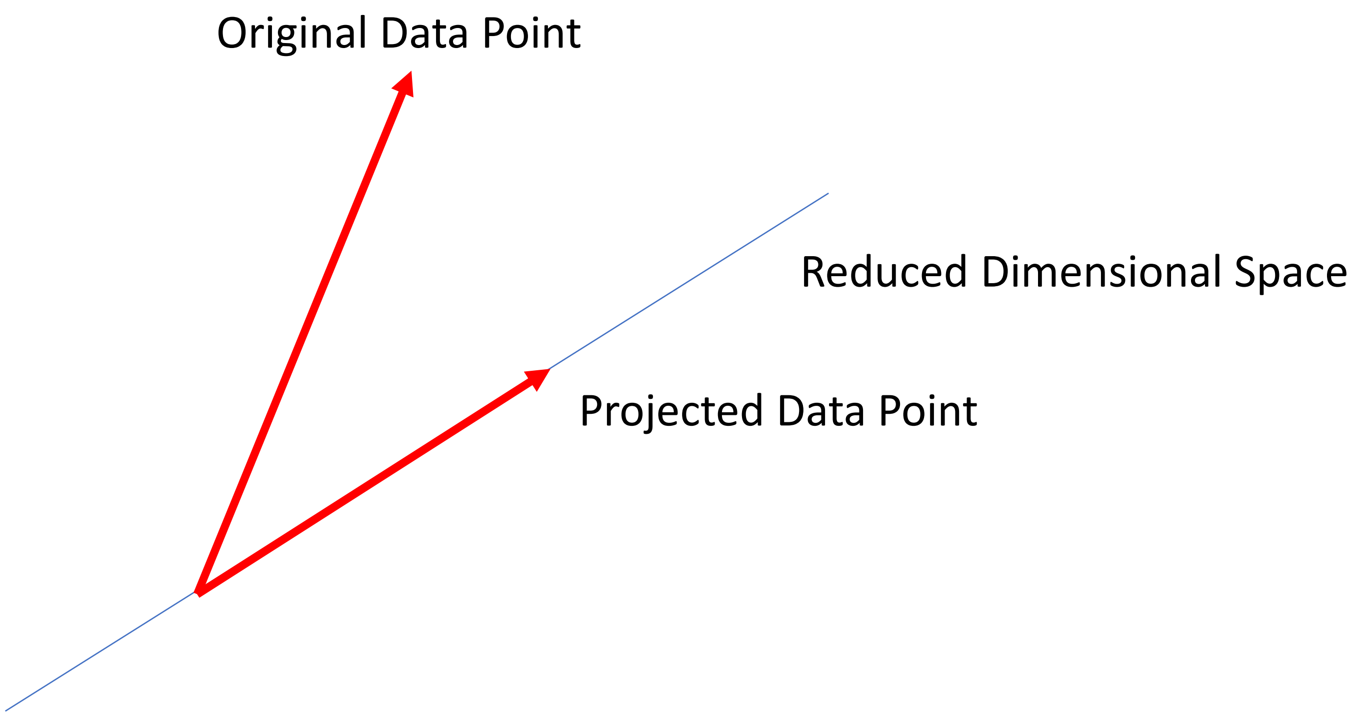
Unsupervised Machine Learning with Python

Section 9.0: Dimension Reduction Overview

Purpose of Dimension Reduction

- Machine learning problems may have datasets with 1000s of features (# features = # of dimensions)
- More dimensions generally means slower computation
- Dimension Reduction attempts to map feature vectors (datasets) into a lower dimensional space while retaining as much information as possible
- See UnsupervisedML_Resources.pdf for links to additional resources

