Maths Preliminaries

COMP9318 @ CSE, UNSW

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Introduction

- This review serves two purposes:
 - Recap relevant maths contents that you may have learned a long time ago (probably not in a CS course and rarely used in any CS course).
 - More importantly, present it in a way that is useful (i.e., giving semantics/motivations) for understanding maths behind Machine Learning.
- Contents
 - Linear Algebra

Note

- You've probability learned Linear Algebra from matrix/system
 of linear equations, etc. We will review key concepts in LA
 from the perspective of linear transformations (think of it as
 functions for now). This perspective provides semantics and
 intuition into most of the ML models and operations.
 - Here we emphasize more on intuitions; We deliberately skip many concepts and present some contents in an informal way.
- It is a great exercise for you to view related maths and ML models/operations in this perspective throughout this course!

A Common Trick in Maths I

Question

Calculate 2^{10} , 2^{-1} , $2^{\ln 5}$ and 2^{4-3i} ?

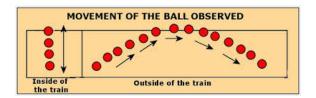
- Properties:
 - $f_a(n) = f_a(n-1) * a$, for $n \ge 1$; $f_a(0) = 1$.
 - f(u) * f(v) = f(u + v).
 - $f(x) = y \Leftrightarrow \ln(y) = x \ln(a) \Leftrightarrow f(x) = \exp\{x \ln a\}.$
 - $e^{ix} = cos(x) + i \cdot sin(x)$.
- The trick:
- Same in Linear algebra



Objects and Their Representations

Goal

- We need to study the objects
- On one side:
 - A good representation helps (a lot)!
- On the other side:
 - Properties of the objects should be independent of the representation!



Basic Concepts I

Algebra

- a set of objects
- two operations and their identity objects (aka. identify element):
 - addition (+); its identity is 0.
 - scalar multiplication (·); its identity is 1.
- constraints:
 - Closed for both operations
 - Some nice properties of these operations:
 - Communicative: a + b = b + a.
 - Associative: (a + b) + c = a + (b + c).
 - Distributive: $\lambda(a + b) = \lambda a + \lambda b$.

Basic Concepts II

Think: What about substraction and division?

Tips

Always use analogy from algebra on integers (\mathbb{Z}) and algebra on Polynomials (\mathcal{P}). § \mathbb{Z}

Why these constraints are natural and useful?

Basic Concepts III

Representation matters?

What if by their polar coordinates?

Consider even geometric vectors: c = a + bWhat if we represent vectors by a column of their coordinates?

Notes

- Informally, the objects we are concerned with in this course are (column) vectors.
- The set of all *n*-dimensional real vectors is called \mathbb{R}^n .



(Column) Vector

Vector

- A *n*-dimensional vector, v, is a $n \times 1$ matrix. We can emphasize its shape by calling it a *column* vector.
 - A row vector is a transposed column vector: v^{\top} .

Operations

- Addition: $v_1 + v_2 =$
- (Scalar) Multiplication: $\lambda v_1 =$

Linearity I

Linear Combination: Generalization of Univariate Linear Functions

• Let $\lambda_i \in \mathbb{R}$, given a set of k vectors v_i ($i \in [k]$), a linear combination of them is

$$\lambda_1 \mathbf{v}_1 + \lambda_2 \mathbf{v}_2 + \ldots + \lambda_k \mathbf{v}_k = \sum_{i \in [k]} \lambda_i \mathbf{v}_i$$

• Later, this is just $V\lambda$, where

$$V = \begin{bmatrix} | & | & | & | \\ v_1 & v_2 & \dots & v_k \\ | & | & | & | \end{bmatrix} \qquad \lambda = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \dots \\ \lambda_k \end{bmatrix}$$

扩张空间, 生成空间

- Span: All linear combination of a set of vectors is the span of them.
- Basis: The minimal set of vectors whose span is exactly the whole \mathbb{R}^n .



Linearity II

Benefit: every vector has a unique decomposition into basis.
 Think: Why uniqueness is desirable?

Examples

- Span of $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ is \mathbb{R}^2 . They are also the basis.
- Span of $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $\begin{bmatrix} 2 \\ 3 \end{bmatrix}$ is \mathbb{R}^2 . But one of them is *redundant*.

Think: Who?

• Decompose $\begin{bmatrix} 4 \\ 6 \end{bmatrix}$



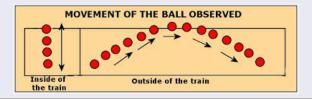
Linearity III

Exercises

- What are the (natural) basis of all (univariate) Polynomials of degrees up to d?
- Decompose $3x^2 + 4x 7$ into *the* linear combination of 2, 2x 3, $x^2 + 1$.

$$3x^2 + 4x - 7 = 3(x^2 + 1) + 2(2x - 3) + (-2)(2).$$

 The "same" polynomial is mapped to two different vectors under two different bases.
 Think: Any analogy?



