Wednesday, September 22, 2021

ECS-230 App Num Linear Algebra

Lecture 2 - Vector Spaces

Convention

- Vectors
  - denoted as bold letters
  - All column vector (row vectors are expressed as $\mathbf{x}^T$)
- 1-based indexing
- Usually suppress *: $\alpha * \mathbf{v} = \alpha\mathbf{v}$

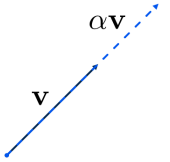
Vector

- Geometric/spatial vectors: oriented line segments defined by a direction and magnitude
- N-tuples (arrays) of real numbers, $\mathbf{x} \in R^n$
- There is a $\mathbf{0}$ vector such that $\mathbf{v} + \mathbf{0} = \mathbf{v}$
- There is a $-\mathbf{v}$ vector such that $\mathbf{v} + (-\mathbf{v}) = \mathbf{0}$
- $1\mathbf{v} = \mathbf{v}$

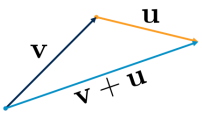
Vector operations

- Scale them by factor α
  - $\alpha(\mathbf{v} + \mathbf{u}) = \alpha\mathbf{v} + \alpha\mathbf{u}$
  - Associative: $(\alpha\beta)\mathbf{v} = \alpha(\beta\mathbf{v})$
- Addition
  - Commutative: $\mathbf{v} + \mathbf{u} = \mathbf{u} + \mathbf{v}$
  - Associative: $(\mathbf{v} + \mathbf{u}) + \mathbf{w} = \mathbf{v} + (\mathbf{u} + \mathbf{w})$

- Geometric vectors



Multiplication by α scales around the tail



Vectors add "tip-to-tail"

- n-tuples scale and add component-wise:

$$\alpha\mathbf{x} = \begin{bmatrix} \alpha x_1 \\ \alpha x_2 \\ \vdots \\ \alpha x_n \end{bmatrix}, \qquad \mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{bmatrix}$$

A *vector space* over a *field* $\mathbb{F}$ is a set of *vectors* V together with two binary operations, $+ : V \times V \to V$ and $* : \mathbb{F} \times V \to V$, satisfying the *axioms*:

1. Addition is commutative: $\mathbf{v} + \mathbf{u} = \mathbf{u} + \mathbf{v} \quad \forall \mathbf{u}, \mathbf{v} \in V$
2. Addition is associative: $(\mathbf{v} + \mathbf{u}) + \mathbf{w} = \mathbf{v} + (\mathbf{u} + \mathbf{w}) \quad \forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in V$
3. Scaling "distributes over" addition:
   i. $\alpha * (\mathbf{v} + \mathbf{u}) = \alpha * \mathbf{v} + \alpha * \mathbf{u} \quad \forall \alpha \in \mathbb{F} \quad \forall \mathbf{u}, \mathbf{v} \in V$
   ii. $(\alpha + \beta) * \mathbf{v} = \alpha * \mathbf{v} + \beta * \mathbf{v} \quad \forall \alpha, \beta \in \mathbb{F} \quad \forall \mathbf{v} \in V$
4. $(\alpha\beta) * \mathbf{v} = \alpha(\beta * \mathbf{v}) \quad \forall \alpha, \beta \in \mathbb{F} \quad \forall \mathbf{v} \in V$
5. Zero vector: $\exists\, \mathbf{0} \in V$ such that $\mathbf{v} + \mathbf{0} = \mathbf{v} \quad \forall \mathbf{v} \in V$
6. Vector negation: $\forall \mathbf{v} \in V,\ \exists (-\mathbf{v}) \in V$ such that $\mathbf{v} + (-\mathbf{v}) = \mathbf{0}$
7. $1\mathbf{v} = \mathbf{v} \quad \forall \mathbf{v} \in V$, where 1 is the multiplicative identity of $\mathbb{F}$

Field $\mathbb{F}$

- Informally: a set of scalars obeying the familiar properties of $\mathbb{R}$.

A field is a set $\mathbb{F}$ along with binary operations $+, * : \mathbb{F} \times \mathbb{F} \to \mathbb{F}$ satisfying the *axioms*:

1. Addition is commutative: $\alpha + \beta = \beta + \alpha \quad \forall \alpha, \beta \in \mathbb{F}$
2. Addition is associative: $\alpha + (\beta + \gamma) = (\alpha + \beta) + \gamma \quad \forall \alpha, \beta \in \mathbb{F}$
3. Additive identity: $\exists\, 0 \in \mathbb{F}$ such that $\alpha + 0 = \alpha \quad \forall \alpha \in \mathbb{F}$
4. Additive inverse: $\forall \alpha \in \mathbb{F}$, $\exists\, (-\alpha) \in \mathbb{F}$ such that $(-\alpha) + \alpha = 0$
5. Multiplicative is commutative: $\alpha * \beta = \beta * \alpha \quad \forall \alpha, \beta \in \mathbb{F}$
6. Multiplicative is associative: $\alpha * (\beta * \gamma) = (\alpha * \beta) * \gamma \quad \forall \alpha, \beta, \gamma \in \mathbb{F}$
7. Multiplicative identity: $\exists\, 1 \in \mathbb{F}$ such that $\alpha * 1 = \alpha \quad \forall \alpha \in \mathbb{F}$
8. Multiplicative inverse: $\forall \alpha \neq 0 \in \mathbb{F}$, $\exists\, \alpha^{-1} \in \mathbb{F}$ such that $\alpha^{-1} * \alpha = 1$
9. Multiplication distributes over addition: $\alpha * (\beta + \gamma) = \alpha * \beta + \alpha * \gamma \quad \forall \alpha, \beta, \gamma \in \mathbb{F}$

Subspaces S

- A subspace is a nonempty subset $S \subseteq V$ of a vector space V over field F that satisfies the condition
  - $\alpha \mathbf{v} \in S, \forall \mathbf{v} \in S, \forall \alpha \in \mathbb{F}$
  - $\mathbf{v} + \mathbf{u} \in S, \forall \mathbf{v}, \mathbf{u} \in S$
- In other words S is closed scalar multiplication and under addition.
- A common and convenient way of building a subspace S is to pick some set of vectors $\tilde{S} \subseteq V$ and then compute their closure under + and *.
  - In other words, for every $\alpha \in \mathbb{F}$ and $\mathbf{v}, \mathbf{u} \in \tilde{S}$, include $\alpha \mathbf{v}$ and $\mathbf{v} + \mathbf{u}$ in S.
  - At the end of this (infinite) process, S is guaranteed to be a subspace by definition.

Span

- Computing the span of the vectors in $\tilde{S}$
  - Given $\{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\} \subseteq V$, we can form **linear combinations** $\alpha_1 \mathbf{v_1} + \alpha_2 \mathbf{v_2} + \ldots + \alpha_n \mathbf{v_n}$ for $\alpha_i \in \mathbb{F}$ using the vector space operations.
  - The set of all linear combinations of $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$ is called the span of $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$ and is denoted: span($\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$)
- Theorem: S:=span($\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$) is a subspace of V.
- Intuition: all linear combinations of vectors

Spanning Sets

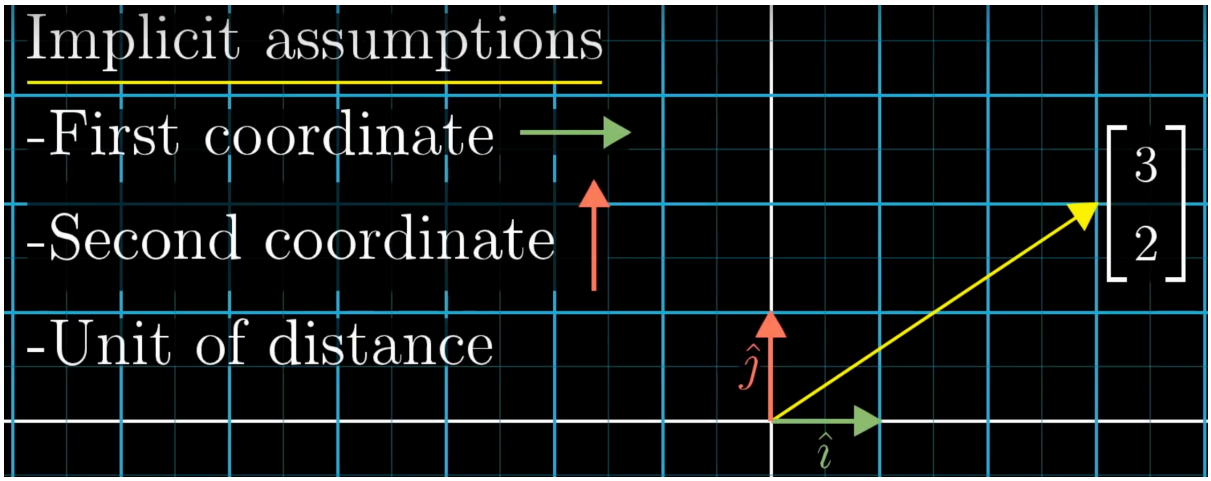
- The set $\{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\} \subseteq V$ is called a spinning set if span($\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$)=V. (i.e. every vector in V can be written as a linear combination of $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$)

Linear Independence

- Vector $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$ are called linearly independent if $c_1\mathbf{v_1} + c_2\mathbf{v_2} + \ldots + c_n\mathbf{v_n} = \mathbf{0}$ implies that $c_1 = \ldots = c_n = 0$.
- On the contrary, if there exists scalars $c_1, \ldots, c_n$ not all zero such that $c_1\mathbf{v_1} + c_2\mathbf{v_2} + \ldots + c_n\mathbf{v_n} = \mathbf{0}$, we call the vectors linearly dependent.
  - In this case, at least one vector is redundant and we can form a smaller spanning set.
  - At least one vector can be a linear transformation of other vectors

Basis

- A set of vectors $\{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\}$ that are linearly independent and span the full vector spaceV, (i.e. span($\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$)=V), are called a **basis** for V.
- Bases are a central concept in linear algebra
  - For a given vector space V there are usually an infinite number of bases to choose from
  - For many problems, the key solution step is transforming into the right basis
- Given a basis $\{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\}$ for V, there is a unique way to write any $\tilde{\mathbf{v}} \in V$ as: $\tilde{\mathbf{v}} = \alpha_1\mathbf{v_1} + \alpha_2\mathbf{v_2} + \ldots + \alpha_n\mathbf{v_n}$



Dimension

- If a vector space V has a basis consisting of n vectors, then V is said to have **dimension** n.

Lecture 3 - Linear Transformations and Matrices

Linear Transformation

- Intuition: https://www.youtube.com/watch?v=kYB8IZa5AuE
- Def: a mapping from vector space $(V, \mathbb{F})$ to vector space $(W, \mathbb{F})$ such that $L(\alpha \mathbf{v} + \beta \mathbf{u}) = \alpha L(\mathbf{v}) + \beta L(\mathbf{u}),\ \forall \alpha, \beta \in \mathbb{F}, \forall \mathbf{v}, \mathbf{u} \in V$
- Some basic properties of a linear map $L : V \to W$
  - $L(\mathbf{0}_V) = \mathbf{0}_W$ (the zero vector of V maps to the zero vector of W)
  - $L(c_1\mathbf{v_1} + c_2\mathbf{v_2} + \ldots + c_n\mathbf{v_n}) = c_1 L(\mathbf{v_1}) + \ldots + c_n L(\mathbf{v_n})$

Image and Kernel (Let $L : V \to W$ be a linear transformation)

In the following definitions, let $\mathcal{L} : V \to W$ be a linear transformation.

The **image** of a subspace $S \subseteq V$ under $\mathcal{L}$ is:

$$\mathcal{L}(S) := \{\mathcal{L}(\mathbf{v}) | \mathbf{v} \in S\}$$

All vectors in W that can be produced by applying $\mathcal{L}$ to a $\mathbf{v} \in S$

The **image** of $\mathcal{L}$ is just the image of V under $\mathcal{L}$:

$$\text{Im}(\mathcal{L}) := \mathcal{L}(V) = \{\mathcal{L}(\mathbf{v}) | \mathbf{v} \in V\}.$$

The **nullspace** or **kernel** of $\mathcal{L}$ is the set of vectors mapping to $\mathbf{0}_W$:

$$\mathcal{N}(\mathcal{L}) := \{\mathbf{v} \in V | \mathcal{L}(\mathbf{v}) = \mathbf{0}_W\}.$$

Representing Linear Transformation

- Evaluating the coordinates of $\mathcal{L}(\mathbf{v})$ in basis C for an arbitrary $\mathbf{v}$:

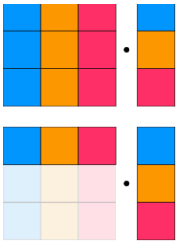
$$\begin{aligned}
[\mathcal{L}(\mathbf{v})]_C &= [\mathcal{L}(x_1\mathbf{v}_1 + \cdots + x_n\mathbf{v}_n)]_C \\
&= \sum_{j=1}^{n} x_j [\mathcal{L}(v_j)]_C = \sum_{j=1}^{n} \begin{bmatrix} a_{1j} \\ \vdots \\ a_{mj} \end{bmatrix} x_j \\
&= \begin{bmatrix} a_{1j} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \\
&:= A[\mathbf{v}]_B,
\end{aligned}$$

  - $A \in \mathbb{F}^{m \times n}$ is the **matrix** representation of A relative to the bases B and C.
  - We have **defined** matrix-vector multiplication $\mathbf{y} = A\mathbf{x}$ to be the operation:

$$y_i = \sum_{j=1}^{n} a_{ij} x_j \quad 1 \le i \le m$$

Interpretation of Matrix-Vector Multiplication

- $\mathbf{a} = A\mathbf{b}$, assume $\hat{e}_1, \ldots, \hat{e}_n$ is the basis of vector space of $\mathbf{b}$, then each column of A is where the transformed vectors of $\hat{e}_1, \ldots, \hat{e}_n$ landed in the vector space of $\mathbf{a}$ (i.e. forming a basis)
    - A linear combination of the columns of A
        - This is why we can use matrix multiplication to represent linear maps!
        - It's also the *most useful interpretation* in this course.
    - A "dot product" of each row of A with $\mathbf{x}$ to produce an entry of $\mathbf{y}$.
        - Each row represents a scalar-valued linear function of $\mathbf{x}$.
        - We'll discuss dot products later this week.

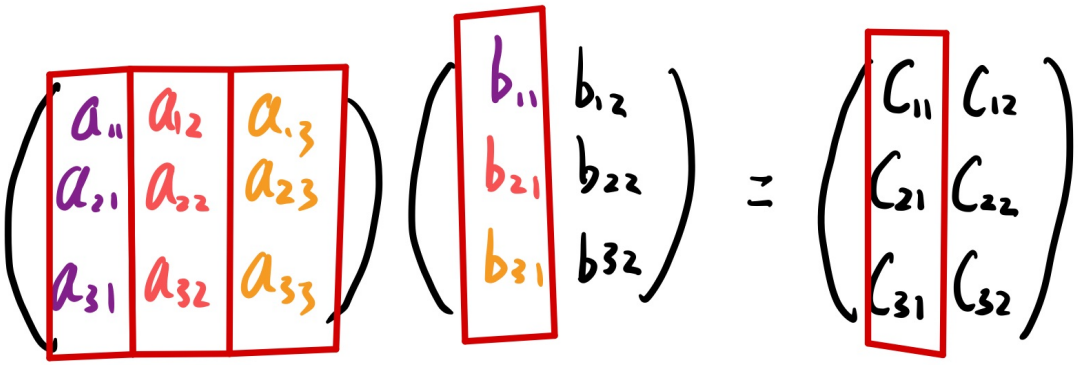


$$\begin{array}{ccc} \mathbf{v} \in V & \xrightarrow{\mathcal{L}} & \mathbf{w} = \mathcal{L}(\mathbf{v}) \in W \\ \updownarrow & & \updownarrow \\ \mathbf{x} = [\mathbf{v}]_B \in \mathbb{F}^n & \xrightarrow[A]{} & A\mathbf{x} = [\mathbf{w}]_C \in \mathbb{F}^m \end{array}$$

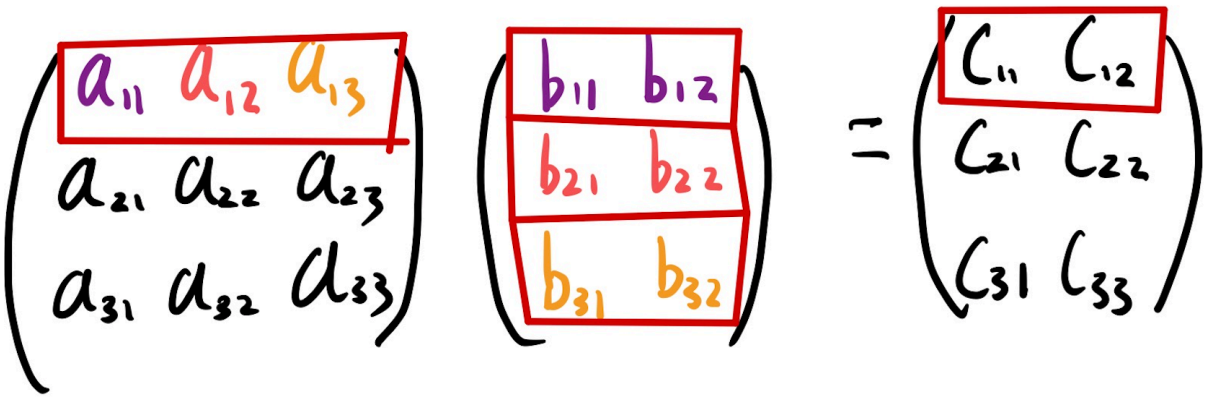
Lecture 4 - Matrix

Matrix Multiplication

- Let $A \in \mathbb{F}^{p \times m}$ and $B \in \mathbb{F}^{m \times n}$. The matrix multiplication operation $C = AB$ is defined as: $c_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj}$
- The matrix dimension should match!
- Each column of C is a linear combination of the columns of A



- Each row of C is a linear combination of the rows of B
- Associative: $A(BC) = (AB)C$



- Not Commutative: $AB \neq BA$
- Interpretation: $\mathbf{u} = AB\mathbf{v} = C\mathbf{v}$ ($C = AB$), matrix complication is the composition of linear transformation, i.e. the effect of first applying linear transformation A, then applying linear transformation B is the same as applying linear transformation C.

