

Linear algebra is the field of mathematics that studies *vectors* and *matrices*.

- A vector is an ordered sequence of numbers

$$\mathbf{v} = (6, 17)$$

- A matrix is a rectangular arrangement of numbers

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix}$$

- A well-known application of linear algebra is solving a set of linear equations

$$\begin{matrix} 2x_1 & + & x_2 & = & 6 \\ x_1 & + & 4x_2 & = & 17 \end{matrix} \quad \Leftrightarrow \quad \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 6 \\ 17 \end{bmatrix}$$

## Vectors

- Vectors are objects with a magnitude and a direction
- We represent vectors with an ordered list of numbers  $\mathbf{v} = (v_1, v_2, \dots, v_n)$
- The number  $n$  (the number of elements or entries of the vector) is its dimension
- We often call an  $n$  dimensional vector as  $n$ -vector
- The vector of  $n$  real numbers is said to be in  $\mathbb{R}^n$  ( $\mathbf{v} \in \mathbb{R}^n$ )
- Typical notation for vectors:

$$\mathbf{v} = \vec{v} = (v_1, v_2, v_3) = \langle v_1, v_2, v_3 \rangle = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$



## Multiplying a vector with a scalar

- For a vector  $\mathbf{v} = (v_1, v_2)$  and a scalar  $a$ ,

$$a\mathbf{v} = (av_1, av_2)$$

- multiplying with a scalar 'scales' the vector
- We can use the notation  $a\mathbf{1}$  for a vector whose all entries are  $a$



## Vector addition and subtraction

For vectors  $\mathbf{v} = (v_1, v_2)$  and  $\mathbf{u} = (u_1, u_2)$

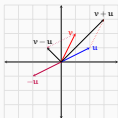
- $\mathbf{v} + \mathbf{u} = (v_1 + u_1, v_2 + u_2)$

$$(1, 2) + (2, 1) = (3, 3)$$

- $\mathbf{v} - \mathbf{u} = \mathbf{v} + (-\mathbf{u})$

$$(1, 2) - (2, 1) = (-1, 1)$$

- For any vector  $\mathbf{v}$ ,  $\mathbf{v} + \mathbf{0} = \mathbf{v}$



## Properties of vector operations

- Vector addition and scalar multiplication is commutative

$$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$$

$$a\mathbf{u} = \mathbf{u}a$$

- Scalar multiplication and vector addition also show the following distributive properties

$$a(\mathbf{u} + \mathbf{v}) = a\mathbf{u} + a\mathbf{v}$$

$$(a + b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}$$

## Dot (inner) product

- Dot product is an operation between two vectors with same dimensions

$$\mathbf{u} \cdot \mathbf{v} = u_1v_1 + u_2v_2 + \dots + u_nv_n$$

- Calculate the dot products for the following vectors

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

- Note that dot product is larger when the vectors are 'similar'

## Properties of dot product

- Commutativity  $\mathbf{u} \cdot \mathbf{v} = \mathbf{v} \cdot \mathbf{u}$

- Distributivity with vector addition  $\mathbf{u} \cdot (\mathbf{v} + \mathbf{w}) = \mathbf{u} \cdot \mathbf{v} + \mathbf{u} \cdot \mathbf{w}$

- Associativity with scalar multiplication  $(a\mathbf{u}) \cdot (\mathbf{v}) = a(\mathbf{u} \cdot \mathbf{v})$

- Note that dot product is not associative, since the result of the dot product is not a vector, but a scalar

## Dot product with unit vectors



- The dot product is larger if the vectors point to the similar directions

## Euclidean distance

- Euclidean distance between two vectors is the L2 norm of their difference

$$D(\mathbf{u}, \mathbf{v}) = \|\mathbf{u} - \mathbf{v}\| = \sqrt{(-6)^2 + (-1)^2}$$