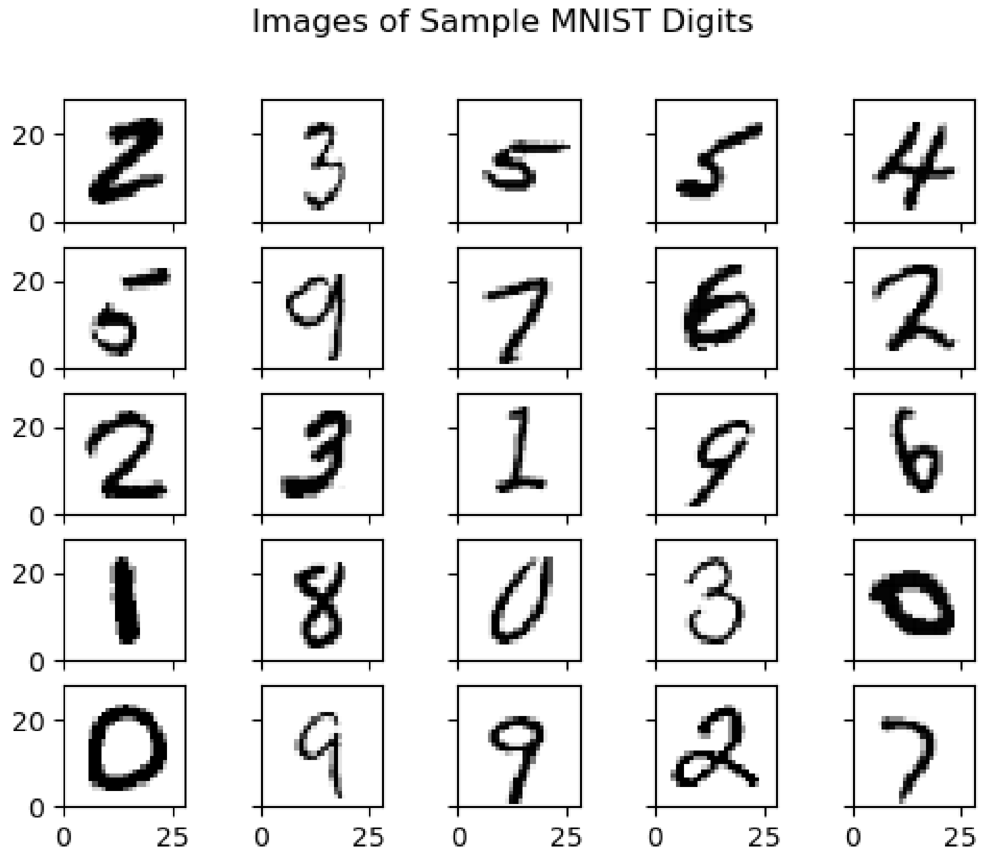
Dimension Reduction



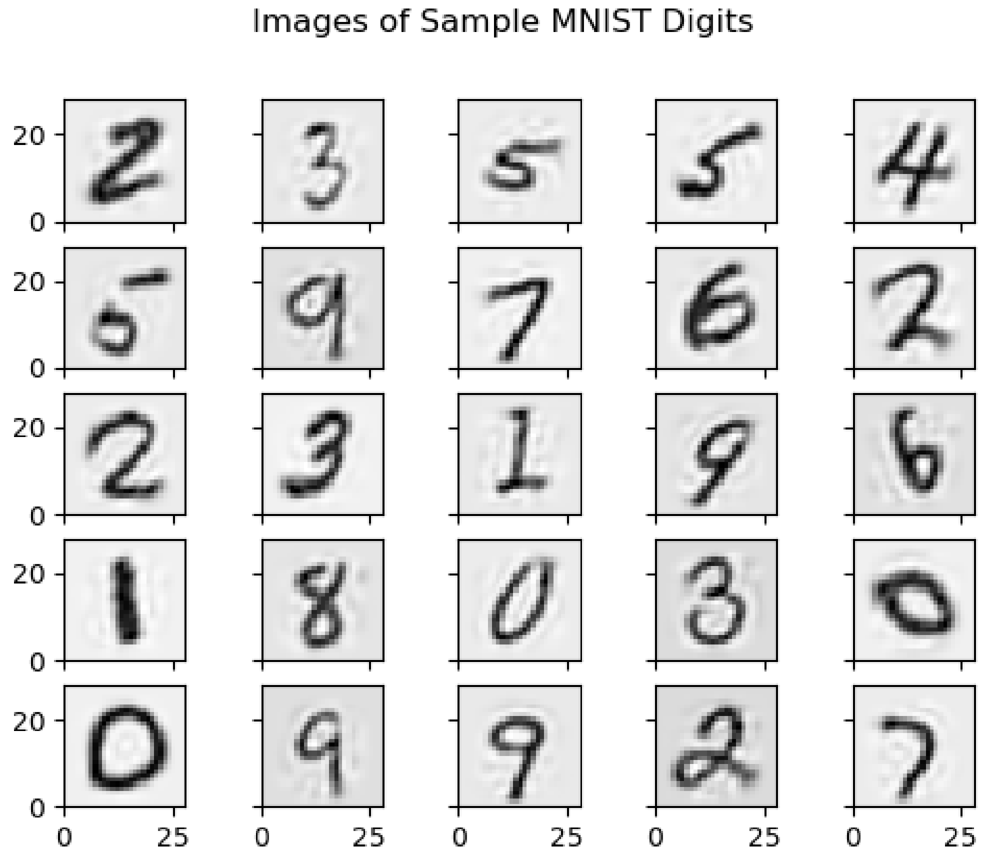
- Picture often seen in Linear Algebra courses
- Use dimension reduction techniques to find Projected Data Point and Reduced Dimensional Space

Dimension Reduction for MNIST Digits

Original Dataset:
28x28 resolution = 784 pixels (dimensions)



Reconstructed Dataset:
Reduce to 78 dimensions then reconstruct images



Dimension Reduction

- Principal Component Analysis (PCA):
  - “Linear” approach
  - Cool application of singular value decomposition to project a dataset onto a lower dimensional space
- Autoencoding:
  - “Nonlinear” approach
  - Uses techniques from supervised learning to learn lower dimensional representation of dataset

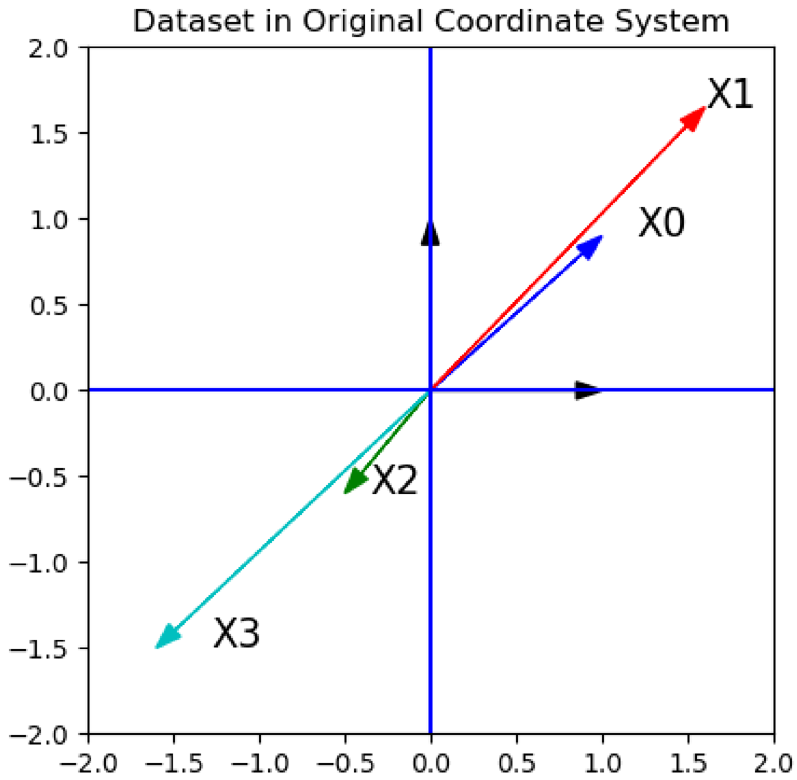
Unsupervised Machine Learning with Python

Section 9.1: Principal Component Analysis Algorithm

Example: 4 Data Points in 2D

- Consider 4 data points in 2 dimensions

$$X = [X_0 \quad X_1 \quad X_2 \quad X_3] = \begin{bmatrix} 1 & 1.6 & -0.5 & -1.6 \\ 0.9 & 1.65 & -0.6 & -1.5 \end{bmatrix}$$



Principal Component Analysis

Basic Idea

- Compute SVD of dataset $X = U\Sigma V^T$
- Let U=[u_0 u_1 … u_{d-1}] be new coordinate system for d dimensional space
- Relevance of each basis vector u_0 u_1 … u_{d-1} is determined by its corresponding singular value, which are ordered in decreasing value
- Project data onto lower dimensional space spanned by first K basis vectors $u_0, u_1, \dots, u_{K-1}$, choosing K to retain sufficient information

SVD of Data Set

- Compute compact SVD of X

$$X = \begin{bmatrix} 1 & 1.6 & -0.5 & -1.6 \\ 0.9 & 1.65 & -0.6 & -1.5 \end{bmatrix}$$

