UVA CS 6316 – Fall 2015 Graduate: Machine Learning

Lecture 2: Algebra and Calculus Review

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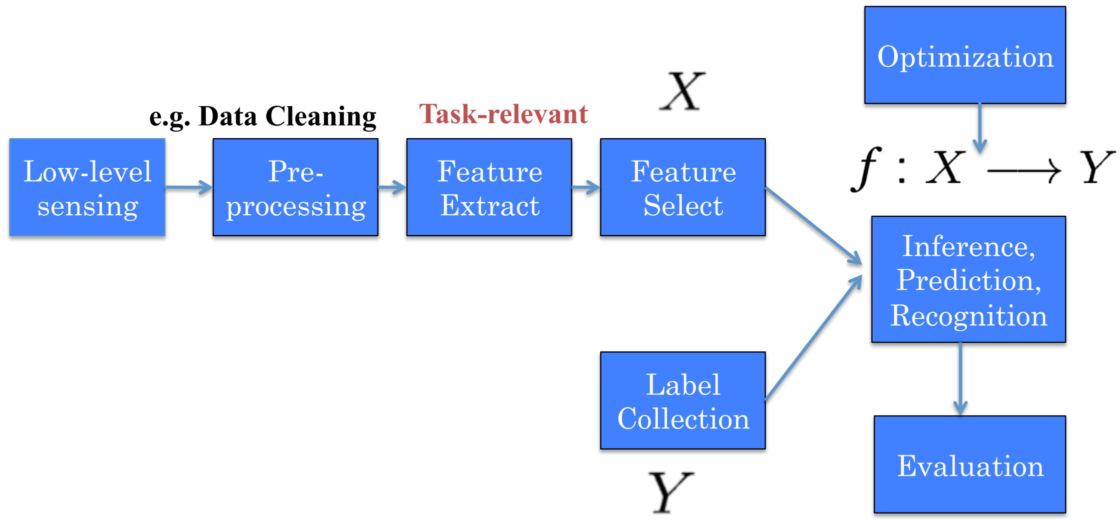
Today:

- ❑ Data Representation
- ❑ Review of Linear Algebra and Matrix Calculus

A Typical Machine Learning Pipeline



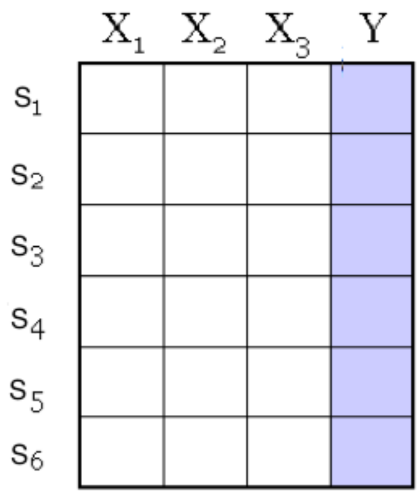
e.g. SUPERVISED LEARNING

$$f : X \longrightarrow Y$$

- Find function to map input space X to output space Y

- Generalisation: learn function / hypothesis from past data in order to "explain", "predict", "model" or "control" new data examples

KEY

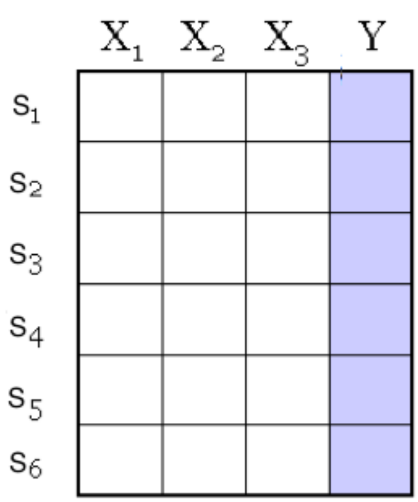


A Dataset

$$f : \boxed{X} \longrightarrow \boxed{Y}$$

- **Data**/*points/instances/examples/samples/records*: [rows]
- **Features**/*attributes/dimensions/independent variables/covariates/ predictors/regressors*: [columns, except the last]
- **Target**/*outcome/response/label/dependent variable*: special column to be predicted [last column]

