

Iterative methods :

Notation and a brief background

- Mathematical background: matrices, inner products and norms
- linear systems of equations
- Iterative processes

Notation & Review of some linear algebra concepts

➤ The set of all linear combinations of a set of vectors $G = \{a_1, a_2, \dots, a_q\}$ of \mathbb{R}^n is a vector subspace called the linear span of G . Notation

$$\text{span}(G), \text{span} \{a_1, a_2, \dots, a_q\}$$

➤ If the a_i 's are linearly independent, then each vector of $\text{span}\{G\}$ admits a unique expression as a linear combination of the a_i 's. The set G is then called a *basis*

➤ Recall: A matrix represents a linear mapping between two vector spaces of finite dimension n and m .

Transposition: If $A \in \mathbb{R}^{m \times n}$ then its transpose is a matrix $C \in \mathbb{R}^{n \times m}$ with entries

$$c_{ij} = a_{ji}, i = 1, \dots, n, j = 1, \dots, m$$

Notation : A^T .

Transpose Conjugate: for complex matrices, the transpose conjugate matrix denoted by A^H is more relevant: $A^H = \bar{A}^T = \overline{A^T}$.

- We consider now only square matrices ($m = n$).
- Spectral radius = The maximum modulus of the eigenvalues

$$\rho(A) = \max_{\lambda \in \lambda(A)} |\lambda|.$$

- Recall: $\lim_{k \rightarrow \infty} A^k = 0$ iff $\rho(A) < 1$.

➤ Trace of A = sum of diagonal elements of A .

$$\text{tr}(A) = \sum_{i=1}^n a_{ii}.$$

➤ $\text{tr}(A)$ = sum of all the eigenvalues of A counted with their multiplicities.

➤ Recall that $\det(A)$ = product of all the eigenvalues of A counted with their multiplicities.

Example: : Trace, spectral radius, and determinant of the matrix:

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

Range and null space

- Range: $\text{Ran}(A) = \{Ax \mid x \in \mathbb{R}^n\}$
- Null Space: $\text{Null}(A) = \{x \in \mathbb{R}^n \mid Ax = 0\}$
- Range = linear span of the columns of A
- Rank of a matrix $\text{rank}(A) = \dim(\text{Ran}(A))$
- $\text{rank}(A)$ = the number of linearly independent columns of A
= the number of linearly independent rows of A .
- A is of *full rank* if $\text{rank}(A) = \min\{m, n\}$. Otherwise it is *rank-deficient*.

Rank+Nullity theorem for an $m \times n$ matrix:

$$\dim(\text{Ran}(A)) + \dim(\text{Null}(A)) = n$$

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Types of matrices (square)

- Symmetric matrices: $A^T = A$.
- Hermitian matrices: $A^H = A$.
- Skew-symmetric matrices: $A^T = -A$.
- Skew-Hermitian matrices: $A^H = -A$.
- Normal matrices: $A^H A = A A^H$.
- Nonnegative matrices: $a_{ij} \geq 0$, $i, j = 1, \dots, n$ (similar definition for nonpositive, positive, and negative matrices).
- Unitary matrices: $Q^H Q = I$.

Note: if Q is unitary then $Q^{-1} = Q^H$.

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Inner products and Norms

- Inner product of 2 vectors x and y in \mathbb{R}^n :

$$x_1 y_1 + x_2 y_2 + \dots + x_n y_n \text{ in } \mathbb{R}^n$$

Notation: (x, y) or $y^T x$

- For complex vectors

$$(x, y) = x_1 \bar{y}_1 + x_2 \bar{y}_2 + \dots + x_n \bar{y}_n \text{ in } \mathbb{C}^n$$

Note: $(x, y) = y^H x$

An important property: Given $A \in \mathbb{C}^{m \times n}$ then

$$(Ax, y) = (x, A^H y) \quad \forall x \in \mathbb{C}^n, \forall y \in \mathbb{C}^m$$

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Vector norms

Norms are needed to measure lengths of vectors and closeness of two vectors. Examples of use: Estimate convergence rate of an iterative method; Estimate the error of an approximation to a given solution; ...

- A vector norm on a vector space \mathbb{X} is a real-valued function on \mathbb{X} , which satisfies the following three conditions:

1. $\|x\| \geq 0$, $\forall x \in \mathbb{X}$, and $\|x\| = 0$ iff $x = 0$.
2. $\|\alpha x\| = |\alpha| \|x\|$, $\forall x \in \mathbb{X}$, $\forall \alpha \in \mathbb{C}$.
3. $\|x + y\| \leq \|x\| + \|y\|$, $\forall x, y \in \mathbb{X}$.

- 3. is called the triangle inequality.

