Spring 2023

SWCON253: Machine Learning

Lecture 02

Review of Linear Algebra

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4. Determinant, Decomposition, Quadratic Forms

References

- *Linear Algebra Review* by J. Zico Kolter (http://www.cs.cmu.edu/~zkolter/course/linalg/)
- *Review of Linear Algebra* by Xinkun Nie & Fereshte Khani (http://cs229.stanford.edu/syllabus-fall2020.html)
- *Linear Algebra for Machine Learning* by Sargur N. Srihari (https://cedar.buffalo.edu/~srihari/CSE574/)

1. Notation & Basic Operations

1. Vector & Matrix
2. Special Matrices
3. Additions & Multiplications
4. Transpose
5. Trace

Vector & Matrix

- By $x \in \mathbb{R}^n$, we denote a vector with n entries.

1-D array of numbers

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}.$$

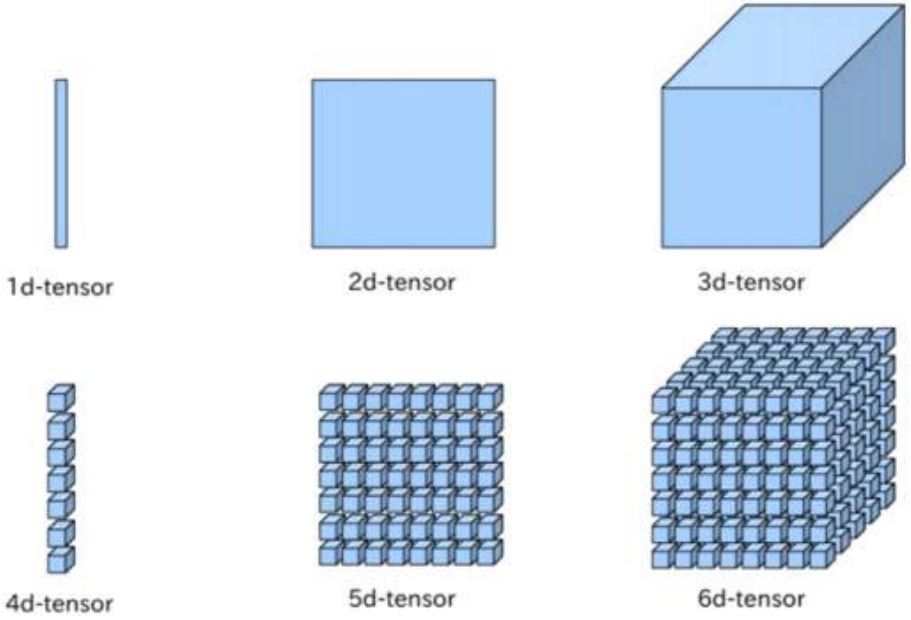
- By $A \in \mathbb{R}^{m \times n}$ we denote a matrix with m rows and n columns, where the entries of A are real numbers.

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} = \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix}.$$

2-D array of numbers *a set of column vectors* *a set of row vectors*

Tensor

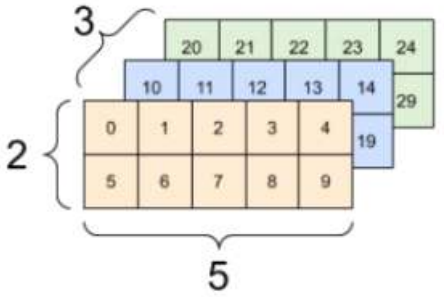
Multi-dimensional array of numbers




```
tf.Tensor(
[[[ 0  1  2  3  4]
  [ 5  6  7  8  9]]

 [[10 11 12 13 14]
  [15 16 17 18 19]]

 [[20 21 22 23 24]
  [25 26 27 28 29]]], shape=(3, 2, 5)
```



Product of Vectors

"row × column"

inner product or ***dot product***

$$x^T y \in \mathbb{R} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^{n} x_i y_i. \qquad = y^T x$$

outer product

$$xy^T \in \mathbb{R}^{m \times n} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & \cdots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \cdots & x_2 y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_m y_1 & x_m y_2 & \cdots & x_m y_n \end{bmatrix}. \qquad = (yx^T)^T$$

Special Matrices – *Zero*

The Zero Matrix

$$0 \in \mathbb{R}^{m \times n} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

Special Matrices – *Identity*

The Identity Matrix

$$I \in \mathbb{R}^{n \times n} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

*~ collection of **unit vectors** in R^n*

Has the property that for any $A \in \mathbb{R}^{m \times n}$

$$AI = A = IA$$

Special Matrices – *Diagonal*

Diagonal Matrices

For $d \in \mathbb{R}^n$

$$\text{diag}(d) \in \mathbb{R}^{n \times n} = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & d_n \end{bmatrix}$$

- For example, the identity is given by $I = \text{diag}(1)$

$$1 \in \mathbb{R}^n = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

Scalar Operations: *aA+b*

A scalar can be added to a matrix.

A matrix can be multiplied by a scalar.

$$B = aA + b \quad \Rightarrow \quad B_{i,j} = aA_{i,j} + b$$

Matrix Addition: *A+B*

- For two matrices *of the same size and type*, $A, B \in \mathbb{R}^{m \times n}$ addition is just sum of corresponding elements

$$A + B = C \in \mathbb{R}^{m \times n} \iff C_{ij} = A_{ij} + B_{ij}$$

Addition is *undefined* for matrices of different sizes $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{p \times q}$

(Note: Numpy's *broadcasting* allows addition of different sized arrays)

Matrix-Vector Multiplication: Ax

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

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

- If we write A by columns, then we have:

$$y = Ax = \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^n \\ | & | & & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \\ a^1 \\ \\ \end{bmatrix} x_1 + \begin{bmatrix} \\ a^2 \\ \\ \end{bmatrix} x_2 + \ldots + \begin{bmatrix} \\ a^n \\ \\ \end{bmatrix} x_n .$$

y is a ***linear combination*** of the *columns* of A.

Vector-Matrix Multiplication: x^TA

- If we write A by columns, then we can express $x^\top A$ as,

$$y^T = x^T A = x^T \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} x^T a^1 & x^T a^2 & \cdots & x^T a^n \end{bmatrix}$$

- expressing A in terms of rows we have:

$$y^T = x^T A = \begin{bmatrix} x_1 & x_2 & \cdots & x_m \end{bmatrix} \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix}$$

$$= x_1 \begin{bmatrix} — & a_1^T & — \end{bmatrix} + x_2 \begin{bmatrix} — & a_2^T & — \end{bmatrix} + \ldots + x_m \begin{bmatrix} — & a_m^T & — \end{bmatrix}$$

y^T is a linear combination of the *rows* of A.

