Iterative solvers for heterogeneous Helmholtz problems

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1. Introduction

The Helmholtz problem is defined as follows

$$-\Delta u - k^2 u = f, \quad \text{in} \quad \Omega,$$
$$\text{Boundary condition} \quad \text{on} \quad \Gamma = \partial\Omega,$$

where:

- $k = k(x, y, z)$ is the wavenumber
- for "solid" boundaries: Dirichlet/Neumann
- for "fictitious" boundaries: Sommerfeld $\frac{du}{dn} - \mathrm{i}ku = 0$

The resulting system

Efficient solution of a linear system,

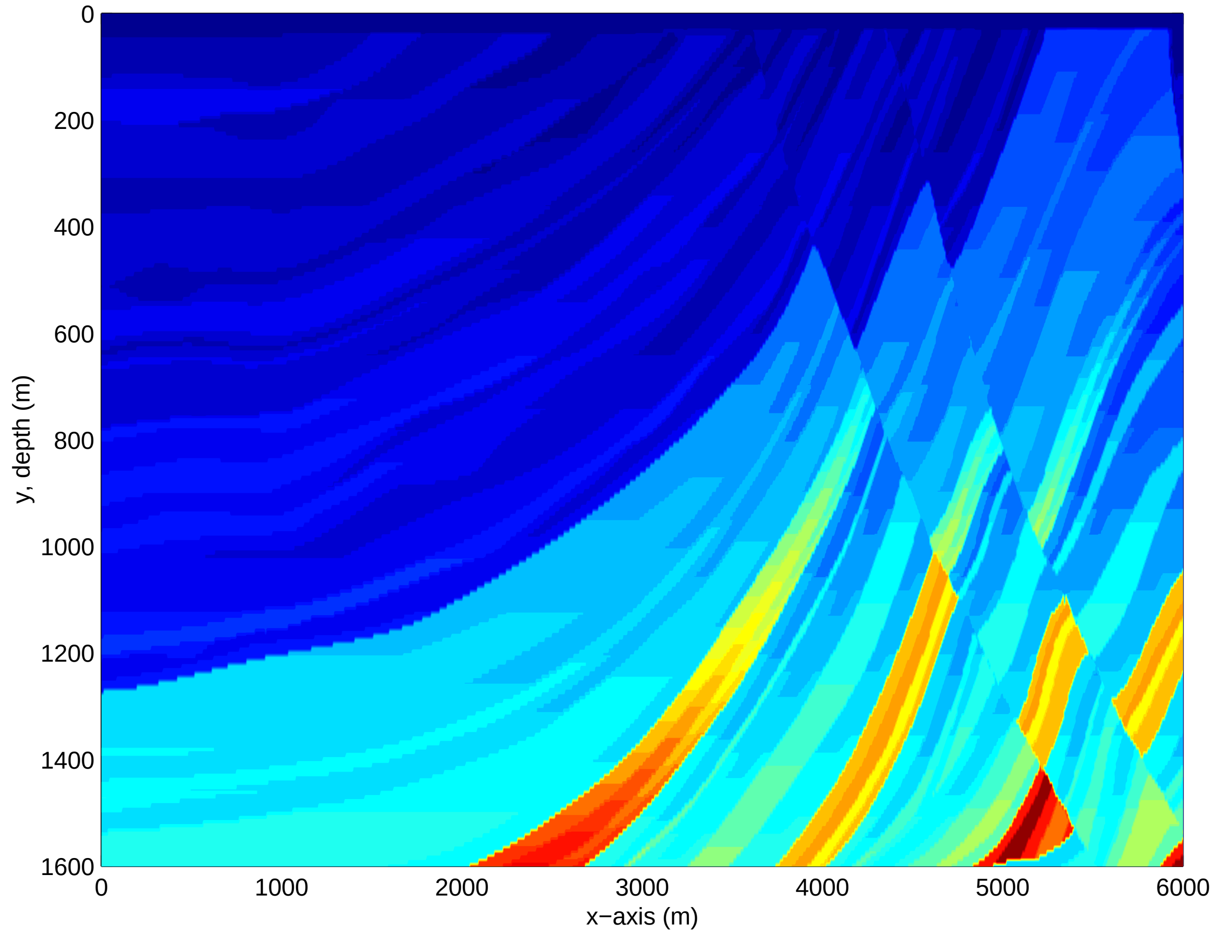
$$Ax = b.$$

Properties: large, sparse, 3 dimensional heterogeneous Helmholtz problems

Solution methods:

- direct solution methods (Gaussian elimination)
- multigrid
- Preconditioned Krylov methods