- Euclidean distance is a metric
  - symmetric  $\|\mathbf{v} - \mathbf{u}\| = \|\mathbf{u} - \mathbf{v}\|$
  - non-negative
  - obeys the triangle inequality  $D(\mathbf{u}, \mathbf{v}) \leq D(\mathbf{u}, \mathbf{w}) + D(\mathbf{w}, \mathbf{v})$  for any  $\mathbf{w}$



## L2 norm

- Euclidean norm, or L2 (or  $L_2$ ) norm is the most commonly used norm

- For  $\mathbf{v} = (v_1, v_2, \dots, v_n)$ ,

$$\|\mathbf{v}\|_2 = \sqrt{v_1^2 + v_2^2 + \dots + v_n^2} = \sqrt{\mathbf{v} \cdot \mathbf{v}}$$

- For example,

$$\|(3, 3)\|_2 = \sqrt{3^2 + 3^2} = \sqrt{18}$$

- L2 norm is the default, we often skip the subscript  $\|\mathbf{v}\|$



## Cosine similarity

- The cosine of the angle between two vectors

$$\cos \theta = \frac{\mathbf{v} \cdot \mathbf{u}}{\|\mathbf{v}\| \cdot \|\mathbf{u}\|}$$

- is called *cosine similarity*

- Unlike dot product, the cosine similarity is not sensitive to the magnitudes of the vectors
- The cosine similarity is bounded in range  $[-1, +1]$



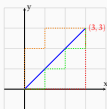
## L1 norm

- Another norm we will often encounter is the L1 norm

$$\|v\|_1 = |v_1| + |v_2|$$

$$\|(3, 3)\|_1 = |3| + |3| = 6$$

- L1 norm is related to Manhattan distance



## Matrix addition and subtraction

Each element is added to (or subtracted from) the corresponding element

$$\begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 4 \end{bmatrix}$$

Note:

- Matrix addition and subtraction are defined on matrices of the same dimensions

## Matrix-vector multiplication

- An  $n \times m$  matrix can be multiplied with a  $m$ -vector to yield a  $n$ -vector
- Example

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \times 0 + 1 \times 1 + 0 \times 1 \\ 1 \times 0 + 0 \times 1 + 1 \times 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- One view of this operation: each entry in the resulting vector is dot product (of rows of the matrix and the vector)
- Another: the result is a linear combination of the columns of the matrix (with the entries in the vector as coefficients)

$$0 \times \begin{bmatrix} 2 \\ 1 \end{bmatrix} + 1 \times \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 0 \times \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

## Transformations by non-square matrices

- Multiplying a vector with (compatible) rectangular matrix results in a vector with different dimensionality
- Example  $\mathbb{R}^3 \rightarrow \mathbb{R}^2$

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- Example  $\mathbb{R}^3 \rightarrow \mathbb{R}^4$

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 2 \\ 1 \end{bmatrix}$$

- Multiplying a vector with a matrix transforms it into the 'column space' of the matrix

## Outer product

The *outer product* of two column vectors is defined as

$$vu^T$$

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \times \begin{bmatrix} 1 & 2 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \end{bmatrix}$$

Note:

- The result is a matrix
- The vectors do not have to be the same length

## Matrix multiplication (demonstration)

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1k} \\ a_{21} & a_{22} & \dots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nk} \end{pmatrix} \times \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1m} \\ b_{21} & b_{22} & \dots & b_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{k1} & b_{k2} & \dots & b_{km} \end{pmatrix}$$

$$c_{1j} = a_{11}b_{1j} + a_{12}b_{2j} + \dots + a_{1k}b_{kj}$$

$$= \begin{pmatrix} c_{11} & c_{12} & \dots & c_{1m} \\ c_{21} & c_{22} & \dots & c_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{n2} & \dots & c_{nm} \end{pmatrix}$$

## Multiplying a matrix with a scalar

Similar to vectors, each element is multiplied by the scalar.

$$2 \begin{bmatrix} 2 & 1 \\ 1 & 4 \end{bmatrix} = \begin{bmatrix} 2 \times 2 & 2 \times 1 \\ 2 \times 1 & 2 \times 4 \end{bmatrix} = \begin{bmatrix} 4 & 2 \\ 2 & 8 \end{bmatrix}$$

## Transpose of a matrix

Transpose of a  $n \times m$  matrix is an  $m \times n$  matrix whose rows are the columns of the original matrix.