Matrix Multiplication: *AB*

- For two matrices $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$, their product is

$$AB = C \in \mathbb{R}^{m \times p} \iff C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}$$

Multiplication is undefined when number of columns in A doesn't equal number or rows in B (one exception: cA for $c \in \mathbb{R}$ taken to mean scaling A by c)

Matrix Multiplication – *Different Views*

1. As a set of vector-vector products

$$C = AB = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix} \begin{bmatrix} | & | & & | \\ b^1 & b^2 & \cdots & b^p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} a_1^T b^1 & a_1^T b^2 & \cdots & a_1^T b^p \\ a_2^T b^1 & a_2^T b^2 & \cdots & a_2^T b^p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^T b^1 & a_m^T b^2 & \cdots & a_m^T b^p \end{bmatrix}.$$

2. As a sum of outer products

$$C = AB = \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^n \\ | & | & & | \end{bmatrix} \begin{bmatrix} — & b_1^T & — \\ — & b_2^T & — \\ & \vdots & \\ — & b_n^T & — \end{bmatrix} = \sum_{i=1}^{n} a^i b_i^T \quad .$$

Matrix Multiplication – *Different Views (cont'd)*

3. As a set of matrix-vector products.

$$C = AB = A \begin{bmatrix} | & | & & | \\ b^1 & b^2 & \cdots & b^p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ Ab^1 & Ab^2 & \cdots & Ab^p \\ | & | & & | \end{bmatrix}. \tag{2}$$

Here the ith column of C is given by the matrix-vector product with the vector on the right, $c_i = Ab_i$. These matrix-vector products can in turn be interpreted using both viewpoints given in the previous subsection.

4. As a set of vector-matrix products.

$$C = AB = \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix} B = \begin{bmatrix} — & a_1^T B & — \\ — & a_2^T B & — \\ & \vdots & \\ — & a_m^T B & — \end{bmatrix}.$$

Matrix Multiplication – *Diagonal Matrix*

- Multiplying $A \in \mathbb{R}^{m \times n}$ by a diagonal matrix $D \in \mathbb{R}^{n \times n}$ on the right scales the *columns* of A

$$AD = \begin{bmatrix} | & | & & | \\ d_1 a_1 & d_2 a_2 & \cdots & d_n a_n \\ | & | & & | \end{bmatrix}$$

→ column scaler
(diagonal on the right)

- Multiplying by a diagonal matrix $D \in \mathbb{R}^{m \times m}$ on the left scales the *rows* of A

$$DA = \begin{bmatrix} — & d_1 a_1^T & — \\ — & d_2 a_2^T & — \\ & \vdots & \\ — & d_m a_m^T & — \end{bmatrix}$$

→ row scaler
(diagonal on the left)

Matrix Multiplication – *Important Properties*

- Associative: $(A \in \mathbb{R}^{n \times n}, B \in \mathbb{R}^{n \times p}, C \in \mathbb{R}^{p \times q})$

$$A(BC) = (AB)C$$

- Distributive: $(A \in \mathbb{R}^{m \times n}, B, C \in \mathbb{R}^{n \times p})$

$$A(B + C) = AB + AC$$

- *NOT* commutative: (the dimensions might not even make sense, but this doesn't hold even when the dimensions are correct)

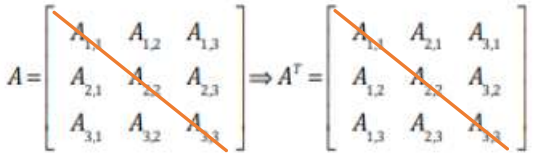
$$AB \neq BA$$

Transpose ~ *flipping*

The ***transpose*** of a matrix results from "flipping" the rows and columns. Given a matrix $A \in \mathbb{R}^{m \times n}$, its transpose, written $A^T \in \mathbb{R}^{n \times m}$, is the $n \times m$ matrix whose entries are given by

$$(A^T)_{ij} = A_{ji}.$$

– The mirror image across a diagonal line



The following properties of transposes are easily verified:

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

Special Matrices – *Symmetric*

Symmetric Matrices

- Symmetric matrix: $A \in \mathbb{R}^{n \times n}$ with $A = A^T$
- Arise naturally in many settings
  - For $A \in \mathbb{R}^{m \times n}$, $A^T A \in \mathbb{R}^{n \times n}$ is symmetric

Gram matrix

Symmetric matrix examples
- distance matrix
- covariance matrix

$$A_{(m \times n)} = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} \rightarrow A^T_{(n \times m)} = \begin{bmatrix} - & a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_n^T & - \end{bmatrix} \rightarrow A^T A_{(n \times n)} = \begin{bmatrix} a_1^T a_1 & a_1^T a_2 & \cdots & a_1^T a_n \\ a_2^T a_1 & a_2^T a_2 & \cdots & a_2^T a_n \\ \vdots & & \ddots & \vdots \\ a_n^T a_1 & a_n^T a_2 & \cdots & a_n^T a_n \end{bmatrix}$$

$(A^T A)^T = A^T A$ ∴ symmetric

$(A A^T)^T = A A^T$ ∴ symmetric

Trace ~ *sum of diagonals*

The ***trace*** of a square matrix $A \in \mathbb{R}^{n \times n}$, denoted $\mathrm{tr}A$, is the sum of diagonal elements in the matrix:

$$\mathrm{tr}A = \sum_{i=1}^{n} A_{ii}.$$

The trace has the following properties:

- For $A \in \mathbb{R}^{n \times n}$, $\mathrm{tr}A = \mathrm{tr}A^T$.
- For $A, B \in \mathbb{R}^{n \times n}$, $\mathrm{tr}(A + B) = \mathrm{tr}A + \mathrm{tr}B$.
- For $A \in \mathbb{R}^{n \times n}$, $t \in \mathbb{R}$, $\mathrm{tr}(tA) = t\,\mathrm{tr}A$.
- For A, B such that AB is square, $\mathrm{tr}AB = \mathrm{tr}BA$.
- For A, B, C such that ABC is square, $\mathrm{tr}ABC = \mathrm{tr}BCA = \mathrm{tr}CAB$, and so on for the product of more matrices.

2. Linear Independence & Inverse

1. Linear Independence
2. Span & Linear Transform
3. Rank & Inverse
4. Solving Linear Equations

Linear Independence

A set of vectors $\{x_1, x_2, \ldots x_n\} \subset \mathbb{R}^m$ is said to be ***(linearly) dependent*** if one vector belonging to the set *can* be represented as a linear combination of the remaining vectors; that is, if

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i$$

for some scalar values $\alpha_1, \ldots, \alpha_{n-1} \in \mathbb{R}$; otherwise, the vectors are ***(linearly) independent***.

Example:

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

are linearly dependent because $x_3 = -2x_1 + x_2$.