Application: geophysical survey, hard Marmousi Model



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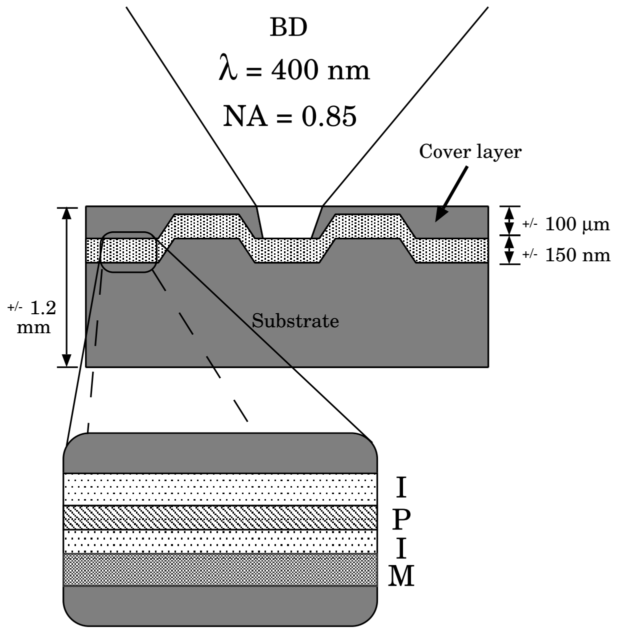
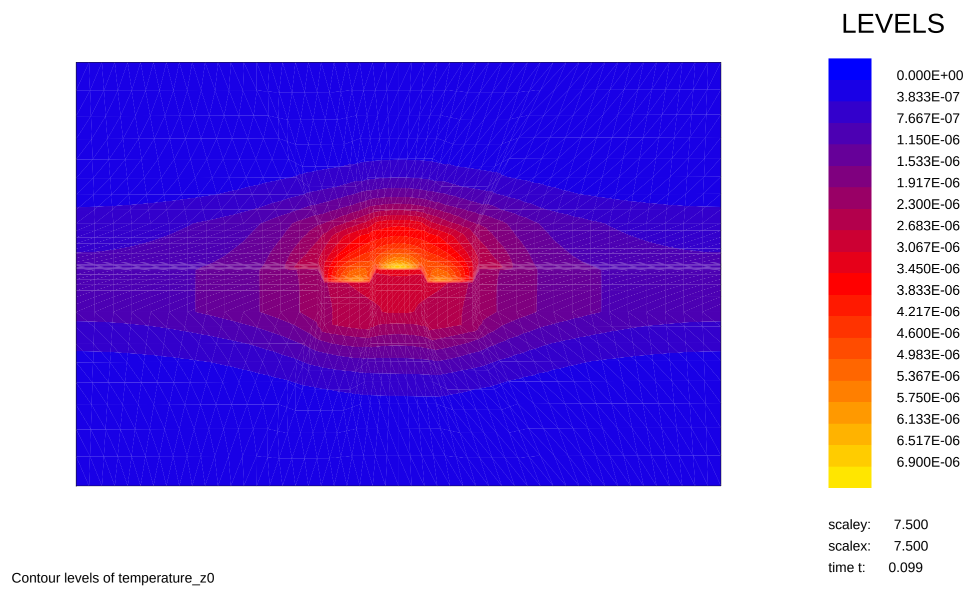
Application: optical storage

Model for Blu-Ray disk





2. Multigrid (standard geometric version)

- Smoothing method reduces high frequency components of an error between numerical approximation and exact discrete solution
- Coarse grid correction handles the low frequency error components.
- Components are easily defined for elliptic equations, like $-u_{xx} - u_{yy} = f$
- Problematic for the Helmholtz equation $-u_{xx} - u_{yy} - k^2 u = f$:
- Depending on k^2, gives rise to both smoothing and coarse grid correction difficulties.

Smoothing

- For $k^2 > \widetilde{\lambda}_h^{1,1}$, the smallest eigenvalue of the Laplace operator, the matrix has positive and negative eigenvalues.

$\Rightarrow$ Jacobi iteration with underrelaxation does not converge, but since its smoothing properties are satisfactory, the convergence will deteriorate gradually for k^2 increasing.

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- By the time k^2 approaches 150, standard multigrid diverges. The Jacobi relaxation now diverges for smooth eigenfrequencies with $\widetilde{\lambda}_h^{\ell,m} < k^2$.

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- The coarsest level limits the convergence: When k^2 gets larger more variables need to be represented on the coarsest level for standard multigrid convergence.

Coarse grid correction

- Discrete eigenvalues close to the origin on a fine grid may undergo a sign change after discretization on a coarser grid.

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- In Elman et al. (2001) multigrid is combined with Krylov subspace iteration methods. GMRES is proposed as a smoother and as a cure for the problematic coarse grid correction. This method is, however, not trivial to implement.
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- For the reasons mentioned above we develop a preconditioner that is not based on a regular splitting of the Helmholtz operator.

Conjugate Gradient Method

A is Symmetric Positive Definite (SPD)

- $A = A^T$,
- $x^T Ax > 0$, for $x \neq 0$.

