UVA CS 4501: Machine Learning

Lecture 2: Algebra and Calculus Review

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$$\left(\begin{array}{cc} -1 & 2 \end{array}\right) \left(\begin{array}{c} 2 \\ 2 \end{array}\right) = ?$$

$$A=\left(egin{array}{cc} 0 & 1 \ 1 & -1 \ 1 & 0 \end{array}
ight) \quad A^T=$$
 ?

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

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

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

Minimum minimum requirement test

Today:

- Data Representation for ML systems
- □ Review of Linear Algebra and Matrix Calculus

e.g. SUPERVISED LEARNING

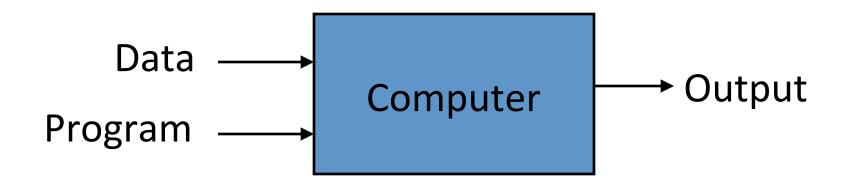
$$f:X\longrightarrow Y$$

 Find function to map input space X to output space Y

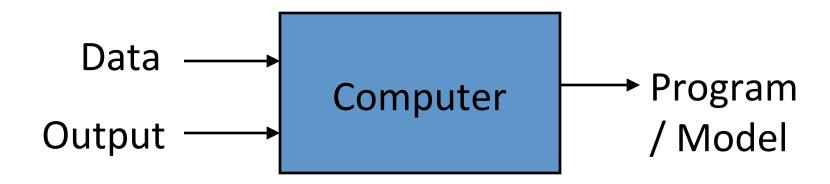
 Generalisation: learn function / hypothesis from past data in order to "explain", "predict", "model" or "control" new data examples



