Numerical Linear Algebra

1 Matrices, Vectors, and Norms

1.1 Matrix-Vector Multiplication

Given a matrix $A \in \mathbb{C}^{m \times n}$ and a vector $x \in \mathbb{C}^n$, the matrix-vector product $Ax = b \in \mathbb{C}^m$ is defined as:

$$b_i = \sum_{j=1}^{n} a_{ij} x_j, \quad \text{for } i = 1, \ldots, m$$

where a_{ij} are the entries of the matrix A.

Observation

The transformation $x \mapsto Ax$ is a linear transformation from $\mathbb{C}^n$ to $\mathbb{C}^m$, i.e., it satisfies:

$$A(x+y) = Ax + Ay, \quad A(\alpha x) = \alpha Ax, \quad \text{for all } x, y \in \mathbb{C}^n, \alpha \in \mathbb{C}$$

1.1.1 A Matrix times a Vector

$$b = Ax = \sum_{j=1}^{n} x_j a_j$$

where a_j is the j-th column of A.

$$\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = x_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix} + x_2 \begin{bmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{m2} \end{bmatrix} + \cdots + x_n \begin{bmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{mn} \end{bmatrix}$$

Example: Vandermonde Matrix

A Vandermonde matrix is defined as:

$$A = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_m & x_m^2 & \cdots & x_m^{n-1} \end{bmatrix} \in \mathbb{C}^{m \times n}$$

Observation

Let fix the sequence $\{x_1, x_2, \ldots, x_m\}$. If p and q are polynomials of degree at most $n-1$ and α is a scalar, then:

1. $(p+q)$ is a polynomial of degree at most $n-1$, and so are $\alpha p, \alpha q$.
2. $(p+q)(x_i) = p(x_i) + q(x_i)$ for $i = 1, \ldots, m$.
3. $(\alpha p)(x_i) = \alpha p(x_i)$ for $i = 1, \ldots, m$.

Observation

Suppose we have a vector $c \in \mathbb{C}^n$ representing the coefficients of a polynomial $p(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_{n-1} x^{n-1}$. Then

$$p(x_i) = (Ac)_i = c_0 + c_1 x_i + c_2 x_i^2 + \cdots + c_{n-1} x_i^{n-1}$$

Any polynomial of degree at most $n-1$ can be represented as

$$p(x) = \begin{bmatrix} 1 & x & x^2 & \cdots & x^{n-1} \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_{n-1} \end{bmatrix}$$

1.2 Matrix-Matrix Multiplication

Given matrices $A \in \mathbb{C}^{l \times m}$ and $C \in \mathbb{C}^{m \times n}$, the matrix-matrix product $B = AC \in \mathbb{C}^{l \times n}$ is defined as:

$$b_{ij} = \sum_{k=1}^{m} a_{ik} c_{kj}, \quad \text{for } i = 1, \ldots, l, j = 1, \ldots, n$$

So,

$$B = \begin{bmatrix} b_1 & b_2 & \cdots & b_n \end{bmatrix} = \begin{bmatrix} a_1 & a_2 & \cdots & a_m \end{bmatrix} \begin{bmatrix} c_1 & c_2 & \cdots & c_n \end{bmatrix}$$

$$b_j = Ac_j = \sum_{k=1}^{m} c_{kj} a_k, \quad j = 1, \ldots, n$$

Example: Outer Product

Given two vectors $u \in \mathbb{C}^{m \times 1}$ and $v \in \mathbb{C}^{1 \times n}$, the outer product $uv^T \in \mathbb{C}^{m \times n}$ is defined as:

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_m \end{bmatrix} \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} = \begin{bmatrix} u_1 v_1 & u_1 v_2 & \cdots & u_1 v_n \\ u_2 v_1 & u_2 v_2 & \cdots & u_2 v_n \\ \vdots & \vdots & \ddots & \vdots \\ u_m v_1 & u_m v_2 & \cdots & u_m v_n \end{bmatrix}$$

Example

Let $B \in \mathbb{C}^{m \times n}$, let $a_1, a_2, \ldots, a_n$ be the columns of $A \in \mathbb{C}^{m \times n}$ and let $R \in \mathbb{C}^{n \times n}$ be an upper triangular matrix with all its superdiagonal entries equal to 1 such that

$$B = \begin{bmatrix} b_1 & b_2 & \ldots & b_n \end{bmatrix} = \begin{bmatrix} a_1 & a_2 & \ldots & a_n \end{bmatrix} \begin{bmatrix} 1 & 1 & \ldots & 1 \\ 0 & 1 & \ldots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{bmatrix}$$

Then,

$$b_j = Ar_j = \sum_{k=1}^{j} a_k, \quad j = 1, \ldots, n$$

which is known as the indefinite integral operation.

1.3 Range and Null Space

Theorem

The range of a matrix $A \in \mathbb{C}^{m \times n}$ is the space spanned by its columns, i.e. it's column space.

"The set of vectors that can be written as Ax for some $x \in \mathbb{C}^n$."

1.3.1 Null Space and Rank

The null space of a matrix $A \in \mathbb{C}^{m \times n}$ is defined as:

$$\text{span}\{x \in \mathbb{C}^n : Ax = 0\}$$

The rank of a matrix $A \in \mathbb{C}^{m \times n}$ is defined as the dimension of its range:

$$\text{rank}(A) = \dim(\text{range}(A))$$

Theorem

For any matrix $A \in \mathbb{C}^{m \times n}, m \geq n$, A has full rank if and only if it maps no two distinct vectors to the same vector:

$$Ax = Ay \implies x = y, \forall x, y \in \mathbb{C}^n \quad \text{and} \quad Ax \neq Ay \implies x \neq y, \forall x, y \in \mathbb{C}^n$$

1.3.2 Non-singular Matrices

A non-singular matrix, or invertible matrix is a square matrix $A \in \mathbb{C}^{n \times n}$ that has full rank.

