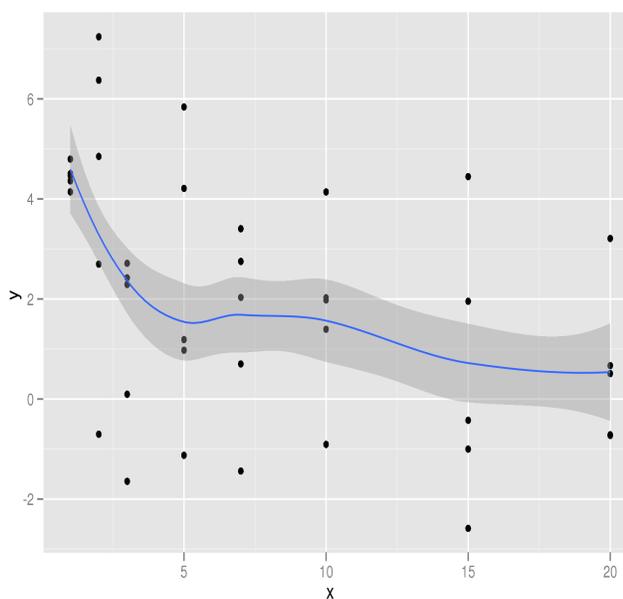


Which of these reveal the hidden structure of data?

```

-----
| 0.5000 0.5040 0.5080 0.5120 0.5160 0.5199 0.5239 0.5279 0.5319 0.5359
| 0.5398 0.5438 0.5478 0.5517 0.5557 0.5596 0.5636 0.5675 0.5714 0.5753
| 0.5793 0.5832 0.5871 0.5910 0.5948 0.5987 0.6026 0.6064 0.6103 0.6141
| 0.6179 0.6217 0.6255 0.6293 0.6331 0.6368 0.6406 0.6443 0.6480 0.6517
| 0.6554 0.6591 0.6628 0.6664 0.6700 0.6736 0.6772 0.6808 0.6844 0.6879
| 0.6915 0.6950 0.6985 0.7019 0.7054 0.7088 0.7123 0.7157 0.7190 0.7224
| 0.7257 0.7291 0.7324 0.7357 0.7389 0.7422 0.7454 0.7486 0.7517 0.7549
| 0.7580 0.7611 0.7642 0.7673 0.7704 0.7734 0.7764 0.7794 0.7823 0.7852
| 0.7881 0.7910 0.7939 0.7967 0.7995 0.8023 0.8051 0.8078 0.8106 0.8133
| 0.8159 0.8186 0.8212 0.8238 0.8264 0.8289 0.8315 0.8340 0.8365 0.8389
| 0.8413 0.8438 0.8461 0.8485 0.8508 0.8531 0.8554 0.8577 0.8599 0.8621
| 0.8643 0.8665 0.8686 0.8708 0.8729 0.8749 0.8770 0.8790 0.8810 0.8830
| 0.8849 0.8869 0.8888 0.8907 0.8925 0.8944 0.8962 0.8980 0.8997 0.9015
| 0.9032 0.9049 0.9066 0.9082 0.9099 0.9115 0.9131 0.9147 0.9162 0.9177
| 0.9192 0.9207 0.9222 0.9236 0.9251 0.9265 0.9279 0.9292 0.9306 0.9319
| 0.9332 0.9345 0.9357 0.9370 0.9382 0.9394 0.9406 0.9418 0.9429 0.9441
| 0.9452 0.9463 0.9474 0.9484 0.9495 0.9505 0.9515 0.9525 0.9535 0.9545
| 0.9554 0.9564 0.9573 0.9582 0.9591 0.9599 0.9608 0.9616 0.9625 0.9633
| 0.9641 0.9649 0.9656 0.9664 0.9671 0.9678 0.9686 0.9693 0.9699 0.9706
| 0.9713 0.9719 0.9726 0.9732 0.9738 0.9744 0.9750 0.9756 0.9761 0.9767
| 0.9772 0.9778 0.9783 0.9788 0.9793 0.9798 0.9803 0.9808 0.9812 0.9817
| 0.9821 0.9826 0.9830 0.9834 0.9838 0.9842 0.9846 0.9850 0.9854 0.9857
| 0.9861 0.9864 0.9868 0.9871 0.9875 0.9878 0.9881 0.9884 0.9887 0.9890
| 0.9893 0.9896 0.9898 0.9901 0.9904 0.9906 0.9909 0.9911 0.9913 0.9916
| 0.9918 0.9920 0.9922 0.9925 0.9927 0.9929 0.9931 0.9932 0.9934 0.9936
| 0.9938 0.9940 0.9941 0.9943 0.9945 0.9946 0.9948 0.9949 0.9951 0.9952
| 0.9953 0.9955 0.9956 0.9957 0.9959 0.9960 0.9961 0.9962 0.9963 0.9964
| 0.9965 0.9966 0.9967 0.9968 0.9969 0.9970 0.9971 0.9972 0.9973 0.9974
| 0.9974 0.9975 0.9976 0.9977 0.9977 0.9978 0.9979 0.9979 0.9980 0.9981
| 0.9981 0.9982 0.9982 0.9983 0.9984 0.9984 0.9985 0.9985 0.9986 0.9986
| 0.9987 0.9987 0.9987 0.9988 0.9988 0.9989 0.9989 0.9989 0.9990 0.9990

```



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## Why learn representations in lower dimensions?



**VISUALIZATION:**  
PROJECTING DATA POINTS ONTO A 2D OR 3D SPACE CAN HELP IN IDENTIFYING PATTERNS, CLUSTERS, OR OUTLIERS.



DIMENSIONALITY REDUCTION CAN SIMPLIFY THE DATA AND MAKE IT MORE MANAGEABLE.



COMPUTATIONAL EFFICIENCY, ESPECIALLY FOR ML ALGORITHMS BASED ON DISTANCE CALCULATIONS CAN LEAD TO FASTER TRAINING AND INFERENCE TIMES.



OVERFITTING MITIGATION BY REDUCING THE COMPLEXITY OF THE MODEL.



LOWER-DIMENSIONAL REPRESENTATIONS CAN BE MORE INTERPRETABLE WHEN TRYING TO UNDERSTAND AND COMMUNICATE THE RESULTS OF A MACHINE LEARNING MODEL.

## More reasons to learn representations in lower dimensions



Data **Compression** beneficial for storage and transmission of data.



Makes it **easier** for **clustering and classification** algorithms to identify patterns and group data points.



Anomalies or **outliers** may become more apparent in lower-dimensional space, aiding in the detection of unusual or suspicious data points.

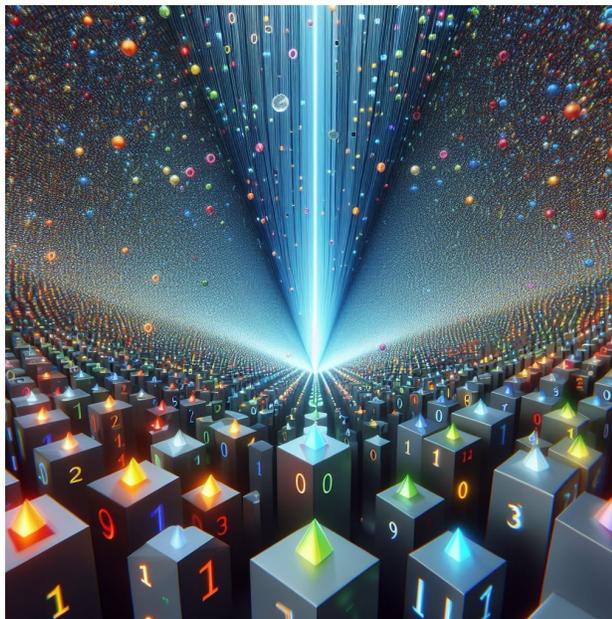


Identifying and retaining the most important features of the data while discarding less important or redundant ones can lead to **more efficient and effective models**.



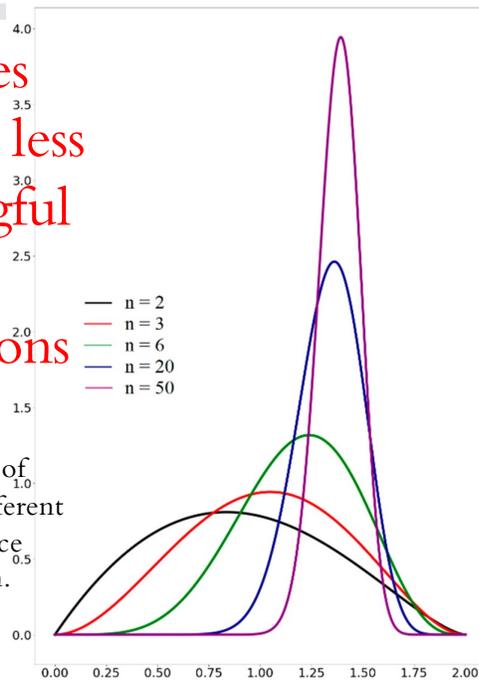
Reduces the impact of **noise or random variations** in the data, making it easier for models to focus on the underlying patterns.

Training data needs  
grow exponentially  
with dimensions  
=> Learning in high  
dimensions is  
intractable

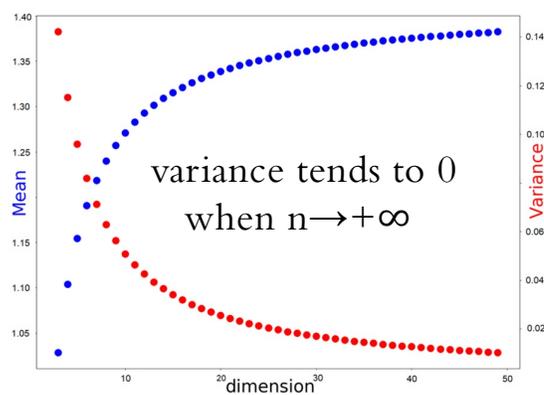


Distances  
become less  
meaningful  
in high  
dimensions

Distribution of  
distances for different  
values of space  
dimension  $n$ .