Range and Nullspace

- The range or column space of $A \in \mathbb{F}^{m \times n}$ is the image of $\mathbb{F}^n$ under A
  - range(A) := $\{A\mathbf{x} \mid \mathbf{x} \in \mathbb{F}^n\}$, i.e. the set of all possible outputs of $A\mathbf{x}$
  - Given our interpretation of matrix-vector multiplication as a linear combination of the columns, it is clear that range(A) = span($a_1, \ldots, a_n$) where a_j are the columns of A. (Column space = the span of columns)
- The nullspace of $A \in \mathbb{F}^{m \times n}$ is the set of vectors mapping to origin $\mathbf{0} \in \mathbb{F}^m$
  - $\mathbb{N}(A) := \{\mathbf{x} \in \mathbb{F}^n \mid A\mathbf{x} = \mathbf{0}\}$
  - Another interpretation: the set of vectors *orthogonal* to each row of A

Matrix Rank

- The **column rank** of $A \in \mathbb{F}^{m \times n}$ is the dimension of the column space range(A)
- The **row rank** of $A \in \mathbb{F}^{m \times n}$ is the dimension of the row space (the span of A's rows)
  - Column and row ranks always equal, so we can simply refer to the rank of a matrix
- **Full rank**: Matrix $A \in \mathbb{F}^{m \times n}$ is full rank if it has the greatest possible rank, *min(m, n)*
  - A **full-rank** matrix $A \in \mathbb{F}^{m \times n}$ with $m \geq n$ must have n linearly independent columns
  - Theorem: a matrix $A \in \mathbb{F}^{m \times n}$ with $m \geq n$ has **full rank** n iff $Ax \neq Ay$, $\forall x \neq y \in \mathbb{F}^n$ (no distinct vectors get mapped to the same vector)
- Intuition: rank = the number of dimensions in the output / column space
  - Rank1: the transformation becomes a line

- Rank2: the transformation becomes a plane

Matrix Inversion

- A^{-1} is called the inverse of A, it inverses the transformation of A
- A **nonsingular** or **invertible** matrix is a square matrix $A \in \mathbb{F}^{m\times m}$ of **full rank**
- A^{-1} is both a left and right inverse: $AA^{-1} = A^{-1}A = I$
- Theorem: the following conditions for $A \in \mathbb{F}^{m\times m}$ are equivalent
  - A has an inverse A^{-1}
  - A is a nonsingular matrix
  - A is of full rank m
  - range(A)=$\mathbb{F}^m$
  - $\mathbb{N}(A) = \{\mathbf{0}\}$
  - 0 is not an eigenvalue of A
  - 0 is not a singular value of A
  - det(A)≠0 (if det(A)=0, then the transformation squishes into lower dimension)
- Interpretation of Linear Systems: see slides 04-11

Matrix Operation

- Multiplication C=AB
- Inversion $B = A^{-1}$
- Addition C=A+B
- Scalar multiplication $B = \alpha A$
- Transposition $B = A^T$

◦ Scalar multiplication

$$\alpha \begin{bmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} = \begin{bmatrix} \alpha A_{11} & \alpha A_{12} & \dots \\ \alpha A_{21} & \alpha A_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

◦ Addition (assuming compatible block sizes)

$$\begin{bmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} + \begin{bmatrix} B_{11} & B_{12} & \dots \\ B_{21} & B_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} = \begin{bmatrix} A_{11}+B_{11} & A_{12}+B_{12} & \dots \\ A_{21}+B_{21} & A_{22}+B_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

◦ Transposition

$$\begin{bmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}^\top = \begin{bmatrix} {A_{11}}^\top & {A_{21}}^\top & \dots \\ {A_{12}}^\top & {A_{22}}^\top & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

Lecture 5 - Block Matrices and Determinants

Block Matrices

- Decompose A into a block matrix, the following operations respect the block structure
  - Scalar multiplication
  - Addition
  - Transposition

- Matrix multiplication

Determinants $A \in \mathbb{F}^{m \times m}$

- The determinant of a square matrix, , measuring the "volume change" produced by the corresponding linear map.
- Intuition: change in volume of the unit hypercube when it is transformed by A
- Three axioms
  - Axiom1: *det(A)* is a multilinear function of the columns of A
    - Intuition: in 3D, scale the length by α then add it by b, the volume changes to $\alpha V + V_b$

$$\det\left(\begin{bmatrix} \mathbf{a}_1 & \cdots & \alpha\mathbf{a}_j + \mathbf{b} & \cdots & \mathbf{a}_m \end{bmatrix}\right) = \alpha \det\left(\begin{bmatrix} \mathbf{a}_1 & \cdots & \mathbf{a}_j & \cdots & \mathbf{a}_m \end{bmatrix}\right) + \det\left(\begin{bmatrix} \mathbf{a}_1 & \cdots & \mathbf{b} & \cdots & \mathbf{a}_m \end{bmatrix}\right)$$

  - Axiom2: *det(A)* vanishes if any columns are repeated
    - Intuition: in 3D, when a dimension collapse, the cube falls into a plane.

$$\mathbf{a}_j = \mathbf{a}_k \text{ for any } j \neq k \implies \det\left(\begin{bmatrix} \mathbf{a}_1 & \cdots & \mathbf{a}_m \end{bmatrix}\right) = 0$$

  - Axiom3: *det(I)*, the determinant of the identity matrix, is 1.
- Properties
  - Property1: Adding a multiple of another column doesn't change the determinant
    - $\det(e_1, \ldots, e_k + \alpha e_j, \ldots, e_m) = \det(e_1, \ldots, e_k, \ldots, e_m) + \underbrace{\alpha \det(e_1, \ldots, e_j, \ldots, e_j, \ldots, e_m)}_{=0}$
  - Property2: Swapping two adjacent columns negates

$$\begin{aligned} 0 &= \det(\mathbf{a}_1, \cdots, (\mathbf{a}_j + \mathbf{a}_{j+1}), (\mathbf{a}_j + \mathbf{a}_{j+1}), \cdots, \mathbf{a}_m) \\ &= \cancelto{0}{\det(\mathbf{a}_1, \cdots, \mathbf{a}_j, \mathbf{a}_j, \cdots, \mathbf{a}_m)} + \det(\mathbf{a}_1, \cdots, \mathbf{a}_j, \mathbf{a}_{j+1}, \cdots, \mathbf{a}_m) + \det(\mathbf{a}_1, \cdots, \mathbf{a}_{j+1}, \mathbf{a}_j, \cdots, \mathbf{a}_m) + \cancelto{0}{\det(\mathbf{a}_1, \cdots, \mathbf{a}_{j+1}, \mathbf{a}_{j+1}, \cdots, \mathbf{a}_m)} \\ \implies & \det(\mathbf{a}_1, \cdots, \mathbf{a}_j, \mathbf{a}_{j+1}, \cdots, \mathbf{a}_m) = -\det(\mathbf{a}_1, \cdots, \mathbf{a}_{j+1}, \mathbf{a}_j, \cdots, \mathbf{a}_m) \end{aligned}$$

  - Property3: det(A) = 0 if A's columns are linearly dependent
    - $\det(e_1, \ldots, e_{m-1}, \sum_{i=1}^{m-1} c_i e_i) = \sum_{i=1}^{m-1} c_i \det(e_1, \ldots, e_{m-1}, e_i) = 0$

$$\det\left(\begin{bmatrix} a_{11} & 0 & \ldots & 0 \\ 0 & a_{22} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & a_{mm} \end{bmatrix}\right) = (a_{11}a_{22}\cdots a_{mm}) \det\left(\begin{bmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{bmatrix}\right) = \prod_{i=1}^{m} a_{ii}$$

- Property4: det(AB)=det(A)det(B)
- Property5: $det(A) = det(A^T)$

- Computing using the Axioms
  - Diagonal matrix (using Axiom1)
  - Upper/lower triangular (using Property1)

$$\det\begin{pmatrix}\begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ 0 & a_{22} & a_{23} & \dots & a_{2m} \\ 0 & 0 & a_{33} & \dots & a_{2m} \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & & a_{mm} \end{bmatrix}\end{pmatrix} = a_{11}\det\begin{pmatrix}\begin{bmatrix} 1 & a_{12} & a_{13} & \dots & a_{1m} \\ 0 & a_{22} & a_{23} & \dots & a_{2m} \\ 0 & 0 & a_{33} & \dots & a_{2m} \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & & a_{mm} \end{bmatrix}\end{pmatrix} = a_{11}\det\begin{pmatrix}\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & a_{22} & a_{23} & \dots & a_{2m} \\ 0 & 0 & a_{33} & \dots & a_{2m} \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & & a_{mm} \end{bmatrix}\end{pmatrix}$$

an do the same procedure for ver-triangular matrices, just "bottom-up."

$$= a_{11}a_{22}\det\begin{pmatrix}\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & a_{23} & \dots & a_{2m} \\ 0 & 0 & a_{33} & \dots & a_{2m} \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & & a_{mm} \end{bmatrix}\end{pmatrix} = \dots = \prod_{i=1}^{m} a_{ii}$$

9

- Calculate: Leibniz Formula

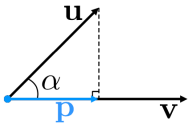
Decomposing the columns of $\det(A)$ in the standard basis $\{\mathbf{e}_i\}$: $\mathbf{a}_j = \sum_{i=1}^{m} a_{ij}\mathbf{e}$ then apply linearity one column at a time:

$$\begin{aligned}
\det(A) &= \det\left(\sum_{i_1=1}^{m} a_{i_1 1}\mathbf{e}_{i_1}, \sum_{i_2=1}^{m} a_{i_2 2}\mathbf{e}_{i_2}, \cdots, \sum_{i_m=1}^{m} a_{i_m m}\mathbf{e}_{i_m}\right) \\
&= \sum_{i_1=1}^{m} a_{i_1 1}\det\left(\mathbf{e}_{i_1}, \sum_{i_2=1}^{m} a_{i_2 2}\mathbf{e}_{i_2}, \cdots, \sum_{i_m=1}^{m} a_{i_m m}\mathbf{e}_{i_m}\right) \\
&= \sum_{i_1=1}^{m} a_{i_1 1}\sum_{i_2=1}^{m} a_{i_2 2}\cdots\sum_{i_m=1}^{m} a_{i_m m}\det\left(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \cdots, \mathbf{e}_{i_m}\right) \\
&= \sum_{i_1,\dots,i_m=1}^{m}\left(\prod_{j=1}^{m} a_{i_j j}\right)\det\left(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \cdots, \mathbf{e}_{i_m}\right) \\
&= \sum_{i_1,\dots,i_m=1}^{m}\det\left(\mathbf{e}_{i_1}, \mathbf{e}_{i_2}, \cdots, \mathbf{e}_{i_m}\right)\prod_{j=1}^{m} a_{i_j j}
\end{aligned}$$

Lecture 6 - Inner Product

Geometric Dot Product

- $\mathbf{u} \cdot \mathbf{v} = len(\mathbf{u}) len(\mathbf{v}) \cos(\alpha)$
- Contains everything we need to measure length, angle, and projections
  - $len(\mathbf{u}) = \sqrt{\mathbf{u} \cdot \mathbf{u}}, \alpha = \cos^{-1}(\frac{\mathbf{u} \cdot \mathbf{v}}{len(\mathbf{u}) len(\mathbf{v})}), \mathbf{p} = \frac{\mathbf{u} \cdot \mathbf{v}}{len(\mathbf{v})^2} \mathbf{v}$
- Properties
  - Commutative: Symmetric with respect to $\mathbf{u}$ and $\mathbf{v}$
  - Linear in each argument: $(\alpha \mathbf{u} + \mathbf{w}) \cdot \mathbf{v} = \alpha \mathbf{u} \cdot \mathbf{v} + \mathbf{w} \cdot \mathbf{v}$



$\mathbf{u} \cdot \mathbf{v} = \text{len}(\mathbf{u}) \text{len}(\mathbf{v}) \cos(\alpha)$

Geometric Dot Product in a Basis

Consider a basis $\{\mathbf{b}_1, \cdots, \mathbf{b}_m\}$ for the m-dimensional geometric vectors. Then we can find the scalar components v_i and u_j in $\mathbb{R}$:

$$\mathbf{v} = \sum_i v_i \mathbf{b}_i, \qquad \mathbf{u} = \sum_j u_j \mathbf{b}_j$$

$$\implies \mathbf{v} \cdot \mathbf{u} = \left(\sum_{i=1}^m v_i \mathbf{b}_i \right) \cdot \left(\sum_{j=1}^m u_j \mathbf{b}_j \right)$$

$$= \sum_{i=1}^m v_i \sum_{j=1}^m (\mathbf{b}_i \cdot \mathbf{b}_j) u_j \quad \text{According to linearity}$$

$$= [v_1 \quad \cdots \quad v_m] B \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix} \quad \text{where } B = \begin{bmatrix} (\mathbf{b}_1 \cdot \mathbf{b}_1) & \cdots & (\mathbf{b}_1 \cdot \mathbf{b}_m) \\ \vdots & & \vdots \\ (\mathbf{b}_m \cdot \mathbf{b}_1) & \cdots & (\mathbf{b}_m \cdot \mathbf{b}_m) \end{bmatrix}$$

- $\boldsymbol{B}$ is a symmetric positive definitive matrix.
- Property 1 of $\boldsymbol{B}$: $B^T = B$ because $b_{ij} = b_i \cdot b_j = b_j \cdot b_i = b_{ji}$
- Property 2 of $\boldsymbol{B}$: Any nonzero $\mathbf{c} \in \mathbb{R}^m$ corresponds to a nonzero geometric vector $\mathbf{v}$ in the basis $\{b_j\}$. So $\mathbf{c}^T B \mathbf{c} = len(\mathbf{v})^2 > 0$

- It turns out that, for $x, y \in \mathbb{R}^m$ the expression $\mathbf{x}^T B \mathbf{y}$ corresponds to a "geometric dot product" iff B is a symmetric positive definitive matrix.
- Very special case (orthonormal case)
  - We call two geometric vector orthogonal if $\mathbf{u} \cdot \mathbf{v} = 0$ which means $\alpha = 90$ degree
  - If the basis vectors are all unit length, $b_i \cdot b_i = 1$, and mutually orthogonal $b_i \cdot b_j = 0, \forall i \neq j$ and $B = I$, so we have $\mathbf{x}^T B \mathbf{y} = \mathbf{x}^T I \mathbf{y} = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^m x_i y_i$

- The standard dot product

General Form of Inner Product

- Definitions

An **inner product** on a vector space $(V, \mathbb{F})$ is an operation $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$ satisfying the following axioms:

1. Linearity in the *second* argument

   $\langle \mathbf{v}, \alpha\mathbf{u} + \beta\mathbf{w} \rangle = \alpha \langle \mathbf{v}, \mathbf{u} \rangle + \beta \langle \mathbf{v}, \mathbf{w} \rangle$

2. *Conjugate* symmetry

   $\langle \mathbf{v}, \mathbf{u} \rangle = \overline{\langle \mathbf{u}, \mathbf{v} \rangle}$ (this is the same as symmetry $\langle \mathbf{v}, \mathbf{u} \rangle = \langle \mathbf{u}, \mathbf{v} \rangle$ when $\mathbb{F} = \mathbb{R}$)

3. Positive definiteness

   $\langle \mathbf{v}, \mathbf{v} \rangle > 0 \quad \forall \mathbf{v} \neq \mathbf{0}$ (by conjugate symmetry: $\langle \mathbf{v}, \mathbf{v} \rangle = \overline{\langle \mathbf{v}, \mathbf{v} \rangle} \in \mathbb{R}$)

WARNING: the inner product is *antilinear* in the first argument:

$$\langle \alpha\mathbf{v} + \beta\mathbf{w}, \mathbf{u} \rangle = \overline{\langle \mathbf{u}, \alpha\mathbf{v} + \beta\mathbf{w} \rangle} = \overline{\alpha \langle \mathbf{u}, \mathbf{v} \rangle + \beta \langle \mathbf{u}, \mathbf{w} \rangle}$$
$$= \overline{\alpha} \langle \mathbf{v}, \mathbf{u} \rangle + \overline{\beta} \langle \mathbf{w}, \mathbf{u} \rangle.$$

Note: conventions differ on which argument is linear/antilinear.

- Inner Product in terms of scalar components in arbitrary basis

$$\mathbf{v} = \sum_i v_i \mathbf{b}_i, \qquad \mathbf{u} = \sum_j u_j \mathbf{b}_j \qquad v_i, u_j \in \mathbb{F}$$

$$\implies \langle \mathbf{v}, \mathbf{u} \rangle = \left\langle \sum_{i=1}^m v_i \mathbf{b}_i, \sum_{j=1}^m u_j \mathbf{b}_j \right\rangle = \sum_{i=1}^m \overline{v_i} \left\langle \mathbf{b}_i, \sum_{j=1}^m \mathbf{b}_j u_j \right\rangle$$

$$= \sum_{i=1}^m \overline{v_i} \sum_{j=1}^m \langle \mathbf{b}_i, \mathbf{b}_j \rangle u_j$$

$$= \begin{bmatrix} \overline{v_1} & \cdots & \overline{v_m} \end{bmatrix} B \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix} \quad \text{where } B = \begin{bmatrix} \langle \mathbf{b}_1, \mathbf{b}_1 \rangle & \cdots & \langle \mathbf{b}_1, \mathbf{b}_m \rangle \\ \vdots & & \vdots \\ \langle \mathbf{b}_m, \mathbf{b}_1 \rangle & \cdots & \langle \mathbf{b}_m, \mathbf{b}_m \rangle \end{bmatrix}$$

- $\boldsymbol{B}$'s properties
  - $B = \overline{B^T} := B^H$, the adjoint of $\boldsymbol{B}$. In other word, $\boldsymbol{B}$ is **hermitian** or **self-joint**.
  - $\forall \mathbf{v} \neq 0$, the corresponding coordinate vector $\mathbf{c} \in \mathbb{F}^m$ must satisfy $< \mathbf{v}, \mathbf{v} > = \mathbf{c}^H B \mathbf{c} > 0$. So B must be a positive definite hermitian matrix.
  - Any inner product can be expressed in this form, and any positive definite B defines an inner product!
- Very special case: orthonormal basis
  - We call two vectors ($\mathbf{u}$, $\mathbf{v}$) **orthogonal** if $\langle \mathbf{v}, \mathbf{u} \rangle = 0$.
  - What if basis vectors are unit length, $\langle \mathbf{b}_i, \mathbf{b}_i \rangle = 1$, and mutually orthogonal $\langle \mathbf{b}_i, \mathbf{b}_j \rangle = 0 \; \forall i \neq j$?
  - $B = I$ and so: $\mathbf{x}^H B \mathbf{y} = \mathbf{x}^H I \mathbf{y} = \boxed{\mathbf{x}^H \mathbf{y} = \sum_{i=1}^m \overline{x_i} y_i.}$

This is the complex dot product formula you probably know. When $\mathbb{F} = \mathbb{R}$ it is just the ordinary dot product.

- Complex Dot Product: $\mathbf{x}^H\mathbf{y} = \sum_{i=1}^{m} \bar{\mathbf{x}}_\mathbf{i}\mathbf{y}_\mathbf{i}$
  - Why conjugate? Since
    $x = a + bi, y = c + di \in \mathbb{C}, \bar{x}y = (a - bi)(c + di) = (ac + bd) + (ad - bc)i$
  - Specifically, $< \mathbf{x}, \mathbf{x} > = \mathbf{x}^H\mathbf{x}$ computes the total squared magnitude.

Decomposition into Components using the Inner Product

- Supposing we are given a vector $\mathbf{v} \in V$ and want to find its coordinates in a basis $\{\mathbf{b_j}\}$
  - Since $\{\mathbf{b_j}\}$ form a basis, we know there exists scalar values $\{x_{ij}\}$ (**the coordinate**) such that $\mathbf{v} = \sum_{j=1}^{m} x_j\mathbf{b_j} = [\mathbf{b_1}\ldots\mathbf{b_m}]\begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$
  - Compute each basis vector with vector $\mathbf{v}$, we have
    $< \mathbf{b_j}, \mathbf{v} > = < \mathbf{b_j}, \sum_{i=1}^{m} x_i\mathbf{b_i} > = \sum_{i=1}^{m} x_i < \mathbf{b_j}, \mathbf{b_i} > \forall i$
  - If we set
    $\mathbf{A} = \begin{bmatrix} < \mathbf{b_1}, \mathbf{b_1} > & \ldots & < \mathbf{b_1}, \mathbf{b_m} > \\ \vdots & \vdots & \vdots \\ < \mathbf{b_m}, \mathbf{b_1} > & \ldots & < \mathbf{b_m}, \mathbf{b_m} > \end{bmatrix}, \mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}, \mathbf{y} = \begin{bmatrix} \sum_{i=1}^{m} x_i < \mathbf{b_1}, \mathbf{b_i} > \\ \vdots \\ \sum_{i=1}^{m} x_i < \mathbf{b_m}, \mathbf{b_i} > \end{bmatrix} = \begin{bmatrix} < \mathbf{b_1}, \mathbf{v} > \\ \vdots \\ < \mathbf{b_m}, \mathbf{v} > \end{bmatrix} \implies \mathbf{Ax} = \mathbf{y}$
  - Thus, our coordinates $\mathbf{x} = \mathbf{A^{-1}y}$
  - Special case: if $\{\mathbf{b_j}\}$ are orthonormal with respect to $< \cdot, \cdot >$
    $\mathbf{A} = I \implies \mathbf{x} = \mathbf{y} = \begin{bmatrix} < \mathbf{b_1}, \mathbf{v} > \\ \vdots \\ < \mathbf{b_m}, \mathbf{v} > \end{bmatrix}$
- Inner products can directly decompose vectors into an orthonormal basis.

Unitary Matrices

- A matrix $Q \in \mathbb{C}^{m\times m}$ is called **unitary** if $Q^HQ = I$, in other words, $Q^{-1} = Q^H$
- Corresponding terminology for real matrices is:
  - A matrix $Q \in \mathbb{R}^{m\times m}$ is called **orthogonal** if $Q^TQ = I$, in other words, $Q^{-1} = Q^T$
- In both, the columns of Q are orthogonal with respect to the standard dot product.

Rank-One Matrices

- A matrix $A \in \mathbb{C}^m$ has rank one if and only if it can be written as $\mathbf{xy^H}$
- A matrix $A \in \mathbb{R}^m$ has rank one if and only if it can be written as $\mathbf{xy^T}$
- Note the action of a rank one matrix on a vector is in general: it takes an inner product with $\mathbf{v}$ and uses the result to scale $\mathbf{u}$

$$(\mathbf{u} \otimes \mathbf{v})\mathbf{x} = (\mathbf{u}\mathbf{v}^H)\mathbf{x} = \mathbf{u}(\mathbf{v}^H\mathbf{x}) = \mathbf{u}\langle \mathbf{v}, \mathbf{x} \rangle$$

Inner Product Properties

- Pythagorean Theorem: If <**v, u**>=0, then $\underbrace{< \mathbf{v}, \mathbf{v} >}_{a^2} + \underbrace{< \mathbf{u}, \mathbf{u} >}_{b^2} = \underbrace{< \mathbf{v}+\mathbf{u}, \mathbf{v}+\mathbf{u} >}_{c^2}$
- Cauchy-Schwarz inequality: $|\langle \mathbf{u}, \mathbf{v} \rangle|^2 \leq \langle \mathbf{u}, \mathbf{u} \rangle \langle \mathbf{v}, \mathbf{v} \rangle$
  - For geometric vectors, $(\mathbf{u} \cdot \mathbf{v})^2 = len^2(\mathbf{u}) len^2(\mathbf{v}) \cos^2(\alpha) \leq len^2(\mathbf{u}) len^2(\mathbf{v})$

Lecture 7 - Norm

Norms

- A **norm** for vector space V is a function $\| \cdot \| : V \to \mathbb{R}$ satisfying the following properties:
  - Positivity: $\|\mathbf{v}\| \geq 0$, with $\|\mathbf{v}\| = 0$ if and only if $\mathbf{v} = 0$
  - Homogeneity: $\|\alpha \mathbf{v}\| = |\alpha| \|\mathbf{v}\|$
  - Triangle inequality: $\|\mathbf{v} + \mathbf{u}\| \leq \|\mathbf{v}\| + \|\mathbf{u}\|$

p-norms

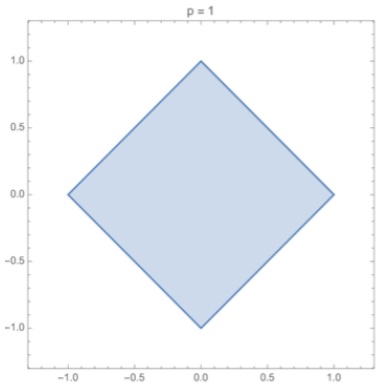
- A very important family of norms for $\mathbb{C}^m$ is called the p or l_p norms.