Span

The ***span*** of a set of vectors $\{x_1, x_2, \ldots x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, \ldots, x_n\}$. That is,

$$\text{span}(\{x_1, \ldots x_n\}) = \left\{ v : v = \sum_{i=1}^{n} \alpha_i x_i, \quad \alpha_i \in \mathbb{R} \right\}.$$

- Note that the ***span*** of n ***linearly independent*** vectors is $\mathbb{R}^n$.

Linear Transform: $v = Ax$

$v = Ax$

- An m x n matrix A maps an n-dimensional vector x into an m-dimensional vector v.

$$x \in \mathbb{R}^n \xrightarrow[A \in \mathbb{R}^{m \times n}]{v = Ax} v \in \mathbb{R}^m$$

- ***linear***, it is called a ***linear transform***.

For $\forall \alpha, \beta \in \mathbb{R}$ and $\forall x_1, x_2 \in \mathbb{R}^n$,

$$A(\alpha x_1 + \beta x_2) = \alpha(Ax_1) + \beta(Ax_2)$$

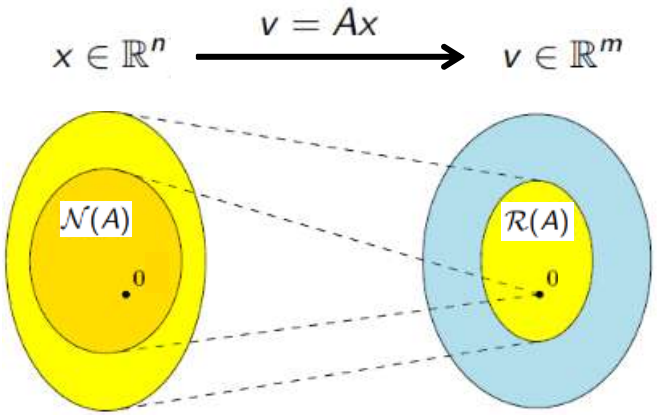
Range & Null Space: $\mathcal{R}(A)$ & $\mathcal{N}(A)$

The ***range*** or the columnspace of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{R}(A)$, is the the span of the columns of A.

$$\mathcal{R}(A) = \{v \in \mathbb{R}^m : v = Ax, x \in \mathbb{R}^n\}.$$ (image)

The ***nullspace*** of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{N}(A)$ is the set of all vectors that equal 0 when multiplied by A, i.e.,

$$\mathcal{N}(A) = \{x \in \mathbb{R}^n : Ax = 0\}.$$ (kernel)



Rank ~ *# of lin. ind. columns (rows)*

The ***column rank*** of a matrix $A \in \mathbb{R}^{m \times n}$ is the size of the largest subset of columns of A that constitute a linearly independent set.

The ***row rank*** is the largest number of rows of A that constitute a linearly independent set.

For any matrix $A \in \mathbb{R}^{m \times n}$, it turns out that the column rank of A is equal to the row rank of A (prove it yourself!), and so both quantities are referred to collectively as the ***rank*** of A, denoted as $\text{rank}(A)$.

Properties of the Rank

- For $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) \leq \min(m, n)$. If $\text{rank}(A) = \min(m, n)$, then A is said to be ***full rank***.
- For $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) = \text{rank}(A^T)$.
- For $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$, $\text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B))$.
- For $A, B \in \mathbb{R}^{m \times n}$, $\text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B)$.

Inverse

The ***inverse*** of a square matrix $A \in \mathbb{R}^{n \times n}$ is denoted A^{-1}, and is the unique matrix such that

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

A^{-1} exists $\iff Ax \neq 0$ for all $x \neq 0$

- We say that A is ***invertible*** or ***non-singular*** if A^{-1} exists and ***non-invertible*** or ***singular*** otherwise.
- In order for a square matrix A to have an inverse A^{-1}, then A must be full rank.

Properties (Assuming $A, B \in \mathbb{R}^{n \times n}$ are non-singular):

- $(A^{-1})^{-1} = A$
- $(AB)^{-1} = B^{-1}A^{-1}$
- $(A^{-1})^T = (A^T)^{-1}$. For this reason this matrix is often denoted A^{-T}.

$(A + B)^{-1} \neq A^{-1} + B^{-1}$

Solving Linear Equations: *Using Inverse*

- **If exists, *the inverse can be used* to solve a system of linear equations**
  - Two linear equations

$$\begin{aligned} 4x_1 - 5x_2 &= -13 \\ -2x_1 + 3x_2 &= 9 \end{aligned}$$

  - In vector form, $Ax = b$, with

$$A = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad b = \begin{bmatrix} -13 \\ 9 \end{bmatrix}$$

  - Solution using inverse

$$\begin{aligned} Ax &= b \\ A^{-1}Ax &= A^{-1}b \\ x &= A^{-1}b \end{aligned}$$

$$Ax = b \iff A^{\top}Ax = A^{\top}b \iff x = (A^{\top}A)^{-1}A^{\top}b$$

- **Note that the inverse may not exists**
- **Even exists, *the inverse is not used* in practice**
  - It cannot be represented with sufficient precision
- **Gaussian elimination also has disadvantages**
  - It has numerical instability (division by small no.)
  - $O(n^3)$ for n x n matrix
- **Iterative algorithms are used instead**
  - Many different decompositions can be used depending on the characteristics of A, x, and b

Solving Linear Equations: *Using Gaussian Elimination*

1. Find a particular solution to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$
2. Find all solutions to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$
3. Combine the solutions from 1. and 2. to the general solution.

A(*m*×*n*): *m* equations with *n* unknowns

- Under-determined: $m < n$
- Over-determined: $m > n$

$$\begin{bmatrix} 1 & 0 & 8 & -4 \\ 0 & 1 & 2 & 12 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 42 \\ 8 \end{bmatrix}$$

Reduced Row Echelon Form

Remark (Gaussian Elimination). *Gaussian elimination* is an algorithm that performs elementary transformations to bring a system of linear equations into reduced row echelon form. ◊

1. a solution is $[42, 8, 0, 0]^\top$
2. $$\begin{bmatrix} 1 & 0 & 8 & -4 \\ 0 & 1 & 2 & 12 \end{bmatrix} \left(\lambda_1 \begin{bmatrix} 8 \\ 2 \\ -1 \\ 0 \end{bmatrix} \right) = \lambda_1(8\boldsymbol{c}_1 + 2\boldsymbol{c}_2 - \boldsymbol{c}_3) = \boldsymbol{0}$$
$$\begin{bmatrix} 1 & 0 & 8 & -4 \\ 0 & 1 & 2 & 12 \end{bmatrix} \left(\lambda_2 \begin{bmatrix} -4 \\ 12 \\ 0 \\ -1 \end{bmatrix} \right) = \lambda_2(-4\boldsymbol{c}_1 + 12\boldsymbol{c}_2 - \boldsymbol{c}_4) = \boldsymbol{0}$$
3. $$\left\{ \boldsymbol{x} \in \mathbb{R}^4 : \boldsymbol{x} = \begin{bmatrix} 42 \\ 8 \\ 0 \\ 0 \end{bmatrix} + \lambda_1 \begin{bmatrix} 8 \\ 2 \\ -1 \\ 0 \end{bmatrix} + \lambda_2 \begin{bmatrix} -4 \\ 12 \\ 0 \\ -1 \end{bmatrix}, \lambda_1, \lambda_2 \in \mathbb{R} \right\}$$

non-pivot columns are expressed as a combination of the *pivot* columns

3. Norm, Orthogonality & Projections

1. Norm
2. Angle
3. Orthogonality
4. Projection & Least Squares

Norm ~ *length of a vector*

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

More formally, a norm is any function $f : \mathbb{R}^n \to \mathbb{R}$ that satisfies 4 properties:

1. For all $x \in \mathbb{R}^n$, $f(x) \geq 0$ (non-negativity).
2. $f(x) = 0$ if and only if $x = 0$ (definiteness).
3. For all $x \in \mathbb{R}^n$, $t \in \mathbb{R}$, $f(tx) = |t|f(x)$ (homogeneity).
4. For all $x, y \in \mathbb{R}^n$, $f(x + y) \leq f(x) + f(y)$ (triangle inequality).

- Note: $\|x - y\|$ is a measure of the "***distance***" of the two vectors.

p-Norms

- ℓ_2 norm (Euclidean norm)

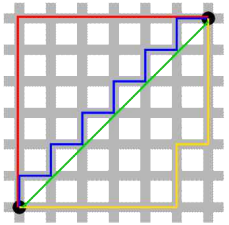
$$\|x\|_2 = \sqrt{x^T x} = \sqrt{\sum_{i=1}^{n} x_i^2}$$

- ℓ_1 norm (Manhattan norm)

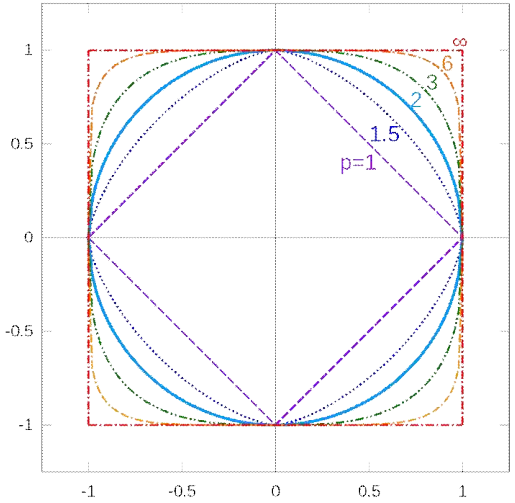
$$\|x\|_1 = \sum_{i=1}^{n} |x_i|$$

- ℓ_∞ norm (Max norm)

$$\|x\|_\infty = \max_{i=1,\ldots,n} |x_i|$$



Illustrations of unit circles in R^2
(length-one vectors from the origin)



In fact, all three norms presented so far are examples of the family of ℓ_p norms, which are parameterized by a real number $p \geq 1$, and defined as

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

Above figure is from: https://commons.wikimedia.org/w/index.php?curid=17428655

Frobenius Norm ~ *a norm for matrices*

$$\mathbb{R}^{m \times n} \rightarrow \mathbb{R}$$

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}^2} = \sqrt{\mathrm{tr}(A^T A)}.$$

Cf. Frobenius norm is used for **regularization**

$$J_R = J + \lambda \sum_{i=1}^{L} \left\| W^{(i)} \right\|_F$$

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & & & \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix}$$

$$a_1^T a_1 = A_{11}^2 + A_{21}^2 + \cdots + A_{m1}^2$$
$$a_2^T a_2 = A_{12}^2 + A_{22}^2 + \cdots + A_{m2}^2$$
$$\vdots$$
$$a_n^T a_n = A_{1n}^2 + A_{2n}^2 + \cdots + A_{mn}^2$$

$$\Rightarrow \quad A^T A = \begin{bmatrix} a_1^T a_1 & a_1^T a_2 & \cdots & a_1^T a_n \\ a_2^T a_1 & a_2^T a_2 & \cdots & a_2^T a_n \\ \vdots & & \ddots & \vdots \\ a_n^T a_1 & a_n^T a_2 & \cdots & a_n^T a_n \end{bmatrix}$$

$$\rightarrow \mathrm{tr}(A^T A) = \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}^2$$

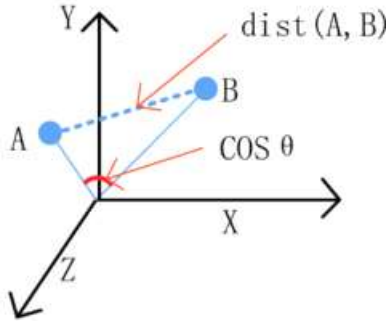
Angle *between Vectors*

Dot product of two vectors can be written in terms of their L^2 norms and angle θ between them

$$x^T y \Rightarrow ||x||_2 ||y||_2 \cos\theta$$

Cosine between two vectors is a measure of their (*orientation*) ***similarity***

$$\cos\theta = \frac{x^T y}{||x||_2 ||y||_2}$$



Orthogonal *Vectors*

- Two vectors $x, y \in \mathbb{R}^n$ are *orthogonal* if

$$x^T y = 0$$

$(\cos(\theta) = 0 \text{ or } \theta = \pi/2)$ $x \perp y$

- They are *orthonormal* if, in addition,

$$\|x\|_2 = \|y\|_2 = 1$$

A vector $x \in \mathbb{R}^n$ is ***normalized*** if $\|x\|_2 = 1$.

Orthogonal *Matrices*

- A matrix $U \in \mathbb{R}^{n \times n}$ is orthogonal if all it's columns are orthonormal, i.e.,

$$U^T U = I = U U^T \quad \Leftrightarrow \quad \text{all its columns are orthogonal to each other}$$

$U^{-1} = U^T$

(linearly independent)

