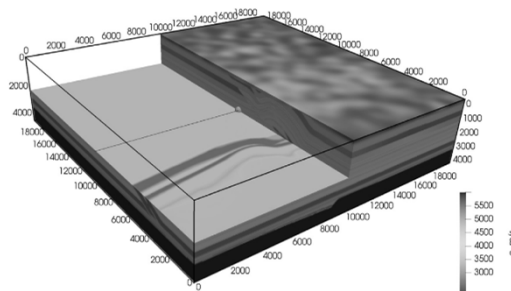


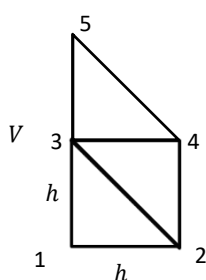
Advanced Solvers for Numerical Partial Differential Equations (PDEs)



Lecture 2

Nikolay Yavich

n.yavich@skoltech.ru



Exercise 1

$$-\Delta u = 1 \text{ в } V,$$

$$\frac{\partial u}{\partial n} = 0 \text{ на } \Gamma$$

Derive the P_1 finite-element system for this domain/problem

Part 1

Introduction to modern iterative solvers

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FD Equation System

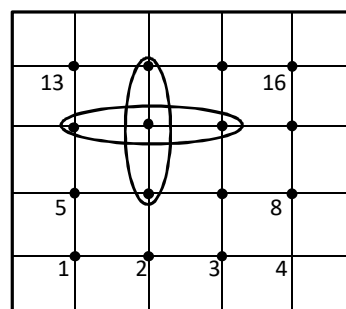
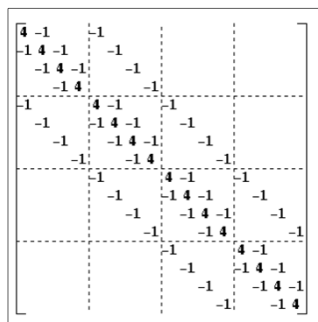
$$\begin{aligned} -\Delta u &= f \text{ in } \Omega \\ u &= \varphi \text{ on } \Gamma \end{aligned}$$

We receive a large equation system

$$A u_h = f_h$$

Its size

$$N = (n_x - 1)(n_y - 1)$$



$$\begin{aligned} n_x &= n_y = 5 \\ N &= 16 \end{aligned}$$

$$A = \begin{pmatrix} C & -I & & \\ -I & C & \ddots & \\ & \ddots & \ddots & \ddots \end{pmatrix}$$

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Overall properties

$$A u_h = g$$

1. Gauss elimination / LU factorization

Computational complexity $Q = O(N^3)$.

2. Block tridiagonal solver

$$D u_{i-1} + C u_i + D u_{i+1} = f_i$$

$$u_i = M_i u_{i+1} + t_i$$

Complexity $Q = O(N^{2.5})$.

$$\begin{pmatrix} C & D & \\ D & C & \ddots \\ & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ u_i \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ f_i \\ \vdots \end{pmatrix}$$

These methods ignore sparsity of the blocks.

Thus iterative solver would be a better fit for this problem.

Single multiplication complexity $O(N)$.

Our goal is thus to design a solver with complexity of

$O(N^2)$, $O(N \log(N))$, or even $O(N)$.

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Iterative solvers

$$A u = f$$

$\varepsilon > 0$ tolerance

u^0 Initial guess

$u^1 \dots u^s \dots$

$A u^s - f$ residual

$u^s - u$ error

Convergence speed ρ

$$\begin{aligned} \|u^s - u\| &\leq \rho \|u^{s-1} - u\| \\ &\leq \rho^s \|u^0 - u\| \leq \varepsilon \|u^0 - u\| \end{aligned}$$