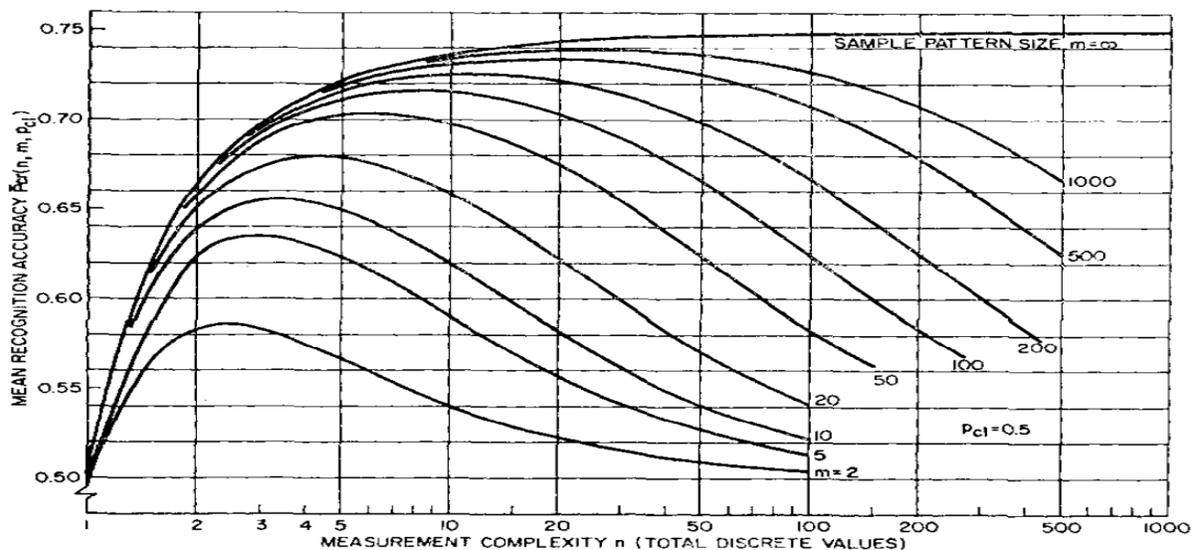


Lellouche, S., & Souris, M. (2019). Distribution of  
distances between elements in a compact set. *Stats*, 3(1),  
1-15.



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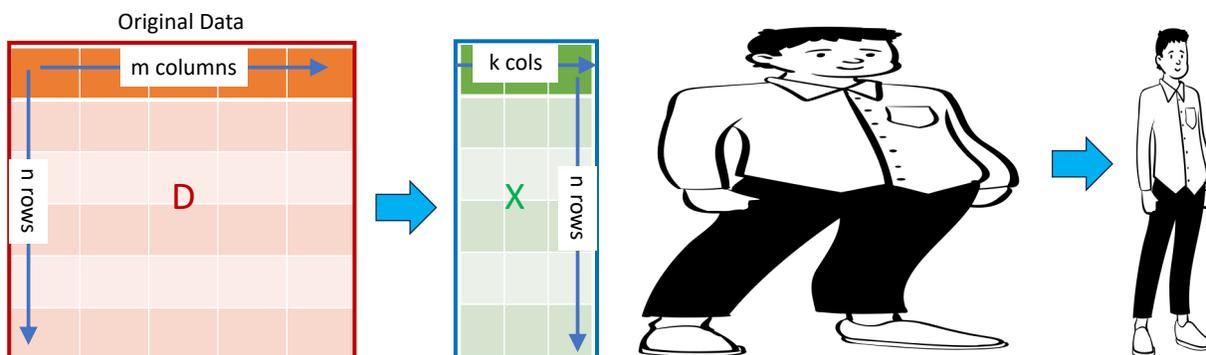
## Curse of dimensionality: Hughes phenomenon



Source: Hughes, G. F. (1968). On the mean accuracy of statistical pattern recognizers. IEEE Transactions on Information Theory, 14(1), 55-63.

## Principal Component Analysis (PCA)

- Does not require labels – **unsupervised**
- Data with many ( $m$ ) features abstracted / condensed into fewer ( $k$ ) principal components ( $k < m$ ) that are **synthetic**



## More Intuition

Movies are shot in 3D but we watch in 2D without much loss of information even when dropping the 3<sup>rd</sup> dimension.

We listen to music when working. But when we need to focus, we drop the music dimension without forgoing much.

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### Class Survey: Rate these on a scale of 1-5

- Everyone in my team contributes to my learning 
- My team provides great insights during discussions 
- Each team member creates a positive environment 

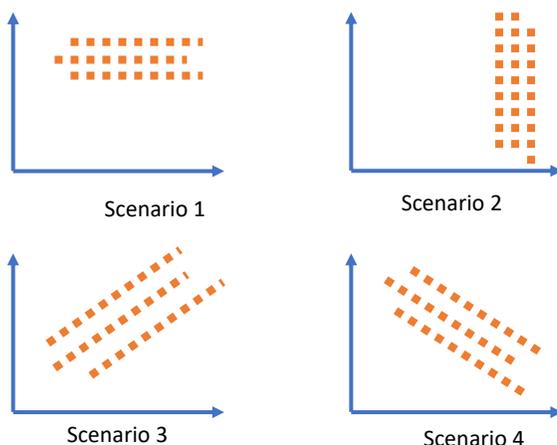
 **Redundancy**

- Can be replaced by

- My team generates great synergy 

 **Latent intent**

Which of the 4 plots is most likely?

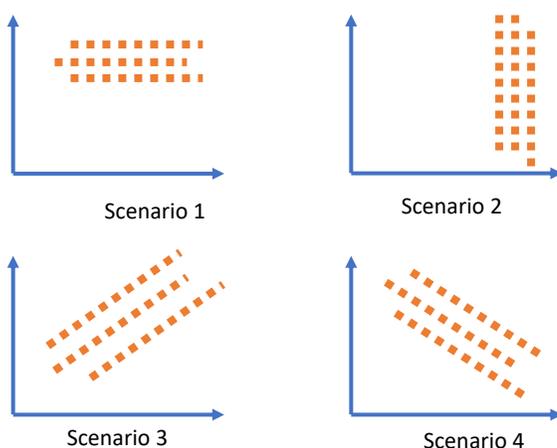


**X-axis:** DATA 245 Score

**Y-axis:** DATA 228 Score

Each vector represents the scores obtained by a student in the MSDA program

If only one subject's grade is available for hiring an RA, what would that subject be?



**X-axis:** DATA 245 Score

**Y-axis:** DATA 228 Score

Each vector represents the scores obtained by a student in the MSDA program

*It is the variance that matters!*



Source: <https://www.flickr.com/photos/grantp/668054637>

A slide with a blue circuit board background. In the top left, there is a scatter plot with a grid and an arrow pointing towards the top right. In the top right, there is a caricature of Barack Obama with a large, smiling mouth and a hand pointing. Below the scatter plot is a green rounded rectangle containing the text "Principal Component Analysis". To the right of that is another green rounded rectangle containing the text "Caricature".

Principal  
Component  
Analysis

Caricature

How do we capture the oddities or unique variations in a dataset?



## Principal Component Analysis (PCA) – A Linear Technique



**Originated** in: Pearson, K. (1901). *On Lines and Planes of Closest Fit to Systems of Points in Space*. *Philosophical Magazine*, 2, 559-572.

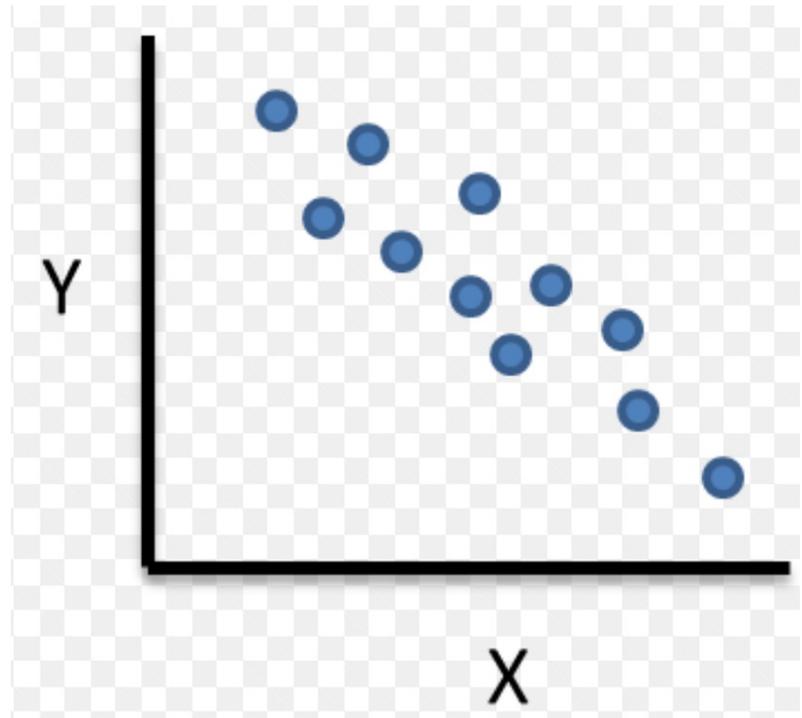


**Significant Improvement:** Hotelling, H. (1933). *Analysis of a Complex of Statistical Variables into Principal Components*. *Journal of Educational Psychology*, 24(6), 417-441.

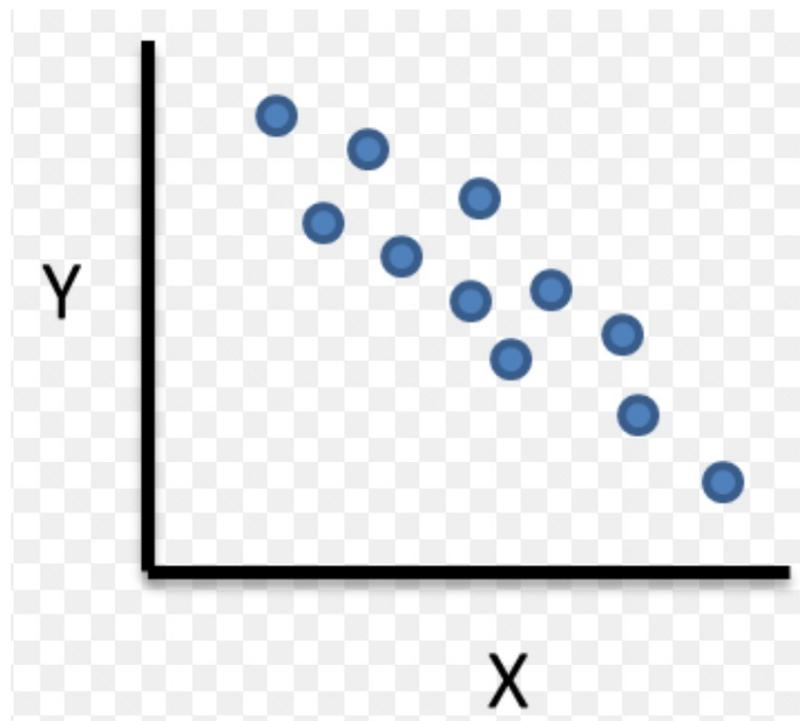


**First application:** Goodall, D. W. (1954). *Objective methods for the classification of vegetation. III. An essay in the use of factor analysis*. *Australian Journal of Botany*, 2(3), 304-324.