Transpose of a matrix  $A$  is denoted with  $A^T$ .

$$\text{If } A = \begin{bmatrix} a & b \\ c & d \\ e & f \end{bmatrix}, A^T = \begin{bmatrix} a & c & e \\ b & d & f \end{bmatrix}.$$

## Matrix multiplication transforms vectors

$$\begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$



- Matrices define a linear operator or function
- Linear transformations scale and/or rotate/reflect a vector

## Dot product as matrix multiplication

In machine learning (and many other disciplines), we treat an  $n$ -vector as an  $n \times 1$  matrix.

Then, the *dot product* of two vectors is

$$u^T v$$

For example,  $u = (2, 2)$  and  $v = (2, -2)$ ,

$$\begin{bmatrix} 2 & 2 \end{bmatrix} \times \begin{bmatrix} 2 \\ -2 \end{bmatrix} = 2 \times 2 + 2 \times -2 = 4 - 4 = 0$$

- This is a  $1 \times 1$  matrix, but matrices and vectors with single entries are often treated as scalars

Question: What is the transformation performed by dot product?

## Matrix multiplication

- If  $A$  is a  $n \times k$  matrix, and  $B$  is a  $k \times m$  matrix, their product  $C$  is a  $n \times m$  matrix
- Elements of  $C$ ,  $c_{ij}$ , are defined as

$$c_{ij} = \sum_{l=1}^k a_{il}b_{lj}$$

- Note:  $c_{ij}$  is the dot product of the  $i^{\text{th}}$  row of  $A$  and the  $j^{\text{th}}$  column of  $B$

## Alternative ways to think about matrix multiplication

If we have  $AB = C$ ,

- Column vectors of  $C$ ,  $c_j = Ab_j$
- Row vectors of  $C$ ,  $c_i^T = a_i^T B$
- $C$  is also the sum of outer product of columns of  $A$  and rows of  $B$

$$C = \sum a_i b_i^T$$

## Properties of matrix multiplication

- Associativity  
 $(AB)C = A(BC)$
- Distributivity  
 $A(B + C) = AB + AC$   
 $(A + B)C = AC + BC$
- Multiplication by Identity  
 $IA = AI = A$
- Matrix multiplication is not commutative  $AB \neq BA$  (in general)
- Matrix multiplication and transpose  
 $(AB)^T = B^T A^T$

## Row reduction and solving systems of linear equations

- $x_1 - x_2 = -1$   
 $2x_1 - x_2 = 1$   $\Leftrightarrow$   $\begin{bmatrix} 1 & -1 \\ 2 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$
- We apply a set of elementary row operations to the augmented matrix to obtain an upper triangle matrix  
 $\begin{bmatrix} 1 & -1 & -1 \\ 2 & -1 & 1 \end{bmatrix}$
- Elementary row operations are
  - Multiply one of the rows with a non-zero scalar
  - Add (or subtract) a multiple of one row from another
  - Swap two rows

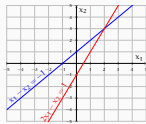
## Solution with row reduction

- $\begin{bmatrix} 1 & -1 & -1 \\ 2 & -1 & 1 \end{bmatrix}$
- Add  $-2 \times$  row 1 to row 2
- This corresponds to:  
 $\begin{bmatrix} 1 & -1 & -1 \\ 0 & 1 & 3 \end{bmatrix}$   
 $x_1 - x_2 = -1$   
 $x_2 = 3$
- where we already see  $x_2 = 3$
- Back-substituting this in the first equation gives the same answer  $x_1 = 2$