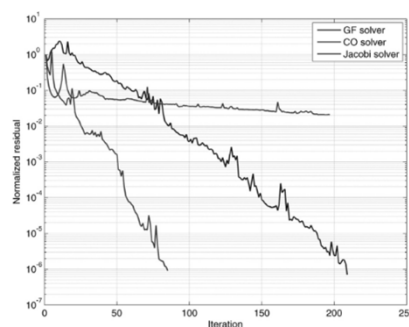
Iteration count to reduce the error in $1/\varepsilon$ times

$$s = \left\lceil \frac{\ln \varepsilon}{\ln \rho} \right\rceil$$

• Fast solver = ρ close to 0

Slow solver = ρ close to 1

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Richardson Iteration

$$Au = f$$

$$A > 0$$

Richardson, 1910

$$u_{k+1} = u_k + \tau(f - Au_k) \quad \tau > 0$$

$$\tau_{opt} = \frac{2}{\lambda_{min} + \lambda_{max}} \quad \rho_{opt} \approx 1 - 2 \frac{\lambda_{min}}{\lambda_{max}}$$

Steepest Descent

$$u_{k+1} = u_k + \tau_k(f - Au_k)$$

$$\phi(u) = \frac{1}{2}(Au, u) - (f, u) \quad \tau_k \text{ s.th. } \phi(u_{k+1}) \rightarrow \min$$

$$\tau_k = \frac{(r_k, r_k)}{(r_k, Ar_k)} \quad \rho \approx 1 - 2 \frac{\lambda_{min}}{\lambda_{max}}$$

Equivalent to $r_{k+1} \perp r_k$

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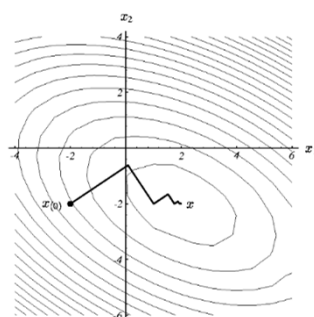
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Conjugate Gradient Method (CG)

$$Au = f \quad A = A^T > 0$$

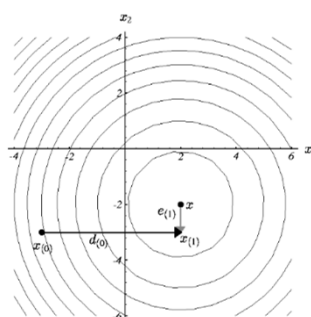
$$\phi(u) = \frac{1}{2}(Au, u) - (f, u) \quad u_k \text{ minimizes } \phi(u) \text{ over } K_m = \text{span}(f, Af, \dots) + u_0$$

Krylov subspace



Steepest Decent

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CG

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Conjugate Gradient Method (CG)

- * Combines SD with Gram-Schmidt orthonormalization
- * Avoids repeating directions

$$\begin{aligned}
 r_k &= Au_k - f \\
 u_{k+1} &= u_k - \beta_k p_k \\
 p_k &= r_k - \alpha_k p_{k-1} \\
 \alpha_k &= \frac{(r_{k-1}, Ap_{k-1})}{(p_{k-1}, Ap_{k-1})} & \beta_k &= \frac{(r_{k-1}, r_{k-1})}{(p_{k-1}, Ap_{k-1})} \\
 \rho &\approx 1 - 2 \sqrt{\frac{\lambda_{\min}}{\lambda_{\max}}}
 \end{aligned}$$

Hestenes & Stiefel, 1952

- * Most commonly used algorithm for problems with SPD matrices

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Complexity of different solvers

Gauss elimination	$O(N^3)$
Block tridiagonal solver	$O(N^{2.5})$
Jacobi and Seidel	$O(N^2 \log \frac{1}{\epsilon})$
Richardson and steepest descent	$O(N^2 \log \frac{1}{\epsilon})$
Conjugate gradient	$O(N^{\frac{3}{2}} \log \frac{1}{\epsilon})$
???	
Optimal estimate	$O(N)$

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Part 2 Introduction to Preconditioning

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Preconditioned Iterative Solvers

For solving $A u = g$ we already discussed

$$u^{k+1} = u^k + \tau(g - Au^k).$$

What if we substitute scalar τ with a matrix B ?

$$u^{k+1} = u^k + B^{-1}(g - Au^k)$$

Two pathological cases

- $B^{-1} = \tau I$, nothing really changes
- $B = A$, convergence in 1 iteration, but complexity is of the original problem.

