Iterative Solvers for Large Linear Systems

Part IIIb: Method of Conjugate Gradients

Andreas Meister

University of Kassel, Department of Analysis and Applied Mathematics

Outline

- Basics of Iterative Methods
- Splitting-schemes
  - Jacobi- u. Gauß-Seidel-scheme
  - Relaxation methods
- Methods for symmetric, positive definite Matrices
  - Method of steepest descent
  - Method of conjugate directions
  - CG-scheme

Outline

- Multigrid Method
  - Smoother, Prolongation, Restriction
  - Twogrid Method and Extension
- Methods for non-singular Matrices
  - GMRES
  - BiCG, CGS and BiCGSTAB
- Preconditioning
  - ILU, IC, GS, SGS, ...

Method of steepest descent

Algorithm:

- Choose $x_0 \in \mathbb{R}^n$
- For $m = 0, 1, \ldots$

$$r_m = b - Ax_m$$

If $r_m \neq 0$

$$\lambda_m = \frac{\|r_m\|_2^2}{(Ar_m, r_m)}$$

$$x_{m+1} = x_m + \lambda_m r_m$$

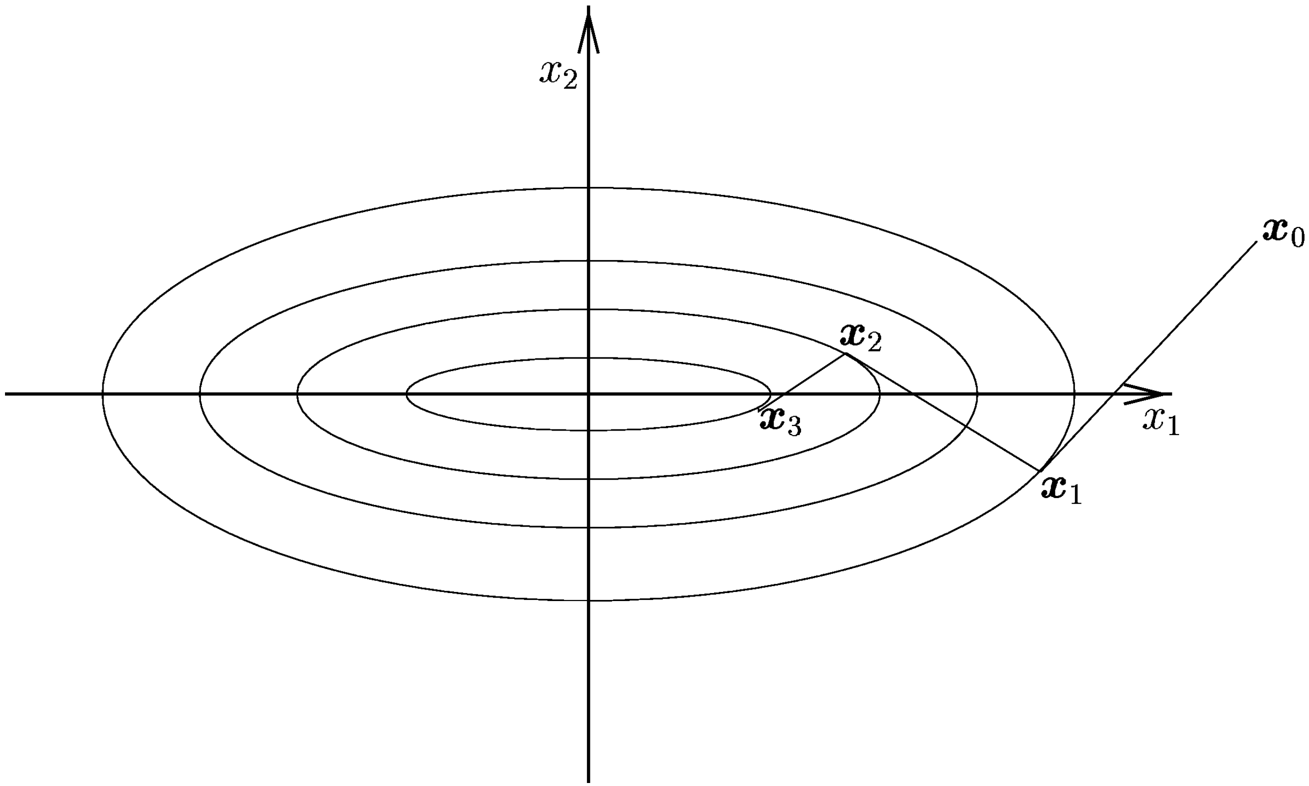
Example

$$A = \begin{pmatrix} 2 & 0 \\ 0 & 10 \end{pmatrix} \quad , \quad b = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad , \quad x_0 = \begin{pmatrix} 4 \\ \sqrt{1.8} \end{pmatrix}$$