1.3.3 Inverse of a Matrix

The matrix $A \in \mathbb{C}^{n \times n}$ is the inverse of Z if and only if:

$$AZ = ZA = I = \begin{bmatrix} e_1 & e_2 & \cdots & e_n \end{bmatrix}$$

where e_i is the i-th standard basis vector. Furthermore, the inverse of a matrix is unique and

$$\text{rank}(A) = n = \text{rank}(Z)$$

Theorem

For $A \in \mathbb{C}^{n \times n}$, the following statements are equivalent:

1. A has an inverse A^{-1}.
2. A has full rank, i.e. $\text{rank}(A) = n$.
3. The columns of A span $\mathbb{C}^n$, i.e. $\text{range}(A) = \mathbb{C}^n$.
4. The columns of A are linearly independent, i.e. $\text{null}(A) = \{0\}$.
5. 0 is not an eigenvalue of A.
6. 0 is not a singular value of A.
7. $|A| \neq 0$.

1.4 Orthogonal Vectors and Matrices

1.4.1 Complex Conjugate and Conjugate Transpose

Given $z \in \mathbb{C}$, the complex conjugate of z is denoted by $\bar{z}$ or z^*, where if $z = x + iy$, then $\bar{z} = x - iy$.
The conjugate transpose of a matrix $A \in \mathbb{C}^{m\times n}$ is denoted by A^*, where $A^* = \bar{A}^T$.

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix} \implies A^* = \begin{bmatrix} \bar{a}_{11} & \bar{a}_{21} & \bar{a}_{31} \\ \bar{a}_{12} & \bar{a}_{22} & \bar{a}_{32} \end{bmatrix}$$

1.4.2 Hermitian Matrices and Skew-Hermitian Matrices

A matrix $A \in \mathbb{C}^{n\times n}$ is called Hermitian if $A^* = A$. (Or $A = A^T$ if $A \in \mathbb{R}^{n\times n}$.)
A matrix $A \in \mathbb{C}^{n\times n}$ is called Skew-Hermitian if $A^* = -A$. (Or $A = -A^T$ if $A \in \mathbb{R}^{n\times n}$.)

1.4.3 Inner Product and Norm

Given two vectors $x, y \in \mathbb{C}^n$, the inner product is defined as:

$$\langle x, y\rangle = y^* x = \sum_{i=1}^{n} \bar{y}_i x_i$$

The norm of a vector $x \in \mathbb{C}^n$ is defined as:

$$\|x\| = \sqrt{\langle x, x\rangle} = \sqrt{\sum_{i=1}^{n} |x_i|^2}$$

The modulus of a complex number $z \in \mathbb{C}$ is defined as:

$$|z| = \sqrt{z\bar{z}} = \sqrt{x^2 + y^2} \quad \text{where } z = x + iy$$

The angle θ between two vectors $x, y \in \mathbb{C}^n$ is defined as:

$$\cos(\theta) = \frac{\langle x, y\rangle}{\|x\|\|y\|}$$

Observation

The inner product is bilinear, which means:

1. $\langle x_1 + x_2, y\rangle = \langle x_1, y\rangle + \langle x_2, y\rangle$
2. $\langle x, y_1 + y_2\rangle = \langle x, y_1\rangle + \langle x, y_2\rangle$
3. $\langle \alpha x, \beta y\rangle = \alpha\bar{\beta}\langle x, y\rangle$ for all $\alpha, \beta \in \mathbb{C}$

For all vectors or matrices A, B of compatible dimensions, we have:

$$(AB)^* = B^* A^*$$

1.4.4 Orthogonal Vectors

Two vectors $x, y \in \mathbb{C}^n$ are orthogonal if $\langle x, y\rangle = 0$.

Observation

If x and y are orthogonal, then they are perpendicular.
With $x = \{x_1, x_2, \ldots, x_n\}$ and $y = \{y_1, y_2, \ldots, y_n\}$, x and y are orthogonal if and only if:

$$\langle x_i, y_j \rangle = 0, \quad \forall i, j = 1, 2, \ldots, n$$

1.4.5 Orthonormal Vectors

A set of vectors $\{x_1, x_2, \ldots, x_n\} \subset \mathbb{C}^n$ is orthonormal if:

$$\langle x_i, x_j \rangle = 0 \text{ for } i \neq j \quad \text{and} \quad \langle x_i, x_i \rangle = \|x_i\|^2 = 1$$

Observation

The vectors in an orthogonal set are linearly independent.

1.4.6 Orthogonal and Unitary Matrices

A matrix $Q \in \mathbb{R}^{n \times n}$ is orthogonal if its columns form an orthonormal set, i.e. $Q^T Q = QQ^T = I$.
A matrix $U \in \mathbb{C}^{n \times n}$ is unitary if its columns form an orthonormal set, i.e. $U^* U = UU^* = I$.

Observation

If $U \in \mathbb{C}^{n \times n}$ is unitary, then $U^{-1} = U^*$ and

$$\begin{bmatrix} u_1^* \\ u_2^* \\ \vdots \\ u_n^* \end{bmatrix} \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

which implies that $\langle u_i, u_j \rangle = \delta_{ij}$ where δ_{ij} is the Kronecker delta, i.e. $\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$.