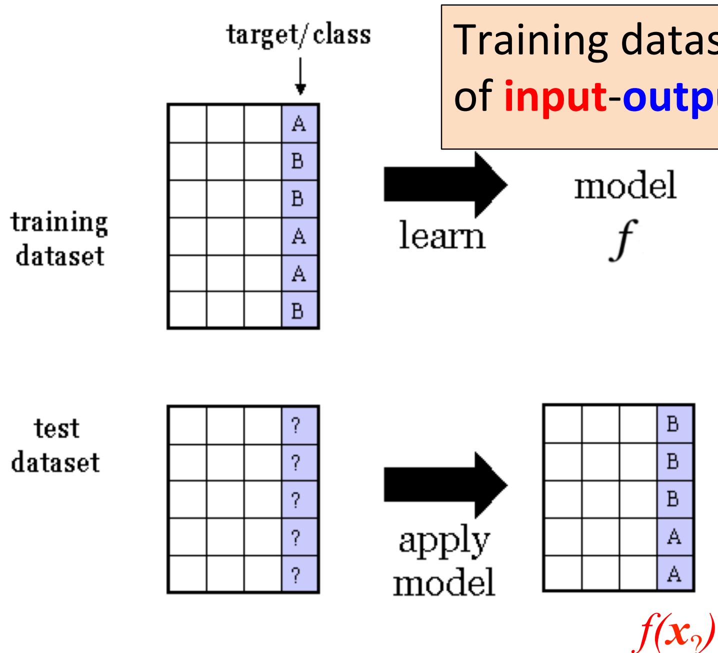
Main Types of Columns



- *Continuous*: a real number, for example, age or height
- *Discrete*: a symbol, like "Good" or "Bad"

e.g. SUPERVISED Classification

Training dataset consists of **input**-**output** pairs



- e.g. Here, target Y is a discrete target variable

Today:

- ❑ **Data Representation**
- ❑ **Review of Linear Algebra and Matrix Calculus**

DEFINITIONS - SCALAR

- a scalar is a number
  - (denoted with regular type: 1 or 22)

DEFINITIONS - VECTOR

- Vector: a single row or column of numbers
  - denoted with **bold small letters**
  - row vector

$$\mathbf{a} = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \end{bmatrix}$$

  - column vector (default)

$$\mathbf{b} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

DEFINITIONS - VECTOR

- Vector in R^n is an ordered set of n real numbers.
  - e.g. $\mathbf{v} = (1,6,3,4)$ is in R^4
  - A column vector: $\begin{pmatrix} 1 \\ 6 \\ 3 \\ 4 \end{pmatrix}$
  - A row vector: $\begin{pmatrix} 1 & 6 & 3 & 4 \end{pmatrix}$

DEFINITIONS - MATRIX

◆ A matrix is an array of numbers

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix}$$

◆ Denoted with a **bold Capital letter**

◆ All matrices have an order (or dimension): that is, the number of rows × the number of columns. So, **A** is 2 by 3 or (2 × 3).

◆ A square matrix is a matrix that has the same number of rows and columns (n × n)

DEFINITIONS - MATRIX

- m-by-n matrix in $R^{m \times n}$ with m rows and n columns, each entry filled with a (typically) real number:

- e.g. 3*3 matrix $\begin{pmatrix} 1 & 2 & 8 \\ 4 & 78 & 6 \\ 9 & 3 & 2 \end{pmatrix}$

Special matrices

$\begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}$ diagonal

$\begin{pmatrix} a & b & c \\ 0 & d & e \\ 0 & 0 & f \end{pmatrix}$ upper-triangular

$\begin{pmatrix} a & b & 0 & 0 \\ c & d & e & 0 \\ 0 & f & g & h \\ 0 & 0 & i & j \end{pmatrix}$ tri-diagonal

$\begin{pmatrix} a & 0 & 0 \\ b & c & 0 \\ d & e & f \end{pmatrix}$ lower-triangular

$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ I (identity matrix)

Special matrices:
Symmetric Matrices

$$A = A^T \quad (a_{ij} = a_{ji})$$

e.g.:
$$\begin{bmatrix} 4 & 5 & -3 \\ 5 & 7 & 2 \\ -3 & 2 & 10 \end{bmatrix}$$

$$\begin{pmatrix} -1 & 2 \end{pmatrix} \begin{pmatrix} 2 \\ 2 \end{pmatrix} = \textbf{?}$$

$$A = \begin{pmatrix} 0 & 1 \\ 1 & -1 \\ 1 & 0 \end{pmatrix} \qquad A^T = \textbf{?}$$

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \text{ and } \mathbf{B} = \begin{bmatrix} 7 & 10 \\ 8 & 11 \\ 9 & 12 \end{bmatrix}$$

C = A – B = ?

C = A + B = ?

$$\left(\begin{pmatrix} 1 & 2 \\ -1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix} \right)^T = \textbf{?}$$

$$\mathbf{A} = \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \text{ and } \mathbf{B} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$$

C = A B = ?

C = B A = ?

$$\left\| \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right\|_2 = \textbf{?}$$

Minimum requirement test

Review of MATRIX OPERATIONS

1) Transposition
2) Addition and Subtraction
3) Multiplication
4) Norm (of vector)
5) Matrix Inversion
6) Matrix Rank
7) Matrix calculus

(1) Transpose

Transpose: You can think of it as
- "flipping" the rows and columns

e.g. $\begin{pmatrix} a \\ b \end{pmatrix}^T = \begin{pmatrix} a & b \end{pmatrix}$

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$$

- $(A^T)^T = A$
- $(AB)^T = B^T A^T$
- $(A+B)^T = A^T + B^T$

(2) Matrix Addition/Subtraction

- Matrix addition/subtraction
  - Matrices must be of same size.

