CS 412 Introduction to Machine Learning

Linear Algebra for Machine Learning

Instructor: Wei Tang

Department of Computer Science
University of Illinois at Chicago
Chicago IL 60607

https://tangw.people.uic.edu tangw@uic.edu

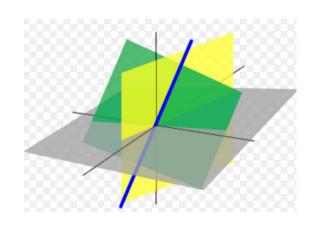
Slides credit: Sargur Srihari

What is linear algebra?

 Linear algebra is the branch of mathematics concerning linear equations such as

$$a_1x_1+\ldots+a_nx_n=b$$

- In vector notation we say $a^{T}x=b$
- Called a linear transformation of x
- Linear algebra is fundamental to geometry, for defining objects such as lines, planes, rotations



Linear equation $a_1x_1+....+a_nx_n=b$ defines a plane in $(x_1,...,x_n)$ space

Why do we need to know it?

- Linear Algebra is used throughout engineering
- Essential for understanding ML algorithms
 - E.g., We convert input vectors $(x_1,...,x_n)$ into outputs by a series of linear transformations
- Here we discuss:
 - Concepts of linear algebra needed for ML
 - Omit other aspects of linear algebra

Linear Algebra Topics

- Scalars, Vectors, Matrices and Tensors
- Multiplying Matrices and Vectors
- Identity and Inverse Matrices
- Linear Dependence and Span
- Norms
- Special kinds of matrices and vectors
- Eigendecomposition
- Singular value decomposition
- The trace operator
- The determinant

Scalar

- Single number
 - In contrast to other objects in linear algebra, which are usually arrays of numbers
- Represented in lower-case italic x
 - They can be real-valued or be integers
 - E.g., let x be the slope of the line
 - Defining a real-valued scalar
 - E.g., let n be the number of units
 - Defining a natural number scalar

Vector

- An array of numbers arranged in order
- Each no. identified by an index
- Written in lower-case bold such as x
 - its elements are in italics lower case, subscripted

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_n \end{bmatrix}$$

- If each element is in R then x is in R^n
- · We can think of vectors as points in space
 - Each element gives coordinate along an axis

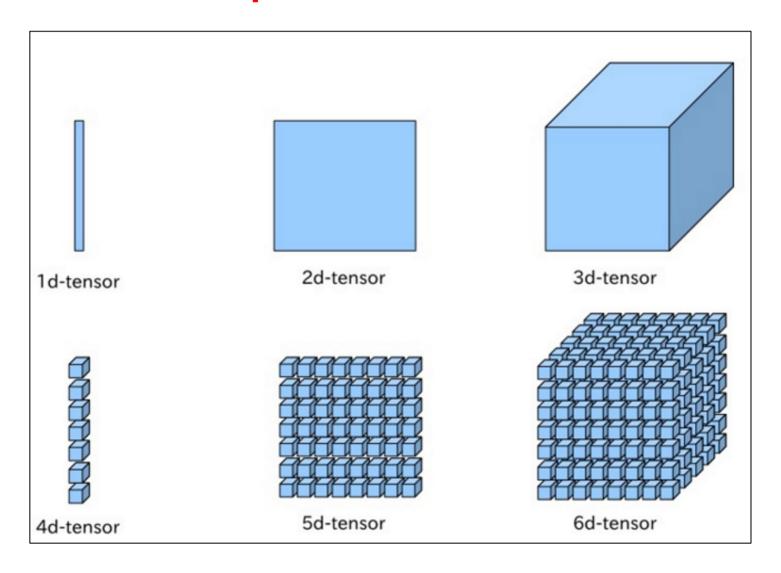
Matrices

- 2-D array of numbers
 - So each element identified by two indices
- Denoted by bold typeface A
 - Elements indicated by name in italic but not bold
 - $A_{1,1}$ is the top left entry and $A_{m,n}$ is the bottom right entry
 - We can identify numbers in vertical column j by writing : for the horizontal coordinate
 - E.g., $A = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix}$
 - $A_{i:}$ is i^{th} row of A, $A_{:j}$ is j^{th} column of A
- If A has shape of height m and width n with real-values then $A \in \mathbb{R}^{m \times n}$

