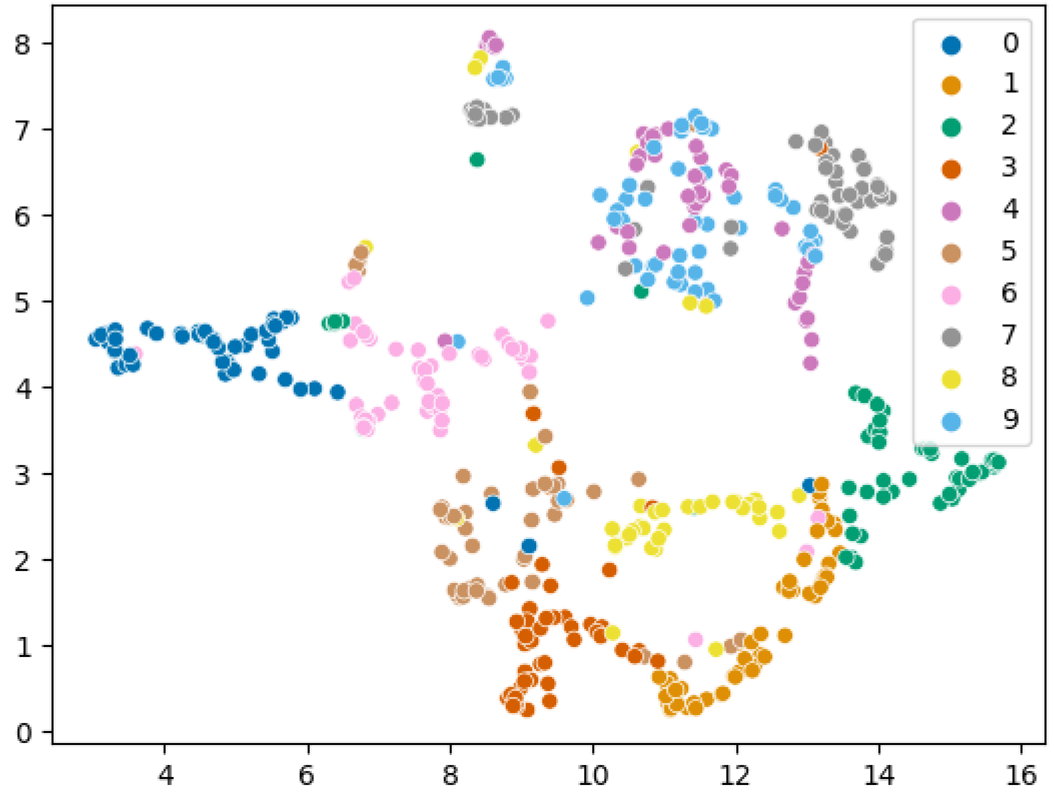


	UMAP	t-SNE	Isomap
Pen Digits (1797x64)	9s	17s	**2s**
COIL20 (1440x16384)	**12s**	22s	58s
COIL100 (7200x49152)	**85s**	810s	3210s
scRNA (21086x1000)	**28s**	258s	923s
Shuttle (58000x9)	**94s**	714s	–
MNIST (70000x784)	**87s**	1450s	–
F-MNIST (70000x784)	**65s**	934s	–
Flow (100000x17)	**102s**	1135s	–
Google News (200000x300)	**361s**	16906s	–