(2) Matrix Addition/Subtraction An Example

- If we have

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 7 & 10 \\ 8 & 11 \\ 9 & 12 \end{bmatrix}$$

then we can calculate **C** = **A** + **B** by

$$\mathbf{C} = \mathbf{A} + \mathbf{B} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} + \begin{bmatrix} 7 & 10 \\ 8 & 11 \\ 9 & 12 \end{bmatrix} = \begin{bmatrix} 8 & 12 \\ 11 & 15 \\ 14 & 18 \end{bmatrix}$$

(2) Matrix Addition/Subtraction
An Example

- Similarly, if we have

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} 7 & 10 \\ 8 & 11 \\ 9 & 12 \end{bmatrix}$$

then we can calculate **C** = **A** - **B** by

$$\mathbf{C} = \mathbf{A} - \mathbf{B} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} - \begin{bmatrix} 7 & 10 \\ 8 & 11 \\ 9 & 12 \end{bmatrix} = \begin{bmatrix} -6 & -8 \\ -5 & -7 \\ -4 & -6 \end{bmatrix}$$

OPERATION on MATRIX

1) Transposition
2) Addition and Subtraction
3) Multiplication
4) Norm (of vector)
5) Matrix Inversion
6) Matrix Rank
7) Matrix calculus

(3) Products of Matrices

- We write the multiplication of two matrices **A** and **B** as **AB**
- This is referred to either as
  - pre-multiplying **B** by **A**

    or
  - post-multiplying **A** by **B**
- So for matrix multiplication **AB**, **A** is referred to as the *premultiplier* and **B** is referred to as the *postmultiplier*

(3) Products of Matrices

$$\underset{m \times n}{\begin{bmatrix} a_{11} & a_{12} & . & a_{1n} \\ a_{21} & a_{22} & . & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{m1} & a_{m2} & . & a_{mn} \end{bmatrix}} \underset{q \times p}{\begin{bmatrix} b_{11} & b_{12} & . & b_{1p} \\ b_{21} & b_{22} & . & b_{2p} \\ \cdots & \cdots & \cdots & \cdots \\ b_{q1} & b_{q2} & . & b_{qp} \end{bmatrix}} = \underset{m \times p}{\begin{bmatrix} c_{11} & c_{12} & . & c_{1p} \\ c_{21} & c_{22} & . & c_{2p} \\ \cdots & \cdots & c_{ij} & \cdots \\ c_{m1} & c_{m2} & . & c_{mp} \end{bmatrix}}$$

Condition: n = q

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \qquad AB \neq BA$$

(3) Products of Matrices

- In order to multiply matrices, they must be conformable (the number of columns in the premultiplier must equal the number of rows in postmultiplier)

- Note that
  - an (m x n) x (n x p) = (m x p)
  - an (m x n) x (p x n) = cannot be done
  - a (1 x n) x (n x 1) = a scalar (1 x 1)

Products of Matrices

- If we have $A_{(3x3)}$ and $B_{(3x2)}$ then

$$\mathbf{AB} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} x \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \\ c_{31} & c_{32} \end{bmatrix} = \mathbf{C}$$

where

$$\begin{aligned}
c_{11} &= a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} \\
c_{12} &= a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} \\
c_{21} &= a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} \\
c_{22} &= a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} \\
c_{31} &= a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31} \\
c_{32} &= a_{31}b_{12} + a_{32}b_{22} + a_{33}b_{32}
\end{aligned}$$

test

Matrix Multiplication An Example

- If we have $\mathbf{A} = \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix}$ and $\mathbf{B} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix}$

  then $\mathbf{AB} = \begin{bmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{bmatrix} \mathrm{x} \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \\ c_{31} & c_{32} \end{bmatrix} = \begin{bmatrix} 30 & 66 \\ 36 & 81 \\ 42 & 96 \end{bmatrix}$

  where
$$
\begin{aligned}
c_{11} &= a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} = 1(1) + 4(2) + 7(3) = 30 \\
c_{12} &= a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32} = 1(4) + 4(5) + 7(6) = 66 \\
c_{21} &= a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} = 2(1) + 5(2) + 8(3) = 36 \\
c_{22} &= a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32} = 2(4) + 5(5) + 8(6) = 81 \\
c_{31} &= a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31} = 3(1) + 6(2) + 9(3) = 42 \\
c_{32} &= a_{31}b_{12} + a_{32}b_{22} + a_{33}b_{32} = 3(4) + 6(5) + 9(6) = 96
\end{aligned}
$$

Some Properties of Matrix Multiplication

- Note that
  - Even if conformable, **AB** does not necessarily equal **BA** (i.e., matrix multiplication is *not commutative*)
  - Matrix multiplication can be extended beyond two matrices
  - matrix multiplication is *associative*, i.e., **A**(**BC**) = (**AB**)**C**

Some Properties of Matrix Multiplication

- Multiplication and transposition

  $(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$

- Multiplication with Identity Matrix

$$AI = IA = A, \text{ where } I = \begin{bmatrix} 1 & 0 & . & 0 \\ 0 & 1 & . & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & . & 1 \end{bmatrix}$$