  $\|\mathbf{x}\|_p = (\sum_{i=1}^{m} |x_i|^p)^{\frac{1}{p}} \quad 1 \leq p \leq \infty$

- Common cases
  - "Taxicab" or "Manhattan distance": $p = 1 \implies \|x\|_1 = \sum_{i=1}^{m} |x_i|$
  - "Euclidean length": $p = 2 \implies \|x\|_2 = \sqrt{\sum_{i=1}^{m} |x_i|^2} = \sqrt{\mathbf{x}^H\mathbf{x}}$

- Taking the limit $p \to \infty$, the largest value dominates. $p = \infty \implies \|x\|_\infty = \max_{1 \le i \le m} |x_i|$

- p-norm visualizations in $\mathbb{R}^2$
  - One way to visualize a norm is to plot its "unit ball," the set of points within distance of the origin according to the norm.
  - When $p = 1$, this is the diamond shape bounded by lines $|x| + |y| = 1$
  - When $p = 2$, this is just a circular disk
  - When $p = \infty$, this is the square bounded by $\max(|x|, |y|) = 1$



1-norm

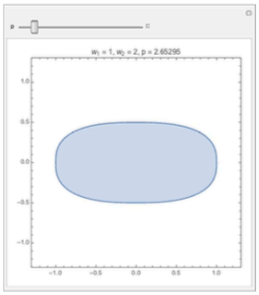
Weighted Norms

- Given a nonsingular matrix W, we can define the norm: $\|\mathbf{x}\|_W = \|W\mathbf{x}\|_p$ using any of the p-norms for the right-hand side.

- In the special case where $W = \text{diag}(w_1, \cdots, w_m)$ is a diagonal matrix and using 2-norm:

$$\| \mathbf{x} \|_W = \left(\sum_{i=1}^{m} |w_i x_i|^2 \right)^{\frac{1}{2}} = \sqrt{\mathbf{x}^H W^H W \mathbf{x}}$$

This is actually norm induced by the inner product whose "B" matrix is (hermitian!) $W^H W$.



- Intuition: entries of x are interpreted as components in the column basis of W

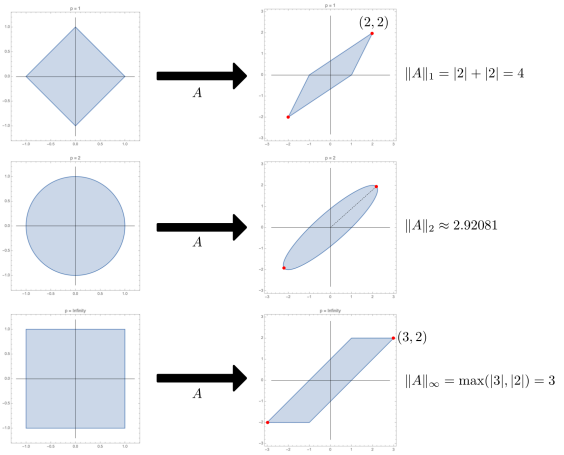
Induced Norms

- Vector norms provide a very useful way to define the norm of a matrix that respects its role as representing a linear transformation.
  - The "size" of a matrix will be the most it can stretch a vector it is applied to.
- Given a pair of vector norms $\|\cdot\|_{(n)}, \|\cdot\|_{(m)}$ for the input and output spaces of $A \in \mathbb{C}^{m \times n}$, the induced matrix norm $\|A\|_{m,n}$ is defined as:

$$\|A\|_{(m,n)} := \max_{\substack{\mathbf{x} \in \mathbb{C}^n \\ \mathbf{x} \neq \mathbf{0}}} \frac{\|A\mathbf{x}\|_{(m)}}{\|\mathbf{x}\|_{(n)}} = \max_{\substack{\mathbf{x} \in \mathbb{C}^n \\ \|\mathbf{x}\|_{(n)} = 1}} \|A\mathbf{x}\|_{(m)}$$

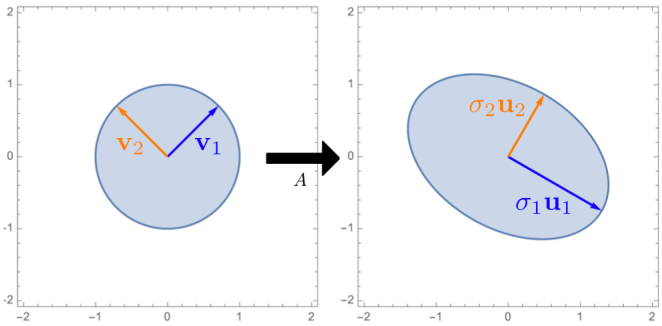
- The second expression is most intuitive: how large can an input vector on the unit circle for $\|\cdot\|_{(n)}$ become?
- If the input and output norms are the same (e.g. (m)=(n)=p), we denote the induced norm just as $\|A\|_p$
- For a diagonal matrix, $\|A\|_p = \max_i a_i$ (proof see picture in the right)

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



Lecture 8 & 9 - Singular Value Decomposition

Induction



- $\mathbf{u_1}, \mathbf{u_2}$ are the **unit** axis vectors for the ellipse
  - Must be orthogonal ($\mathbf{u_1}^H\mathbf{u_2} = \mathbf{0}$)
- $\sigma_1\mathbf{u_1}, \sigma_2\mathbf{u_2}$ are the the ellipse's semi-major and semi-minor axes
- $\mathbf{v_1}, \mathbf{v_2}$ are the **unit** pre-images of $\sigma_1\mathbf{u_1}, \sigma_2\mathbf{u_2}$: $A\mathbf{v_1} = \sigma_1\mathbf{u_1}, A\mathbf{v_2} = \sigma_2\mathbf{u_2}$
  - Must be orthogonal ($\mathbf{v_1}^H\mathbf{v_2} = \mathbf{0}$)
- Organizing these facts into a matrix equation:

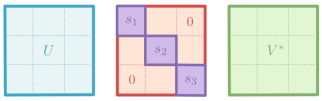
$$\underbrace{\left[\mathbf{u_1} \,|\, \mathbf{u_2}\right]}_{U} \underbrace{\begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}}_{\Sigma} = \left[\sigma_1\mathbf{u_1} \,|\, \sigma_2\mathbf{u_2}\right] = A \underbrace{\left[\mathbf{v_1} \,|\, \mathbf{v_2}\right]}_{V}$$

- Because both U and V are **unitary** $U^HU = V^HV = I_{2\times 2}$ since $\mathbf{u_j}$ and $\mathbf{v_j}$ are orthonormal
- We have $A = U\Sigma V^H$, it implies applying A can be decomposed into following steps
  - Rotate/reflects V^H
  - Applies axis-aligned scale Σ
  - Rotate/reflects again U

SVD

- Singular values are $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_p \geq 0$, p=$min(m, n)$, diagonal entries in Σ

The Singular Value Decomposition



Given $A \in \mathbb{C}^{m \times n}$, a **singular value decomposition (SVD)** of A is a factorization:

$$A = U\Sigma V^H \quad \text{where} \quad \begin{cases} U \in \mathbb{C}^{m \times m} & \text{is unitary,} \\ \Sigma \in \mathbb{C}^{m \times n} & \text{is diagonal,} \\ V \in \mathbb{C}^{n \times n} & \text{is unitary.} \end{cases}$$

Following the standard convention, we assume the **nonnegative** diagonal entries σ_j of Σ are ordered $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, where $p = \min(m, n)$.

- Note: the columns of V and U form an *orthonormal basis* for the input and output spaces $\mathbb{C}^n$ and $\mathbb{C}^m$, respectively.
  - Columns of U are called "left singular vectors" $\mathbf{u}_j$ and columns of V are called "right singular vectors" $\mathbf{v}_j$.

- The columns of V and U form an orthonormal basis for the input and output space $\mathbb{C}^n$ and $\mathbb{C}^m$
  - Columns of U are called "left singular vectors" u_j
  - Columns of V are called "right singular vectors" v_j

SVD's Power

- Easily compute determinants when m=n

$$|det(A)| = |det(U\Sigma V^H)| = |det(U)||det(\Sigma)||det(V^H)| = 1 * |det(\Sigma) * 1 = \sum_{i=1}^{m} \sigma_{mm}$$

- Easily computer inverse: $A^{-1} = (U\Sigma V^H)^{-1} = (V^H)^{-1}\Sigma^{-1}U^{-1} = V\Sigma^{-1}U^H$, with $\Sigma^{-1} = diag(1/\sigma_1, \ldots, 1/\sigma_m)$
- Prove row rank=column rank
- Reveals normal bases for the **nullspace** and **range** of A
  - span($u_1, \ldots, u_r$) = range(A)
  - span($v_{r+1}, \ldots, v_n$=$\mathcal{N}(A)$

- Reveals that row rank = column rank! Suppose the singular values are $\sigma_1 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_p = 0$.

$$A = \left[\begin{array}{c|c|c|c|c} \mathbf{u}_1 & \cdots & \mathbf{u}_r & \mathbf{u}_{r+1} & \cdots \end{array}\right] \begin{bmatrix} \sigma_1 & & & & \\ & \ddots & & & \\ & & \sigma_r & & \\ & & & 0 & \\ & & & & \ddots \end{bmatrix} \left[\begin{array}{c} \mathbf{v}_1^H \\ \hline \vdots \\ \hline \mathbf{v}_r^H \\ \hline \mathbf{v}_{r+1}^H \\ \hline \vdots \end{array}\right]$$

$$= \underbrace{\left[\begin{array}{c|c|c} \mathbf{u}_1 & \cdots & \mathbf{u}_r \end{array}\right]}_{\hat{U}} \underbrace{\begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{bmatrix}}_{\hat{\Sigma}} \underbrace{\left[\begin{array}{c} \mathbf{v}_1^H \\ \hline \vdots \\ \hline \mathbf{v}_r^H \end{array}\right]}_{\hat{V}^H}$$

Because SVD lets us determine rank by counting the nonzero singular values, it is called "rank-revealing."

  - A's ***column rank*** is r
    - $A's$ columns are a linear combination of $\{\mathbf{u}_1, \cdots, \mathbf{u}_r\}$ $\implies$ ***column rank*** $\leq r$
    - Any $\mathbf{u} \in \text{span}(\mathbf{u}_1, \cdots, \mathbf{u}_r)$ can be written as $A\mathbf{x}$ with $\mathbf{x} = \hat{V}\hat{\Sigma}^{-1}\hat{U}^H\mathbf{u}$ $\implies$ ***column rank*** $\geq r$
  - A's **row rank** is r
    - A's rows are a linear combination of $\{\mathbf{v}_1^H, \cdots, \mathbf{v}_r^H\}$, $\implies$ ***row rank*** $\leq r$
    - Any vector $\mathbf{v} \in \text{span}(\mathbf{v}_1, \cdots, \mathbf{v}_r)$ can be written as $A^H\mathbf{x}$ with $\mathbf{x} = \hat{U}\hat{\Sigma}^{-1}\hat{V}^H\mathbf{v}$ $\implies$ ***row rank*** $\geq r$

Proof of Existence & Uniqueness of SVD

- An unique **SVD** exists for **any** $A \in \mathbb{C}^{m \times n}$ (Proof See slides 09-03)

SVD vs. Eigendecomposition

SVD vs. Eigendecomposition

$$A = \underbrace{U\Sigma V^H}_{\text{SVD}} \quad \text{vs.} \quad A = \underbrace{X\Lambda X^{-1}}_{\text{Eigendecomposition}}$$

- You may remember that eigenvalue decompositions also diagonalize matrices.
- Some key differences:
  - The eigendecomposition insists on using the ***same*** change of basis for the input and output space.
  - Consequently, the eigendecomposition only exists for ***square matrices***—and ***not even all square matrices***!
  - X is not a unitary matrix in general.
- However, you can compute the SVD via an eigendecomposition:
  - Consider the "square" of the singular value decomposition, $A^HA = V\Sigma^\top U^H U\Sigma V^H = V\Sigma^\top \Sigma V^H$
  - The right-hand side is actually an eigendecomposition with $\Lambda = \Sigma^\top\Sigma$, $X = V$
    - The singular values are the square root of these eigenvalues.
    - The right-singular vectors are the eigenvectors.
    - The left singular vectors can be found from AV.

Lecture 10 - Conditioning of Computational Problems

Generic Computation Problem

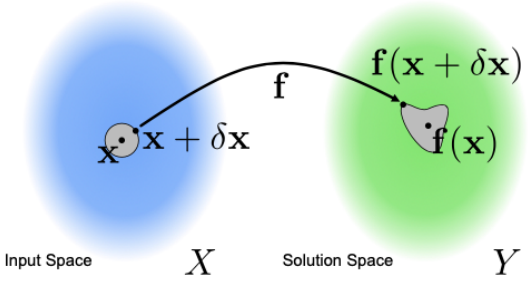
- Abstract viewpoint: all computational problems can be interpreted as a ***nonlinear*** function ***f*** mapping from inputs to outputs
  - Assume inputs and outputs live in vector spaces X and Y
  - Assume we have norms for both X and Y
- We will call computing **f(x)** "solving a problem instance."
- Central question: how accurately can we evaluate **f(x)** on a computer?

Conditioning

- How does an inaccuracy/roundoff error in **x** affect the computed result **f(x)** assuming all results are computed exactly?
  - Given a "small" perturbation to the input δx, how large can the perturbation to the output $\delta f := f(x + \delta x) - f(x)$ be?
  - Stated differently: "How much does **f** magnify errors/uncertainties?"
  - This will give us a bound on how accurately we can expect to solve a problem instance.

Relative and Absolute Error Measures

- How do we define the "size" of perturbations?
  - We assumed X and Y are normed vector spaces, so we can use each space's norm, $\|\cdot\|_X$ and $\|\cdot\|_Y$
  - **Absolute** perturbation/error magnitude:
    - $\|(x + \delta x) - x\|_X = \|\delta x\|_X$
    - $\|f(x + \delta x) - f(x)\|_Y = \|\delta f\|_Y$
  - **Relative** perturbation/error magnitude:
    - $\dfrac{\|(x + \delta x) - x\|_X}{\|x\|_X} = \dfrac{\|\delta x\|_X}{\|x\|_X}$
    - $\dfrac{\|f(x + \delta x) - f(x)\|_Y}{\|f(x)\|_Y} = \dfrac{\|\delta f\|_Y}{\|f(x)\|_Y}$

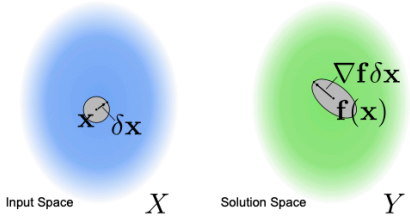


Absolute Condition Numbers

- Definition: $\hat{\kappa} := \lim_{h \to 0} \max_{\substack{\delta x \\ 0 < \|\delta x\| \leq h}} \frac{\|\delta f\|}{\|\delta x\|}$
- Using **absolute** error measures: Given a 'small' perturbation to the input δx, how large can the perturbation to the output $\delta f := f(x + \delta x) - f(x)$ be?
- Worst-case analysis: meaning we must maximize over all input possible perturbations.
- When f is differentiable, we have $\hat{\kappa} = \|\nabla f\|$ (proof see below)

Relative Condition Numbers

- Definition: $\kappa := \lim_{h \to 0} \max_{\substack{\delta x \\ 0 < \|\delta x\| \leq h}} \frac{\|\delta f\|}{\|f(x)\|} / \frac{\|\delta x\|}{\|x\|}$
- Using **relative** error measures: Given a 'small' perturbation to the input δx, how large can the perturbation to the output $\delta f := f(x + \delta x) - f(x)$ be?
- When f is differentiable, we have $\kappa = \frac{\|\nabla f\|}{\|f(x)\| / \|x\|}$ (proof see below)



$$\hat{\kappa} := \lim_{h \to 0} \max_{\substack{\delta \mathbf{x} \\ 0 < \|\delta \mathbf{x}\| \leq h}} \frac{\|\delta \mathbf{f}\|}{\|\delta \mathbf{x}\|}$$

- If $\mathbf{f}(\mathbf{x})$ is differentiable, we can construct a first-order Taylor approximation:

$$\mathbf{f}(\mathbf{x} + \delta \mathbf{x}) = \mathbf{f}(\mathbf{x}) + \nabla \mathbf{f}(\mathbf{x}) \delta \mathbf{x} + O(\|\delta \mathbf{x}\|^2) \quad \Longrightarrow \quad \delta \mathbf{f}(\mathbf{x}) = \nabla \mathbf{f}(\mathbf{x}) \delta \mathbf{x} + O(\|\delta \mathbf{x}\|^2),$$

  where $\nabla \mathbf{f}$ is the **Jacobian** matrix whose $(i, j)^{\text{th}}$ entry holds $\frac{\partial f_i}{\partial x_j}$.
- Note: after linearizing, the map from $\delta \mathbf{x}$ to $\delta \mathbf{f}$ is just the matrix-vector multiplication $\delta \mathbf{f} \approx \nabla \mathbf{f} \delta \mathbf{x} = \sum_j \frac{\partial f_i}{\partial x_j} \delta x_j$

Absolute Condition Numbers Proof (1)

III-Conditioned Problems

$$\underbrace{\hat{\kappa} = \|\nabla \mathbf{f}\|}_{\text{Absolute}}, \qquad \underbrace{\kappa = \frac{\|\nabla \mathbf{f}\|}{\|\mathbf{f}(\mathbf{x})\| / \|\mathbf{x}\|}}_{\text{Relative}}$$

- We will use the ***relative*** condition number κ in this course.
  It is a dimensionless quantity and compatible with the relative error introduced by floating point.
- Given a relative uncertainty $\|\delta \mathbf{x}\| / \|\mathbf{x}\| \leq \epsilon$, we can only expect to compute $\mathbf{f}(\mathbf{x})$ with accuracy:

$$\frac{\|\delta \mathbf{f}\|}{\|\mathbf{f}(x)\|} \leq \kappa \epsilon.$$

- If $\kappa \gg 1$ (e.g., 10^6 or 10^{16}), we may not be able to meaningfully solve the problem! Such problems are called ill-conditioned. Problems with $= 1, 10^2$, etc. are called well-conditioned.

Lecture 11 - Matrix Condition Numbers

Condition Number of a Matrix

- The condition number of a square matrix $A \in \mathbb{C}^{m \times m}$ relative to a norm $\|\cdot\|$ is defined as $\kappa(A) := \|A\|\|A^{-1}\|$ (Proof see below)
  - This condition number is attached to matrix A itself, not to a particular problem
  - If $\kappa(A)$ is small, A is "well-conditioned"
  - If $\kappa(A)$ is large, A is "ill-conditioned"
  - If A is singular, we write $\kappa(A) = \infty$
- When using the 2-norm for $\|\cdot\|$, we have $\|A\|_2 = \sigma_1$, $\|A^{-1}\|_2 = \sigma_m$ and can conclude $\kappa(A) = \dfrac{\sigma_1}{\sigma_m}$ (for $\|\cdot\| = \|\cdot\|_2$)

Condition Numbers: Matrix Multiplication

- Important example: consider matrix multiplication $\mathbf{f}(\mathbf{x}) = A\mathbf{x}$ for $A \in \mathbb{C}^{m \times n}$
  - In this case $\nabla \mathbf{f} = A$
  - Let $\|\mathbf{x}\|$, $\|A\mathbf{x}\|$ denote arbitrary norms for $\mathbb{C}^n$ and $\mathbb{C}^m$, and $\|A\|$ the corresponding induced matrix norm.
  - Then for a given $\mathbf{x}$:

$$\kappa = \frac{\|\nabla \mathbf{f}\|}{\|\mathbf{f}(\mathbf{x})\| / \|\mathbf{x}\|} = \frac{\|A\|}{\|A\mathbf{x}\| / \|\mathbf{x}\|} = \|A\| \frac{\|\mathbf{x}\|}{\|A\mathbf{x}\|}.$$

  - When A is square and nonsingular, we can use the fact that $\frac{\|\mathbf{x}\|}{\|A\mathbf{x}\|} = \frac{\|A^{-1}\mathbf{b}\|}{\|\mathbf{b}\|} \leq \|A^{-1}\|$ to say that **for any** $\mathbf{x}$:

$$\kappa \leq \|A\|\|A^{-1}\|,$$

  and there exists some $\mathbf{x}$ for which this upper bound is attained ($\kappa = \|A\|\|A^{-1}\|$).

