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 $G = \{a_1, a_2, \ldots, a_q\}$ of $\mathbb{R}^n$ is a vector subspace called the linear span of $G$. Notation $\text{span}(G)$, $\text{span} \{a_1, a_2, \ldots, a_q\}$

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

Notation: $A^T$.

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

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

**Trace of $A$** = sum of diagonal elements of $A$. $\text{tr}(A) = \sum_{i=1}^{n} a_{ii}$.

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

- Recall that $\det(A) = \text{product of all the eigenvalues of } A \text{ counted with their multiplicities}$.

**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** \( \text{rank}(A) = \text{dim}(\text{Ran}(A)) \)

**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:

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

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:** \( A^H A = AA^H \).
- **Nonnegative matrices:** \( a_{ij} \geq 0 \), \( i,j = 1,...,n \) (similar definition for nonpositive, positive, and negative matrices).
- **Unitary matrices:** \( Q^H Q = I \).

Note: if \( Q \) is unitary then \( Q^{-1} = Q^H \).

Inner products and Norms

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

\[
x_1 y_1 + x_2 y_2 + \cdots + x_n y_n \text{ in } \mathbb{R}^n
\]

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

For complex vectors

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

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

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

\[
(Ax, y) = (x, A^H y) \text{ } \forall \text{ } x \in \mathbb{C}^n, \forall y \in \mathbb{C}^m
\]

**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 \( X \) is a real-valued function on \( X \), which satisfies the following three conditions:

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

**3. is called the triangle inequality.**
Example: Euclidean norm on $X = \mathbb{C}^n$,

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

- Most common vector norms in numerical linear algebra:
  
  $$\|x\|_1 = |x_1| + |x_2| + \cdots + |x_n|,$$
  
  $$\|x\|_2 = [|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2]^{1/2},$$
  
  $$\|x\|_\infty = \max_{i=1,\ldots,n} |x_i|.$$ 

- The Cauchy-Schwartz inequality (important) is:

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

Convergence of vector sequences

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

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

- 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: $\lim_{k \to \infty} x^{(k)} = x$

- Note: $x^{(k)}$ converges to $x$ iff each component $x^{(k)}_i$ 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
  \[ \|A\|_F = \left( \sum_{j=1}^n \sum_{i=1}^m |a_{ij}|^2 \right)^{1/2}. \]
- This norm is also consistent [but not induced from a vector norm]

Important equalities:

- \( \|A\|_1 = \max_{j=1,...,n} \sum_{i=1}^m |a_{ij}| \),
- \( \|A\|_{\infty} = \max_{i=1,...,m} \sum_{j=1}^n |a_{ij}| \),
- \( \|A\|_2 = \left[ \rho(A^HA) \right]^{1/2} = \left[ \rho(AA^H) \right]^{1/2}, \)
- \( \|A\|_F = \left[ \text{Tr}(A^HA) \right]^{1/2} = \left[ \text{Tr}(AA^H) \right]^{1/2}. \)

Positive-Definite Matrices

- A real matrix is said to be positive definite if
  \[ (Au, u) > 0 \text{ for all } u \neq 0 \quad \forall u \in \mathbb{R}^n \]
- 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

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 \( X^TAX \) 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:
  \[ \|x\|_A = (Ax, x)^{1/2} = \sqrt{x^TAX} \]
- \( A \) admits the Cholesky factorization \( A = LL^T \) where \( L \) is lower triangular
**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 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 \( A \)
  - \( F = \) 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 \( j = 1, 2, \ldots, n \).

**Basic relaxation techniques**

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

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:
\[
\omega A = (D - \omega E) - (\omega F + (1 - \omega)D)
\]

\[\rightarrow\] 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

\[ x^{(k+1)} = M x^{(k)} + f \]

- Jacobi
  \[ M_{Jac} = D^{-1}(E + F) = I - D^{-1}A \]
- Gauss-Seidel
  \[ M_{GS} = (D - E)^{-1}F = I - (D - E)^{-1}A \]
- SOR
  \[ M_{SOR} = (D - \omega E)^{-1}(\omega F + (1 - \omega)D) = I - (\omega^{-1}D - E)^{-1}A \]
- SSOR
  \[ M_{SSOR} = I - \omega(2 - \omega)(D - \omega F)^{-1}D(D - \omega E)^{-1}A \]

**General convergence result**

Consider the iteration:

\[ x^{(k+1)} = G x^{(k)} + f \]

(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
  \[ |a_{ii}| > \sum_{j \neq i} |a_{ij}|, i = 1, \ldots, n \]
- SOR converges for \( 0 < \omega < 2 \) for SPD matrices
- The optimal \( \omega \) 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 \( 2 \times 2 \) block matrix whose diagonal blocks are diagonal.

\[ P A P^T = \begin{bmatrix} D_1 & E \\ E^T & D_2 \end{bmatrix} \]

- Let \( A \) be a matrix which has property A. Then the eigenvalues \( \lambda \) of the SOR iteration matrix and the eigenvalues \( \mu \) of the Jacobi iteration matrix are related by
  \[ (\lambda + \omega - 1)^2 = \lambda \omega^2 \mu^2 \]

- The optimal \( \omega \) 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.
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.