Method of steepest descent

m	$x_{m,1}$	$x_{m,2}$	$\varepsilon_m := \|x_m - x^*\|_A$	$\varepsilon_m/\varepsilon_{m-1}$
0	4.000000e+00	1.341641e+00	7.071068e+00	
1	2.987552e+00	-3.562863e-01	4.372680e+00	6.183904e-01
2	1.529627e+00	5.130523e-01	2.704023e+00	6.183904e-01
3	1.142460e+00	-1.362463e-01	1.672142e+00	6.183904e-01
4	5.849394e-01	1.961946e-01	1.034036e+00	6.183904e-01
5	4.368842e-01	-5.210148e-02	6.394382e-01	6.183904e-01
6	2.236847e-01	7.502613e-02	3.954224e-01	6.183904e-01
7	1.670674e-01	-1.992395e-02	2.445254e-01	6.183904e-01
8	8.553851e-02	2.869049e-02	1.512122e-01	6.183904e-01
9	6.388768e-02	-7.619051e-03	9.350814e-02	6.183904e-01
10	3.271049e-02	1.097143e-02	5.782453e-02	6.183904e-01
20	2.674941e-04	8.972025e-05	4.728673e-04	6.183904e-01
30	2.187466e-06	7.336985e-07	3.866930e-06	6.183904e-01
40	1.788827e-08	5.999910e-09	3.162230e-08	6.183904e-01
50	1.462836e-10	4.906500e-11	2.585953e-10	6.183904e-01
60	1.196252e-12	4.012351e-13	2.114695e-12	6.183904e-01
70	9.782499e-15	3.281150e-15	1.729318e-14	6.183904e-01
71	7.306431e-15	-8.713427e-16	1.069393e-14	6.183904e-01
72	3.740893e-15	1.254734e-15	6.613026e-15	6.183904e-01

Method of steepest descent



Contour lines (level curves) of $F(x) = \frac{1}{2}(Ax, x) - (b, x)$ w.r.t. the example

$$A = \begin{pmatrix} 2 & 0 \\ 0 & 10 \end{pmatrix}, \quad b = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

are determined by $F(x) = \frac{1}{2}(Ax, x) - (b, x) = x_1^2 + 5x_2^2$.

Method of steepest descent

Problem:

Forgetfulness

- During the calculation of the new search direction p_m we do not take into account any old search direction $p_0, \dots, p_{m-1}$.

Aim:

- Choose linear independent $p_0, p_1, \dots \in \mathbb{R}^n$
- Search into the direction p_m and find the

  optimal approximation $x_{m+1} \in \mathbb{R}^n$ w.r.t. $x_0 + \text{span}\{p_0, \dots, p_m\}$

Effect:

- At least for $m = n$ we obtain $x_m = A^{-1}b$

Method of steepest descent

Optimality:

Let $F : \mathbb{R}^n \longrightarrow \mathbb{R}$. A vector $x \in \mathbb{R}^n$ is called

1. optimal w.r.t. $p \in \mathbb{R}^n \setminus \{0\}$, if
$$F(x) \leq F(x + \lambda p) \quad \forall \lambda \in \mathbb{R}.$$
2. optimal w.r.t. $U \subset \mathbb{R}^n$, if
$$F(x) \leq F(x + \xi) \quad \forall \xi \in U.$$

Method of steepest descent

How to investigate the opitimalty of $x \in \mathbb{R}^n$ w.r.t. $U \subset \mathbb{R}^n$?

