Scientific Computing II

Relaxation Methods and the Smoothing Property

Michael Bader

Summer 2013

Part I

Relaxation Methods

The Residual Equation

- we consider a system of linear equations: $Ax = b$
- for which we compute a sequence of approximate solutions $x^{(i)}$
- the **residual** $r^{(i)}$ shall then be defined as:

$$r^{(i)} = b - Ax^{(i)}$$

- short computation:

$$r^{(i)} = b - Ax^{(i)} = Ax - Ax^{(i)} = A(x - x^{(i)}) = Ae^{(i)}.$$

- relates the residual $r^{(i)}$ to the **error** $e^{(i)} := x - x^{(i)}$
  (note that $x = x^{(i)} + e^{(i)}$);
- we will call this equation the **residual equation**:

$$Ae^{(i)} = r^{(i)}$$

Residual Based Correction

Solve $Ax = b$ using the residual equation $Ae^{(i)} = r^{(i)}$

- r (which can be computed) is an indicator for the size of the error e (which is not known).
- use residual equation to compute a *correction* to $x^{(i)}$
- basic idea: solve a modified (easier) SLE:

$$B\,\hat{e}^{(i)} = r^{(i)} \qquad \text{where} \quad B \sim A$$

- use $\hat{e}^{(i)}$ as an approximation for $e^{(i)}$, and set

$$x^{(i+1)} = x^{(i)} + \hat{e}^{(i)}.$$

Relaxation

How should we choose B?

- $B \sim A$ (B should be "similar" to A),
  more precisely $B^{-1} \approx A^{-1}$,
  or at least $B^{-1}y \approx A^{-1}y$ for most vectors y.
- $Be = r$ should be easy/fast to solve

Examples:

- $B = \mathrm{diag}(A) = D_A$ (diagonal part of A)
  $\Rightarrow$ Jacobi iteration
- $B = L_A$ (lower triangular part of A)
  $\Rightarrow$ Gauss-Seidel iteration

Jacobi Relaxation

Iteration formulas in matrix-vector notation:

1. residual notation:

$$x^{(i+1)} = x^{(i)} + D_A^{-1} r^{(i)} = x^{(i)} + D_A^{-1} \left(b - A x^{(i)} \right)$$

2. for implementation:

$$x^{(i+1)} = D_A^{-1} \left(b - (A - D_A) x^{(i)} \right)$$

3. for analysis:

$$x^{(i+1)} = \left(I - D_A^{-1} A \right) x^{(i)} + D_A^{-1} b =: M x^{(i)} + N b$$

Jacobi Relaxation – Algorithm

- based on: $x^{(i+1)} = D_A^{-1}\left(b - (A - D_A)x^{(i)}\right)$

```
for i from 1 to n do
    xnew[i] := ( b[i]
         - sum( A[i,j]*x[j], j=1..i-1)
         - sum( A[i,j]*x[j], j=i+1..n)
        ) / A[i,i];
end do;
for i from 1 to n do
    x[i] := xnew[i];
end do;
```

- **properties:**
  - additional storage required (`xnew`)
  - `x`, `xnew` can be computed **in any order**
  - `x`, `xnew` can be computed **in parallel**

Gauss-Seidel Relaxation

Iteration formulas in matrix-vector notation:

1. residual notation:

$$x^{(i+1)} = x^{(i)} + L_A^{-1} r^{(i)} = x^{(i)} + L_A^{-1} \left(b - A x^{(i)} \right)$$

2. for implementation:

$$x^{(i+1)} = L_A^{-1} \left(b - (A - L_A) x^{(i)} \right)$$

3. for analysis:

$$x^{(i+1)} = \left(I - L_A^{-1} A \right) x^{(i)} + L_A^{-1} b =: M x^{(i)} + N b$$

Gauss-Seidel Relaxation – Algorithm

- based on: $x^{(i+1)} = L_A^{-1}\left(b - (A - L_A)x^{(i)}\right)$
- solve $L_A x^{(i+1)} = b - (A - L_A)x^{(i)}$
  via backwards substitution:

```
for i from 1 to n do
    x[i] := ( b[i]
         - sum( A[i,j]*x[j], j=1..i-1)
         - sum( A[i,j]*x[j], j=i+1..n)
        ) / A[i,i];
end do;
```

- **properties:**
  - no additional storage required
  - inherently **sequential** computation of `x`
  - usually faster convergence than Jacobi

Successive-Over-Relaxation (SOR)

- observation: Gauss-Seidel corrections are "too small"
- add an over-relaxation-factor α:

```
for i from 1 to n do
    x[i] := x[i] + alpha * ( b[i]
         - sum( A[i,j]*x[j], j=1..n)
        ) / A[i,i];
end do;
```

- for 2D-Poisson: optimal α ($\approx$ 1.7) improves convergence: $\mathcal{O}(n^2) \to \mathcal{O}(n^{3/2})$

Does It Always Work?