Special Uses for Matrix Multiplication

- Products of Scalars & Matrices → Example, If we have

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \quad \text{and} \quad b = 3.5$$

then we can calculate b**A** by

$$\mathbf{bA} = 3.5\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} = \begin{bmatrix} 3.5 & 7.0 \\ 10.5 & 14.0 \\ 17.5 & 21.0 \end{bmatrix}$$

- Note that b**A** = **A**b if b is a scalar

Special Uses for Matrix Multiplication

- Dot (or Inner) Product of two Vectors
  - Premultiplication of a column vector **a** by conformable row vector **b** yields a single value called the *dot product* or *inner product* - If

$$\mathbf{a}^{\mathbf{T}} = \begin{bmatrix} 3 & 4 & 6 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix}$$

then **their inner product** gives us

$$\mathbf{a}^{\mathbf{T}}\mathbf{b} = \mathbf{a} \bullet \mathbf{b} = \begin{bmatrix} 3 & 4 & 6 \end{bmatrix} \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix} = 3(5) + 4(2) + 6(8) = 71 = \mathbf{b}^{\mathbf{T}}\mathbf{a}$$

which is the sum of products of elements in similar positions for the two vectors

Special Uses for Matrix Multiplication

- Outer Product of two Vectors
  - Postmultiplication of a column vector **a** by conformable row vector **b** yields a matrix containing the products of each pair of elements from the two matrices (called the *outer product*) - If

$$\mathbf{a}^{\mathbf{T}} = \begin{bmatrix} 3 & 4 & 6 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix}$$

then $\mathbf{ab}^{\mathbf{T}}$ gives us

$$\mathbf{ab}^{\mathbf{T}} = \begin{bmatrix} 3 \\ 4 \\ 6 \end{bmatrix} \begin{bmatrix} 5 & 2 & 8 \end{bmatrix} = \begin{bmatrix} 15 & 6 & 24 \\ 20 & 8 & 32 \\ 30 & 12 & 48 \end{bmatrix}$$

Special Uses for Matrix Multiplication

- Outer Product of two Vectors, e.g. a special case :

As an example of how the outer product can be useful, let $\mathbf{1} \in \mathbb{R}^n$ denote an n-dimensional vector whose entries are all equal to 1. Furthermore, consider the matrix $A \in \mathbb{R}^{m \times n}$ whose columns are all equal to some vector $x \in \mathbb{R}^m$. Using outer products, we can represent A compactly as,

$$A = \begin{bmatrix} | & | & & | \\ x & x & \cdots & x \\ | & | & & | \end{bmatrix} = \begin{bmatrix} x_1 & x_1 & \cdots & x_1 \\ x_2 & x_2 & \cdots & x_2 \\ \vdots & \vdots & \ddots & \vdots \\ x_m & x_m & \cdots & x_m \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \begin{bmatrix} 1 & 1 & \cdots & 1 \end{bmatrix} = x\mathbf{1}^T.$$

Special Uses for Matrix Multiplication

- Sum the Squared Elements of a Vector
  - Premultiply a column vector **a** by its transpose
    – If

$$\mathbf{a} = \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix}$$

then premultiplication by a row vector **a**^{T}

$$a^T = \begin{bmatrix} 5 & 2 & 8 \end{bmatrix}$$

will yield the sum of the squared values of elements for **a**, i.e.

$$a^T\mathbf{a} = \begin{bmatrix} 5 & 2 & 8 \end{bmatrix} \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix} = 5^2 + 2^2 + 8^2 = 93$$

Special Uses for Matrix Multiplication

- Matrix-Vector Products (I)

Given a matrix $A \in \mathbb{R}^{m\times n}$ and a vector $x \in \mathbb{R}^n$, their product is a vector $y = Ax \in \mathbb{R}^m$.

If we write A by rows, then we can express Ax as,

$$y = Ax = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix} x = \begin{bmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_m^T x \end{bmatrix}.$$

Special Uses for Matrix Multiplication

- Matrix-Vector Products (II)

Alternatively, let's write A in column form. In this case we see that,

$$y = Ax = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_1 \end{bmatrix} x_1 + \begin{bmatrix} a_2 \end{bmatrix} x_2 + \ldots + \begin{bmatrix} a_n \end{bmatrix} x_n \ .$$

In other words, y is a ***linear combination*** of the *columns* of A, where the coefficients of the linear combination are given by the entries of x.

Special Uses for Matrix Multiplication

- Matrix-Vector Products (III)

to multiply on the left by a row vector. This is written, $y^T = x^T A$ for $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^m$, and $y \in \mathbb{R}^n$.

$$y^T = x^T A = x^T \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} x^T a_1 & x^T a_2 & \cdots & x^T a_n \end{bmatrix}$$

which demonstrates that the ith entry of y^T is equal to the inner product of x and the ith *column* of A.