Consider

$$f_{x,\xi}(\lambda) = F(x + \lambda\xi)$$

$$f'_{x,\xi}(\lambda) = (Ax - b, \xi) + \lambda(A\xi, \xi)$$

x is optimal w.r.t. $U \ni \xi \neq 0$

$$\iff f'_{x,\xi}(0) = 0$$

$$\iff (Ax - b, \xi) = 0$$

$$\iff \boxed{r \perp U}$$

Method of steepest descent

How to maintain optimality ?

Let $x_m \in x_0 + \underbrace{\text{span}\{p_0, \dots, p_{m-1}\}}_{U_m :=}$.

If x_m is optimal w.r.t. U_m and

$$x_{m+1} = x_m + \lambda_m p_m \quad , \quad \xi \in U_m$$

$$\Longrightarrow \quad (b - Ax_{m+1}, \xi) = \underbrace{(b - Ax_m, \xi)}_{=0} - \lambda_m (Ap_m, \xi)$$

Condition:

$$\boxed{(Ap_m, p_i) = 0 \quad \text{für } i = 0, \dots, m-1}$$

Method of steepest descent

Conjugate vectors

The vectors $p_0, \ldots, p_m \in \mathbb{R}^n \setminus \{0\}$ are called

pairwise conjugated or A-orthogonal,

if

$$(Ap_j, p_i) = 0 \text{ for all } i \neq j.$$

How to obtain optimality w.r.t. U_{m+1}?

Optimality w.r.t. U_m:

$$(Ap_m, p_i) = 0, \quad i = 0, \dots, m-1$$

Optimality w.r.t. p_m: $\quad (U_{m+1} = \{U_m, p_m\} := \text{span}\{p_0, \dots, p_{m-1}, p_m\})$

$$0 = (b - Ax_{m+1}, p_m) = (b - Ax_m, p_m) - \lambda_m (Ap_m, p_m)$$

$$\Longrightarrow \qquad \lambda_m = \frac{(b - Ax_m, p_m)}{(Ap_m, p_m)}$$

Method of steepest descent

Eastern and Christmas simultaneously?

or in other words

Are pairwise conjugated vectors always linear independent?

Proof by contradiction: Assume:
$p_0, \ldots, p_m \in \mathbb{R}^n \backslash \{0\}$ pairw. conjugated, $p_m \in \text{span}\{p_0, \ldots, p_{m-1}\}$

$$\Longrightarrow p_m = \sum_{j=0}^{m-1} \alpha_j p_j$$

$$\Longrightarrow 0 = (Ap_m, p_i) = \left(A \sum_{j=0}^{m-1} \alpha_j p_j, p_i \right) = \sum_{j=0}^{m-1} \alpha_j (Ap_j, p_i) = \alpha_i \underbrace{(Ap_i, p_i)}_{\neq 0}$$

holds for i=0,...,m-1 $\Longrightarrow p_m = 0$ Contradiction!!!

Answer: Yes, in the case that the matrix A is positive definite!

Method of conjugate directions

Summary:

- Choose pairwise conjugated search directions $p_0, \ldots, p_{n-1}$
- Calculate

$$\lambda_m = \frac{(b - Ax_m, p_m)}{(Ap_m, p_m)} \quad , m = 0, \ldots, n-1$$

$\Longrightarrow$ Hence, one obtains at least $x_n = A^{-1}b$.

Method of conjugate directions

Algorithm (Method of conjugate directions)

- Choose $x_0 \in \mathbb{R}^n$ and $p_0, \ldots, p_{n-1}$ pairwise conjugated
- $r_0 = b - Ax_0$
- For $m = 0, \ldots, n-1$

$$\begin{aligned}
\lambda_m &= \frac{(r_m, p_m)}{(Ap_m, p_m)} \\
x_{m+1} &= x_m + \lambda_m p_m \\
r_{m+1} &= r_m - \lambda_m A p_m
\end{aligned}$$

Problems

- Calculation of $p_0, \ldots, p_{n-1}$
- error reduction (convergence history)

Method of conjugate gradients (CG)

Method of steepest descent

Basis	: Gradients as search directions
Advantage	: Associated w.t. problem
Disadvant.	: Forgetfulness

Method of conjugate directions

Basis	: Search directions are conjugated
Advantage	: Optimality
Disadvant.	: Convergence history

Method of conjugate gradients

Basis	: Use gradients for the calculation of conjugated search directions
Advantage	: Associated with the problem Optimality