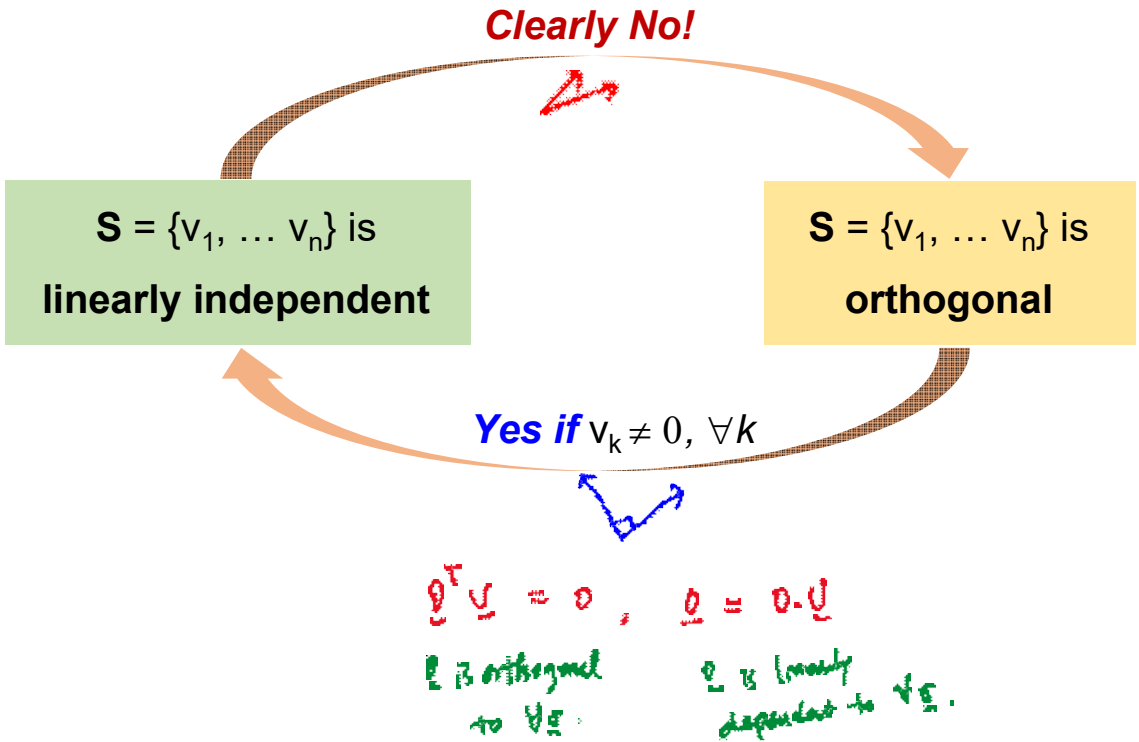
Transformations with orthogonal matrices preserve Euclidean ***distances*** and ***angles***!

$$\|\boldsymbol{A}\boldsymbol{x}\|^2 = (\boldsymbol{A}\boldsymbol{x})^\top(\boldsymbol{A}\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{x} = \boldsymbol{x}^\top \boldsymbol{I}\boldsymbol{x} = \boldsymbol{x}^\top \boldsymbol{x} = \|\boldsymbol{x}\|^2$$

$$\cos\omega = \frac{(\boldsymbol{A}\boldsymbol{x})^\top(\boldsymbol{A}\boldsymbol{y})}{\|\boldsymbol{A}\boldsymbol{x}\|\,\|\boldsymbol{A}\boldsymbol{y}\|} = \frac{\boldsymbol{x}^\top \boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{y}}{\sqrt{\boldsymbol{x}^\top \boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{x}\boldsymbol{y}^\top \boldsymbol{A}^\top \boldsymbol{A}\boldsymbol{y}}} = \frac{\boldsymbol{x}^\top \boldsymbol{y}}{\|\boldsymbol{x}\|\,\|\boldsymbol{y}\|}$$

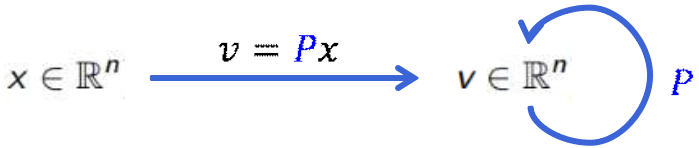
Linear Independence vs. *Orthogonality*

Consider a set of vectors **S** = $\{v_1, \ldots v_n\}$



Projection

- Definition: *Idempotence*
  - A ***projection matrix*** P is a linear transformation from a vector space to itself such that $P^2 = P$.
  - Such mapping is called a ***projection***.



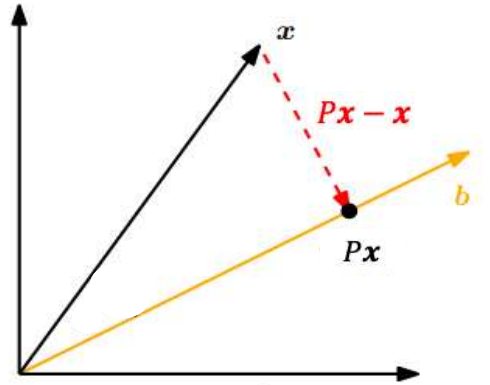
- Examples

$$P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$P = \begin{bmatrix} 0 & 0 \\ \alpha & 1 \end{bmatrix}$$

Projection onto 1-D Subspaces

Assume we are given a line (1-dimensional subspace) through the origin with basis vector $\boldsymbol{b} \in \mathbb{R}^n$. The line is a one-dimensional subspace $U \subseteq \mathbb{R}^n$ spanned by $\boldsymbol{b}$. When we project $\boldsymbol{x} \in \mathbb{R}^n$ onto U, we seek the vector $\boldsymbol{v} = P\boldsymbol{x} \in U$ that is closest to $\boldsymbol{x}$.



(a) Projection of $\boldsymbol{x} \in \mathbb{R}^2$ onto a subspace U with basis vector $\boldsymbol{b}$.

The projection $\boldsymbol{v} = P\boldsymbol{x}$ is closest to $\boldsymbol{x}$.

$\Longrightarrow$ $\|P\boldsymbol{x} - \boldsymbol{x}\|$ is minimal.

$\Longrightarrow$ $(P\boldsymbol{x} - \boldsymbol{x})$ is orthogonal to $\boldsymbol{b}$.

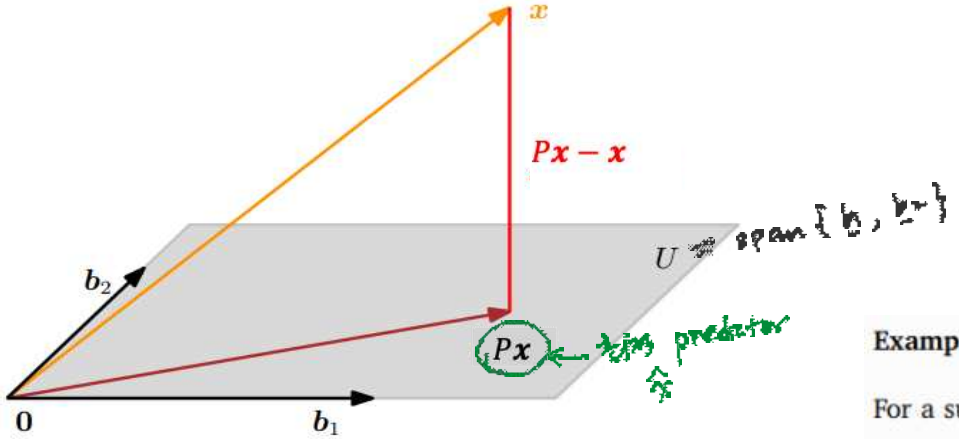
$$\Longrightarrow P = \frac{\boldsymbol{b}\boldsymbol{b}^T}{\|\boldsymbol{b}\|^2}$$