## Solving systems of linear equations

Geometric interpretation (1)

- The solution is the intersection of the lines defined by the equations

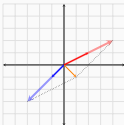


## Solving systems of linear equations

Geometric interpretation (2)

- The solution satisfies the linear combination of the column vectors

$$2 \begin{bmatrix} 2 \\ 1 \end{bmatrix} + 3 \begin{bmatrix} -1 \\ -1 \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$



## Singular matrices and matrix rank

- If the elimination results in one or more rows with all zeros, the matrix is said to be singular
- This means – effectively – we have fewer equations than unknowns
- If a square matrix is not singular, we can find a unique solution for any right-hand side
- The systems of equations with a singular matrix results in either none or an infinite number of solutions
- The number of columns (or rows) with a pivot is called the rank of the matrix
- A non-singular square matrix is said to be full-rank

## Systems of equations with singular matrices

- What is the rank of the following matrix?

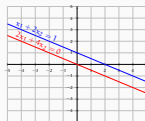
$$A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$$

- Can we solve  $Ax = b$

$$\begin{aligned} \text{– for } b = \begin{bmatrix} 1 \\ 0 \end{bmatrix} ? \\ \text{– for } b = \begin{bmatrix} 3 \\ 6 \end{bmatrix} ? \end{aligned}$$

## Systems of equations with singular matrices

Demonstration of no solution

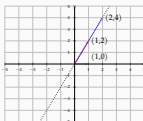


$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \Rightarrow \begin{aligned} 2x_1 + x_2 &= 1 \\ 4x_1 + 2x_2 &= 0 \end{aligned}$$

- Lines are parallel to each other: no intersection, no solution

## Systems of equations with singular matrices

Demonstration of no solution (another view)

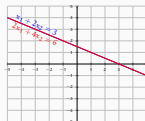


$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \Rightarrow x_1 \begin{bmatrix} 1 \\ 2 \end{bmatrix} + x_2 \begin{bmatrix} 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- All linear combinations of  $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$  and  $\begin{bmatrix} 2 \\ 4 \end{bmatrix}$  bound to be on the dotted line: no linear combination can produce  $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

## Systems of equations with singular matrices

Demonstration of infinite number of solutions



$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 6 \end{bmatrix} \Rightarrow \begin{aligned} 2x_1 + x_2 &= 3 \\ 4x_1 + 2x_2 &= 6 \end{aligned}$$

- Lines are identical: any point on the line is a solution

## Systems of equations with singular matrices

Demonstration of infinite number of solutions (another view)



$$\begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 6 \end{bmatrix} \Rightarrow x_1 \begin{bmatrix} 1 \\ 2 \end{bmatrix} + x_2 \begin{bmatrix} 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 3 \\ 6 \end{bmatrix}$$

- There are many  $(x_1, x_2)$  combinations that satisfy the equation. An obvious one:  $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$
- More?

## Matrix inverse

- If we have a single linear equation with a single unknown:  $ax = b$ , the solution is

$$x = \frac{1}{a}b \text{ or } x = a^{-1}b$$

- We can use an analogous method with systems of linear equations

$$\text{if } Ax = b \text{ then, } x = A^{-1}b$$

- Matrix inverse is only defined for square matrices (and not all square matrices are invertible)
- When it exists,  $A^{-1}A = AA^{-1} = I$
- If a square matrix is invertible, a version of elimination can be used to find the inverse
  - Create the augmented matrix  $[A|I]$
  - Use elementary row operations to obtain  $[I|B]$
  - If successful,  $B = A^{-1}$

## Systems of equations with rectangular matrices

wide matrices (more columns than rows)

- This means  $n \times m$  rectangular matrices with  $n < m$ .
- Note: the rank of such a matrix is always  $\leq n$
- Exercise: solve

$$\begin{bmatrix} 4 & 2 & 4 \\ 2 & 2 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 10 \\ 4 \end{bmatrix}$$

