Unsupervised Machine Learning with Python

Section 3.0: Review of Mathematical Concepts

Review of Mathematical Concepts

Section	Contents
3.1	What is the Data in Unsupervised Machine Learning? -Demo on text processing and creating word clouds
3.2	Computational Complexity -Discussion describing language of complexity, used to quantify resources required by algorithms -Demo on measuring complexity
3.3	Distance Measures -Review of formulas for distance between points and sets of points -Demo on computing distances between data points
3.4	Singular Value Decomposition -Math underlying principal component analysis for reducing number of dimensions in data -Demo on computing and visualizing SVD
3.5	Mean, Variance, and Covariance -Review of formulas -Demo on computing mean, variance, and covariance

See UnsupervisedML_Resources.pdf for links to additional resources

Unsupervised Machine Learning with Python

Section 3.1: What is the Data in Unsupervised Learning?

Unsupervised Machine Learning

- Goal of Unsupervised ML is to find patterns in data
- Question: what is the data?

Data and Datasets

- Typically, a data point is a vector in d dimensions

$$\begin{bmatrix} x_0 \\ \dots \\ x_{d-1} \end{bmatrix}$$

Data point often called feature vector as each entry represents a feature

- Let $X_0, X_1, \dots, X_{M-1}$ denote the M data points, then dataset is represented as a matrix of dimensions d rows and M columns

$$X = [X_0 \quad \dots \quad X_{M-1}]$$

Throughout course we will call X the dataset or the feature matrix

Example: Customer Segmentation

Data point consists of features of customer

Example: 4 features

- age = 27
- # of credit cards = 4
- salary = 60,000
- # of purchases = 10
- Data point represented as:

$$\begin{bmatrix} 27 \\ 4 \\ 60000 \\ 10 \end{bmatrix}$$

- Combine feature vectors for multiple customers to create feature matrix

Example: Natural Language Processing

- How do we convert text into a feature matrix?
- Simple approach is word count
    - Create dictionary of all words (case insensitive)
    - Count number of times each word appears in each document
- Consider 3 messages:

"Call me soon", "CALL to win", "Pick me up soon"

Words

$$\begin{matrix} call \\ me \\ pick \\ soon \\ to \\ up \\ win \end{matrix}$$

Feature Matrix

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Example: Natural Language Processing

- Term Frequency Inverse Document Frequency (Tfidf) approach
  - Term frequency: number of times word appears in document
  - Inverse document frequency: inverse of number of documents in which word appears
  - Tfidf is term frequency multiplied by inverse document frequency (with scaling)
  - Logic: if word appears in many documents, then its importance/weighting is lowered
- Messages:

"Call me soon", "CALL to win", "Pick me up soon"

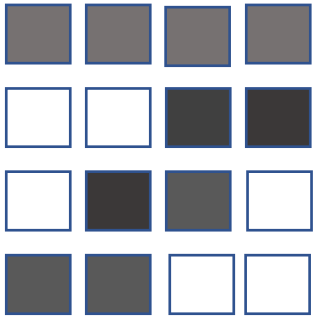
$$
\begin{array}{c c}
\text{Words} & \text{Feature Matrix} \\
\begin{array}{c} call \\ me \\ pick \\ soon \\ to \\ up \\ win \end{array} &
\begin{bmatrix}
0.58 & 0.47 & 0.00 \\
0.58 & 0.00 & 0.43 \\
0.00 & 0.00 & 0.56 \\
0.58 & 0.00 & 0.43 \\
0.00 & 0.62 & 0.00 \\
0.00 & 0.00 & 0.56 \\
0.00 & 0.62 & 0.00
\end{bmatrix}
\end{array}
$$

Example: Images

- Images typically are composed of rectangular arrays of pixels
- For black and white images, intensity of greyscale for each pixel is represented by a number between 0 and 255 (0=white, 255=black)
- Feature vector for image is vector of intensities for all pixels
- For colour images, each pixel represented by 3 values – intensities of red, blue, and green components for that pixel – feature vector in colour case vector will be 3 times longer than in black and white case