Projection onto General Subspaces

$\boldsymbol{x} \in \mathbb{R}^n$

lower-dimensional subspaces $U \subseteq \mathbb{R}^n$ with $\dim(U) = m$

Assume that $(\boldsymbol{b}_1, \ldots, \boldsymbol{b}_m)$ is an ordered basis of U.



$$\boldsymbol{B} = [\boldsymbol{b}_1, \ldots, \boldsymbol{b}_m] \in \mathbb{R}^{n \times m},$$

$$\boldsymbol{P} = \boldsymbol{B}(\boldsymbol{B}^\top \boldsymbol{B})^{-1} \boldsymbol{B}^\top.$$

Example 3.11 (Projection onto a Two-dimensional Subspace)

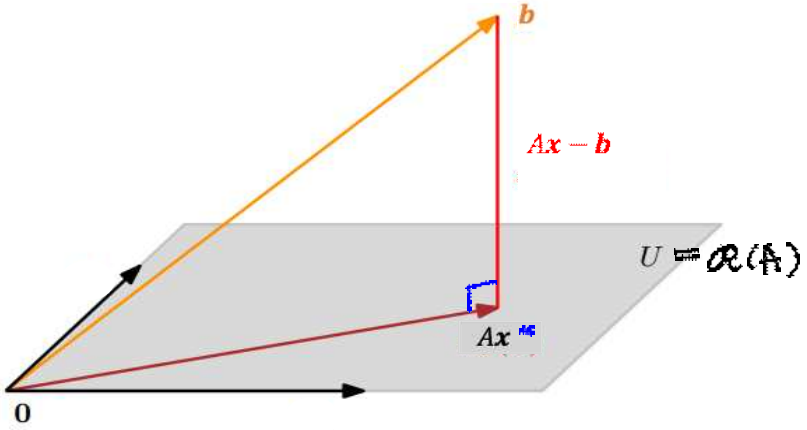
For a subspace $U = \text{span}\left[\begin{bmatrix}1\\1\\1\end{bmatrix}, \begin{bmatrix}0\\1\\2\end{bmatrix}\right] \subseteq \mathbb{R}^3$ and $\boldsymbol{x} = \begin{bmatrix}6\\0\\0\end{bmatrix} \in \mathbb{R}^3$

$$\boldsymbol{B} = \begin{bmatrix}1 & 0\\1 & 1\\1 & 2\end{bmatrix} \qquad \hat{\boldsymbol{x}} = \boldsymbol{P}\boldsymbol{x} = \begin{bmatrix}5\\2\\-1\end{bmatrix}.$$

Projection & Least Squares

Using projections, we can find approximate solutions to linear equations A$\boldsymbol{x}$ = $\boldsymbol{b}$.

- Suppose $\boldsymbol{b}$ does not lie in the span of A. Given that the linear equation cannot be solved exactly.
- We can find an approximate solution by computing the ***orthogonal projection*** of $\boldsymbol{b}$ onto the span of A.



$A\boldsymbol{x}^* \perp \boldsymbol{b}$

This problem arises often in practice, and the solution is called the ***least-squares solution*** of an over-determined system.

$$\begin{bmatrix} & A & \\ & & \end{bmatrix} \begin{bmatrix} x \\ \end{bmatrix} = \begin{bmatrix} b \\ \end{bmatrix}$$

Squared Error

$$\|Ax-b\|^2 = (Ax-b)^T(Ax-b)$$
$$= x^TA^TAx - b^TAx - x^TA^Tb + b^Tb$$

$$\frac{\partial}{\partial x}\|Ax-b\|^2 = 2A^TAx - 2A^Tb = 0$$

Orthogonality: $(A\boldsymbol{x})^T(A\boldsymbol{x}-\boldsymbol{b}) = \boldsymbol{0}$

$$\Longrightarrow \boxed{\boldsymbol{x}^* = (A^TA)^{-1}A^T\boldsymbol{b}}$$

$$\Longrightarrow \boxed{\boldsymbol{x} = (A^TA)^{-1}A^T\boldsymbol{b}}$$

→ Least Square Solution ($\frac{\partial}{\partial x}=0$)

4. Determinant, Decomposition, Quadratic Forms

1. Determinant
2. Eigenvector & Eigenvalue
3. Eigendecomposition
4. Quadratic Forms
5. Positive Definite
6. Singular Value Decomposition (SVD)

Determinant ~ *volume*

The ***determinant*** of a square matrix $A \in \mathbb{R}^{n \times n}$,

is a function $\det : \mathbb{R}^{n \times n} \to \mathbb{R}$, and is denoted $|A|$ or $\det A$.

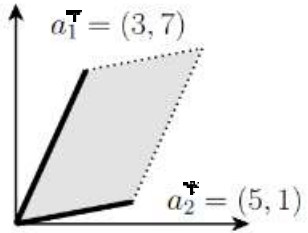
Measures how much multiplication by the matrix expands or contracts space

Given a matrix $\begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_n^T & — \end{bmatrix}$, consider the set of points $S \subset \mathbb{R}^n$ as follows:

$$S = \{v \in \mathbb{R}^n : v = \sum_{i=1}^{n} \alpha_i a_i \text{ where } 0 \leq \alpha_i \leq 1, i = 1, \ldots, n\}.$$

The absolute value of the determinant of A,

is a measure of the "volume" of the set S



$$A = \begin{bmatrix} 3 & 7 \\ 5 & 1 \end{bmatrix}$$

$|\det A|$ is the area of the parallelogram

Determinant: *Definition*

- Can be formally defined by three properties

1. Determinant of identity is one: $\det I = 1$

2. Multiplying a row by scalar $t \in \mathbb{R}$ scales determinant:

$$\det \begin{bmatrix} — & ta_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_n^T & — \end{bmatrix} = t \det A$$

3. Swapping rows negates determinant:

$$\det \begin{bmatrix} — & a_2^T & — \\ — & a_1^T & — \\ & \vdots & \\ — & a_n^T & — \end{bmatrix} = -\det A$$

In case you are wondering, it is not immediately obvious that a function satisfying the above three properties exists. In fact, though, such a function does exist, and is unique (which we will not prove here).

Determinant: *Properties*

- Important properties

  For $A, B \in \mathbb{R}^{n \times n}$,

  - $\det A = \det A^T$
  - $\det AB = \det A \det B$
  - $\det A = 0 \Leftrightarrow$ A singular (non-invertible)
  - $\det A^{-1} = 1/\det A$

Determinant: *Formula*

Let $A \in \mathbb{R}^{n \times n}$, $A_{\setminus i,\setminus j} \in \mathbb{R}^{(n-1)\times(n-1)}$ be the *matrix* that results from deleting the ith row and jth column from A.