- In this case we have
  - no solution if rank  $r < n$  (number of rows)
  - infinitely many solution if rank  $r = n$

## Systems of equations with rectangular matrices

tall matrices (more rows than columns)

- This means  $n \times m$  rectangular matrices with  $m < n$ .
- Note: the rank of such a matrix is always  $\leq m$
- Exercise: solve

$$\begin{bmatrix} 4 & 2 \\ 2 & 2 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 10 \\ 4 \\ 4 \end{bmatrix}$$

- In this case we have
  - a unique solution if the right-hand side is in the column space of the matrix
  - no solution otherwise
- We will work with this case more often

## Determinant

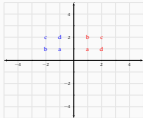
- The determinant of a square matrix is a number that provides a lot of information about the matrix
  - Whether the matrix has an inverse or not
  - Calculating eigenvalues and eigenvectors
  - Solving systems of linear equations
  - Determining the (signed) 'change of volume' caused by the linear transformation defined by the matrix

## Determinant

example geometric interpretation (1)

$$A = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$\det(A) = ?$$

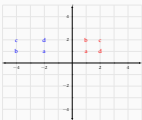


## Determinant

example geometric interpretation (2)

$$A = \begin{bmatrix} 0 & -1 \\ 2 & 0 \end{bmatrix}$$

$$\det(A) = ?$$

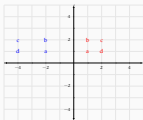


## Determinant

example geometric interpretation (3)

$$A = \begin{bmatrix} -2 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\det(A) = ?$$

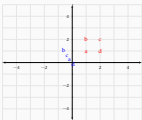


## Determinant

example geometric interpretation (3)

$$A = \begin{bmatrix} \cos 120^\circ & \sin 120^\circ \\ 0.25 & -0.43 \\ -0.43 & 0.75 \end{bmatrix} \times \begin{bmatrix} \cos 120^\circ & \sin 120^\circ \\ 0.25 & -0.43 \\ -0.43 & 0.75 \end{bmatrix}$$

$$\det(A) = ?$$



## Eigenvalues and eigenvectors

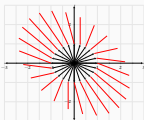
- We can view any linear transformation as a combination of scaling and rotation (and reflection)
- The linear transformation defined by a matrix does not change the directions of some vectors, vectors in these directions are called the *eigenvectors*
- The scaling factor in these directions is called *eigenvalues*
- More formally, if  $v$  is an eigenvector of  $A$  with corresponding eigenvalue  $\lambda$ ,

$$Av = \lambda v$$

- Independent eigenvectors of a symmetric are orthogonal

## Eigenvalues and eigenvectors

visualization



## Diagonalization

(eigenvalue decomposition)

- An  $n \times n$  with  $n$  independent eigenvalues can be *diagonalized* using eigenvalues and eigenvectors
- We take the matrix  $S$  whose columns are the eigenvectors of  $A$ , and the diagonal matrix  $\Lambda$  with eigenvalues of  $A$ , then

$$AS = SA$$

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

$$S^{-1}AS = \Lambda$$

## Matrix powers and matrix inverse

- Matrix powers can be easily calculated with diagonalization

$$Ax = \lambda x$$

$$AAx = \lambda Ax$$

$$A^2x = \lambda^2 x$$

- In general,

$$A^2 = SAS^{-1}AS^{-1}$$

$$= SA^2S^{-1}$$

$$A^k = SA^kS^{-1}$$

- Inverse is also easy to obtain after eigendecomposition

$$A^{-1} = SA^{-1}S^{-1}$$

## Singular Value Decomposition

- Singular value decomposition (SVD) of an  $n \times m$  matrix  $X$  is

$$X = U\Sigma V^T$$

$U$  is a  $n \times n$  orthogonal matrix

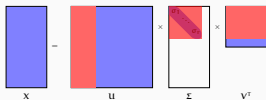
$\Sigma$  is a  $n \times m$  diagonal matrix of singular values

$V^T$  is a  $m \times m$  orthogonal matrix.