B is a preconditioner. The goal is to design B , **close** to A , yet easier to invert.

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Jacobi Preconditioner

Take

$$u^{k+1} = u^k + B^{-1}(g - Au^k)$$

$$B = \text{diag}(A).$$

How good will such a solver for the model problem?

For that we have to analyze $S = I - B^{-1}A$

Note $B_{ii} = \frac{4}{h^2}$.

Studying the eigenvalue problem

$$(I - B^{-1}A)v = \lambda v$$

Leads to

$$\lambda_{km} = 1 - \frac{h^2}{4} \frac{4}{h^2} \left[\sin^2\left(\frac{\pi kh}{2}\right) + \sin^2\left(\frac{\pi mh}{2}\right) \right].$$

Thus

$$\rho = 1 - 2\sin^2\left(\frac{\pi h}{2}\right) \approx 1 - \frac{\pi^2 h^2}{2},$$

- Arithmetical complexity $Q = cN^2 \ln \frac{1}{\varepsilon}$

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Part 3 FFT solver as a direct method

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Motivation

$$\begin{aligned} -\Delta u &= f \quad \text{в } \mathbb{R}^2 \\ u &= 0 \quad \text{при } |x| + |y| \rightarrow \infty \end{aligned}$$

Apply double Fourier transform

$$U(k_x, k_y) = \iint_{-\infty}^{\infty} e^{-2\pi i(k_x x + k_y y)} u(x, y) dx dy$$

$$F(k_x, k_y) = \iint_{-\infty}^{\infty} e^{-2\pi i(k_x x + k_y y)} f(x, y) dx dy$$

$$(2\pi)^2 (k_x^2 + k_y^2) U(k_x, k_y) = F(k_x, k_y)$$

Apply inverse double Fourier transform $U(k_x, k_y)$

$$u(x, y) = \iint_{-\infty}^{\infty} e^{2\pi i(k_x x + k_y y)} U(k_x, k_y) dx dy$$

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Discrete Fourier Transform

$$v_k = \sum_{n=0}^{N-1} e^{-\frac{2\pi i k n}{N}} p_n \quad k = 0..n-1$$

This summation has a complexity $O(N^2)$

Cooley Tukey, 1965 г.
Fast Fourier Transform
 $O(N \log(N))$

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Separation-by-variable Solver

$$\begin{aligned} -\Delta u &= f & \text{в } (0,1)^2, \\ u &= 0 & \text{на } \Gamma \end{aligned} \quad A u = g$$

Spectral decomposition

$$A = W D W^{-1}$$

Solution could be written

$$u = W D^{-1} W^{-1} g.$$

This would be practical if we could multiply by W and W^{-1} efficiently.

Unfortunately, W is dense thus single multiplication takes $O(N^2)$.

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Separation-by-variable Solver

We know entries of W

$$W_{ij} = C \sin(\pi i_x j_x h) \sin(\pi i_y j_y h),$$

i_x and i_y are indices of node i

$$i = (i_y - 1)(n - 1) + i_x$$

Multiplication $v = Wp$ is equivalent to

$$v_i = \sum_{j=1}^N W_{ij} p_j = C \sum_{j_y=1}^{n-1} \sin(\pi i_y j_y h) \sum_{j_x=1}^{n-1} \sin(\pi i_x j_x h) p_{(j_y-1)(n-1)+j_x}$$

This is discrete double sine transform!

Both forward and inverse could be performed in $O(N \log N)$ using FFT

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Separation-by-variable Solver

Thus solution

$$u = W D^{-1} W^{-1} g$$

computed as

- 1) $v = W^{-1}g$ (inverse 2D DST);
- 2) $p = D^{-1}v$ (diagonal matrix scaling)
- 3) $u = Wp$ (forward 2D DST).

