Maths Preliminaries

Wei Wang @ CSE, UNSW

February 27, 2019

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} ?

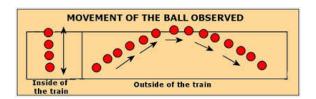
- Properties:
 - $f_a(n) = f_a(n-1) * a$, for $n \ge 1$; $f_a(0) = 1$.
 - f(u) * f(v) = f(u + v).
 - $f(x) = y \Leftrightarrow \ln(y) = x \ln(a) \Leftrightarrow f(x) = \exp\{x \ln a\}.$
 - $e^{ix} = cos(x) + i \cdot sin(x)$.
- The trick:
- Same in Linear algebra



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 (\cdot); its identity is 1.
- constraints:
 - Closed for both operations
 - Some nice properties of these operations:
 - Communicative: $\mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}$.
 - Associative: $(\mathbf{a} + \mathbf{b}) + \mathbf{c} = \mathbf{a} + (\mathbf{b} + \mathbf{c})$.
 - Distributive: $\lambda(\mathbf{a} + \mathbf{b}) = \lambda \mathbf{a} + \lambda \mathbf{b}$.

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}).

Why these constraints are natural and useful?

Basic Concepts III

Representation matters?

Consider even geometric vectors: $\mathbf{c} = \mathbf{a} + \mathbf{b}$

What if we represent vectors by a column of their coordinates?

What if by their polar coordinates? 极坐标

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

3*4的矩阵为三行四列,

列向量就是一个colum 行向量就是一个row 列向量的转置矩阵为行向量 行向量的转置矩阵为列向量

Vector

- A *n*-dimensional vector, \mathbf{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: \mathbf{v}^{\top} .

Operations

- Addition: $\mathbf{v}_1 + \mathbf{v}_2 =$
- (Scalar) Multiplication: $\lambda \mathbf{v}_1 =$
- n linear algebra, a column vector or column matrix is an m × 1 matrix, that is, a matrix consisting of a single column of m elements.

Linearity I

单变量 Linear Combination: Generalization of Univariate Linear Functions

• Let $\lambda_i \in \mathbb{R}$, given a set of k vectors \mathbf{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

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

- 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 $\begin{bmatrix} 4 \\ 6 \end{bmatrix}$

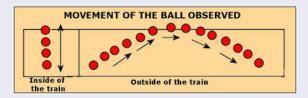
Linearity III

Exercises

- What are the (natural) basis of all (univariate) Polynomials of degrees up to d?
- Decompose $3x^2 + 4x 8$ 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? 类推



Matrix I

Linear Transformation 线件转换

• 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:
 - $(f_1 + f_2)(x) = f_1(x) + f_2(x)$
 - $(\lambda f)(x) = \lambda \cdot f(x)$
 - 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
 - $f(\mathbf{x}) = \mathbf{y} \implies \mathbf{M} \mathbf{x} = \mathbf{y}$, where matrix-vector multiplication is defined as: $y_i = \sum_k M_{ik} \cdot x_k$
 - MoutDimxinDim
 - 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:

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

矩阵乘法

$$\mathbf{y} = x_1 \mathbf{M}_{\bullet 1} + \ldots + x_n \mathbf{M}_{\bullet n}$$

• 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

矩阵乘法

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

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

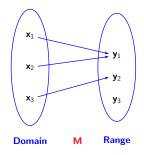
矩阵乘法

$$y_{1} = M_{11}x_{1} + M_{12}x_{2} y_{2} = M_{21}x_{1} + M_{22}x_{2} y_{3} = M_{31}x_{1} + M_{32}x_{2} \implies \begin{bmatrix} y_{1} \\ y_{2} \\ y_{3} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \\ M_{31} & M_{32} \end{bmatrix} \begin{bmatrix} x_{1} \\ x_{2} \end{bmatrix} \mathbf{y} = \mathbf{M}\mathbf{x}$$

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



System of Linear Equations II



The above transformation is injective, but not surjective.

单射

满射

A Matrix Also Specifies a (Generalized) Coordinate System

Yet another interpretation

- $y = Mx \implies ly = Mx$.
- with respect to 关于 坐标系

 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**?

A Matrix Also Specifies a (Generalized) Coordinate System II

Example for polynomials

for 1
for
$$x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
 \Longrightarrow M: for $x = \begin{bmatrix} 3 & -1 & -4 \\ 0 & 1 & 5 \\ 0 & 0 & 2 \end{bmatrix}$
Let $\mathbf{x} = \begin{bmatrix} 1 \\ -2 \\ 3 \end{bmatrix}$ \Longrightarrow M $\mathbf{x} = \mathbf{I} \begin{bmatrix} -7 \\ 13 \\ 6 \end{bmatrix}$

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: $\langle \mathbf{x}, \mathbf{y} \rangle$.
 - In \mathbb{R}^n , usually called dot product: $\mathbf{x} \cdot \mathbf{y} \stackrel{\text{def}}{=} \mathbf{x}^\top \mathbf{y} = \sum_i x_i y_i$.
 - 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: $\langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{y}, \mathbf{x} \rangle$
 - linearity in the first argument: $\langle a\mathbf{x} + \mathbf{y}, \mathbf{z} \rangle = a \langle \mathbf{x}, \mathbf{z} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle$
 - positive definitiveness: $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$; $\langle \mathbf{x}, \mathbf{x} \rangle \Leftrightarrow \mathbf{x} = \mathbf{0}$;
- 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 orthogonal to each other.
- $\mathbf{C} = \mathbf{A}^{\top} \mathbf{B}$: $C_{ij} = \langle A_i, B_i \rangle$
 - Special case: $\mathbf{A}^{\top}\mathbf{A}$.



Eigenvalues/vectors and Eigen Decomposition

"Eigen" means "characteristic of" (German)

- A (right) eigenvector of a square matrix **A** is **u** such that $\mathbf{A}\mathbf{u} = \lambda \mathbf{u}$.
- Not all matrices have eigenvalues. Here, we only consider "good" matrices. Not all eigenvalues need to be distinct.
- Traditionally, we normalize \mathbf{u} (such that $\mathbf{u}^{\top}\mathbf{u} = 1$).
- We can use all eigenvectors of **A** to construct a matrix **U** (as columns). Then $\mathbf{A}\mathbf{U} = \mathbf{U}\boldsymbol{\Lambda}$, or equivalently, $\mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{-1}$. 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 $\mathbf{A} \sim \mathbf{B}$) if there exists an invertible $n \times n$ matrix **P** such that $\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{B}$.
- **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.)

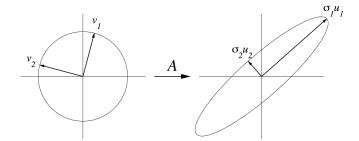
Singular Vector Decomposition

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

Geometric Illustration of SVD

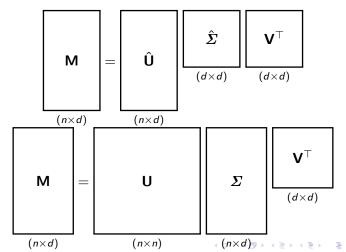
Geometric Meaning

• $\mathbf{M} \mathbf{v}_i = \sigma_i \mathbf{u}_i$



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 \mathbf{V}^{\top} are the basis of \mathbb{R}^d

SVD Applications I

Relationship between Singular Values and Eigenvalues

- What are the eigenvalues of M[⊤]M?
- Hint: $\mathbf{M} = \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^{\top}$ and \mathbf{U} and \mathbf{V} are unitary (i.e., rotations)

Related to PCA (Principle Component Analysis)

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