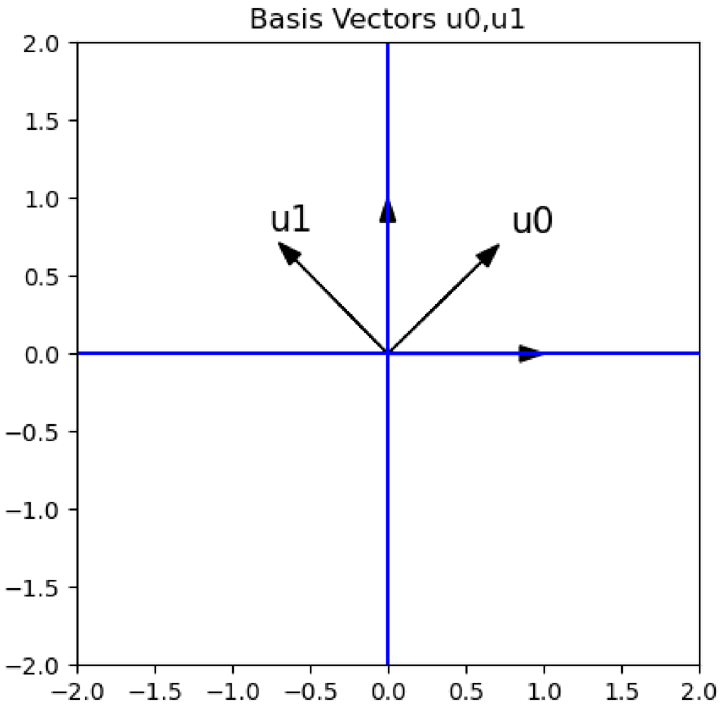
$$X = U\Sigma V^T = [u_0 \quad u_1] \begin{bmatrix} \sigma_0 & 0 \\ 0 & \sigma_1 \end{bmatrix} \begin{bmatrix} v_0^T \\ v_1^T \end{bmatrix}$$

$$X = \begin{bmatrix} 0.71 & -0.70 \\ 0.70 & 0.71 \end{bmatrix} \begin{bmatrix} 3.54 & 0 \\ 0 & 0.12 \end{bmatrix} \begin{bmatrix} 0.38 & 0.65 & -0.22 & -062 \\ -0.47 & 0.46 & -0.63 & 0.41 \end{bmatrix}$$

New Coordinate system with basis u0 and u1

- Consider new coordinate system using u0 and u1 as basis

$$u_0 = \begin{bmatrix} 0.71 \\ 0.70 \end{bmatrix} \quad u_1 = \begin{bmatrix} -0.70 \\ 0.71 \end{bmatrix}$$



Notes:

- Basis vectors of original system typically correspond to physical or measurable quantity: (word count, pixel intensity, features of a house)
- New basis vectors u_0, u_1, … typically don't correspond to physical or measurable quantities

Data points in u0-u1 Coordinate System

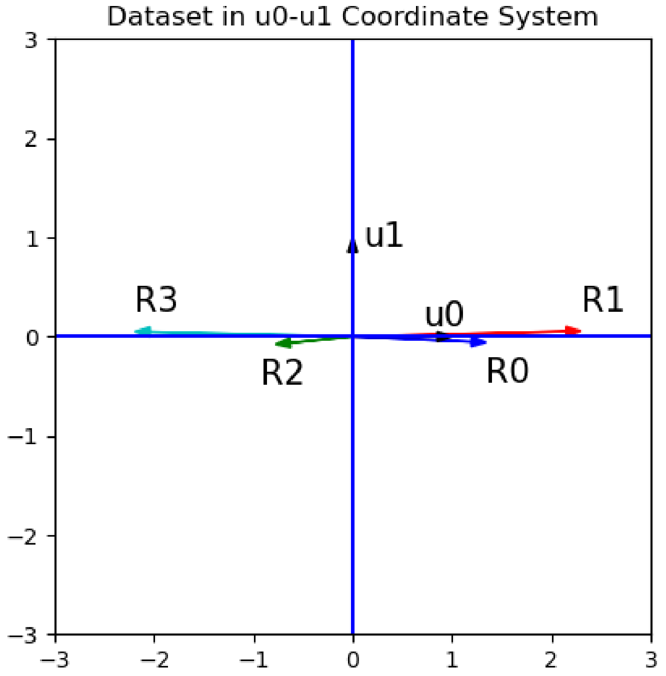
- Data points in u0 and u1 coordinate system

$$\Sigma V^T = \begin{bmatrix} 3.54 & 0 \\ 0 & 0.12 \end{bmatrix} \begin{bmatrix} 0.38 & 0.65 & -0.22 & -062 \\ -0.47 & 0.46 & -0.63 & 0.41 \end{bmatrix}$$

$$\Sigma V^T = [R_0 \quad R_1 \quad R_2 \quad R_3] = \begin{bmatrix} 1.34 & 2.30 & -0.78 & -2.19 \\ -0.06 & 0.06 & -0.08 & 0.05 \end{bmatrix}$$

Units of u0 for each data point

Units of u1 for each data point



Reduce Dimensions

- Only keep information in u0 direction (1 dimension)
- Data points in reduced number of dimensions

Units of u0 for each data point

$$R = [\sigma_0][v_0^T] = [3.54][0.38 \quad 0.65 \quad -0.22 \quad -0.62] = [1.34 \quad 2.30 \quad -078 \quad -2.19]$$