Can we use just one dimension for this 2D data?



What's the statistical parameter that is indicative of the direction?



## PCA: Ideas



Capture as much **important** information in a dataset, but using fewer features (dimensions)



Transform the feature space: From correlated features to entirely uncorrelated, **orthogonal**, synthetic features



Drop **least important** features so generated; importance is indicative of the **variance** in the data the new feature captures



Result: Original dataset is now projected in a fewer dimensional space



Keywords: variance; orthogonal; relative importance



Think: covariance matrix; eigen vectors (orthogonal for symmetric matrices like the covariance matrix); eigen values

## The notion of variance and correlation

- One variable,  $\text{Var}(x) = \frac{\sum_{i=1}^N (x_i - \bar{x})^2}{n}$  Two Variables,  $\text{Cov}(x,y) = \frac{\sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})}{n}$

$x$  and  $y$  are independent  $\Rightarrow \text{cov}(x,y) = 0$ ; directly correlated  $\Rightarrow \text{cov}(x,y) > 0$

inversely correlated  $\Rightarrow \text{cov}(x,y) < 0$

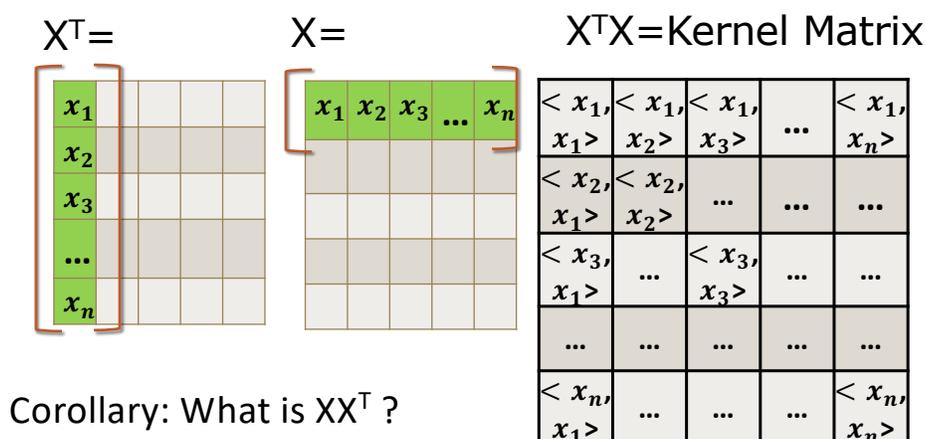
$$\text{Correlation Coefficient} = \frac{\text{cov}(x,y)}{\sqrt{\text{Var}(x) \cdot \text{Var}(y)}}$$

- Three or more variables, Covariance Matrix:

$\text{Cov}(x,x) = \text{var}(x)$	$\text{Cov}(x,y)$	$\text{Cov}(x,z)$
$\text{Cov}(y,x)$	$\text{Cov}(y,y) = \text{var}(y)$	$\text{Cov}(y,z)$
$\text{Cov}(z,x)$	$\text{Cov}(z,y)$	$\text{Cov}(z,z) = \text{var}(z)$

*If the data is already mean adjusted, what is the covariance?*

## Kernel Matrix vs Covariance Matrix



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## Eigenvalues and Eigenvectors

Eigenvalues ( $\lambda$ ) are scalar values that represent how a linear transformation (represented by a matrix) stretches or compresses space.

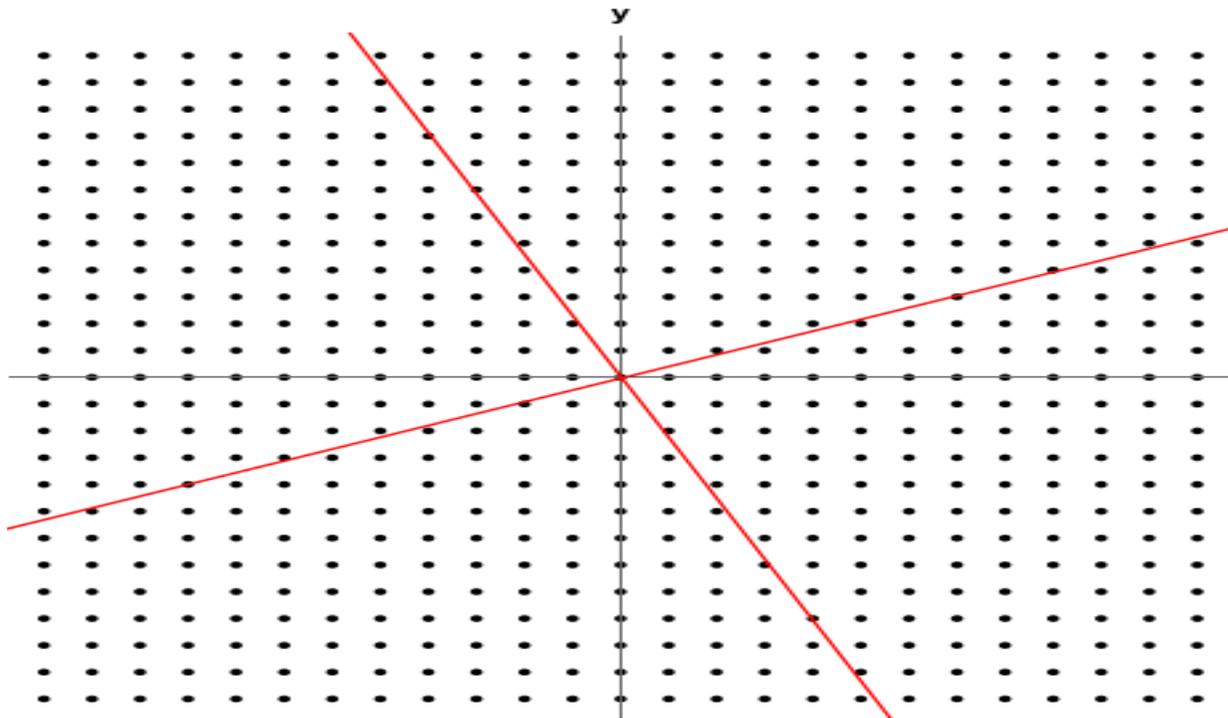
For a given eigenvalue, there may be multiple eigenvectors. The set of all eigenvectors corresponding to a particular eigenvalue is called the eigenspace.

If  $A$  is a square matrix,  $\lambda$  is an eigenvalue of  $A$  if there exists a non-zero eigenvector  $v$  such that  $Av = \lambda v$ .

Eigenvectors are non-zero vectors that only change by a scalar factor,  $\lambda$  (direction does not change) when a linear transformation,  $A$  is applied

Two properties useful for PCA:

- Orthogonality: Eigenvectors corresponding to distinct eigenvalues are orthogonal (linearly independent) for symmetric matrices
- Eigenbasis: Eigenvectors can form a basis for a vector space



Jacopo Bertolotti, CC0, via Wikimedia Commons

## Finding Eigenvalues and Eigenvectors

- Characteristic equation: Determinant of  $(A - \lambda I) = 0$ , where  $A$  is the matrix,  $\lambda$  is the eigenvalue, and  $I$  is the identity matrix of the same size as  $A$ .
- Why?  $Ax = \lambda x \Rightarrow (Ax - \lambda x) = 0 \Rightarrow (A - \lambda I)x = 0$  and by definition, eigenvectors are non-zero, so  $\det(A - \lambda I) = 0$
- Solve the characteristic equation for  $\lambda$  to find the eigenvalues.
- To find the eigenvectors, for each eigenvalue  $\lambda$ :
  - Substitute  $\lambda$  back into the equation  $(A - \lambda I)v = 0$ , where  $v$  is the eigenvector.
  - Solve the resulting system of linear equations to find the eigenvector  $v$ .

## Finding eigenvectors: 2x2 matrix example

- Matrix A:  $\begin{bmatrix} 4 & 2 \\ 3 & -1 \end{bmatrix}$
- Characteristic equation: :  

$$\begin{bmatrix} 4 - \lambda & 2 \\ 3 & -1 - \lambda \end{bmatrix} = 0$$

$$\Rightarrow (4 - \lambda)(-1 - \lambda) - 6 = 0$$

$$\lambda^2 - 3\lambda - 10 = 0 \Rightarrow (\lambda - 5)(\lambda + 2) = 0$$
- Eigenvalues:  $\lambda = 5, -2$
- **Eigenvector for  $\lambda = 5$ :**
- $(A - 5I)v = 0$
- $\begin{bmatrix} -1 & 2 \\ 3 & -6 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 0$
- $\Rightarrow -x + 2y = 0$  and  $3x - 6y = 0$
- Both the equations are identical to  $x = 2y$
- Solving this system gives many eigenvectors such as  $v = [2, 1]$ .
- **Eigenvector for  $\lambda = -2$ :**
- $(A + 2I)v = 0$
- $\begin{bmatrix} 6 & 2 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 0$
- Again, the resulting equations are identical to  $y = -3x$
- Many eigenvectors like  $[1, -3], [2, -6]$

## Finding eigenvectors: 3x3 symmetric matrix

- Matrix A:  $\begin{bmatrix} 2 & 1 & 3 \\ 1 & 2 & 3 \\ 3 & 3 & 20 \end{bmatrix}$
- Characteristic equation:
- $$\begin{bmatrix} 2 - \lambda & 1 & 3 \\ 1 & 2 - \lambda & 3 \\ 3 & 3 & 20 - \lambda \end{bmatrix} = 0$$
- Expand the determinant using cofactor expansion:
- Choose a row or column to expand along. For this example, let's expand along the first row:
- $$(2 - \lambda) * (\text{submatrix determinant}) - 1 * (\text{submatrix determinant}) + 3 * (\text{submatrix determinant}) = 0$$
- Evaluate each 2x2 submatrix determinant:
- $$(2 - \lambda)[(2 - \lambda)(20 - \lambda) - 9] - 1[(1)(20 - \lambda) - 9] + 3[(1)(3) - (2 - \lambda)(3)]$$
- $$\Rightarrow \lambda^3 - 25\lambda^2 + 114\lambda - 120 = 0$$
- $$\Rightarrow (\lambda - 1)(\lambda - 5)(\lambda - 20) = 0$$
- $\lambda = 1, 5, 20$
- Eigenvectors can be found like before



What if the eigen values cannot be found or are not real numbers?