Tensor

- Sometimes need an array with more than two axes
 - E.g., an RGB color image has three axes
- A tensor is an array of numbers arranged on a regular grid with variable number of axes
 - See figure next
- Denote a tensor with this bold typeface: A
- Element (i,j,k) of tensor denoted by $A_{i,j,k}$

Shapes of Tensors



Transpose of a Matrix

- An important operation on matrices
- The transpose of a matrix A is denoted as AT
- Defined as

$$(\mathbf{A}^{\mathrm{T}})_{i,j} = A_{j,i}$$

- The mirror image across a diagonal line
 - · Called the main diagonal, running down to the right starting from upper left corner

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,1} & A_{3,2} & A_{3,3} \end{bmatrix} \Rightarrow A^{T} = \begin{bmatrix} A_{1,1} & A_{2,1} & A_{3,1} \\ A_{1,2} & A_{2,2} & A_{3,2} \\ A_{1,3} & A_{2,3} & A_{3,3} \end{bmatrix} \Rightarrow A^{T} = \begin{bmatrix} A_{1,1} & A_{2,1} & A_{3,1} \\ A_{1,2} & A_{2,2} & A_{3,2} \\ A_{1,3} & A_{2,3} & A_{3,3} \end{bmatrix}$$

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \\ A_{3,1} & A_{3,2} \end{bmatrix} \Rightarrow A^{T} = \begin{bmatrix} A_{1,1} & A_{2,1} & A_{3,1} \\ A_{1,2} & A_{2,2} & A_{3,2} \end{bmatrix}$$

Vectors as special case of matrix

- Vectors are matrices with a single column
- Often written in-line using transpose

$$\boldsymbol{x} = [x_1, ..., x_n]^T$$

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \\ \boldsymbol{x}_n \end{bmatrix} \Rightarrow \boldsymbol{x}^T = [\boldsymbol{x}_1, \boldsymbol{x}_2, ... \boldsymbol{x}_n]$$

A scalar is a matrix with one element

$$a = a^{\mathrm{T}}$$

Matrix Addition

- We can add matrices to each other if they have the same shape, by adding corresponding elements
 - If A and B have same shape (height m, width n)

$$C = A + B \Rightarrow C_{i,j} = A_{i,j} + B_{i,j}$$

• A scalar can be added to a matrix or multiplied by a scalar $D = aB + c \Rightarrow D_{i,j} = aB_{i,j} + c$

Multiplying Matrices

- For product C = AB to be defined, A has to have the same no. of columns as the no. of rows of B
 - If A is of shape mxn and B is of shape nxp then matrix product C is of shape mxp

$$C = AB \Rightarrow C_{i,j} = \sum_{k} A_{i,k} B_{k,j}$$

- Note that the standard product of two matrices is not just the product of two individual elements
 - Such a product does exist and is called the element-wise product or the Hadamard product A ¤ B

Multiplying Vectors

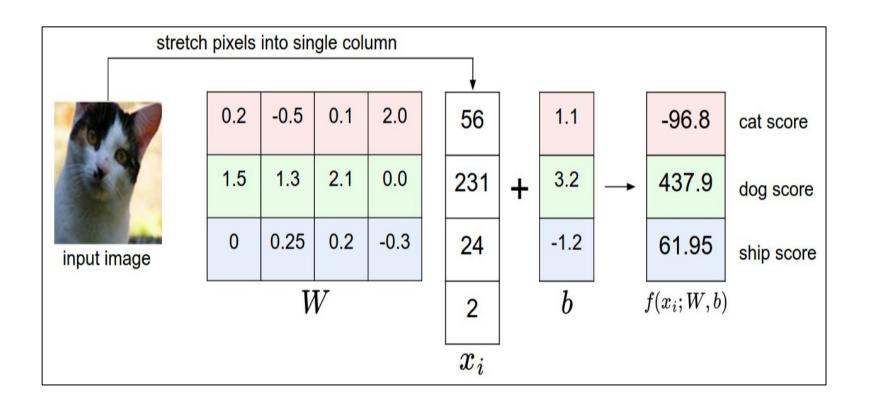
- Dot product between two vectors x and y of same dimensionality is the matrix product x^Ty
- We can think of matrix product C=AB as computing C_{ij} the dot product of row i of A and column j of B

