Scientific Computing II

Michael Bader

Outlines

Part I: Smoothing Property of Relaxation Methods Part II: Multigrid Methods Part II: Components of Multigrid Methods

Scientific Computing II Towards Multigrid Methods

Michael Bader

Summer term 2012

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Part I: Smoothing Property of Relaxation Methods



Convergence of Relaxation Methods





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Part II: Multigrid Methods

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- More Multigrid Schemes
- 10 Speed of Convergence

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Convergence of Relaxation Methods

The Model Problem – 1D Poisson

The Smoothing Property

Part I

Smoothing Property of Relaxation Methods

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Convergence of Relaxation Methods

Observation

- slow convergence
- high frequency error components are damped more efficiently
- smooth error components are reduced very slowly

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Convergence of Relaxation Methods

The Model Problem – 1D Poisson

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 **consistent** scheme, x is a fixpoint of the iteration (x = Mx - Nb)

hence:

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

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

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Convergence of Relaxation Methods

The Model Problem – 1D Poisson

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:

$$M\mathbf{v}_{j} = \lambda_{j}\mathbf{v}_{j} \Rightarrow M(\sum_{j} \alpha_{j}\mathbf{v}_{j}) = \sum_{j} \lambda_{j}\alpha_{j}\mathbf{v}_{j}$$
$$\Rightarrow M^{i}e^{(0)} = M^{i}(\sum_{j} \alpha_{j}\mathbf{v}_{j}) = \sum_{j} \lambda_{j}^{i}\alpha_{j}\mathbf{v}_{j}$$

• convergence, if all $|\lambda_j| < 1$

• speed of convergence dominated by largest λ_j

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Convergence of Relaxation Methods

The Model Problem – 1D Poisson

The Smoothing Property

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The Model Problem

1D Poisson equation:

•
$$-u''(x) = f(x)$$
 on $\Omega = (0, 1)$

- u = 0 on $\partial \Omega$ (hom. Dirichlet boundaries)
- 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, ..., (n-1)
- system matrix A_h built from 3-point stencil:

$$\frac{1}{h^2}[-1 \quad 2 \quad -1]$$

• A_h a tridiagonal (n-1) imes (n-1)-matrix

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The Model Problem – 1D Poisson

The Smoothing Property

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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: $v^{(k)} = (\sin(k\pi j/n))_{j=1,\dots,n-1}$ - 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*: $\mu_k := 1 2\sin^2(\frac{k\pi h}{2})$
- $|\mu_k| < 1$ 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 $\mathcal{O}(1-h^2)$

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Convergence of Relaxation Methods

The Model Problem – 1D Poisson

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:
$$v^{(k)} = (\sin(k\pi j/n))_{j=1,\dots,n-1}$$

- both for $k = 1, \dots, (n-1)$

For weighted Jacobi relaxation:

- iteration matrix $M = I \omega D_A^{-1} A = I \frac{\hbar^2}{2} \omega A$
- eigenvalues of $M: 1 2\omega \sin^2(\frac{k\pi h}{2})$
- $\mu_1 \in \mathcal{O}(1-h^2)$: 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 $O(1 n^{-2})$ (slower than normal Jacobi due to ω)

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Convergence of Relaxation Methods

The Model Problem – 1D Poisson

The Smoothing Property (2)

"Fourier mode analysis"

- decompose the error e⁽ⁱ⁾ into eigenvectors (for 1D Poisson: sin(kπx_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"

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The Model Problem – 1D Poisson

The Smoothing Property (2)

"Fourier mode analysis"

- decompose the error e⁽ⁱ⁾ into eigenvectors (for 1D Poisson: sin(kπx_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"

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Convergence of Relaxation Methods

The Model Problem – 1D Poisson

Part II Multigrid Methods

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Aultigrid Idea No.

Multigrid Idea No. 2

A Two-Grid Method

Correction Scheme – Components

The Multigrid V-Cycle

More Multigrid Schemes

Speed of Convergence

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Multigrid Idea No. 1

- additional result from convergence analysis:
 "high-frequency error" is relative to mesh size
- on a sufficiently coarse grid, even very low frequencies can be "high-frequency" (if the mesh size is big)

"Multigrid":

- use multiple grids to solve the system of equations
- on each grid, a certain range of error frequencies will be reduced efficiently

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Multigrid Idea No. 1

Multigrid Idea No. 2

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More Multigrid Schemes

Nested Iteration

Solve the problem on a coarser grid:

- will be comparably (very) fast
- can give us a good initial guess:
- nested iteration/ "poor man's multigrid"

Algorithm:

- Start on a very coarse grid with mesh size $h = h_0$; guess an initial solution x_h
- 2 Iterate over $A_h x_h = b_h$ using **relaxation** method \Rightarrow approximate solution x_h
- **3** interpolate the solution x_h to a finer grid $\Omega_{h/2}$
- proceed with step 2 (now with mesh size h := h/2) using interpolated $x_{h/2}$ as initial solution

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Multigrid Idea No. 1

Multigrid Idea No. 2

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More Multigrid Schemes

Multigrid Idea No. 2

Observation for nested iteration:

- error in interpolated initial guess also includes low frequencies
- relaxation therefore still slow
- can we go "back" to a coarser grid later in the algorithm?