Traditional Programming

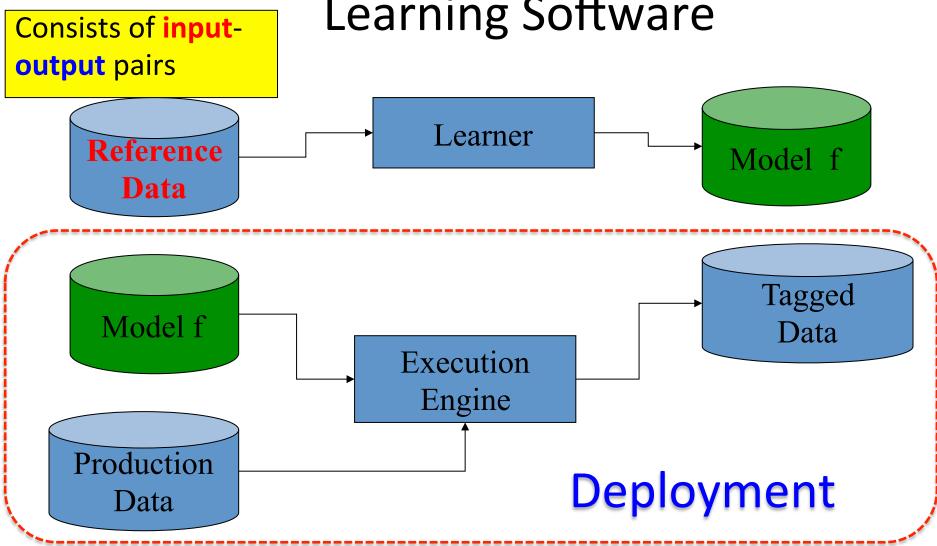


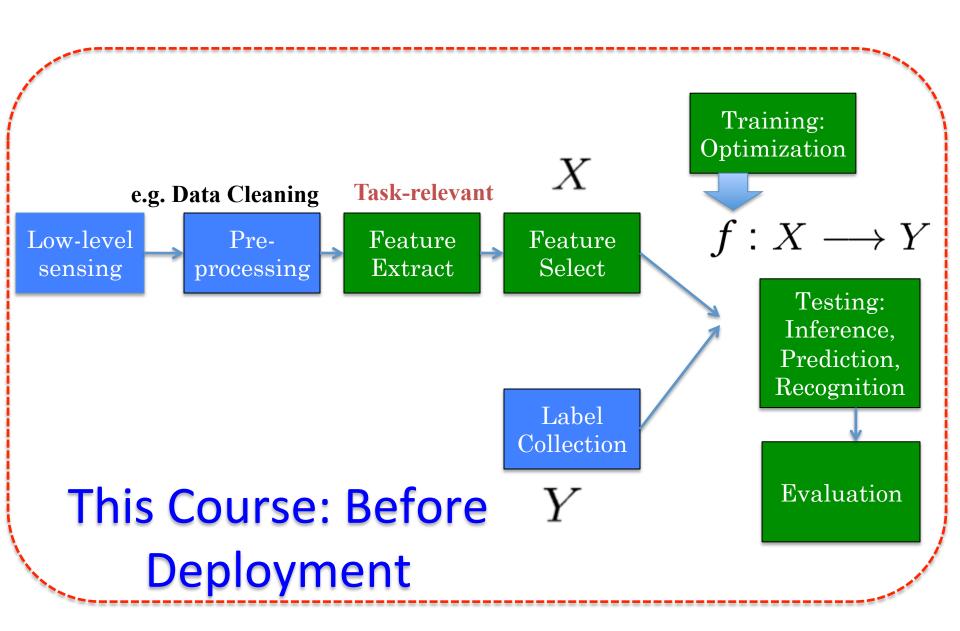
Machine Learning

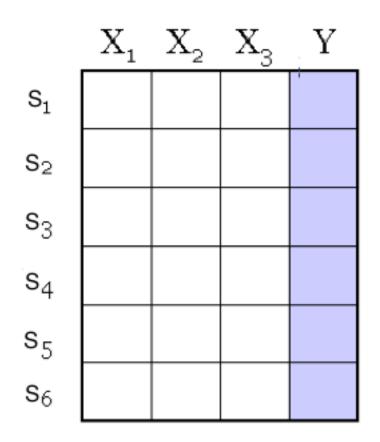


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An Operational Model of Machine Learning Software





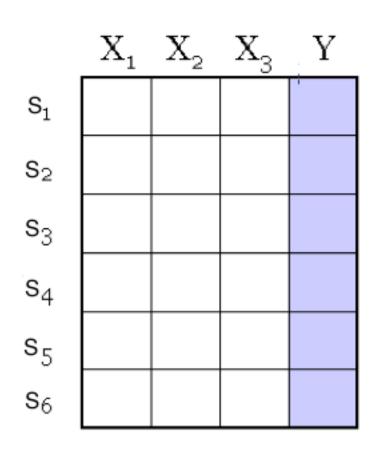


A Dataset

$$f:[X] \longrightarrow [Y]$$

- 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]

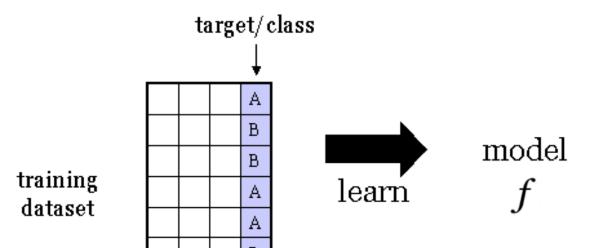
Main Types of Columns



 Continuous: a real number, for example, weight

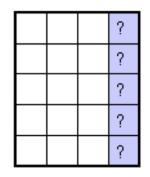
 Discrete: a symbol, like "Good" or "Bad"

e.g. SUPERVISED Classification

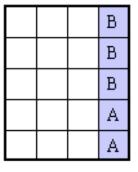


Training dataset consists of input-output pairs

test dataset





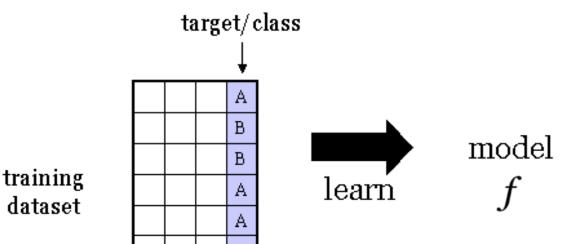


)