- Singular vectors in  $U$  are the eigenvectors of  $XX^T$

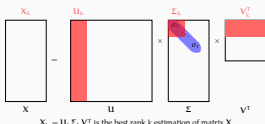
- Singular vectors in  $V^T$  are the eigenvectors of  $X^TX$

## Singular Value Decomposition



- Since  $n = r$  rows and  $m = r$  rows of  $\Sigma$  is 0, the decomposition does need the full matrices

## Low rank estimation of a matrix



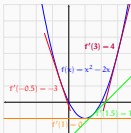
$$X_k = U_k \Sigma_k V_k^T \text{ is the best rank } k \text{ estimation of matrix } X$$

## Derivatives

- Derivative of a function  $f(x)$  is another function  $f'(x)$  indicating the rate of change in  $f(x)$
- Alternatively:  $f'(x) = \frac{df}{dx}(x)$
- When derivative exists, it determines the tangent line to the function at a given point
- Example from physics: velocity is the derivative of the position
- Our main interest:
  - the points where the derivative is 0.00 are the stationary points (maxima, minima, inflection points)
  - the derivative evaluated at other points indicate the direction and steepness of the curve defined by the function

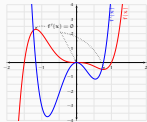
## Example: derivatives

- $f'(x)$  is negative when  $f(x)$  is decreasing, positive when it is increasing
- The absolute value of  $f'(x)$  indicates how fast  $f(x)$  changes when  $x$  changes
- $f'(x) = 0$  when at a stationary point
- $f'(a)$  is a (good) approximation to the  $f(x)$  near the  $a$



## Derivatives and extrema

- Derivative of a function is 0 at minimum, maximum and inflection points
- Derivative is useful for optimization (minimization of maximization) problems
- We need additional tests to determine the type of critical points



## Partial derivatives and gradient

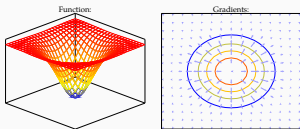
- In ML, we are often interested in (error) functions of many variables
- A partial derivative is derivative of a multivariate function with respect to a single variable, noted  $\frac{\partial f}{\partial x_i}$
- A very useful quantity, called *gradient*, is the vector of partial derivatives with respect to each variable

$$\nabla f(x_1, \dots, x_n) = \left( \frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n} \right)$$

- Gradient points to the direction of the steepest change
- Example: if  $f(x, y) = x^2 + yx$

$$\nabla f(x, y) = (2x^2 + y, x)$$

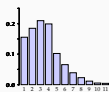
## Gradient visualization



## Probability mass function

Example: probabilities for sentence length in words

- Probability mass function (PMF) of a discrete random variable (X) maps every possible (x) value to its probability ( $P(X = x)$ ).

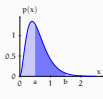


x	P(X = x)
1	0.155
2	0.185
3	0.210
4	0.194
5	0.102
6	0.066
7	0.039
8	0.023
9	0.012
10	0.005
11	0.004

## Probability density function (PDF)

- Continuous variables have *probability density functions*
- $p(x)$  is not a probability (note the notation: we use lowercase  $p$  for PDF)
- Area under  $p(x)$  sums to 1.00
- $P(X = x) = 0$
- Non zero probabilities are possible for ranges:

$$P(a \leq x \leq b) = \int_a^b p(x) dx$$



## Joint and marginal probability

Two or more random variables form a *joint probability distribution*.