2 Vector Spaces

A vector space $\mathcal{V}$ over a field $\mathbb{F}$ (usually $\mathbb{R}$ or $\mathbb{C}$) is a set of objects called vectors, along with two operations: vector addition and scalar multiplication, satisfying the following axioms for all $u, v, w \in \mathcal{V}$ and $\alpha, \beta \in \mathbb{F}$:

1. (Closure under addition) $u + v \in \mathcal{V}$
2. (Commutativity) $u + v = v + u$
3. (Associativity) $(u + v) + w = u + (v + w)$
4. (Existence of additive identity) There exists an element $0 \in \mathcal{V}$ such that $u + 0 = u$
5. (Existence of additive inverses) For each $u \in \mathcal{V}$, there exists an element $-u \in \mathcal{V}$ such that $u + (-u) = 0$
6. (Closure under scalar multiplication) $\alpha u \in \mathcal{V}$
7. (Distributivity of scalar multiplication with respect to vector addition) $\alpha(u + v) = \alpha u + \alpha v$
8. (Distributivity of scalar multiplication with respect to field addition) $(\alpha + \beta)u = \alpha u + \beta u$
9. (Associativity of scalar multiplication) $\alpha(\beta u) = (\alpha\beta)u$
10. (Existence of multiplicative identity) $1u = u$ where 1 is the multiplicative identity in $\mathbb{F}$

2.1 Linear Subspaces

A subset $\mathcal{W}$ of a vector space $\mathcal{V}$ is a subspace if $\mathcal{W}$ is itself a vector space under the operations of addition and scalar multiplication defined on $\mathcal{V}$:

1. (Closure under addition) $u + v \in \mathcal{W}$
2. (Closure under scalar multiplication) $\alpha u \in \mathcal{W}$

2.2 Linear Independence

A set of vectors $\{v_1, v_2, \dots, v_k\} \subset \mathcal{V}$ is linearly independent if the only solution to

$$\alpha_1 v_1 + \alpha_2 v_2 + \cdots + \alpha_k v_k = 0$$

is $\alpha_1 = \alpha_2 = \cdots = \alpha_k = 0$. If there exists a non-trivial solution, the set is linearly dependent.

2.3 Basis and Dimension

A basis of a vector space $\mathcal{V}$ is a set of linearly independent vectors that spans $\mathcal{V}$. The dimension of $\mathcal{V}$, denoted $\dim(\mathcal{V})$, is the number of vectors in any basis of $\mathcal{V}$.

2.4 Inner Product and Norms

An inner product on a vector space $\mathcal{V}$ over $\mathbb{F}$ is a function $\langle \cdot, \cdot \rangle : \mathcal{V} \times \mathcal{V} \to \mathbb{F}$. The standard inner product on $\mathbb{C}^n$ is defined as:

$$\langle x, y \rangle = y^* x = \sum_{i=1}^{n} \bar{y}_i x_i$$

A norm on a vector space $\mathcal{V}$ is a function $\| \cdot \| : \mathcal{V} \to \mathbb{R}$ satisfying:

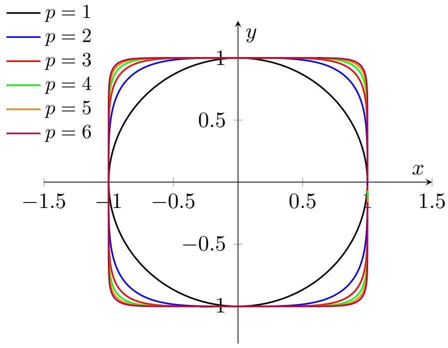
1. (Non-negativity) $\|v\| \geq 0$
2. (Definiteness) $\|v\| = 0$ if and only if $v = 0$
3. (Homogeneity) $\|\alpha v\| = |\alpha| \|v\|$ for all $\alpha \in \mathbb{F}$ and $v \in \mathcal{V}$
4. (Triangle inequality) $\|u + v\| \leq \|u\| + \|v\|$ for all $u, v \in \mathcal{V}$

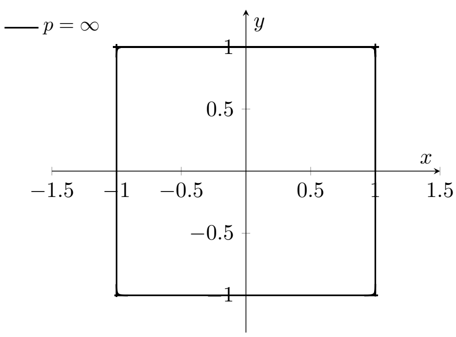
The p-norm on $\mathbb{C}^n$ is defined as:

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

for $1 \leq p < \infty$, and the ∞-norm is defined as:

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





2.4.1 Lemma

Let $\|\cdot\|_\alpha$ and $\|\cdot\|_\beta$ be two norms on a finite-dimensional vector space $\mathcal{V}$. Then there exist positive constants c_1 and c_2 such that for all $v \in \mathcal{V}$:

$$c_1\|v\|_\alpha \leq \|v\|_\beta \leq c_2\|v\|_\alpha$$

$\|\cdot\|_\alpha$ and $\|\cdot\|_\beta$ are said to be equivalent norms. In $\mathbb{R}^n$:

$$\|x\|_2 \leq \|x\|_1 \leq \sqrt{n}\|x\|_2$$

$$\|x\|_\infty \leq \|x\|_2 \leq \sqrt{n}\|x\|_\infty$$

$$\|x\|_\infty \leq \|x\|_1 \leq n\|x\|_\infty$$

3 Matrix Norms

A matrix norm is a function $\|\cdot\| : \mathbb{C}^{m\times n} \to \mathbb{R}$ satisfying:

1. (Non-negativity) $\|A\| \geq 0$
2. (Definiteness) $\|A\| = 0$ if and only if $A = 0$
3. (Homogeneity) $\|\alpha A\| = |\alpha|\|A\|$ for all $\alpha \in \mathbb{C}$ and $A \in \mathbb{C}^{m\times n}$
4. (Triangle inequality) $\|A + B\| \leq \|A\| + \|B\|$ for all $A, B \in \mathbb{C}^{m\times n}$
5. (Sub-multiplicativity) $\|AB\| \leq \|A\|\|B\|$ for all $A \in \mathbb{C}^{m\times n}$ and $B \in \mathbb{C}^{n\times p}$

3.1 Frobenius Norm

The Frobenius norm of a matrix $A \in \mathbb{C}^{m\times n}$ is defined as:

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} |a_{ij}|^2} = \sqrt{\text{trace}(A^*A)}$$

3.2 Induced Norms

The induced norm (or operator norm) of a matrix $A \in \mathbb{C}^{m\times n}$ is defined as:

$$\|A\| = \sup_{x\neq 0} \frac{\|Ax\|}{\|x\|} = \sup_{\|x\|=1} \|Ax\|$$

3.3 Consistent Norms

Let $\|\cdot\|_{m\times n}, \|\cdot\|_{n\times p}$ and $\|\cdot\|_{m\times p}$ be three matrix norms on $\mathbb{C}^{m\times n}, \mathbb{C}^{n\times p}$ and $\mathbb{C}^{m\times p}$ respectively. They are said to be consistent if:

$$\|AB\|_{m\times p} \leq \|A\|_{m\times n}\|B\|_{n\times p}, \quad \forall A \in \mathbb{C}^{m\times n}, B \in \mathbb{C}^{n\times p}$$

3.4 Properties of Induced Norms

1. $\|Ax\| \le \|A\|\|x\|$ for all $A \in \mathbb{C}^{m\times n}$ and $x \in \mathbb{C}^n$
2. $\|AB\| \le \|A\|\|B\|$ for all $A \in \mathbb{C}^{m\times n}$ and $B \in \mathbb{C}^{n\times p}$
3. $\|A\|_\infty = \max_{1\le i\le m} \sum_{j=1}^{n} |a_{ij}|$ (maximum absolute row sum)
4. $\|A\|_1 = \max_{1\le j\le n} \sum_{i=1}^{m} |a_{ij}|$ (maximum absolute column sum)
5. $\|A\|_2 = \sqrt{\lambda_{\max}(A^*A)}$ (with $\lambda_{\max}$ the largest eigenvalue)
6. $\|A\|_2 = \|A^T\|_2$
7. $\|A\|_2 = \max|\lambda_i(A)|$ if A is normal (i.e. $A^*A = AA^*$)
8. $\|A\|_F = \sqrt{\text{trace}(A^*A)}$

So, in general,

$$\|A\|_\alpha = \max_{x\neq 0} \frac{\|Ax\|_\alpha}{\|x\|_\alpha} = \max_{\|x\|_\alpha=1} \|Ax\|_\alpha$$

The Frobenius norm is consistent with the euclidean vector norm, but it is not an induced norm.

3.5 Equivalence of Matrix Norms

Let $\|\cdot\|_\alpha$ and $\|\cdot\|_\beta$ be two matrix norms on $\mathbb{C}^{m\times n}$. Then there exist positive constants c_1 and c_2 such that for all $A \in \mathbb{C}^{m\times n}$:

$$c_1\|A\|_\alpha \le \|A\|_\beta \le c_2\|A\|_\alpha$$

4 Conditioning and Stability

4.1 Conditioning

The conditioning is a measure of how the output value of a function changes with respect to small changes in the input value.

$$f : X \to Y$$

With a small perturbation in the input x to $x + \delta x$, the output changes from $f(x)$ to $f(x + \delta x)$. We define

$$\delta f = f(x + \delta x) - f(x)$$

We want to measure how large δf is relative to $f(x)$ when δx is small relative to x.

4.1.1 Absolute Condition Number

The normwise absolute condition number of a function f at a point x is defined as:

$$\hat{\kappa}_f(x) = \lim_{\delta x\to 0} \sup_{\|\delta x\|\le\delta} \frac{\|\delta f\|}{\|\delta x\|} \approx \sup_{\|\delta x\|<\delta} \frac{\|\delta f\|}{\|\delta x\|}$$

If f is differentiable at x, then

$$\hat{\kappa}_f(x) = \lim_{\delta x\to 0} \sup_{\|\delta x\|\le\delta} \frac{\|\delta f(x)\|}{\|\delta x\|} = \|J_f(x)\|$$

where $J_f(x)$ is the Jacobian of f at x.

4.1.2 Relative Condition Number

The normwise relative condition number of a function f at a point x is defined as:

$$\kappa_f(x) = \lim_{\delta x \to 0} \sup_{\frac{\|\delta x\|}{\|x\|} \leq \delta} \frac{\|\delta f\|/\|f(x)\|}{\|\delta x\|/\|x\|} \overset{f \text{ differentiable}}{=} \frac{\|J_f(x)\|\|x\|}{\|f(x)\|}$$

Example

Let $f : \mathbb{R} \setminus \{0\} \to \mathbb{R}$ be defined as $f(x) = \dfrac{1}{x}$. Then $f'(x) = -\dfrac{1}{x^2}$ and

$$\hat{\kappa}_f(x) = |f'(x)| = \frac{1}{|x|^2}, \quad \kappa_f(x) = \frac{|f'(x)||x|}{|f(x)|} = 1$$

As $x \to 0$, $\hat{\kappa}_f(x) \to \infty$ but $\kappa_f(x) = 1$. This means that $f(x) = \frac{1}{x}$ is well-conditioned for all $x \neq 0$ in the relative sense, but it is ill-conditioned as $x \to 0$ in the absolute sense.