Method of conjugate gradients (CG)

Ansatz:

$$p_0 = r_0$$

$$p_m = r_m + \sum_{j=0}^{m-1} \alpha_j p_j \quad , \qquad m = 1, \ldots, n-1$$

- m degrees of freedom
- Calculation of $\alpha_0, \ldots, \alpha_{m-1}$

$$0 = (Ap_m, p_i) = (Ar_m, p_i) + \sum_{j=0}^{m-1} \alpha_j \underbrace{(Ap_j, p_i)}_{=0 \quad i \neq j}$$

$$\alpha_i = -\frac{(Ar_m, p_i)}{(Ap_i, p_i)} \quad , \; i = 0, \ldots, m-1$$

Method of conjugate gradients (CG)

Algorithm

- Choose $x_0 \in \mathbb{R}^n$ and define $p_0 = r_0 = b - Ax_0$
- For $m = 0, \ldots, n-1$

$$
\begin{aligned}
\lambda_m &= \frac{(r_m, p_m)}{(Ap_m, p_m)} \\
x_{m+1} &= x_m + \lambda_m p_m \\
r_{m+1} &= r_m - \lambda_m A p_m \\
p_{m+1} &= r_{m+1} - \sum_{j=0}^{m} \frac{(Ar_{m+1}, p_j)}{(Ap_j, p_j)} p_j
\end{aligned}
$$

Disadvantages

- Break down for $p_m = 0$
- Inapplicable in the case of large, sparse matrices
- Computational effort increasing from iteration step to iteration step

Properties and consequences

1. $U_m := \text{span}\{p_0, \ldots, p_{m-1}\} = \text{span}\{r_0, Ar_0, \ldots, A^{m-1} r_0\}$

   - $x_m = x_{m-1} + \lambda_{m-1} p_{m-1} = \ldots = x_0 + \sum_{j=0}^{m-1} \lambda_j p_j$

   $\Longrightarrow \quad x_m \in x_0 + U_m \; = \; x_0 + K_m$

2. $r_m \perp U_m$

   - $r_m = b - Ax_m \perp U_m = K_m$

   $\Longrightarrow$ Orthogonal Krylov subspace method

Method of conjugate gradients (CG)

Properties and consequences

1. $x_m = A^{-1}b \Longleftrightarrow r_m = 0 \Longleftrightarrow p_m = 0$
   - $p_m = 0 \;\equiv$ Stopping criterion
2. $(Ar_{m+1}, p_j) = 0 \quad , j = 0, \ldots, m-1$
   - $$p_{m+1} = r_{m+1} - \sum_{j=0}^{m} \frac{(Ar_{m+1}, p_j)}{(Ap_j, p_j)} p_j = r_{m+1} - \frac{(Ar_{m+1}, p_m)}{(Ap_m, p_m)} p_m$$
   - Applicable for large sparse systems
   - Low computational effort

Method of conjugate gradients (CG)

Algorithm

- Choose $x_0 \in \mathbb{R}^n$ and define $p_0 = r_0 = b - Ax_0$
- For $m = 0, \ldots, n-1$

If $p_m \neq 0$ then

$$\begin{aligned}
\lambda_m &= \frac{(r_m, p_m)}{(Ap_m, p_m)} \\
x_{m+1} &= x_m + \lambda_m p_m \\
r_{m+1} &= r_m - \lambda_m A p_m \\
p_{m+1} &= r_{m+1} - \frac{(Ar_{m+1}, p_m)}{(Ap_m, p_m)} p_m
\end{aligned}$$

else STOP

Method of conjugate gradients (CG)