\Rightarrow Idea No. 2: use the residual equation:

- solve Ae = r on a coarser grid
- leads to an approximation of the error e
- add this approximation to the fine-grid solution

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Multigrid Idea No. 1

Multigrid Idea No. 2

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More Multigrid Schemes

A Two-Grid Method

Algorithm:

- relaxation/smoothing on the fine level system \Rightarrow solution x_h
- **2** compute the **residual** $r_h = b_h A_h x_h$
- **I estriction** of r_h to the coarse grid Ω_H
- compute a **solution** to $A_H e_H = r_H$
- interpolate the coarse grid solution e_H to the fine grid Ω_h
- add the resulting correction to x_h
- again, relaxation/smoothing on the fine grid

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Multigrid Idea No. 1

Aultigrid Idea No.

A Two-Grid Method

Correction Scheme – Components

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More Multigrid Schemes

Correction Scheme - Components

smoother: reduce the high-frequency error components, and get a smooth error restriction: transfer residual from fine grid to coarse grid, for example by injection • (full) weighting coarse grid equation: (acts as) discretisation of the PDE on the coarse grid interpolation: transfer coarse grid solution/correction from coarse grid to fine grid

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Multigrid Idea No. 1

Multigrid Idea No. 2

A Two-Grid Method

Correction Scheme - Components

The Multigrid V-Cycle

More Multigrid Schemes

The Multigrid V-Cycle

- smoothing on the fine level system \Rightarrow solution x_l
- 2 compute the residual $r_I = b_I A_I x_I$
- restriction of r_l to the coarse grid Ω_{l-1}
- solve coarse grid system $A_{l-1}e_{l-1} = r_{l-1}$ by a recursive call to the V-cycle algorithm
- interpolate the coarse grid solution e_{l-1} to the fine grid Ω_l
- add the resulting correction to x_l
- post-smoothing on the fine grid

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Multigrid Idea No. 1

Multigrid Idea No. 2

A Two-Grid Method

Correction Scheme – Components

The Multigrid V-Cycle

More Multigrid Schemes

V-Cycle – Implementation

- on the coarsest grid: direct solution
- number of smoothing steps is typically very small (1 or 2)

Cost (storage and computing time):

• 1D:
$$c \cdot n + c \cdot n/2 + c \cdot n/4 + \ldots \leq 2c \cdot n$$

- 2D: $c \cdot n + c \cdot n/4 + c \cdot n/16 + ... \le 4/3c \cdot n$
- 3D: $c \cdot n + c \cdot n/8 + c \cdot n/64 + \ldots \le 8/7c \cdot n$
- overall costs are dominated by the costs of the finest grid

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Multigrid Idea No. 1

Multigrid Idea No. ?

A Two-Grid Method

Correction Scheme – Components

The Multigrid V-Cycle

More Multigrid Schemes

The W-Cycle

• perform two coarse grid correction steps instead of one



- more expensive
- useful in situations where the coarse grid correction is not very accurate

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Multigrid Idea No.

A Two-Grid Method

More Multigrid Schemes

The Full Multigrid V-Cycle (FMV)

Recursive algorithm:

- combines nested iteration and V-cycle
- (recursively!) perform an **FMV-cycle** on the next coarser grid to get a good initial solution
- interpolate this initial guess to the current grid
- perform a V-cycle to improve the solution



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Multigrid Idea No. 1

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Correction Scheme – Components

The Multigrid V-Cycle

More Multigrid Schemes

Speed of Convergence

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Speed of Convergence

- fastest method around (if all components are chosen carefully)
- "textbook multigrid efficiency":

 $\left\|\boldsymbol{e}^{(m+1)}\right\| \leq \gamma \left\|\boldsymbol{e}^{(m)}\right\|,$

where convergence rate $\gamma < 1$ (esp. $\gamma << 1)$ is independent of the number of unknowns

- ⇒ constant number of multigrid steps to obtain a given number of digits
- ⇒ overall computational work increases only linearly with the number of unknowns

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Multigrid Idea No. 1

Multigrid Idea No. 2

A Two-Grid Method

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The Multigrid V-Cycle

More Multigrid Schemes

Convergence Rates (2)

For the "Model Problem" (i.e., Poisson Problem):

- $\mathcal{O}(n)$ to solve up to "level of truncation"
- "level of truncation": $O(h^2)$ (discretisation error)
- O(n) is achieved by FMV-Cycle (1 or 2 cycles sufficient)

For Other Problems:

- OK for strongly elliptic problems
- multigrid variants for non-linear problems, parabolic/hyperbolic, ...
- achieving "textbook efficiency" usually a demanding task

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Multigrid Idea No. 1

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Part III

Components of Multigrid Methods

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Smoothers

For the Poisson problem (see tutorials):

- Gauss-Seidel
- red-black Gauss-Seidel
- damped $(\omega = \frac{2}{3})$ Jacobi
- how about Jacobi (non-weighted) and SOR?
 - ightarrow do not work well