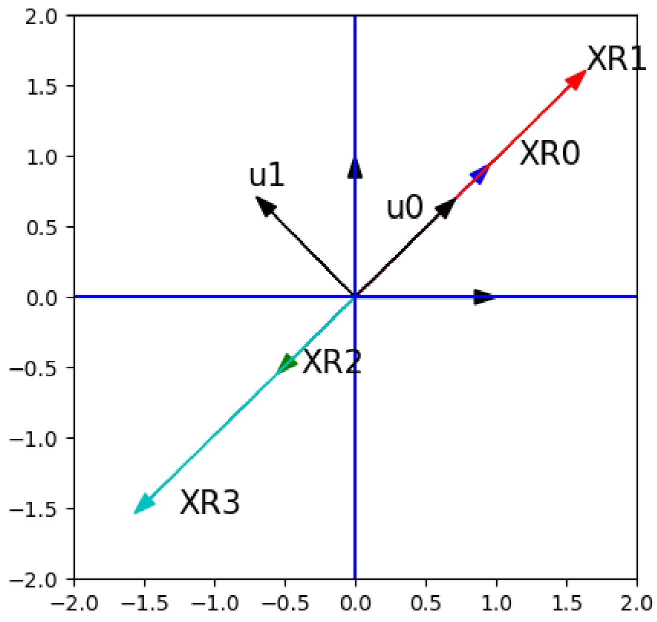
Reconstruct in Original Space

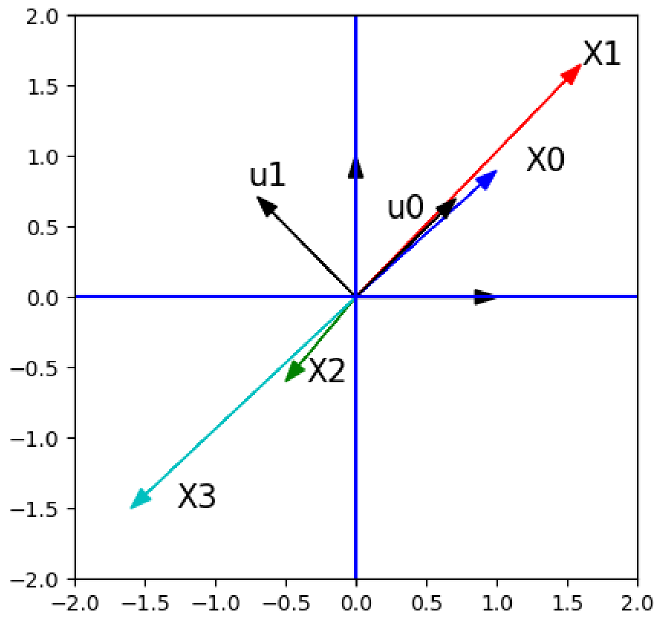
- Can reconstruct data points in original coordinate system using information in u0 direction only

$$X_R = [u_0]\ R = [u_0][\sigma_0][v_0^T]$$

$$X_R = \begin{bmatrix} 0.71 \\ 0.70 \end{bmatrix} [3.54][0.38 \quad 0.65 \quad -0.22 \quad -0.62]$$

$$X_R = \begin{bmatrix} 0.96 & 1.64 & -0.55 & -1.56 \\ 0.94 & 1.61 & -0.54 & -1.54 \end{bmatrix} \qquad X = \begin{bmatrix} 1 & 1.6 & -0.5 & -1.6 \\ 0.9 & 1.65 & -0.6 & -1.5 \end{bmatrix}$$





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PCA Algorithm

PCA Algorithm:

- Start with data matrix X (d features x M samples) (here d < M)

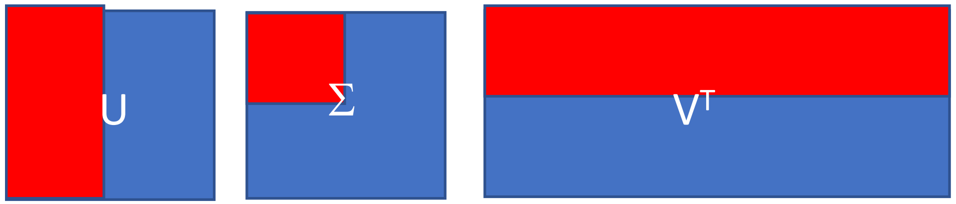
(1) Subtract mean of data $X - X_{mean}$ (translate data points by same amount)

(2) Compute the compact version of SVD of $\bar{X} = X - X_{mean} = U\Sigma V^T$

$$\bar{X}\ (\text{dxM}) = U\ (\text{dxd})\ \ \Sigma\ (\text{dxd})\ \ V^T\ (\text{dxM})$$

PCA Algorithm

(3) Pick K<d principal components



(first K columns of U, first K diagonal entries of Σ, first K rows of V^T)

(4) Data points in K dimensional $(u_0, \dots, u_{K-1})$ coordinate system given by:

$$R = \begin{bmatrix} \sigma_0 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_{K-1} \end{bmatrix} \begin{bmatrix} v_0^T \\ \vdots \\ v_{K-1}^T \end{bmatrix}$$

PCA Algorithm

(5) Reconstructed $\bar{X}_R$ in original space(keeping only K principal components)

$$\bar{X}_R = [u_0 \quad \cdots \quad u_{K-1}]R = [u_0 \quad \cdots \quad u_{K-1}]\begin{bmatrix} \sigma_0 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_{K-1} \end{bmatrix}\begin{bmatrix} v_0^T \\ \vdots \\ v_{K-1}^T \end{bmatrix}$$

(6) Add back mean to get reconstructed X (based on K principal components)

$$X_R = \bar{X}_R + X_{mean}$$

- SVD is connected to L2 distance measure theoretically, so use L2 distance measure when computing distances for consistency

Principal Component Analysis: Choosing K

- Covariance matrix for dataset:

$$Cov = \frac{1}{M}(X - X_{mean})(X - X_{mean})^{T}$$

- Total variance is sum of eigenvalues of Covariance matrix, which is same as sum of squares of singular values of $(X - X_{mean})$, divided by M
- Define

$$Variance(K) = \frac{1}{M}\sum_{k=0}^{K-1}\sigma_k^2$$

- Instead of specifying K directly, choose smallest number of principal components so that Variance(K)/Variance(N) is at least as large as specified percentage

Example: Choosing K

- Assume M = 4 data points
- Assume singular values are: $\sigma_0 = 4, \sigma_1 = 3, \sigma_2 = 2, \sigma_3 = 1$
- Recall: $Variance(K) = \frac{1}{M}\sum_{k=0}^{K-1} \sigma_k^2$

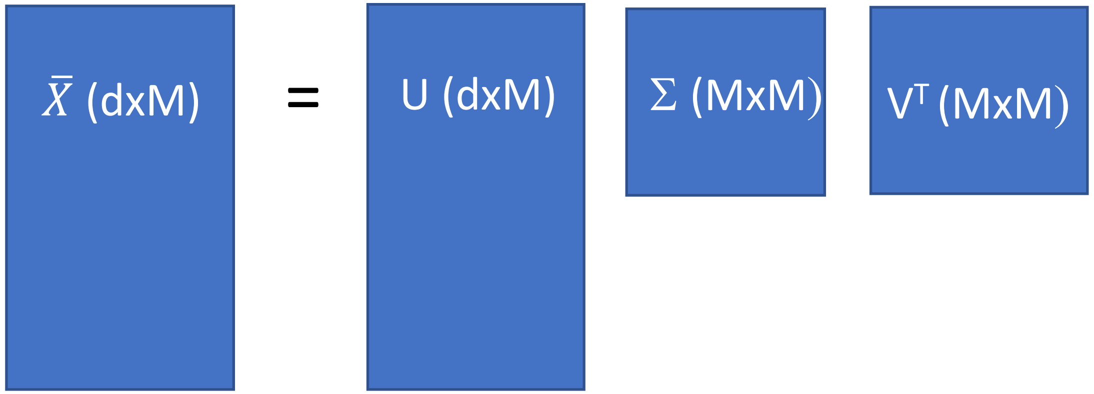
	K = 1	K = 2	K = 3	K = 4
Variance(K)	4.00	6.25	7.25	7.50
Variance(K)/Variance(M)	0.5333	0.8333	0.9666	1.0000

- In this example, only need K=2 principal components to capture 83% of total variance

More Dimensions than Data Points

PCA Algorithm in case number of dimensions d > number of samples M

- Compute the compact version of SVD of $\bar{X} = X - X_{mean} = U\Sigma V^T$



- Suppose we retain M principal components

$$R = \begin{bmatrix} \sigma_0 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sigma_{M-1} \end{bmatrix} \begin{bmatrix} v_0^T \\ \vdots \\ v_{M-1}^T \end{bmatrix}$$

- R is in M<d dimensions and no information is lost
- (L2) distances between data points same in original and reduced dimensional space since U has orthogonal columns of length 1.