Converting Image to Feature Vector

Original Image:
Greyscale 4x4 =16 pixels



Intensity Matrix
4x4 (white=0 to 255=black)

$$\begin{bmatrix} 190 & 190 & 190 & 190 \\ 0 & 0 & 220 & 220 \\ 0 & 220 & 200 & 0 \\ 200 & 200 & 0 & 0 \end{bmatrix}$$

Feature Vector 16x1
Standard to divide by 255

$$\begin{bmatrix} 190 \\ 190 \\ 190 \\ 190 \\ 0 \\ 0 \\ 220 \\ 220 \\ 0 \\ 220 \\ 200 \\ 0 \\ 200 \\ 200 \\ 0 \\ 0 \end{bmatrix}$$

Websites for Data

sklearn Toy Datasets
- https://scikit-learn.org/stable/datasets/toy_dataset.html
- 7 easy to use datasets

University of California, Irvine Machine Learning Data Repository
- https://archive.ics.uci.edu/ml/index.php
- Contains 100s of freely available machine learning datasets

Kaggle
- www.kaggle.com
- Site for data science competitions (often with prize money) with freely available data
- Can learn from tutorials and notebooks created by others
- You will need to create a free account to access Kaggle resources (not needed for this course)

3.1 sklearn Text Processing DEMO

Jupyter Notebook for demo:

- UnsupervisedML/Examples/Section03/SklearnText.ipynb

Course Resources at:

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

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Section 3.2: Computational Complexity

Computational Complexity

- Complexity of an algorithm is amount of resources (number of operations, memory, etc) to run it
- Typically, represent complexity as a function of the size of the input
  - For sorting, represent complexity in terms of number of elements in list
  - For matrix multiplication, represent complexity in terms of size of input matrices
- In this course, we provide complexity estimates for amount of time to run clustering algorithms, usually in terms of number of data points
- Complexity is a useful metric for comparing algorithms

Language of Complexity: Big O Notation

Example:

- $f(M) = O(M^2)$ as $M \to \infty$, means that $|f(M)| \approx CM^2$ as $M \to \infty$

General Definition:

- A function $f(M) = O\big(g(M)\big)$ as M$\to \infty$ if

$$|f(M)| \approx C|g(M)| \quad as\ M \to \infty$$

See Section 3 of file UnsupervisedML_Resources.pdf for links to additional resources

Examples

- Well known result from computer science is that sorting of a list of M elements can be done in $O(MlogM)$ operations as $M \to \infty$
- If X and Y are vectors of length M, then computation of dot product X^TY requires M multiplications and M-1 additions, hence it requires $O(M)$ operations as $M \to \infty$

Work Complexity	Implication
$O(M)$ as $M \to \infty$	If M increases by factor of 2, then amount of work increases by factor of 2
$O(M^2)$ as $M \to \infty$	If M increases by factor of 2, then amount of work increases by factor of 4
$O(M^3)$ as $M \to \infty$	If M increases by factor of 2, then amount of work increases by factor of 8

Estimating Complexity Power from Data

- Let us assume the amount of work for an algorithm is $O(M^p)$ as $M \to \infty$. How can we estimate p?
- Note: $W = CM^p$, then $\log W = \log C + p \log M$

Estimate p as follows:

Assume work is measured by amount of time to run algorithm

(1) Collect data for Time as a function of M for the algorithm to run

(2) Take log of M and log of Time data

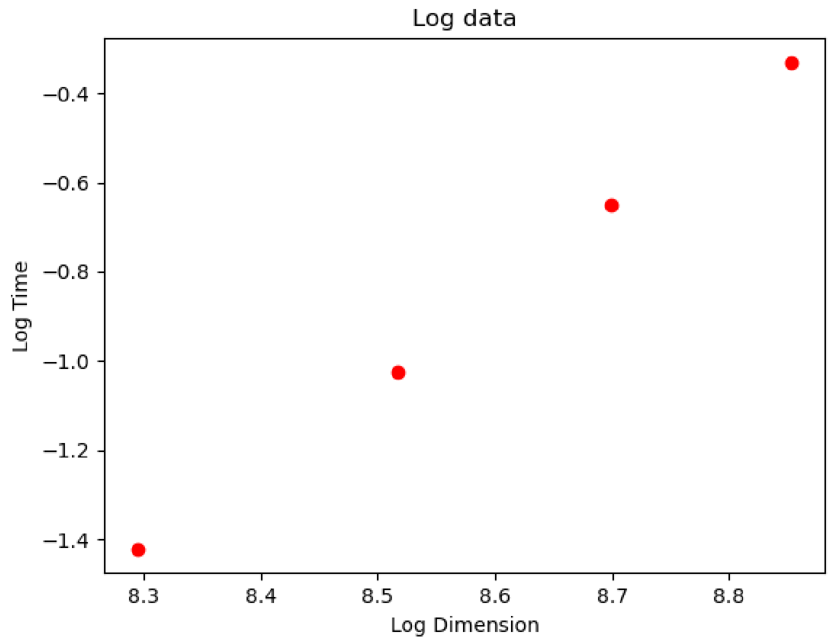
(3) Fit a straight line to log M vs log Time data

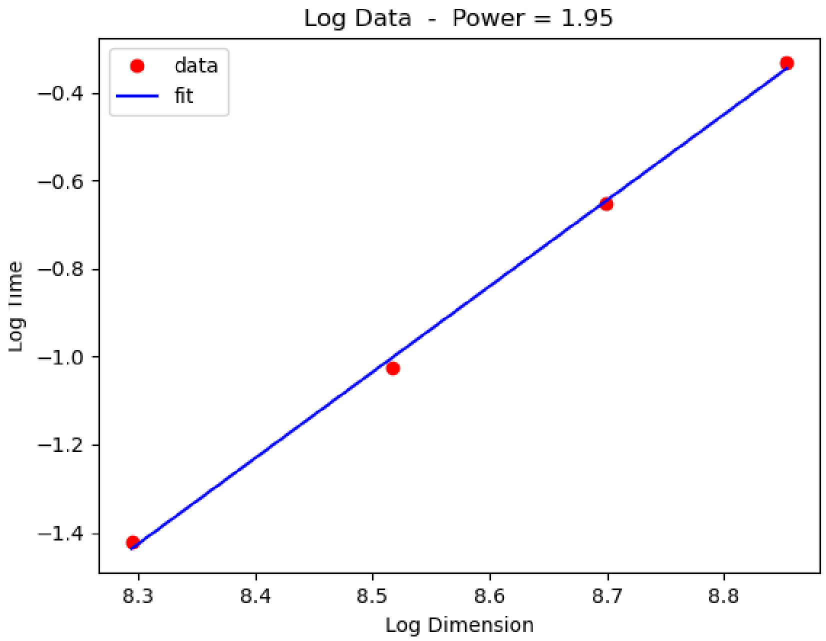
(4) Slope of line is p

(5) Intercept is $\log C$

Example: Estimating Complexity Power from Data

Dimension (M)	4000	5000	6000	7000
Time (T)	0.2413	0.3590	0.5216	0.7181
Log Dimension	8.294	8.517	8.700	8.854
Log Time	-1.422	-1.024	-0.651	-0.331





- Here: $T = O(M^{1.95})$
- This is only an estimate of behaviour as $M \to \infty$, as test M values only go to 7000.
- Timings may be affected by other processes taking place, vectorization versus looping, memory issues, etc

3.2 Computing Complexity DEMO

Jupyter Notebook for demo:

- UnsupervisedML/Examples/Section03/Complexity.ipynb

Course Resources at:

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

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Section 3.3: Distance Measures

Why is a Distance Measure Needed?