Matrix I

Linear Transformation

• is a "nice" linear function that maps a vector in \mathbb{R}^n to another vector in \mathbb{R}^m .

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \stackrel{f}{\longrightarrow} \quad \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

• The general form:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \xrightarrow{f} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \xrightarrow{y_1 = M_{11}x_1 + M_{12}x_2} y_1 = M_{21}x_1 + M_{22}x_2 y_3 = M_{31}x_1 + M_{32}x_2$$

Matrix II

Nonexample

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \xrightarrow{f} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \xrightarrow{y_1 = \alpha x_1^2 + \beta x_2} y_1 = \alpha x_1^2 + \beta x_1 + \tau x_2 y_2 = \gamma x_1^2 + \theta x_1 + \tau x_2 y_3 = \cos(x_1) + e^{x_2}$$

Why Only Linear Transformation?

- Simple and nice properties:
 - $(f_1 + f_2)(x) = f_1(x) + f_2(x)$
 - $\bullet (\lambda f)(x) = \lambda \cdot f(x)$
 - What about f(g(x))?
- Useful



Matrix I

Definition

- A $m \times n$ matrix corresponds to a linear transformation from \mathbb{R}^n to \mathbb{R}^m
 - $f(x) = y \implies Mx = y$, where matrix-vector multiplication is defined as: $y_i = \sum_k M_{ik} \cdot x_k$
 - MoutDim×inDim
 - Transformation or Mapping emphasizes more on the mapping between two sets, rather than the detailed specification of the mapping; the latter is more or less the *elementary* understanding of a *function*. These are all specific instances of morphism in category theory.

Semantic Interpretation



Matrix II

Linear combination of columns of M:

$$\begin{bmatrix} \begin{vmatrix} & & & & & & \\ M_1 & M_2 & \dots & M_n \\ & & & & & \end{bmatrix} \begin{bmatrix} | & & & & \\ | & & & & \\ | & & & & & \end{bmatrix} \begin{bmatrix} | & & & & \\ | & & & & \\ | & & & & & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

$$y = x_1 M_{\bullet 1} + \ldots + x_n M_{\bullet n}$$

• Example:

$$\begin{bmatrix} 1 & 2 \\ -4 & 9 \\ 25 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 10 \end{bmatrix} = 1 \begin{bmatrix} 1 \\ -4 \\ 25 \end{bmatrix} + 10 \begin{bmatrix} 2 \\ 9 \\ 1 \end{bmatrix} = \begin{bmatrix} 21 \\ 86 \\ 35 \end{bmatrix}$$

Matrix III

$$\begin{bmatrix} 1 & 2 \\ -4 & 9 \end{bmatrix} \begin{bmatrix} 1 \\ 10 \end{bmatrix} = 1 \begin{bmatrix} 1 \\ -4 \end{bmatrix} + 10 \begin{bmatrix} 2 \\ 9 \end{bmatrix} = \begin{bmatrix} 21 \\ 86 \end{bmatrix}$$

Think: What does M do for the last example?

- Rotation and scaling
- When x is also a matrix,

$$\begin{bmatrix} 1 & 2 \\ -4 & 9 \\ 25 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 10 & 20 \end{bmatrix} = \begin{bmatrix} 21 & 42 \\ 86 & 172 \\ 35 & 70 \end{bmatrix}$$

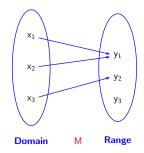
System of Linear Equations I

$$y_{1} = M_{11}x_{1} + M_{12}x_{2} y_{2} = M_{21}x_{1} + M_{22}x_{2} y_{3} = M_{31}x_{1} + M_{32}x_{2}$$
 \Longrightarrow
$$\begin{bmatrix} y_{1} \\ y_{2} \\ y_{3} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \\ M_{31} & M_{32} \end{bmatrix} \begin{bmatrix} x_{1} \\ x_{2} \end{bmatrix} y = Mx$$

- Interpretation: find a vector in \mathbb{R}^2 such that its image (under M) is exactly the given vector $y \in \mathbb{R}^3$.
- How to solve it?



System of Linear Equations II



A Matrix Also Specifies a (Generalized) Coordinate System

Yet another interpretation

- $y = Mx \implies Iy = Mx$.
- The vector y wrt standard coordinate system, I, is the same as x wrt the coordinate system defined by column vectors of M.

Think: why columns of M?

Example for polynomials

Exercise I

- What if y is given in the above example?
- What does the following mean?

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

• Think about representing polynomials using the basis: $(x-1)^2$, x^2-1 , x^2+1 .