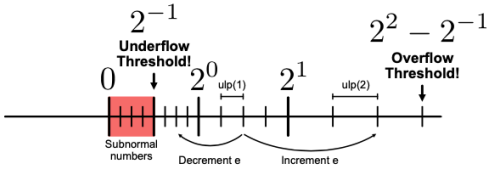
Lecture 12 & 13 - Floating Point

Floating Point Representation

$$\underbrace{3.\overbrace{14159}^{\text{fraction}}}_{\text{significand}} \times \underbrace{10}_{\text{base}}{}^{\overbrace{-5}^{\text{exponent}}}$$

- A floating point representation is defined by its:
  - Base β (there are standards for $\beta \in \{2,10,16\}$, but essentially all computation uses binary $\beta = 2$)
  - Precision $p \in \mathbb{Z}^+$, the number of bits/digits for storing the significand; and
  - Range for the integer exponent, $[e_{min}, e_{max}]$
- To ensure a unique encoding, we use "**normalized**" or "**normal**" floating point numbers wherever possible. This means shifting the significand and adjusting the exponent so that the significand looks like $1.f$.
- In binary ($\beta = 2$) the "**normal**" numbers are in the form: (where f is a *(p-1)* bits integer)
  $(-1)^s 1.f \times 2^e, \quad f \in \{0,\ldots,2^{p-1}-1\}, \quad s \in \{0,1\}, \quad e \in \{e_{min}, \ldots, e_{max}\}$
- ± 0 and the "**subnormal**" or " **denormal**" numbers are in the form:
  $(-1)^s 0.f \times 2^{e_{min}}, \quad f \in \{0,\ldots,2^{p-1}-1\}, \quad s \in \{0,1\}, \quad e = e_{min} - 1$

- Let's consider the space of of floating point numbers in the system $\beta = 2, p = 3, e_{\min} = -1, e_{\max} = 1$
  - The "normal" numbers are in the form:
    $$(-1)^s 1.f \times 2^e \qquad f \in \{00, \cdots, 11\}, \quad s \in \{0,1\}, \quad e \in \{-1,0,1\},$$
    here s is the "sign bit."
  - When $s = 0$, the normal numbers look like
    $$(1+\underbrace{0\times 2^{-2}}_{.00})\times 2^e,\ (1+\underbrace{1\times 2^{-2}}_{.01})\times 2^e,\ (1+\underbrace{2\times 2^{-2}}_{.10})\times 2^e,\ (1+\underbrace{3\times 2^{-2}}_{.11})\times 2^e$$
  - The "gap" between numbers is $2^{-2}\times 2^e = 2^{e-2}$. In general, this is $2^{e-(p-1)}$.
    This quantity is called the **unit in the last place** or **ulp**(2^e).
    - Increasing e doubles the gaps between numbers, decreasing e halves them:



- We can represent "**subnormal**" or "**denormal**" numbers by setting $e = e_{\min} - 1$.
  - In this mode, the number is interpreted as $(-1)^s 0.f \times 2^{e_{\min}}$ (note the leading 0).
  - "± 0" can then be represented as $f = 0, e = e_{\min} - 1$.
  - "± 0" is always represented like this, but denormal numbers *can be disabled* for performance reasons.

Unit in the last place and Machine ϵ

$$\hat{x} = (-1)^s 1.\underbrace{[f_{p-1}\ldots f_1]}_{p-1 \text{ bit integer } f} \times \beta^e$$

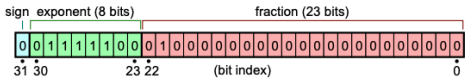
- **Unit in the last place ("Gap")**
  - The next floating number after $\hat{x}$ is found by incrementing f.
  - The "gap" between these numbers is the "**unit in the last place**" $ulp(\hat{x})$
  - This is the "place value" of f_1: $ulp(\hat{x}) = ulp(2^e) = \beta^{-(p-1)}\beta^e = \beta^{e-(p-1)}$
  - The maximum *absolute error* in rounding a real number in $[\hat{x}, \hat{x} + ulp(\hat{x})]$ is $\frac{ulp(\hat{x})}{2}$
  - The maximum *relative error* occurs around $f = 0 \implies \hat{x} = \beta^e$ (the smallest magnitude with exponent e), when rounding $\hat{x} + \overline{0.4999}ulp(\hat{x})$

$$\frac{|x - fl(x)|}{|x|} \leq \frac{|(\beta^e + ulp(\hat{x})/2) - \beta^e|}{|\beta^e + ulp(\hat{x})/2|} < \frac{|ulp(\hat{x})/2|}{|\beta^e|} = \frac{|\beta^{e-(p-1)}/2|}{|\beta^e|} = \beta^{1-p}/2 = ulp(1)/2$$

    - This is our definition of **machine epsilon** $\epsilon = \beta^{1-p}/2 = ulp(1)/2$
    - When $\beta = 2$, this simplifies to $\epsilon = 2^{-p}$

IEEE 754 Floating Point: Single Precision & Double Precision

IEEE 754 Floating Point: Single Precision



- IEEE 754 single precision floating point numbers (`float`) are defined by :
  - $\beta = 2$
  - $p = 24$ (so that 23 bits are used to represent the *fraction* of the significand $1.f$)
  - $e_{\min} = -126, e_{\max} = 127$ ($\approx 10^{-38}$ to 10^{38})
- To represent both negative and positive exponents as a bit string, IEEE 754 uses a somewhat unusual "bias" approach (instead of "sign + magnitude" or two's complement).
  - For single precision, store $\hat{e} \in \{0, \cdots, 255\}$ and define: $e = \hat{e} - 127$.
  - $\{e_{\min}, \cdots, e_{\max}\}$ correspond to $\hat{e} \in \{1, \cdots, 254\}$
  - $\hat{e} = 0$ indicates zeros/denormals.
  - $\hat{e} = 255$ signals $\pm\infty$ when $f = 0$ (e.g., result of $\frac{1}{\pm 0}$), or `NaN` (not a number!) when $f \neq 0$ (e.g., result of $\frac{0}{0}, \infty - \infty$).
  - This is so positive floats sort in the correct order if we reinterpret the bitstring as an integer (simplifies comparison
- The gap between floating point numbers with exponent e is $\text{ulp}(2^e) = 2^{e-(p-1)} = 2^{e-23}$
  - The *relative rounding error* is thus bounded by $\epsilon = \text{ulp}(1)/2 = 2^{-23}/2 = 2^{-24} \approx 6 \times 10^{-8}$.
  - We call this the "**machine epsilon**." Note: some references define $\epsilon = \text{ulp}(1)$ instead...

Single Precision

Fundamental Axiom of Floating Point Arithmetic

- For any $x \in \pm [2^{e_{min}}, 2^{e_{max}}] \subset \mathbb{R}$, the nearest floating point representation satisfies: $fl(x) = x(1 + \delta) \qquad |\delta| \leq \epsilon,$ where $|\delta|$ is the **relative error** $|fl(x) - x|/|x|$.

- Single precision represents numbers with 7-8 digits of accuracy, Double precision gives 16 digits
- IEEE 754 guarantees that the floating point result of, e.g., $x + y$ of two floating point numbers x and y is the exact result rounded to the nearest floating point number.
  - **Fundamental Axiom of Floating Point Arithmetic**: For all floating point numbers $fl(x), fl(y)$, there exists δ with $|\delta| \leq \epsilon$ such that:
    $fl(x) \circledast fl(y) = (fl(x) * fl(y))(1 + \delta)$, where * stands for any of the arithmetic operators +, -, /, ×, and $\circledast$ is the floating point operator.

Floating Point Peculiarities

- Floating point numbers do not behave exactly like real numbers
  - Additive inverses ($\pm n$) are always exactly representable (flip s), but multiplicative inverses ($n, \frac{1}{n}$) are not!
  - Operations are commutative:
    - $a \oplus b = b \oplus a$
    - $a \otimes b = b \otimes a$
  - Operations are not associative (use parentheses carefully)
    - $a \oplus (b \oplus c) \neq (a \oplus b) \oplus c$
    - $a \otimes (b \otimes c) \neq (a \otimes b) \otimes c$

      - Does the following statement hold?

        $$x \neq y \implies (x - y) \neq 0$$

      - Actually, yes! But only with denormals/subnormals enabled...
      - Example: $1.1 \times 2^{e_{min}} - 1.0 \times 2^{e_{min}} = 0.1 \times 2^{e_{min}}$
        Underflows to 0 if denormals are disabled/unsupported.

Because basic identities like $(x * (1/x) = 1$ fail to hold in floating point, you should **almost never** test "$x = y$" for two floating point numbers.

Prefer tests like "$|x - y| <$ `tol`" for some tolerance parameter `tol`.

Error Propagation

- Multiplication
  $z = (x(1 + \delta x)) \otimes (y(1 + \delta y)) = (x(1 + \delta x) * y(1 + \delta y)) * (1 + \delta) \quad |\delta| \leq \epsilon$
  - The **relative** error in this approximation is
    $\frac{|z - xy|}{|xy|} = \frac{|xy(1 + \delta x)(1 + \delta y)(1 + \delta) - xy|}{|xy|} = |(1 + \delta x)(1 + \delta y)(1 + \delta) - 1| = \delta x + \delta y + \delta +$ higher order terms

- Therefore, when multiplying and dividing, the **relative** errors **add**.
- Consequently, multiplication and division are safe since accurate inputs give similarly accurate outputs.

- Addition $z = (x(1+\delta x)) \oplus (y(1+\delta y)) = (x(1+\delta x) + y(1+\delta y)) * (1+\delta) \quad |\delta| \leq \epsilon$
  - The **absolute** error in this approximation is $|z - (x+y)| = |(x + x\delta x + y + y\delta y) + O(\delta) - x - y| = |x\delta x + y\delta y + O(\delta)|$
  - Here, the **absolute** errors of the input $x\delta x$ and $y\delta y$ **add**.
  - This is dangerous since adding two inputs with low relative error can produce an output with high relative error when $|x+y| \ll \max(|x|, |y|)$
  - This is the so called **catastrophic cancellation** phenomenon
  - *Example: calculate* $1 - \sqrt{1-c}$ *(see picture below)*
- **Loss of Digits**
  - We also run into problems when adding numbers of widely-differing magnitude
  - $1.0010 + 0.00013000 = 1.0011$
  - Only registers one of the digits of the smaller number!
  - *Example: harmonic numbers (see picture below)*

Catastrophic Cancellation

- Catastrophic cancellation example:

$$1.23456 \pm 5 \times 10^{-6} - 1.23455 \pm 5 \times 10^{-6} = 0.00001 \pm 5 \times 10^{-6}$$

  - Relative error is now $5 \times 10^{-6} / 1 \times 10^{-5} = 50\%$ despite good accuracy in the inputs.
- Consider trying to solve $x^2 - 2x + c = 0$ for $|c| \ll 1$
  - One of the roots is $1 - \sqrt{1-c}$
  - What's dangerous about this expression?

Floating Point "Exceptions"

- By default, calculations proceed silently, even with unusual inputs:
  - Dividing $x \neq 0$ by zero: $x/0$ gives $\text{sign}(x) * \infty$.
  - $1/\infty$ gives 0
  - Operations like $\sqrt{-1}, 0/0, \infty/\infty, \infty * 0$ produce `NaN`
  - Any operation involving `NaN` produces a `NaN`, ensuring if a `NaN` ever originates in a computation, it propagates to the final result.
  - IEEE 754 comparison rules for `NaN`s may look strange at first glance:
    `NaN cmp NaN` is `false` for any comparison `cmp` in $\{=, \neq, <, >, \leq, \geq\}$
    - Despite associativity, $a + b == b + a$ can be false if a or b is `NaN`!
- Usually verifying the final result is not `NaN` suffices, but IEEE standard provides mechanisms for notifying us immediately when things go wrong.
  - Exception flags `FE_DIVBYZERO, FE_INVALID, FE_INEXACT, FE_OVERFLOW, FE_UNDERFLOW` can be checked after a calculation.
  - On many platforms, exception handling can be enabled so that some or all of these errors "trap" and invoke a custom handler function. (e.g., `feenableexcept` on Linux)

IEEE 754 Rounding Modes

- By default, numbers that cannot be represented exactly are rounded to the **nearest** floating point number.
- However, IEEE 754 requires that three other rounding modes can be selected:
  - Round toward 0
  - Round toward $+\infty$ (analogous to "ceiling")
  - Round toward $-\infty$ (analogous to "floor")
- These modes also modify overflow behavior:
  - Round toward 0 or $-\infty$: overflowing ***positive*** values round down to the largest representable value.
  - Round toward 0 or $+\infty$: overflowing ***negative*** values round up to the most negative representable value.
- Application: *interval arithmetic*
  - Compute lower and upper bounds l, u for the exact result $x \in [l, u]$ of every operation
  - At the end of a computation, you know the exact answer must be within the computed bounds.
  - Small interval $\Rightarrow$ answer known precisely. However, bounds are often overly pessimistic/conservative.

Lecture 14 - C++ Types

Types in C++

- Every variable and expression in C/C++ has a **static** (known at compile-time) type.
  - Floating point:

`float`	IEEE 754 single-precision (32-bit)
`double`	IEEE 754 double-precision (64-bit)

  - Signed/Unsigned integers:

`short, unsigned short`	*usually* 16-bit
`int, unsigned int`	*usually* 32-bit
`long, unsigned long`	64-bit on modern Linux machines, 32-bit on Windows...

  - Fixed-width integer types: `#include <cstdint>`

`int{8,16,32,64}_t`	signed integer with **exactly** 8, 16, ... bits.
`uint{8,16,32,64}_t`	unsigned integer with **exactly** 8, 16, ... bits.

Type Conversions in C++

- See more rules here.
  - For binary operators with mismatched types, one operand converts to the other's type.
  - What are the following expressions' types?
    - `1.0f / 2` `float`
    - `1.0f / 2.0` `double`
    - `1u + (-2)` `unsigned int` (value is `4294967295`)
    - `1u + (-2ll)` `long long` (value is `-1`)
  - Conversion rules:
    - Integers are *always* promoted to floating point.
    - Narrower types are converted to wider types.
    - Signed integers of the "same width" as unsigned are converted to unsigned.
    - See more rules here.
  - These implicit conversions can be counterintuitive/unexpected and lead to bugs!
    - It is best to be **explicit** when it matters (using **casts**)!

Casting in C++

- Values can be explicitly converted to another type using casts.
- In C++ there are several different kinds of casts with varying degrees of safety:

`(float)(1)`	C-style cast: most powerful/dangerous; attempt C++ casts below in increasing order of danger.
`float(1)`	Functional cast: "syntactic sugar" for C-style cast (equivalent)
`const_cast<T>(expr)`	Add/remove `const` qualifier
`static_cast<T>(expr)`	Apply any available implicit conversion rules, cast base pointer to derived pointer, etc.
`reinterpret_cast<T>(expr)`	Reinterpret bits as if they were of type `T`. This can be used to inspect bits of a `float`.

- More on this
- For numerical expressions, we can generally use C-style or functional casts.

- How to check if a value v stored in a *double* is representable by a *float*?
  - Cast to float and then back to double: test if *double(float(v)) == v*.
- Functional Argument Type
  - For function calls, the compiler tries to implicitly convert arguments to the accepted types (see right)

```
#include<iostream>
int f(int i) {
    return i;
}

int main() {
    std::cout << f(1.98) << std::endl;
    return 0;
}
```

print 1

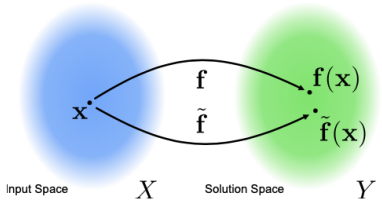
- Templates in C++
  - Templates enable us to write generic code that can be instantiated for different types (and much more…)
  - The compiler automatically generates a distinct functions for each T used.

Lecture 15 - Stability

How to analyze error accumulated when computing $f(x + \delta x)$?

Accuracy of Algorithms

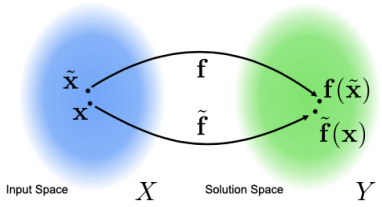
- We view an algorithm for problem f as another nonlinear function $\tilde{f} : X \to Y$
- Evaluating $\tilde{f}(x)$ to solve a problem instance $f(x)$ entails:
  - Rounding true input **x** to the computer's number representation; and then
  - Executing a finite sequence of arithmetic operations (a computer program implementing some numerical method), accumulating roundoff error in every step.



- Def: Ideally $\tilde{f}$ is "close" to f, achieving a low relative error (high accuracy) for all inputs $x \in X$: $\dfrac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|} = O(\epsilon)$

Stability

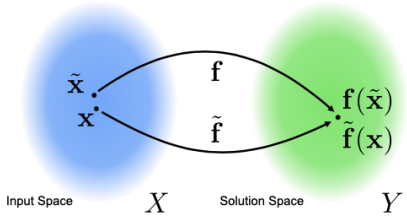
- Accuracy is too much to ask for. Stability is a weaker, more realistic goal.
- Def: An algorithm $\tilde{f}$ is **stable** if for each $x \in X$: $\dfrac{\|\tilde{f}(x) - f(\tilde{x})\|}{\|f(\tilde{x})\|} = O(\epsilon)$ for some $\tilde{x}$ such that $\dfrac{\|x - \tilde{x}\|}{\|x\|} = O(\epsilon)$



- It computes almost the right solution to almost the right problem.
- It's sometimes called "mixed stability" since both the problem instance and the solution are allowed to perturb.
- Accurate algorithms are clearly stable since $\frac{\|\tilde{f}(x) - f(\tilde{x})\|}{\|f(x)\|} = O(\epsilon)$ holds for $\tilde{x} = x$

Backward Stability

- Stronger but simpler condition than stability.
- Def: Algorithm $\tilde{f}$ is **backward stable** if $\forall x \in X$: $\tilde{f}(x) = f(\tilde{x})$ for some $\tilde{x}$ such that $\frac{\|x - \tilde{x}\|}{\|x\|} = O(\epsilon)$.



- It computes the exact solution to almost the right problem.
- $\frac{\|x - \tilde{x}\|}{\|x\|}$ is called the (relative) backward error. (How much the input must change to make our approximate solution exact)

Meaning of $O(\epsilon)$

- The statement that an expression is $O(\epsilon)$ refers to the limit $\epsilon \to 0$.That is, we consider a sequence of higher- and higher-precision number systems.

Example: Floating Point Addition

- We saw earlier that floating point addition $\oplus$ is ***dangerous*** because *absolute* errors add and relative errors are not kept under control.
  - In other words, there are inputs for which the result of addition will not be **accurate** when cancellation occurs.
  - This is due to the conditioning of the problem $f(x_1, x_2) = x_1 + x_2$. We shouldn't blame the algorithm!
- The algorithm $\tilde{f}(x_1, x_2) = \mathrm{fl}(x_1) \oplus \mathrm{fl}(x_2)$ is still *backward stable* (and thus *stable*):

$$
\begin{aligned}
\tilde{f}(x_1, x_2) &= \mathrm{fl}(x_1) \oplus \mathrm{fl}(x_2) \\
&= x_1(1+\delta_1) \oplus x_2(1+\delta_2) && |\delta_1|, |\delta_2| \leq \epsilon \\
&= (x_1(1+\delta_1) + x_2(1+\delta_2))(1+\delta_3) && |\delta_1| \leq \epsilon \quad \text{(Fundamental axiom of fp arithmetic)} \\
&= x_1(1+\delta_4) + x_2(1+\delta_5) \\
&= f(x_1(1+\delta_4), x_2(1+\delta_5)) \\
&\quad \text{with} \quad \delta_4 = (1+\delta_1)(1+\delta_3) - 1 = \delta_1 + \delta_3 + \delta_1\delta_3 \quad |\delta_4| \leq 2\epsilon + \epsilon^2 \\
&\quad \text{with} \quad \delta_5 = (1+\delta_2)(1+\delta_3) - 1 = \delta_2 + \delta_3 + \delta_2\delta_3 \quad |\delta_5| \leq 2\epsilon + \epsilon^2.
\end{aligned}
$$

$\tilde{f}(x_1, x_2)$ computes the exact result for perturbed inputs $\tilde{\mathbf{x}} = \begin{bmatrix} x_1(1+\delta_4) \\ x_2(1+\delta_5) \end{bmatrix}$, with $\|\tilde{\mathbf{x}} - \mathbf{x}\| = \left\| \begin{bmatrix} x_1\delta_4 \\ x_2\delta_5 \end{bmatrix} \right\| \leq \|\mathbf{x}\|(2\epsilon + \epsilon^2) \leq C\epsilon\|\mathbf{x}\|$.

- $\frac{\|x - \tilde{x}\|}{\|x\|} = O(\epsilon)$ really means that for all ϵ small enough: $\|x - \tilde{x}\| = C\epsilon\|x\|$
  - constant C independent of the input x
  - moving $\|x\|$ to right side handles $\|x\| = 0$
  - In other words, the backward error for even the worst x must eventually shrink proportionally to ϵ (or faster).

What Norm?

- It doesn't matter.

Algorithm $\tilde{\mathbf{f}}$ is **backward stable** if $\forall \mathbf{x} \in X$:

$$\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}}) \quad \text{for some} \quad \tilde{\mathbf{x}} \quad \text{such that} \quad \|\mathbf{x} - \tilde{\mathbf{x}}\| \leq C\epsilon \|\mathbf{x}\|.$$

- Which vector norm should we use to measure stability (or accuracy)?
- It does not matter. All finite-dimensional vector norms are equivalent!
  - By this we mean for any two norms $\|\cdot\|_a$ and $\|\cdot\|_b$, there are positive constants C_1 and C_2 such that:

    $$C_1 \|\mathbf{x}\|_a \leq \|\mathbf{x}\|_b \leq C_2 \|\mathbf{x}\|_a \qquad \forall \mathbf{x}$$

  - Therefore, after proving backward stability using $\|\cdot\|_a$:

    $$\|\mathbf{x} - \tilde{\mathbf{x}}\|_a \leq C\epsilon \|\mathbf{x}\|_a,$$

    we can conclude:

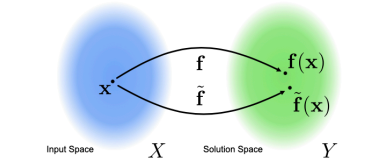
    $$\|\mathbf{x} - \tilde{\mathbf{x}}\|_b \leq C_2 \|\mathbf{x} - \tilde{\mathbf{x}}\|_a \leq C_2 C\epsilon \|\mathbf{x}\|_a \leq C_2 C\epsilon \frac{\|\mathbf{x}\|_b}{C_1},$$

    proving backward stability under $\|\cdot\|_b$ just with a different constant $\frac{C_2}{C_1}C$.