Example: 1-D Poisson-Equation $x'' = b$

$D = [0,1] \quad , \quad h = 1/8 \quad , \quad N = 7$

$\mathbb{R}^{7\times 7} \ni A = \text{tridiag}\{-64, 128, -64\}$

$\mathbb{R}^{7} \ni b = (128, -448, 704, -832, 512, 128, 320)^T, \quad x_0 = 0$

Method of conjugate gradients (CG)								
m	$x_{m,1}$	$x_{m,2}$	$x_{m,3}$	$x_{m,4}$	$x_{m,5}$	$x_{m,6}$	$x_{m,7}$	$\|\vec{r}_m\|_2$
0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1336.36
1	0.58	-2.04	3.21	-3.79	2.33	0.58	1.46	363.57
2	-0.39	-1.72	2.81	-4.57	3.00	4.99	4.26	252.76
3	-0.01	-2.38	2.06	-3.53	4.87	6.07	6.25	153.30
4	-0.14	-2.88	2.57	-2.13	6.50	7.48	5.93	117.64
5	-0.70	-2.18	3.53	-1.12	7.65	7.81	6.27	103.52
6	0.13	-1.14	5.40	0.54	8.23	8.54	6.98	89.70
7	1.00	0.00	6.00	1.00	9.00	9.00	7.00	0.00

Convection-Diffusion Equation

Governing Equation

$$\beta \cdot \nabla u(x,y) - \epsilon\, \Delta u(x,y) = 0 \ \text{ on } \ D = (0,1) \times (0,1)$$

with

$$\beta = \alpha \begin{pmatrix} \cos\frac{\pi}{4} \\ \sin\frac{\pi}{4} \end{pmatrix} \quad \alpha, \epsilon \in \mathbb{R}_0^+$$

Boundary Conditions

$$u(x,y) = x^2 + y^2 \ \text{ for } \ (x,y) \in \partial D$$

Mesh

$$x_i = i \cdot h \ \text{ and } \ y_j = j \cdot h \ \text{ for } \ j = 0, \ldots, N+1, \quad h = \frac{1}{N+1}$$

Convection-Diffusion Equation

Discretization of Laplacian (Central Difference)

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_j) \approx \frac{1}{h^2}(u_{i+1,j} - 2u_{ij} + u_{i-1,j})$$
$$\frac{\partial^2 u}{\partial y^2}(x_i, y_j) \approx \frac{1}{h^2}(u_{i,j+1} - 2u_{ij} + u_{i,j-1})$$

Discretization of convective part (Backward Difference)

$$\frac{\partial u}{\partial x}(x_i, y_j) \approx \frac{1}{h}(u_{i,j} - u_{i-1,j})$$
$$\frac{\partial u}{\partial y}(x_i, y_j) \approx \frac{1}{h}(u_{i,j} - u_{i,j-1})$$