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

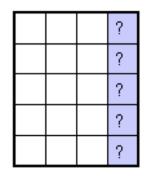
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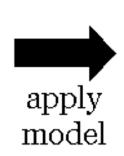
e.g. SUPERVISED Regression

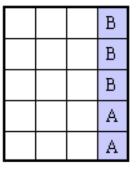


Training dataset consists of input-output pairs

test dataset



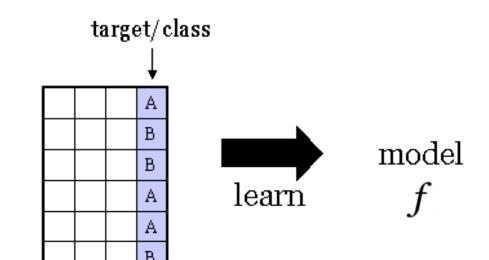






 e.g. Here, target Y is a continuous target variable

SUPERVISED LEARNING



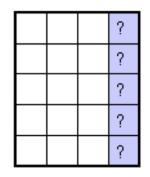
Training dataset consists of input-output pairs

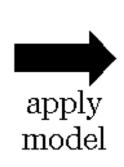
test dataset

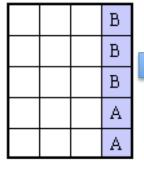
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training

dataset







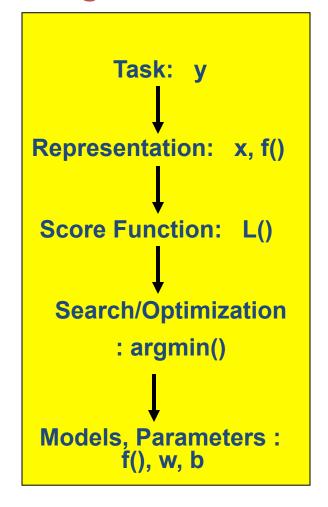
Evaluation

Measure Loss on pair \rightarrow Error $(f(x_2), y_2)$

 $f(\mathbf{x})$

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Machine Learning Variations in a Nutshell



ML grew out of work in Al

Optimize a performance criterion using example data or past experience,

Aiming to generalize to unseen data

Today:

- Data Representation for ML systems
- ☐ Review of Linear Algebra and Matrix Calculus

DEFINITIONS - SCALAR

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

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DEFINITIONS - VECTOR

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

$$a = [1 \ 2 \ 3 \ 4 \ 5]$$

- column vector (default)

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

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DEFINITIONS - VECTOR

Vector in real space Rⁿ is an ordered set of n real numbers.

$$- e.g. \mathbf{v} = (1,6,3,4)^{T} is in R^{4}$$

– A column vector:

 $-\mathbf{v}^{\mathsf{T}}$ as a row vector:

 $\begin{array}{c|c}
\bullet & 0 \\
3 & 4
\end{array}$

 $\begin{pmatrix} 1 & 6 & 3 & 4 \end{pmatrix}$

DEFINITIONS - MATRIX

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

Square matrix

DEFINITIONS - MATRIX

◆ We normally write the entry of a matrix as

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

- ◆ Denoted with a **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)

Special matrices

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

$$\left(egin{array}{cccccc} a & b & c \ 0 & d & e \ 0 & 0 & f \end{array}
ight)$$

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

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

Special matrices: Symmetric Matrices

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

Column or Row Views to Denote

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

• We denote the jth column of A by a_j or $A_{:,j}$:

$$A = \left[\begin{array}{cccc} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{array} \right].$$

• We denote the *i*th row of A by a_i^T or $A_{i,:}$:

$$A = \left[egin{array}{cccc} - & a_1^T & - \ - & a_2^T & - \ & dots \ - & a_2^T & - \ \end{array}
ight].$$

• Note that these definitions are ambiguous (for example, the a_1 and a_1^T in the previous two definitions are *not* the same vector). Usually the meaning of the notation should be obvious from its use.