The overall complexity is $O(N \log N)$,

For comparison, with the CG we had $O\left(N^{\frac{3}{2}} \log \frac{1}{\varepsilon}\right)$

- This is a **direct** method
- We looked at uniform grids, constant coefficients.
- Let us check few generalizations

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Kronecker Product Representation

$$\begin{aligned} -\Delta u &= f & \text{in } (0,1)^2, \\ u &= 0 & \text{on } \Gamma \end{aligned} \quad A u = g$$

APPENDIX B: KRONECKER PRODUCT AND ITS PROPERTIES

Given an $m \times n$ matrix $\mathbf{A} = \{a_{ij}\}$ and some matrix \mathbf{B} , their Kronecker product matrix $\mathbf{A} \otimes \mathbf{B}$ is a block matrix defined as

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{pmatrix}. \quad (\text{B1})$$

We used the following properties of this product within this note:

$$(\mathbf{A} \otimes \mathbf{B})^T = \mathbf{A}^T \otimes \mathbf{B}^T, \quad (\text{B2})$$

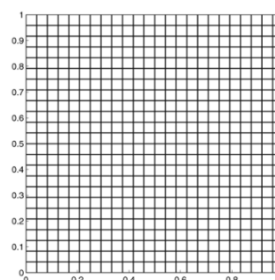
$$(\mathbf{A} \otimes \mathbf{B})^{-1} = \mathbf{A}^{-1} \otimes \mathbf{B}^{-1}, \quad (\text{B3})$$

$$(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{AC}) \otimes (\mathbf{BD}). \quad (\text{B4})$$

The identity (B3) holds under the assumption that \mathbf{A} and \mathbf{B} are invertible, while (B4) holds under the assumption that the respective matrix products are well defined.

Yavich & Zhdanov, 2020

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$$A = I_y \otimes L_{xx} + L_{yy} \otimes I_x$$

$$\text{Eigenvector matrix } W = W_y \otimes W_x$$

$$L_{xx} \quad L_{yy} \quad \text{tridiagonal}$$

$$W A W^T W u = W g$$

$$T \tilde{u} = \tilde{g}$$

$$T \text{ diagonal !}$$

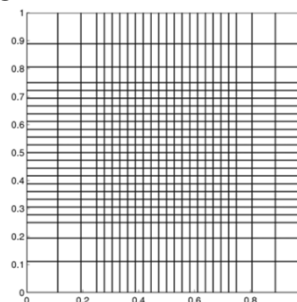
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Non-uniform Grids

The system and eigenvector matrices still admit this representations

$$A = I_y \otimes L_{xx} + L_{yy} \otimes I_x$$

$$W = W_y \otimes W_x$$



Although W_x and W_y are not sines any more

Yet we can perform spectral decomposition of L_{xx} and L_{yy} and find W_x and W_y

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1D coefficients

$$-\frac{\partial}{\partial x} \left(a(x) \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(b(y) \frac{\partial u}{\partial y} \right) = g \text{ в } V = (0,1)^2$$

$$u = 0 \text{ на } \Gamma$$

The system and eigenvector matrices still admit this representations

$$A = I_y \otimes L_{xx} + L_{yy} \otimes I_x$$

$$W = W_y \otimes W_x$$

with W_x and W_y easy to compute

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Part 4

FFT solver as a preconditioner

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Preconditioned Richardson Method

$$A u = g$$

u^0 initial guess

B some preconditioner

ε tolerance

residual

$$u^{k+1} = u^k + \tau B^{-1}(g - Au^k)$$

$$\|g - Au^k\| < \varepsilon ?$$

How fast the convergence will be / how many iterations will be needed?

u^* exact solution

$$z^k = u^* - u^k \text{ error}$$

$$z^{k+1} = z^k - \tau B^{-1} A z^k$$

$$= (I - \tau B^{-1} A) z^k$$

$$\|z^{k+1}\| \leq \|S\| \|z^k\|$$

Convergence depends
on the norm/largest eigenvalue of
 $S = I - \tau B^{-1} A$

The smaller the faster convergence!