Stability Summary

An algorithm $\tilde{\mathbf{f}}$ is **accurate** if $\forall \mathbf{x} \in X$:

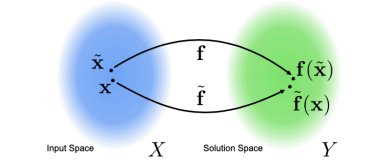
$$\frac{\|\tilde{\mathbf{f}}(\mathbf{x}) - \mathbf{f}(\mathbf{x})\|}{\|\mathbf{f}(\mathbf{x})\|} = O(\epsilon).$$



Accuracy: Approximate answer to the original problem.

An algorithm $\tilde{\mathbf{f}}$ is **stable** if $\forall \mathbf{x} \in X$:

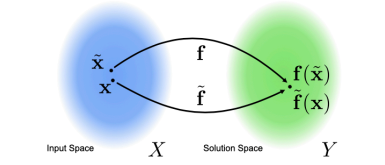
$$\frac{\|\tilde{\mathbf{f}}(\mathbf{x}) - \mathbf{f}(\tilde{\mathbf{x}})\|}{\|\mathbf{f}(\tilde{\mathbf{x}})\|} = O(\epsilon) \quad \text{for some } \tilde{\mathbf{x}} \text{ such that } \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} = O(\epsilon).$$



Stability: Approximate answer to a nearby problem.

Algorithm $\tilde{\mathbf{f}}$ is **backward stable** if $\forall \mathbf{x} \in X$:

$$\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}}) \quad \text{for some } \tilde{\mathbf{x}} \text{ such that } \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} = O(\epsilon).$$



Backward Stability: Exact answer to a nearby problem.

Accuracy vs. Backward Stability

- Algorithms mapping from lower-dimensional input space X to higher-dimensional input space Y generally cannot be backward stable.
  - Arbitrarily small roundoff error can perturb the result outside the image $f(X) \subset Y$

- For $\kappa \ll 1$we can hope for accuracy but not backward stability.
- For $\kappa \gg 1$ we can hope for backward stability but not accuracy.
- In both cases, we can hope for stable algorithms.
- When an algorithm is stable, its accuracy reflects the condition number.

Accuracy of a Backward-Stable Algorithm

- This leads us to consider the connection between backward stability and accuracy: how accurate will a backward stable algorithm $\tilde{\mathbf{f}}(\mathbf{x})$ be?
- By definition of backward stability, for all $\mathbf{x}$ there exists some $\tilde{\mathbf{x}}$ such that:

$$\tilde{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\tilde{\mathbf{x}}), \qquad \text{and} \qquad \frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|} = O(\epsilon).$$

  - Recall the definition of the condition number for a problem instance $\mathbf{f}(\mathbf{x})$:

$$\kappa(\mathbf{x}) = \lim_{h \to 0} \max_{\|\delta\mathbf{x}\| \le h} \frac{\|\mathbf{f}(\mathbf{x} + \delta\mathbf{x}) - \mathbf{f}(\mathbf{x})\|}{\|\mathbf{f}(\mathbf{x})\|} \Big/ \frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|}.$$

$$\implies \max_{\|\delta\mathbf{x}\| \le h} \frac{\|\mathbf{f}(\mathbf{x} + \delta\mathbf{x}) - \mathbf{f}(\mathbf{x})\|}{\|\mathbf{f}(\mathbf{x})\|} \Big/ \frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|} = \kappa(\mathbf{x}) + o(1)$$

$o(1)$ denotes terms shrinking to zero as $\|\delta\mathbf{x}\| \to 0$.

  - Perturbation $\delta\mathbf{x} = \tilde{\mathbf{x}} - \mathbf{x}$ can be no worse than the maximizer for $h = \|\tilde{\mathbf{x}} - \mathbf{x}\|$:

$$\frac{\|\mathbf{f}(\mathbf{x} + (\tilde{\mathbf{x}} - \mathbf{x})) - \mathbf{f}(\mathbf{x})\|}{\|\mathbf{f}(\mathbf{x})\|} \le (\kappa(\mathbf{x}) + o(1)) \frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|}.$$

  - But $\mathbf{f}(\mathbf{x} + (\tilde{\mathbf{x}} - \mathbf{x})) = \mathbf{f}(\tilde{\mathbf{x}}) = \tilde{\mathbf{f}}(\mathbf{x})$, and we conclude $\tilde{\mathbf{f}}(\mathbf{x})$ has accuracy:

$$\frac{\|\tilde{\mathbf{f}}(\mathbf{x}) - \mathbf{f}(\mathbf{x})\|}{\|\mathbf{f}(\mathbf{x})\|} \le (\kappa(\mathbf{x}) + o(1)) \frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|} = \kappa(\mathbf{x}) O(\epsilon).$$

When an algorithm is stable, its accuracy reflects the condition number.

Lecture 16 - Triangular Linear Systems

Triangular Linear Systems

- Triangular systems are a special type of linear system that can be solved with a very simple, efficient, and stable algorithm.
  - Efficient approaches for solving general linear systems factor a matrix into a product of matrices where at least one is triangular and then apply a triangular system solver.
    - LU decomposition factors into the product of lower and upper triangular matrices.
    - QR decomposition factors into the product of a unitary matrix and an upper triangular matrix.

- Example: Lower Triangular(or "Left Triangular")

$$\begin{aligned} l_{11}x_1 &= b_1 \\ l_{21}x_1 + l_{22}x_2 &= b_2 \\ l_{31}x_1 + l_{32}x_2 + l_{33}x_3 &= b_3 \\ &\vdots \\ l_{m1}x_1 + l_{m2}x_2 + l_{m3}x_3 + \cdots + l_{mm}x_m &= b_m \end{aligned} \quad \Longrightarrow \quad \underbrace{\begin{bmatrix} l_{11} & & & & \\ l_{21} & l_{22} & & & \\ l_{31} & l_{32} & l_{33} & & \\ \vdots & & & \ddots & \\ l_{m1} & l_{m2} & l_{m3} & \cdots & l_{mm} \end{bmatrix}}_{L} \mathbf{x} = \mathbf{b}$$

Lower/Left Triangular

Forward / Backward Substitution

- Both are backward stable (Proof see Slides 15b-6)

Forward Substitution

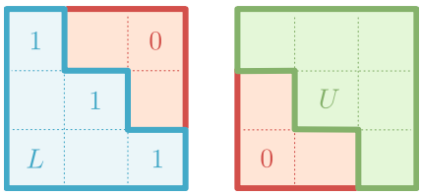
- We can efficiently solve a *lower* triangular system by rearranging:

$$\begin{aligned} l_{11}x_1 &= b_1 \\ l_{21}x_1 + l_{22}x_2 &= b_2 \\ l_{31}x_1 + l_{32}x_2 + l_{33}x_3 &= b_3 \\ &\vdots \\ l_{m1}x_1 + l_{m2}x_2 + l_{m3}x_3 + \cdots + l_{mm}x_m &= b_m \end{aligned} \quad \Longrightarrow \quad \begin{aligned} x_1 &= b_1/l_{11} \\ x_2 &= (b_2 - l_{21}x_1)/l_{22} \\ x_3 &= (b_3 - l_{31}x_1 - l_{32}x_2)/l_{33} \\ &\vdots \\ x_i &= \left(b_i - \sum_{j=1}^{i-1} l_{ij}x_j\right) \Big/ l_{ii} \end{aligned}$$

- Solving for $x_1, x_2, \cdots, x_m$ in sequence, the RHS expression contains known quantities at every step.
- This process is called "**forward substitution**" since solved values are substituted into the next equation.
- Rearranged equations are still "lower triangular" in shape, needing a $\ominus$ and $\otimes$ at each position. Thus roughly m^2 floating point operations must be performed.

Lecture 16 - LU Decomposition

LU Decomposition



- Factor a matrix $A \in \mathbb{C}^{m \times m}$ into the form: $A=LU$, where L is lower triangular and U is upper triangular.
  - The algorithm is Gaussian elimination with careful bookkeeping
- Motivation
  - Motivation: computing determinants

$$\det(A) = \det(LU) = \det(L)\det(U) = \left(\prod_{i=1}^{m} l_{ii}\right)\left(\prod_{i=1}^{m} u_{ii}\right) = \prod_{i=1}^{m} u_{ii} \quad (L \text{ is *unit* lower triangular})$$

  - Motivation: solving linear systems

$$A\mathbf{x} = \mathbf{b} \implies L\underbrace{U\mathbf{x}}_{\mathbf{y}} = \mathbf{b}$$

    - Solve $L\mathbf{y} = \mathbf{b}$ (forward substitution: fast $(O(m^2))$ and stable)
    - Solve $U\mathbf{x} = \mathbf{y}$ (back substitution: $(O(m^2))$ and stable)
    - LU with *pivoting* (next lecture) is the standard approach for solving linear systems.

Gaussian Elimination

- General definition (pic 1)
- Example (pic 2-4)
- General Case (pic 5-7)

- Zero out entries below the diagonal, one column at a time:

$$\underbrace{\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}}_{A} \xrightarrow{L_1} \underbrace{\begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \end{bmatrix}}_{L_1 A} \xrightarrow{L_2} \underbrace{\begin{bmatrix} * & * & * & * \\ & * & * & * \\ & 0 & * & * \\ & 0 & * & * \end{bmatrix}}_{L_2 L_1 A} \xrightarrow{L_3} \underbrace{\begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & 0 & * \end{bmatrix}}_{U = L_3 L_2 L_1 A}$$

- This is accomplished by multiplying by a sequence of lower triangular matrices:

$$L_{m-1} \cdots L_1 A = U,$$

  where L_k subtracts multiples of row k from the rows below.
- Therefore: $A = (L_{m-1} \cdots L_1)^{-1} U = LU \qquad L = L_1^{-1} \cdots L_{m-1}^{-1}$
  - Facts used from homework 0:
    - The inverse of a lower triangular matrix is lower triangular.
    - Product of lower triangular matrices $L_{m-1} \cdots L_1$ is lower triangular.

Gaussian Elimination

- Complexity

Complexity of Gaussian Elimination

The **LU decomposition algorithm** operating on an input matrix $A \in \mathbb{C}^{m\times m}$ is:

```
algorithm lu(A):
    L, U = I, A                          # U will hold (L_1^{-1} ... L_k^{-1}) A after step k.
    for k=1 to m - 1:                    # Run m - 1 elimination steps.
        for i=k + 1 to m:                # Cancel zeros in row i > k.
            L(i, k) = U(i, k) / U(k, k)  # Determine and store multiplier l_ik.
            for j=k + 1 to m:
                U(i, j) -= L(i, k) * U(k, j) # Subtract multiple of row k.
    return L, U
```

- Work is dominated by the multiplication and subtraction in the innermost loop.
  - For each outermost iteration k, we do a "double-for" loop over the $m-k$ indices $\{k+1,\cdots,m\}$. Thus, the innermost line runs $(m-k)^2$ times, performing two operations each time:

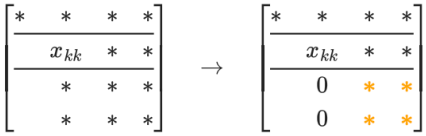
$$\sum_{k=1}^{m-1} 2(m-k)^2 = \sum_{k'=1}^{m-1} 2(k')^2, \quad \text{with } k' = m-k$$
$$= 2\frac{(m-1)m(2m-1)}{6} = 2\frac{m^3}{3} - m^2 + \frac{m}{6} \sim \frac{2}{3}m^3.$$

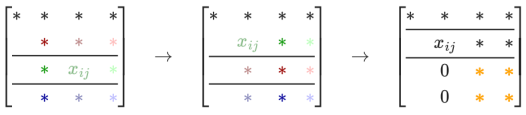
  - Therefore roughly $\frac{2}{3}m^3$ floating point operations are needed.

Lecture 17 - LU Decomposition with Pivoting

Pivots

- The version of Gaussian elimination presented is neither backward stable nor stable — very dangerous
- The backward stability issue is closely related to zeros on the diagonal leading to $l_{ik} = \dfrac{a_{ik}}{0}$
  - Solution: swap the rows/columns (pivoting)
  - Pivoting brings backward stability
- Step k of Gaussian elimination looks like
  - The k^{th} row is used to eliminate the entries below it in column k.
  - Entry x_{kk} is called the "pivot" in this operation
  - We subtract x_{ik}/x_{kk} times row k from each row $i > k$. (Dividing by $x_{kk} \approx 0$ will be problematic)
  - It's not necessary to choose x_{kk} as the pivot.
  - For stability, pick largest value as pivot, then exchanging rows/columns.
  - This process of exchanging rows/columns can be interpreted as reordering the variables/equations and is called pivoting.





Pivoting

The **LU decomposition algorithm** operating on an input matrix $A \in \mathbb{C}^{m \times m}$ is:

```
algorithm lu(A):
    L, U = I, A                          # U will hold (L_1^{-1} ... L_k^{-1}) A after step k.
    for k=1 to m - 1:                    # Run m - 1 elimination steps.
        for i=k + 1 to m:                # Cancel zeros in row i > k.
            L(i, k) = U(i, k) / U(k, k)  # Determine and store multiplier l_ik.
            for j=k + 1 to m:
                U(i, j) -= L(i, k) * U(k, j) # Subtract multiple of row k.
    return L, U
```

Choosing Pivots: Complete Pivoting

- At step k, we ideally pick the largest magnitude value in block $i, j \geq k$ as the pivot.
- Require searching through the $(m - k + 1)^2$ entries for each step $1 \leq k < m$, it means $O(m^3)$ work for selecting pivots, a nontrivial cost on top of $\frac{2}{3}m^3$ operations of plain lu.

Choosing Pivots: Partial Pivoting

- Only reorder the **rows**. Choose the largest entry from column k as the pivot: x_{ik} $(i \geq k)$
- Require searching through the $(m - k + 1)$ entries for each step $1 \leq k < m$: only $O(m^2)$ work
- Almost as stable as complete pivoting in practice.

$$\begin{bmatrix} * & * & * & * \\ & * & * & * \\ \hline & x_{ik} & * & * \\ \hline & * & * & * \end{bmatrix}$$

Permutation Matrix in Partial Pivoting

- The row exchange operation can be written as a multiplication by a simple permutation matrix
- Permutation matrices P are orthogonal: $P^{-1} = P^T$ and "binary"

$$P_k = P_k\, I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Because P_k just exchanges two rows: P_k is an **involution**: $P_k P_k = I$ and **symmetric**: $P_k = P_k^{-1} = P_k^T$
- After all steps $k \in \{1, \ldots, m-1\}$ we have: $L_{m-1}P_{m-1}\ldots L_2 P_2 L_1 P_1 A = U$
- To make $L_{m-1}P_{m-1}\ldots L_2 P_2 L_1 P_1$ a lower triangular, we can "shift" later row exchanges P_k past earlier elimination matrices $L_j (j < k)$ to collect them on the right.
  - This simply reorders the rows modified by L_j but does not change the typical lower triangular "elimination step" instructor of L_j
  - The multipliers l_{ij} in column j are just reordered by the permutation $P_k \ldots P_{j+1}$ to obtain entries l'_{ij} of L'_j
  - At the end of this process: $L'_{m-1}\ldots L'_1 P_{m-1}\ldots P_1 A = U$

- Finally, $L'_{m-1}\ldots L'_1 P_{m-1}\ldots P_1 A = U \implies P_{m-1}\ldots P_1 A = L_1^{'-1}\ldots L_{m-1}^{'-1} U \implies PA = LU$
  - This can be interpreted as applying P to A and running the ordinary lu algorithm. (But it determines P computes the LU decomposition of PA all at once).
  - LU with partial pivoting even works for all square matrices—**even singular ones**!
  - L is always unit lower triangular ($\det(L)=1$).
  - But when A is singular, U has zeros on its diagonal ($\det(U)=\det(A)=0$).

Gaussian elimination with partial pivoting operating $A \in \mathbb{C}^{m\times m}$ is the algorithm:

```
algorithm lu_partial_pivot(A):
    L, U, P = I, A, I
    for k=1 to m - 1:                       # Run m - 1 elimination steps.
        imax = argmax_{i ≥ k}(|U(i, k)|)    # Select largest element (imax, k) as pivot
        swap(U(k, k:m), U(imax, k:m))       # Exchange row imax and k of U
        swap(L(k, 1:k-1), L(imax, 1:k-1))   # Permute the multipliers from earlier steps
        swap(P(k, :), P(imax, :))           # Record the permutation: P = P_k P
        for i=k + 1 to m:                   # Do standard elimination step using pivot (k, k) (like in `lu`)
            L(i, k) = U(i, k) / U(k, k)
            for j=k + 1 to m:
                U(i, j) -= L(i, k) * U(k, j)
    return L, U, P
```

Partial Pivoting Example

Partial Pivoting Example

- We run LU with partial pivoting on the same example matrix from last lecture:

$$A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

- Step 1a: choose pivot entry $(3,1)$ and exchange

$$\underbrace{\begin{bmatrix} & & 1 & \\ & 1 & & \\ 1 & & & \\ & & & 1 \end{bmatrix}}_{P_1} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ 4 & 3 & 3 & 1 \\ 2 & 1 & 1 & 0 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

- Step 1b: eliminate

$$\underbrace{\begin{bmatrix} 1 & & & \\ -\frac{1}{2} & 1 & & \\ -\frac{1}{4} & & 1 & \\ -\frac{3}{4} & & & 1 \end{bmatrix}}_{L_1} \begin{bmatrix} 8 & 7 & 9 & 5 \\ 4 & 3 & 3 & 1 \\ 2 & 1 & 1 & 0 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & -\frac{1}{2} & -\frac{3}{2} & -\frac{3}{2} \\ & -\frac{3}{4} & -\frac{5}{4} & -\frac{5}{4} \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \end{bmatrix}$$

Lecture 18 - Stability of LU

Without Pivoting

- In our pathological example for LU without pivoting:

$$A = \begin{bmatrix} 10^{-30} & 1 \\ 1 & 1 \end{bmatrix} \implies L = \begin{bmatrix} 1 & 0 \\ 10^{30} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 10^{-30} & 1 \\ 0 & 1 - 10^{30} \end{bmatrix}$$
$$\implies \tilde{L} = \begin{bmatrix} 1 & 0 \\ 10^{30} & 1 \end{bmatrix}, \quad \tilde{U} = \begin{bmatrix} 10^{-30} & 1 \\ 0 & -10^{30} \end{bmatrix}$$

  we observed a large relative backward error $\frac{\|A-\tilde{L}\tilde{U}\|}{\|A\|} = \frac{\left\|\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}\right\|}{\|A\|}$ that caused a completely wrong answer to "$A\mathbf{x} = \mathbf{b}$" via forward/back substitution.

- LU without pivoting is **not** backward stable
  - We said this was linked to the huge entry 10^{30} in the L factor, which we could avoid with pivoting.
  - It turns out large backward errors are *always* due to large entries in either U or L

Backward Stability Theorem

Suppose $A = LU$ for a nonsingular $A \in \mathbb{C}^{m\times m}$ is computed by Gaussian elimination ***without pivoting*** to obtain $\tilde{L}$ and $\tilde{U}$. If the LU factorization exists, and the computer obeys the fundamental axiom of FPA:

$$\tilde{L}\tilde{U} = A + \delta A \qquad \frac{\|\delta A\|}{\|L\|\|U\|} = O(\epsilon)$$

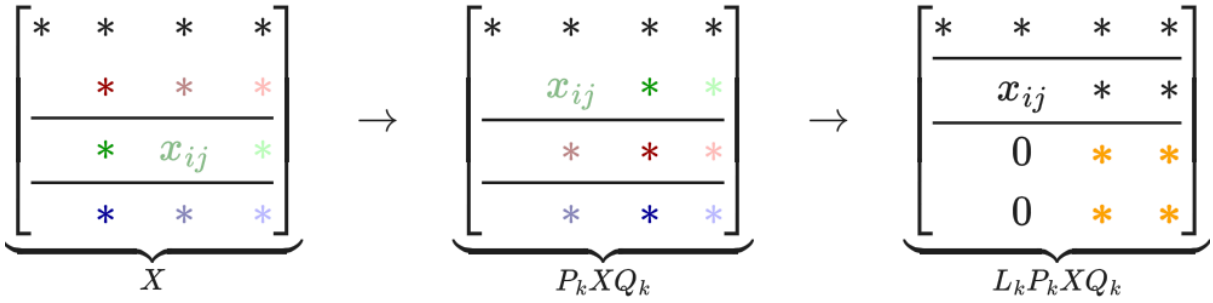
Warning: $\|L\|\|U\|$ in the denominator, not $\|A\|$!!!

for some $\delta A \in \mathbb{C}^{m\times m}$.

- This also applies to Gaussian elimination ***with pivoting*** if we first apply P to A.
- Recall, for backward stability, we require $\frac{\|\delta A\|}{\|A\|} = O(\epsilon)$.
  - This is only true if $\|L\|\|U\| = O(\|A\|)$.
  - If $\|L\|\|U\| > O(\|A\|)$ we expect backward instability.
  - Without pivoting, entries in L and U can become unbounded in magnitude.
  - With partial pivoting, we know L has entries of magnitude ≤ 1 (formed by dividing a smaller column k entry by the pivot x_{kk}) and thus $\|L\| = O(1)$.
    - The condition for stability is thus $\frac{\|\delta A\|}{\|U\|} = O(\epsilon)$ or $\|U\| = O(\|A\|)$.