Example

Let $f : \mathbb{R}^2 \to \mathbb{R}$ be defined as $f(x, y) = x - y$. Then, f is differentiable and

$$J_f(x, y) = \begin{bmatrix} 1 & -1 \end{bmatrix}$$

So,

$$\hat{\kappa}_f(x, y) = \|J_f(x, y)\|_2 = \sqrt{2}, \quad \|\kappa_f(x, y)\|_1 = \frac{\|J_f(x, y)\|_1 \|(x, y)\|_1}{|f(x, y)|} = \frac{2(|x| + |y|)}{|x - y|}$$

As $x \to y$, $\kappa_f(x, y) \to \infty$. This means that $f(x, y) = x - y$ is ill-conditioned when x is close to y.

Example

Let $f : \mathbb{R}^2 \to \mathbb{R}$ be defined as $f(x, y) = \dfrac{x}{y}$. Then

$$\|\kappa_f(x, y)\|_2 = \left|\frac{x}{y}\right| + \left|\frac{y}{x}\right|$$

As $y \to 0$ or $x \to 0$, $\kappa_f(x, y) \to \infty$. This means that $f(x, y) = \dfrac{x}{y}$ is ill-conditioned when y or x is close to 0.

4.2 Stability

An algorithm is stable if it produces an output that is close to the exact solution of a problem. Formally, an algorithm $\hat{f}$ for the problem $f : X \to Y$ is **numerically stable** if for every input $x \in X$, there exists $\hat{x} = x + \delta x \in X$ such that

$$\frac{\|\hat{f}(x) - f(\hat{x})\|}{\|f(x)\|} = O(\epsilon_{\text{mach}}) \quad \text{and} \quad \frac{\|x - \hat{x}\|}{\|x\|} = O(\epsilon_{\text{mach}})$$

where ϵ_{mach} is the machine precision.
An algorithm is **backward stable** if for every input $x \in X$, there exists $\hat{x} = x + \delta x \in X$ such that

$$\hat{f}(x) = f(\hat{x}) \quad \text{and} \quad \frac{\|x - \hat{x}\|}{\|x\|} = O(\epsilon_{\text{mach}})$$

4.3 Accuracy

An algorithm $\hat{f}$ is said to be **accurate** if it produces results that are close to the true solution $f(x)$ for all inputs $x \in X$. Formally, this means that for every input $x \in X$, the following holds:

$$\frac{\|\hat{f}(x) - f(\hat{x})\|}{\|f(x)\|} = O(\epsilon_{\text{mach}})$$

Observation

A numerically stable algorithm or a backward stable algorithm is accurate if the problem it solves is well-conditioned.

$$\begin{aligned}\frac{\|\hat{f}(x) - f(\hat{x})\|}{\|f(x)\|} &= \frac{\|f(\hat{x}) + \Delta y - f(x)\|}{\|f(x)\|} \le \frac{\|f(x+\Delta x) - f(x)\|}{\|f(x)\|} + \frac{\|\Delta y\|}{\|f(x)\|} \cdot \|y\| \\ &\le \frac{\|f(x+\Delta x) - f(x)\|/\|f(x)\|}{\|\Delta x\|/\|x\|} \cdot \frac{\|\Delta x\|}{\|x\|} + O(\epsilon_{\text{mach}}) = O(\kappa_f(x)\epsilon_{\text{mach}})\end{aligned}$$

where $\Delta x = \hat{x} - x$ and $\Delta y = \hat{f}(x) - f(\hat{x})$.

5 Solving Linear Systems

Let

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

where L is a lower triangular matrix and U is an upper triangular matrix. Now, we define x_k as the k-th column of A:

$$x_k = \begin{bmatrix} x_{1k} \\ \vdots \\ x_{kk} \\ \vdots \\ x_{nk} \end{bmatrix} \longrightarrow L_k \cdot x_k = \begin{bmatrix} x_{1k} \\ \vdots \\ x_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \text{where} \quad L_k = \begin{bmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & -l_{k+1,k} & 1 & & \\ & & \vdots & & \ddots & \\ & & -l_{n,k} & & & 1 \end{bmatrix}$$

with $l_{ik} = \dfrac{x_{ik}}{x_{kk}}$ for $k < i \le n$. Thus, we can write

$$L_k = I - l_k e_k^T$$

where $l_k = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ l_{k+1,k} \\ \vdots \\ l_{n,k} \end{bmatrix}$ and $e_k = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$ (1 at the k-th position).