Special Uses for Matrix Multiplication

- Matrix-Vector Products (IV)

$$\begin{aligned} y^T &= x^T A \\ &= \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix} \\ &= x_1 \begin{bmatrix} — & a_1^T & — \end{bmatrix} + x_2 \begin{bmatrix} — & a_2^T & — \end{bmatrix} + \ldots + x_n \begin{bmatrix} — & a_n^T & — \end{bmatrix} \end{aligned}$$

so we see that y^T is a linear combination of the *rows* of A, where the coefficients for the linear combination are given by the entries of x.

MATRIX OPERATIONS

1) Transposition
2) Addition and Subtraction
3) Multiplication
4) Norm (of vector)
5) Matrix Inversion
6) Matrix Rank
7) Matrix calculus

(4) Vector norms

A norm of a vector ||x|| is informally a measure of the "length" of the vector.

$$\|x\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

- Common norms: L_1, L_2 (Euclidean)

$$\|x\|_1 = \sum_{i=1}^{n} |x_i| \qquad \|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$$

- $L_{infinity}$

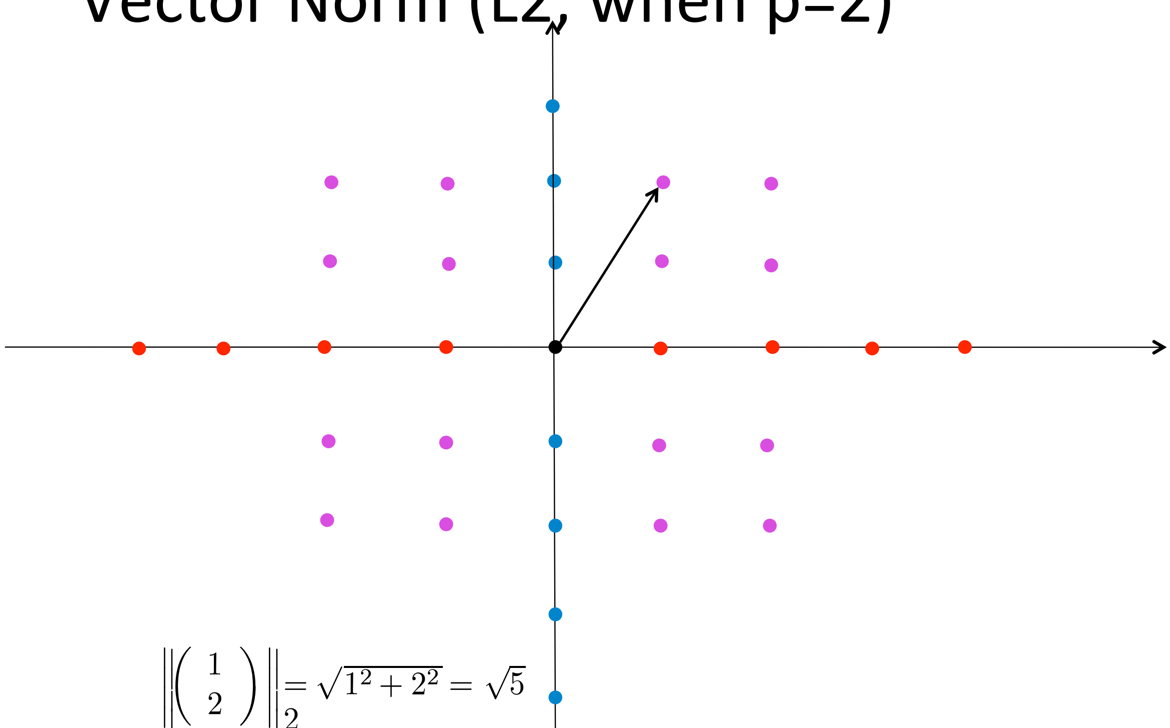
$$\|x\|_\infty = \max_i |x_i|$$

More General : Norm

- A norm is any function g() that maps vectors to real numbers that satisfies the following conditions:

- **Non-negativity**: for all $\boldsymbol{x} \in \mathbb{R}^D$, $g(\boldsymbol{x}) \geq 0$
- **Strictly positive**: for all $\boldsymbol{x}$, $g(\boldsymbol{x}) = 0$ implies that $\boldsymbol{x} = \boldsymbol{0}$
- **Homogeneity**: for all $\boldsymbol{x}$ and a, $g(a\boldsymbol{x}) = |a|\, g(\boldsymbol{x})$, where $|a|$ is the absolute value.
- **Triangle inequality**: for all $\boldsymbol{x}, \boldsymbol{y}$, $g(\boldsymbol{x} + \boldsymbol{y}) \leq g(\boldsymbol{x}) + g(\boldsymbol{y})$

Vector Norm (L2, when p=2)



$$\left\| \begin{pmatrix} 1 \\ 2 \end{pmatrix} \right\|_2 = \sqrt{1^2 + 2^2} = \sqrt{5}$$

Orthogonal & Orthonormal

Inner Product defined between column vector **x** and **y** , as

➔ x•y= $x^T y \in \mathbb{R} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ x_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^{n} x_i y_i.$

