Numerical Linear Algebra for Computational Science and Information Engineering

Lecture 08
Classical Iterative Methods for Linear Systems

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Outline

Towards iterative methods to solve linear systems

- So far, we saw how **direct methods** can be used **to solve linear systems**:
  1. **Factorize** the matrix (e.g., LU or Cholesky factorization) with cost $\mathcal{O}(n^3)$
  2. **Solve** the system using the computed factors with cost $\mathcal{O}(n^2)$
- **Direct methods** are very stable and accurate.

  However, they can have a very high computational cost.

  In general, direct methods are **not suitable for very large** n.
- As a potentially more efficient way to solve linear systems, we will explore **iterative methods**.

  Iterative methods are **inexact** in the sense that they rely on the generation of a sequence of approximate solutions which **converges towards the solution**, but the sequence is stopped at finite accuracy.

  In general, iterative methods **do not require explicit access to the matrix** and they **rely on** the **matrix-vector kernel** $x \mapsto Ax$.

  Iterative methods are particularly **recommended** for cases **where** the **matrix-vector product can be efficiently deployed**, e.g., as it is the case for sparse matrices.

Splitting methods

Section 7.1 in Darve & Wootters (2021)

General splitting methods

- Splitting methods are simple iterative methods to solve linear systems.
- Consider the $A = M - N$ splitting of a matrix A, where M is non-singular.
- The linear system $Ax = b$ can be recast as follows:

$$\begin{aligned} Mx - Nx &= b \\ x - M^{-1}Nx &= M^{-1}b \\ x &= Gx + M^{-1}b \end{aligned}$$

  so that x is a **fixed point** of $f : x \mapsto M^{-1}Nx + M^{-1}b$, i.e., $x = f(x)$, and where $G := M^{-1}N$ is the **iteration matrix**.
- To solve a fixed point problem, one can start with any point x, and compute $f(x)$. Then compute $f(f(x))$, then $f(f(f(x)))$ and so on, until the sequence converges. In particular, we consider the following

Splitting method update rule

Given a matrix $A = M - N$ where M is non-singular, the update rule for a general splitting method with a given $x^{(0)}$ is

$$x^{(k+1)} := Gx^{(k)} + M^{-1}b \quad \text{where} \quad G := M^{-1}N.$$

General splitting methods, cont'd$_1$

- The error $e^{(k+1)} := x^{(k+1)} - x$ is such that

$$\begin{aligned} e^{(k+1)} &= Gx^{(k)} + M^{-1}b - Gx - M^{-1}b \\ &= Gx^{(k)} - Gx \\ &= Ge^{(k)} \end{aligned}$$

  so that $e^{(k)} = G^k e^{(0)}$.
- The convergence theory depends on the iteration matrix $G = M^{-1}N$:

Theorem (Convergence of splitting methods)

Given b and $A = M - N$ with non-singular A and M, the iteration

$$x^{(k+1)} = Gx^{(k)} + M^{-1}b \;\; \textit{where} \;\; G := M^{-1}N$$

converges for any starting $x^{(0)}$ if and only if

$$\rho(G) < 1$$

where $\rho(G)$ is the spectral radius, i.e., the largest modulus of eigenvalue of the iteration matrix G.

General splitting methods, cont'd$_2$

- Even though analyzing the spectrum of the iteration matrix G is generally difficult, it is understood that, the smaller the modulus $\rho(G)$, the faster the convergence.
- How should we pick M and N?

  The selection of M and N may be guided by two desirable properties:
  - Linear systems of the form $Mz = d$ are easy to solve.

    This suggest good choices for M are diagonal or triangular.
  - The spectral radius $\rho(G)$ is less than 1.
- We will see several examples of splitting methods, namely
  - Jacobi method
  - Gauss-Seidel method
  - Over-relaxation method

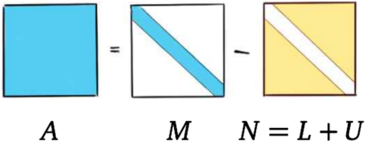
Jacobi method

Section 7.2 in Darve & Wootters (2021)

Jacobi method

- Let $A = D - L - U$ where
  - D is diagonal
  - L is strictly lower-triangular, i.e., with zeros on the diagonal
  - U is strictly upper-triangular

  Then, the splitting is clearly unique given A as we choose $M = D$ and $N = L + U$:



- The Jacobi splitting leads to the following iteration

Jacobi iterations

Suppose $A = D - U - L$ as above. The update formula for Jacobi iteration is given by

$$Dx^{(k+1)} = (L + U)x^{(k)} + b.$$

Jacobi method, cont'd

- The convergence of Jacobi iterations is as follows:

Theorem (Convergence of Jacobi iterations)

If A is strictly diagonally dominant, i.e.,

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|$$

for $i = 1, 2 \ldots, n$, then Jacobi iterations converge for any initial guess $x^{(0)}$.