- For clustering algorithms, one needs to compute distances between data points or distances between groups of data points
- We need a formula to compute such distances

Euclidean Distance Formula

- Define:

$$X = \begin{bmatrix} x_0 \\ \dots \\ x_{d-1} \end{bmatrix} \qquad Y = \begin{bmatrix} y_0 \\ \dots \\ y_{d-1} \end{bmatrix}$$

- L2 or Euclidean distance measure between X and Y defined as

$$dist(X,Y) = \left[\sum_{i=0}^{d-1} (x_i - y_i)^2\right]^{1/2}$$

L1 and Lp Distance Formulas

- L1 or Taxicab distance measure between X and Y defined as

$$dist(X,Y) = \sum_{i=0}^{d-1} |x_i - y_i|$$

- p norm ($p \geq 1$) or Minkowski distance between X and Y is a general distance measure that incorporates L1 and L2 measures as special cases:

$$dist(X,Y) = \left[\sum_{i=0}^{d-1} |x_i - y_i|^p\right]^{1/p}$$

Computational Complexity

- Confirm for yourself that number of operations and memory to compute L1, L2, Lp distances between 2 vectors of dimension d are $O(d)$ as $d \rightarrow \infty$

Distance Between Clusters

- Suppose $\{X_j\}$ j=0,…,M-1 is a set of points in a cluster

$$X = [X_0 \quad \dots \quad X_{M-1}] = \begin{bmatrix} X_{00} & \cdots & X_{0,M-1} \\ \vdots & \cdots & \vdots \\ X_{d-1,0} & \cdots & X_{d-1,M-1} \end{bmatrix}$$

- Define cluster mean as

$$C = \frac{1}{M} \sum_{j=0}^{M-1} X_j \qquad or \quad C_i = \frac{1}{M} \sum_{j=0}^{M-1} X_{ij} \quad i = 0, \dots, d-1$$

- Suppose $\{X_j\}$ and $\{Y_j\}$ are two clusters and let C_X and C_Y denote their means

- Distance between clusters defined as distance between the cluster means:

$$dist(\{X_j\}, \{Y_j\}) = dist(C_X, C_Y)$$

3.3 Distance Computation DEMO

Jupyter Notebook for demo:

- UnsupervisedML/Examples/Section03/Distance.ipynb

Course Resources at:

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

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Section 3.4: Singular Value Decomposition

