## Introduction to Data Science

## Linear Algebra

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## Matrix representation

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- A row represents an example
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- Graphs \& Networks - City network, chemical structure, etc.
- Rearrangements - Permutation of given set of elements


## Geometry \& Vectors

- Vectors - A $1 \times d$ dimension matrix. In geometry sense a ray from the origin through the given point in $d$ dimension
- Normalization - In many scenarios the vectors are normalized to have unit norm
- Dot Product -
- Useful to reduce vector to scalar
- Can be used to measure angle


## Matrix operations

- Addition: $\mathrm{C}=\mathrm{A}+\mathrm{B}, C_{i j}=A_{i j}+B_{i j}$
- Scalar multiplication: $\mathrm{A}^{\prime}=c \mathrm{~A}, A_{i j}^{\prime}=c \cdot A_{i j}$
- Linear combination: $\alpha \mathrm{A}+(1-\alpha) \mathrm{B}$



## Matrix Transpose

- Let M be a matrix and $\mathrm{M}^{T}$ be the transpose of M , then $M_{i j}=M_{i j}^{\prime}$
- $\left(\mathrm{A}^{T}\right)^{T}=\mathrm{A}$
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## Matrix multiplication

- It is an aggregated version of the vector dot or inner product
- $x \cdot y=\sum_{i} x_{i} y_{i}$
- Matrix product $X Y^{\top}$ produces $1 \times 1$ matrix which contains dot product $X \cdot Y$
- $\mathrm{C}=\mathrm{AB}, C_{i j}=\sum_{k} A_{i k} B_{k j}$
- It does not commute, usually $A B \neq B A$
- It is associative, $A(B C)=(A B) C$
- Consider the following matrixes: $A_{1 \times n}, B_{n \times n}, C_{n \times n}, D_{n \times 1}$. Which of the following is better - $(A B)(C D)$ or $(A(B C)) D$ ?


## Covariance matrix

- Multiplication by transpose matrix is common ie. $A \cdot A^{T}$
- Both $A \cdot A^{T}$ and $A^{T}$. $A$ are compatible for multiplications
- Let $A_{n \times d}$ be a feature matrix, each row represents an item and each column denotes a feature
- $C=A A^{T}$ is a $n \times n$ matrix dot products
- $C_{i j}$ is a measure how similar item $i$ is to item $j$ (in syncness)
- $D=A^{T} A$ is a $d \times d$ dot products in syncness among the features
- $D_{i j}$ represents the similarity between feature $i$ and feature $j$
- Covariance formula: $\operatorname{Cov}(X, Y)=\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)\left(Y_{i}-\bar{Y}\right)$


## Covariance matrix (contd)

- $A, A \cdot A^{T}, A^{T} \cdot A$



## Matrix multiplication \& Paths

- Square matrix can be multiplied without transposition
- A matrix can represent the connectivity of nodes in a given network
- Let $A_{n \times n}$ can represent adjacency matrix

$$
A_{i j}^{2}=\sum_{k=1}^{n} A_{i k} A_{k j}
$$

## Matrix multiplication \& Permutations

- Multiplication is often used to rearrange the oder of the elements in a particular matrix
- Multiplication with identity matrix ( $/$ ) does not arrange anything new
- I contains exactly one non-zero element in each row and each column
- Matrix with this property is known as permutation matrix
- For example, multiplication with $P_{(2431)}$

$$
P_{(2431)}=\left[\begin{array}{llll}
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0
\end{array}\right], \quad M=\left[\begin{array}{llll}
11 & 12 & 13 & 14 \\
21 & 22 & 23 & 24 \\
31 & 32 & 33 & 34 \\
41 & 42 & 43 & 44
\end{array}\right], \quad P M=\left[\begin{array}{llll}
31 & 32 & 33 & 34 \\
11 & 12 & 13 & 14 \\
41 & 42 & 43 & 44 \\
21 & 22 & 23 & 24
\end{array}\right]
$$

## Permutations Example



$$
\begin{array}{c:c:c:c}
x_{2} \\
\hdashline & \hdashline & & \\
& & A & \\
& & A=\left[\begin{array}{ll}
1 & 3 \\
2 & 1
\end{array}\right] \quad x=\left[\begin{array}{l}
2 \\
1
\end{array}\right]
\end{array}
$$

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\hdashline & & & A x=\left[\begin{array}{l}
1 \\
2
\end{array}\right] \times 2+\left[\begin{array}{l}
3 \\
1
\end{array}\right] \times 1=\left[\begin{array}{l}
5 \\
5
\end{array}\right]
\end{array}
$$

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& & \\
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## Linear transformation

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2 \\
1
\end{array}\right] \\
& A x=\left[\begin{array}{l}
1 \\
2
\end{array}\right] \times 2+\left[\begin{array}{l}
3 \\
1
\end{array}\right] \times 1=\left[\begin{array}{l}
5 \\
5
\end{array}\right]
\end{aligned}
$$



## Rotating points in space

- Multiplying with the right matrix can rotate a set of points about the origin by angle $\theta$
$R_{\theta}=\left[\begin{array}{cc}\cos (\theta) & -\sin (\theta) \\ \sin (\theta) & \cos (\theta)\end{array}\right]$
- $\left[\begin{array}{l}x^{\prime} \\ y^{\prime}\end{array}\right]=R_{\theta}\left[\begin{array}{l}x \\ y\end{array}\right]=\left[\begin{array}{cc}x \cos (\theta) & -y \sin (\theta) \\ x \sin (\theta) & y \cos (\theta)\end{array}\right]$