Example

- Dataset X: 2 data points in 4 dimensions

$$X_0 = \begin{bmatrix} 1 \\ 3 \\ 5 \\ 7 \end{bmatrix} \quad X_1 = \begin{bmatrix} 2 \\ 4 \\ 6 \\ 8 \end{bmatrix} \quad X = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \\ 7 & 8 \end{bmatrix}$$

- Compute L2 (Euclidean) distance between points

$$dist(X_0, X_1) = 2.646$$

Example

- SVD

$$X = U\Sigma V^T = \begin{bmatrix} -0.16 & -0.49 \\ -0.36 & -0.13 \\ -0.52 & -0.63 \\ -0.76 & 0.59 \end{bmatrix} \begin{bmatrix} 13.93 & 0 \\ 0 & 0.92 \end{bmatrix} \begin{bmatrix} -0.62 & -0.79 \\ 0.79 & -0.62 \end{bmatrix}$$

- R in 2 dimensional space (keep both components):

$$R = \Sigma V^T = \begin{bmatrix} 13.93 & 0 \\ 0 & 0.92 \end{bmatrix} \begin{bmatrix} -0.62 & -0.79 \\ 0.79 & -0.62 \end{bmatrix} = \begin{bmatrix} -8.63 & -10.94 \\ 0.72 & -0.57 \end{bmatrix}$$

$$R_0 = \begin{bmatrix} -8.63 \\ 0.72 \end{bmatrix} \quad R_1 = \begin{bmatrix} -10.94 \\ -0.57 \end{bmatrix} \quad dist(R_0, R_1) = 2.646$$

Principal Component Analysis DEMO

Jupyter Notebook for demo:

- UnsupervisedML/Examples/Section09/PCA.ipynb

Course Resources at:

- https://github.com/satishchandrareddy/UnsupervisedML/

Unsupervised Machine Learning with Python

Section 9.2: Principal Component Analysis Code Design

PCA Code Design

- This section contains design information for the PCA Code based on algorithm presented in Section 9.1
- Code located at UnsupervisedML/Code/Programs
- Stop video here, if you would like to do code design yourself

PCA Code Design

Create PCA class with methods for:

- Performing SVD
- Computing dataset in reduced number of dimensions
- Computing reconstructed dataset
- Plotting cumulative variance proportion

pca class: Principal Variables

Variable	Type	Description
self.Xmean	2d numpy array	X_{mean} of dataset (column vector of dimension d x 1)
self.dimension	integer	Number of dimensions in dataset
self.nsample	Integer	Number of data points
self.U	2d numpy array	U from SVD of $X - X_{mean}$ (d x N) N = min(d,M)
self.Sigma	1d numpy array	Singular values of $X - X_{mean}$ (N entries)
self.Vt	2d numpy array	V^T from SVD of $X - X_{mean}$ (N x M)
self.cumulative_ variance_ proportion	1d numpy array	Cumulative variance proportion (N entries)

pca class – Key Methods

Method	Input	Description
__init__		Constructor for pca class
fit	X (2d np.array)	Computes compact SVD of X – Xmean and stores results in self.U, self.Sigma, and self.Vt Return: nothing
get_dimension	variance_capture (float)	Computes minimum number of principal components to retain at least variance_capture proportion of total variance Return: number of principal components K
data_reduced_ dimension	**kwargs reduced_dim (integer) variance_capture (float)	Computes the dataset in U coordinate system with reduced number of dimensions. User specifies either reduced_dim directly or the proportion of variance to be captured. Return: R (2d numpy array)
data_reconstructed	**kwargs reduced_dim (integer) variance_capture (float)	Computes the reconstructed dataset in original coordinate system with reduced number of dimensions. User specifies either reduced_dim directly or the proportion of variance to be captured. Return: X_R (2d numpy array)
plot_cumulative_ variance_ proportion		Plots the cumulative variance proportion Return: nothing

Unsupervised Machine Learning with Python

Section 9.3: Principal Component Analysis Code Walkthrough

PCA Code Walkthrough

Code located at:

- UnsupervisedML/Code/Programs

Files to Review	Description
pca.py	class for principal component analysis

Course Resources at:

- https://github.com/satishchandrareddy/UnsupervisedML/

- Stop video if you would like to implement code yourself first

Unsupervised Machine Learning with Python

Section 9.4: PCA Applied to MNIST Digits Dataset

MNIST Digits Dataset

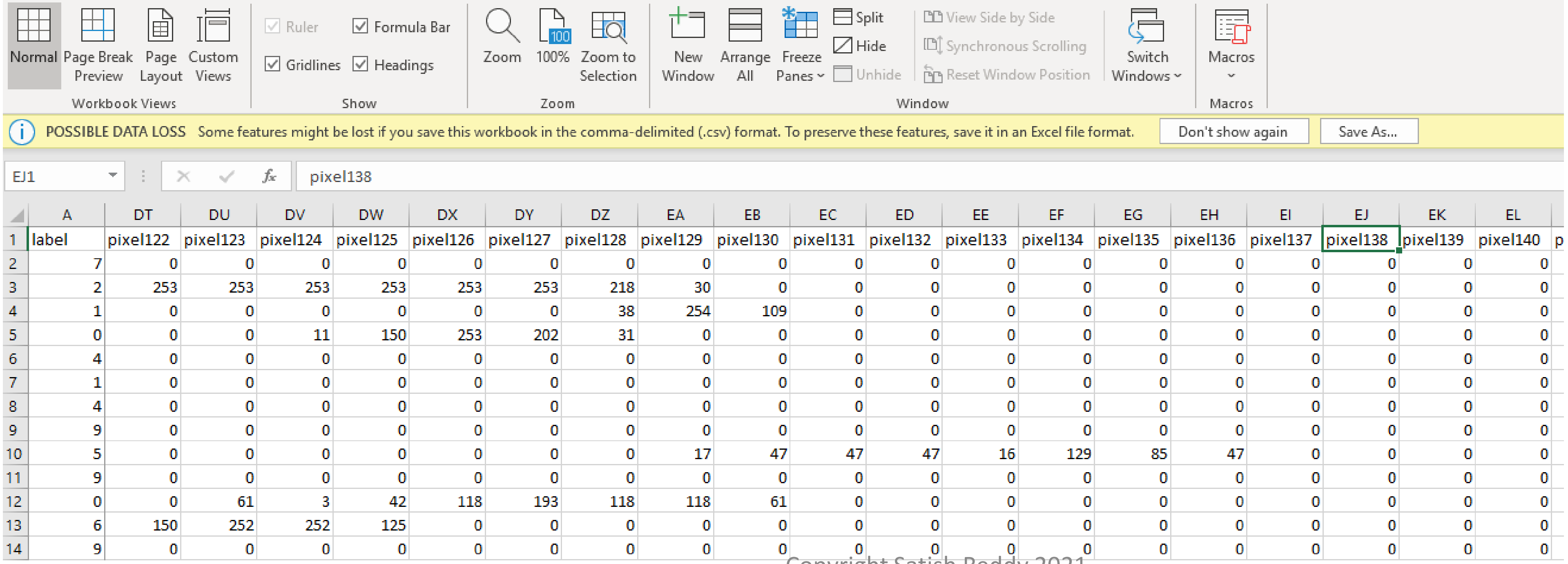
- Thousands of handwritten digit images with 28x28 resolution
- Data Source: http://yann.lecun.com/exdb/mnist/
- Used in machine learning research and teaching