The general (recursive) formula for the determinant is

$$\begin{aligned} |A| &= \sum_{i=1}^{n} (-1)^{i+j} a_{ij} |A_{\setminus i,\setminus j}| \quad \text{(for any } j \in 1, \ldots, n) \\ &= \sum_{j=1}^{n} (-1)^{i+j} a_{ij} |A_{\setminus i,\setminus j}| \quad \text{(for any } i \in 1, \ldots, n) \end{aligned}$$

with the initial case that $|A| = a_{11}$ for $A \in \mathbb{R}^{1\times 1}$. If we were to expand this formula completely for $A \in \mathbb{R}^{n \times n}$, there would be a total of $n!$ (n factorial) different terms. For this reason, we hardly ever explicitly write the complete equation of the determinant for matrices bigger than 3×3.

However, the equations for determinants of matrices up to size 3×3 are fairly common, and it is good to know them:

$$\begin{aligned} |[a_{11}]| &= a_{11} \\ \left|\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\right| &= a_{11}a_{22} - a_{12}a_{21} \end{aligned}$$

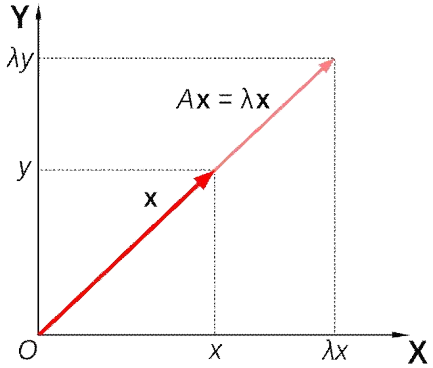
$$\left|\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}\right| = \begin{aligned} &a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ &- a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} - a_{13}a_{22}a_{31} \end{aligned}$$

Eigenvector & Eigenvalue

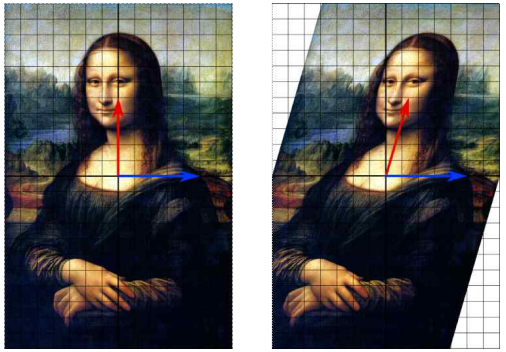
Given a square matrix $A \in \mathbb{R}^{n \times n}$, we say that $\lambda \in \mathbb{C}$ is an ***eigenvalue*** of A and $x \in \mathbb{C}^n$ is the corresponding ***eigenvector*** if

$$Ax = \lambda x, \quad x \neq 0.$$

Intuitively, this definition means that multiplying A by the vector x results in a new vector that points in the same direction as x, but scaled by a factor λ.



Matrix A acts by stretching the vector x, not changing its direction, so x is an eigenvector of A.



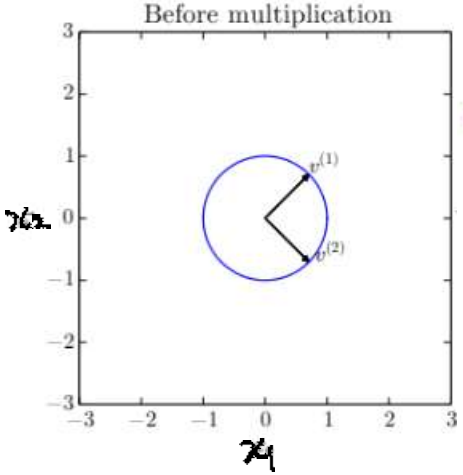
In this shear mapping, the red arrow changes direction, but the blue arrow does not. Thus the blue arrow is an eigenvector of this mapping.

Figures are from https://en.wikipedia.org/wiki/Eigenvalues_and_eigenvectors

Eigenvector & Eigenvalue (cont'd)

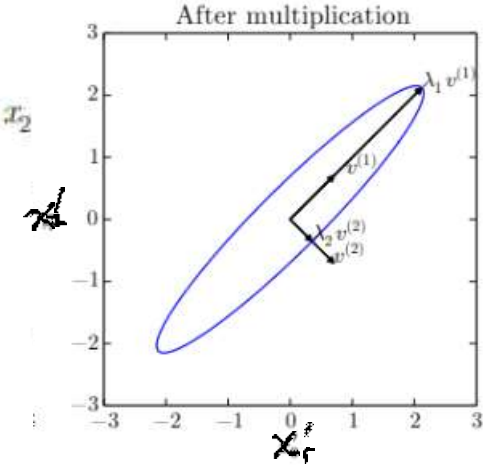
- Example of 2×2 matrix
- Matrix A with two orthonormal eigenvectors
  - $v^{(1)}$ with eigenvalue λ_1, $v^{(2)}$ with eigenvalue λ_2

Plot of unit vectors $\boldsymbol{u} \in \mathbb{R}^2$ (circle)



with two variables x_1 and x_2

Plot of vectors $A\boldsymbol{u}$ (ellipse)



Characteristic Polynomial

We can rewrite the equation above to state that (λ, x) is an eigenvalue-eigenvector pair of A if,

$$(\lambda I - A)x = 0, \quad x \neq 0.$$

But $(\lambda I - A)x = 0$ has a non-zero solution to x if and only if $(\lambda I - A)$ has a non-empty nullspace, which is only the case if $(\lambda I - A)$ is singular, i.e.,

$$|(\lambda I - A)| = 0. \quad = (\lambda_1\text{-}\lambda)(\lambda_2\text{-}\lambda)\ldots(\lambda_n\text{-}\lambda)$$

We can now use the previous definition of the determinant to expand this expression $|(\lambda I - A)|$ into a (very large) polynomial in λ, where λ will have degree n. It's often called the characteristic polynomial of the matrix A.