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Spectrally-equivalent preconditioner

$$A u = g$$

a preconditioner B e.g. in

$$u^{k+1} = u^k + \tau B^{-1}(g - Au^k)$$

spectrally-equivalent if

$$C_1 Bv \cdot v \leq Av \cdot v \leq C_2 Bv \cdot v \quad \forall v$$

with C_1 and C_2 independent of problem size

$$S = I - \tau B^{-1}A$$

$$\rho(S) \text{ independent of } h!$$

With such a preconditioner iteration count depends only
 C_1, C_2 и ε !

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Anisotropic Diffusion Equation

$$-\frac{\partial}{\partial x} \left(a(x, y) \frac{\partial u}{\partial x} \right) - \frac{\partial}{\partial y} \left(b(x, y) \frac{\partial u}{\partial y} \right) = g \text{ в } V = (0, 1)^2$$

$$u = 0 \text{ на } \Gamma$$

$$a(x, y), b(x, y) > 0$$

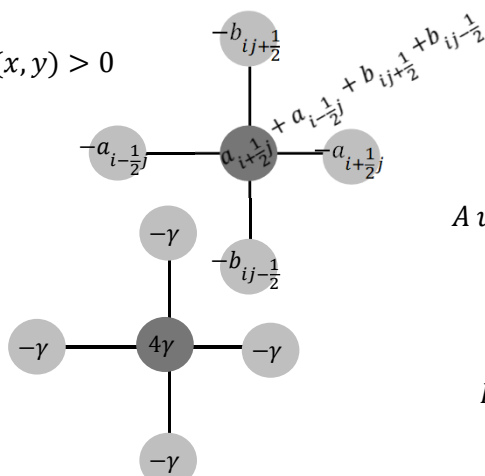
uniform grid

$$-\gamma \Delta u = f \text{ в } V$$

$$u = 0 \text{ на } \Gamma$$

$$\gamma > 0 - \text{const}$$

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$$A u = g$$

$$B u = f$$

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FFT as preconditioner

- Matrices A and B are of the same size
- Vector $B^{-1}v$ could be computed with FFT

$$u^{k+1} = u^k + \tau B^{-1}(g - Au^k)$$

Claim. Assume

$$c_1 \gamma \leq a(x, y) \leq c_2 \gamma \quad \forall x, y \in V$$

$$c_1 \gamma \leq b(x, y) \leq c_2 \gamma$$

then B is spectrally-equivalent A with constants c_1 and c_2

i.e. solver convergence speed will depend on closeness of $a(x, y)$ and $b(x, y)$ to γ .

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FFT as preconditioner

□

$$Av \cdot v =$$

$$\frac{1}{h^2} \left(\dots a_{i-\frac{1}{2}j} (v_{i-1j} - v_{ij}) \dots a_{i-\frac{1}{2}j} (v_{ij} - v_{i+1j}) \dots \right) \cdot \\ (\dots v_{i-1j} v_{ij} \dots) =$$

$$\dots \frac{a_{i-\frac{1}{2}j}}{h^2} (v_{ij} - v_{i-1j})^2 \dots \leq \\ \dots \frac{c_2 \gamma}{h^2} (v_{ij} - v_{i-1j})^2 \dots =$$

$$= c_2 Bv \cdot v$$

Similarly,

$$Av \cdot v \geq c_1 Bv \cdot v$$

■

We thus designed a solver with complexity $O\left(N \log N \log \frac{1}{\varepsilon}\right)$

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Part 2

Multigrid Method

R. Fedorenko, 1961

A. Brand, 1973

W. Hackbusch, 1977

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Motivation

Model problem

$$\begin{aligned} -\Delta u &= g \text{ в } V \\ u &= 0 \text{ на } \Gamma \end{aligned}$$

$$A_h u_h = g_h$$

Why the Jacobi solver is so slow?