Not Possible for Covariance matrices!

## Eigen vectors of a Symmetric Matrix

If all the values in the symmetric matrix ( $S^T = S$ ) are real, then eigen values and eigen vectors are **real** numbers as well.

Eigen vectors of a real symmetric matrix are **orthogonal**

**Spectral decomposition**:  $S = Q\Lambda Q^T$  where  $Q$  is an orthogonal matrix

$Q$ 's columns are eigen vectors of  $S$

$\Lambda$  is a diagonal matrix of eigen values of  $S$

All the eigen values of a **positive definite symmetric matrix** are positive

## Why are the eigenvalues of the Gram matrices nonnegative?

Let  $\lambda$  be any eigenvalue of  $K = X^T X$  and the corresponding eigen vector,  $v$ . Then,

$$\begin{aligned}(X^T X)v &= \lambda v \\ v^T X^T X v &= v^T \lambda v \\ (Xv)^T (Xv) &= \lambda v^T v \\ (Xv)^T (Xv) \text{ and } v^T v &\text{ are both norms} \\ &\text{so have to be positive} \\ \|Xv\|^2 &= \lambda \|v\|^2 \\ \Rightarrow \lambda &> 0\end{aligned}$$

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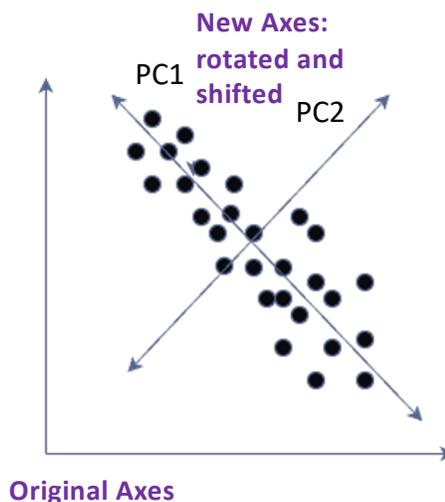
### Other interesting properties

- The eigenvalues of the covariance matrix,  $XX^T$  can also be similarly proved to be  $> 0$
- The Gram matrices  $XX^T$  and  $X^T X$  share the same nonzero eigenvalues (why?).

$$\begin{aligned}X^T X u &= \lambda u \\ XX^T X u &= X \lambda u \\ XX^T (X u) &= \lambda (X u) \\ XX^T \tilde{u} &= \lambda \tilde{u}\end{aligned}$$

## Principal Components

- Sort the absolute |eigenvalues|
- PC1: Direction of maximum spread (variance) – the direction of the 1<sup>st</sup> eigenvector corresponding to the largest absolute |eigenvalue|
- PC2: 2<sup>nd</sup> eigenvector direction covering maximum residual variation left in the data, orthogonal to PC1
- PC3 (if the original data has 3+ dimensions): 3<sup>rd</sup> eigenvector direction with maximum spread left in data after PC1 and PC2, orthogonal to PC1 and PC2
- So on and so forth
- Observation: PC1 covers most the spread; PC2 is almost redundant
- PC2 can be dropped without losing significant information that the data conveys



## Equations of the new axes in terms of the old

- Original features:  $x_1, x_2, x_3, \dots, x_m$     New **uncorrelated** PCs:  $z_1, z_2, z_3, \dots, z_m$
- $PC_1$  (direction of the **most spread**):  $z_1 = k_{11}x_1 + k_{12}x_2 + \dots + k_{1m}x_m$
- $[k_{11}, k_{12}, k_{13}, \dots, k_{1m}]$  is the 1st **eigenvector** of the **covariance** matrix
- $PC_2$  (direction of 2<sup>nd</sup> eigenvector):  $z_2 = k_{21}x_1 + k_{22}x_2 + \dots + k_{2m}x_m$
- $[k_{21}, k_{22}, k_{23}, \dots, k_{2m}]$  is the 2nd eigenvector of the **covariance** matrix
- ...
- $PC_m$ :  $z_m = k_{m1}x_1 + k_{m2}x_2 + \dots + k_{mm}x_m$
- The PCs capture **all** of the information in the original features
- Usually, the 1<sup>st</sup> few PCs capture most of the information; rest are redundant
- If so, keep the 1<sup>st</sup> few and drop the rest => dimensionality reduction

## PCA: Dimensionality Reduction

- Cattell, Raymond B. (1966). "The Scree Test For The Number Of Factors". *Multivariate Behavioral Research*. 1 (2): 245–276.
- Scree Test: procedure of finding statistically significant factors
- Y-axis: eigenvalues represent the percentage of variance explained by each PC

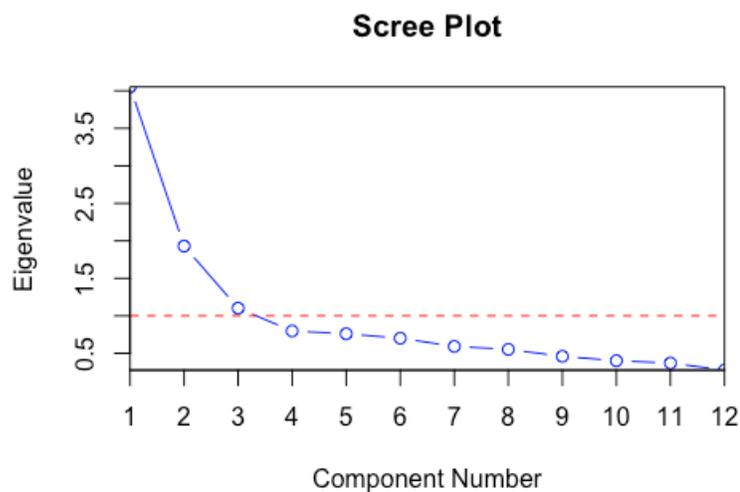
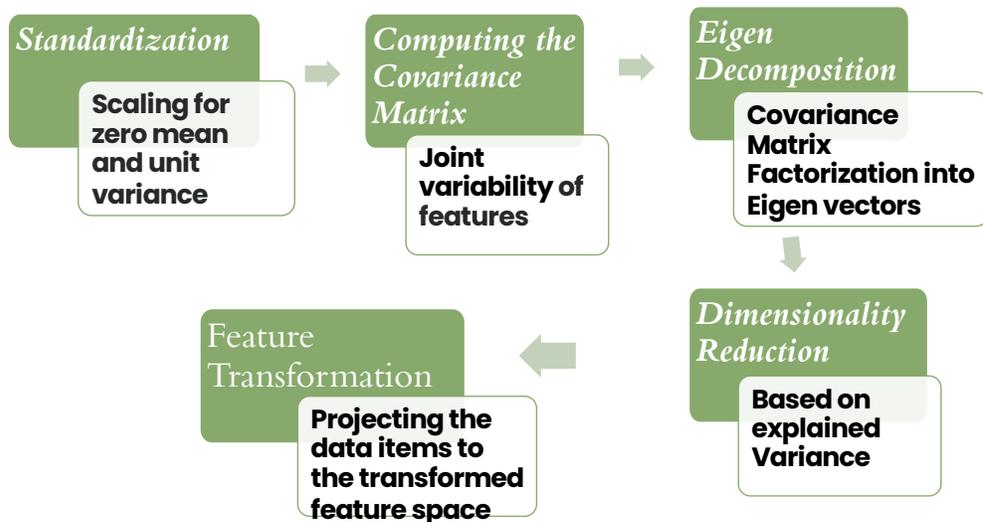


Figure By Staticshakedown - Own work, CC BY-SA 4.0, <https://commons.wikimedia.org/w/index.php?curid=75715167>

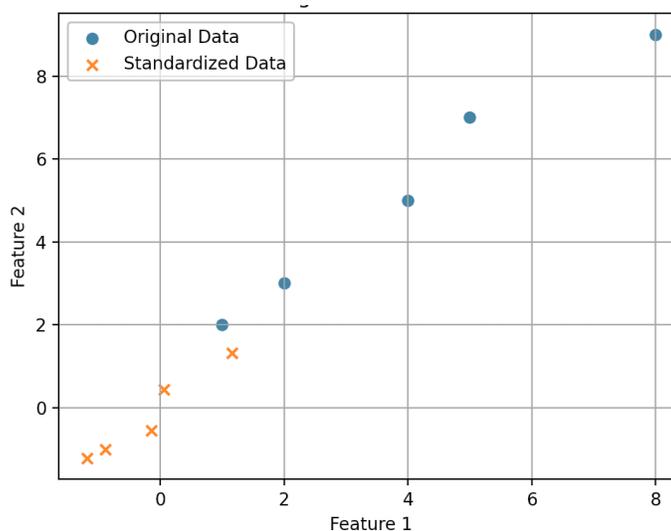
## PCA – The Process



## PCA: Implementation

- Data (2 features, 5 observations):
- $X = [[1, 2], [2, 3], [4, 5], [5, 7], [8, 9]]$
- $\text{std\_X} = \text{np.std}(X, \text{axis}=0)$ 
  - # [2.44948974 2.56124969]
- $Z = (X - \text{mean\_X}) / \text{std\_X}$
- Standardization: Calculate the mean and standard deviation for each variable:
  - $\text{mean\_X} = \text{np.mean}(X, \text{axis}=0)$ 
    - # [4.0, 5.2]
    - #  $\text{mean\_X1} = (1 + 2 + 4 + 5 + 8) / 5 = 4.0$
    - #  $\text{mean\_X2} = (2 + 3 + 5 + 7 + 9) / 5 = 5.2$
  - # Standardized data
  - $Z = [[-1.22474487 \ -1.2493901 \ ]$
  - $[-0.81649658 \ -0.85895569]$
  - $[0. \quad -0.07808688]$
  - $[0.40824829 \ 0.70278193]$
  - $[1.63299316 \ 1.48365074]]$

Effect of  
Standardization  
of Data



## PCA: Implementation (contd)

- covariance matrix of the standardized data:
 

```
Zt = np.transpose(Z)
cov_matrix = np.cov(Zt)
Σ = [[1.25    1.23530488]
      [1.23530488  1.25]]
```
- eigenvalues, eigenvectors = np.linalg.eig(cov\_matrix)
 