Complete Pivoting

- Complete pivoting can avoid backward instability. But in practice, complete pivoting is almost never done since choosing pivots takes $O(m^3)$ work, and partial pivoting nearly always achieves low backward error.
- Nevertheless, it can still be written in matrix form:



$$
\begin{aligned}
&(L_{m-1}P_{m-1}\dots L_2P_2L_1P_1)AQ_1Q_2\dots Q_{m-1} = U \\
\implies &\underbrace{(L'_{m-1}\dots L'_2L'_1)}_{L^{-1}}\underbrace{P_{m-1}\dots P_2P_1}_{P}A\underbrace{Q_1Q_2\dots Q_{m-1}}_{Q} = U \\
&\implies PAQ = LU
\end{aligned}
$$

Partial Pivoting

- With partial pivoting, L has entries of magnitude ≤ 1, thus $\|L\| = O(1)$
- The condition for stability is $\dfrac{\|\delta A\|}{\|U\|} = O(\epsilon)$ or $\|U\| = O(\|A\|)$
- Growth factor

Backward Stability Theorem Partial Pivoting

- With partial pivoting, the condition for stability is $\frac{\|\delta A\|}{\|U\|} = O(\epsilon)$ or $\|U\| = O(\|A\|)$.
  - To reason about this, we introduce the **growth factor**:

    $$\rho := \frac{\max_{i,j}|u_{ij}|}{\max_{i,j}|a_{ij}|},$$

    so that $\|U\| = O(\rho\|A\|) = \|A\|O(\rho)$.
  - Therefore, we can state the following corollary to the general backward stability condition:

Suppose $A = LU$ for a nonsingular $A \in \mathbb{C}^{m\times m}$ is computed by Gaussian elimination ***with partial pivoting*** to obtain $\tilde{P}$, $\tilde{L}$, and $\tilde{U}$. If the the computer obeys the fund. axiom of FPA:

$$\tilde{L}\tilde{U} = \tilde{P}A + \delta A \qquad \frac{\|\delta A\|}{\|A\|} = O(\rho\epsilon)$$

for some $\delta A \in \mathbb{C}^{m\times m}$, where ρ is the growth factor for A. If $|l_{ij}|$ for each $i > j$ (so that there are no ties in pivot selection in exact arithmetic) then $\tilde{P} = P$ for sufficientlly small ϵ.

- Gaussian elimination with partial pivoting is thus stable if $\rho = O(1)$ for all A of dimension m.

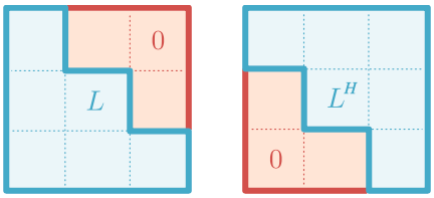
- Using an informal, more practical definition of the stability as the growth of ρ as we increase matrix size m, we see that in the worst case, Gaussian elimination is horribly unstable. However, the worst case seldom happens in real applications.
- Conclusion: Partial Pivoting is truly helpful and appears to be sufficient for acceptable (non-exponential) growth factors except in vanishingly rare pathological cases.

Lecture 19 - Cholesky Factorization

Motivation

- LU decomposition without pivoting $A = LU$, not backward stable
- LU decomposition with partial pivoting $PA = LU$, technically backward stable, though theoretically with backward error growing exponentially as we enlarge the matrix $\rho = 2^{m-1}$
- LU decomposition with complete pivoting $PAQ = LU$, keep backward error under control at an extra cost
- What if A is symmetric or hermitian? Can we come up with a faster algorithm?

Cholesky Factorization



- $A = LL^H$ or $A = RR^H$ with positive **real** diagonal entries $L_{ii} > 0$
- If $A \in \mathbb{C}^{m\times m}$ is hermitian/symmetric, it seems natural for LU to respect this symmetry.
  - The product of two upper/lower triangular is upper/lower triangular
  - By this, we mean $U = L^H$
  - No extra time and space needed to calculate U in LU decomposition
- *A is called* ***positive definite*** *(正定矩阵) if* $A \in \mathbb{R}^{m\times m}$ *we have* $x^T Ax > 0 \quad \forall x \neq 0$
- *A is called* ***hermitian positive definite*** *(hermitian正定矩阵) if* $A \in \mathbb{C}^{m\times m}$ *we have* $A = A^H, \quad x^H Ax > 0 \quad \forall x \neq 0$
- Is this always possible? Consider the vector $\mathbf{y} = L^H\mathbf{x}$ for an arbitrary *nonzero* $\mathbf{x} \in \mathbb{C}^m$.
  - We can compute the ℓ_2 (Euclidean) norm of $\mathbf{y}$: $0 \leq \|\mathbf{y}\|_2^2 = \mathbf{y}^H\mathbf{y} = \mathbf{x}^H LL^H\mathbf{x} = \mathbf{x}^H A\mathbf{x}$.
  - Furthermore, if we are hoping to solve linear systems, $\det(A) \neq 0$, meaning L^H has linearly independent columns and $\mathbf{y} \neq \mathbf{0} \implies \|\mathbf{y}\|_2^2 > 0 \iff \mathbf{x}^H A\mathbf{x} > 0 \quad \forall \mathbf{x} \neq 0$.

In other words, A must be hermitian ***positive definite***.

Hermitian Positive Definite Matrices

$A = A^H, \quad x^H Ax > 0 \quad \forall x \neq 0$

- If $X \in \mathbb{C}^{m\times n}$ is full rank with $m \geq n$, then A is hermitian positive definite $\implies X^H AX$ is hermitian positive definite. (Proof see Slide 19-5)
- Every diagonal of A must be strictly positive ($a_{ii} = e_i^H Ae_i > 0$)
- Every "principal submatrix" is positive definite

Symmetric Gaussian Elimination

- Suppose that a hermitian positive definite matrix A happens to be in the block form:

$$A = \begin{bmatrix} 1 & \mathbf{w}^H \\ \mathbf{w} & K \end{bmatrix}.$$

  - Consider the first step of Gaussian elimination:

$$A = \underbrace{\begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{w} & I \end{bmatrix}}_{L_1} \begin{bmatrix} 1 & \mathbf{w}^H \\ \mathbf{0} & K - \mathbf{w}\mathbf{w}^H \end{bmatrix}$$

  - To maintain conjugate symmetry, we can use the leftmost column to eliminate $\mathbf{w}^H$ in the top row:

$$A = \underbrace{\begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{w} & I \end{bmatrix}}_{L_1} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & K - \mathbf{w}\mathbf{w}^H \end{bmatrix} \underbrace{\begin{bmatrix} 1 & \mathbf{w}^H \\ \mathbf{0} & I \end{bmatrix}}_{L_1^H}$$

  - Now ideally we repeat, multiplying by L_k and L_k^H on the left/right until the working matrix becomes I.

Cholesky Factorization

- After m steps of symmetric Gaussian elimination, the working matrix becomes I and: $A = \underbrace{L_1 L_2 \ldots L_m}_{L} \underbrace{L_m^H \ldots L_2^H L_1^H}_{L^H}$ with positive real diagonal entries $L_{ii} > 0$
  - This can also be written as $A = R^H R$ with $R = L^H$
  - This process can never break down! Diagonal pivots are always strictly positive by positive definiteness.
  - Furthermore, each L_k is uniquely determined by the algorithm, making the entire factorization unique.
- **Every** hermitian positive definite matrix $A \in \mathbb{C}^{m \times m}$ has a **unique** Cholesky factorization.
  - Formal proof see Slide 19-9
- Algorithm
  - Time complexity: $\frac{m^3}{3}$ operations
- Cholesky Factorization is backward stable

$$A = \begin{bmatrix} a_{11} & \mathbf{w}^H \\ \mathbf{w} & K \end{bmatrix} = \begin{bmatrix} \sqrt{a_{11}} & \mathbf{0} \\ \mathbf{w}/\sqrt{a_{11}} & I \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & K - \mathbf{w}\mathbf{w}^H/a_{11} \end{bmatrix} \begin{bmatrix} \sqrt{a_{11}} & \mathbf{w}^H/\sqrt{a_{11}} \\ \mathbf{0} & I \end{bmatrix}$$

- Using Cholesky factorization, we only need to look at/operate on "half" of the input (either upper or lower triangle).
  - The other triangle is just a conjugate transpose.
  - We can avoid half the arithmetic and potentially half the storage (using a compressed representation).

Cholesky factorization for any Hermitian positive definite matrix A. Compare to LU.

```
algorithm cholesky(A):
    L = A                                   # We operate in-place, replacing the k^th column of A with the k^th column of L
    for k = 1 to m:
        alpha = sqrt(L(k, k))
        for i = k + 1 to m:
            beta = L(i, k) / L(k, k)        # Multiplier used for row i.
            for j = i to m:                 # (Conceptually) eliminate "w" by subtracting beta * row k from row i. But only
                L(i, j) -= beta * L(k, j) #    actually modify the upper tri of the "K" block; keep "w" in the leftmost column.
            L(i, k) /= alpha                # k^th column of L is just the k^th column of the working matrix divided by alpha
            L(k, i) = 0                     # Zero out k^th row of upper tri (optional if upper tri of result is ignored)
        L(k, k) = alpha
    return L, U, P
```

Algorithm

LDL^H Factorization

- What if we want to solve $A\mathbf{x} = \mathbf{b}$ for a symmetric non-positive-definite matrix A?
  - Can we still use Cholesky?
    - No: we proved $A = LL^H$ implies A is positive definite.
    - Practically: one of the a_{ii} will become nonpositive.
  - Can we still exploit symmetry?
    - Sometimes. We can avoid the square root by leaving the a_{ii} factors on the diagonal to obtain

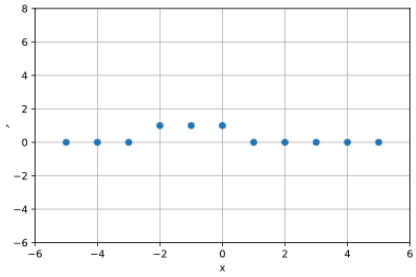
      $$A = LDL^H$$

      with L *unit* lower triangular and some entries D being zero or negative. (This of course can be done for positive definite matrices too if you want to avoid the square root.)
    - However this doesn't *always* work for indefinite matrices (with positive and negative eigenvalues). One sufficient condition: all "leading principal minors" are nonsingular.

Lecture 20 - Least Squares

Least Squares

- Suppose we have n points $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ and wish to fit the polynomial



$$p(x) = a_0 + a_1 x + \cdots + a_d x^d = \sum_{j=0}^{d} a_j x^j$$

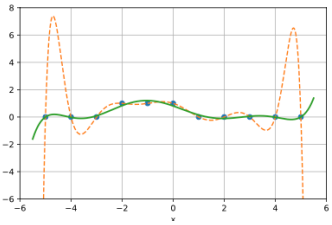
- We can find a polynomial passing through each point by solving a linear system, but this is usually a bad idea!
  - Notice that $p(x)$ is a linear combination of the "basis monomials" x^j. Evaluating at each point x_i:

$$p(x_i) = \sum_{j=0}^{d} a_j x_i^j = \begin{bmatrix} 1 & x_i & \cdots & x_i^d \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_d \end{bmatrix} \implies \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 & \cdots & x_1^d \\ \vdots & \vdots & & \vdots \\ 1 & x_n & \cdots & x_n^d \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_d \end{bmatrix}$$

  - When $d = n - 1$, This is the square, nonsingular Vandermonde matrix, meaning we can solve for unique coefficients.
    - But this usually becomes a badly ill-conditioned system and produces a highly oscillatory polynomial.

Solution: Cholesky Factorization

- Cholesky is generally fastest (but not most robust) method for solving least-squares problems.
- It's much better to use a smaller degree $d < n - 1$ and **minimize the residual** of the

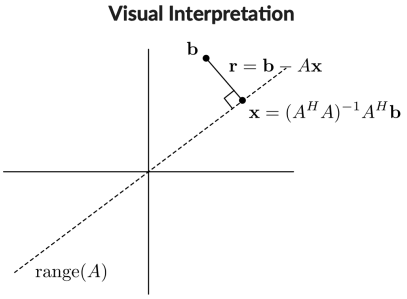


$$\min_{\mathbf{a}} \left\| \begin{bmatrix} 1 & x_1 & \cdots & x_1^d \\ \vdots & \vdots & & \vdots \\ 1 & x_n & \cdots & x_n^d \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_d \end{bmatrix} - \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \right\|^2$$

overdetermined system

- **General Statement**
  - In general, the least-squares problem seeks to solve: $A\,x = b$ with rectangular $A \in \mathbb{C}^{m \times n}$, $b \in \mathbb{C}^m$, $x \in \mathbb{C}^n$, and $m > n$
  - Because there are more equations than unknowns (overdetermined), we cannot expect an exact solution.
  - Instead, we seek the best solution by minimizing the **residual** (or "error vector"): $r := b - A\,x \in \mathbb{C}^m$

- The simplest, most efficient formulation is to measure **r** using the 2-norm: $\min_x \|b - Ax\|_2^2$
  - We seek the vector **x** such that **Ax** is the closest point in **range(A)** to **b** in Euclidean distance



- Solve $\min_x \|b - Ax\|_2^2 = \min_x (b - Ax)^H (b - Ax)$ with Calculus
  - Using some matrix calculus:
    $$0 = \frac{\partial (b - Ax)^H (b - Ax)}{\partial x} = 2\frac{\partial (b - Ax)^H}{\partial x}(b - Ax) = 2A^H(b - Ax) \iff A^H Ax = A^H b$$
  - Thus, when A has **full rank** *min(m, n)=n*, we have $A^H A$ is nonsingular
  - Because A has **full rank**, we have $\forall x \neq 0$, we have $Ax \neq 0 \implies 0 < \|Ax\|_2^2 = x^H (A^H A) x$ (why), thus $A^H A$ is hermitian positive definite
  - In conclusion, when A has **full rank**, we have unique optimal $x = (A^H A)^{-1} A^H b$ to get $\min_x \|b - Ax\|_2^2$
  - Detail proof of uniqueness and pseudoinverse, see Slide 20.6-7
- Because the normal equations $A^H Ax = A^H b$ involve a **positive definite** hermitian matrix $A^H A$, we can use the Cholesky factorization.

> Cholesky Factorization Approach to Least Squares Problem $\min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|_2$
> 1. Construct the normal equations matrix $A^H A$ and right-hand side vector $A^H \mathbf{b}$.
> 2. Compute the Cholesky factorization $A^H A = LL^H$.
> 3. Solve $L\mathbf{y} = \mathbf{b}$ with forward-substitution for $\mathbf{y}$.
> 4. Solve $L^H \mathbf{x} = \mathbf{y}$ with back-substitution for $\mathbf{x}$.

  - Floating point operations: (dominated by building $A^H A$ and Cholesky factorization)
    - mn^2 operations to construct $A^H A$ leveraging symmetry (half the work of generic matrix-matrix mult.).
    - $\sim n^3/3$ operations to compute Cholesky factorization.
    - Total work is thus $\sim mn^2 + \frac{1}{3}n^3$ arithmetic operations.

- This is the most efficient algorithm (and the classical choice), but suffers from robustness problems.
  - Condition number $\kappa(A^H A) = \frac{\sigma_{\max}(A^H A)}{\sigma_{\min}(A^H A)} = \frac{\sigma_{\max}(A)^2}{\sigma_{\min}(A)^2} = \kappa(A)^2$ (why?)is squared, impacting accuracy.

Other Approaches

- Cholesky Factorization: the most efficient algorithm (and the classical choice), but suffers from robustness problems

- QR Factorization: more robust, and the "modern classical" approach
- SVD: even more robust than QR

Lecture 21 - QR Factorization

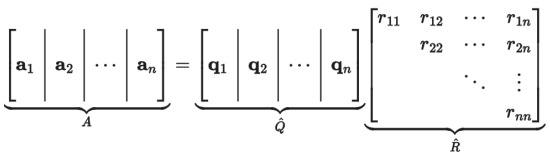
Motivation

- Least squares for *overdetermined systems*: "$A\mathbf{x} = \mathbf{b}$" for $A \in \mathbb{C}^{m\times n}$, $m > n$.
  - Solving $\min_{\mathbf{x}} \|A\mathbf{x} - \mathbf{b}\|_2^2$ with the Cholesky factorization means solving the **normal equations**:
    $$A^H A\mathbf{x} = A^H\mathbf{b},$$
    whose condition number is as bad as $\kappa(A^H A) = \kappa(A)^2$.
  - "Squaring" A impacts accuracy, and the QR factorization avoids this.
- *Underdetermined* systems: solving $A\mathbf{x} = \mathbf{b}$ for $A \in \mathbb{C}^{m\times n}$, $m < n$.
  - The full QR decomposition of A^H will look like:
    $$A^H = \begin{bmatrix}\hat{Q} & Q_{\mathcal{N}}\end{bmatrix}\begin{bmatrix}\hat{R}\\ 0\end{bmatrix}$$
    where $\hat{R}$ is square upper tri. and $\hat{Q}$ and $Q_{\mathcal{N}}$ hold orthonormal bases for the rowspace and nullspace of A.
  - The underdetermined linear system then looks like:
    $$\mathbf{b} = \begin{bmatrix}\hat{R}^H & 0\end{bmatrix}\begin{bmatrix}\hat{Q}^H\\ Q_{\mathcal{N}}^H\end{bmatrix}\mathbf{x} = \hat{R}^H\tilde{\mathbf{x}} + 0\,\mathbf{x}_{\mathcal{N}} \quad \text{with} \quad \tilde{\mathbf{x}} = \hat{Q}^H\mathbf{x}, \quad \mathbf{x}_{\mathcal{N}} = Q_{\mathcal{N}}^H\mathbf{x}$$
  - All vectors of the form $\hat{Q}\hat{R}^{-H}\mathbf{b} + Q_{\mathcal{N}}\mathbf{x}_{\mathcal{N}}$ are solutions, and $\hat{Q}\hat{R}^{-H}\mathbf{b}$ has the smallest norm.

More generally: constructing an orthonormal basis for range(A) and $\mathcal{N}(A^H)$.

QR Factorization

- Starting points
  - Successive spaces spanned by the columns a_j of $A \in \mathbb{C}^{m\times n}, m \geq n$: $span(a_1) \subseteq span(a_1, a_2) \subseteq span(a_1, a_2, a_3) \subseteq \cdots$
  - Idea: construct a sequence of orthonormal vectors $q_1, q_2, \cdots, q_n$ whose prefixes span these spaces.
  - In other words, if A has full rank n, the first j vectors should satisfy: $span(q_1, q_2, \cdots, q_j) = span(a_1, a_2, \cdots, a_j), j = 1, \cdots, n$, and the first j columns of A can be written as a linear combination of $q_1, q_2, \cdots, q_n$
  - Expressing this fact in matrix form (diagram in the right)
  - When A isn't full rank, some of the r_{jj} will be 0 ($span(q_1, \cdots, q_j) \supset span(a_1, \cdots, a_j)$)

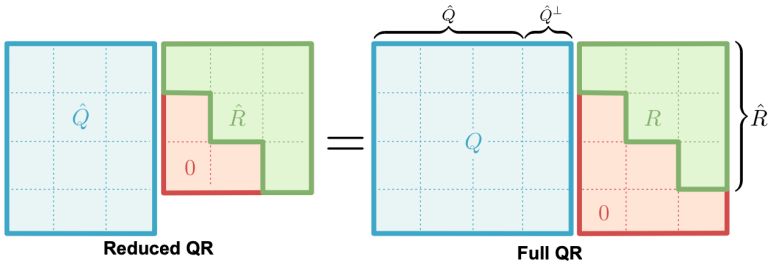


- Reduced QR Factorization
  - We have just shown $A = \hat{Q}\hat{R}$ with

$\hat{Q} \in \mathbb{C}^{m \times n}$ and $\hat{R} \in \mathbb{C}^{n \times n}$

- Where $\hat{R}$ is a square upper triangular matrix and the columns of $\hat{Q}$ hold an orthonormal basis for *range(A)*: $q_i^H q_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$
- This is called the **reduced** QR factorization, since $\hat{Q}$ contains only a basis for *range(A)* rather than $\mathbb{C}^m$. (It is rectangular rather than square)

Reduced vs. Full QR



- The reduced QR decomposition of a "tall" matrix $A \in \mathbb{C}^{m \times n}$ has "tall" $\hat{Q}$ and square $\hat{R}$
- We can augment the columns of $\hat{Q}$ with additional orthonormal vectors to form the full QR decomposition $A=QR$ with a square unitary matrix Q and a "tall" R.
- The reduced decomposition is recovered from the full decomposition by slicing off the zero rows at the boom of R and the corresponding columns $\hat{Q}^\perp$
- When A is of full rank min(m, n)=n
  - Columns of $\hat{Q}$ form an orthonormal basis for ***range(A)***
  - Columns of $\hat{Q}^\perp$ form an orthonormal basis for ***range***$(A^\perp)$ (the space of vectors **orthogonal** to all columns of ***A***). This also the null space of A^H: $\mathcal{N}(A^H)$

Gram-Schmidt

$$\underbrace{\begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_n \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_n \end{bmatrix}}_{\hat{Q}} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}}_{\hat{R}}$$

- Inspecting the individual equations:

$$\begin{aligned} \mathbf{a}_1 &= r_{11}\mathbf{q}_1 \\ \mathbf{a}_2 &= r_{12}\mathbf{q}_1 + r_{22}\mathbf{q}_2 \\ &\vdots \\ \mathbf{a}_n &= r_{1n}\mathbf{q}_1 + r_{2n}\mathbf{q}_2 + \cdots + r_{nn}\mathbf{q}_n \end{aligned} \qquad \begin{aligned} \mathbf{q}_1 &= \mathbf{a}_1 / r_{11} \\ \mathbf{q}_2 &= (\mathbf{a}_2 - r_{12}\mathbf{q}_1)/r_{22} \\ &\vdots \\ \mathbf{q}_n &= (\mathbf{a}_n - r_{1n}\mathbf{q}_1 - r_{2n}\mathbf{q}_2 + \cdots + r_{n-1,n}\mathbf{q}_{n-1})/r_{nn} \end{aligned}$$

  - We can find **unit** vector $\mathbf{q}_1$ by normalizing $\mathbf{a}_1$ $(r_{11} = /\|\mathbf{a}_1\|)$.
  - We can find **orthogonal unit** vector $\mathbf{q}_2$ by normalizing $\mathbf{a}_2 - r_{12}\mathbf{q}_1$, picking r_{12} to make $\mathbf{q}_2$ orthogonal.
  - We can find **orthogonal unit** vector $\mathbf{q}_j$ by making $\mathbf{a}_j$ orthogonal to $\mathbf{q}_1, \cdots, \mathbf{q}_{j-1}$:

$$\mathbf{a}_j - \underbrace{(\mathbf{q}_1^H \mathbf{a}_j)}_{r_{1j}}\mathbf{q}_1 - \underbrace{(\mathbf{q}_2^H \mathbf{a}_j)}_{r_{2j}}\mathbf{q}_2 - \cdots - \underbrace{(\mathbf{q}_{j-1}^H \mathbf{a}_j)}_{r_{j-1,j}}\mathbf{q}_{j-1}$$

  and then normalizing. It is easy to verify that the complex dot product with $\mathbf{q}_1, \cdots, \mathbf{q}_{j-1}$ is zero.