Error of
initial guess



Error after 5
iterations



Error after 10
iterations

U. Trottenberg (2001)

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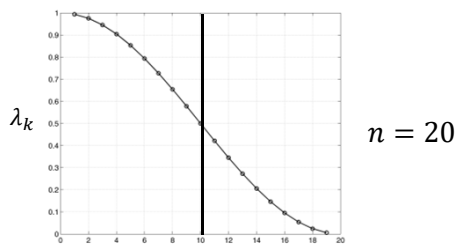
Motivation

Why Jacobi solver smooths out the error?

$$S = E - D^{-1}A$$

$$D = \text{diag}(A)$$

$$\lambda_k = 1 - \sin\left(\frac{\pi kh}{2}\right)^2 \quad u_{k,j}^h = \sin(\pi jkh)$$



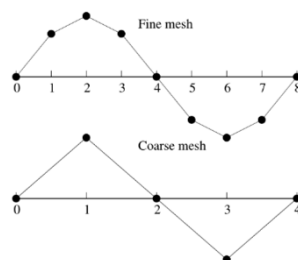
We can form two groups of frequencies:

- Low frequencies $k < n/2, \frac{1}{2} < \lambda < 1$
- High frequencies $\frac{n}{2} \leq k, \lambda \leq 1/2$

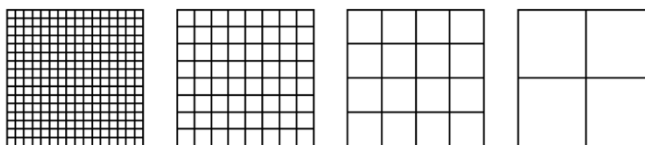
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Motivation

- High-frequency error components smoothed out well on fine grids
- Low-frequency error components represented well on coarse grids

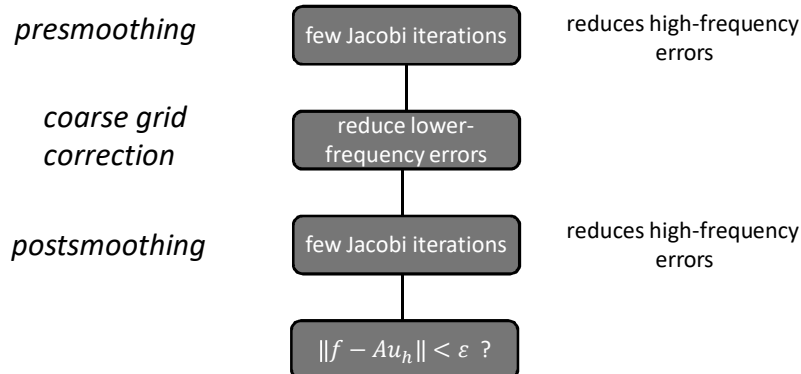


- Coarser problems are easier to solve



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The Big Idea of Multigrid



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Coarse grid correction

$$A_h u_h = g_h$$

u_h^* exact sol-n

u_h current guess

$$r_h = g_h - A_h u_h$$

$$e_h = u_h^* - u_h$$

Note:

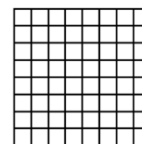
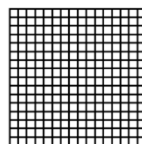
$$e_h = A_h^{-1} r_h$$

If we were able to compute the sum

$$u_h := u_h + e_h = u_h^*$$

then the problem would be solved

$$A_h e_h = r_h \longrightarrow \begin{aligned} &\bullet \quad r_H = R r_h \\ &\bullet \quad A_H d_H = r_H \\ &\bullet \quad d_h = P d_H \\ &\bullet \quad u_h := u_h + d_h \end{aligned}$$



h

$H = 2h$

We need to define

- restriction operator R
- coarse grid operator A_H
- prolongation operator P

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Prolongation Operator

$$v_{h,2i} = v_{2h,i}$$

$$v_{h,2i+1} = \frac{1}{2}(v_{2h,i} + v_{2h,i+1})$$

$$v_h = P v_{2h}$$

$$P = \frac{1}{2} \begin{bmatrix} 1 & & & & \\ 2 & 1 & & & \\ 1 & 2 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 2 \\ & & & & 1 \end{bmatrix}$$