If u•v=0, $||u||_2$!= 0, $||v||_2$!= 0

→ *u and v are orthogonal*

If u•v=0, $||u||_2 = 1$, $||v||_2 = 1$

→ *u and v are orthonormal*

Orthogonal matrices

- Notation:

$$A = \begin{bmatrix} a_{11} & a_{12} & . & a_{1n} \\ a_{21} & a_{22} & . & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{m1} & a_{m2} & . & a_{mn} \end{bmatrix}, \quad \begin{matrix} u_1^T = [a_{11}\ a_{12} \cdots a_{1n}] \\ u_2^T = [a_{21}\ a_{22} \cdots a_{2n}] \\ \cdots \\ u_m^T = [a_{m1}\ a_{m2} \cdots a_{mn}] \end{matrix} \quad A = \begin{bmatrix} u_1^T \\ u_2^T \\ \cdots \\ u_m^T \end{bmatrix}$$

- A is orthogonal if:

$$u_j . u_k = 0, \text{ for every } j \neq k \ (u_j \text{ is perpendicular to } u_k)$$

Example: $\begin{bmatrix} cos(\theta) & -sin(\theta) \\ sin(\theta) & cos(\theta) \end{bmatrix}$

Orthonormal matrices

- A is orthonormal if:

(1) $u_k . u_k = 1$ or $||u_k|| = 1$, for every k

(2) $u_j . u_k = 0$, for every $j \neq k$ (u_j is perpendicular to u_k)

- Note that if A is orthonormal, it easy to find its inverse:

$$AA^T = A^T A = I \qquad (\text{i.e., } A^{-1} = A^T)$$

Property: $||Av|| = ||v||$ (does not change the magnitude of v)

MATRIX OPERATIONS

1) Transposition
2) Addition and Subtraction
3) Multiplication
4) Norm (of vector)
5) Matrix Inversion
6) Matrix Rank
7) Matrix calculus

(5) Inverse of a Matrix

- The inverse of a matrix **A** is commonly denoted by $\mathbf{A}^{-1}$ or inv **A**.
- The inverse of an *n x n* matrix **A** is the matrix $\mathbf{A}^{-1}$ such that $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I} = \mathbf{A}^{-1}\mathbf{A}$
- The matrix inverse is analogous to a scalar reciprocal
- A matrix which has an inverse is called *nonsingular*

(5) Inverse of a Matrix

- For some *n x n* matrix **A** , an inverse matrix $\mathbf{A}^{-1}$ *may not exist*.
- A matrix which does not have an inverse is singular.
- An inverse of *n x n* matrix **A** exists iff $|\mathbf{A}| \neq 0$

THE DETERMINANT OF A MATRIX

- The determinant of a matrix A is denoted by $|\mathbf{A}|$ (or det(**A**)).
- Determinants exist only for square matrices.
- E.g. If A = $\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$

$$|A| = a_{11}a_{22} - a_{12}a_{21}$$

THE DETERMINANT OF A MATRIX

2 x 2

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \quad det(A) = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{21}a_{12}$$

3 x 3

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{21} \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix} + a_{31} \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix}$$

n x n

$$det(A) = \sum_{j=1}^{m} (-1)^{j+k} a_{jk} det(A_{jk}), \text{ for any } k\text{: } 1 \le k \le m$$

THE DETERMINANT OF A MATRIX

$$det(AB) = det(A)det(B)$$

$$det(A+B) \neq det(A) + det(B)$$

diagonal matrix: If $A = \begin{bmatrix} a_{11} & 0 & . & 0 \\ 0 & a_{22} & . & 0 \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ 0 & 0 & . & a_{nn} \end{bmatrix}$, then $det(A) = \prod_{i=1}^{n} a_{ii}$

HOW TO FIND INVERSE MATRIXES? An example,

- If
- $\boldsymbol{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ and $|\mathbf{A}| \neq 0$

$$\boldsymbol{A}^{-1} = \frac{1}{\det(\boldsymbol{A})} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

Matrix Inverse

- The inverse A^{-1} of a matrix A has the property:

  $$\boldsymbol{AA^{-1}=A^{-1}A=I}$$

- A^{-1} exists only if $det(A) \neq 0$

- Terminology
  - **Singular matrix:** A^{-1} does not exist
  - **Ill-conditioned matrix:** A is close to being singular

PROPERTIES OF INVERSE MATRICES

- $$(\boldsymbol{AB})^{-1} = \boldsymbol{B}^{-1}\boldsymbol{A}^{-1}$$
- $$\left(\boldsymbol{A}^{T}\right)^{-1} = \left(\boldsymbol{A}^{-1}\right)^{T}$$
- $$\left(\boldsymbol{A}^{-1}\right)^{-1} = \boldsymbol{A}$$

Inverse of special matrix

- For diagonal matrices $\mathbf{D}^{-1} = \mathrm{diag}\{d_1^{-1}, \ldots, d_n^{-1}\}$

- For orthonormal matrices $\mathbf{A}^{-1} = \mathbf{A}^{\mathsf{T}}$
  - a square matrix with real entries whose columns and rows are orthogonal unit vectors (i.e., orthonormal vectors)