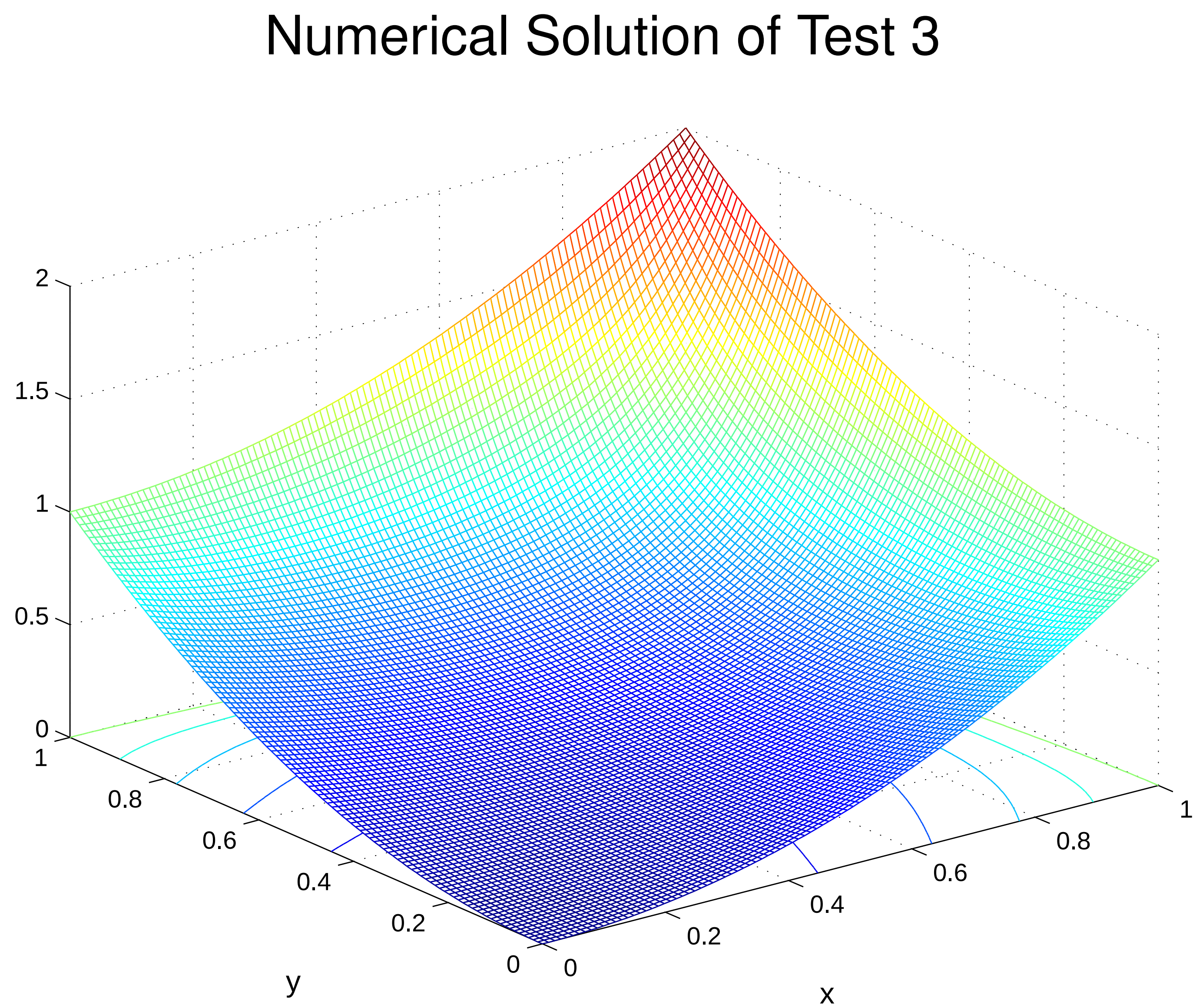
Convection-Diffusion Equation

Testcases

	α	ϵ	Matrix properties
Test 1	0	1	Symmetric, positive definite
Test 2	0.1	1	Non-symmetric, non-singular
Test 3	1	0.1	Non-symmetric, non-singular

- Number of unknowns: $100 \times 100 = 10000 \quad (N = 100)$
- Stopping criterion: $\|r_j\|_2 < 10^{-12}\|b\|$

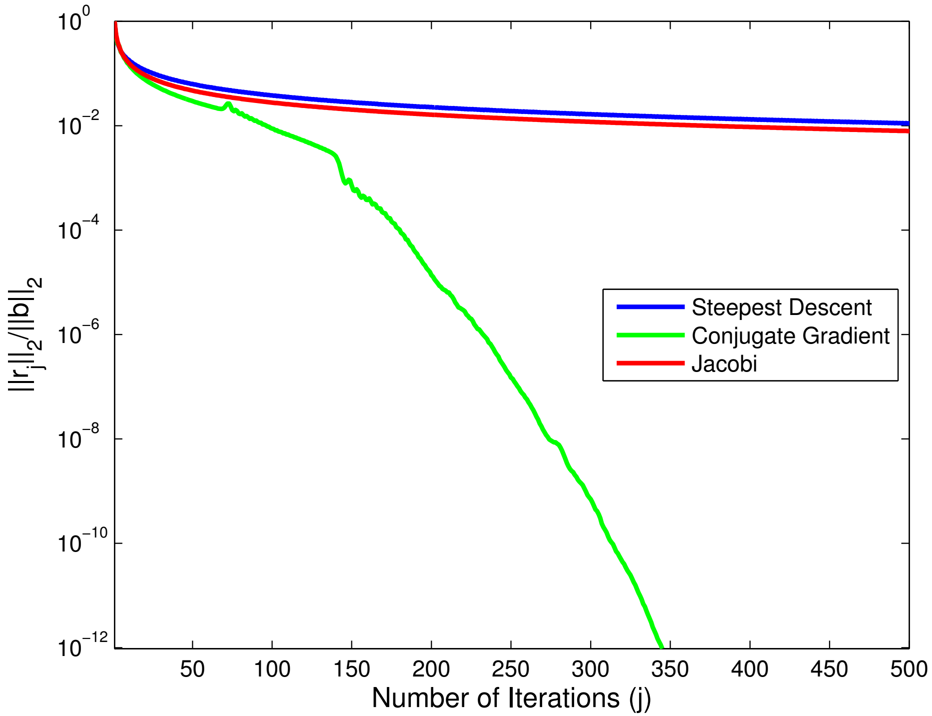
Convection-Diffusion Equation



Steepest Descent vs. Conjugate Gradient method

Test 1: Pure Diffusion ($\alpha = 0$, $\epsilon = 1$)