Compact Singular Value Decomposition

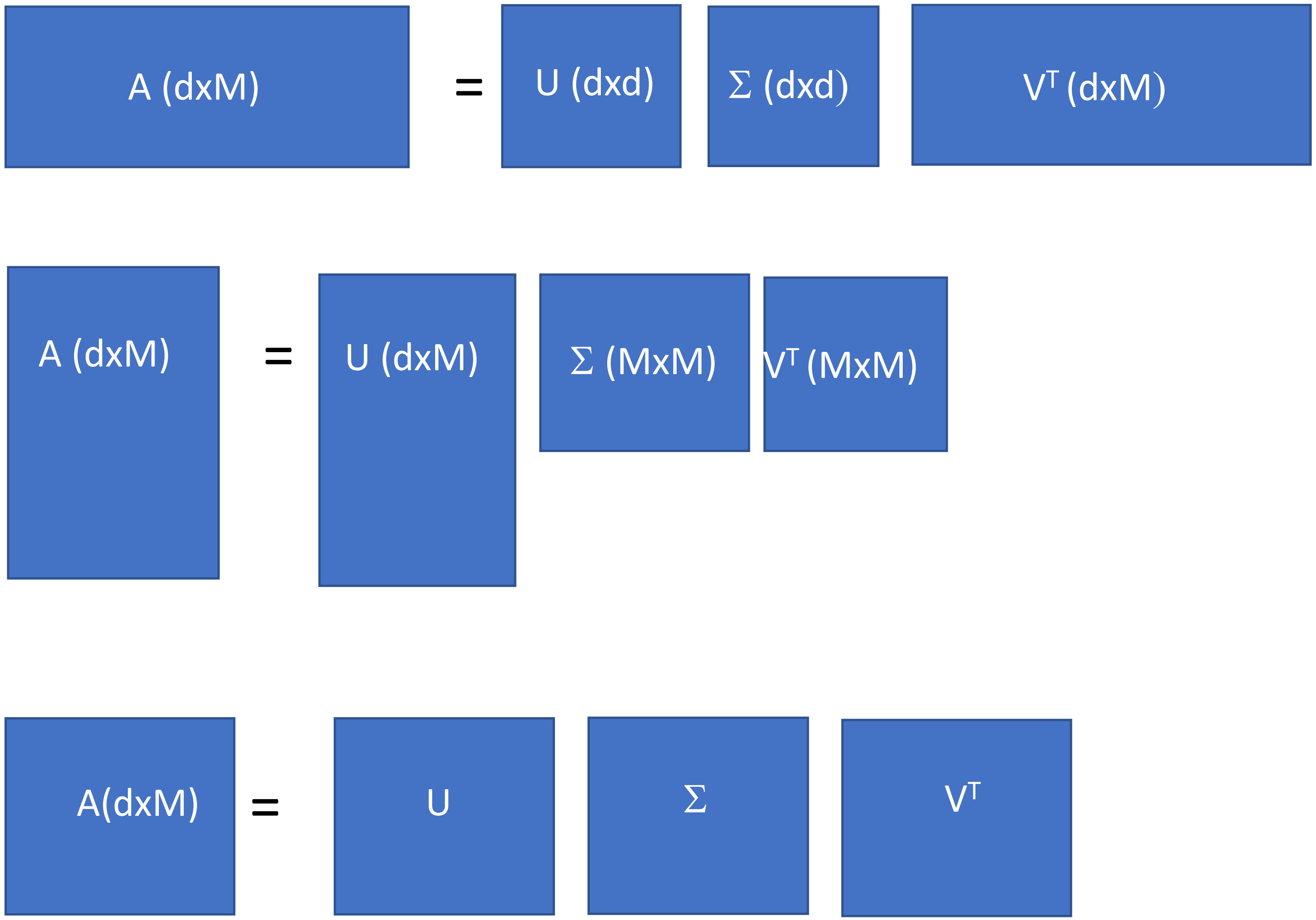
Compact version of SVD

- EVERY MATRIX A (dxM) can be decomposed as A = UΣV^T
- N = min(d,M)
- $U = [u_0 \quad \dots \quad u_{N-1}]$ U is dxN
  - Vectors $u_0, \dots, u_{N-1}$ are in d dimensions, have L2 length =1 and are orthogonal (pairwise dot products = 0)
- $\Sigma = diag(\sigma_0, \dots, \sigma_{N-1})$

Singulars values $\sigma_0, \dots, \sigma_{N-1}$ are non-negative and arranged in descending order

- $V^T = \begin{bmatrix} v_0^T \\ \dots \\ v_{N-1}^T \end{bmatrix}$ V is NxM
  - Vectors $v_0, \dots, v_{N-1}$ are in M dimensions, have L2 length=1 and are orthogonal (pairwise dot products = 0)

Singular Value Decomposition (Compact)



