

Gauss-Seidel & SOR Methods

Solvers for Symmetric Positive
Definite Systems

Outline

- Review
- Gaussian Seidel iteration
- The algorithm
- Convergence conditions
- The Successive Over Relaxation (SOR) method
- Optimal SOR

Review

- Linear system: $Ax = b$,
- General form of iterative method:

$$A = N - P, N \approx A, P = N - A.$$

$$Ax = b \rightarrow Nx = b + Px.$$

$$Nx^{(k+1)} = b + Px^{(k)}.$$

- The convergence condition

$$e^{(k)} = x - x^{(k)}.$$

$$e^{(k+1)} = (N^{-1}P)e^{(k)}, M = N^{-1}P.$$

$$e^{(k)} = M^k e^{(0)}.$$

$$\|e^{(k)}\| = \|M^k e^{(0)}\| \leq \|M^k\| \cdot \|e^{(0)}\| \leq \|M\|^k \|e^{(0)}\|.$$

$$\|M\| < 1.$$

Gauss-Seidel Iteration

- N is the lower triangular matrix and P is the strictly upper triangular matrix of A .

$$n_{ij} = \begin{cases} a_{ij}, i \geq j. \\ 0, \text{otherwise.} \end{cases}$$

$$p_{ij} = \begin{cases} -a_{ij}, i < j, \\ 0, \text{otherwise.} \end{cases}$$

The shape of A , N , and P

$$A = N - P$$

$$\bullet \quad A = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\bullet \quad N = \begin{bmatrix} a_{00} & 0 & 0 & 0 \\ a_{10} & a_{11} & 0 & 0 \\ a_{20} & a_{21} & a_{22} & 0 \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\bullet \quad P = \begin{bmatrix} 0 & -a_{01} & -a_{02} & -a_{03} \\ 0 & 0 & -a_{12} & -a_{13} \\ 0 & 0 & 0 & -a_{23} \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Gauss-Seidel Iteration

- N is the lower triangular matrix and P is the strictly upper triangular matrix of A .

- The iteration:

$$Nx^{(k)} = b + Px^{(k-1)}.$$

//consider the i^{th} equation:

$$\sum_{j=0}^i a_{ij}x_j^{(k)} = b_i - \sum_{j=i+1}^{n-1} a_{ij}x_j^{(k-1)},$$

$$a_{i0}x_0^{(k)} + \cdots + a_{ii-1}x_{i-1}^{(k)} + a_{ii}x_i^{(k)} = b_i - \sum_{j=i+1}^{n-1} a_{ij}x_j^{(k-1)},$$

$$x_i^{(k)} = \frac{1}{a_{ii}} \left[b_i - \sum_{j=0}^{i-1} a_{ij}x_j^{(k)} - \sum_{j=i+1}^{n-1} a_{ij}x_j^{(k-1)} \right]$$

$$A = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$N = \begin{bmatrix} a_{00} & 0 & 0 & 0 \\ a_{10} & a_{11} & 0 & 0 \\ a_{20} & a_{21} & a_{22} & 0 \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$P = \begin{bmatrix} 0 & -a_{01} & -a_{02} & -a_{03} \\ 0 & 0 & -a_{12} & -a_{13} \\ 0 & 0 & 0 & -a_{23} \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The Pseudo-Codes

//Initialize the solution.

x[] = {0.0};

err = ∞;

//Iterate until being converged

while(err>ε){

 for(i=0;i≤n-1;i++){

 sum = b[i];

 for(j=0;j≤n-1;j++) if(j!=i) sum = sum - A[i][j]*x[j];

 x[i] = sum/A[i][i];

 }

//Compute the residual

r[] = b[] - A[][]*x[];

err = norm_inf(r, n); //Compute the norm

}

return (x[]);

$$x_i^{(k)} = \frac{1}{a_{ii}} \left[b_i - \sum_{j=0}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n-1} a_{ij} x_j^{(k-1)} \right]$$

Convergence of Gauss-Seidel

- Theorem1: Gauss-Seidel converges, if A is diagonal dominant.
 - See the proof of convergence of Jacobi method.
 $M = N^{-1}P, \|M\| < 1$. //using ∞ norm.
- Theorem2: Gauss-Seidel converges, if A is **Symmetric Positive Definite (SPD)**.
- Definition of SPD: if A is SPD, then A is symmetric and $x^T A x > 0, \forall x \in R^n, x \neq 0$.