Therefore,

$$e_k^T l_k = 0 \quad \text{and} \quad (I - l_k e_k^T)(I + l_k e_k^T) = I \implies L_k^{-1} = I + l_k e_k^T$$

Example

Let $A = L \cdot U = (L_1^{-1} L_2^{-1} L_3^{-1}) \cdot U$ where

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

Then,

$$L_1 = \begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ -4 & & 1 & \\ -3 & & & 1 \end{bmatrix}, \quad L_2 = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & -3 & 1 & \\ & -4 & & 1 \end{bmatrix}, \quad L_3 = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & -1 & 1 \end{bmatrix}$$

Consider $L_k^{-1} \cdot L_{k+1}^{-1} = (I + l_k e_k^T)(I + l_{k+1} e_{k+1}^T) = I + l_k e_k^T + l_{k+1} e_{k+1}^T$ because $e_k^T l_{k+1} = 0$. Thus,

$$L_1^{-1} \cdots L_{n-1}^{-1} = L = \begin{bmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ l_{31} & l_{32} & 1 & & \\ \vdots & \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{bmatrix}$$

5.1 Forward Elimination

Consider the Forward Elimination algorithm:

$$\text{Input: } A \in \mathbb{R}^{n \times n}, \bar{b} \in \mathbb{R}^n$$

$$\text{Output: } U \in \mathbb{R}^{n \times n}, \bar{b}^* \in \mathbb{R}^n \text{ such that } LA = U \text{ and } L\bar{b} = \bar{b}^*$$

Algorithm 1: Forward Elimination

Input: $A \in \mathbb{R}^{n \times n}, \bar{b} \in \mathbb{R}^n$

Output: $U \in \mathbb{R}^{n \times n}, \bar{b}^* \in \mathbb{R}^n$ such that $LA = U$ and $L\bar{b} = \bar{b}^*$

```
for k = 1 to n − 1 do
    for i = k + 1 to n do
        l_ik = a_ik / a_kk;
        for j = k to n do
            a_ij = a_ij − l_ik a_kj;
        b_i = b_i − l_ik b_k;
```

So, the output is

$$L \left[A \;\middle|\; \bar{b} \right] = \left[U \;\middle|\; \bar{b}^* \right]$$

5.2 Backward Substitution

Consider the Backward Substitution algorithm:

$$R\bar{x} = \bar{b}, \quad R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}$$

$$r_{nn}x_n = b_n \quad \text{and} \quad r_{n-1,n}x_{n-1} + r_{n-1,n}x_n = b_{n-1}$$

$$x_n = \frac{b_n}{r_{nn}} \quad \text{and} \quad x_i = \frac{b_i - \sum_{j=i+1}^{n} r_{ij}x_j}{r_{ii}}, \quad i = n-1, n-2, \ldots, 1$$

Algorithm 2: Backward Substitution

Input: $U \in \mathbb{R}^{n\times n}$ (upper triangular), $\bar{b} \in \mathbb{R}^n$
Output: $\bar{x} \in \mathbb{R}^n$ such that $U\bar{x} = \bar{b}$

$x_n = \dfrac{b_n}{r_{nn}}$;
for $i = n-1$ ***down to*** 1 **do**
  $x_i = b_i$;
  for $j = i+1$ ***to*** n **do**
    $x_i = x_i - r_{ij}x_j$;
  $x_i = \dfrac{x_i}{r_{ii}}$;

5.3 Solving Triangular Systems

With $D\overline{x} = \bar{b}$, D diagonal $(d_{11}, d_{22}, \ldots, d_{nn}) \in \mathbb{R}^{n\times n}$, we can solve for $\overline{x}$ as follows:

$$x_i = \frac{b_i}{d_{ii}}, \quad i = 1, 2, \ldots, n$$

With $U\overline{x} = \bar{b}$, L upper triangular, we can solve for $\overline{x}$ using backward substitution:

$$\begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$u_{nn}x_n = b_n \quad \text{and} \quad u_{n-1,n}x_{n-1} + u_{n-1,n}x_n = b_{n-1}$$

$$x_n = \frac{b_n}{u_{nn}} \quad \text{and} \quad x_i = \frac{b_i - \sum_{j=i+1}^{n} u_{ij}x_j}{u_{ii}}, \quad i = n-1, n-2, \ldots, 1$$

We can define the algorithm for solving $U\overline{x} = \bar{b}$ where U is a upper triangular matrix as follows:

Algorithm 3: Solve Upper Triangular System

Input: $U \in \mathbb{R}^{n\times n}$ (upper triangular), $\bar{b} \in \mathbb{R}^n$
Output: $\bar{x} \in \mathbb{R}^n$ such that $U\bar{x} = \bar{b}$

$x_n = \dfrac{b_n}{u_{nn}}$;
for $i = n-1$ ***down to*** 1 **do**
  $x_i = b_i$;
  for $j = i+1$ ***to*** n **do**
    $x_i = x_i - u_{ij}x_j$;
  $x_i = \dfrac{x_i}{u_{ii}}$;

The cost of this algorithm is as follows:

$$\textbf{Flops} = \sum_{i=1}^{n-1}\left(1 + 2\sum_{j=i+1}^{n} 1\right) = \cdots = \frac{(n-2)n}{2} \sim \mathcal{O}(n^2)$$

5.4 Gaussian Elimination

The Gaussian Elimination algorithm can be defined as follows:

Algorithm 4: Gaussian Elimination

Input: $A \in \mathbb{R}^{n \times n}, \bar{b} \in \mathbb{R}^n$

Output: $U \in \mathbb{R}^{n \times n}, \bar{b}^* \in \mathbb{R}^n$ such that $LA = U$ and $L\bar{b} = \bar{b}^*$

for $k = 1$ ***to*** $n - 1$ **do**
- **for** $i = k + 1$ ***to*** n **do**
  - $t = \dfrac{a_{ik}}{a_{kk}}$; `// t is a factor`
  - **for** $j = k$ ***to*** n **do**
    - $a_{ij} = a_{ij} - t a_{kj}$;
  - $b_i = b_i - t b_k$;

The cost of this algorithm is as follows:

$$\textbf{Flops} = \mathcal{O}(n^3)$$

5.5 LU Factorization

With $A \in \mathbb{R}^{n \times n}$ non-singular, we can factor A as $A = L \cdot U$ where L is a lower triangular matrix with unit diagonal and U is an upper triangular matrix:

$$L = I + \sum_{k=1}^{n-1} l_k e_k^T$$

Observation

If an $n \times n$ matrix A has an LU factorization, then it is unique. Furthermore, if we relax the condition that L has a unit diagonal (i.e., normalized), then there are infinitely many LU factorizations of A.