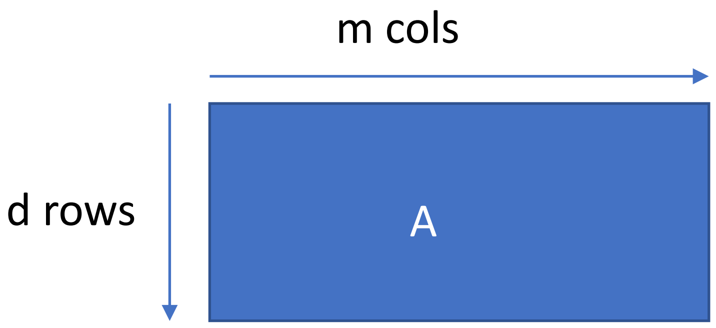
$d < M$

$d > M$

A (dxM) $d = M$

Matrix as a Mapping

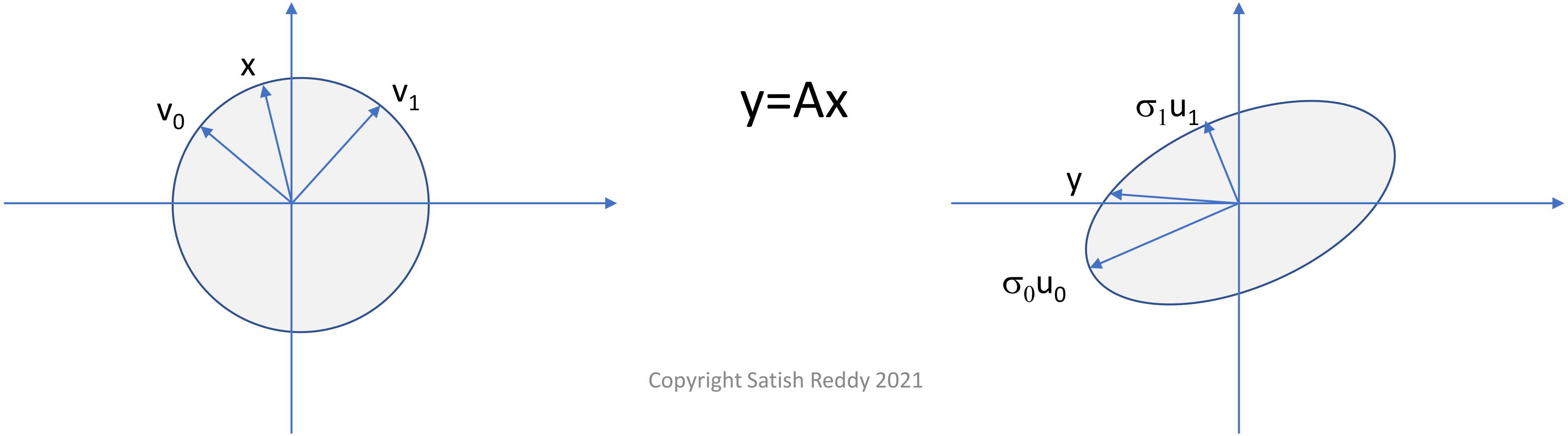
- Consider a matrix A (d rows and M columns)



- If $y = Ax$, then x point in R^M (M dimensional space) is mapped to y point in R^d (d dimensional space)
- A represents mapping from R^M to R^d

Matrix A as a Mapping and SVD

- Consider A is 2x2
- $A = \begin{bmatrix} u_0 & u_1 \end{bmatrix} \begin{bmatrix} \sigma_0 & 0 \\ 0 & \sigma_1 \end{bmatrix} \begin{bmatrix} v_0^T \\ v_1^T \end{bmatrix}$
- A maps v_0 to $\sigma_0 u_0$ and v_1 to $\sigma_1 u_1$
- v_0 and v_1 form an orthonormal basis for input space
- x can be decomposed as a linear combination of v_0 and v_1
- y=Ax can be decomposed as a linear combination of $\sigma_0 u_0$ and $\sigma_1 u_1$
- u_0 and u_1 form an orthonormal basis for output space
- A maps the unit disk in input space to the elliptical region in output space