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Example: Euclidean norm on $\mathbb{X} = \mathbb{C}^n$,

$$\|x\|_2 = (x, x)^{1/2} = \sqrt{|x_1|^2 + |x_2|^2 + \dots + |x_n|^2}$$

➤ Most common vector norms in numerical linear algebra:

$$\begin{aligned}\|x\|_1 &= |x_1| + |x_2| + \dots + |x_n|, \\ \|x\|_2 &= [|x_1|^2 + |x_2|^2 + \dots + |x_n|^2]^{1/2}, \\ \|x\|_\infty &= \max_{i=1, \dots, n} |x_i|.\end{aligned}$$

➤ The Cauchy-Schwartz inequality (important) is:

$$|(x, y)| \leq \|x\|_2 \|y\|_2.$$

Convergence of vector sequences

A sequence of vectors $x^{(k)}$, $k = 1, \dots, \infty$ converges to a vector x with respect to the norm $\|\cdot\|$ if, by definition,

$$\lim_{k \rightarrow \infty} \|x^{(k)} - x\| = 0$$

➤ **Important point:** because all norms in \mathbb{R}^n are equivalent, the convergence of $x^{(k)}$ w.r.t. a given norm implies convergence w.r.t. any other norm.

➤ **Notation:** $\lim_{k \rightarrow \infty} x^{(k)} = x$

➤ **Note:** $x^{(k)}$ converges to x iff each component $x_i^{(k)}$ of $x^{(k)}$ converges to the corresponding component x_i of x

Matrix norms

➤ Can define matrix norms by considering $m \times n$ matrices as vectors in \mathbb{R}^{mn} . These norms satisfy the usual properties of vector norms, i.e.,

1. $\|A\| \geq 0$, $\forall A \in \mathbb{C}^{m \times n}$, and $\|A\| = 0$ iff $A = 0$
2. $\|\alpha A\| = |\alpha| \|A\|$, $\forall A \in \mathbb{C}^{m \times n}$, $\forall \alpha \in \mathbb{C}$
3. $\|A + B\| \leq \|A\| + \|B\|$, $\forall A, B \in \mathbb{C}^{m \times n}$.

➤ However, these will lack (in general) the right properties for composition of operators (product of matrices).

➤ The case of $\|\cdot\|_2$ yields the Frobenius norm of matrices.

➤ Given a matrix A in $\mathbb{C}^{m \times n}$, define the set of **matrix norms**

$$\|A\|_p = \max_{x \in \mathbb{C}^n, x \neq 0} \frac{\|Ax\|_p}{\|x\|_p}.$$

➤ These norms satisfy the usual properties of vector norms (see previous page).

➤ The matrix norm $\|\cdot\|_p$ is **induced** by the vector norm $\|\cdot\|_p$.

➤ Again, important cases are for $p = 1, 2, \infty$.

Consistency

- A fundamental property is consistency

$$\|AB\|_p \leq \|A\|_p \|B\|_p.$$

- Consequence: $\|A^k\|_p \leq \|A\|_p^k$
- A^k converges to zero if *any* of its p -norms is < 1
- The Frobenius norm is defined by

$$\|A\|_F = \left(\sum_{j=1}^n \sum_{i=1}^m |a_{ij}|^2 \right)^{1/2}.$$

- Same as the 2-norm of the column vector in \mathbb{C}^{mn} consisting of all the columns (respectively rows) of A .
- This norm is also consistent [but not induced from a vector norm]

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Important equalities:

$$\|A\|_1 = \max_{j=1,\dots,n} \sum_{i=1}^m |a_{ij}|,$$

$$\|A\|_\infty = \max_{i=1,\dots,m} \sum_{j=1}^n |a_{ij}|,$$

$$\|A\|_2 = [\rho(A^H A)]^{1/2} = [\rho(AA^H)]^{1/2},$$

$$\|A\|_F = [\text{Tr}(A^H A)]^{1/2} = [\text{Tr}(AA^H)]^{1/2}.$$

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Positive-Definite Matrices

- A real matrix is said to be positive definite if

$$(Au, u) > 0 \text{ for all } u \neq 0, u \in \mathbb{R}^n$$

- Let A be a real positive definite matrix. Then there is a scalar $\alpha > 0$ such that

$$(Au, u) \geq \alpha \|u\|_2^2,$$

- Consider now the case of Symmetric Positive Definite (SPD) matrices.
- Consequence 1: A is nonsingular
- Consequence 2: the eigenvalues of A are (real) positive

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A few properties of Symmetric Positive Definite matrices

- Diagonal entries of A are positive. More generally, ...
- Diagonal block $A(k:l, k:l)$, ($k < l$), is SPD
- For any $n \times k$ matrix X of rank k , the matrix $X^T A X$ is SPD.
- The mapping :

$$x, y \rightarrow (x, y)_A \equiv (Ax, y)$$

is a proper inner product on \mathbb{R}^n . The associated norm, denoted by $\|\cdot\|_A$, is called the **energy norm**:

$$\|x\|_A = (Ax, x)^{1/2} = \sqrt{x^T A x}$$

- A admits the Cholesky factorization $A = LL^T$ where L is lower triangular

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Iterative processes for linear systems

In contrast with “direct” methods (Gaussian Elimination) iterative methods compute a sequence of approximations $x^{(k)}$ to the solution x . Ideally, a good approximation is obtained in a few iterations of the process. Convergence measured by some norm.