Collage of 160 individual digit images

By Josef Steppan - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=64810040

MNIST Digits – Format of Data Files

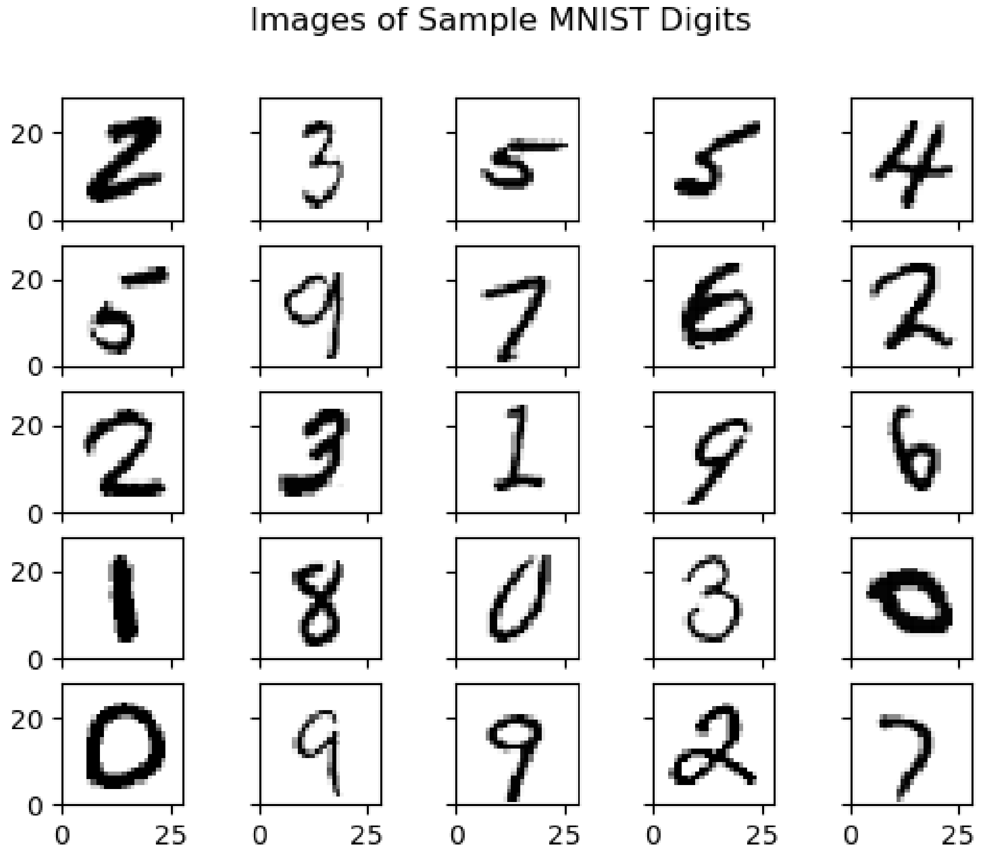
- Each row contains data for one image
  - First column is the digit label (0,1,…,9)
  - Columns 2 – 785 are the intensities (integers between 0=white and 255=black)
  - 784 dimensions
  - Take transpose to convert feature matrix to (dimension x sample) format
  - Standard practice is to divide pixel values by 255 so between 0 and 1



	A	DT	DU	DV	DW	DX	DY	DZ	EA	EB	EC	ED	EE	EF	EG	EH	EI	EJ	EK	EL
1	label	pixel122	pixel123	pixel124	pixel125	pixel126	pixel127	pixel128	pixel129	pixel130	pixel131	pixel132	pixel133	pixel134	pixel135	pixel136	pixel137	pixel138	pixel139	pixel140
2	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	2	253	253	253	253	253	253	218	30	0	0	0	0	0	0	0	0	0	0	0
4	1	0	0	0	0	0	0	38	254	109	0	0	0	0	0	0	0	0	0	0
5	0	0	0	11	150	253	202	31	0	0	0	0	0	0	0	0	0	0	0	0
6	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	5	0	0	0	0	0	0	0	17	47	47	47	16	129	85	47	0	0	0	0
11	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	61	3	42	118	193	118	118	61	0	0	0	0	0	0	0	0	0	0
13	6	150	252	252	125	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Example MNIST Digits

Original Dataset: 60000 images
Plot 25 randomly chosen images



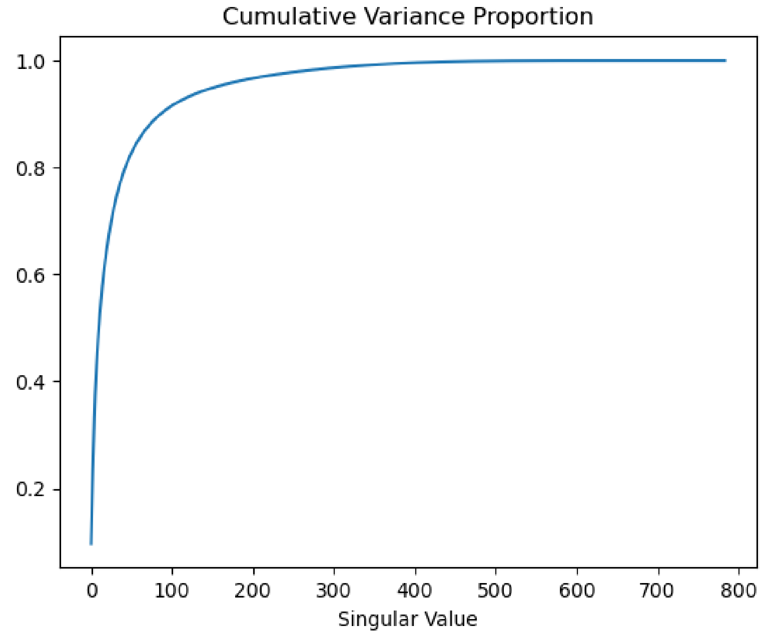
PCA for MNIST Digits Dataset

Perform PCA for MNIST Digits Dataset

- Dataset X: d = 784 dimensions and M = 60000 images
- Compute compact SVD of $\bar{X} = X - X_{mean} = U\Sigma V^T$