The A-inner product is defined by $$(y, z)_A = y^T Az,$$

and the A-norm by $$\|y\|_A = \sqrt{(y, y)_A} = \sqrt{y^T Ay}.$$

Krylov subspace: $K^k(A; r_0) = span\{r_0, Ar_0, ..., A^{k-1}r_0\}$

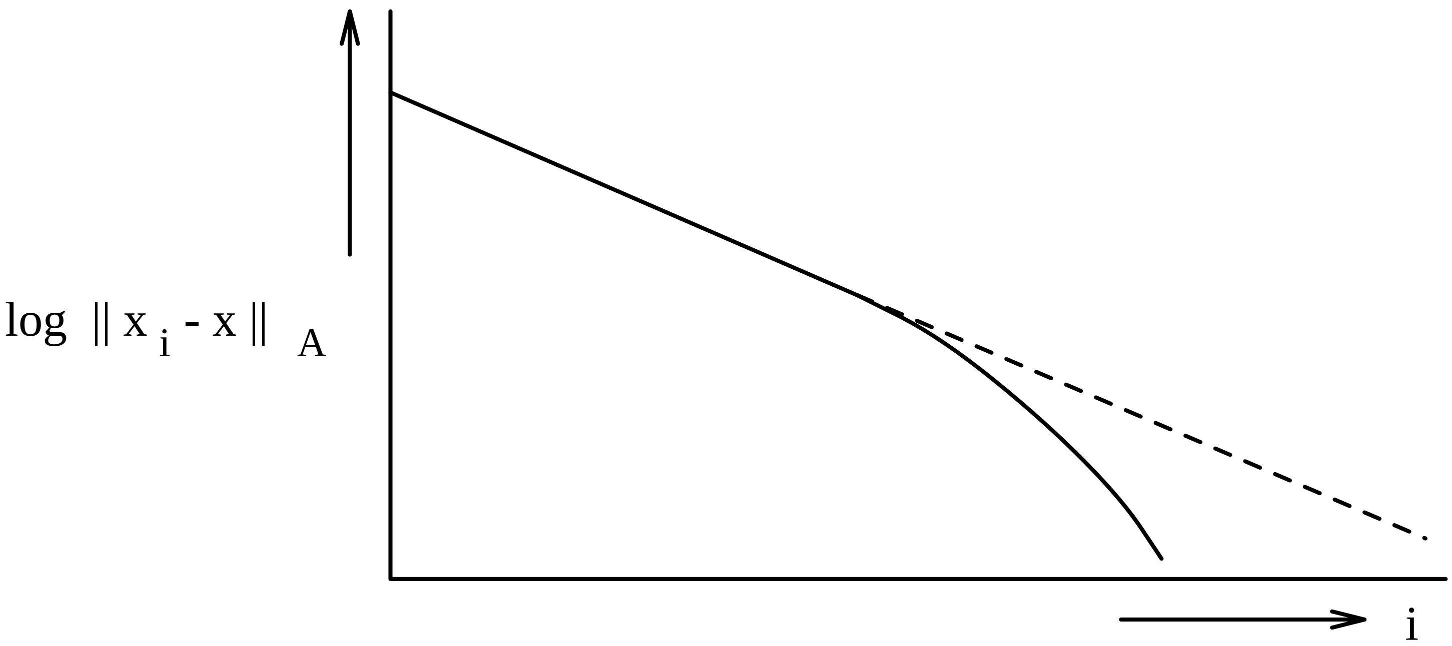
The Conjugate Gradient Method computes a solution such that

$$\|x - x_k\|_A = \min_{y \in K^k(A; r_0)} \|x - y\|_A$$

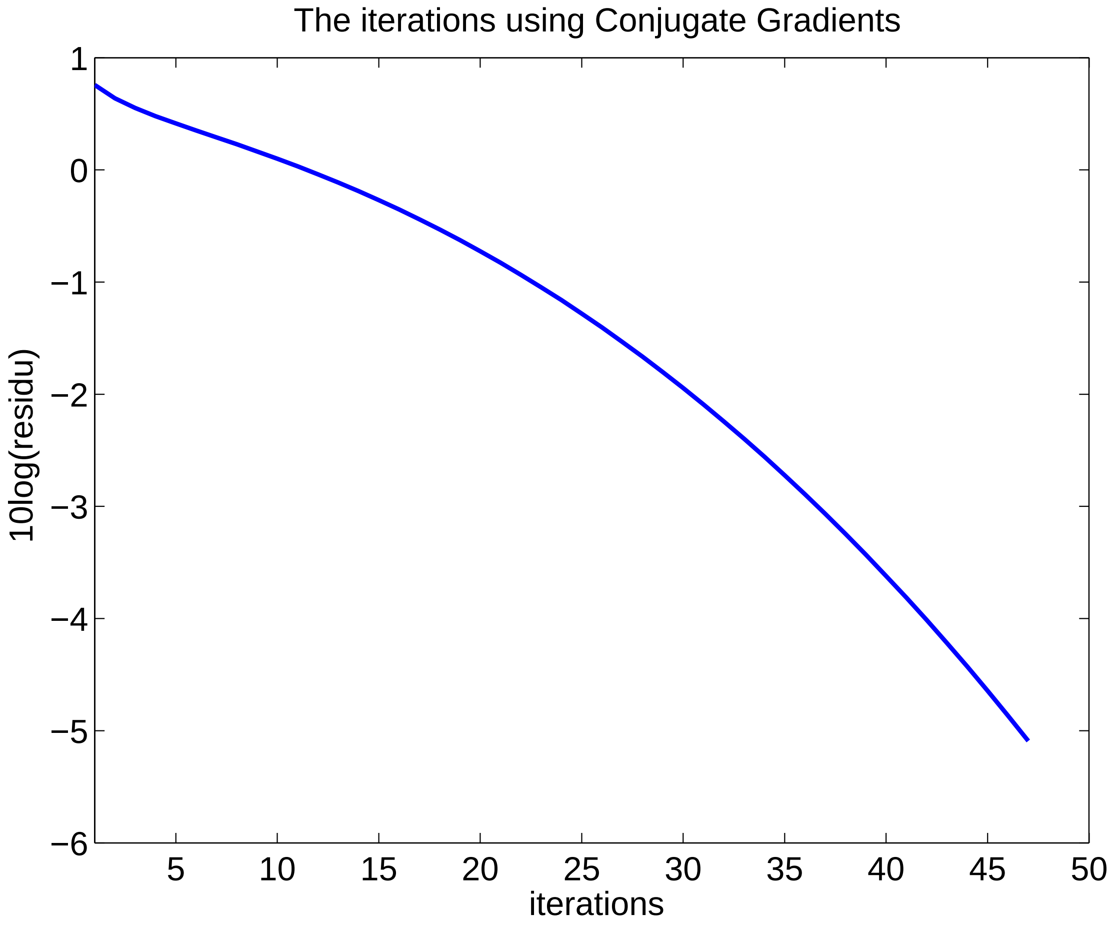
Conjugate Gradient Method Convergence

The x_k obtained from CG satisfy the following inequality:

$$\|x - x_k\|_A \leq 2 \left(\frac{\sqrt{K_2(A)} - 1}{\sqrt{K_2(A)} + 1} \right)^k \|x - x_0\|_A .$$