  Note that this condition is not necessary to ensure convergence.

  The necessary condition to ensure convergence remains that the iteration matrix $G_{\text{Jacobi}} = D^{-1}(L + U)$ has a spectral radius smaller than one.

- The Jacobi method is especially simple to implement.

  It is also well-suited for parallel implementation as we have

$$x_i^{(k+1)} = \left(b_i + (L + U)[i, :]x^{(k)}\right) / d_{ii}$$

$$x_i^{(k+1)} = \left(b_i - (A - D)[i, :]x^{(k)}\right) / d_{ii}.$$

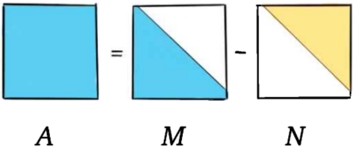
Gauss-Seidel method

Section 7.3 in Darve & Wootters (2021)

Gauss-Seidel method

- Let $A = D - L - U$ where
  - D is diagonal
  - L is strictly lower-triangular, i.e., with zeros on the diagonal
  - U is strictly upper-triangular

  Then, the splitting is clearly unique given A as we choose $M = D - L$ and $N = U$:



- The Gauss-Seidel splitting leads to the following iteration

Gauss-Seidel iterations

Suppose $A = D - U - L$ as above. The update formula for Gauss-Seidel iteration is given by

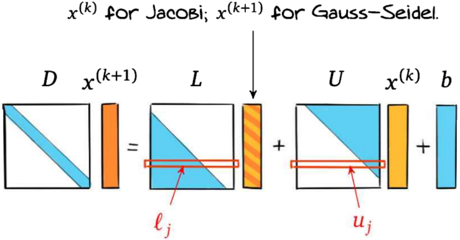
$$(D - L)x^{(k+1)} = Ux^{(k)} + b.$$

Gauss-Seidel method, cont'd$_1$

- Intuitively, "putting more information in M" should help with convergence of the method, and this is indeed the case, i.e., $\rho(G_{\mathrm{GS}}) = \rho(G_{\mathrm{Jacobi}})^2$.
- On the other hand, solving triangular systems with $M = D - L$ is more involved than solving diagonal systems with $M = D$.
- We can compare Gauss-Seidel to Jacobi iterations as follows:

$$\begin{aligned}(D-L)x^{(k+1)} &= Ux^{(k)} + b \\ Dx^{(k+1)} &= Lx^{(k+1)} + Ux^{(k)} + b \text{ (Gauss-Seidel)} \\ Dx^{(k+1)} &= Lx^{(k)} + Ux^{(k)} + b \quad \text{(Jacobi)}\end{aligned}$$

and see they are very similar except for one term:



Gauss-Seidel method, cont'd$_2$

- The convergence of Gauss-Seidel iterations is as follows:

Theorem (Convergence of Gauss-Seidel iterations)

If A

- *is strictly diagonally dominant, or*
- *is symmetric positive definite (SPD)*

then Gauss-Seidel iterations converge irrespective of the initial guess $x^{(0)}$.

Note that these conditions are not necessary to ensure convergence.

The necessary condition to ensure convergence remains that the iteration matrix $G_{\mathrm{GS}} = (D-L)^{-1}U$ has a spectral radius smaller than one.

Successive over-relaxation

Section 7.4 in Darve & Wootters (2021)

Successive over-relaxation

- Successive over-relaxation (SOR) consists of introducing a parameter to a splitting method in order to get a handle of the speed of convergence.
- In particular, we use a parameter ω to boost convergence.