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \qquad |A - \lambda I| = \begin{bmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{bmatrix} = 3 - 4\lambda + \lambda^2$$

λ=1,
λ=3

$$v_{\lambda=1} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, v_{\lambda=3} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Eigendecomposition

- Suppose that matrix A has n linearly independent eigenvectors $\{\boldsymbol{v}^{(1)},..,\boldsymbol{v}^{(n)}\}$ with eigenvalues $\{\lambda_1,..,\lambda_n\}$
- Concatenate eigenvectors to form matrix V
- Concatenate eigenvalues to form vector $\lambda=[\lambda_1,..,\lambda_n]$
- Eigendecomposition of A is given by

$$A = V\text{diag}(\lambda)\, V^{-1}$$

$$A\begin{bmatrix} | & & | \\ \boldsymbol{v}^{(1)} & \cdots & \boldsymbol{v}^{(n)} \\ | & & | \end{bmatrix} = \begin{bmatrix} | & & | \\ \lambda_1\boldsymbol{v}^{(1)} & \cdots & \lambda_n\boldsymbol{v}^{(n)} \\ | & & | \end{bmatrix}$$

$$AV = V\begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}$$

column scalar (diagonal on the right)

$$\Rightarrow A = V\Lambda V^{-1}$$

$$\begin{cases} A\boldsymbol{v}_1 = \lambda_1\boldsymbol{v}_1 \\ A\boldsymbol{v}_2 = \lambda_2\boldsymbol{v}_2 \\ \vdots \\ A\boldsymbol{v}_n = \lambda_n\boldsymbol{v}_n \end{cases}$$

Properties of Eigenvalues

- $\text{tr}\, A = \sum_{i=1}^{n} \lambda_i$
- $\det A = \prod_{i=1}^{n} \lambda_i$
- $\text{rank}(A) =$ number of non-zero eigenvalues

  Matrix is singular $\iff$ any eigenvalue is zero

- Eigenvalues of A^{-1} are $1/\lambda_i, i = 1, \ldots, n$, eigenvectors are the same

$\because \; tr(V \Lambda V^{-1}) = tr(\Lambda V^{-1} V) = tr(\Lambda)$

$\because \; \det(V \Lambda V^{-1}) = \det V \cdot \det \Lambda \cdot \det V^{-1}$

$= \det \Lambda$

$\left(\det V^{-1} = \frac{1}{\det V} \right)$

$\because \; Ax = \lambda x$

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

$\frac{1}{\lambda} x = A^{-1} x$

Eigendecomposition of *Real Symmetric Matrices*

let's assume that A is a symmetric real matrix

- Every real symmetric matrix A can be decomposed into real-valued eigenvectors and eigenvalues

$$A = Q \Lambda Q^{\mathrm{T}}$$

where Q is an orthogonal matrix composed of eigenvectors of A: $\{\boldsymbol{v}^{(1)}, .., \boldsymbol{v}^{(n)}\}$

Λ is a diagonal matrix of eigenvalues $\{\lambda_1, .., \lambda_n\}$

- By convention order entries of Λ in descending order:
- Decomposition is not unique when two eigenvalues are the same

Quadratic Forms

Given a square matrix $A \in \mathbb{R}^{n \times n}$ and a vector $x \in \mathbb{R}^n$, the scalar value $x^T Ax$ is called a ***quadratic form***. Written explicitly, we see that

$$x^T Ax = \sum_{i=1}^{n} x_i (Ax)_i = \sum_{i=1}^{n} x_i \left(\sum_{j=1}^{n} A_{ij} x_j \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \ .$$

$$x^T A x = A_{11} x_1^2 + A_{12} x_1 x_2 + A_{13} x_1 x_3 + \cdots$$
$$+ A_{21} x_2 x_1 + A_{22} x_2^2 + A_{23} x_2 x_3 + \cdots$$
$$+ A_{31} x_3 x_1 + A_{32} x_3 x_2 + A_{33} x_3^2 + \cdots$$
$$+ \cdots$$

a ***quadratic form*** is a polynomial with terms all of degree two

$$4x^2 + 2xy - 3y^2 = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} 4 & 1 \\ 1 & -3 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$N(\mathbf{x} \mid \boldsymbol{\mu}, \Sigma) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\Sigma|^{1/2}} \exp\left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\}$$

$\mathbf{x}^T$ A $\mathbf{x}$

Positive Definite

A symmetric matrix $A \in \mathbb{S}^n$ is:

- ***positive definite*** (PD), denoted $A \succ 0$ if for all non-zero vectors $x \in \mathbb{R}^n$, $x^T Ax > 0$.
- ***positive semidefinite*** (PSD), denoted $A \succeq 0$ if for all vectors $x^T Ax \geq 0$.
- ***negative definite*** (ND), denoted $A \prec 0$ if for all non-zero $x \in \mathbb{R}^n$, $x^T Ax < 0$.
- ***negative semidefinite*** (NSD), denoted $A \preceq 0$) if for all $x \in \mathbb{R}^n$, $x^T Ax \leq 0$.
- ***indefinite***, if it is neither positive semidefinite nor negative semidefinite — i.e., if there exists $x_1, x_2 \in \mathbb{R}^n$ such that $x_1^T Ax_1 > 0$ and $x_2^T Ax_2 < 0$.

One important property of positive definite and negative definite matrices is that they are always full rank, and hence, invertible.

Given any matrix $A \in \mathbb{R}^{m \times n}$ (not necessarily symmetric or even square), the matrix $G = A^T A$ (sometimes called a ***Gram matrix***) is always positive semidefinite. Further, if $m \geq n$ and A is full rank, then $G = A^T A$ is positive definite.

$\|Ax\|^2 \geq 0$

$= (Ax)^T Ax$

$= x^T A^T A x$

Definiteness & Eigenvalue Signs

1. If all $\lambda_i > 0$, then the matrix A s positivedefinite

2. If all $\lambda_i \geq 0$, it is positive semidefinite

3. Likewise, if all $\lambda_i < 0$ or $\lambda_i \leq 0$, then A is negative definite or negative semidefinite respectively.

4. Finally, if A has both positive and negative eigenvalues, say $\lambda_i > 0$ and $\lambda_j < 0$, then it is indefinite.

Singular Value Decomposition (SVD)

- SVD is more general than eigendecomposition
  - If A is not square, eigendecomposition is undefined
  - Every real matrix has a SVD

$$A = UDV^{\top}$$

- U and V are orthogonal matrices
- D is a diagonal matrix not necessarily square
  - Elements of Diagonal of D are called *singular values of* A
  - Columns of U are called *left singular vectors*
  - Columns of V are called *right singular vectors*
- Left singular vectors of A are eigenvectors of AA^{T}
- Right singular vectors of A are eigenvectors of $A^{\mathrm{T}}A$
- Nonzero singular values of A are square roots of eigen values of $A^{\mathrm{T}}A$. Same is true of AA^{T}

Use of SVD in ML

1. SVD is used in generalizing matrix inversion
   - Moore-Penrose inverse (discussed next)
2. Used in Recommendation systems
   - Collaborative filtering (CF)

Moore-Penrose Pseudoinverse

- [illegible] $A^+ = VD^+U^\top$

- Solution to y = Ax (using the pseudoinverse): $\boldsymbol{x} = \boldsymbol{A}^+\boldsymbol{y}$

If the equation has:

- Exactly one solution: this is the same as the inverse.
- No solution: this gives us the solution with the smallest error $||\boldsymbol{A}\boldsymbol{x} - \boldsymbol{y}||_2$.
- Many solutions: this gives us the solution with the smallest norm of $\boldsymbol{x}$.