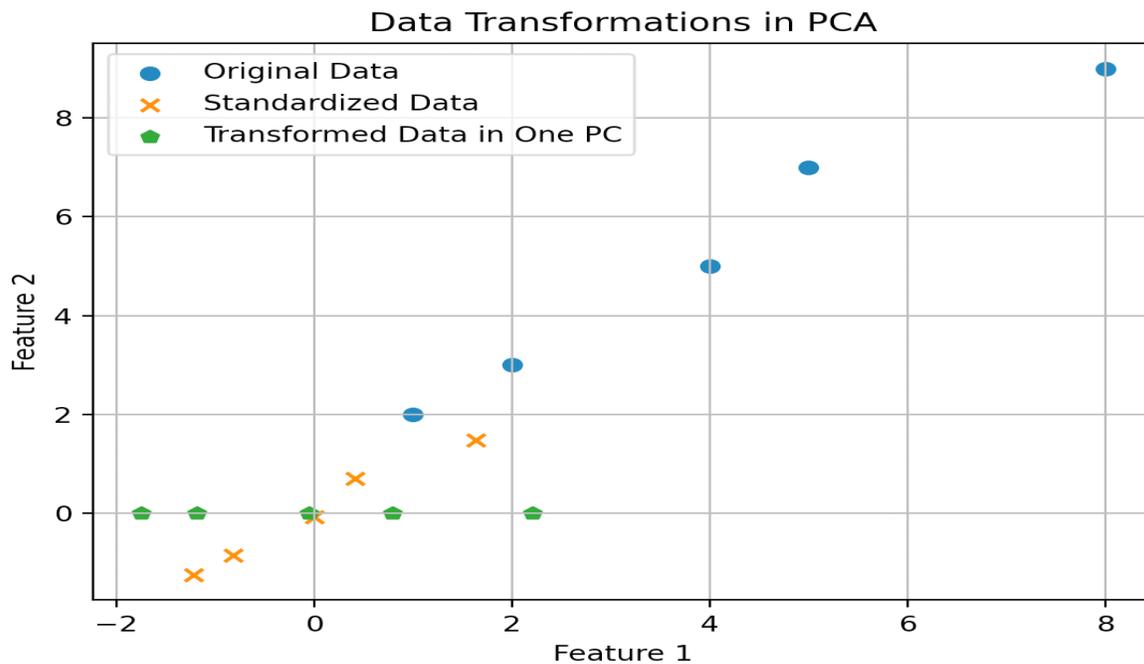
```
Eigenvalues: λ1 = 2.48530488, λ2 = 0.01469512
Eigenvectors: v1 = [0.70710678, 0.70710678], v2 = [-0.70710678, 0.70710678]
```
- sorted\_indices = np.argsort(eigenvalues)[::-1]
- sorted\_eigenvectors = eigenvectors[:, sorted\_indices]
- Choose the top k (=1, in this example) eigenvectors as principal components:
  - principal\_component = sorted\_eigenvectors[:, 0] # First PC
 

```
principal_component = [0.70710678, 0.70710678]
```

## PCA: Implementation (contd)

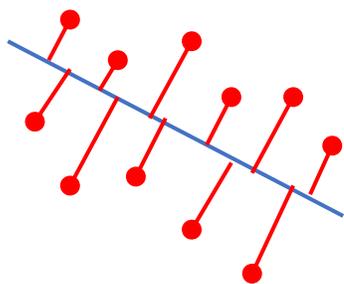
- Project the original data onto the selected principal component:
  - transformed\_data = Z.dot(principal\_component)
 

```
[-1.74947761 -1.18472366 -0.05521576  0.785617  2.20380004]
```
- The transformed data now has a single dimension, representing the projection of the original data onto the principal component
- This lower-dimensional representation captures the most significant variance in the data.



## Relation to Linear Regression

Linear Regression: Minimizing Least Squares

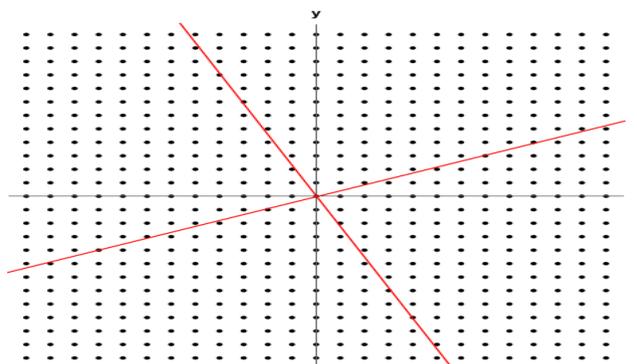


Minimizing this side (least square)



Is same as maximizing this side (projection)

PCA: Maximizing the stretch of the projection



Both are equivalent due to Pythagoras theorem



How can we reduce the  
dimensionality of this dataset?

This figure by Unknown Author is licensed under CC BY-SA

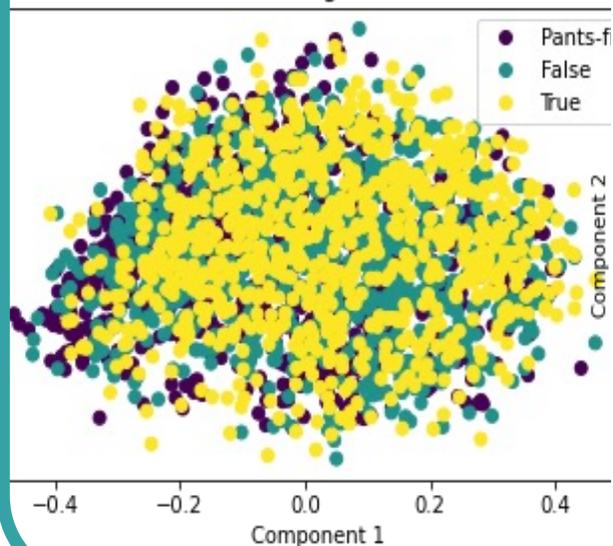
## Application of PCA

Pendyala, Vishnu S., and Foroozan Sadat Akhavan Tabatabaie. "Spectral analysis perspective of why **misinformation containment** is still an unsolved problem." *2023 IEEE Conference on Artificial Intelligence (CAI)*. IEEE, 2023.

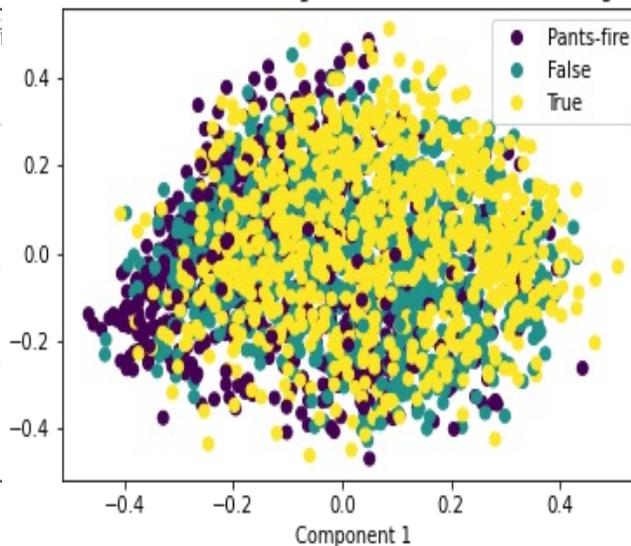


Pendyala, Vishnu S., and Foroozan Sadat Akhavan Tabatabaai. "Spectral analysis perspective of why misinformation containment is still an unsolved problem." 2023 IEEE Conference on Artificial Intelligence (CAI). IEEE, 2023.

PCA on SBERT Embeddings on Balanced Dataset

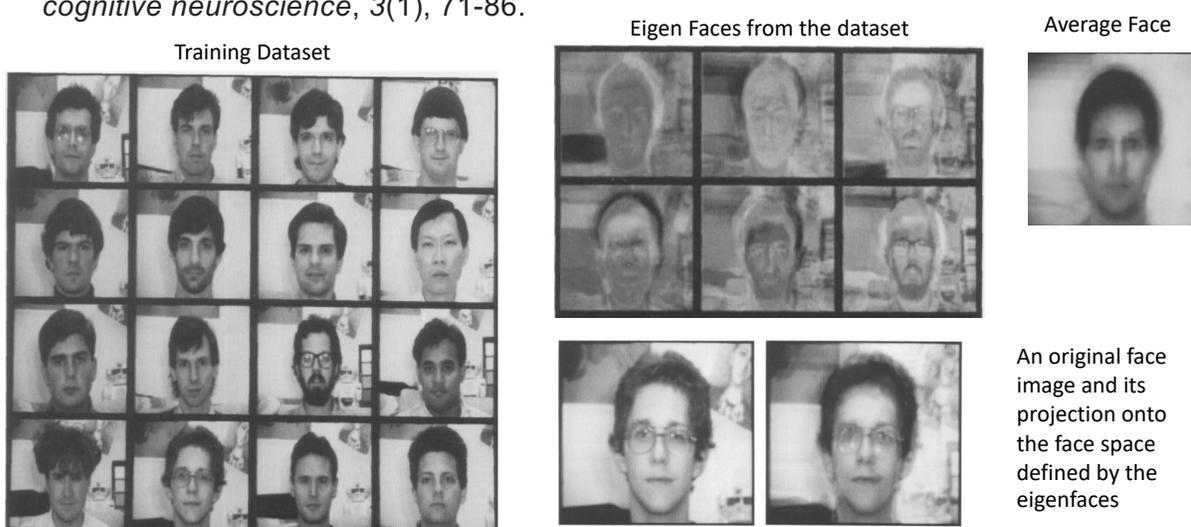


PCA on SBERT Embeddings on Balanced Dataset Using SVM

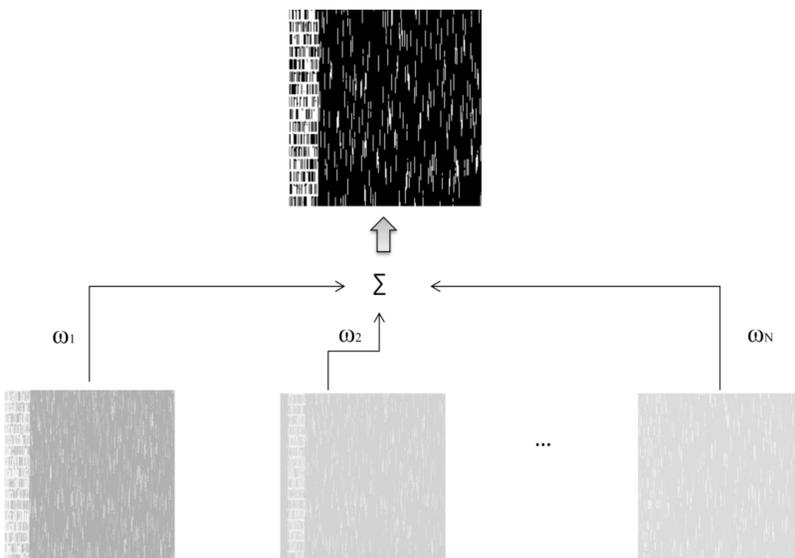


## More Interesting Applications of PCA

Source: Turk, M., & Pentland, A. (1991). **Eigenfaces** for recognition. *Journal of cognitive neuroscience*, 3(1), 71-86.