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

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

$$\bullet \ (A^T)^T = A$$

$$\bullet \ (AB)^T = B^T A^T$$

•
$$(AB)^T = B^T A^T$$

• $(A+B)^T = A^T + B^T$

(2) Matrix Addition/Subtraction

- Matrix addition/subtraction
 - Matrices must be of same size.
 - Entry-wise operation across all entries

(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

Products of Matrices

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

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

$$c_{11} = a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31}$$

$$c_{12} = a_{11}b_{12} + a_{12}b_{22} + a_{13}b_{32}$$

$$c_{21} = a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31}$$

$$c_{22} = a_{21}b_{12} + a_{22}b_{22} + a_{23}b_{32}$$

$$c_{31} = a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31}$$

$$c_{32} = a_{31}b_{12} + a_{32}b_{22} + a_{33}b_{32}$$

Matrix Multiplication An Example

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

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

where
$$c_{11} = a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} = 1(1) + 4(2) + 7(3) = 30$$

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

Products of Matrices

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

Condition: $\mathbf{n} = \mathbf{q}$ $c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$

$$c_{ij} = \sum_{k=1}^{\mathbf{n}} a_{ik} b_{kj}$$

$$AB \neq BA$$

(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 $(1 \times n) \times (n \times 1) = a \text{ scalar } (1 \times 1)$

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 $(AB)^T = B^TA^T$

◆Multiplication with Identity Matrix

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

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Special Uses for Matrix Multiplication

Products of Scalars & Matrices → Example, If we have

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

then we can calculate bA 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 bA = Ab if b is a scalar

- 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
$$\mathbf{b} = \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix} \qquad \mathbf{a}^{\mathsf{T}} = \begin{bmatrix} 3 & 4 & 6 \end{bmatrix}$$

then their inner product gives us

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

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

- 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

 $\mathbf{a} = \begin{bmatrix} 3 \\ 4 \\ 6 \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} 5 \\ 2 \\ 8 \end{bmatrix}$

then **ab**^T gives us

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

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Outer Product of two Vectors, e.g. a special

case:

As an example of how the outer product can be useful, let $1 \in \mathbb{R}^n$ 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,

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,

$$y=Ax=\left[egin{array}{cccc} -&a_1^T&-\ -&a_2^T&-\ dots&dots\ -&a_m^T&- \end{array}
ight]x=\left[egin{array}{cccc} a_1^Tx\ a_2^Tx\ dots\ dots\ a_m^Tx \end{array}
ight].$$

Matrix-Vector Products (II)

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

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.

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 $y \in \mathbb{R}^n$.

$$y^T=x^TA=x^T\left[egin{array}{ccccc} ert & ert & ert \ a_1 & a_2 & \cdots & a_n \ ert & ert & ert \end{array}
ight]=\left[egin{array}{cccc} x^Ta_1 & x^Ta_2 & \cdots & x^Ta_n \end{array}
ight]$$

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

Matrix-Vector Products (IV)

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.