Theorem

If all the leading principal minors of A are non-zero, i.e., $\det(A_k) \neq 0$ for $k = 1, 2, \ldots, n-1$ where A_k is the $k \times k$ leading principal submatrix of A, then A has an LU factorization. In particular, if A is strictly diagonally dominant or symmetric positive definite, then A has an LU factorization.

Proof. We will prove this by induction on n. The base case $n = 1$ is trivial since any non-zero scalar can be factored as $1 \cdot a_{11}$. A matrix with k row operations already done can be written as

$$A^{(k)} = \begin{bmatrix} a_{11} & a_{12} & \cdots & \cdots & a_{1n} \\ 0 & a_{22}^{(2)} & \cdots & \cdots & a_{2n}^{(2)} \\ 0 & 0 & a_{kk}^{(k)} & \cdots & a_{kn}^{(k)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n2}^{(k)} & \cdots & a_{nn}^{(k)} \end{bmatrix}$$

where every superindex (k) indicates that k row operations have been performed. Note that the leading principal submatrix of order k of $A^{(k)}$ is the same as that of A. Thus, $\det(A^{(k)}) = \det(A_k) \neq 0$. Hence, the next step is possible. $\square$

Theorem

If an invertible matrix $A \in \mathbb{R}^{n \times n}$ has an LU factorization, then it is unique.

Proof. Suppose $A = L_1 U_1 = L_2 U_2$ where L_1, L_2 are lower triangular with unit diagonal and U_1, U_2 are upper triangular. Then,

$$L_2^{-1} L_1 = U_2 U_1^{-1}$$

The left-hand side is lower triangular with unit diagonal, and the right-hand side is upper triangular. Thus, both sides must be equal to the identity matrix. Therefore, $L_1 = L_2$ and $U_1 = U_2$. $\square$

5.6 Pivoting

We use pivoting to avoid division by zero or small numbers during the elimination process. There are three types of pivoting:

1. Partial row pivoting: We interchange rows to ensure that the pivot element is the largest in its column.
$$|a_{lk}| = \max_{k \leq i \leq n} |a_{ik}^{(k)}|$$
2. Partial column pivoting: We interchange columns to ensure that the pivot element is the largest in its row.
$$|a_{kl}| = \max_{k \leq j \leq n} |a_{kj}^{(k)}|$$
3. Total pivoting: We interchange both rows and columns to ensure that the pivot element is the largest in the remaining submatrix.
$$|a_{lm}| = \max_{k \leq i,j \leq n} |a_{ij}^{(k)}|$$

Total pivoting is the most stable but also the most expensive. It yields the complete LU factorization. The cost of partial pivoting is $\mathcal{O}(n^2)$, while the cost of total pivoting is $\mathcal{O}(n^3)$.

The LU factorization with partial pivoting algorithm can be defined as follows:

Algorithm 5: LU Factorization with Partial Pivoting

Input: $A \in \mathbb{R}^{n \times n}, b \in \mathbb{R}^n$
Output: P, L, U such that $PA = LU$

for $k = 1$ ***to*** $n - 1$ **do**
  $l = \arg\max_{k \leq i \leq n} |a_{ik}^{(k)}|$;
  Swap rows k and l of A and b;
  for $i = k + 1$ ***to*** n **do**
    $t = \dfrac{a_{ik}}{a_{kk}}$;
    for $j = k$ ***to*** n **do**
      $a_{ij} = a_{ij} - t a_{kj}$;
    $b_i = b_i - t b_k$;

5.7 The role of L and U in Backward Stability

Let $A \in \mathbb{R}^{n\times n}$ be a non-singular matrix with LU factorization $A = LU$. Then,

$$\hat{L}\hat{U} = A + \delta A, \quad \frac{\|\delta A\|}{\|L\|\|U\|} = \mathcal{O}(\varepsilon_{\text{mach}})$$

where $\hat{L}$ and $\hat{U}$ are the computed factors of A, and δA is the perturbation in A due to rounding errors.

Now, let us introduce partial pivoting. Let P be a permutation matrix such that $PA = LU$. Then,

$$L = \begin{bmatrix} \ddots & & & & \\ l_{ik} & \ddots & & & \\ \vdots & \vdots & \ddots & & \\ l_{nk} & l_{n,k+1} & \cdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & l_{n,n-1} & 1 \end{bmatrix} \implies \|L\| = \mathcal{O}(1)$$

Thus, the stability of the LU factorization with partial pivoting depends on $\|U\|$ relative to $\|A\|$. This ratio is known as the growth factor:

$$\rho = \frac{\max |u_{ij}|}{\max |a_{ij}|}$$

With $PA = LU$, we have

$$\hat{L}\hat{U} = PA + \delta A, \quad \frac{\|\delta A\|}{\|P\|\|A\|} = \mathcal{O}(\varepsilon_{\text{mach}}) \implies \frac{\|\delta A\|}{\|A\|} = \mathcal{O}(\rho\varepsilon_{\text{mach}})$$