Source: Saleh, Mostafa E., A. Baith Mohamed, and A. Abdel Nabi. "Eigenviruses for metamorphic virus recognition." *IET information security* 5.4 (2011): 191-198.



- Eigenviruses are vectors that span across the most important features in the sample virus files
- Euclidean distance used to find the nearest neighbor for classification (recognition) of the virus

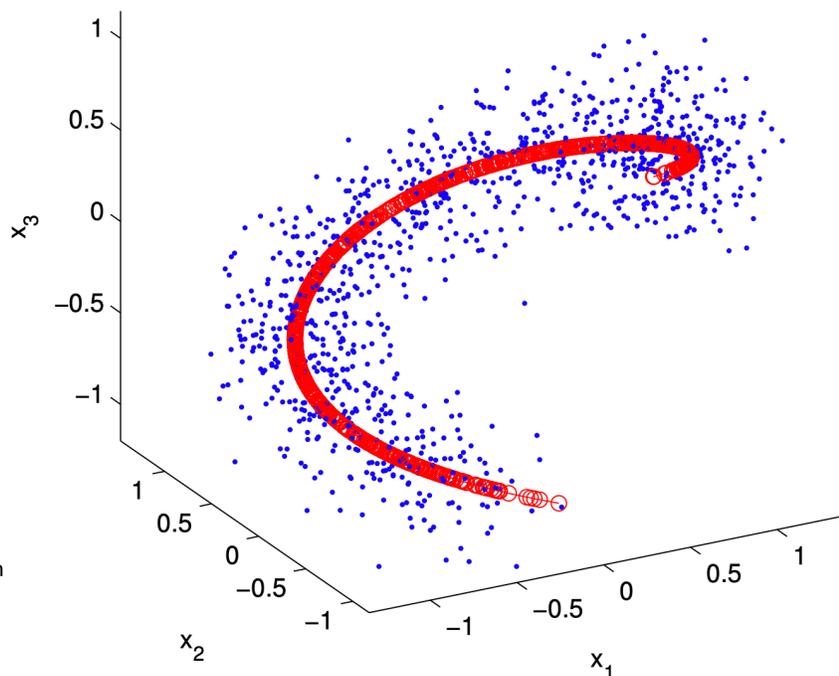
### Other eigen\* applications of PCA (contd)

- Speaker recognition and verification: Captures principal components of speech signals to create representative "eigenvoices."
  - Kuhn, Roland, et al. "Rapid speaker adaptation in eigenvoice space." *IEEE Transactions on Speech and Audio Processing* 8.6 (2000): 695-707.
  - Kwok, J., Mak, B., & Ho, S. (2003). Eigenvoice speaker adaptation via composite kernel principal component analysis. *Advances in Neural Information Processing Systems*, 16.
- Hand gesture recognition: principal components from hand images or videos to generate "eigenhands."
  - Birk, Henrik, Thomas B. Moeslund, and Claus B. Madsen. "Real-time recognition of hand alphabet gestures using principal component analysis." *Proceedings of the Scandinavian conference on image analysis*. Vol. 1. Proceedings published by various publishers, 1997.

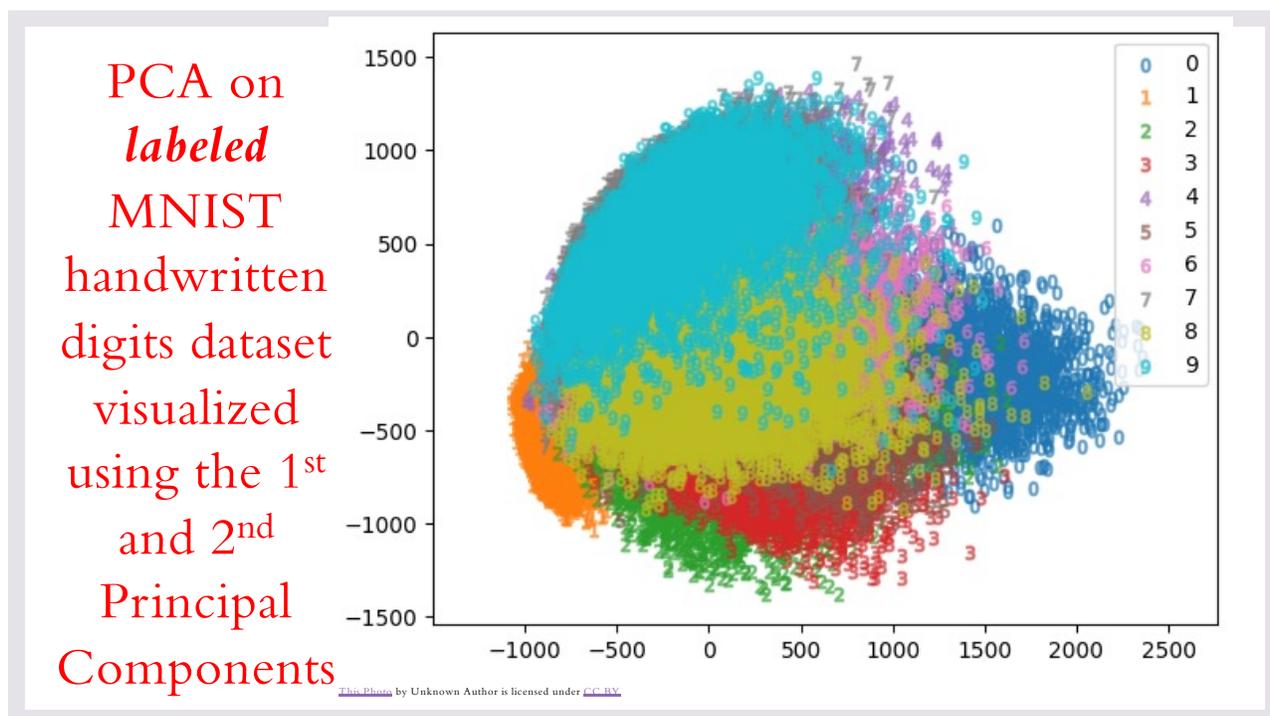
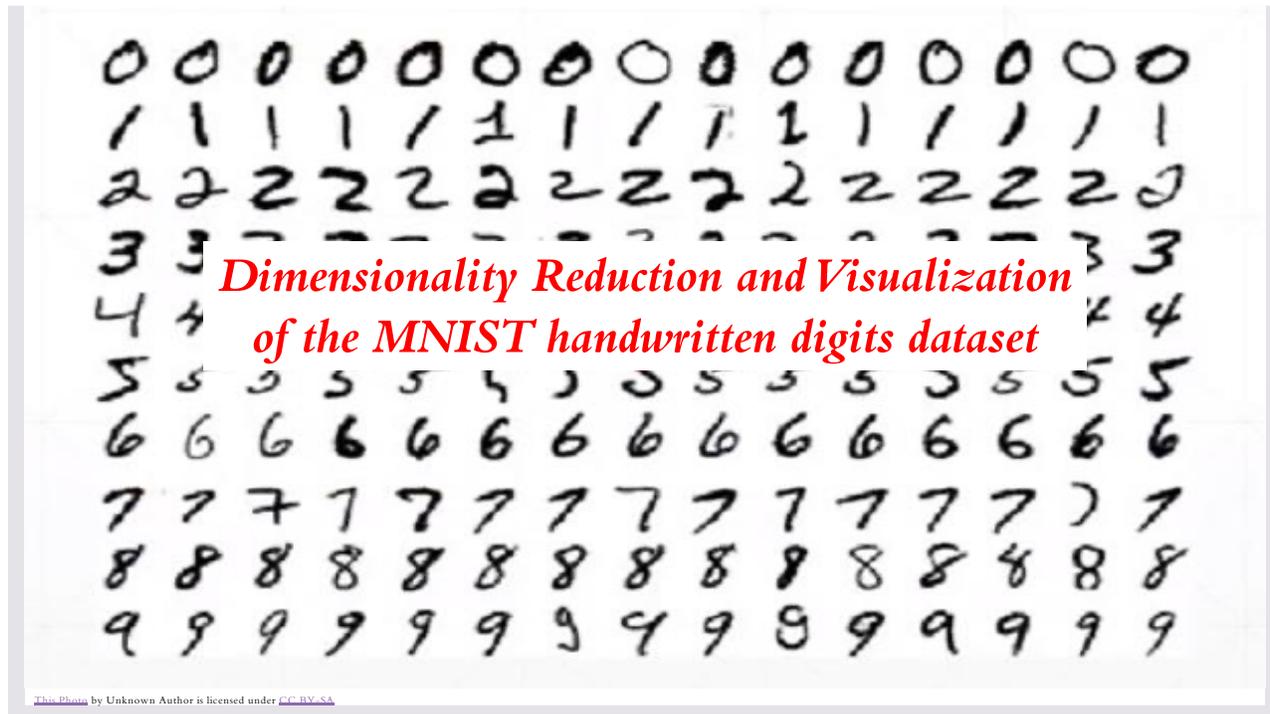
## Other eigen\* applications of PCA (contd)

- Gesture recognition in general: Captures principal directions of variation in gesture data to create "eigengestures."
  - Nakajima, Masato, et al. "Motion prediction based on eigen-gestures." Proc. of the 1st First Korea-Japan Joint Workshop on Pattern Recognition. 2006.
  - Gawron, Piotr, et al. "Eigengestures for natural human computer interface." Man-Machine Interactions 2. Springer Berlin Heidelberg, 2011.
- Texture analysis and synthesis: principal components of texture patterns to create "eigentextures."
  - Vasilescu, M. A. O., & Terzopoulos, D. (2004). TensorTextures: Multilinear image-based rendering. In ACM SIGGRAPH 2004 Papers (pp. 336-342).
- General image compression and representation: Computes eigenvectors of image covariance matrices to form a basis for representing images
  - Abadpour, A., & Kasaei, S. (2008). Color PCA eigenimages and their application to compression and watermarking. Image and Vision Computing, 26(7), 878-890.