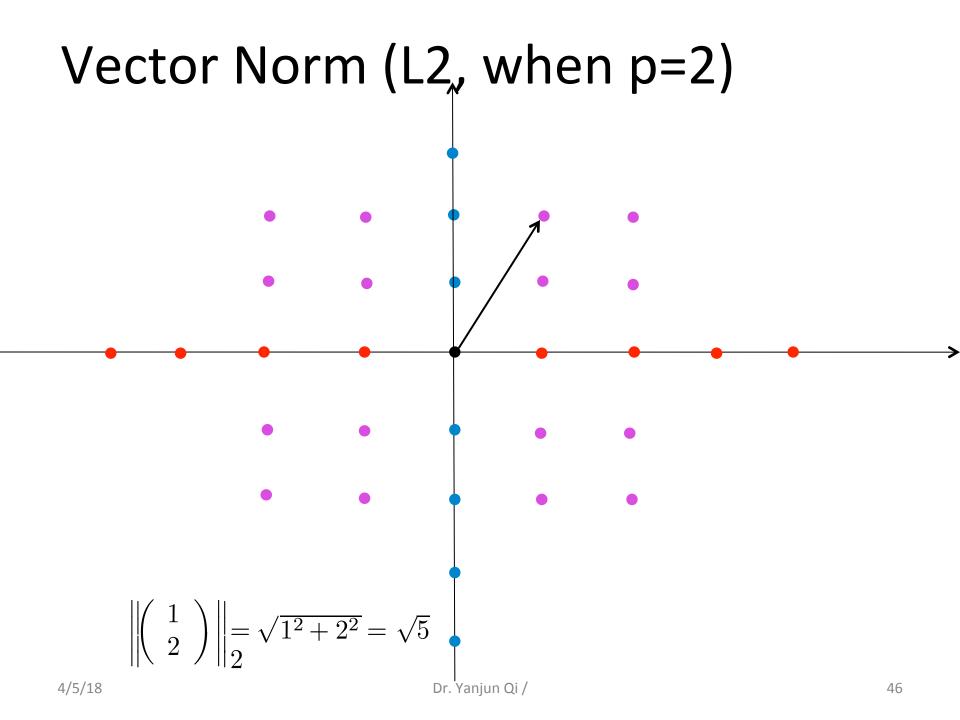
$$||x||_p = \left(\sum_{i=1}^n |x_i|^p\right)^{1/p}$$

Common norms: L₁, L₂ (Euclidean)

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

L_{infinity}

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



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

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

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

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

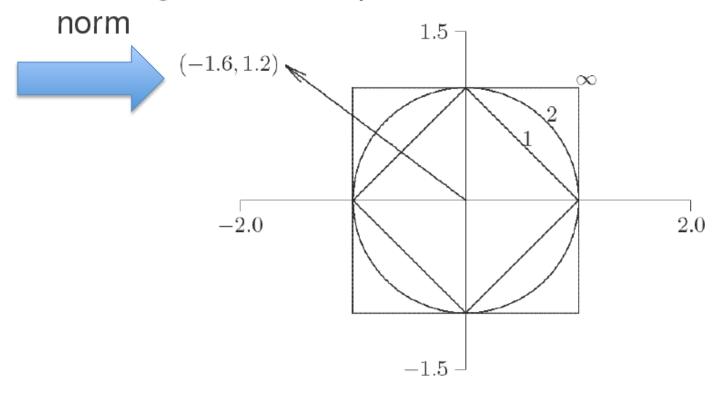
will yield the sum of the squared values of elements for **a**, i.e.

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

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Vector Norms (e.g.,)

Drawing shows unit sphere in two dimensions for each



Norms have following values for vector shown

$$\|\boldsymbol{x}\|_1 = 2.8 \quad \|\boldsymbol{x}\|_2 = 2.0 \quad \|\boldsymbol{x}\|_{\infty} = 1.6$$

In general, for any vector x in \mathbb{R}^n , $||x||_1 \ge ||x||_2 \ge ||x||_\infty$

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 x, g(x) = 0 implies that x = 0
- Homogeneity: for all x and a, g(ax) = |a| g(x), where |a| is the absolute value.
- Triangle inequality: for all $x, y, g(x + y) \le g(x) + g(y)$