- This process is a very old idea and is known as Gram-Schmidt orthogonalization.

Existence and Uniqueness

- **Theorem**: Every $A \in \mathbb{C}^{m\times n}(m \geq n)$ has a full QR factorization A=QR (and hence also a reduced QR factorization).
- **Theorem**: Every $A \in \mathbb{C}^{m\times n}(m \geq n)$ of full rank has a unique reduced QR factorization $A = \hat{Q}\hat{R}$ with positive real diagonal entries $r_{jj} > 0$.

Solving using QR Factorization

Solving Ax = b

- The QR factorization is a stable and easy method for solving $A\mathbf{x} = \mathbf{b}$ with a nonsingular square matrix $A \in \mathbb{C}^{m\times m}$:

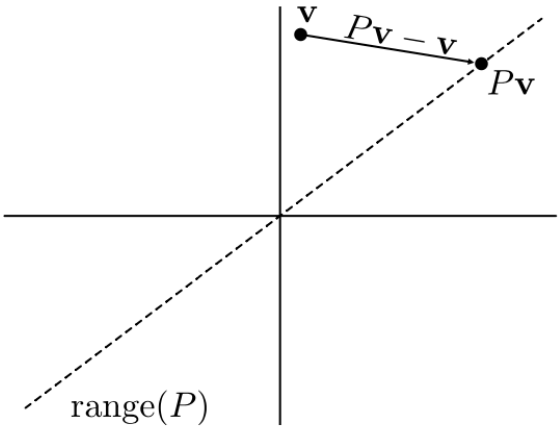
QR Factorization Approach to solve $A\mathbf{x} = \mathbf{b}$:
1. Compute the QR factorization $A = QR$.
2. Compute right-hand-side vector $\mathbf{y} = Q^H\mathbf{b}$.
3. Solve $R\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$ with back substitution.

- Generally not used because LU takes about half the work.

Lecture 22 - QR Factorization Pt2

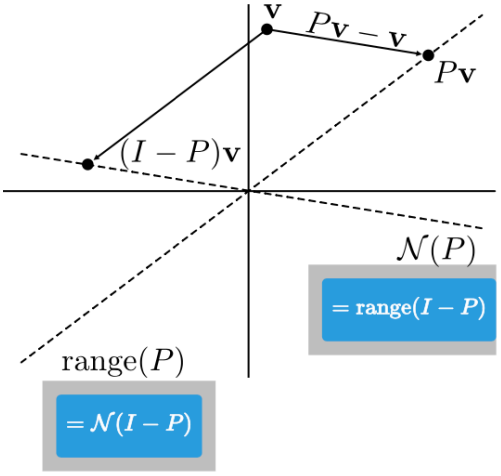
Projector Matrices

- A **projector** is a **square matrix** P that satisfies: PP=P
  - Another term: **P** is an idempotent matrix
  - After projecting a vector v to x=$PV \in$ *range(P)*, subsequent projection do nothing: $\mathbf{Px = PPv = Pv = x}$
  - We say that **P** projects onto **range(P)**
  - Visually: **Pv** is the "shadow" cast by **v** when illuminated by a directional light pointing along **Pv-v**.
    - The light direction may depend on **v** but lies in **P**'s nullspace:
      $\mathbf{P(Pv - v)} = \underbrace{\mathbf{PPV}}_{\mathbf{P}} \mathbf{- Pv = 0}$



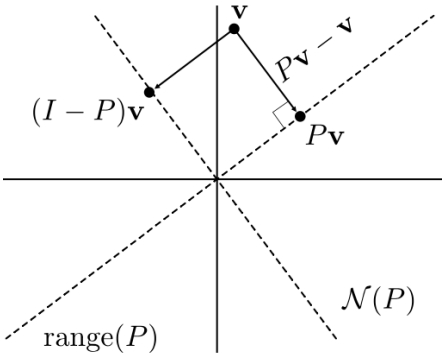
Complementary Projectors

- If P is a projector, then I-P is a projector as well: *(I-P)(I-P)=I-2P+PP=I-2P+P=I-P*
  - ***I-P*** is called the **complementary projector** to ***P***.
  - It projects onto the nullspace of P. Specifically, *range(I-P)=*$\mathcal{N}(P)$
  - Because *P=I-(I-P)*, *P* is the complementary projector to *(I-P)* and thus *range(P)=* $\mathcal{N}(I-P)$
- Complementary subspaces: A projector partitions $\mathbb{C}^m$ into two "disjoint", complementary subspaces:
  - range(P) + range(I-P) = $\mathbb{C}^m$
  - range(P) ∩ range(I-P) = {0}



Orthogonal Projectors

- An orthogonal projector P projects onto a subspace *range(P)=*S_1 along a subspace *range(I-P)=*S_2 where S_1 and S_2 are orthogonal.
- A projector ***P*** is orthogonal if and only if $P = P^H$



- First direction: $P = P^H \Longrightarrow$ any $\mathbf{u} \in S_1$ and $\mathbf{v} \in S_2$ are orthogonal. Note: $\mathbf{u} = P\mathbf{x}, \mathbf{v} = (I-P)\mathbf{y}$ for some $\mathbf{x}, \mathbf{y}$.

$$\mathbf{u}^H\mathbf{v} = \mathbf{x}^H P^H (I-P)\mathbf{y} = \mathbf{x}^H (P - PP)\mathbf{y} = 0.$$

- Second direction: $S_1 \perp S_2 \Longrightarrow P = P^H$.
  - Construct orthonormal bases $\{\mathbf{q}_1, \cdots \mathbf{q}_n\}$ for range S_1 (n-dim) and $\{\mathbf{q}_{n+1}, \cdots \mathbf{q}_m\}$ for nullspace S_2 ($(m-n)$-dim).
  - Concatenate them into a full orthonormal basis for $\mathbb{C}^m$ in Q:

$$Q^H P Q = Q^H \left[\begin{array}{c|c|c|c|c|c} \mathbf{q}_1 & \cdots & \mathbf{q}_n & \mathbf{0} & \cdots & \mathbf{0} \end{array}\right] = \begin{bmatrix} I_{n\times n} & 0 \\ 0 & 0 \end{bmatrix} := \Sigma$$

  - Hence $P = Q\Sigma Q^H$, which is clearly Hermitian.

This

QR Factorization in Projector Form

- Details see slide 22-7~11

Orthogonal Projectors with an Orthonormal Basis

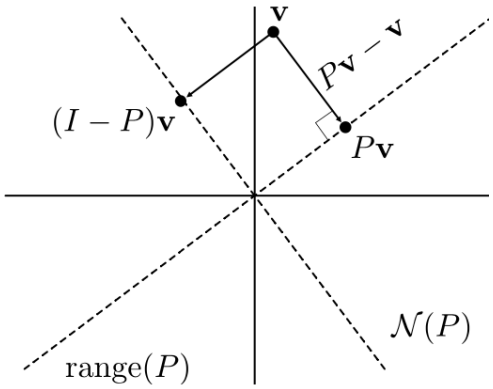
We have shown that an orthogonal projector P can be written using *orthonormal bases* $\hat{Q}$ for $\mathbf{range}(P)$ and $\hat{Q}^\perp$ for $\mathcal{N}(P)$ simply as:

$$P = Q\Sigma Q^H = \begin{bmatrix}\hat{Q} & \hat{Q}^\perp\end{bmatrix}\begin{bmatrix}I_{n\times n} & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}\hat{Q} & \hat{Q}^\perp\end{bmatrix}^H,$$

- The $\hat{Q}^\perp$ blocks do not contribute to P (multiplied by 0). We can drop them and conclude: $P = \hat{Q}\hat{Q}^H$.

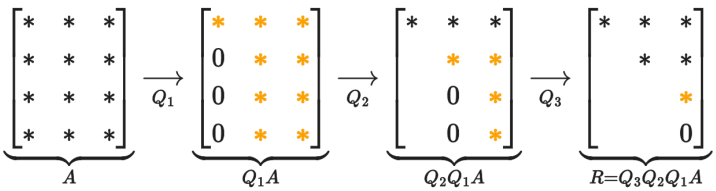
Given any n orthonormal vectors $\{\mathbf{q}_1, \cdots, \mathbf{q}_n\}$ collected in the columns of $\hat{Q}$, the matrix $\hat{Q}\hat{Q}^H$ represents an orthogonal projection onto $\mathbf{range}(\hat{Q})$.

- In sum form: $\hat{Q}\hat{Q}^H = \sum_{i=1}^n \mathbf{q}_i\mathbf{q}_i^H$
- Complementary projector onto $\mathbf{range}(\hat{Q}^\perp)$ is $I - \hat{Q}\hat{Q}^H$.
- Special case: Rank-1 orthogonal projection $P_\mathbf{q} = \mathbf{q}\mathbf{q}^H$ for unit-norm $\mathbf{q}$ and its complement $P_{\perp\mathbf{q}} = I - \mathbf{q}\mathbf{q}^H$.



Lecture 23 - QR Householder Triangularization

- Gram-Schmidt vs. Householder
  - Gram-Schmidt is a "triangular orthogonalization" process: it transforms $\boldsymbol{A}$'s columns into $\hat{Q}$'s orthonormal columns by multiplying a sequence of upper triangular matrices.
    - $AR_1R_2\ldots R_n = \hat{Q} \implies A = \hat{Q}\hat{R}$
  - Householder is a "orthogonal triangularization" process: it reduces $\boldsymbol{A}$ to upper triangular form by multiplying a sequence of unitary matrices
    - $\underbrace{Q_n\ldots Q_2Q_1}_{Q^H}A = R \implies A = QR$
- Key idea: pick **Householder reflector** matrices Q_k to zero out entries below the diagonal.
  - Q_1 operates on all rows, introducing zeros in the first column.
  - Q_2 operates on all rows after the **first**, introducing zeros in the second column.
    - Since entries 2, 3, 4 of the first column are all zeros, they **remain zero** when a linear combination is formed.
  - Q_k operates on rows k to m, introducing zeros in the <u>*k-th*</u> column.
- Details see slide 23



Lecture 24 - Eigenvalues and Eigenvectors

Eigenvalue and Eigenvector

- Definition: Given a square matrix $A \in \mathbb{C}^{m \times m}$ a nonzero vector $\mathbf{x} \in \mathbb{C}^m$ is an **eigenvector**, and $\lambda \in \mathbb{C}$ is its corresponding **eigenvalue**, if: $A\mathbf{x} = \lambda \mathbf{x}$
- Why only for square matrices? $A\mathbf{x}$ must live in the same space as $\mathbf{x}$.
- Intuitively: $\mathbf{A}$ acts just like scalar multiplication on certain subspaces $S \subseteq \mathbb{C}^m$
  - Intuitive video
  - These are called eigenspaces of A
  - Any nonzero vector $\mathbf{x} \in S$ is an eigenvector with the same eigenvalue.
  - These S are generally 1-dimensional, but they can be higher dimension (example: αI)
- The set of all eigenvalues of A is called the matrix **spectrum** $\Lambda(A)$

Eigenvalue Decomposition

- Given a square matrix $A \in \mathbb{C}^{m \times m}$, an eigenvalue decomposition is a factorization: $A = X\Lambda X^{-1} \iff AX = X\Lambda$ where X is a nonsingular matrix.

$$A \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_m \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_m \end{bmatrix} \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_m \end{bmatrix}$$

  - Does not always exist!
- Comparison of Eigenvalue Decomposition and Singular Value Decomposition:
  - SVD always exists!
  - Singular values are positive and real, while eigenvalues can be general complex numbers.
  - Singular vectors are orthogonal, while eigenvectors generally are not.
  - Left and right singular vectors can be completely decoupled; Right eigenvectors (rows of X^{-1}) are orthogonal to corresponding left eigenvector (columns of X).

Eigenvector Basis

- If $Ax = b$ and $A = X\Lambda X^{-1}$ then:

$$b = X\Lambda X^{-1}\mathbf{x} \iff (X^{-1}b) = \Lambda(X^{-1}\mathbf{x})$$

- $X^{-1}b$ and $X^{-1}x$ are the coefficients of **b** and **x** in the eigenvector basis.
  - They express **b** and **x** as linear combinations of the columns of **X**
- After this change of basis, the multiplication by A simply scales each coefficient by the corresponding λ_i

- An **eigenbasis** is a basis of $\mathbb{R}^n$ consisting of eigenvectors of A.
- A's inverse (if it exists) has the same eigenvectors and reciprocal eigenvalues:

$$A^{-1} = (X\Lambda X^{-1})^{-1} = X\Lambda^{-1}X^{-1}$$

- We can solve the linear system $Ax = b$ easily in the eigenvector basis: $(X^{-1}\mathbf{x}) = \Lambda^{-1}(X^{-1}b)$, just dividing each coefficient of B by the corresponding λ_i

---

Characteristic Polynomial

- By definition: λ is an eigenvalue of $A \in \mathbb{C}^{m\times m}$ if and only if:

$$A\mathbf{x} = \lambda\mathbf{x} \text{ for some nonzero } \mathbf{x} \iff (\lambda I - A)\mathbf{x} = 0 \iff det(\lambda I - A) = 0$$

- The **characteristic polynomial** of A is the degree m polynomial defined by: $p_A(z) = det(zI - A)$, where the sign was chosen so that the leading term is always z^m rather than $(-z)^m$.
- In fact, you can show that $p_A(z) = z^m - tr(A)z^{m-1} + \cdots$
- λ is an eigenvalue if and only if it is a root of the characteristic polynomial: $p_A(\lambda) = 0$

$$det(\begin{bmatrix}\lambda - a_{11} & a_{12} \\ a_{21} & \lambda - a_{22}\end{bmatrix}) = 0 \iff (\lambda - a_{11})(\lambda - a_{22}) - a_{12}a_{21} = \lambda^2 - (a_{11} + a_{22})\lambda + a_{11}a_{22} - a_{12}a_{21} = 0$$

Algebraic Multiplicity

- Eigenvalues (roots of p_A) are not necessarily distinct. An eigenvalue λ_j may appear more than once in $\Lambda(A)$.
- The **algebraic multiplicity** of an eigenvalue λ of A is its multiplicity as a root of p_A. An eigenvalue is called **simple** if it is of algebraic multiplicity 1.
  - $A \in \mathbb{C}^{m\times m}$ has exactly m eigenvalues when counted with multiplicity; it will have distinct eigenvalues iff all eigenvalues are simple.
  - Every matrix has at least one eigenvalue.
    Some matrices have only one (distinct) eigenvalue: e.g. αI

Eigenspaces and Geometric Multiplicity

- The set of eigenvectors corresponding to a single eigenvalue λ, together with the zero vector, forms a subspace $E_\lambda \subseteq \mathbb{C}^m$ called an **eigenspace**.

- The dimension of the eigenspace, $\dim(E_\lambda)$, is the number of linearly independent eigenvectors with eigenvalue λ.
  - The dimension is known as the **geometric multiplicity** of λ.
  - Geometric multiplicity is always **less than or equal to** algebraic multiplicity. (Proof see slide 24-14)
  - **Defective matrix** has a **defective eigenvalue** whose algebraic multiplicity exceeds its geometric multiplicity.

Similarity Transformation

- Let $A, B, Y \in \mathbb{C}^{m\times m}$ and suppose Y is nonsingular. Then A and B are said to be **similar** if:

$$B = Y^{-1}AY,$$

And transformation $A \mapsto Y^{-1}AY$ is called a similarity transformation.

- Furthermore, A and B have the same characteristic polynomial, eigenvalues, and algebraic/geometric multiplicity. (Proof see slide 24-13)

Diagonalizability

- A matrix $A \in \mathbb{C}^{m\times m}$ has an eigenvalue decomposition $A = X\Lambda X^{-1}$ if and only if it is non defective (geometric multiplicity=algebraic multiplicity for all eigenvalues)

Determinant and Trace

- $det(A) = \prod_{j=1}^{m} \lambda_j$
- $tr(A) = \sum_{j=1}^{m} \lambda_j$
- Proof see slide 24-16

Unitary Diagonalizability

- A matrix $A \in \mathbb{C}^{m\times m}$ is called **unitarily diagonalizable** if there exists a unitary matrix Q such that: $A = Q\Lambda Q^H$
- These special eigenvalue decompositions are also SVDs (up to signs/ordering of Λ).
- Hermitian matrices are unitarily diagonalizable and have all real eigenvalues!
- A is unitarily **diagonalizable** if and only if $A^H A = A A^H$. Matrices satisfying this are called **normal**.

Schur Factorization

- A very important factorization forming the basis of eigenvalue algorithms:

  A **Shur factorization** of a matrix $A \in \mathbb{C}^{m \times m}$ is a factorization:

  $$A = QTQ^H$$

  where Q is unitary and T is upper-triangular.

  - Because A and T are similar, $\Lambda(A) = \Lambda(T) = t_{ii}$.
  - We therefore call the Shur Factorization an **eigenvalue revealing** factorization.
  - If A is Hermitian:

    $$A^H = (QTQ^H)^H = QT^HQ^H = A = QTQ^H$$

    - Thus $T = T^H$ and T must actually be a diagonal matrix with ***real*** entries.
    - In other words A is unitarily diagonalizable and has real eigenvalues!

- ***Every*** square matrix has a Schur factorization!
  (Even defective ones–this is why the factorization is so powerful.)

Schur Factorization

Lecture 25~26 - Eigenvalue Solvers

Eigenvalue Algorithms

- Algorithms for getting all eigenvalues are generally based on computing a Schur factorization $A = QTQ^H$.
  - When is Hermitian, the Schur factorization is really the eigenvalue decomposition (eigenvectors are the columns of Q).
  - When A is not Hermitian, the eigenvalues are still the diagonal entries t_{ii}.
    - We don't get the eigenvectors directly in this case.
    - However, we will find there are fast algorithms for finding the eigenvectors once you know the eigenvalues.
- A fundamental difficulty: uncomputability!
  - It is actually impossible to compute the eigenvalues (or the Schur factorization) of a general matrix of size in a finite number of arithmetic steps.

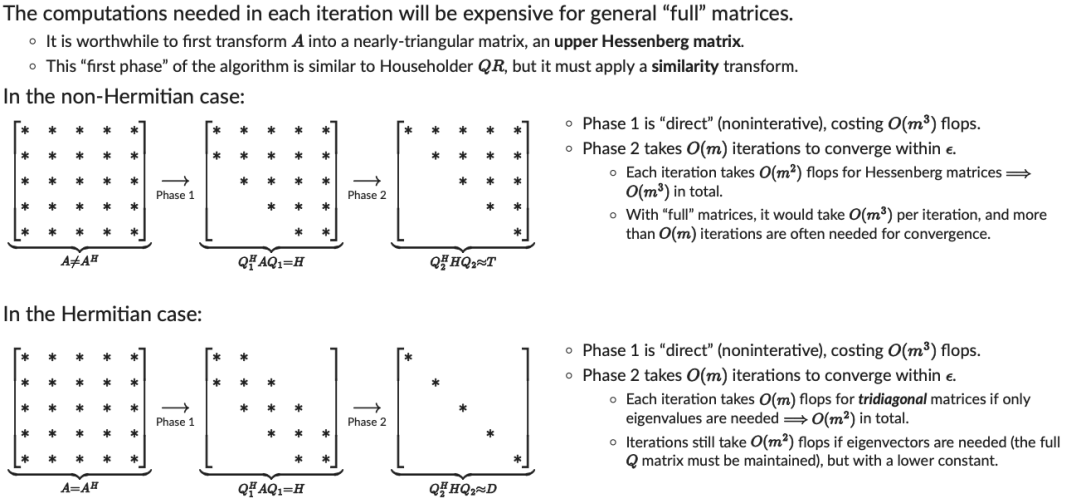
- Proof: a reduction from computing the roots of degree polynomials, which is known to be impossible for certain polynomials of degree in a finite number of arithmetic steps (Galios theory). *Proof see slide 25-7*
- Thus, eigenvalue solvers fundamentally must be **iterative**.