## Principal Components of Non-linear Data

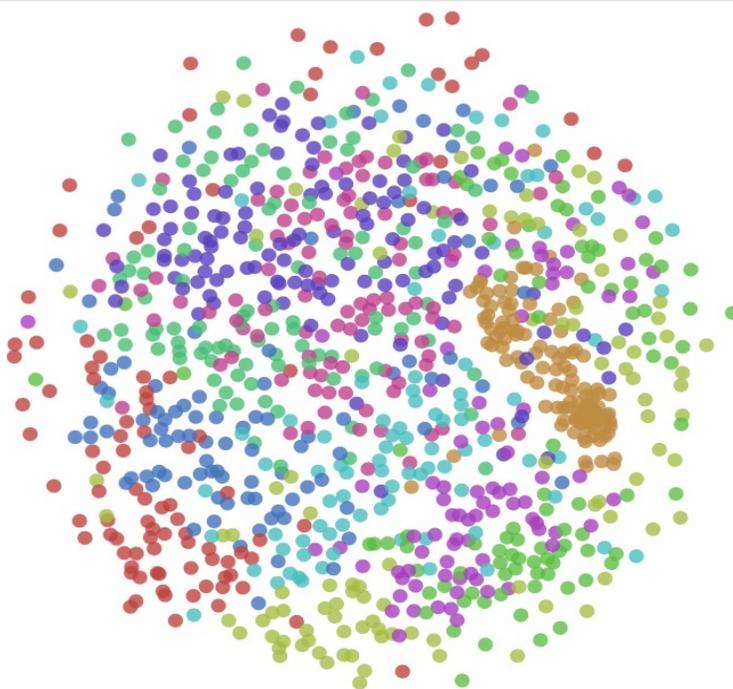


Source: Scholz, M. (2012). Validation of nonlinear PCA. *Neural processing letters*, 36(1), 21-30.



Multidimensional  
scaling  
(MDS) on *labeled*  
MNIST  
handwritten  
digits dataset  
visualized using  
the 1<sup>st</sup> and 2<sup>nd</sup>  
Principal  
Components

Source: <https://colah.github.io/posts/2014-10-Visualizing-MNIST/>

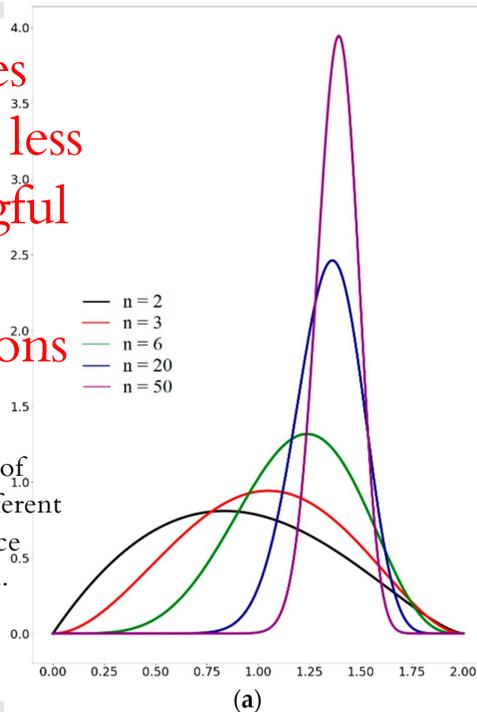


MDS is a spectral  
method that  
preserves the pair-  
wise distances  
between data items

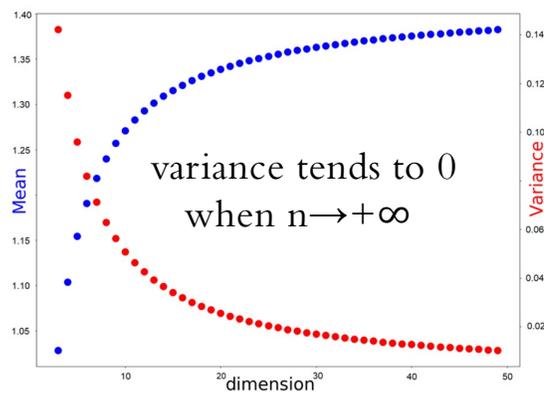
*What is the problem  
with the approach?*

Distances  
become less  
meaningful  
in high  
dimensions

Distribution of  
distances for different  
values of space  
dimension  $n$ .



Lellouche, S., & Souris, M. (2019). Distribution of distances between elements in a compact set. *Stats*, 3(1), 1–15.



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## Solution: t-distributed stochastic neighbor embedding (t-SNE)

Preserve only the smaller pairwise distances between data items (think neighbors within a group)

Good at identifying clusters and anomalies, visualization of very high dimensional data

Not good at preserving global distances like PCA does

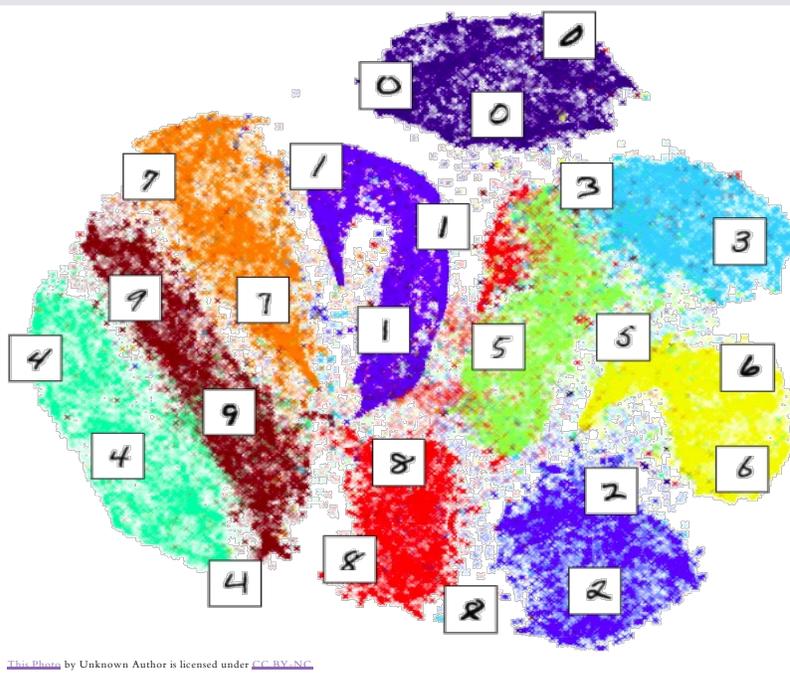
Handles non-linear relationships among data well

Computation intensive

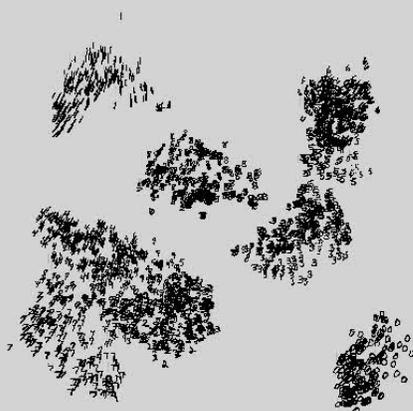
Stochastic elements: initialization, stochastic gradient descent

Highly configurable via hyperparameters and non-deterministic

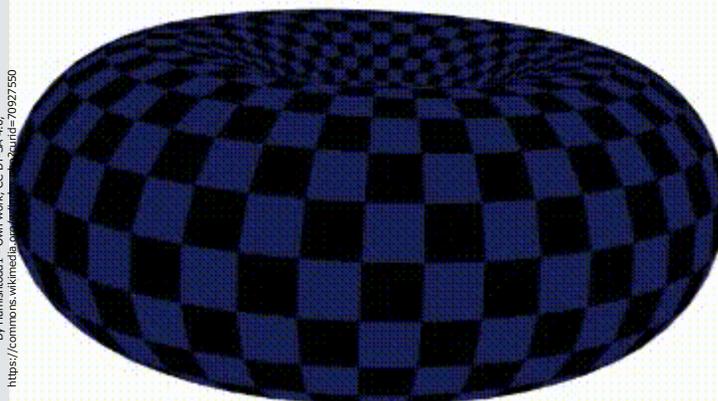
T-SNE on  
*labeled*  
 MNIST  
 handwritten  
 digits dataset  
 visualized  
 using the 1<sup>st</sup>  
 and 2<sup>nd</sup>  
 Principal  
 Components



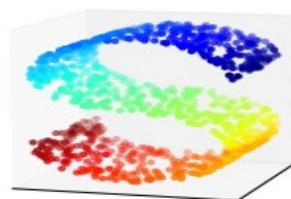
T-SNE on  
*unlabeled*  
 MNIST  
 handwritten  
 digits dataset  
 visualized  
 using the 1<sup>st</sup>  
 and 2<sup>nd</sup>  
 Principal  
 Components



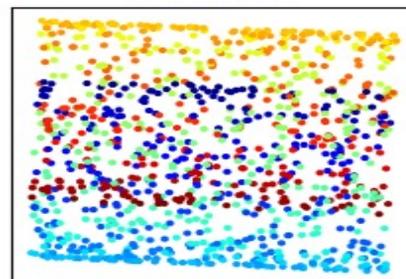
Isomap  
uses  
Geodesic –  
the  
shortest  
distance  
between  
two points  
on a  
manifold  
surface,  
honoring  
the shape