Properties

- P1, If A is SPD, then $a_{ii} > 0$.

Proof by contradiction:

- Assume $a_{ii} \leq 0$ for some i .
- Select $e = [0, \dots, 0, 1, 0, \dots, 0]^T$, $e[i] = 1$, and $e[j] = 0$, $i \neq j$.
- Then $e^T A e = a_{ii} \leq 0$.
- Thus A is not SPD, a contradiction!

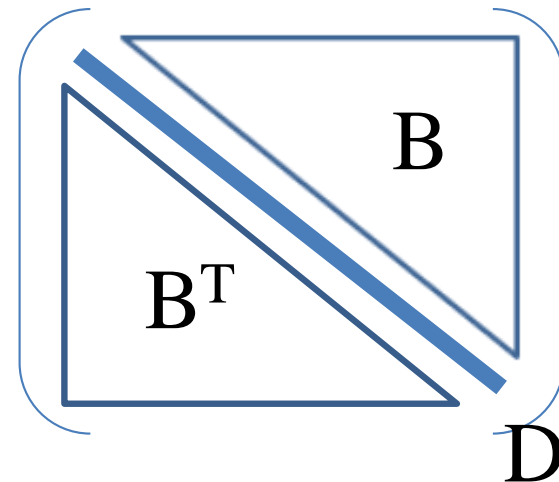
- P2, if A is SPD, then its eigenvalues $\lambda > 0$.

Proof:

- Let w be an eigenvector of A and λ the corresponding eigenvalue.
 $Aw = \lambda w$.
- $w^T Aw = \lambda w^T w = \lambda \|w\|^2 > 0$, //by definition of SPD
- It implies $\lambda > 0$.

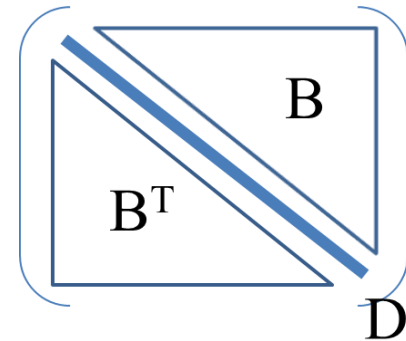
Properties

- P3, Let $D = \text{diag}(A)$, the diagonal matrix of A , then D is SPD.
 - Using property P1.
- P4, If A is SPD, then $N = D + B^T$, where B is the strictly upper triangle matrix of A .
 - See the right figure. $B^T \sim B$.
- P5, $D = A - B - B^T$
- P6, $w^T B w = w^T B^T w$.
 - Proof by expanding the equation and using $B_{ij} = B_{ji}$.
- A is SPD and it is divided into 3 parts in Gaussian-Seidel method.



Spectral Radius of the Correction Matrix

- Lemma: In Gauss-Seidel method, eigenvalues of $M=N^{-1}P$ are in the range of $(-1,1)$, if A is SPD.
- Proof:
 - In Gauss-Seidel iteration $(A - B)x^{(k+1)} = b - Bx^{(k)}$.
 $x^{(k+1)} = (A - B)^{-1}b - (A - B)^{-1}Bx^{(k)}$.
 - Thus $M = N^{-1}P = -(A - B)^{-1}B$.
 - Let w and λ be an eigenvector and an eigenvalue of M .
 - $Mw = \lambda w$, $-(A - B)^{-1}Bw = \lambda w$.
 - Multiply both sides by $(A-B)$, we have $-Bw = \lambda(A - B)w$.
 - Inner-product both sides with w : $-w^T Bw = \lambda w^T (A - B)w = \lambda w^T Aw - \lambda w^T Bw$.
 - $w^T Bw = \lambda w^T Bw - \lambda w^T Aw$. $(1 - \lambda)w^T Bw = -\lambda w^T Aw$.
 - Thus, $w^T Bw = \frac{\lambda}{\lambda-1} w^T Aw$. ----- (1).