Orthogonal & Orthonormal

Inner Product defined between

column vector
$$\mathbf{x}$$
 and \mathbf{y} , as $x^T y \in \mathbb{R} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ x_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^n x_i y_i. = \mathbf{x} \bullet \mathbf{y}$

If $u \cdot v = 0$, $||u||_2! = 0$, $||v||_2! = 0$ → u and v are orthogonal

If $u \cdot v = 0$, $||u||_2 = 1$, $||v||_2 = 1$ \rightarrow u and v are orthonormal

Orthogonal matrices

Notation:

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

A is orthogonal 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)

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

Orthogonal matrices

•If square A is orthogonal, it is easy to find its inverse:

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

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

Matrix Norm

 Definition: Given a vector norm ||x||, the matrix norm defined by the vector norm is given by:

$$||A|| = \max_{x \neq 0} \frac{||Ax||}{||x||}$$

- What does a matrix norm represent?
- It represents the maximum "stretching" that A does to a vector x -> (Ax).

Matrix 1- Norm

Theorem A: The matrix norm corresponding to 1-norm is maximum absolute column sum:

$$||A||_1 = \max_j \sum_{i=1}^n |a_{ij}|$$

Proof: From previous slide, we can have $||A||_1 = \max_{\|x\|=1} ||Ax||_1$

Also,
$$Ax = x_1 A_1 + x_2 A_2 + \dots + x_n A_n = \sum_{j=1}^{n} x_j A_j$$

where A_i is the j-th column of A.

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 A⁻¹ or inv A.
- The inverse of an $n \times n$ 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

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(5) Inverse of a Matrix

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

THE DETERMINANT OF A MATRIX

- ◆The determinant of a matrix A is denoted by |A| (or det(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

 2×2

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

3 x 3

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

 $n \times n$

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

THE DETERMINANT OF A MATRIX

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

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

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

then
$$det(A) = \prod_{i=1}^{n} a_{ii}$$

HOW TO FIND INVERSE MATRIXES? An example,

and |A| not 0

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

Matrix Inverse

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

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

• A^{-1} exists if 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

$$(\mathbf{A}\mathbf{B})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$$

Inverse of special matrix

• For diagonal matrices $\mathbf{D}^{-1} = \operatorname{diag}\{d_1^{-1}, \dots, d_n^{-1}\}$

- For orthogonal 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:

 $A^{+}A = I$ (provided that $(A^{T}A)^{-1}$ 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.

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

$$x_3 = -2 x_1 + x_2$$

→ NOT linearly independent

(6) Rank: Linear independence

• Alternative definition: Vectors $v_1,...,v_k$ are linearly independent if $c_1v_1+...+c_kv_k=0$ implies $c_1=...=c_k=0$

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
 - $\operatorname{rank}(A) \le \min(m,n)$
 - 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

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

(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

We can use row reduction to calculating Rank of a matrix

The following complexity figures assume that arithmetic with individual elements has complexity O(1), as is the case with fixed-preci operations on a finite field.

From Wik

Operation	Input	Output	Algorithm	Complexity
Matrix multiplication	Two <i>n×n</i> matrices	One <i>n</i> × <i>n</i> matrix	Schoolbook matrix multiplication	O(n ³)
			Strassen algorithm	$O(n^{2.807})$
			Coppersmith–Winograd algorithm	O(n ^{2.376})
			Optimized CW-like algorithms ^{[14][15][16]}	$O(n^{2.373})$
Matrix multiplication	One $n \times m$ matrix & one $m \times p$ matrix	One <i>n</i> × <i>p</i> matrix	Schoolbook matrix multiplication	O(nmp)
Matrix inversion*	One <i>n</i> × <i>n</i> matrix	One <i>n</i> × <i>n</i> matrix	Gauss-Jordan elimination	O(n ³)
			Strassen algorithm	$O(n^{2.807})$
			Coppersmith-Winograd algorithm	$O(n^{2.376})$
			Optimized CW-like algorithms	$O(n^{2.373})$
Singular value decomposition	One <i>m</i> × <i>n</i> matrix	One $m \times m$ matrix, one $m \times n$ matrix, & one $n \times n$ matrix		$O(mn^2)$ $(m \le n)$
		One <i>m×r</i> matrix, one <i>r×r</i> matrix, & one <i>n×r</i> matrix		
Determinant	One <i>n</i> × <i>n</i> matrix	One number	Laplace expansion	O(n!)
			Division-free algorithm ^[17]	O(n ⁴)
			LU decomposition	O(n ³)
			Bareiss algorithm	O(n ³)
			Fast matrix multiplication ^[18]	$O(n^{2.373})$
Back substitution	Triangular matrix	n solutions	Back substitution ^[19]	O(n ²)