Pseudo-inverse

- The pseudo-inverse A^+ of a matrix A (could be non-square, e.g., m x n) is given by:

$$A^+ = (A^T A)^{-1} A^T$$

- It can be shown that:

$$A^+ A = I \quad \text{(provided that } (A^T A)^{-1} \text{ exists)}$$

MATRIX OPERATIONS

1) Transposition
2) Addition and Subtraction
3) Multiplication
4) Norm (of vector)
5) Matrix Inversion
6) Matrix Rank
7) Matrix calculus

(6) Rank: Linear independence

- A set of vectors is linearly independent if none of them can be written as a linear combination of the others.

$$x_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \quad x_2 = \begin{bmatrix} 4 \\ 1 \\ 5 \end{bmatrix} \quad x_3 = \begin{bmatrix} 2 \\ -3 \\ -1 \end{bmatrix}$$

x3 = −2x1 + x2

→ NOT linearly independent

(6) Rank: Linear independence

- **<u>Alternative definition:</u>** Vectors $v_1,\ldots,v_k$ are linearly independent if $c_1v_1+\ldots+c_kv_k = 0$ implies $c_1=\ldots=c_k=0$

$$\begin{pmatrix} | & | & | \\ v_1 & v_2 & v_3 \\ | & | & | \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

e.g.

$$\begin{pmatrix} 1 & 0 \\ 2 & 3 \\ 1 & 3 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

(u,v)=(0,0), i.e. the columns are linearly independent.

(6) Rank of a Matrix

- rank(A) (the rank of a m-by-n matrix A) is
  = The maximal number of linearly independent columns
  =The maximal number of linearly independent rows

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 2 & 1 \\ 4 & 2 \end{pmatrix}$$

Rank=? **Rank=?**

- If A is n by m, then
  - rank(A)<= min(m,n)
  - If n=rank(A), then A has full row rank
  - If m=rank(A), then A has full column rank

(6) Rank of a Matrix

- Equal to the dimension of the largest square sub-matrix of A that has a non-zero determinant

Example: $\begin{bmatrix} 4 & 5 & 2 & 14 \\ 3 & 9 & 6 & 21 \\ 8 & 10 & 7 & 28 \\ 1 & 2 & 9 & 5 \end{bmatrix}$ has rank 3

$$det(A) = 0, \text{ but } det(\begin{bmatrix} 4 & 5 & 2 \\ 3 & 9 & 6 \\ 8 & 10 & 7 \end{bmatrix}) = 63 \neq 0$$

(6) Rank and singular matrices

If A is nxn, $rank(A) = n$ iff A is nonsingular (i.e., invertible).

If A is nxn, $rank(A) = n$ iff $det(A) \neq 0$ (**full rank**).

If A is nxn, $rank(A) < n$ iff A is singular

MATRIX OPERATIONS

1) Transposition
2) Addition and Subtraction
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6) Matrix Rank
7) Matrix calculus

Review: Derivative of a Function

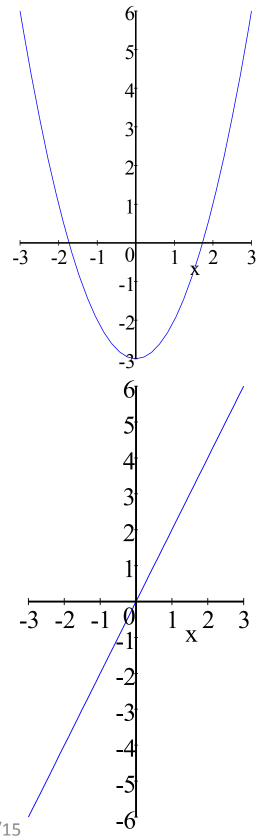
$$\lim_{h\to 0}\frac{f(a+h)-f(a)}{h}$$ is called the derivative of f at a.

We write: $$f'(x)=\lim_{h\to 0}\frac{f(x+h)-f(x)}{h}$$

"The derivative of f with respect to x is ..."

There are many ways to write the derivative of $y=f(x)$

➔ e.g. define the slope of the curve y=f(x) at the point x



Review: Derivative of a Quadratic Function

$$y = x^2 - 3$$

$$y' = \lim_{h \to 0} \frac{(x+h)^2 - 3 - (x^2 - 3)}{h}$$

$$y' = \lim_{h \to 0} \frac{\cancel{x^2} + 2x\cancel{h} + h^{\cancel{2}} - \cancel{x^2}}{\cancel{h}}$$

$$y' = \lim_{h \to 0} 2x + \underbrace{\cancel{h}}_{0}$$

$$y' = 2x$$

Some important rules for taking derivatives

- Scalar multiplication: $\partial_x[af(x)] = a[\partial_x f(x)]$
- Polynomials: $\partial_x[x^k] = kx^{k-1}$
- Function addition: $\partial_x[f(x) + g(x)] = [\partial_x f(x)] + [\partial_x g(x)]$
- Function multiplication: $\partial_x[f(x)g(x)] = f(x)[\partial_x g(x)] + [\partial_x f(x)]g(x)$
- Function division: $\partial_x \left[\frac{f(x)}{g(x)}\right] = \frac{[\partial_x f(x)]g(x) - f(x)[\partial_x g(x)]}{[g(x)]^2}$
- Function composition: $\partial_x[f(g(x))] = [\partial_x g(x)][\partial_x f](g(x))$
- Exponentiation: $\partial_x[e^x] = e^x$ and $\partial_x[a^x] = \log(a)e^x$
- Logarithms: $\partial_x[\log x] = \frac{1}{x}$