Matrix Product Properties

- Distributivity over addition: A(B+C)=AB+AC
- Associativity: A(BC)=(AB)C
- Not commutative: AB = BA is not always true
- Dot product between vectors is commutative: $x^Ty=y^Tx$
- Transpose of a matrix product has a simple form: $(AB)^T = B^TA^T$

Example flow of tensors in ML

A linear classifier y = Wx + b



Identity and Inverse Matrices

- Matrix inversion is a powerful tool to analytically solve Ax=b
- Needs concept of Identity matrix
- Identity matrix does not change value of vector when we multiply the vector by identity matrix
 - Denote identity matrix that preserves n-dimensional vectors as I_n
 - Formally $I_n \in \mathbb{R}^{n \times n}$ and $\forall \mathbf{x} \in \mathbb{R}^n, I_n \mathbf{x} = \mathbf{x}$
 - Example of I_3 $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

Matrix Inverse

 $A^{-1}A = I$ Inverse of square matrix A defined as

$$A^{-1}A = I$$

• We can now solve Ax=b as follows:

$$Ax = b$$

$$A^{-1}Ax = A^{-1}b$$

$$I_n x = A^{-1}b$$

$$x = A^{-1}b$$

- This depends on being able to find A^{-1}
- If A-1 exists there are several methods for finding it

Solving Simultaneous equations

```
Ax = b
where A is N x N
x is N x 1: set of weights to be determined
b is N x 1
```

Closed-form solutions

- Two closed-form solutions
 - 1. Matrix inversion $x = A^{-1}b$
 - 2. Gaussian elimination

Linear Equations: Closed-Form Solutions

1. Matrix Formulation: Ax = b

Solution: $x = A^{-1}b$

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n = b_m$$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

2. Gaussian Elimination followed by back-substitution

$$x + 3y - 2z = 5$$
$$3x + 5y + 6z = 7$$
$$2x + 4y + 3z = 8$$

$$\begin{bmatrix} 3x + 5y + 6z = 7 \\ 2x + 4y + 3z = 8 \end{bmatrix} \begin{bmatrix} 1 & 3 & -2 & 5 \\ 3 & 5 & 6 & 7 \\ 2 & 4 & 3 & 8 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & 5 \\ 0 & -4 & 12 & -8 \\ 2 & 4 & 3 & 8 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & 5 \\ 0 & -4 & 12 & -8 \\ 0 & -2 & 7 & -2 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & 5 \\ 0 & 1 & -3 & 2 \\ 0 & -2 & 7 & -2 \end{bmatrix}$$

$$\sim \begin{bmatrix} 1 & 3 & -2 & 5 \\ 0 & 1 & -3 & 2 \\ 0 & 0 & 1 & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & -2 & 5 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 3 & 0 & 9 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 0 & -15 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{bmatrix}$$

Disadvantage of closed-form solutions

- If A^{-1} exists, the same A^{-1} can be used for any given \boldsymbol{b}
 - But A⁻¹ cannot be represented with sufficient precision
 - It is not used in practice
- Gaussian elimination also has disadvantages
 - numerical instability (division by small no.)
 - $-O(n^3)$ for $n \times n$ matrix
- Software solutions use value of b in finding x
 - E.g., difference (derivative) between b and output is used iteratively

Span of a set of vectors

- Span of a set of vectors: set of points obtained by a linear combination of those vectors
 - A linear combination of vectors $\{v^{(1)},...,v^{(n)}\}$ with coefficients c_i is $\sum c_i \mathbf{v}^{(i)}$
 - System of equations is Ax = b

$$A x = \sum_{i} x_{i} A_{:,i}$$

- This is a linear combination of vectors
- Thus determining whether Ax=b has a solution is equivalent to determining whether b is in the span of columns of A
 - This span is referred to as column space or range of A

Use of a Vector in Regression

- A sample matrix
 - N samples, D features



- Feature vector has three dimensions
- This is a regression problem

Norms

- Used for measuring the size of a vector
- Norms map vectors to non-negative values
- Norm of vector $x = [x_1,...,x_n]^T$ is distance from origin to x
 - It is any function f that satisfies:

$$f(x) = 0 \Rightarrow x = 0$$

$$f(x + y) \le f(x) + f(y)$$
 Triangle Inequality
$$\forall \alpha \in R \quad f(\alpha x) = |\alpha| f(x)$$