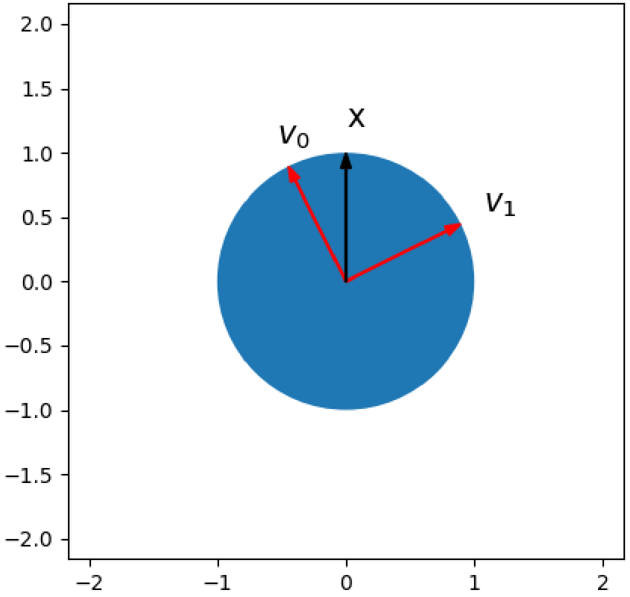


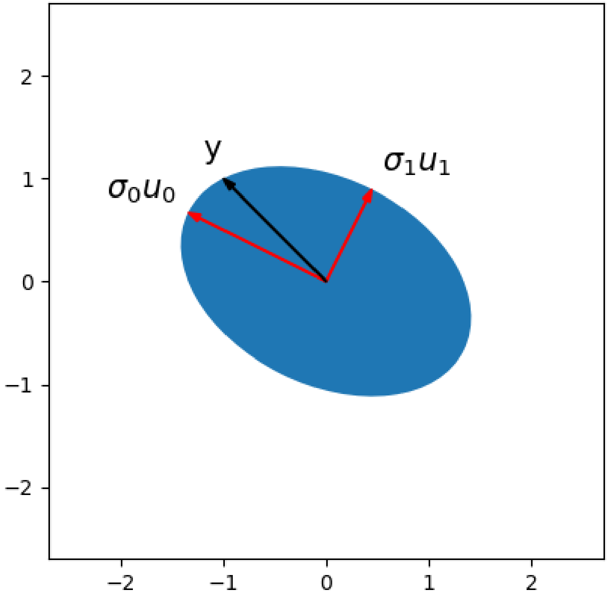
Example: 2x2 matrix

$$A = \begin{bmatrix} 1 & -1 \\ 0.5 & 1 \end{bmatrix}$$

$$A = U\Sigma V^T = \begin{bmatrix} -0.8944 & 0.4472 \\ 0.4472 & 0.8944 \end{bmatrix} \begin{bmatrix} 1.5 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -0.4472 & 0.8944 \\ 0.8944 & 0.4472 \end{bmatrix}$$

$$Ax = \begin{bmatrix} 1 & -1 \\ 0.5 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$





Singular Value Decomposition: Computation

- Eigenvalues of $A^T A$ are squares of singular values of A
- Usually one computes singular values, U, and V using a numerical approach without directly computing $A^T A$
- No exact formula for SVD so use iterative approach
- Use linalg.svd() function in numpy with appropriate settings to get compact version of SVD
- For dxd matrix SVD computation requires $O(d^3)$ operations as $d \rightarrow \infty$

Singular Value Decomposition in this Course

We will use SVD for

- Visualization/Animation of contours of normal probability density function for the Gaussian Mixture Model
  - Take SVD of covariance matrix
- Dimension Reduction using Principal Component Analysis
  - Take SVD of feature matrix X

3.4 Singular Value Decomposition DEMO

Jupyter Notebook for demo:

- UnsupervisedML/Examples/Section03/SVD.ipynb

Course Resources at:

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

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Section 3.5: Mean, Variance, and Covariance

Mean, Variance, and Covariance

- Mean of data points will be computed for various clustering algorithms
- Covariance of datasets will be used in Gaussian Mixture Model algorithm for clustering and in Principal Component Analysis algorithm for dimension reduction

Mean and Variance

Let $x_0, x_1, \ldots, x_{M-1}$ be a data series with M values

- Row vector form $x = [x_0 \quad \ldots \; x_{M-1}]$
- Sample mean is defined as:

$$\mu = \frac{1}{M}\sum_{j=0}^{M-1} x_j$$

- Sample variance defined as:

$$v = \frac{1}{M-1}\sum_{j=0}^{M-1}(x_j - \mu)^2 = \frac{1}{M-1}(x-\mu)(x-\mu)^T$$