Spectral Radius of the Correction Matrix

- Lemma: In Gauss-Seidel method, eigenvalues of $M=N^{-1}P$ are in the range of $(-1,1)$, if A is SPD.

Shape of B^T , D , and B .

- Proof: (continued)

- Since D is SPD,

$$0 < w^T D w = w^T (A - B - B^T) w.$$

- Using (1) and P6,

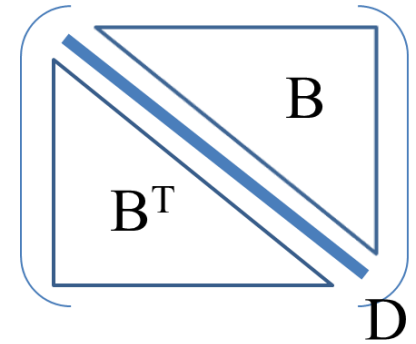
$$0 < w^T A w - w^T B w - w^T B^T w = (1 - 2 \frac{\lambda}{\lambda-1}) w^T A w.$$

- Since A is SPD, $w^T A w > 0$ and

$$0 < 1 - 2 \frac{\lambda}{\lambda-1} = 1 - \frac{2\lambda(\lambda-1)}{(\lambda-1)^2} = \frac{1-\lambda^2}{(\lambda-1)^2}.$$

- Thus,

$$1 - \lambda^2 > 0, -1 < \lambda < 1.$$



Convergence of SPD Systems

- Theorem: If A is SPD, Gauss-Seidel converges.
- Proof:
 - Define $e^{(k)} = x - x^{(k)}$.
 $e^{(k+1)} = (N^{-1}P)e^{(k)}$, $M = N^{-1}P$.
 - From a previous proof, $e^{(k)} = M^k e^{(0)}$
 $\|e^{(k)}\| = \|M^k e^{(0)}\| \leq \|M^k\| \cdot \|e^{(0)}\| \leq \|M\|^k \|e^{(0)}\|.$
 - By the previous lemma, if A is SPD then $\|M\| < 1$,
 - Thus, $\lim_{k \rightarrow \infty} \|M\|^k = 0$.
 - The Gauss-Seidel iteration converges.

Relaxation

- In Gauss-Seidel method

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left[b_i - \sum_{j=0}^{i-1} a_{ij} x_j^{(k+1)} + \sum_{j=i+1}^{n-1} a_{ij} x_j^{(k)} \right].$$

- Adding and subtracting $a_{ii}x_i^{(k)}$ in the right side

$$x_i^{(k+1)} = \color{red}{x_i^{(k)}} + \frac{1}{a_{ii}} \left[b_i - \sum_{j=0}^{i-1} a_{ij} x_j^{(k+1)} + \sum_{j=i}^{n-1} \color{red}{a_{ij} x_j^{(k)}} \right].$$

- The 2nd term of the right side contains an approximation of the residual $\color{violet}{r = b - Ax}$.
 - We modify the value of x by using the approximation.
- It is called a *relaxation*.

Successive Over Relaxation

- The relaxation of Gauss-Seidel

$$x_i^{(k+1)} = x_i^{(k)} + \frac{1}{a_{ii}} \left[b_i - \sum_{j=0}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i}^{n-1} a_{ij} x_j^{(k)} \right].$$

- By parameterizing the **relaxation** part

$$x_i^{(k+1)} = x_i^{(k)} + \frac{\omega}{a_{ii}} \left[b_i - \sum_{j=0}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i}^{n-1} a_{ij} x_j^{(k)} \right].$$

- If $\omega = 1.0$, we have Gauss-Seidel Iteration.
- If $1 < \omega < 2$, we have **Successive Over-Relaxation (SOR)** method.
- If $0 < \omega < 1$, we have **under-relaxation**.