(do not smooth high frequencies efficiently)

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Smoothers Interpolation Restriction Coarse Grid Operator

Smoothers (2) – other problems

anisotropic Poisson eq.: $u_{xx} + \epsilon u_{yy} = f$

- Strong dependency in *x*-direction, weak dependency in *y*-direction
- Good smoothing of the error only in x-direction
- "semi-coarsening" (coarsen only in "smooth" direction) → see tutorials
- line smoothers: perform a column-wise Gauss-Seidel = solve each "column" (or row) simultaneously (direct, tridiagonal solver):

$$u_{i-1,j}^{(n+1)} - 4u_{ij}^{(n+1)} + u_{i+1,j}^{(n+1)} = f_{ij} - u_{i,j-1}^{(n)} - u_{i,j+1}^{(n)}$$

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Smoothers (3) – other problems

1D Convection-Diffusion eq.: $\epsilon u_{xx} + u_x = f$, $\epsilon \ll 1$

- "upwind discretisaton": $\frac{\epsilon}{h^2}(u_{n-1}-2u_n+u_{n+1})+\frac{1}{h}(u_n-u_{n-1})=f_n$
- (weighted) Jacobi and red-black Gauss-Seidel: no smoothing, basically updates one grid point per iteration
- Gauss-Seidel (relaxation from "left to right"): almost an exact solver
- in general: Gauss-Seidel smoothing in "downwind" order

 \rightarrow difficult to do in 2D and 3D

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Interpolation (aka "Prolongation")

For Poisson problem:

- (bi-)linear interpolation:
 in 1D: resembles homogeneous (f = 0) solution
- constant (in general too small approximation order): sometimes used for cell-based coarsening (unknowns located in cell centers)
- quadratic, cubic, etc.: often too costly, more smoothing steps are cheaper and can eliminate the disadvantage of a lower order interpolation
- **but:** in FMV-cycle interpolation to finer grid (after a completed V-cycle) should be higher-order

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Interpolation – Matrix Notation

For linear interpolation (1D):

$$\begin{pmatrix} \frac{1}{2} & 0 & 0\\ 1 & 0 & 0\\ \frac{1}{2} & \frac{1}{2} & 0\\ 0 & 1 & 0\\ 0 & \frac{1}{2} & \frac{1}{2}\\ 0 & 0 & 1\\ 0 & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} x_1\\ x_2\\ x_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(0+x_1)\\ x_1\\ \frac{1}{2}(x_1+x_2)\\ x_2\\ \frac{1}{2}(x_1+x_2)\\ x_2\\ \frac{1}{2}(x_2+x_3)\\ x_3\\ \frac{1}{2}(x_3+0) \end{pmatrix}$$

Notation: $I_{2h}^h x_{2h} = x_h$ or $P_{2h}^h x_{2h} = x_h$

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Restriction

For Poisson problem:

- "injection": pick values at corresp. coarse grid points
- "full weighting" = transpose of bilinear interpolation (safer, more robust convergence), see illustration below for the 1D case



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Restriction – Matrix Notation

For full weighting (1D):

$$\begin{pmatrix} \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 & 0 & 0\\ 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} & 0 & 0\\ 0 & 0 & 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} x_1\\ x_2\\ x_3\\ x_4\\ x_5\\ x_6\\ x_7 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(x_1 + 2x_2 + x_3)\\ \frac{1}{2}(x_3 + 2x_4 + x_5)\\ \frac{1}{2}(x_5 + 2x_6 + x_7) \end{pmatrix}$$

Notation: $I_h^{2h}x_h = x_{2h}$ or $R_h^{2h}x_h = x_{2h}$

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Coarse Grid Operator

Coarse Grid Operator

Two main options:

- discretise PDE on grid Ω_h to obtain A_h
- "Galerkin approach": $A_{2h} := R_h^{2h} A_h P_{2h}^h$ \rightarrow compare effect on vector x_{2h} :

$$A_{2h}x_{2h} := R_h^{2h} A_h P_{2h}^h x_{2h}$$

- \rightarrow evaluate from right to left:
 - interpolate x_2h to $\hat{x}_h := P_{2h}^h x_{2h}$
 - apply fine-grid operator A_h to interpolated \hat{x}_h
 - restrict resulting matrix-vector product to Ω_{2h}

Exercise:

• Compute
$$A_{2h} := R_h^{2h} A_h P_{2h}^h$$
 for $A_h := \frac{1}{h^2}$ tridiag $(-1, 2, -1)$

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Literature

General:

- Gander, Hrebicek: Solving Problems in Scientific Computing Using Maple and MATLAB.
- Golub, Ortega: *Scientific Computing and Differential Equations.*
- Dongarra, et. al.: Numerical linear algebra for high-performance computers.

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Restriction

Coarse Grid Operator

Literature (2)

Multigrid:

• Briggs, Henson, McCormick: *A Multigrid Tutorial* (2nd ed.).

Conjugate Gradients:

• Shewchuk: An Introduction to the Conjugate Gradient Method Without the Agonizing Pain.

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