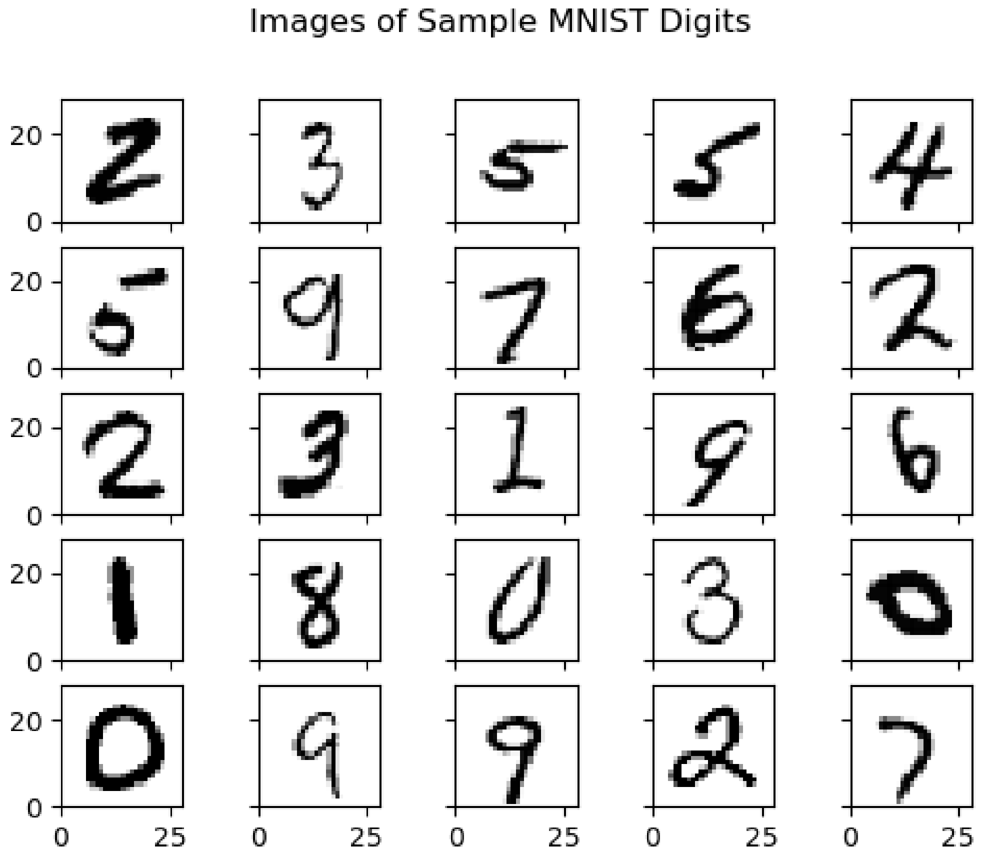
Cumulative Variance Proportion

$\bar{X}$ (dxM) = U (dxd) Σ (dxd) V^T (dxM)

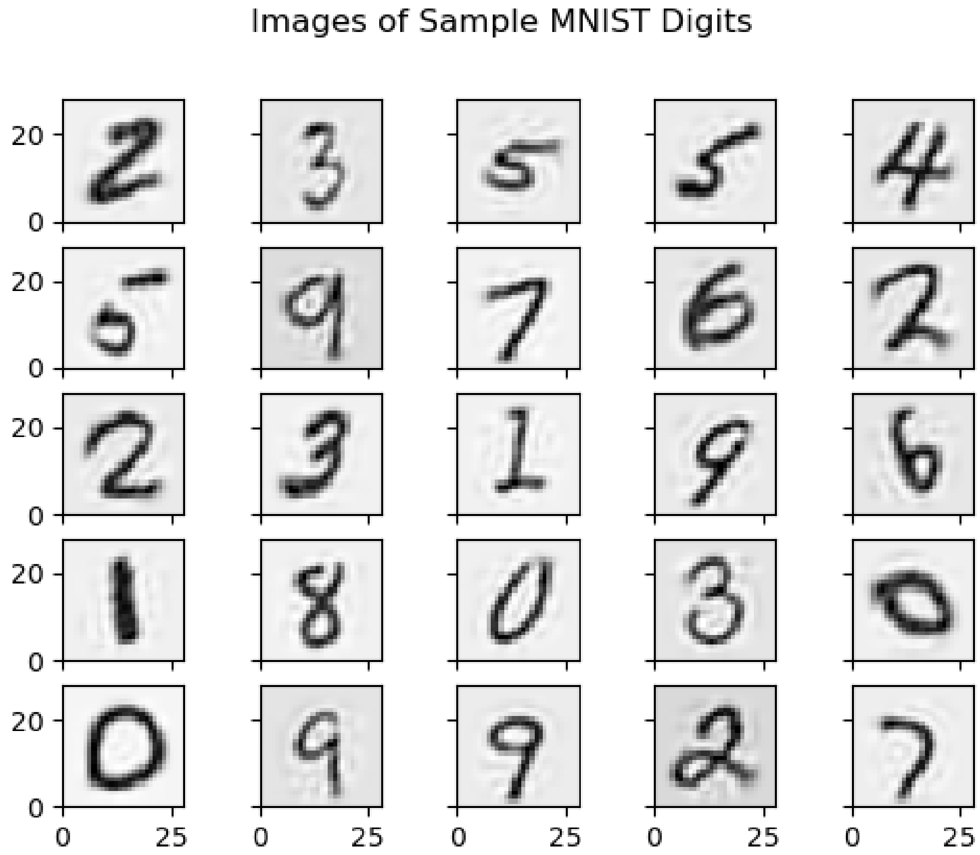


PCA for MNIST: Original and Reconstructed

Original Dataset:
Plot 25 randomly chosen images



Reconstructed Dataset:
90% variance capture (87 dimensions)



mnist class Code Design

Method	Input	Description
__init__		Constructor for mnist class – saves data directory Return: nothing
load_train	nsample (integer)	Loads nsample (maximum 60,000) images and corresponding class labels from the train dataset Return: X (2d numpy array), class_label (1d numpy array)
load_valid	nsample (integer)	Loads nsample (maximum 10,000) images and corresponding class labels from the validation dataset Return: X (2d numpy array), class_label (1d numpy array)
plot	X (2d numpy array) seed (integer)	Creates figure of 25=5x5 images randomly chosen from the dataset X. seed is used to set up the seed for the random number generator. Return: nothing