SOR Algorithm

//Initialize the solution.

x[] = {0.0};

err = ∞;

//Iterate until being converged

while(err>ε){

 for(i=0;i≤n-1;i++){

 sum = b[i];

 for(j=0;j≤n-1;j++) sum = sum - A[i][j]*x[j];

 x[i] = x[i] + ω*sum/A[i][i];

 }

//Compute the residual

r[] = b[] - A[][]*x[];

err = norm_inf(r, n); //Compute the norm of the residual

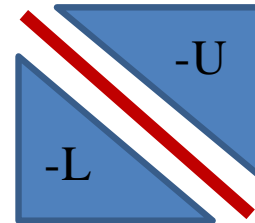
}

return (x[]);

$$x_i^{(k+1)} = x_i^{(k)} + \frac{\omega}{a_{ii}} \left[b_i - \sum_{j=0}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i}^{n-1} a_{ij} x_j^{(k)} \right]$$

Relaxation Parameter

- The best ω is hard to compute.
 - But some results are known.
- P1, if A is SPD and $0 < \omega < 2$, SOR converges.
- P2, SOR can converge only if $0 < \omega < 2$.
- P3, Optimal ω :
 - Split the coefficient matrix $A = D - L - U$.
 - Let $T = D^{-1}(L+U)$
$$\omega = \frac{2}{1 + \sqrt{1 - \rho^2}},$$
 - where ρ is the spectral radius of T ,
 $\rho = |\lambda_{\max}|.$



ADI Method

- In Jacobi, Gauss-Seidel, and SOR methods, we update $x[]$ from $x[0]$ to $x[n-1]$ in each iteration.
- In Altered Direction Iteration (ADI) method,
 - We update $x[]$ from $x[0]$ to $x[n-1]$ in most cases.
 - But, in some iterations, we update $x[]$ from $x[n-1]$ to $x[0]$.
- SSOR (Symmetric Successive Over-Relaxation) method:
 - Using SOR to solve the system.
 - Update $x[]$ from $x[0]$ to $x[n-1]$ in odd-numbered iterations.
 - Update $x[]$ from $x[n-1]$ to $x[0]$ in even-numbered iterations.
- SSOR may be slower than SOR.
- SSOR is used as a preconditioner for other iterative methods.
 - What is a preconditioner?

Preconditioners

- The original system $Ax = b$ has a large condition number.
- Modify the system as follows
 $(PA)x = Pb$. Then solve the system.
- Or with more efforts
 - Solve $(AP)y = b$ at first.
 - Then solve $P^{-1}x = y$ later to obtain the solution.
- Method: left precondition and right precondition.
- Criteria:
 - **P** should be simple
 - Don't form **AP** or **PA** explicitly. Why? Think about the time complexity of matrix-multiplication.

Reminder

- Hilbert matrix is symmetric positive definite,
$$a_{ij} = \frac{1}{i+j+1}, 0 \leq i, j \leq n-1.$$
- However, linear systems with Hilbert matrices as coefficient matrices are almost intractable by using Gauss-Seidel method.
- Why?
- Answer:
 - The condition number $\text{cond}(A) = O\left(\frac{(1+\sqrt{2})^{4n}}{\sqrt{n}}\right)$ is exponentially grows with the dimension n .
 - Numerical errors (perturbations) prevent the computation from converge.

References

- Broyden, C. G. (1964). On convergence criteria for the method of successive over-relaxation. *Mathematics of Computation*, 18(85), 136-141.
 - Symmetric matrix, $0 < \omega < 2$ converges
 - Positive definite & low-triangular dominant \rightarrow convergence
- James, K. R., & Riha, W. (1975). Convergence criteria for successive overrelaxation. *SIAM Journal on Numerical Analysis*, 12(2), 137-143.
 - Convergence criteria of SOR method for general and special matrices
 - Most referenced paper about SOR.
- Yang, S., & Gobbert, M. K. (2009). The optimal relaxation parameter for the SOR method applied to the Poisson equation in any space dimensions. *Applied Mathematics Letters*, 22(3), 325-331.
 - Optimal ω for Poisson equations (PDE, elliptic PDE)