Questions which arise:

- Why not use a direct method [always works!]
- Under which condition (s) will the method converge?
- When to stop?
- Can we estimate costs?

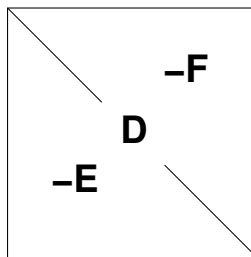
Basic relaxation techniques

- Relaxation methods: Jacobi, Gauss-Seidel, SOR
- Basic convergence results
- Optimal relaxation parameter for SOR
- See Chapter 4 of text for details.

Basic relaxation schemes

- **Relaxation schemes:** methods that modify one component of current approximation at a time

- Based on the decomposition $A = D - E - F$ with:
 $D = \text{diag}(A)$, $-E =$ strict lower part of A and $-F =$ its strict upper part.



Gauss-Seidel iteration for solving $Ax = b$:

- corrects j -th component of current approximate solution, to zero the $j - th$ component of residual for $j = 1, 2, \dots, n$.

- Gauss-Seidel iteration can be expressed as:

$$(D - E)x^{(k+1)} = Fx^{(k)} + b$$

Can also define a **backward** Gauss-Seidel Iteration:

$$(D - F)x^{(k+1)} = Ex^{(k)} + b$$

and a Symmetric Gauss-Seidel Iteration: forward sweep followed by backward sweep.

Over-relaxation is based on the decomposition:

$$\omega A = (D - \omega E) - (\omega F + (1 - \omega)D)$$

→ successive overrelaxation, (SOR):

$$(D - \omega E)x^{(k+1)} = [\omega F + (1 - \omega)D]x^{(k)} + \omega b$$

Iteration matrices

Jacobi, Gauss-Seidel, SOR, & SSOR iterations are of the form

$$x^{(k+1)} = Mx^{(k)} + f$$

$$M_{Jac} = D^{-1}(E + F) = I - D^{-1}A$$

$$M_{GS} = (D - E)^{-1}F = I - (D - E)^{-1}A$$

$$M_{SOR} = (D - \omega E)^{-1}(\omega F + (1 - \omega)D) \\ = I - (\omega^{-1}D - E)^{-1}A$$

$$M_{SSOR} = I - \omega(2 - \omega)(D - \omega F)^{-1}D(D - \omega E)^{-1}A$$

General convergence result

Consider the iteration: $x^{(k+1)} = Gx^{(k)} + f$

(1) Assume that $\rho(G) < 1$. Then $I - G$ is non-singular and G has a fixed point. Iteration converges to a fixed point for any f and $x^{(0)}$.

(2) If iteration converges for any f and $x^{(0)}$ then $\rho(G) < 1$.

Example: Richardson's iteration

$$x^{(k+1)} = x^{(k)} + \alpha(b - Ax^{(k)})$$

 Assume $\Lambda(A) \subset \mathbb{R}$. When does the iteration converge?

A few well-known results

➤ Jacobi and Gauss-Seidel converge for diagonal dominant matrices, i.e., matrices such that

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|, i = 1, \dots, n$$

➤ SOR converges for $0 < \omega < 2$ for SPD matrices

➤ The optimal ω is known in theory for an important class of matrices called **2-cyclic matrices** or **matrices with property A**.

➤ A matrix has property **A** if it can be (symmetrically) permuted into a 2×2 block matrix whose diagonal blocks are diagonal.

$$PAP^T = \begin{bmatrix} D_1 & E \\ E^T & D_2 \end{bmatrix}$$

➤ Let A be a matrix which has property **A**. Then the eigenvalues λ of the SOR iteration matrix and the eigenvalues μ of the Jacobi iteration matrix are related by

$$(\lambda + \omega - 1)^2 = \lambda \omega^2 \mu^2$$

➤ The optimal ω for matrices with property **A** is given by

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \rho(B)^2}}$$

where B is the Jacobi iteration matrix.

An observation Introduction to Preconditioning

► The iteration $x^{(k+1)} = Mx^{(k)} + f$ is attempting to solve $(I - M)x = f$. Since M is of the form $M = I - P^{-1}A$ this system can be rewritten as

$$P^{-1}Ax = P^{-1}b$$

where for SSOR, we have

$$P_{SSOR} = (D - \omega E)D^{-1}(D - \omega F)$$

referred to as the SSOR 'preconditioning' matrix.

In other words:

Relaxation iter. \iff *Preconditioned Fixed Point Iter.*