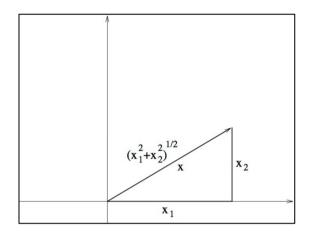
L^P Norm

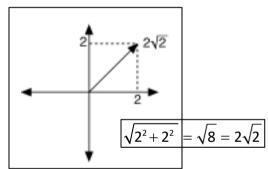
Definition:

$$\left|\left|\mathbf{x}\right|\right|_{p} = \left(\sum_{i} \left|x_{i}\right|^{p}\right)^{\frac{1}{p}}$$

- L² Norm
 - Called Euclidean norm
 - Simply the Euclidean distance
 between the origin and the point x
 - written simply as |x|
 - Squared Euclidean norm is same as x^Tx







$$\|x\|_{\infty} = \max_{i} |x_{i}|$$

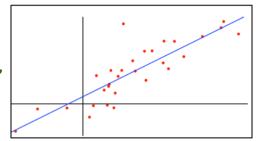
Called max norm

Use of norm in Regression

Linear Regression

x: a vector, w: weight vector

$$y(x, w) = w_0 + w_1 x_1 + ... + w_d x_d = w^T x$$



Loss Function

$$\tilde{E}(\boldsymbol{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(\boldsymbol{x}_n, \boldsymbol{w}) - t_n\}^2$$

Size of a Matrix: Frobenius Norm

• Similar to L^2 norm

$$\left\|\left|A\right|\right|_F = \left(\sum_{i,j} A_{i,j}^2\right)^{\frac{1}{2}}$$

- Frobenius in ML
 - Layers of neural network involve matrix multiplication
 - Regularization:
 - minimize Frobenius of weight matrices ||W(i)|| over L layers

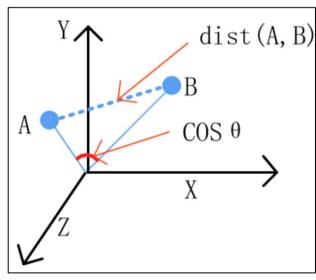
$$J_R = J + \lambda \sum_{i=1}^{L} \left\| W^{(i)} \right\|_F$$

Angle between Vectors

• Dot product of two vectors can be written in terms of their L^2 norms and angle θ between them $x^T y \Rightarrow ||x||_p ||y||_p \cos \theta$

 Cosine between two vectors is a measure of their similarity

$$ext{similarity} = \cos(heta) = rac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = rac{\sum\limits_{i=1}^n A_i B_i}{\sqrt{\sum\limits_{i=1}^n A_i^2} \sqrt{\sum\limits_{i=1}^n B_i^2}},$$



Special kind of Matrix: Diagonal

- Diagonal Matrix has mostly zeros, with nonzero entries only in diagonal
 - E.g., identity matrix, where all diagonal entries are 1
 - E.g., covariance matrix with independent features

$$Cov(X,Y) = \sigma_{XY} = E[(X - \mu_X)(Y - \mu_Y)] \qquad \qquad \sigma_1^2 \quad 0 \quad \dots \quad 0$$

$$Covariance = \frac{\sum(x_i - x_{avg})(y_i - y_{avg})}{n-1}$$

$$Covariance = \frac{-64.57}{8}$$

$$Covariance = \begin{bmatrix} -8.07 \end{bmatrix}$$

If
$$Cov(X, Y) = 0$$
 then $E(XY) = E(X)E(Y)$

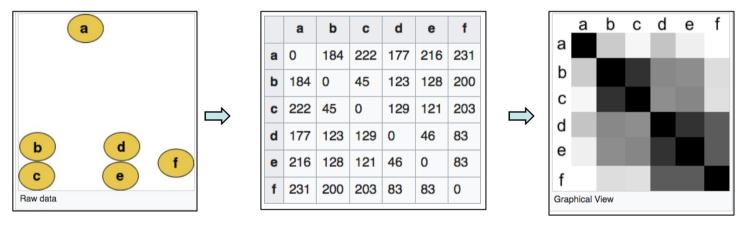
$$N(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{\mid \boldsymbol{\Sigma} \mid^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