Superlinear Convergence Examples



eigenvalues $1, 2, ..., 100$

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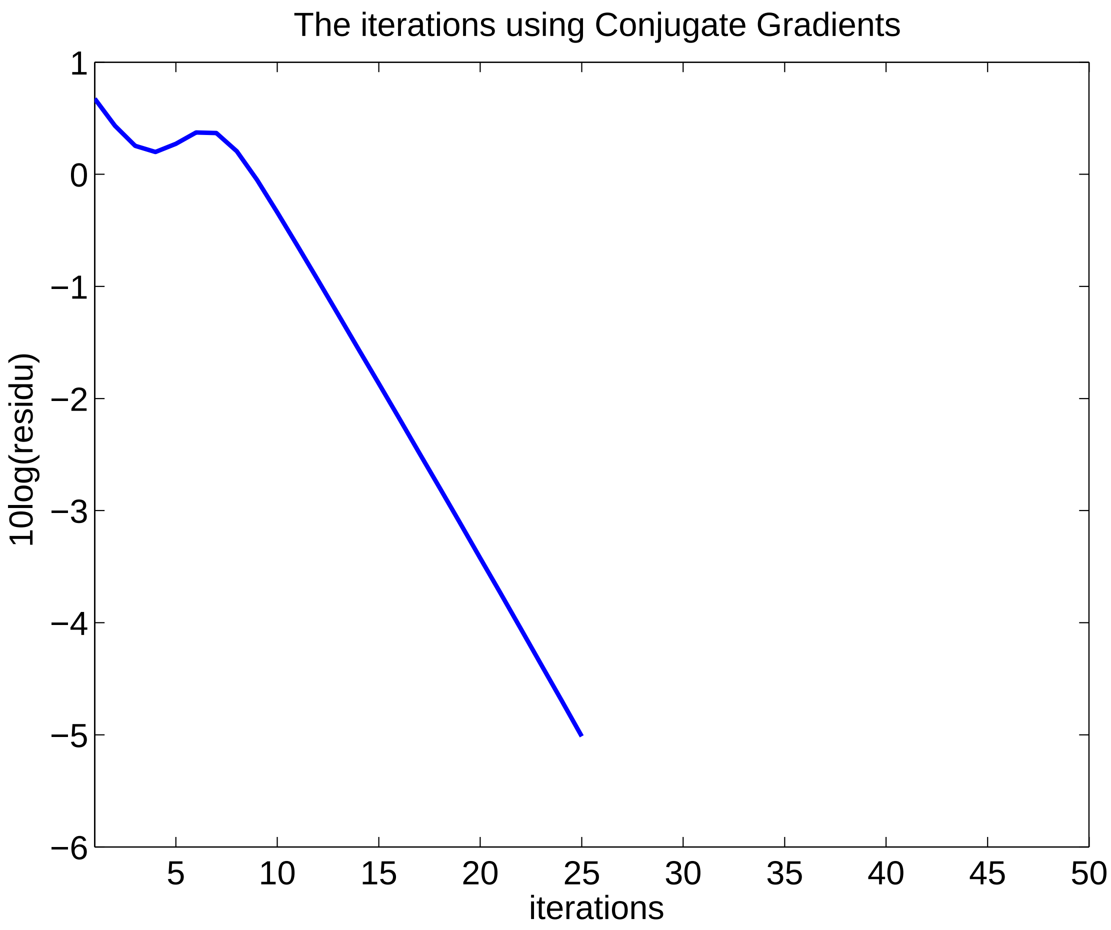
Superlinear Convergence Examples