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MATRIX OPERATIONS

- 1) Transposition
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Review: Derivative of a Function

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

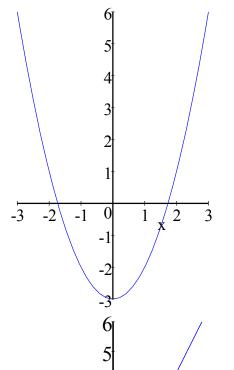
We write:
$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

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

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

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

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Review: Derivative of a Quadratic Function

$$y = x^2 - 3$$

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

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

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

$$y' = 2x$$

-3 -2 -1

 $1_{x}2$ 3

Single Var-Func to Multivariate

Single Var- Function	Multivariate Calculus	
Derivative	Partial Derivative	
Second-order	Gradient	
derivative	Directional Partial Derivative	
	Vector Field	
	Contour map of a function	
	Surface map of a function	
	Hessian matrix	
	Jacobian matrix (vector in / vector out)	

Some important rules for taking (partial) 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

$$\nabla_A f(A) \in \mathbb{R}^{m \times n} =$$

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

$$\frac{\partial f(A)}{\partial A_{11}} \quad \frac{\partial f(A)}{\partial A_{12}} \quad \dots \quad \frac{\partial f(A)}{\partial A_{1n}} \\
\frac{\partial f(A)}{\partial A_{21}} \quad \frac{\partial f(A)}{\partial A_{22}} \quad \dots \quad \frac{\partial f(A)}{\partial A_{2n}} \\
\vdots \qquad \vdots \qquad \vdots \qquad \vdots \\
\frac{\partial f(A)}{\partial A_{m1}} \quad \frac{\partial f(A)}{\partial A_{m2}} \quad \dots \quad \frac{\partial f(A)}{\partial A_{mn}}$$

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

 Size of gradient is always the same as the size of

→ Denominator layout

$$abla_x f(x) = \left[egin{array}{c} rac{\partial f(x)}{\partial x_1} \ rac{\partial f(x)}{\partial x_2} \ dots \ rac{\partial f(x)}{\partial x_n} \end{array}
ight] \in \mathbb{R}^n \quad ext{if } x \in \mathbb{R}^n$$

For Examples

Exercise: a simple example

$$f(w) = w^{T} a = \begin{bmatrix} w_{1}, w_{2}, w_{3} \end{bmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = w_{1} + 2w_{2} + 3w_{3}$$



$$\frac{\partial f}{\partial w_1} = 1$$

$$\frac{\partial f}{\partial w_2} = 2$$

$$\frac{\partial f}{\partial w_3} = 3$$

→ Denominator layout

$$\frac{\partial \overline{\partial w_1}}{\partial f} = 1$$

$$\frac{\partial f}{\partial w_2} = 2$$

$$\frac{\partial f}{\partial w} = \frac{\partial w^T a}{\partial w} = a = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