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- For matrix, we say $A^{-1}$ is multiplicative inverse if $A \cdot A^{-1}=I$
- for $2 \times 2$ matrix, $A^{-1}=\left[\begin{array}{ll}a & b \\ c & d\end{array}\right]^{-1}=\frac{1}{a d-b c}\left|\begin{array}{cc}d & -b \\ c & a\end{array}\right|$


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- Matrix that is not invertible is known as singular matrix
- Gaussian elimination can be used to find the inverse


## Inversion Example

- Inverse of Lincoln image and $M \cdot M^{-1}$



## Linear Systems, Matrix Rank

- Linear systems
- Consider the following linear equation: $y=c_{0}+c_{1} x_{1}+\cdots+c_{m-1} x_{m-1}$
- Thus the coefficient of $n$ such linear equations can be represented as a matrix $C$ of size $n \times m$ $C X=Y \Rightarrow X=C^{-1} Y$
- What will happen if inverse does not exist?
- Matrix Rank
- A rank of a matrix measures the number of linearly independent rows
- Rank can be determined using Gaussian elimination


## Factoring matrices

- Factoring matrix $A$ into matrices in $B$ and $C$ represents particular aspect of division
- Non-singular matrix has an inverse $I=M \cdot M^{-1}$
- Matrix factorization is an important abstraction in data science, leading to feature representation in a compact way
- Suppose matrix $A$ can be factored as $A \approx B C$ where the size of $A$ is $n \times m, B-n \times k, C$ - $k \times m$ where $k<\min (n, m)$


[^0]
## Eigenvalues \& Eigenvectors

- Multiplying a vector $U$ by a matrix $A$ can have the same effect as multiplying it by scalar $\lambda$

$$
\left[\begin{array}{cc}
-5 & 2 \\
2 & -2
\end{array}\right] \cdot\left[\begin{array}{c}
2 \\
-1
\end{array}\right]=-6\left[\begin{array}{c}
2 \\
-1
\end{array}\right],\left[\begin{array}{cc}
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\end{array}\right] \cdot\left[\begin{array}{l}
1 \\
2
\end{array}\right]=-1\left[\begin{array}{l}
1 \\
2
\end{array}\right]
$$

- $\lambda$ is eigenvalue, $U$ is eigen vector
- Together, the eigenvector and eigenvalue must encode a lot of information about the matrix A
- Properties
- Each eigenvalue has an associated eigenvector
- There are in general $n$ eigenvector-eigenvalue pairs for every full rank $n \times n$ matrix
- Every pair of eigenvectors of symmetric matrix are mutually orthogonal
- Two vectors are orthogonal if the dot product is 0
- The eigenvectors can play the role of dimensions or bases in some $n$ dimensional space


## Example



$$
\mathrm{A}=\left[\begin{array}{ll}
1.25 & 0.75 \\
0.75 & 1.25
\end{array}\right]
$$

Example
$\xrightarrow{\text { (2) }}$

Example
A $=\left[\begin{array}{ll}1.25 & 0.75 \\ 0.75 & 1.25\end{array}\right]$
$\mathrm{v}_{1}=\left[\begin{array}{c}0.707 \\ 0.707\end{array}\right], \lambda_{1}=2.0$
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## Eigenvalue decomposition

- Any $n \times n$ symmetric matrix $M$ can be decomposed into the sum of its $n$ eigenvector products
- Let $\left(\lambda_{i}, U_{i}\right)$ be the eigen pairs $i=1, \ldots, n$ and assume $\lambda_{i} \geq \lambda_{i+1}$
- Each eigenvector $U_{i}$ is an $n \times 1$ matrix, multiplying it by its transpose yields an $n \times n$ matrix, product $U_{i} U_{i}^{T}$ same dimension as $M$
- Linear combination of these matrices weighted by its corresponding eigenvalue gives the original matrix $M=\sum_{i=1}^{n} \lambda_{i} U_{i} U_{i}^{T}$
- It holds for symmetric matrices
- Can be applied on covariance matrix
- Using only the vector associated with the largest eigenvalues, a good approximation of the matrix can be made


## Example

- Covariance of Lincoln \& $M-U_{1} U_{1}^{T}$



## Error plot

- Reconstructing the Lincoln memorial from the one, five, fifty eigenvectors


[^1]
## Singular Value Decomposition

- Eigen value decomposition is good but works for symmetric matrix
- Singular value decomposition is more general matrix factorization approach
- SVD of an $n \times m$ matrix $M$ factors into three matrices $U_{n \times n}, D_{n \times m}, V_{m \times m}$ ie. $M=U D V^{T}$, $D$ is a diagonal matrix
- The product $U$ • D has the effect of multiplying $U_{i j}$ by $D_{j j}$
- Relative importance of each column of $U$ is provided by $D$
- $D V^{\top}$ provides relative importance of each row of $V^{T}$
- The weight of $D$ are known as singular values of $M$


## Singular Value Decomposition

- Let $X$ and $Y$ be vectors of size $n \times 1$ and $1 \times m$, then matrix outer product $P=X \otimes Y$ is $n \times m$ matrix, $P_{j k}=X_{j} Y_{K}$
- Traditional matrix multiplication can be expressed as $C=A \cdot B=\sum_{k} A_{k} \otimes B_{k}^{T}$
- $A_{k}-k$ th column of $A, B_{k}^{T}-k$ th row of $B$
- $M$ can be expressed as the sum of outer product of vectors resulting from SVD namely $(U D)_{k}$, $V_{k}^{T}$


## Example

- Vectors associated with first 50 singular values, MSE of reconstruction




## Example

- Reconstruction with $k=5,50$, and error for $k=50$



[^0]:    image source: Data Science Design Manual

[^1]:    image source: Data Science Design Manual

