

Iterative methods for large and sparse linear systems

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January 5, 2026

Outline

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What this course is

Overall, this course will talk about

- Mathematics
- (Numerical) Linear algebra
- Linear systems
- Empirical evaluations through implementations
- Basic programming

This is a week long project-based course: progress on your own, as we slowly detail things.

What this course is not

Remember this course is not

- A CS / programming course – Even though implementation is an integral part of the deliverables expected, the emphasis is not on clean code or good IT practices
- A proof-heavy course
- An exhaustive presentation of all methods for solving linear systems
- targetting a precise application

Course setting

Plan:

- M./Tu./F. 8am-12-noon; 1:30pm-5:30pm
- W. 1:30pm-5:30pm
- Th. 8am-12 noon
- Group evaluation on Friday afternoon

Evaluation:

- Groups of 3 – to be chosen among yourselves and notified to us by Monday afternoon
- Work presentation : 10 minutes / group + 5 minutes of questions
- Deliverables sent to us no later than Friday 9/01/25, 12 noon:
 - All codes as an archived file (LastName1_LastName2_SLS.tar or zip)
 - A brief report describing your results
 - A small presentation used as a support for the oral presentation

More on the evaluation

What is the absolute minimum (= passing grade) the report should contain:

- Solutions to in-slides question "Now you try"
- Comments on convergence

What is the absolute minimum your code should contain:

- All routines/codes asked for in the slides
- All code used for generating your report and presentation's contents

To get over the top, be creative in analysing methods. You may include

- Study of convergence (with respect to time, number of iterations, type of structure CSR vs COO)
- Cases of convergence of the various methods (in terms of types of matrices, spectral radius)
- Memory limitations
- and much more....
- Why not invent your own method?!

Linear System Definition

- Given a square matrix A of size $n \times n$ and a vector b of size $n \times 1$, find a vector x of size $n \times 1$ that satisfies:

$$Ax = b$$

- Applications:

- Engineering: Structural analysis, fluid dynamics, heat transfer
- Physics: Electromagnetism, quantum mechanics
- Computer Graphics: Image processing, computer vision
- Machine Learning: Solving linear regression problems

Direct approach cost

- The direct way is to solve the system $Ax = b$ as

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

- This involves computing the inverse of matrix A , A^{-1} .
- Computing the inverse of a general matrix A has a computational cost of $O(n^3)$ using standard algorithms.
- For large systems (large values of n), this cubic complexity can lead to prohibitively long computation times.
- Memory requirements: storing and manipulating the entire matrix can be memory-intensive, especially for sparse matrices
- Numerical issues (like round-off errors) can accumulate during the inversion process, potentially leading to inaccurate results.

Why iterative methods?

Iterative methods as an alternative

- Avoid the explicit computation of the matrix inverse
- Can provide approximate solutions within a desired tolerance, which may be sufficient for many practical applications
- Often exploit the structure of the matrix (e.g., sparsity) to reduce computational cost and memory usage

Fixed Point Problem: A Simple Analogy

- **Imagine a mirror:** You stand in front of a mirror. Your image in the mirror is a "reflection" of you.
- **A fixed point** In this analogy, the fixed point is the position where you and your image perfectly overlap. You are "fixed" in that position relative to your reflection.
- **Finding the fixed point**
 - You might initially stand slightly off-center.
 - You then adjust your position slightly to try and align with your image.
 - You continue making small adjustments until you find the position where you and your image perfectly coincide.

Fixed Point Problem: A Simple Analogy

- A fixed point of a function $G(x)$ is a value x^* such that:

$$G(x^*) = x^*$$

- Choose an initial guess $x^{(0)}$.
- for $k = 0, 1, 2, \dots$

$$x^{(k+1)} = G(x^{(k)})$$

- Stop the iteration when:

$$\lim_{k \rightarrow \infty} \|x^{(k+1)} - x^{(k)}\| = 0$$

where $\|\cdot\|$ denotes a suitable norm (e.g., Euclidean norm).

- In the context of linear systems, iterative methods work similarly.
- Reformulate the linear system $Ax = b$ as a fixed-point problem:
$$x = G(x).$$
- We start with an initial guess for the solution.
- We refine this guess by applying a specific rule "G" until we converge to the "fixed point"

General Formula for Iterative Methods

Let $A \in \mathbb{R}^{n \times n}$ be invertible and $b \in \mathbb{R}^n$. We denote by $\bar{x} = A^{-1}b \in \mathbb{R}^n$ **the solution to the linear system $Ax = b$.**

Iterative methods work by constructing a sequence of estimates (or approximations) $x^{(k)}$, $k \in \mathbb{N}$ as follows

- Initialisation: Pick an initial value $x^{(0)} \in \mathbb{R}^n$.
- Iterate: For any $k \in \mathbb{N}$, $k > 0$, compute

$$x^{(k+1)} = G(x^{(k)})$$

where $G : \mathbb{R}^n \rightarrow \mathbb{R}^n$ maps one estimate to the next one.