Review: Definitions of gradient (Matrix_calculus / Scalar-by-matrix)

Suppose that $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ is a function that takes as input a matrix A of size $m \times n$ and returns a real value. Then the ***gradient*** of f (with respect to $A \in \mathbb{R}^{m\times n}$) is the matrix of

➔ *Denominator layout*

$$\nabla_A f(A) \in \mathbb{R}^{m\times n} = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

In principle, gradients are a natural extension of partial derivatives to functions of multiple variables.

Review: Definitions of gradient (Matrix_calculus / Scalar-by-vector)

- Size of gradient is always the same as the size of

➔ *Denominator layout*

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix} \in \mathbb{R}^n \quad \text{if } x \in \mathbb{R}^n$$

For Examples

$$\boxed{\frac{\partial \mathbf{x}^T \mathbf{a}}{\partial \mathbf{x}} = \frac{\partial \mathbf{a}^T \mathbf{x}}{\partial \mathbf{x}} = \mathbf{a}}$$

$$\frac{\partial \mathbf{a}^T \mathbf{X} \mathbf{b}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{b}^T$$

$$\frac{\partial \mathbf{a}^T \mathbf{X}^T \mathbf{b}}{\partial \mathbf{X}} = \mathbf{b}\mathbf{a}^T$$

$$\frac{\partial \mathbf{a}^T \mathbf{X} \mathbf{a}}{\partial \mathbf{X}} = \frac{\partial \mathbf{a}^T \mathbf{X}^T \mathbf{a}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{a}^T$$

$$\frac{\partial \mathbf{x}^T \mathbf{B} \mathbf{x}}{\partial \mathbf{x}} = (\mathbf{B} + \mathbf{B}^T)\mathbf{x}$$

Exercise: a simple example

$$f(w) = w^T x = [w_1, w_2, w_3] \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = w_1 + 2w_2 + 3w_3$$

→ ***Denominator layout***

$$\frac{\partial f}{\partial w_1} = 1 \quad \frac{\partial f}{\partial w_2} = 2 \quad \frac{\partial f}{\partial w_3} = 3$$

$$\Rightarrow \quad \frac{\partial f}{\partial w} = \frac{\partial w^T x}{\partial w} = x = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

Even more general Matrix Calculus: Types of Matrix Derivatives

	Scalar	Vector	Matrix
Scalar	$\frac{\mathrm{d}y}{\mathrm{d}x}$	$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}x} = \left[\frac{\partial y_i}{\partial x}\right]$	$\frac{\mathrm{d}\mathbf{Y}}{\mathrm{d}x} = \left[\frac{\partial y_{ij}}{\partial x}\right]$
Vector	$\frac{\mathrm{d}y}{\mathrm{d}\mathbf{x}} = \left[\frac{\partial y}{\partial x_j}\right]$	$\frac{\mathrm{d}\mathbf{y}}{\mathrm{d}\mathbf{x}} = \left[\frac{\partial y_i}{\partial x_j}\right]$	
Matrix	$\frac{\mathrm{d}y}{\mathrm{d}\mathbf{X}} = \left[\frac{\partial y}{\partial x_{ji}}\right]$		

By Thomas Minka. Old and New Matrix Algebra Useful for Statistics

Review: Hessian Matrix / n==2 case

Singlevariate → multivariate

$$f(x,y)$$

- 1st derivative to gradient,

$$g = \nabla f = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{pmatrix}$$

- 2nd derivative to Hessian

$$H = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix}$$

Review: Hessian Matrix

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is a function that takes a vector in $\mathbb{R}^n$ and returns a real number. Then the ***Hessian*** matrix with respect to x, written $\nabla_x^2 f(x)$ or simply as H is the $n \times n$ matrix of partial derivatives,

$$\nabla_x^2 f(x) \in \mathbb{R}^{n\times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}.$$

Today Recap

- ❑ **Data Representation**
- ❑ **Linear Algebra and Matrix Calculus Review**

References

- http://www.cs.cmu.edu/~zkolter/course/linalg/index.html
- Prof. James J. Cochran's tutorial slides "Matrix Algebra Primer II"
- http://www.cs.cmu.edu/~aarti/Class/10701/recitation/LinearAlgebra_Matlab_Rev iew.ppt
- Prof. Alexander Gray's slides
- Prof. George Bebis' slides
- Prof. Hal Daum´e III' notes