Example

Let

$$A = \begin{bmatrix} 1 & & & & 1 \\ -1 & 1 & & & 1 \\ -1 & -1 & 1 & & 1 \\ -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 \end{bmatrix} = L \cdot U = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ -1 & -1 & 1 & & \\ -1 & -1 & -1 & 1 & \\ -1 & -1 & -1 & -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & & & & 1 \\ & 1 & & & 2 \\ & & 1 & & 4 \\ & & & 1 & 8 \\ & & & & 16 \end{bmatrix}$$

Then, $\rho = 16 = 2^{n-1}$, which is not bounded. Then,

$$\frac{\|\delta A\|}{\|A\|} = \mathcal{O}(2^{n-1}\varepsilon_{\text{mach}})$$

6 Least Squares

To compute the QR factorization of a matrix $A \in \mathbb{R}^{m \times n}$ with $m \geq n$, we can use different methods such as Gram-Schmidt, given rotations, or Householder reflections. The QR factorization decomposes A into an orthogonal matrix $Q \in \mathbb{R}^{m \times m}$ and an upper triangular matrix $R \in \mathbb{R}^{m \times n}$:

$$A = QR$$

where

$$Q = \begin{bmatrix} q_1 & q_2 & \cdots & q_m \end{bmatrix}, \quad R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

6.1 Gram-Schmidt Process

Given a matrix $A \in \mathbb{R}^{m \times n}$ with linearly independent columns, the Gram-Schmidt process constructs an orthonormal basis for the column space of A.

$$A = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}, \quad \text{span}\{a_1, a_2, \ldots, a_n\} = \text{span}\{q_1, q_2, \ldots, q_n\}$$

The Gram-Schmidt process can be defined as follows:

$$\begin{aligned}
v_1 &= a_1 & &\longrightarrow & q_1 &= \frac{v_1}{\|v_1\|} \\
v_2 &= a_2 - (a_2^T \cdot q_1) \cdot q_1 & &\longrightarrow & q_2 &= \frac{v_2}{\|v_2\|} \\
v_3 &= a_3 - (a_3^T \cdot q_2) \cdot q_2 - (a_3^T \cdot q_1) \cdot q_1 & &\longrightarrow & q_3 &= \frac{v_3}{\|v_3\|} \\
&\vdots \\
v_n &= a_n - \sum_{j=1}^{n-1} (a_n^T \cdot q_j) \cdot q_j & &\longrightarrow & q_n &= \frac{v_n}{\|v_n\|}
\end{aligned}$$

The coefficients q_k satisfy the following:

$$q_i \cdot q_j = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

The matrix R can be constructed as follows:

$$R = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix} = \begin{bmatrix} \|v_1\| & q_1^T a_2 & \cdots & q_1^T a_n \\ 0 & \|v_2\| & \cdots & q_2^T a_n \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \|v_n\| \end{bmatrix}$$

where

$$r_{ij} = \begin{cases} q_i^T a_j & i < j \\ \|v_i\| & i = j \\ 0 & i > j \end{cases}$$

With this, we can express a_k as follows:

$$
\begin{aligned}
a_1 &= q_1 r_{11} = q_1\|v_1\| \\
a_2 &= q_1 r_{12} + q_2 r_{22} = q_1(q_1^T a_2) + q_2|v_2\| \\
a_3 &= q_1 r_{13} + q_2 r_{23} + q_3 r_{33} = q_1(q_1^T a_3) + q_2(q_2^T a_3) + q_3\|v_3\| \\
&\vdots \\
a_n &= q_1 r_{1n} + q_2 r_{2n} + \cdots + q_n r_{nn} = q_1(q_1^T a_n) + q_2(q_2^T a_n) + \cdots + q_n\|v_n\|
\end{aligned}
$$

The Gram-Schmidt algorithm can be summarized as follows:

Algorithm 6: Gram-Schmidt Process

Input: $A \in \mathbb{R}^{m\times n}$ with linearly independent columns
Output: $Q \in \mathbb{R}^{m\times n}$ with orthonormal columns, $R \in \mathbb{R}^{n\times n}$ upper triangular

for $k = 1$ ***to*** n **do**
  $v_k = a_k$;
  for $j = 1$ ***to*** $k-1$ **do**
    $r_{jk} = q_j^T a_k$;
    $v_k = v_k - r_{jk} q_j$;
  $r_{kk} = \|v_k\|$;
  $q_k = \dfrac{v_k}{r_{kk}}$;

This algorithm can be modified to improve numerical stability, resulting in the Modified Gram-Schmidt algorithm:

Algorithm 7: Modified Gram-Schmidt Process

Input: $A \in \mathbb{R}^{m\times n}$ with linearly independent columns
Output: $Q \in \mathbb{R}^{m\times n}$ with orthonormal columns, $R \in \mathbb{R}^{n\times n}$ upper triangular

for $k = 1$ ***to*** n **do**
  $v_k = a_k$;
  $r_{kk} = \|v_k\|$;
  $q_k = \dfrac{v_k}{r_{kk}}$;
  for $j = k+1$ ***to*** n **do**
    $r_{kj} = q_k^T a_j$;
    $a_j = a_j - r_{kj} q_k$;

Remark

The matrix R is invertible if and only if the columns of A are linearly independent. The reduced QR factorization is unique up to a sign.

6.2 Householder Transformations

A Householder transformation is a linear transformation that reflects a vector about a plane or hyperplane. It is defined as follows:
Given a vector $v \in \mathbb{R}^n$, the Householder transformation H is defined as:

$$H = I - 2\frac{uu^T}{\|u\|}$$

where $u = v - \alpha e_1$, $\alpha = \|v\|$, and e_1 is the first standard basis vector in $\mathbb{R}^n$.