Even more general Matrix Calculus: Types of Matrix Derivatives

	Scalar	Vector	Matrix
Scalar	<u>df</u> dx	$\frac{dF}{dx} = \left[\frac{\partial F_i}{\partial x}\right]$	$\frac{dF}{dx} = \left[\frac{\partial F_{ij}}{\partial x}\right]$
Vector	$\frac{df}{dX} = \left[\frac{df}{dX_i}\right]$	$\left \frac{dF}{dX} = \left[\frac{\partial F_i}{\partial X_j} \right] \right $	
Matrix	$\frac{df}{dX} = \left[\frac{df}{dX_{ij}}\right]$		

Adapted from Thomas Minka. Old and New Matrix Algebra Useful for Statistics

Review: Hessian Matrix / n=2 case

Singlevariate

→ multivariate

f(x,z)

1st derivative to gradient,

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

2nd derivative to Hessian

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

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

Notation

- Inputs
 - X_i (jth element of vector X): random variables written in capital letter
 - p #inputs, N #observations
 - X : matrix written in bold capital
 - Vectors are assumed to be column vectors
 - Discrete inputs often described by characteristic vector (dummy variables)
- Outputs
 - quantitative Y
 - qualitative C (for categorical)
- Observed variables written in lower case
 - The i-th observed value of X is x_i and can be a scalar or a vector

Extra

- The following topics are covered by handout, but not by this slide (some will be covered ...)
 - Trace()
 - Eigenvalue / Eigenvectors
 - Positive definite matrix , Gram matrix
 - Quadratic form
 - Projection (vector on a plane, or on a vector)

Best Place to Review: Khan Academy

< MATH

Linear algebra



Vectors and spaces

0 of 45 complete

Let's get our feet wet by thinking in terms of vectors and spaces.

Vectors

Linear combinations and spans

Linear dependence and independence

Subspaces and the basis for a subspace

Vector dot and cross products

Matrices for solving systems by elimina...

Null space and column space



Matrix transformations

0 of 58 complete

Understanding how we can map one set of vectors to another set. Matrices used to define linear transformations.

Functions and linear transformations

Linear transformation examples

Transformations and matrix multiplicati...

Inverse functions and transformations

Finding inverses and determinants

More determinant depth

Transpose of a matrix



Alternate coordinate systems (bases)

0 of 39 complete

We explore creating and moving between various coordinate systems.

Orthogonal complements

Orthogonal projections

Change of basis

Orthonormal bases and the Gram-Sch...

Eigen-everything

Best Place to Review: Khan Academy

< MATH

Multivariable calculus



Thinking about multivariable functions

2 of 22 complete

The only thing separating multivariable calculus from ordinary calculus is this newfangled word "multivariable". It means we will deal with functions whose inputs or outputs live in two or more dimensions. Here we lay the foundations for thinking about and visualizing multivariable functions.

Introduction to multivariable calculus

Visualizing scalar-valued functions

Visualizing vector-valued functions

Transformations

Visualizing multivariable functions (artic...



Derivatives of multivariable functions

6 of 72 complete

What does it mean to take the derivative of a function whose input lives in multiple dimensions? What about when its output is a vector? Here we go over many different ways to extend the idea of a derivative to higher dimensions, including partial derivatives, directional derivatives, the gradient, vector derivatives, divergence, curl, etc.

Partial derivatives

Gradient and directional derivatives

Partial derivative and gradient (articles)

Differentiating parametric curves

Multivariable chain rule

Curvature

Partial derivatives of vector-valued fun...

Differentiating vector-valued functions (...

Divergence

Curl

Divergence and curl (articles)

Laplacian

Jacobian



Applications of multivariable derivatives

1 of 37 complete

The tools of partial derivatives, the gradient, etc. can be used to optimize and approximate multivariable functions. These are very useful in practice, and to a large extent this is why people study multivariable calculus.

Tangent planes and local linearization

Quadratic approximations

Optimizing multivariable functions

Optimizing multivariable functions (artic...

Lagrange multipliers and constrained o...

Constrained optimization (articles)

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 Review.ppt ☐ Prof. Alexander Gray's slides ☐ Prof. George Bebis' slides □ Prof. Hal Daum e III' notes ■ Khan Academy