PCA for MNIST Digits Code Walkthrough

Programs and data located at

- UnsupervisedML/Code/Programs
- UnsupervisedML/Code/Data_MNIST

Files to Review	Description
Programs/data_mnist.py	Class for loading and plotting mnist digits dataset
Programs/driver_pca_mnist.py	Driver for performing pca for mnist dataset
Data_MNIST/MNIST_valid_10K.csv	Validation dataset (10000 images)

Course Resources at:

- https://github.com/satishchandrareddy/UnsupervisedML/

- Stop video if you would like to implement code yourself first

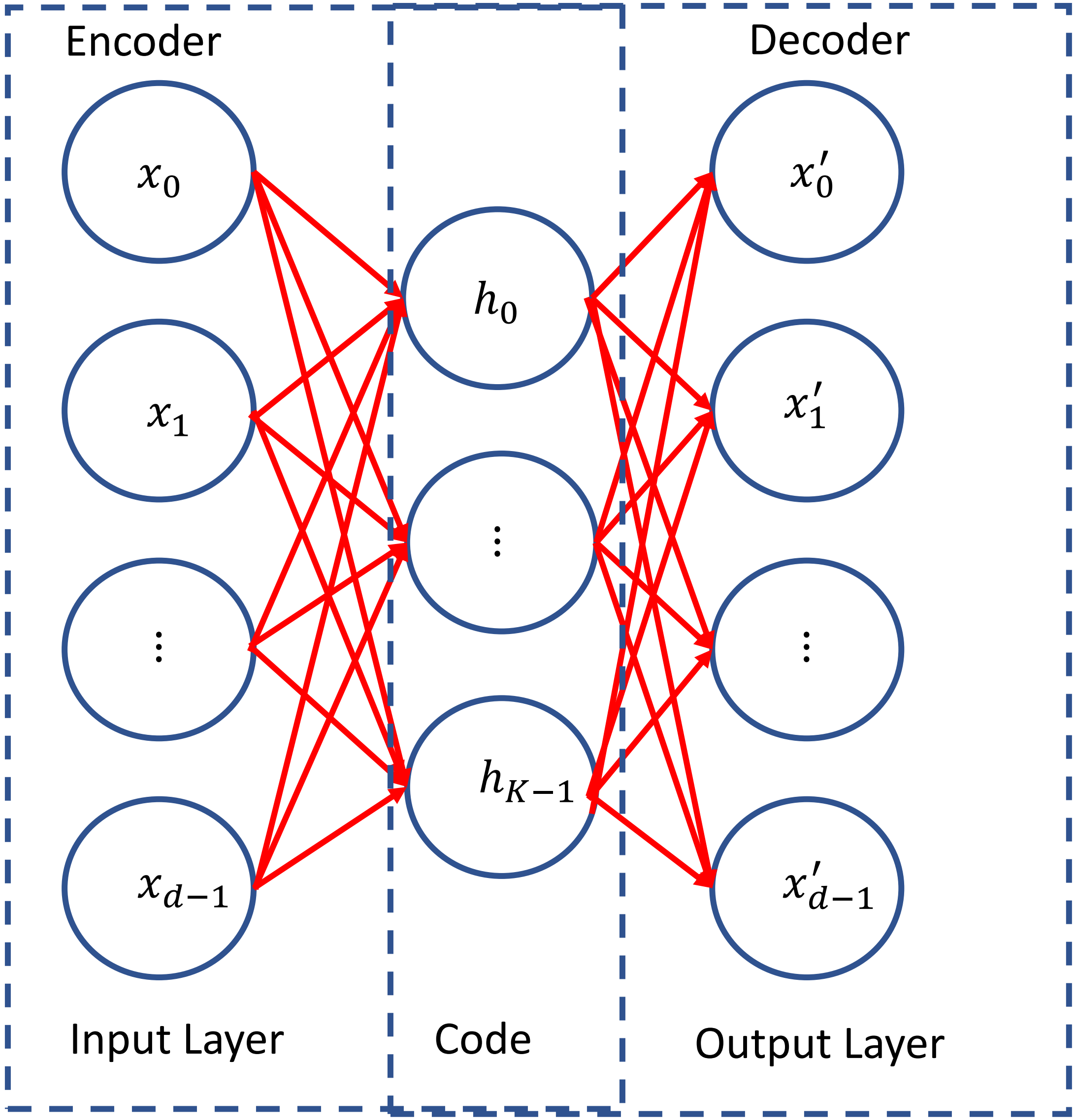
Unsupervised Machine Learning with Python

Section 9.5: Autoencoders

What is an Autoencoder?

- An Autoencoder is type of Artificial Neural Network for learning efficient representations of the feature vector
- Can be used to reduce dimensions
- Whereas PCA (based on SVD) is linear, Autoencoder can use a nonlinear approach

Sample Autoencoder Neural Network



- Input: (d dimensions)

$$X = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{d-1} \end{bmatrix}$$

- Encoder: Map X to H (K dimensions). "Code" H is a new feature vector representation of X

$$H = \begin{bmatrix} h_0 \\ \vdots \\ h_{K-1} \end{bmatrix}$$

- Decoder: Map H to X' (d dimensions). X' is a reconstructed version of X

$$X' = \begin{bmatrix} x'_0 \\ x'_1 \\ \vdots \\ x'_{d-1} \end{bmatrix}$$

Autoencoder: Determining Mappings

- Encoder:

$$H = f(WX + b)$$

X (d dimensions) is data point, W is Kxd matrix, b is Kx1 vector, f is activation function, H is (K dimensions) reduced dimension version of data point

- Decoder:

$$X' = g(W'H + b')$$

X’ is (d dimensions) reconstructed data point, W’ is dxK matrix, b’ is dx1 vector, g is activation function

- Given a dataset of M datapoints $X_0, X_1, \ldots, X_{M-1}$ and pre-specified activation functions f, g: Determine unknown W, b, W’, b’ by minimizing mean squared error loss function:

$$Loss = \frac{1}{M}\sum_{i=0}^{M-1} dist(X_i', X_i)^2$$

Autoencoder: Notes

- Autoencoder set up is similar to Supervised Learning
  - Key difference is that there is no label Y for each data point
- Determine W, b, W', b' using optimizer such as Gradient Descent and backpropagation to determine derivatives
- Can use familiar activation functions such as sigmoid, Relu for f and g
- "Code" representation H is related nonlinearly to X (if nonlinear activation functions used)
- Code representation H is equivalent to reduced dimension version R from Principal Component Analysis