An example with letter bigrams:									
	a	b	c	d	e	f	g	h	
a	0.04	0.02	0.02	0.03	0.05	0.01	0.02	0.06	0.23
b	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.04
c	0.02	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.05
d	0.02	0.00	0.00	0.01	0.02	0.00	0.01	0.02	0.08
e	0.06	0.02	0.01	0.03	0.08	0.01	0.01	0.07	0.29
f	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.02
g	0.01	0.00	0.00	0.01	0.02	0.00	0.01	0.02	0.07
h	0.08	0.00	0.00	0.01	0.10	0.00	0.01	0.02	0.22
	0.23	0.04	0.05	0.08	0.29	0.02	0.07	0.22	

## Self information / surprisal

*Self information (or surprisal)* associated with an event  $x$  is

$$I(x) = \log \frac{1}{P(x)} = -\log P(x)$$

- If the event is certain, the information (or surprise) associated with it is 0.00
- Low probability (surprising) events have higher information content
- Base of the log determines the unit of information
  - 2.00 bits
  - e nats
  - 10.00 dit, ban, hartley

## Entropy

Entropy is a measure of the uncertainty of a random variable:

$$H(X) = - \sum_x P(x) \log P(x)$$

- Entropy is the lower bound on the best average code length, given the distribution  $P$  that generates the data
- Entropy is average surprisal:  $H(X) = E[-\log P(x)]$
- It generalizes to continuous distributions as well (replace sum with integral)

Entropy is about a distribution, while surprisal is about individual events

## Pointwise mutual information

Pointwise mutual information (PMI) between two events is defined as

$$\text{PMI}(x, y) = \log_2 \frac{P(x, y)}{P(x)P(y)}$$

- Reminder:  $P(x, y) = P(x)P(y)$  if two events are independent PMI
  - 0 if the events are independent
  - + if events cooccur more than they would occur by chance
  - if events cooccur less than they would occur by chance
- Pointwise mutual information is symmetric  $\text{PMI}(X, Y) = \text{PMI}(Y, X)$
- PMI is often used as a measure of association (e.g., between words) in computational/corpus linguistics

## Conditional entropy

Conditional entropy is the entropy of a random variable conditioned on another random variable.

$$\begin{aligned} H(X|Y) &= - \sum_{y \in Y} P(y) H(X|Y=y) \\ &= - \sum_{x \in X, y \in Y} P(x, y) \log P(x|y) \end{aligned}$$

- $H(X|Y) = H(X)$  if random variables are independent
- Conditional entropy is lower if random variables are dependent

## Cross entropy

Cross entropy measures entropy of a distribution  $P$ , under another distribution  $Q$ .

$$H(P, Q) = - \sum_x P(x) \log Q(x)$$

- It often arises in the context of approximation:
  - if we approximate the true distribution  $P$  with  $Q$
- It is always larger than  $H(P)$ : It is the (non-optimum) average code-length of  $P$  coded using  $Q$
- It is a common *error function* in ML for categorical distributions

Note: the notation  $H(X, Y)$  is also used for *joint entropy*.

## KL-divergence / relative entropy

For two distribution  $P$  and  $Q$  with same support, Kullback-Leibler divergence of  $Q$  from  $P$  (or relative entropy of  $P$  given  $Q$ ) is defined as

$$D_{\text{KL}}(P||Q) = - \sum_x P(x) \log_2 \frac{P(x)}{Q(x)}$$

- $D_{\text{KL}}$  measures the amount of extra bits needed when  $Q$  is used instead of  $P$
- $D_{\text{KL}}(P||Q) = H(P, Q) - H(P)$
- Used for measuring the difference between two distributions
- Note: it is not symmetric (not a distance measure)

## Some sources of information

On Linear algebra:

- A classic reference book in the field is Strang (2009)
- Also video lectures from the author: <https://www.youtube.com/playlist?list=PLUu0b0uVTDQ3r5K-rj53D0uVRWYD3t5Yz>
- A nice video series by 3Blue1Brown (also some calculus): <https://www.youtube.com/playlist?list=PLUu0b0uVTDQ3r5K-rj53D0uVRWYD3t5Yz>
- Shifrin and Adams (2011) and Farin and Hansford (2014) are textbooks with a more practical/graphical orientation.
- Cherney, Denton, and Waldron (2013) and Beezer (2014) are two textbooks that are freely available.