$$\text{Stencil } P = \frac{1}{2} \begin{bmatrix} 1 & 2 & 1 \end{bmatrix}$$

$$P = \frac{1}{4} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$$

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Restriction Operator

$$(u_H, Rv_h)_H = (Pu_H, v_h)_h$$

$$v_{2h,i} = \frac{1}{4}(v_{h,2i-1} + 2v_{h,2i} + v_{h,2i+1})$$

$$v_{2h} = R v_h$$

$$R = \frac{1}{4} \begin{bmatrix} 1 & 2 & 1 & & & \\ & 1 & 2 & 1 & & \\ & & 1 & 2 & 1 & \\ & & & \ddots & \ddots & \ddots \\ & & & & 1 & 2 & 1 \end{bmatrix}$$

$$R = \frac{1}{4} \begin{bmatrix} 1 & 2 & 1 \end{bmatrix}$$

$$R = \frac{1}{16} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$$

$$P = 2 \quad R^T \quad \text{in 1D}$$

$$P = 4 \quad R^T \quad \text{in 2D}$$

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Coarse Grid Operator

- Direct method
 A_H – approximation of the differential operator on grid H
- Galerkin projection method

$$A_H = R A_h P$$
 Yet the product should be computed implicitly, e.g.

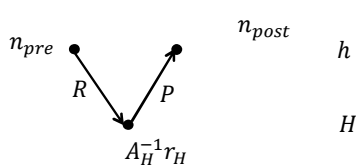
$$A_H v = (R (A_h (P v)))$$

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Two-grid Algorithm

$$A_h u_h = g_h$$



Algorithm u_h^0, A_h, g_h

$u_h := \text{Jacobi_Iter}(n_{pre}, u_h^0, A_h, g_h)$ *presmoothing*

$r_h = g_h - A_h u_h$

$r_H = R r_h$

Restriction of the residual

Solve $A_H d_H = r_H$

Coarse grid problem

$d_h = P d_H$

Prolongation

$u_h := u_h + d_h$

$u_h := \text{Jacobi_Iter}(n_{post}, u_h, A_h, g_h)$ *postsmoothing*

$\|g_h - A_h u_h\| < \varepsilon ?$

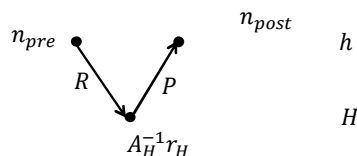
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Two-grid Algorithm

$$A_h u_h = g_h$$

$$D = \text{diag}(A_h)$$



Iteration matrix

$$S = (I - D^{-1}A_h)^{n_{post}} (I - PA_H^{-1}RA_h)(I - D^{-1}A_h)^{n_{pre}}$$

Theorem

$\rho(S) < \frac{1}{2}$ is independent of h , but depends on n_{post}, n_{pre}

$$n_{post} + n_{pre} > 0$$

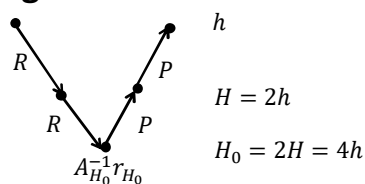
We designed a spectrally-equivalent preconditioner,

- although we have solve $A_H e_H = r_H \dots$

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Multigrid algorithm

$$A_h u_h = g_h$$



Algorithm $u_h = \text{V-cycle}(u_h^0, A_h, g_h)$

$$u_h := \text{Jacobi_Iter}(n_{pre}, u_h^0, A_h, g_h)$$

$$r_h = g_h - A_h u_h$$

$$r_H = R r_h$$

if $H \neq H_0$ $e_H = \text{V-cycle}(0, A_H, r_H)$

Recursion

else solve $A_H e_H = r_H$

We are on the coarsest grid

$$e_h = P e_H$$

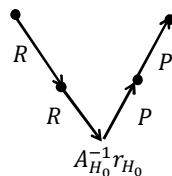
$$u_h := u_h + e_h$$

$$u_h := \text{Jacobi_Iter}(n_{post}, u_h, A_h, g_h)$$

Return u_h

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Computational Complexity



Assume the coarsest problem has size of $O(1)$

Then complexity of a single iteration is

$$1D: N + \frac{1}{2}N + \frac{1}{4}N + \dots = O(N)$$

$$2D: N + \frac{1}{4}N + \frac{1}{16}N + \dots = O(N)$$

i.e. multigrid had linear computational complexity

What will be the convergence speed?