Iterative Eigenvalue Solvers

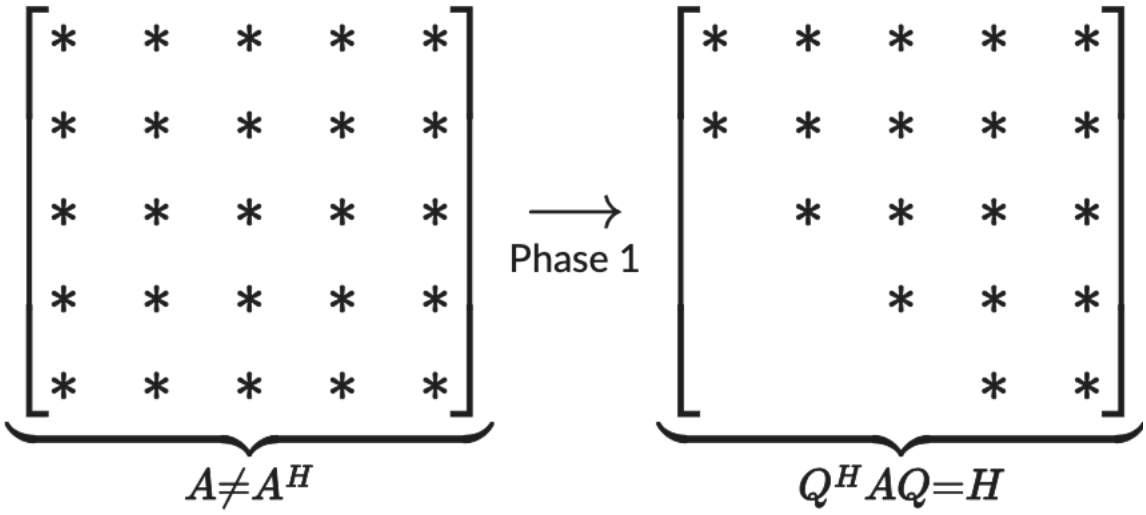
- We can still develop extremely effective, fast eigenvalue solvers.
  - They simply must be iterative: produce a sequence of better and better approximations to the solution.
    - This is fine since we cannot represent the exact solutions in floating point anyway!
    - Stop when we determine the error is on the order of the machine epsilon (or sooner if less accuracy is needed).
  - The best algorithms for individual eigenvalues converge **cubically** in most cases, **quadratically** worst-case.
    - Cubically: the number of correct digits in the eigenvalue estimates triples with each iteration.
    - Quadratically: the number of correct digits doubles with each iteration.
- Most eigenvalue solvers used today approximate a Schur factorization by iteratively applying a sequence of unitary similarity transformations $X \to Q_j^H X Q_j$ to obtain:

$$A_j := \underbrace{Q_j^H \cdots Q_2^H Q_1^H}_{Q^H} A \underbrace{Q_1 Q_2 \cdots Q_j}_{Q}$$

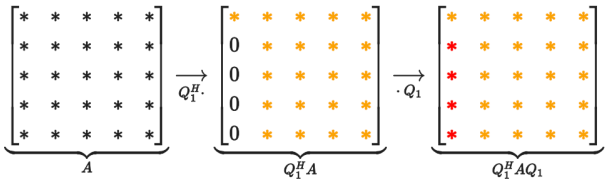
  where A_j approaches an upper-triangular matrix T as $j \to \infty$.
  - Remember: even if A is real, these Schur factors can be complex!
  - If $A = A^H$, then T_j converges to a real diagonal matrix.
- Two Phases Iterative Eigenvalue Solvers



Phase 1: Reduce to Hessenberg matrix



- Idea: use Householder reflections to zero out entries below **sub**-diagonal via similarity transforms.
- Why can't we just zero out all elements below the diagonal and obtain T directly?
  - The uncomputability theorem says this is impossible!
  - If we try, applying the Householder transformation also on the right (needed for similarity transform) undoes progress:
    - Multiplying by Q_1 on the right replaces all columns by a linear combination of all columns, destroying the newly inserted zeros.
    - However, the new entries (red) are typically smaller than before. This will form the basis of the QR algorithm to be studied later.



- Detail see slide 25. 10~15

Phase 2: Power Iteration

- In a word: 不停地用矩阵A乘以向量v，$A^k v$会收敛到对应最大特征值的特征向量。
- Let $A = Q \Lambda Q^T$ with $\Lambda = diag(\lambda_i)$ sorted $|\lambda_1| \geq |\lambda_2| \geq \cdots |\lambda_m|$
- Consider an arbitrary vector $v \in \mathbb{R}^m$ decomposed in A's eigenbasis: $v = a_1 q_1 + a_2 q_2 + \cdots + a_m q_m$
- we have

$$A^k v = \lambda_1^k (a_1 q_1 + a_2 (\frac{\lambda_2}{\lambda_1})^k q_2 + \cdots + a_m (\frac{\lambda_m}{\lambda_1})^k q_m)$$

- If $a_1 \neq 0$, $v_k := \frac{A^k v}{\|A^k v\|}$ approaches $\pm q_1$ since $\frac{\lambda_i}{\lambda_1}$ approaches 0 as $k \to \infty$
  - Thus, repeatedly applying A gives us an **estimate of the eigenvector** corresponding to the largest magnitude eigenvalue
  - What if $a_1 = 0$? Highly unlikely if **v** is chosen randomly!
- What about an eigenvalue estimate?

$$v_k := \frac{A^k v}{\|A^k v\|} \approx \pm q_1 \implies \lambda_1 = q_1^T A q_1 \approx v_k^T A v_k \text{ (Rayleigh Quotient)}$$

- Convergence:
  - The relative eigenvector error is: $\|(\pm v_k) - q_1\| := \|\delta q_1\| = O(|\frac{\lambda_1}{\lambda_2}|)$ as $k \to \infty$
  - The component orthogonal to q_1 gets shrunk by factor $|\frac{\lambda_1}{\lambda_2}|$ at each iteration. (Linear convergence)
  - In a word: too slow

Inverse Iteration & Rayleight Quotient Iteration

- In a word
  - Inverse Iteration: 对$(A - \mu I)^{-1}$使用power iteration可以更快地收敛到q_j和λ_j
  - Rayleigh Quotient Iteration: 对$(A - \lambda I)^{-1}$使用power iteration，更快收敛

Inverse Iteration

- Suppose A has eigenvalues $\{\lambda_j\}$
- If $\mu \notin \{\lambda_j\}$ is not exactly an eigenvalue of A, then

$$\begin{aligned}(A - \mu I)^{-1} &= (Q \Lambda Q^\top - \mu I)^{-1} = (Q \Lambda Q^\top - \mu Q Q^\top)^{-1} \\ &= (Q\,(\Lambda - \mu I)\,Q^\top)^{-1} == (Q\,\mathrm{diag}(\lambda_j - \mu)\,Q^\top)^{-1} \\ &= Q\,\mathrm{diag}(\lambda_j - \mu)^{-1}\,Q^\top,\end{aligned}$$

  has the same eigenvectors as A and eigenvalues $\left\{\frac{1}{\lambda_j - \mu}\right\}$.
  - By picking μ very close to eigenvalue λ_J, we expect $|(\lambda_J - \mu)^{-1}|$ to be much larger than $|(\lambda_j - \mu)^{-1}|$ for all $\lambda_j \neq \lambda_J$.
  - Hence, if we apply power iteration to $(A - \mu I)^{-1}$ we expect it to converge quickly to $\mathbf{q}_J$.

```
algorithm inverse_power_iteration(A, μ):
    v = arbitrary unit-norm vector
    for k = 1, 2, ...:
        v = normalize((A - μ I) \ v)
        λ = dot(v, A * v)
```

- The operation `(A - μ I) \ v` means solve the linear system $(A - \mu I)\mathbf{x} = \mathbf{v}$.
  - Since the matrix doesn't change, we can factorize $(A - \mu I)$ once and reuse it.
  - If $\mu \approx \lambda_J$, $A - \mu I$ is ill-conditioned (nearly singular), but actually this is fine!

- Quicker convergence

Lecture 27 - QR Algorithm for Eigenvalues

QR Algorithm

- An algorithm to compute the **entire** eigenvalue decomposition of a symmetric real matrix.
- The most basic form

```
algorithm pure_qr_algorithm(A):
    for k = 1, 2, ...:
        Q R = A     # Compute the QR factorization of A
        A = R Q     # Recombine the factors in the reverse order.
```

- For it to work, we must have two properties:
  1. The working matrix remains similar to the input matrix with every iteration.
     - $Q_k R_k = A_{k-1}$, $A_k = R_k Q_k \implies Q_k A_k = Q_k(R_k Q_k) = A_{k-1} Q_k \implies A_k = Q_k^{-1} A_{k-1} Q_k$
  2. The working matrix converges to a diagonal matrix.
     - $Q_k R_k = A_{k-1}$, $A_k = R_k Q_k \implies Q_k R_k = A_k = R_{k-1} Q_{k-1}$

$$
\begin{aligned}
A &= Q_1 R_1 \\
A^2 &= (Q_1 R_1)(Q_1 R_1) = Q_1 Q_2 R_2 R_1 \\
A^3 &= (Q_1 R_1)(Q_1 Q_2 R_2 R_1) = Q_1 Q_2 R_2 Q_2 R_2 R_1 = Q_1 Q_2 Q_3 R_3 R_2 R_1 \\
&\vdots \\
A^k &= Q_1 R_1 (Q_1 \cdots Q_{k-1} R_{k-1} \cdots R_1) = \cdots = Q_1 Q_2 \cdots Q_k R_k \cdots R_1
\end{aligned}
$$

- Conclusion: It's a QR factorization of A^k where $\underline{Q_k} := Q_1 Q_2 \ldots Q_k$, $\underline{R_k} := R_k \cdots R_2 R_1$

Block Power Iteration

- To better understand how the QR factorization $A^k = \underline{Q_k}\underline{R_k}$ is helpful, consider applying power iteration to several vectors at once:
  - Suppose we start with a set of m linearly independent vectors $\mathbf{v}_1, \cdots, \mathbf{v}_m$ and apply A^k
  - We have argued that the ordinary power iteration $A^k \mathbf{v}$ converges to a vector parallel to $\mathbf{q}_1$:

$$
\begin{aligned}
A^k \mathbf{v}_1 &= \lambda_1^k \left(a_{11}\mathbf{q}_1 + a_{21}(\lambda_2/\lambda_1)^k \mathbf{q}_2 + \cdots + a_{m1}(\lambda_m/\lambda_1)^k \mathbf{q}_m \right) \\
A^k \mathbf{v}_2 &= \lambda_1^k \left(a_{12}\mathbf{q}_1 + a_{22}(\lambda_2/\lambda_1)^k \mathbf{q}_2 + \cdots + a_{m2}(\lambda_m/\lambda_1)^k \mathbf{q}_m \right) \\
&\cdots
\end{aligned}
$$

    as long as the initial component along $\mathbf{q}_1$, $a_{1*} \neq 0$. Apparently all vectors will converge to be parallel to $\mathbf{q}_1$ ☹.
  - But what if we ***force*** $a_{12} = 0$? Then the $\mathbf{q}_2$ term must dominate (assuming $|\lambda_2| > |\lambda_3|$):

$$
A^k \mathbf{v}_2 = \lambda_2^k \left(a_{22}\mathbf{q}_2 + a_{32}(\lambda_3/\lambda_2)^k \mathbf{q}_3 + \cdots + a_{m2}(\lambda_m/\lambda_2)^k \mathbf{q}_m \right),
$$

    so that $\frac{A^k \mathbf{v}_2}{\|A^k \mathbf{v}_2\|} \to \pm \mathbf{q}_2$ linearly as $k \to \infty$, with error $O\left(\left| \frac{\lambda_3}{\lambda_2} \right|^k \right)$.

    We can apply this same projection process to make $\frac{\|A^k \mathbf{v}_3\|}{\|A^k \mathbf{v}_3\|} \to \pm \mathbf{q}_3, \cdots, \frac{\|A^k \mathbf{v}_m\|}{\|A^k \mathbf{v}_m\|} \to \pm \mathbf{q}_m$ as $k \to \infty$.

  - We can force this by projecting out the component of $\mathbf{v}_2$ along $\mathbf{q}_1 \approx \frac{A^k \mathbf{v}_1}{\|A^k \mathbf{v}_1\|}$ at the start.
  - In exact arithmetic, this is equivalent to projecting out $A^k \mathbf{v}_2$'s component along $\mathbf{q}_1$ (both simply zero out the a_{12} term).

    This is exactly what the QR factorization does: it projects out the second column's component along the first!

    5

- According to above proof, the column of $\underline{Q_k}$ in $A^k = \underline{Q_k}\underline{R_k}$ will converge linearly to the eigenvectors, and A^k converges to Λ.

Accelerating the QR Algorithm (Inverse & Rayleigh Quotient Iteration)

- Details see slide 27.8~11

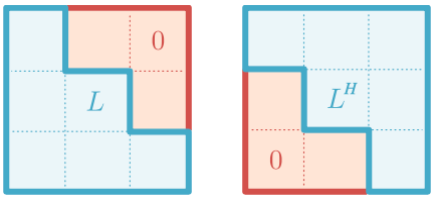
Review

Factorization

LU Factorization

- Definition: Factor a matrix into the form: $A=LU$, where L is lower triangular and U is upper triangular.
- Existence:
  - Without pivoting, might not exist
  - With partial pivoting, we can always construct LUP decomposition
- What do they reveal?
- What can they be used for?
- What algorithms exits for computing them?
  - Gaussian elimination, $A=LU$
    - neither backward stable nor stable, why: 0 on the diagonal)
  - Complete pivoting, $PAQ=LU$ (P, Q are permutation matrix)
    - pick the largest x_{ij} in submatrix $i, j \geq k$, reordering rows and columns
    - Backward stable
  - Partial pivoting, $PA=LU$ (P are permutation matrix)
    - pick the largest x_{ik} in column k ($i \geq k$), only reorder rows
    - Backward stable

Cholesky Factorization

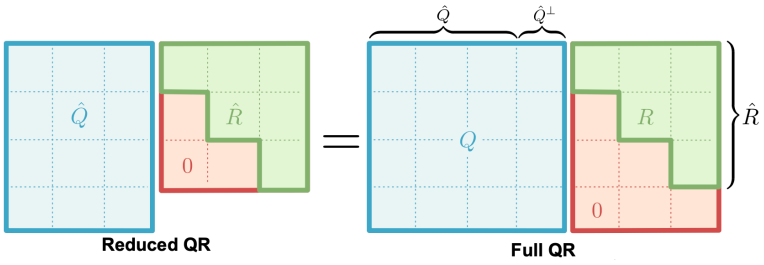


- $A = LL^H$ or $A = RR^H$ with positive **real** diagonal entries $L_{ii} > 0$
- Existence: ***A*** must be hermitian positive definite matrix
- Uniqueness: **Every** hermitian positive definite matrix $A \in \mathbb{C}^{m \times m}$ has a **unique** Cholesky factorization.
- What do they reveal?
- What can they be used for?
- What algorithms exits for computing them?
  - Symmetric Gaussian Elimination

- Backward stable (No pivoting needed)

QR Factorization

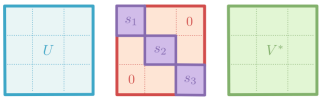
- Reduced QR: $A = \hat{Q}\hat{R}$ with $\hat{Q} \in \mathbb{C}^{m\times n}$ and $\hat{R} \in \mathbb{C}^{n\times n}$, where $\hat{R}$ is a square upper triangular matrix and the columns of $\hat{Q}$ hold an orthonormal basis for *range(A)*:
  $q_i^H q_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$
- Full QR: We can augment the columns of $\hat{Q}$ with additional orthonormal vectors to form the full QR decomposition with a square unitary matrix Q and a "tall" R.



- Existence: ***always exists***
- Uniqueness: **Reduced QR** is unique if we require R's diagonal to be real and positive.
- What do they reveal?
- What can they be used for?
- What algorithms exits for computing them?
  - Gram-Schmidt (unstable, q_j quickly loses orthogonality due to round off error)
  - Householder (backward stable)

Singular Value Decomposition (SVD)

The Singular Value Decomposition



Given $A \in \mathbb{C}^{m\times n}$, a **singular value decomposition (SVD)** of A is a factorization:

$$A = U\Sigma V^H \quad \text{where} \quad \begin{cases} U \in \mathbb{C}^{m\times m} & \text{is unitary,} \\ \Sigma \in \mathbb{C}^{m\times n} & \text{is diagonal,} \\ V \in \mathbb{C}^{n\times n} & \text{is unitary.} \end{cases}$$

Following the standard convention, we assume the **nonnegative** diagonal entries σ_j of Σ are ordered $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p \geq 0$, where $p = \min(m, n)$.

- Note: the columns of V and U form an *orthonormal basis* for the input and output spaces $\mathbb{C}^n$ and $\mathbb{C}^m$, respectively.
  - Columns of U are called "left singular vectors" $\mathbf{u}_j$ and columns of V are called "right singular vectors" $\mathbf{v}_j$.

- Given $A \in \mathbb{C}^{m \times n}$, a singular value decomposition of A is a factorization: $A = U \Sigma V^H$, where $U \in \mathbb{C}^{m \times m}$ is unitary, $\Sigma \in \mathbb{C}^{m \times n}$ is diagonal, and $V \in \mathbb{C}^{n \times n}$ is unitary.
- Existence: ***always exists***
- What do they reveal?
  - determinants when m=n
  - Easily compute the inverse
  - Prove row rank = column rank
  - Reveal normal bases for the nullspace and range of A
- Not backward stable. SVD algorithms are doomed to fail backward stability since an arbitrarily small roundoff error can make $\hat{U}$ and $\hat{V}$ non-unitary: in this case, they cannot be an exact SVD of any matrix.

Schur Factorization

- Given a square matrix $A \in \mathbb{C}^{m \times m}$, a Schur Factorization is a factorization: $A = QTQ^H$ where $\boldsymbol{Q}$ is a unitary matrix and $\boldsymbol{T}$ is an upper triangular.
- Existence: always exists

Eigenvalue Decomposition

- Given a square matrix $A \in \mathbb{C}^{m \times m}$, an eigenvalue decomposition is a factorization: $A = X \Lambda X^{-1} \iff AX = X\Lambda$ where $\boldsymbol{X}$ is a nonsingular matrix.
- Existence: ***not always exists***
- Computing Eigenvalues?
  - "Direct" reduction to upper Hessianberg (similar to householder)
  - Iterative reduction to upper triangular (power iteration)
- Computing full eigenvalue decomposition of a symmetric real matrix A
  - QR algorithm

Solving Linear System

Ax=b

Solving Least Squares

$\min_x \|Ax - b\|_2$ for $A \in \mathbb{C}^{m \times n}$, $m \geq n$

- Cholesky (normal equations)
  - $A^H A x = A^H b, \quad A^H A = L L^H$
- Reduced QR
  - $A = \hat{Q}\hat{R}, Ax = b \implies \underbrace{\hat{R}^H \hat{Q}^H}_{A^H} \underbrace{\hat{Q}\hat{R}}_{A} x = \underbrace{\hat{R}^H \hat{Q}^H}_{A^H} b \implies \hat{R}x = \hat{Q}^H b$
- Reduced SVD
  - $A = \hat{U}\hat{\Sigma}V^H, Ax = b \implies \underbrace{V\hat{\Sigma}\hat{U}^H}_{A^H} \underbrace{\hat{U}\hat{\Sigma}V^H}_{A} x = \underbrace{V\hat{\Sigma}\hat{U}^H}_{A^H} b \implies x = V\hat{\Sigma}^{-1}\hat{U}^H b$

Lemma

Triangular Matrix

- The product of two upper/lower triangular matrix is still upper/lower triangular. (HW0 - Prob 5)
- The inverse of upper/lower triangular matrix, if it exists, is still upper/lower triangular. (HW0 - Prob 6)

Orthogonal Square Matrix

- $A^T = A^{-1}$
- $AA^T = I$
- A^T is orthogonal
- det(A)=± 1 (Proof: $det(I) = det(A^T A) = det(A^T)det(A) = 1$)

Rank

- Rank-One: The rank of a matrix $A \in \mathbb{R}^{m \times n}$ equals 1 if and only if it can be written in the form xy^T. (HW0 - Prob 3)
- Full-Rank: A matrix $A \in \mathbb{F}^{m \times n}$ with $m \geq n$ has full rank n iff $Ax \neq Ay$, $\forall x \neq y \in \mathbb{F}^n$
  - $\implies \forall x \neq 0$, we have $Ax \neq 0$
- rank(AB)$\leq$min(rank(A), rank(B))

Determinant

- det(A)=0 if A's columns are linearly dependent
- det(I)=1
- det(triangular matrix)=$\prod_{i=1}^{m} a_{ii}$
- det(αA)=α^mdet(A)
- det(A^T)=det(A)
- det(AB)=det(A)det(B)
- det(A^{-1})=$\frac{1}{det(A)}$

Inverse Matrix

- Theorem: the following conditions for square matrix $A \in \mathbb{F}^{m \times m}$ are equivalent
  - A has an inverse A^{-1}
  - A is a nonsingular matrix
  - det(A)≠0 (if det(A)=0, then the transformation squishes into lower dimension)
  - A is of full rank m
  - range(A)=$\mathbb{F}^m$
  - $\mathbb{N}(A) = \{\mathbf{0}\}$
  - 0 is not an eigenvalue of A
  - 0 is not a singular value of A

Positive Definite

- A hermitian matrix (i.e. $A = A^H$) is positive definite if $x^H A x > 0 \quad \forall x \neq 0$