Efficiency of Diagonal Matrix

- diag (v) denotes a square diagonal matrix with diagonal elements given by entries of vector v
- Multiplying vector x by a diagonal matrix is efficient
 - To compute $\operatorname{diag}(v)x$ we only need to scale each x_i by v_i $\operatorname{diag}(v)x = v \odot x$
- Inverting a square diagonal matrix is efficient
 - Inverse exists iff every diagonal entry is nonzero, in which case diag $(v)^{-1}$ =diag $([1/v_1,...,1/v_n]^T)$

Special kind of Matrix: Symmetric

- A symmetric matrix equals its transpose: $A = A^T$
 - E.g., a distance matrix is symmetric with $A_{ij}=A_{ji}$



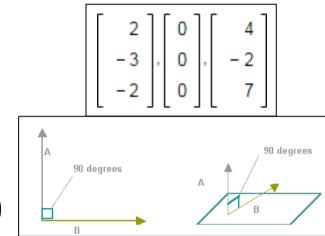
E.g., covariance matrices are symmetric

Special Kinds of Vectors

- Unit Vector
 - -A vector with unit norm

$$|x|_2 = 1$$

- Orthogonal Vectors
 - A vector x and a vector y are orthogonal to each other if $x^Ty=0$



- If vectors have nonzero norm, vectors at 90 degrees to each other
- Orthonormal Vectors
 - Vectors are orthogonal & have unit norm
 - Orthogonal Matrix
 - A square matrix whose rows are mutually orthonormal: $A^{T}A = AA^{T} = I$
 - $-A^{-1}=A^{T}$

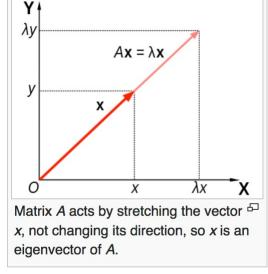
Orthogonal matrices are of interest because their inverse is very cheap to compute

Eigenvector

An eigenvector of a square matrix
 A is a non-zero vector v such that
 multiplication by A only changes
 the scale of v

$$Av = \lambda v$$

- The scalar λ is known as eigenvalue
- If v is an eigenvector of A, so is any rescaled vector sv. Moreover sv still has the same eigen value.
 Thus look for a unit eigenvector



Wikipedia

Eigenvalue and Characteristic Polynomial

- Consider Av=w
- If v and w are scalar multiples, i.e., if $Av = \lambda v$
 - then v is an eigenvector of the linear transformation A and the scale factor λ is the eigenvalue corresponding to the eigen vector
- This is the eigenvalue equation of matrix A
 - Stated equivalently as $(A-\lambda I)v=0$
 - This has a non-zero solution if $|A-\lambda I|=0$ as
 - The polynomial of degree n can be factored as

$$|A-\lambda I| = (\lambda_1 - \lambda)(\lambda_2 - \lambda)...(\lambda_n - \lambda)$$

• The $\lambda_1, \lambda_2...\lambda_n$ are roots of the polynomial and are eigenvalues of A

Example of Eigenvalue/Eigenvector

Consider the matrix

$$A = \left| egin{array}{ccc} 2 & 1 \ 1 & 2 \end{array}
ight|$$

• Taking determinant of $(A-\lambda I)$, the char poly is

$$egin{array}{c|c} A-\lambda I \models \left[egin{array}{cc} 2-\lambda & 1 \ 1 & 2-\lambda \end{array}
ight] = 3-4\lambda+\lambda^2 \end{array}$$

- It has roots $\lambda=1$ and $\lambda=3$ which are the two eigenvalues of A
- The eigenvectors are found by solving for v in $Av=\lambda v$, which are $\begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$

$$egin{bmatrix} v_{_{\lambda=1}} = igg [& 1 \ -1 & \end{bmatrix}, v_{_{\lambda=3}} = igg [& 1 \ 1 & \end{bmatrix} igg]$$