## Some sources of information (cont.)

- Beezer, Robert A. (2014). *A First Course in Linear Algebra*. version 3.40. Congruent Press. isbn: 9780984417351. url: <http://linear.ups.edu/>.
- Cherney, David, Tom Denton, and Andrew Waldron (2013). *Linear algebra*. math.ucdavis.edu. url: <https://www.math.ucdavis.edu/~linear/>
- Farin, Gerald E. and Dianne Hansford (2014). *Practical linear algebra: a geometry toolbox*. Third edition. CRC Press. isbn: 978-1-4665-7958-3.
- Goldwater, Sharon (2018). *Basic probability theory*. url: [https://homepages.inf.ed.ac.uk/sgwater/teaching/general/probability\\_T20pdf](https://homepages.inf.ed.ac.uk/sgwater/teaching/general/probability_T20pdf).
- Grinstead, Charles Miller and James Laurie Snell (2012). *Introduction to probability*. American Mathematical Society. isbn: 9780821894149. url: [http://www.dartmouth.edu/~chance/teaching\\_aids/books\\_articles/probability\\_book/book.html](http://www.dartmouth.edu/~chance/teaching_aids/books_articles/probability_book/book.html)
- Jaynes, Edwin T. (2007). *Probability Theory: The Logic of Science*. Ed. by G. Larry Bretthorst. Cambridge University Press. isbn: 978-05-2199-271-0.

## Mutual information

Mutual information measures mutual dependence between two random variables

$$MI(X, Y) = \sum_x \sum_y P(x, y) \log_2 \frac{P(x, y)}{P(x)P(y)}$$

- MI is the average (expected value of) PMI
- PMI is defined on events, MI is defined on distributions
- Note the similarity with the covariance (or correlation)
- Unlike correlation, mutual information is
  - also defined for discrete variables
  - also sensitive to the non-linear dependence

## Entropy, mutual information and conditional entropy



## Perplexity

Perplexity is the exponential version of (cross) entropy:

$$PP(X) = 2^{H(X)}$$

- Perplexity 'undoes' the logarithmic scaling
- Perplexity easier to interpret in some contexts
- Especially for language models, its interpretation is the average 'branching factor'

Predict the next word: (S) The perplexity of a random variable (/S)

## Final remarks

- The knowledge most if these topics are assumed, and important for understanding modern methods in ML
- For math (and also for programming), it is difficult to master the concepts with passive participation. You need to practice

Next:

- Recap: regression
- Recap: classification

## Some sources of information (cont.)

On probability theory:

- Please read, and follow the exercises in Goldwater (2018)
- See Grinstead and Snell (2012) a more conventional introduction to probability theory. This book is also freely available
- For an influential, but not quite conventional approach, see Jaynes (2007)

For information theory:

- MacKay (2003): a freely available textbook with further topics in ML, also includes probability theory,
- Shannon (1948)

In general for math:

- Many open books on math: <https://www.openculture.com/free-math-textbooks>

## Some sources of information (cont.)

- MacKay, David J. C. (2003). *Information Theory, Inference and Learning Algorithms*. Cambridge University Press. isbn: 978-05-2164-298-9. url: <http://www.inference.phy.cam.ac.uk/itprn/book.html>
- Shannon, Claude E. (1948). "A mathematical theory of communication". In: *Bell Systems Technical Journal* 27, pp. 379-423, 623-656.
- Shifrin, Theodore and Malcolm R Adams (2011). *Linear Algebra: A Geometric Approach*. 2nd. W. H. Freeman. isbn: 978-1-4292-1521-3.
- Strang, Gilbert (2009). *Introduction to Linear Algebra, Fourth Edition*. 4th ed. Wellesley Cambridge Press. isbn: 9780980232714.