UMAP on MNIST



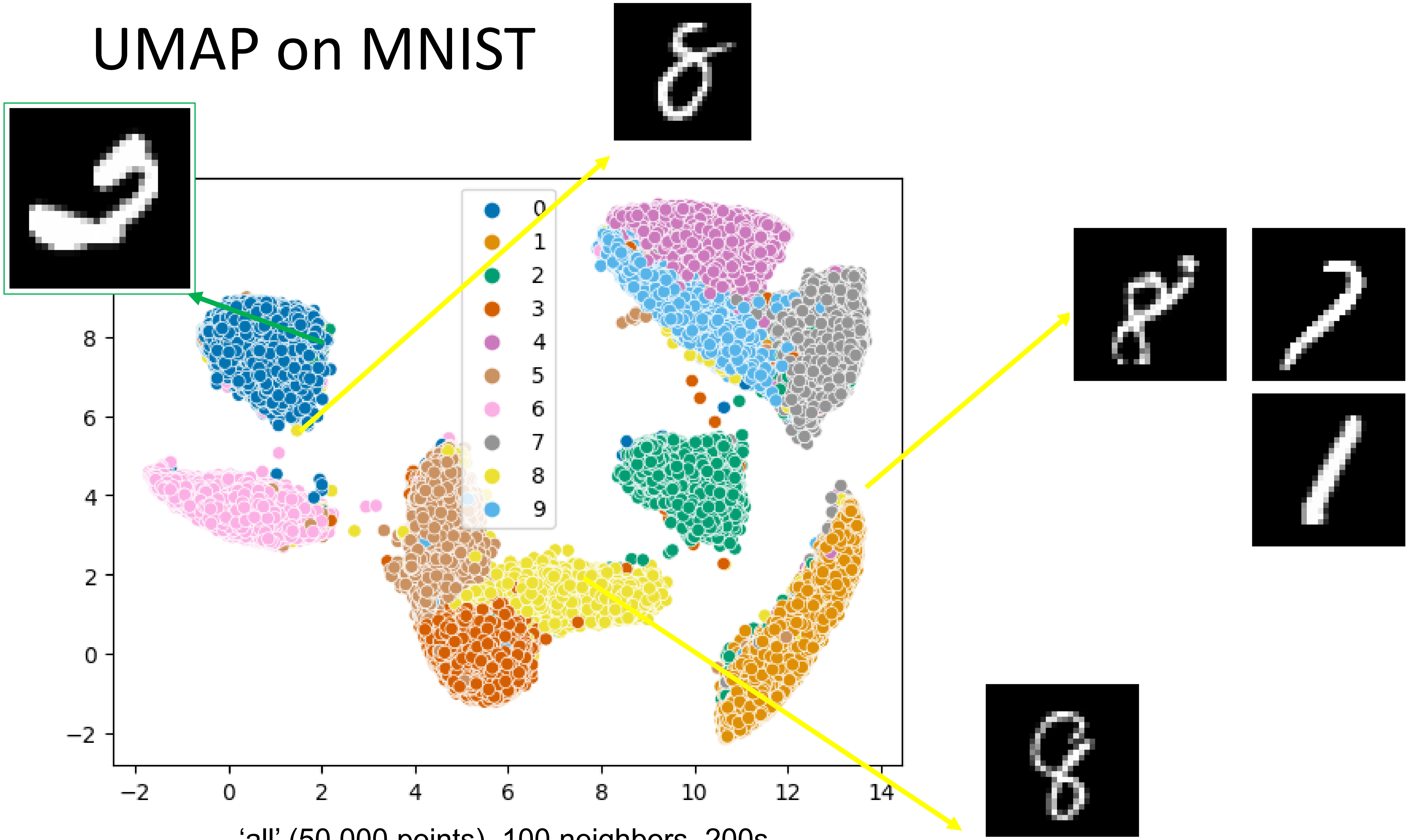
‘m’ (5000 points), 100 neighbors, 34s



‘s’ (500 pts), 10 neighbors

```
#!pip install umap-learn
from umap import UMAP
ind = train_indices['s']
x_umap = UMAP(n_components=2, n_neighbors=100).fit_transform(x[ind, :30])
sns.scatterplot(x=x_umap[ind,0],y=x_umap[ind,1], hue=y_train[ind], palette="colorblind")
```

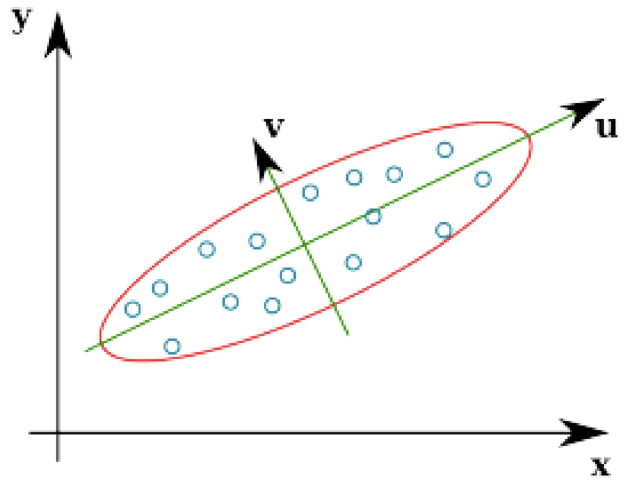
UMAP on MNIST



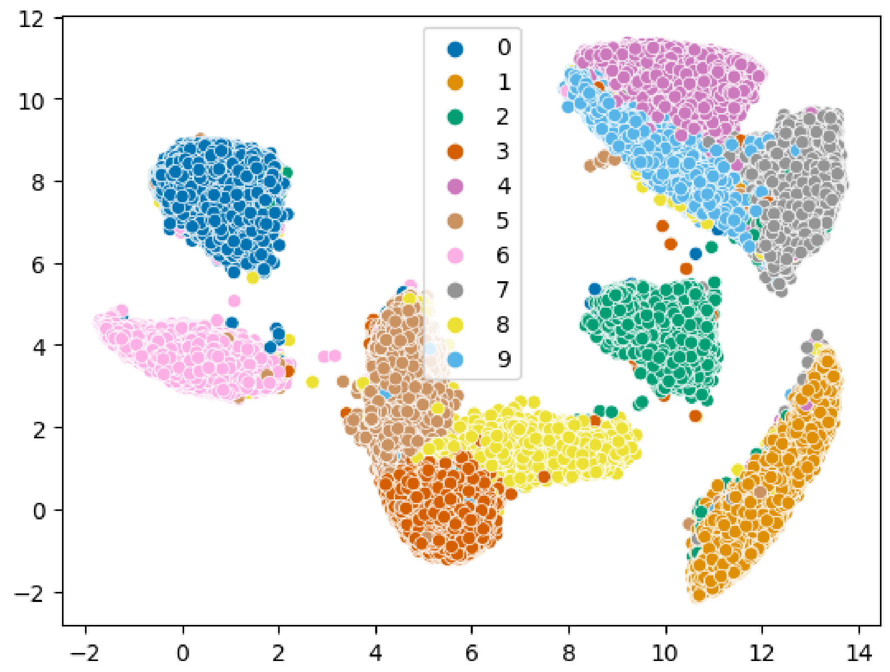
'all' (50,000 points), 100 neighbors, 200s

Things to remember

- PCA reduces dimensions by linear projection
  - Preserves variance to reproduce data as well as possible, according to mean squared error
  - May not preserve local structure or discriminative information



- Other methods try to preserve relationships between points
  - MDS: preserve pairwise distances
  - IsoMap: MDS but using a graph-based distance
  - t-SNE: preserve a probabilistic distribution of neighbors for each point (also focusing on closest points)
  - UMAP: incorporates k-nn structure, spectral embedding, and more to achieve good embeddings relatively quickly



Next class: Topic Modeling

Topic Modeling

- LDA
- LSA
- BertTopic
  - https://blog.deepgram.com/python-topic-modeling-with-a-bert-model/
  - https://www.pinecone.io/learn/bertopic/ (also covers umap)