Jacobi Method: Introduction

- Consider the system of linear equations:

$$Ax = b$$

$$\bullet \quad A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}, \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \text{ and } x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- Find an iterative method to approximate the solution vector x .

Decomposition of Matrix A= D-L-U

Diagonal matrix $D = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix}$

Strictly Lower Triangular (L) $-L = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ a_{21} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix}$

Strictly Upper Triangular (U) $-U = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ 0 & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$

Jacobi Iteration

$$(D - L - U)x = b$$

$$Dx = b + (L + U)x$$

$$x = D^{-1}b + D^{-1}(L + U)x$$

- Jacobi Iteration Formula

$$x^{(k+1)} = D^{-1}(L + U)x^{(k)} + D^{-1}b$$

where:

- $x^{(k)}$ is the current approximation of the solution vector at iteration k .
- $x^{(k+1)}$ is the updated approximation at iteration $k + 1$.

- Component-wise Form:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j^{(k)} \right) \quad \text{for } i = 1, 2, \dots, n$$

Convergence of the Jacobi Method

- Sufficient condition for convergence

- The Jacobi method is guaranteed to converge if the matrix A is strictly diagonally dominant
- A matrix A is strictly diagonally dominant if:

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}| \quad \text{for all } i = 1, 2, \dots, n$$

- This means the absolute value of each diagonal element must be greater than the sum of the absolute values of the other elements in its row.
- Necessary and sufficient condition:
 - A more general condition for convergence is that the "spectral radius" of the iteration matrix $T = D^{-1}(L + U)$ must be less than 1:

$$\rho(T) < 1$$

where $\rho(T)$ is the spectral radius of T , which is defined as the maximum eigenvalue of T in absolute value.

Theoretical convergence of Jacobi: Now you try

Compute the first 4 iterates through Jacobi's method starting at $x_0 = 0$ of the following systems and conclude on the convergence. (assuming the true solution x^* is the vector filled with 1's, i.e. $b_i = A_i x^*$)

$$A_0 = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} \quad A_1 = \begin{bmatrix} 3 & 0 & 4 \\ 7 & 4 & 2 \\ -1 & 1 & 2 \end{bmatrix} \quad A_2 = \begin{bmatrix} -3 & 3 & -6 \\ -4 & 7 & -8 \\ 5 & 7 & -9 \end{bmatrix}$$
$$A_3 = \begin{bmatrix} 4 & 1 & 1 \\ 2 & -9 & 0 \\ 0 & -8 & -6 \end{bmatrix} \quad A_4 = \begin{bmatrix} 7 & 6 & 9 \\ 4 & 5 & -4 \\ -7 & -3 & 8 \end{bmatrix}$$

Jacobi Method Convergence Investigation: Now you try

Consider the linear system $Ax = b$, where matrix A has the following structure

$$a_{ii} = 5(i + 1) \text{ for } i = 1, 2, \dots, n \text{ and } a_{ij} = -1 \text{ for } i \neq j$$

The right-hand side vector b is a random vector of dimension n .

- Investigate the convergence behavior of the Jacobi iterative method for this specific system for various values of n . Does strict diagonal dominance hold in this case? Will the Jacobi method always converge for this type of matrix structure?

Jacobi Method Convergence Investigation: (Minimum) Expected outcome in file jacobi_dense.py

- A function named *jacobi_method* with 5 inputs
 - a numpy array A , the matrix,
 - a numpy array b , the right hand side,
 - a numpy array x_0 , the first estimate,
 - a float tol with default value $1E^{-5}$ which will stop the iterations once the error gets below, and
 - a float max_iter to represent a maximum number of iterations
- and returns three outputs
 - a numpy array x , the approximate solution,
 - the number of iterations done (an int), and
 - the list of errors in the estimates at each iteration (list of float)
- a function *generate_linear_system* taking a single input
 - an integer n representing the dimension of the system
- and returning two outputs
 - the matrix A generated (a numpy array) and
 - the right hand side generated (a numpy array)

Sparse Matrices: Introduction

- A sparse matrix is a matrix with a high proportion of zero elements.
- Most of the entries in the matrix are zero.
- Examples:
 - Network adjacency matrices (social networks, transportation networks)
 - Finite element method (FEM) matrices
 - Discretization of partial differential equations
- Memory Efficiency (Only non-zero elements are stored)
- Many matrix operations can be performed more efficiently by exploiting the sparsity.
- Only non-zero elements need to be considered in calculations.

Importance of Sparse Matrices

- Large-scale simulations:
 - Essential for solving large systems of equations arising in scientific and engineering applications.
- Machine learning:
 - Used in various machine learning algorithms, such as support vector machines and graph neural networks.
- Data analysis:
 - Efficiently handling and analyzing large datasets with sparse representations.