- simple answer: no (life is not that easy ...)
- Jacobi: matrix A needs to be *diagonally dominant*
- Gauß-Seidel: matrix A needs to be *positive definite*
- How about performance?
  $\rightarrow$ usually quite slow

Our next topics:

1. How slow are the methods exactly?
2. What is the underlying reason?
3. Is there a fix?

Part II

Smoothing Property of Relaxation Methods

The Model Problem – 1D Poisson

1D Poisson equation:

- $-u''(x) = 0$ on $\Omega = (0, 1)$, $u(0) = u(1) = 0$ (thus: $u(x) = 0$)
- discretised on a uniform grid of mesh size $h = \frac{1}{n}$
- compute approximate values $u_j \approx u(x_j)$
  at grid points $x_j := jh$, with $j = 1, \dots, (n-1)$
- system matrix A_h built from 3-point stencil:

$$\frac{1}{h^2}\begin{bmatrix} -1 & 2 & -1 \end{bmatrix}$$

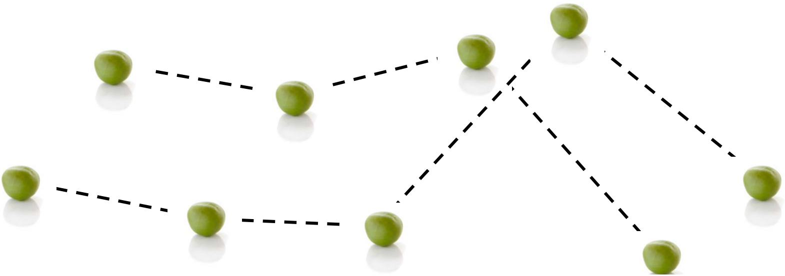
- A_h a tridiagonal $(n-1) \times (n-1)$-matrix

1D Poisson: Jacobi Relaxation

Iterative scheme for Jacobi relaxation:

- leads to relaxation scheme $u_j^{(i+1)} = \frac{1}{2}\left(u_{j+1}^{(i)} + u_{j-1}^{(i)}\right)$
- start with initial guess $u_j^{(0)} \neq 0$
- in this case: $e_j^{(i)} = u_j - u_j^{(i)} = -u_j^{(i)}$

Visualisation of relaxation process:

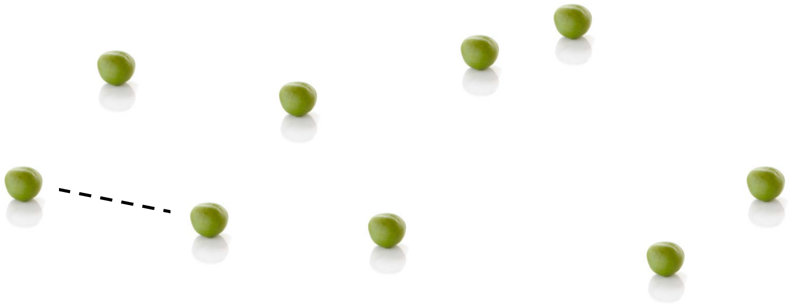


1D Poisson: Gauß-Seidel Relaxation

Iterative scheme for Gauß-Seidel relaxation:

- leads to relaxation scheme $u_j^{(i+1)} = \frac{1}{2}\left(u_{j+1}^{(i)} + u_{j-1}^{(i)}\right)$
- start with initial guess $u_j^{(0)} \neq 0$
- in this case: $e_j^{(i)} = u_j - u_j^{(i)} = -u_j^{(i)}$

Visualisation of relaxation process:



Convergence of Relaxation Methods

Observation (see also tutorials)

- slow convergence
- smooth error components are reduced very slowly
- high frequency error components are damped more efficiently (esp. for Gauß-Seidel relaxation)