  The idea is to start with the Gauss-Seidel update step as follows:

$$\begin{aligned} Dx_{\mathrm{GS}}^{(k+1)} &= Lx_{\mathrm{GS}}^{(k+1)} + Ux^{(k)} + b \\ x_{\mathrm{GS}}^{(k+1)} &= D^{-1}\left(Lx_{\mathrm{GS}}^{(k+1)} + Ux^{(k)} + b\right) \\ x_{\mathrm{GS}}^{(k+1)} &= x^{(k)} + \left[D^{-1}\left(Lx_{\mathrm{GS}}^{(k+1)} + Ux^{(k)} + b\right) - x^{(k)}\right] \end{aligned}$$

so that $x_{\mathrm{GS}}^{(k+1)} = x^{(k)} + \Delta x_{\mathrm{GS}}^{(k)}$ where

$$\Delta x_{\mathrm{GS}}^{(k)} = D^{-1}\left(Lx_{\mathrm{GS}}^{(k+1)} + Ux^{(k)} + b\right) - x^{(k)}$$

is the update to $x^{(k)}$ in a Gauss-Seidel iteration.

In SOR, the idea is to scale this correction by a parameter $0 < \omega < 2$:

$$x_{\mathrm{SOR}}^{(k+1)} = x^{(k)} + \omega\Delta x_{\mathrm{GS}}^{(k)}.$$

Successive over-relaxation, cont'd

- When $\omega \approx 0$, we are very cautious and only make small corrections to $x^{(k)}$.

  When $\omega = 1$, we recover a Gauss-Seidel iteration.

  When $\omega \approx 2$, we are very confident in the Gauss-Seidel correction and apply it twice instead of once.
- The update formula of the SOR sequence is given as follows:

$$\begin{aligned} x_{\text{SOR}}^{(k+1)} &= x_{\text{SOR}}^{(k)} + \omega \left[D^{-1} \left(L x_{\text{SOR}}^{(k+1)} + U x_{\text{SOR}}^{(k)} + b \right) - x_{\text{SOR}}^{(k)} \right] \\ &= (1-\omega) x_{\text{SOR}}^{(k)} + \omega \left[D^{-1} \left(L x_{\text{SOR}}^{(k+1)} + U x_{\text{SOR}}^{(k)} + b \right) \right] \end{aligned}$$

  which yields the following iterations:

SOR iterations

Let $\omega \in (0, 2)$, and suppose $A = D - L - U$ as above. The update formula for SOR iterations is

$$(D - \omega L) x_{\text{SOR}}^{(k+1)} = ((1-\omega) D + \omega U) x_{\text{SOR}}^{(k)} + \omega b.$$

Successive over-relaxation, cont'd

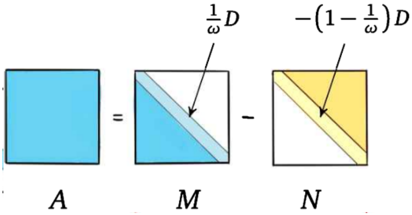
- Since the update formula can written as

$$\left(\frac{1}{\omega}D - L\right)x_{\text{SOR}}^{(k+1)} = \left(\left(\frac{1}{\omega} - 1\right)D + U\right)x_{\text{SOR}}^{(k)} + b$$

and that we have

$$\left(\frac{1}{\omega}D - L\right) - \left(\left(\frac{1}{\omega} - 1\right)D + U\right) = D - L - U = A$$

we can say that SOR is a splitting method with $M = \frac{1}{\omega}D - L$ and $N = (\frac{1}{\omega} - 1)D + U$ such that $A = M - N$:



Successive over-relaxation, cont'd

- Although SOR is a heuristic, it can lead to significant improvements in the convergence rate when ω is chosen appropriately.

Theorem (Convergence of SOR iterations)

If A is symmetric positive definite (SPD), then SOR iterations converge irrespective of the initial guess $x^{(0)}$, for any $\omega \in (0, 2)$.

Note that this condition is not necessary to ensure convergence.

The necessary condition to ensure convergence remains that the iteration matrix

$$\begin{aligned} G &= \left(\frac{1}{\omega}D - L\right)^{-1}\left((\frac{1}{\omega} - 1)D + U\right) \\ &= (D - \omega L)^{-1}((1-\omega)D + \omega U) \end{aligned}$$

has a spectral radius smaller than one.

Homework problems

Homework problem

Turn in **your own** solution to the following problem:

Pb. 18 Let $A = \begin{bmatrix} 1 & 2 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$. Analyze the spectrum of the iteration matrix and show whether

(a) A Jacobi iteration would converge.

(b) A Gauss-Seidel iteration would converge.

(c) A SOR iteration would converge with $\omega = 1/2$.

Practice session

Practice session

1. Implement Jacobi, Gauss-Seidel and SOR iterations.
2. Benchmark your implementations.