Sparse Matrices: An Example

Tridiagonal Matrix Example

A tridiagonal matrix is a sparse matrix with non-zero elements only on the main diagonal, the diagonal above it (superdiagonal), and the diagonal below it (subdiagonal).

$$A = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ 0 & -1 & 2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{bmatrix}$$

This structure arises frequently in numerical methods for solving differential equations, such as those encountered in finite difference methods.

Sparse Matrix Storage Formats

- Compressed Row Storage (CSR):
 - Store non-zero elements in a single array.
 - Store an array of cumulative numbers of non zero entries per row.
 - Store column indices of the non-zero elements in a third array.
- Compressed Column Storage (CSC):
 - Similar to CSR, but stores non-zero elements and indices column-wise.
- Coordinate List (COO):
 - Stores the row and column indices of each non-zero element along with its value.

Storing a Tridiagonal Matrix in COO Format

- Tridiagonal Matrix

$$\begin{bmatrix} 5 & 1 & 0 & 0 & 0 \\ 1 & 5 & 1 & 0 & 0 \\ 0 & 1 & 5 & 1 & 0 \\ 0 & 0 & 1 & 5 & 1 \\ 0 & 0 & 0 & 1 & 5 \end{bmatrix}$$

- Stores non-zero values [5, 5, 5, 5, 5, 1, 1, 1, 1, 1, 1]
- row indices of non-zero values: [0, 1, 2, 3, 4, 0, 1, 2, 3, 1, 2, 3, 4]
- column indices of non-zero values: [0, 1, 2, 3, 4, 1, 2, 3, 4, 0, 1, 2, 3]

Storing a Tridiagonal Matrix in COO Format

- Sparse matrix

Coords	Values
(0, 0)	5
(0, 1)	1
(1, 0)	1
(1, 1)	5
(1, 2)	1
(2, 1)	1
(2, 2)	5
(2, 3)	1
(3, 2)	1
(3, 3)	5
(3, 4)	1
(4, 3)	1
(4, 4)	5

Storing a Tridiagonal Matrix in CSR and CSC formats

The previous matrix

$$\begin{bmatrix} 5 & 1 & 0 & 0 & 0 \\ 1 & 5 & 1 & 0 & 0 \\ 0 & 1 & 5 & 1 & 0 \\ 0 & 0 & 1 & 5 & 1 \\ 0 & 0 & 0 & 1 & 5 \end{bmatrix}$$

can be written as

- CSR:

- Data: [5, 1, 1, 5, 1, 1, 5, 1, 1, 5, 1, 1, 5]
- Row indices: [0, 2, 5, 8, 11, 13]
- Col indices: [0, 1, 0, 1, 2, 1, 2, 3, 2, 3, 4, 3, 4]

- CSC:

- Data: [5, 1, 1, 5, 1, 1, 5, 1, 1, 5, 1, 1, 5]
- Row indices: [0, 1, 0, 1, 2, 1, 2, 3, 2, 3, 4, 3, 4]
- Col indices: [0, 2, 5, 8, 11, 13]

Storing matrices in sparse format: Now you try

Convert the following three matrices in all three of the format introduced

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 5 & 6 & 7 \\ 0 & 0 & 8 & 9 \\ 0 & 0 & 0 & 10 \end{bmatrix}$$

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

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

Comment on the memory usage of each approaches. When is one advantageous over another? Over a plain dense matrix? Generalise your results in the case of triangular matrices and tridiagonal matrices of size n .

Preconditioning

- Preconditioning is a technique used to accelerate the convergence of iterative methods for solving linear systems of the form $Ax = b$.
- The core idea is to transform the original system into an equivalent system that is better conditioned, meaning it converges more rapidly under iterative methods.
- We introduce a "preconditioner matrix" C (invertible) and transform the original system as follows:

$$Ax = b$$

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

Examples for preconditioning

- Jacobi: $C = D$, where D is the diagonal of matrix A

$$D^{-1}(D - (L + U))x = D^{-1}b$$

$$(I - D^{-1}(L + U))x = D^{-1}b$$

$$x = D^{-1}b + D^{-1}(L + U)x$$

Iterative form

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j^{(k)} \right) \quad \text{for } i = 1, 2, \dots, n$$

Sparse and dense Jacobi: Now you try, file dense_sparse_jacobi.py

- Two functions named *jacobi_dense* (similar to the previous one) and *jacobi_sparse* with 5 inputs as before (except the *A* matrix should be a *csr* matrix in the case of the sparse implementation) and returning three outputs
 - a numpy array *x*, the approximate solution,
 - the number of iterations done (an int), and
 - the time taken for the solution
- a function *generate_corrected_sparse_tridiagonal_matrix* generating a tridiagonal matrix, taking two inputs
 - an integer *n* representing the dimension of the system
 - two floats, the first one for the diagonal entries, and the second for the upper and lower diagonaland returning three outputs
 - the sparse matrix *A* generated as a *csr_matrix* and
 - the equivalent dense matrix (a numpy array, implemented via a for loop, not with *to_array*)
 - a random right hand side *b*