Convergence Analysis

- remember iteration scheme: $x^{(i+1)} = Mx^{(i)} + Nb$
- derive iterative scheme for the error $e^{(i)} := x - x^{(i)}$:

$$e^{(i+1)} = x - x^{(i+1)} = x - Mx^{(i)} - Nb$$

- for a **consistent** scheme, x is a fixpoint of the iteration equation: $x = Mx - Nb$
- hence:

$$\begin{aligned} e^{(i+1)} &= Mx + Nb - Mx^{(i)} - Nb = Me^{(i)} \\ &= Mx - Mx^{(i)} = Me^{(i)} \\ \Rightarrow e^{(i)} &= M^i e^{(0)}. \end{aligned}$$

Convergence Analysis (2)

- iteration equation for error: $e^{(i)} = M^i e^{(0)}$
- consider eigenvalues λ_j and eigenvectors v_j of iteration matrix M:

$$Mv_j = \lambda_j v_j \quad \Rightarrow \quad M\Big(\sum_j \alpha_j v_j\Big) = \sum_j \lambda_j \alpha_j v_j$$

- write error as combination of eigenvectors: $e^{(0)} = \sum_j \alpha_j v_j$, then:

$$M^i e^{(0)} = M^i \Big(\sum_j \alpha_j v_j\Big) = \sum_j (\lambda_j)^i \alpha_j v_j$$

- convergence, if all $\left|\lambda_j\right| < 1$
- speed of convergence dominated by largest λ_j

The Smoothing Property

Eigenvalues and -vectors of A_h:

- eigenvalues: $\lambda_k = \frac{4}{h^2}\sin^2\left(\frac{k\pi}{2n}\right) = \frac{4}{h^2}\sin^2\left(\frac{k\pi h}{2}\right)$
- eigenvectors: $v^{(k)} = \left(\sin(k\pi j/n)\right)_{j=1,\dots,n-1}$
  – both for $k = 1, \dots, (n-1)$

For Jacobi relaxation:

- iteration matrix $M = I - D_A^{-1}A = I - \frac{h^2}{2}A$
- eigenvalues of M: $\mu_k := 1 - 2\sin^2\left(\frac{k\pi h}{2}\right)$
- $|\mu_k| < 1$ for all k, but $|\mu_k| \approx 1$ if $k = 1$ or $k = n-1$
- $\mu_1 \in \mathcal{O}(1 - h^2)$: slow convergence of smooth errors
- $\mu_{n-1} \approx -1$: "sign-flip" (but slow reduction) of "zig-zag" error components
- convergence factor determined by $\mathcal{O}(1 - h^2)$

The Smoothing Property

Eigenvalues and -vectors of A_h:

- eigenvalues: $\lambda_k = \frac{4}{h^2} \sin^2\left(\frac{k\pi}{2n}\right) = \frac{4}{h^2} \sin^2\left(\frac{k\pi h}{2}\right)$
- eigenvectors: $v^{(k)} = \big(\sin(k\pi j/n)\big)_{j=1,\dots,n-1}$
  – both for $k = 1, \dots, (n-1)$

For weighted Jacobi relaxation:

- iteration matrix $M = I - \omega D_A^{-1} A = I - \frac{h^2}{2} \omega A$
- eigenvalues of M: $1 - 2\omega \sin^2\left(\frac{k\pi h}{2}\right)$
- $\mu_1 \in \mathcal{O}(1 - h^2)$: slow convergence of smooth errors
- $\mu_{n-1} \approx 0$ for $\omega = \frac{1}{2}$; $\mu_{n-1} \approx -\frac{1}{3}$ for $\omega = \frac{2}{3}$
  thus quick reduction of high-frequency errors
- convergence determined by $\mathcal{O}(1 - n^{-2})$
  (slower than normal Jacobi due to ω)

The Smoothing Property (2)

"Fourier mode analysis"

- decompose the error $e^{(i)}$ into eigenvectors (for 1D Poisson: $\sin(k\pi x_j)$,)
- determine convergence factors for "eigenmodes"

Observation for weighted Jacobi and Gauß-Seidel:

- The *high* frequency part (with respect to the underlying grid) is reduced quite quickly.
- The *low* frequency part (w.r.t. the grid) decreases only very slowly; actually the slower, the finer the grid is.

$\Rightarrow$ **"smoothing property"**

The Smoothing Property (2)

“Fourier mode analysis”

- decompose the error $e^{(i)}$ into eigenvectors (for 1D Poisson: $\sin(k\pi x_j)$,)
- determine convergence factors for “eigenmodes”

Another Observation:

- the smoothest (slowest converging) component corresponds to the smallest eigenvalue of A ($k = 1$)
- remember residual equation: $Ae = r$:
  if $e = v^{(1)}$, then $r = \lambda_1 v^{(1)}$

$\Rightarrow$ **“small residual, but large error”**