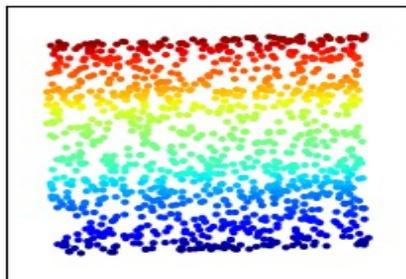
## PCA vs Manifold Learning



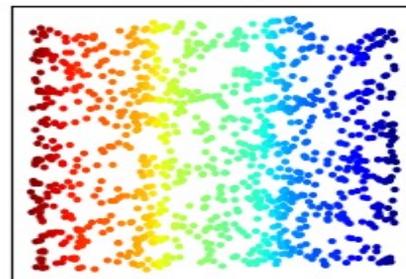
PCA projection



LLE projection



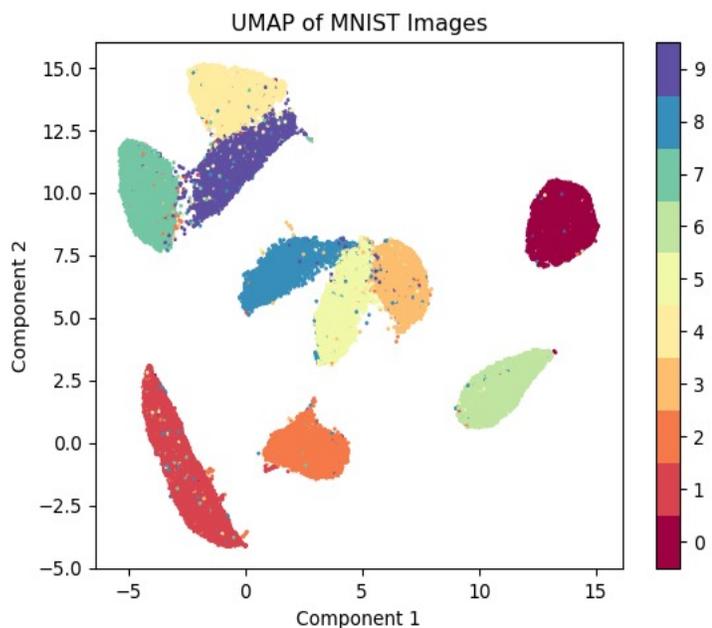
IsoMap projection



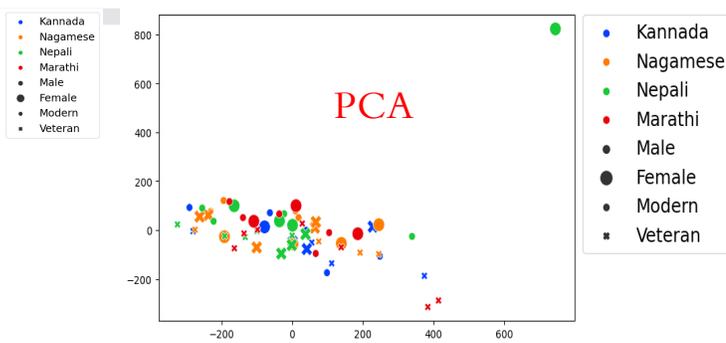
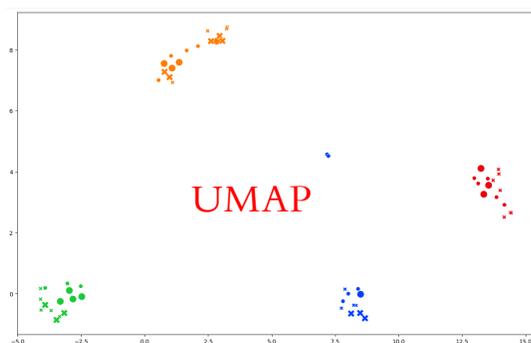
Source: [https://www.astroml.org/\\_images/fig\\_S\\_manifold\\_PCA\\_1.png](https://www.astroml.org/_images/fig_S_manifold_PCA_1.png)

## Uniform Manifold Approximation and Projection (UMAP)

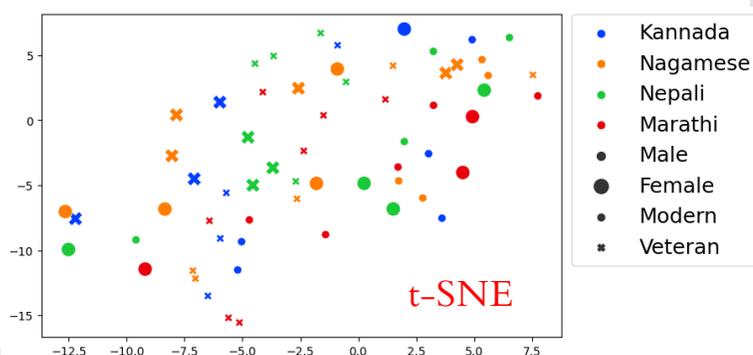
- Builds a topological representation of data
- Preserves both local and global structure
- Based on manifold learning, graph theory
- Can capture non-linear relationships in the data
- Computationally efficient compared to t-SNE



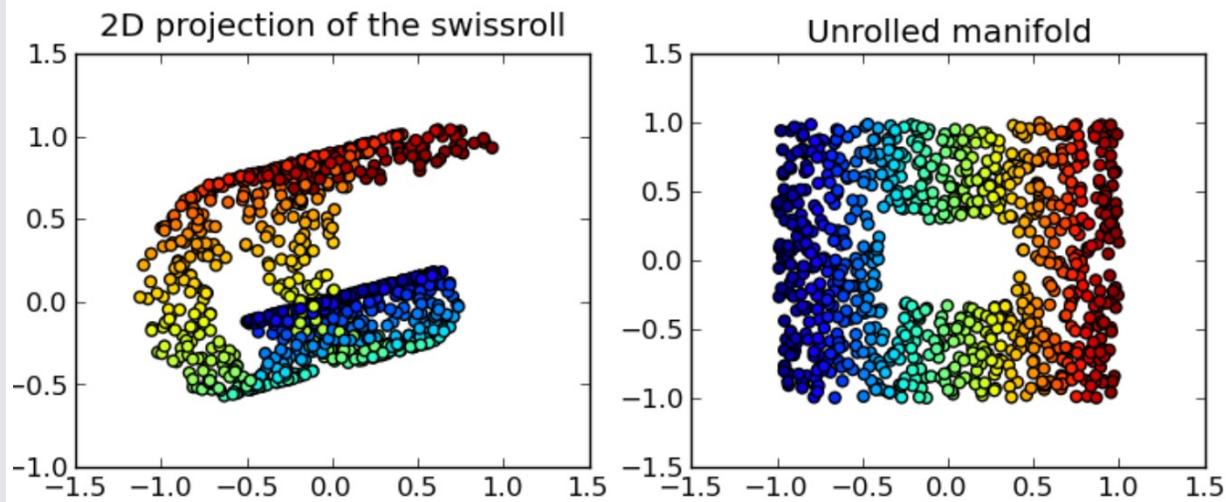
Source: Tezuka, Naoya, et al. "Resilience of Wireless Ad Hoc Federated Learning against Model Poisoning Attacks." 2022 IEEE 4th International Conference on Trust, Privacy and Security in Intelligent Systems, and Applications (TPS-ISA). IEEE, 2022.



Source: Pendyala, Vishnu, Konduri Samhita, and Pendyala, Kriti, "Analysis of Multilanguage Regional Music Tracks using Representation Learning Techniques in Lower Dimensions." In *10th International Conference On Mathematics And Computing ICMC 2024*. Springer. [Best paper award]



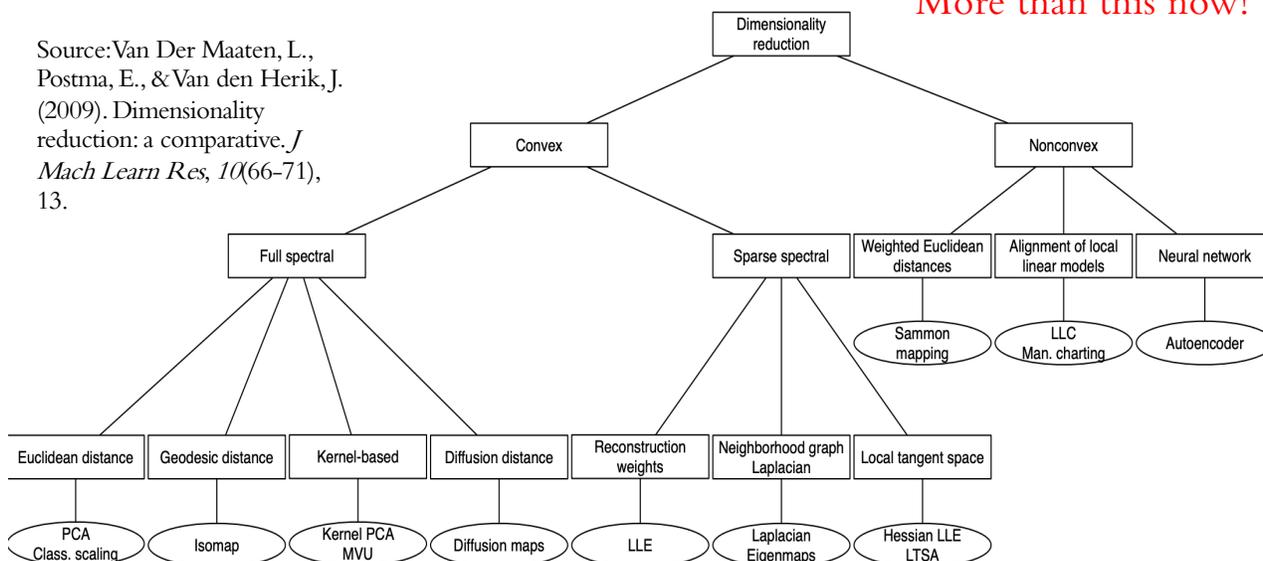
## Many algorithms for non-linear dimensionality reduction



Source: [https://en.wikipedia.org/wiki/Nonlinear\\_dimensionality\\_reduction#/media/File:Lle\\_hlle\\_swissroll.png](https://en.wikipedia.org/wiki/Nonlinear_dimensionality_reduction#/media/File:Lle_hlle_swissroll.png) CC BY 3.0

## Taxonomy of dimensionality reduction techniques (2009)

More than this now!



## Kernel PCA

**Increase** the dimensions:  
Transform the non-linear data into higher dimensional space

**Reduce** the dimensions: Run PCA in higher dimensional space

Finding the eigen values of the kernel matrix is equivalent to finding those of the covariance matrix

Use the kernel matrix in place of covariance matrix and compute the principal components in the transformed space

The feature vector  $x$  is transformed as:

$$\sum_{i=1}^N \alpha_i K(x, x^{(i)}).$$

$\alpha_i$  are the respective weights (values in the eigen vectors of the kernel matrix)

**Demo time:**  
**Tensorflow**  
**Embedding**  
**Projector**