Eigendecomposition

- Suppose that matrix A has n linearly independent eigenvectors $\{v^{(1)},...,v^{(n)}\}$ with eigenvalues $\{\lambda_1,...,\lambda_n\}$
- Concatenate eigenvectors to form matrix V
- Concatenate eigenvalues to form vector $\lambda = [\lambda_1,...,\lambda_n]$
- Eigendecomposition of A is given by

$$A = V \operatorname{diag}(\lambda) V^{-1}$$

Decomposition of Symmetric Matrix

 Every real symmetric matrix A can be decomposed into real-valued eigenvectors and eigenvalues

$$A = Q\Lambda Q^{T}$$

where Q is an orthogonal matrix composed of eigenvectors of A: $\{v^{(1)},...,v^{(n)}\}$

orthogonal matrix: components are orthogonal or $v^{(i)T}v^{(j)}=0$

 Λ is a diagonal matrix of eigenvalues $\{\lambda_1,...,\lambda_n\}$

- We can think of A as scaling space by λ_i in direction $v^{(i)}$
 - See figure on next slide

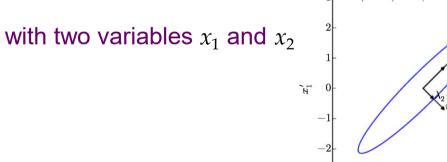
Effect of Eigenvectors and Eigenvalues

- Example of 2 × 2 matrix
- Matrix A with two orthonormal eigenvectors
 - $v^{(1)}$ with eigenvalue λ_1 , $v^{(2)}$ with eigenvalue λ_2

Plot of unit vectors $u \in \mathbb{R}^{2}$ (circle)

Plot of vectors Au (ellipse)

After multiplication



Eigendecomposition is not unique

- Eigendecomposition is $A = Q\Lambda Q^T$
 - where Q is an orthogonal matrix composed of eigenvectors of A
- Decomposition is not unique when two eigenvalues are the same
- By convention order entries of Λ in descending order:
 - Under this convention, eigendecomposition is unique if all eigenvalues are unique

What does eigendecomposition tell us?

- Tells us useful facts about the matrix:
 - 1. Matrix is singular if & only if any eigenvalue is zero
 - 2. Useful to optimize quadratic expressions of form

$$f(x) = x^T A x$$
 subject to $|x||_2 = 1$

Whenever x is equal to an eigenvector, f is equal to the corresponding eigenvalue

Maximum value of f is max eigen value, minimum value is min eigen value

Positive Definite Matrix

- A matrix whose eigenvalues are all positive is called positive definite
 - Positive or zero is called positive semidefinite
- If eigen values are all negative it is negative definite
 - Positive definite matrices guarantee that $x^TAx \ge 0$

Singular Value Decomposition (SVD)

- Eigendecomposition has form: $A = V \operatorname{diag}(\lambda) V^{-1}$
 - If A is not square, eigendecomposition is undefined
- SVD is a decomposition of the form A=UDV^T
- SVD is more general than eigendecomposition
 - Used with any matrix rather than square ones
 - Every real matrix has a SVD
 - Same is not true of eigen decomposition

SVD Definition

- Write A as a product of 3 matrices: $A=UDV^{T}$
 - If A is $m \times n$, then U is $m \times m$, D is $m \times n$, V is $n \times n$
- Each of these matrices have a special structure
 - U and V are orthogonal matrices
 - D is a diagonal matrix not necessarily square
 - Elements of Diagonal of D are called singular values of A
 - Columns of *U* are called *left singular vectors*
 - Columns of V are called right singular vectors
- SVD interpreted in terms of eigendecomposition
 - Left singular vectors of A are eigenvectors of AA^T
 - Right singular vectors of A are eigenvectors of A^TA
 - Nonzero singular values of A are square roots of eigenvalues of $A^{T}A$. Same is true of AA^{T}

Trace of a Matrix

 Trace operator gives the sum of the elements along the diagonal

$$Tr(A) = \sum_{i,i} A_{i,i}$$

Frobenius norm of a matrix can be represented as

$$\left\|\left|A\right|\right|_F = \left(Tr(A)\right)^{\frac{1}{2}}\right|$$

Determinant of a Matrix

- Determinant of a square matrix det(A) is a mapping to a scalar
- It is equal to the product of all eigenvalues of the matrix
- Measures how much multiplication by the matrix expands or contracts space