Inner Product

THE binary operator – some kind of "similarity"

- Type signature: vector \times vector \rightarrow scalar: $\langle x, y \rangle$.
 - In \mathbb{R}^n , usually called dot product: $x \cdot y \stackrel{\text{def}}{=} x^\top y = \sum_i x_i y_i$.
 - For certain functions, $\langle f,g\rangle=\int_a^b f(t)g(t)\,\mathrm{d}t.$ \Rightarrow leads to the Hilbert Space
- Properties / definitions for \mathbb{R} :
 - conjugate symmetry: $\langle x, y \rangle = \langle y, x \rangle$
 - linearity in the first argument: $\langle ax + y, z \rangle = a \langle x, z \rangle + \langle y, z \rangle$
 - positive definitiveness: $\langle x, x \rangle \ge 0$; $\langle x, x \rangle \Leftrightarrow x = 0$;
- Generalizes many geometric concepts to vector spaces: angle (orthogonal), projection, norm
 - $\langle \sin nt, \sin mt \rangle = 0$ within $[-\pi, \pi]$ $(m \neq n) \Rightarrow$ they are 正交的 orthogonal to each other.
- $C = A^T B$: $C_{ij} = \langle A_i, B_j \rangle$
 - Special case: $A^{T}A$.

Eigenvalues/vectors and Eigen Decomposition

特征值

特征分解

"Eigen" means "characteristic of" (German)

- A (right) eigenvector of a square matrix A is u such that $Au = \lambda u$.
- Not all matrices have eigenvalues. Here, we only consider "good" matrices. Not all eigenvalues need to be distinct.
- Traditionally, we normalize u (such that $u^{\top}u = 1$).
- We can use all eigenvectors of A to construct a matrix U (as columns). Then $AU = U\Lambda$, or equivalently, $A = U\Lambda U^{-1}$. This is the Eigen Decomposition.
 - We can interpret U as a transformation between two coordinate systems. Note that vectors in U are not necessarily orthogonal.
 - A as the scaling on each of the directions in the "new" coordinate system.

Similar Matrices

Similar Matrix

- Let A and B be two $n \times n$ matrix. A is similar to B (denoted as A \sim B) if there exists an invertible $n \times n$ matrix P such that $P^{-1}AP = B$.
- **Think:** What does this mean?
 - Think of P as a *change of basis* transformation.
 - Relationship with the Eigen decomposition.
- Similar matrices have the same value wrt many properties (e.g., rank, trace, eigenvalues, determinant, etc.)

SVD

Singular Vector Decomposition 奇异向量分解

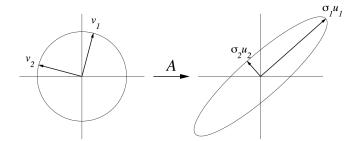
- Let M be $n \times d$ $(n \ge d)$.
- Reduced SVD: $M = \hat{U}\hat{\Sigma}V^{\top}$ exists for any M, such that
 - $\hat{\Sigma}$ is a diagonal matrix with diagonal elements σ_i (called singular values) in decreasing order
 - $\hat{\mathbb{U}}$ consists of an (incomplete) set of basis vectors \mathbf{u}_i (left singular vectors in \mathbb{R}^n) $(n \times d)$: original space as M)
 - \hat{V} consists of a set of basis vectors v_i (right singular vectors in \mathbb{R}^d) ($d \times d$: reduced space)
- Full SVD: $M = U\Sigma V^{\top}$:
 - Add the remaining (n-d) basis vectors to $\hat{\mathbb{U}}$ (thus becomes $n \times n$).
 - Add the n-d rows of 0 to $\hat{\Lambda}$ (thus becomes $n \times d$).



Geometric Illustration of SVD

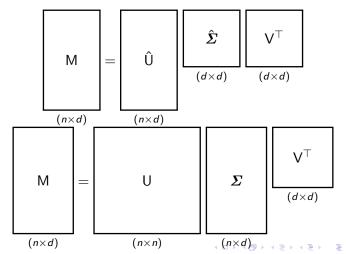
Geometric Meaning

• $Mv_i = \sigma_i u_i$



Graphical Illustration of SVD I

Figure: Reduced SVD vs Full SVD



Graphical Illustration of SVD II

Meaning:

- Columns of U are the basis of \mathbb{R}^n
- Rows of V^{\top} are the basis of \mathbb{R}^d

SVD Applications I

Relationship between Singular Values and Eigenvalues

- What are the eigenvalues of M^TM ?
- Hint: $M = U\Sigma V^{T}$ and U and V are unitary (i.e., rotations)

References and Further Reading I

- Gaussian Quadrature:
 https://www.youtube.com/watch?v=k-yUdqRXijo
- Linear Algebra Review and Reference.
 http://cs229.stanford.edu/section/cs229-linalg.pdf
- Scipy LA tutorial. https://docs.scipy.org/doc/scipy/reference/tutorial/linalg.html
- We Recommend a Singular Value Decomposition. http://www.ams.org/samplings/feature-column/fcarc-svd