eigenvalues $1, 10, ..., 100$

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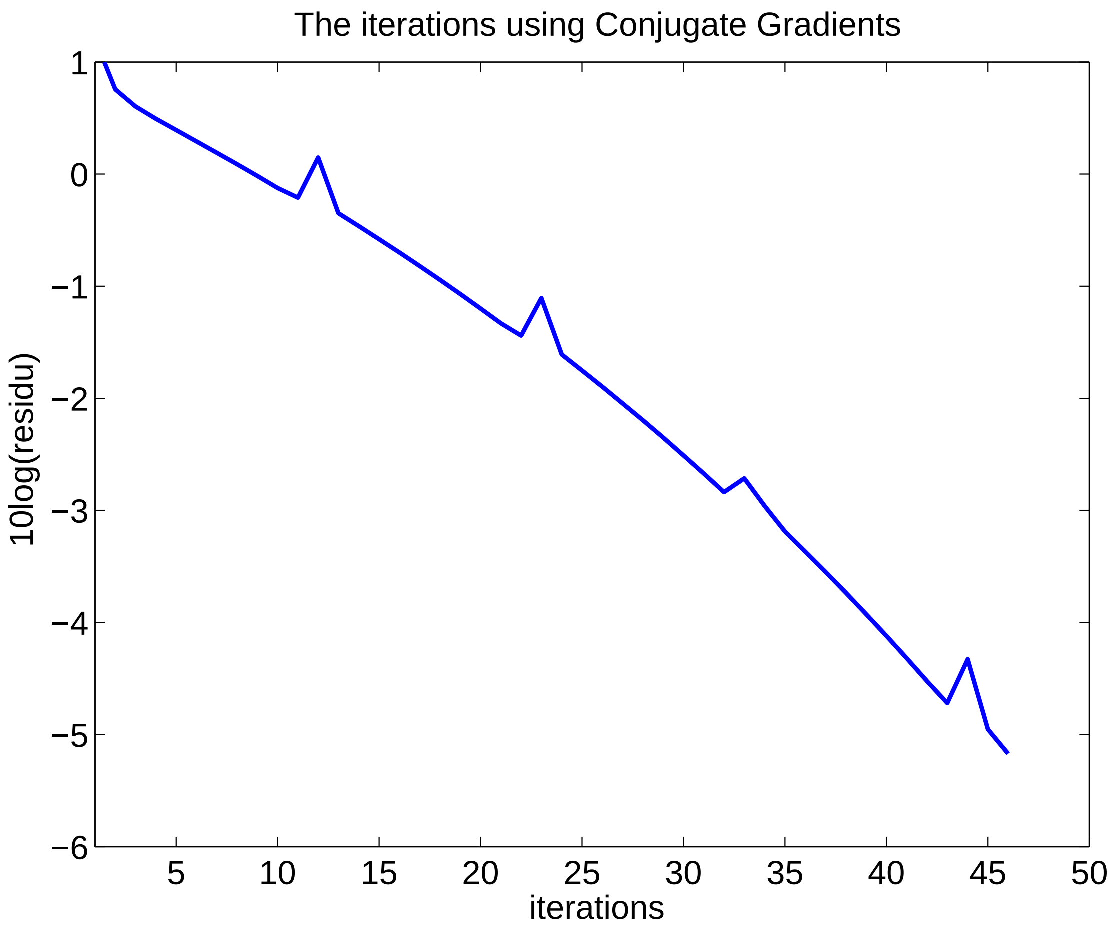


eigenvalues $1, ..., 10, 100$

Krylov methods for general matrices

Properties of the CG method:

- based on the Krylov subspace: $K^k(A; r_0)$
- the error is minimal in some norm (optimality)
- short recurrences

For general matrices, there is no method with all these properties!

CGNR
Apply CG to the normal equations: $A^T Ax = A^T b$

Drawbacks:

slow convergence, bad behavior with respect to rounding errors

BiCG methods

No optimality

BiCG

$r_0, ..., r_{k-1}$ is a basis for $K^k(A; r_0)$ and $s_0, ..., s_{k-1}$ is a basis for $K^k(A; s_0)$. The sequences $\{r_i\}$ and $\{s_i\}$ are bi-orthogonal.

Drawbacks:

breakdown possible, A^T is used, weak behavior with respect to rounding errors

BiCG methods (faster variants)

No optimality

CGS
Two times as fast, A^T is not used.

Bi-CGSTAB
More stable than CGS

Drawbacks:

breakdown possible, weak behavior with respect to rounding errors

GMRES type methods (GCR)

Long recurrences, several variants available.

Suppose that A is diagonalizable so that $A = XDX^{-1}$ and let

$$\varepsilon^{(k)} = \min_{\substack{p \in P_k \\ p(0)=1}} \max_{\lambda_i \in \sigma} |p(\lambda_i)|$$

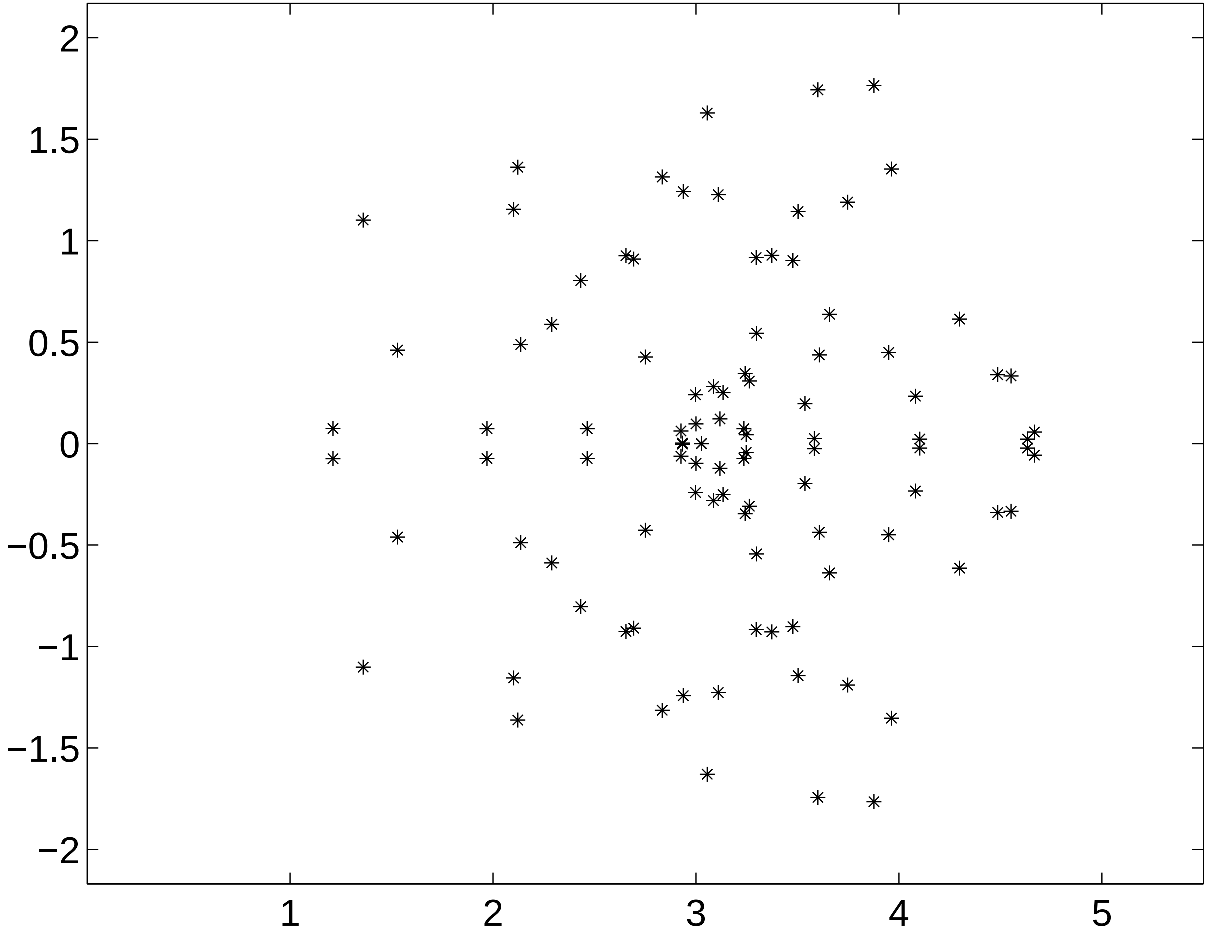
Then the residual norm of the k-th iterate satisfies:

$$\|r_k\|_2 \leq K(X)\varepsilon^{(k)}\|r_0\|_2$$

where $K(X) = \|X\|_2\|X^{-1}\|_2$. If furthermore all eigenvalues are enclosed in a circle centered at $C \in \mathbb{R}$ with $C > 0$ and having radius R with $C > R$, then

$$\varepsilon^{(k)} \leq \left(\frac{R}{C}\right)^k .$$

Illustration of the theorem



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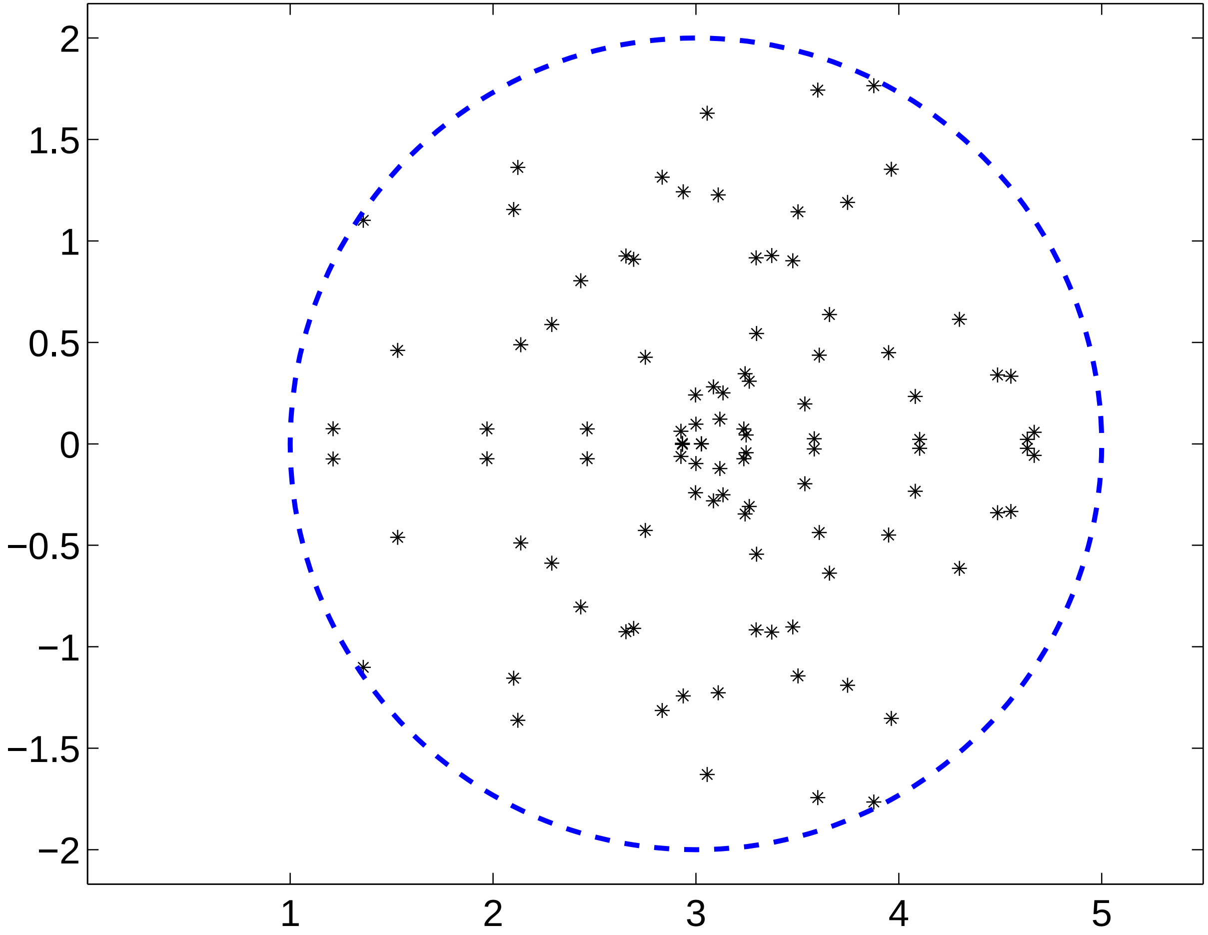