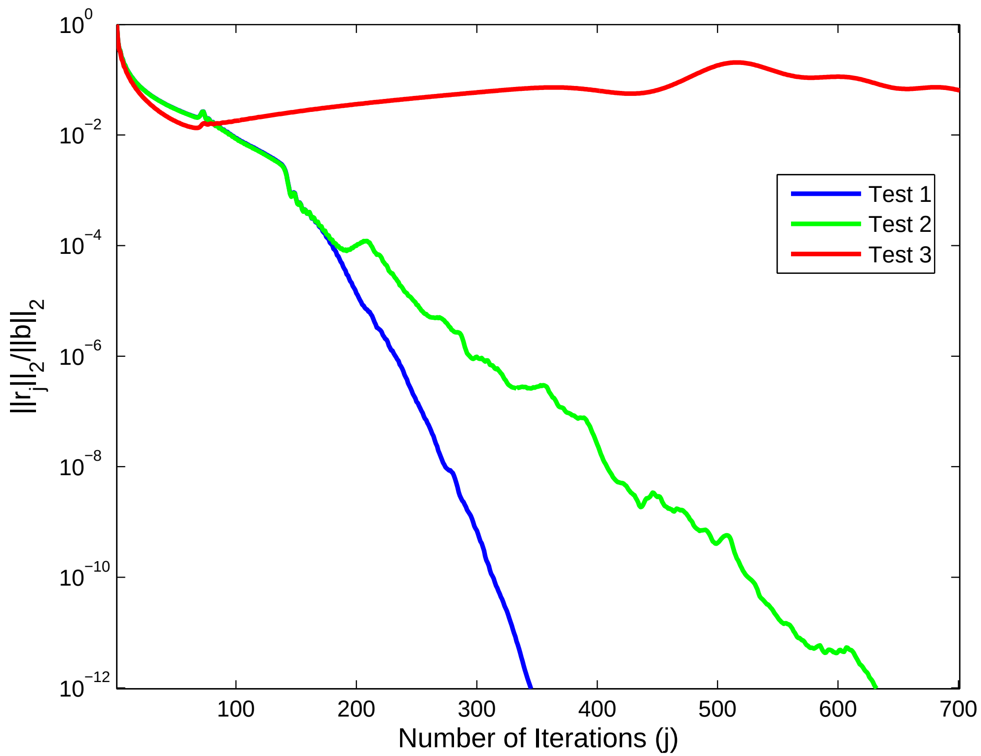
	Number of Iterations	CPU Time (%)
Conjugate Gradient	344	100
Steepest Descent	47258	12222
Jacobi Method	46582	14806



Conjugate Gradients for Non-SPD Systems

Comparison of CG method for all three test case

	α	ϵ	Number of Iterations
Test 1	0	1	344
Test 2	0.1	1	631
Test 3	1	0.1	Convergence failed



Convergence properties of the CG-method

Theorem

Let $A \in \mathbb{R}^{n \times n}$ be symmetric and positive definite. Then the error estimate

$$\|e_m\|_A \leq 2 \left(\frac{\sqrt{cond_2(A)} - 1}{\sqrt{cond_2(A)} + 1} \right)^m \|e_0\|_A,$$

holds with $e_m = x_m - A^{-1}b$, $\quad x_m =$ approximate solution.

Properties: (A symm., positive definite)

1. Eigenvalues: $\lambda_n \geq ... \geq \lambda_1 > 0$,
   Eigenvectors: $\{v_1, ..., v_n\}$ ONB of $\mathbb{R}^n$
2. Condition number: $c := cond_2(A) = ||A||_2 \, ||A^{-1}||_2 = \frac{\lambda_n}{\lambda_1}$
3. Weighted vector norm (energy norm):

$$||x||_A = \sqrt{(Ax, x)}$$