Mean and Variance Example

- Consider the series: $x = [1\ \ -2\ 3\ 4\ 4]$
- Sample mean given by:

$$\mu = \frac{1}{M}\sum_{j=0}^{M-1} x_j = \frac{1}{5}(1 - 2 + 3 + 4 + 4) = 2$$

- For sample variance: $x - \mu = x - 2 = [-1\ \ -4\ 1\ 2\ 2]$

$$v = \frac{1}{M-1}(x-\mu)(x-\mu)^T = \frac{1}{4}[-1\ \ -4\ 1\ 2\ 2]\begin{bmatrix}-1\\-4\\1\\2\\2\end{bmatrix} = 6.5$$

Covariance

- Let: $x_0, x_1, \ldots, x_{M-1}$ and $y_0, y_1, \ldots, y_{M-1}$ be two series
- Let μ_x and μ_y be the sample means for the x and y series
- Covariance given by:

$$Cov(x,y) = \frac{1}{M-1}\sum_{j=0}^{M-1}(x_j - \mu_x)(y_j - \mu_y)$$

- Represent series x and series y as row vectors, then we can write the covariance as a matrix multiplication

$$Cov(x,y) = \frac{1}{M-1}(x - \mu_x)(y - \mu_y)^T$$

Covariance Example

- Consider: x series: $1, -2,3,4,4$ y series: 2,-3,3,3,5
- Can show means are: $\mu_x = 2$ and $\mu_y = 2$
- Covariance:

$$Cov = \frac{1}{4}(x - \mu_x)\left(y - \mu_y\right)^T = \frac{1}{4}[-1\ \ -4\ 1\ 2\ 2]\begin{bmatrix} 0 \\ -5 \\ 1 \\ 1 \\ 3 \end{bmatrix} = 7.25$$

Mean and Covariance Matrix for a Dataset

- Consider dataset (d features and M samples)

$$X = [X_0 \quad \dots \quad X_{M-1}] = \begin{bmatrix} X_{00} & \cdots & X_{0,M-1} \\ \vdots & \cdots & \vdots \\ X_{d-1,0} & \cdots & X_{d-1,M-1} \end{bmatrix}$$

- Sample mean (mean of each row)

$$\mu = \begin{bmatrix} \mu_0 \\ \vdots \\ \mu_{d-1} \end{bmatrix} \qquad \mu_i = \frac{1}{M} \sum_{j=0}^{M-1} X_{ij}$$

- Sample covariance matrix of dataset: $CovMat_{mn} = Cov\left(X_{Row\ m,} X_{Row\ n}\right)$
- Full covariance matrix:

$$CovMat = \frac{1}{M-1} (X - \mu)(X - \mu)^T$$

- Note for Gaussian Mixture Model covariance matrix formula has division by M

Mean and Covariance Matrix for a Dataset

- Consider dataset:

$$X = \begin{bmatrix} 1 & -2 & 3 & 4 & 4 \\ 2 & -3 & 3 & 3 & 5 \end{bmatrix}$$

- Can show that the mean is $\mu = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$
- For $X - \mu$, subtract μ from each column of X

$$X - \mu = \begin{bmatrix} -1 & -4 & 1 & 2 & 2 \\ 0 & -5 & 1 & 1 & 3 \end{bmatrix}$$

$$CovMat = \frac{1}{4}(X-\mu)(X-\mu)^T = \frac{1}{4}\begin{bmatrix} -1 & -4 & 1 & 2 & 2 \\ 0 & -5 & 1 & 1 & 3 \end{bmatrix}\begin{bmatrix} -1 & 0 \\ -4 & -5 \\ 1 & 1 \\ 2 & 1 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} 6.5 & 7.25 \\ 7.25 & 9 \end{bmatrix}$$

3.5 Mean, Variance, and Covariance DEMO

Jupyter Notebook for demo:

- UnsupervisedML/Examples/Section03/MeanCovariance.ipynb

Course Resources at:

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