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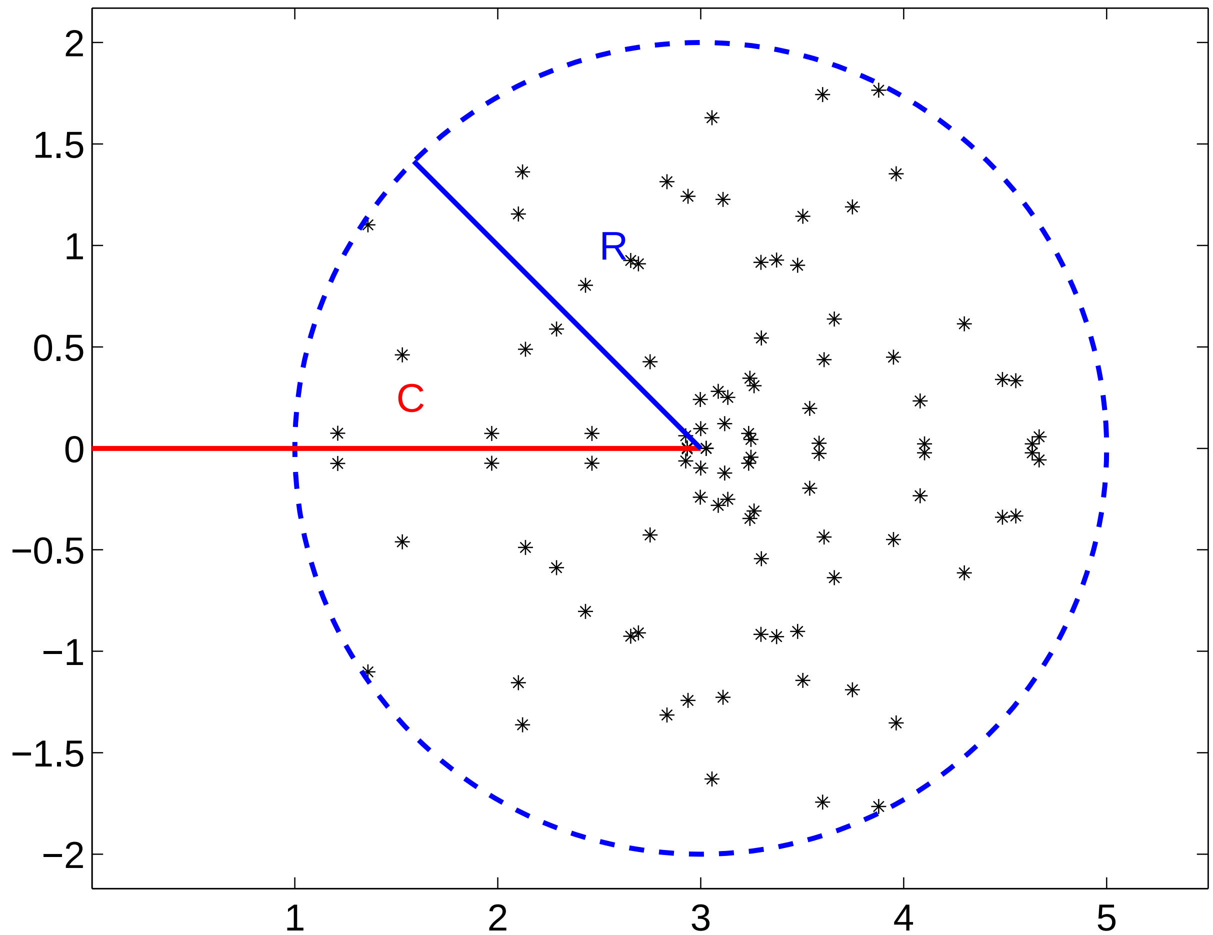


Convergence of GMRES

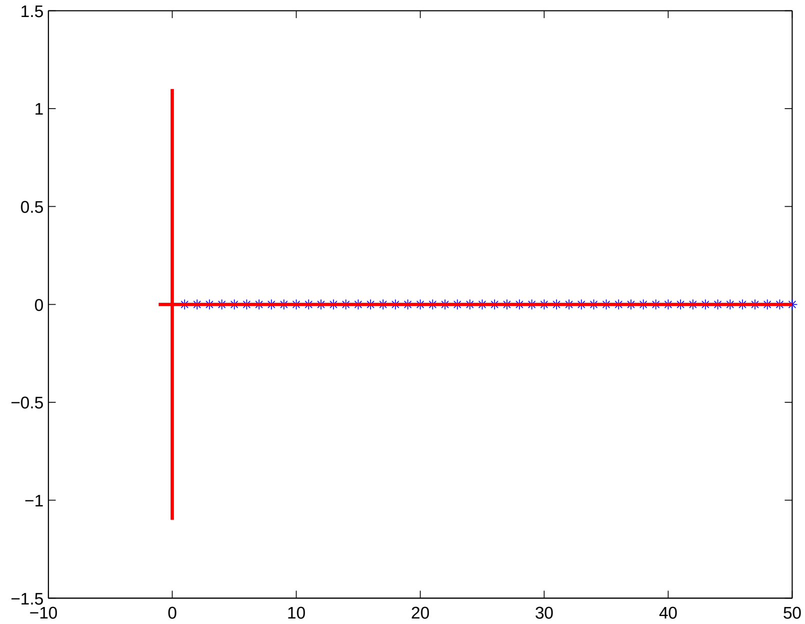
GMRES has also superlinear convergence.