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Multigrid Iteration Matrix

Assume we L grids from $k = L$ (fine) to $k = 1$ (coarsest)

A_k system matrix
 S_k iteration matrix

$R_{k \rightarrow k-1}$

$P_{k-1 \rightarrow k}$

$$S_1 = 0$$

$$S_k = (I - D_k^{-1}A_k)^{n_{post}} \left(I - P_{k-1 \rightarrow k} (I - S_{k-1}) A_{k-1}^{-1} R_{k \rightarrow k-1} A_k \right) (I - D_k^{-1}A_k)^{n_{pre}}$$

Full iteration matrix $S = S_L$

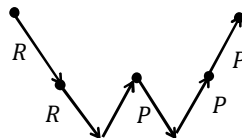
$$\rho(S) = 0.05 \dots 0.5 \text{ for model problems}$$

Spectrally-equivalent preconditioner

Solver with optimal complexity $O(N \log \frac{1}{\epsilon})$

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W-cycles



Algorithm $u_h = \text{W-cycle}(u_h^0, A_h, g_h)$

$u_h := \text{Jacobi_Iter}(n_{pre}, u_h^0, A_h, g_h)$

$r_h = g_h - A_h u_h$

$r_H = R r_h$

if $H \neq H_0$ $e_H = \text{W-cycle}(0, A_H, r_H)$

Two recursion calls

$e_H = \text{W-cycle}(e_H, A_H, r_H)$

else solve $A_H e_H = r_H$

We are on the coarsest grid

$e_h = P e_H$

$u_h := u_h + e_h$

$u_h := \text{Jacobi_Iter}(n_{post}, u_h, A_h, g_h)$

Return u_h

- More robust than V-cycle
- Also there is also FMG.

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Complexity of different solvers

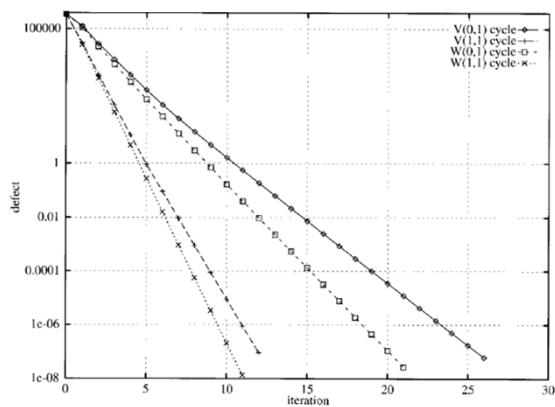
Gauss elimination	$O(N^3)$
Jacobi and Seidel	$O(N^2 \log \frac{1}{\epsilon})$
Richardson and steepest descent	$O(N^2 \log \frac{1}{\epsilon})$
Conjugate gradient	$O(N^{\frac{3}{2}} \log \frac{1}{\epsilon})$
FFT-based	$O(N \log N)$
Multigrid V-cycle	$O(N \log \frac{1}{\epsilon})$
Optimal estimate	$O(N)$

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Example

$$\begin{aligned} -\Delta u &= g \text{ в } V \\ u &= 0 \text{ на } \Gamma \end{aligned}$$

$$h = \frac{1}{256}$$



Trottenberg et al, 2001 ●45

Resumé on Multigrid

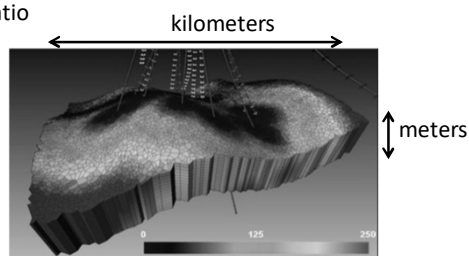
- Solver with optimal complexity
- Has many generalization (nonlinear equations etc)

The concept we discusses is only robust for

- Square grids
- Heterogeneous equations but isotropic coefficients

These cases require special treatment

- Stretched grids / high aspect ratio
- Anisotropic coefficients



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