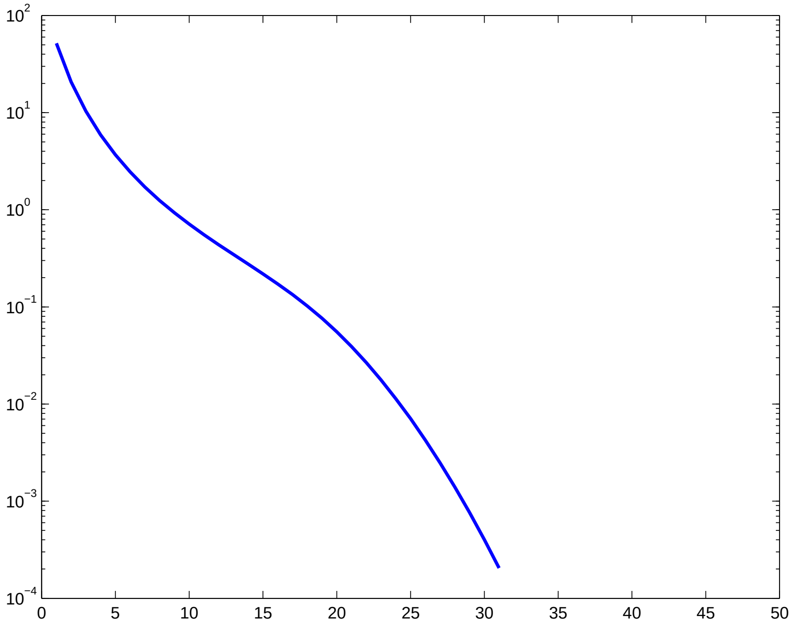
But eigenvalue information can be useless for nonnormal matrices.

- a set of eigenvalues
- a non-increasing sequence

Claim: there exists a matrix A and a right-hand-side vector b such that A has the specified eigenvalues and if GMRES is applied to the corresponding system the norm of the residuals are equal to the non-increasing sequence.

Convergence of GMRES for a real spectrum





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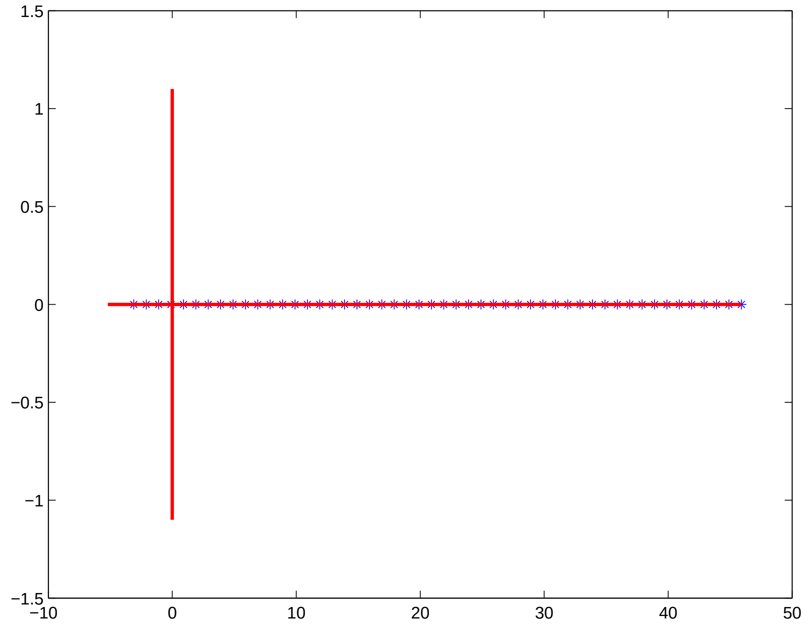

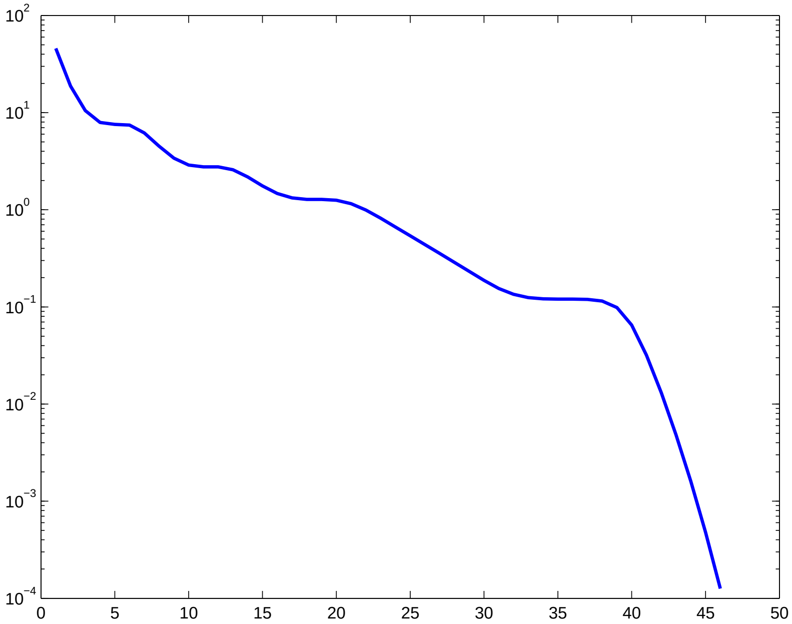

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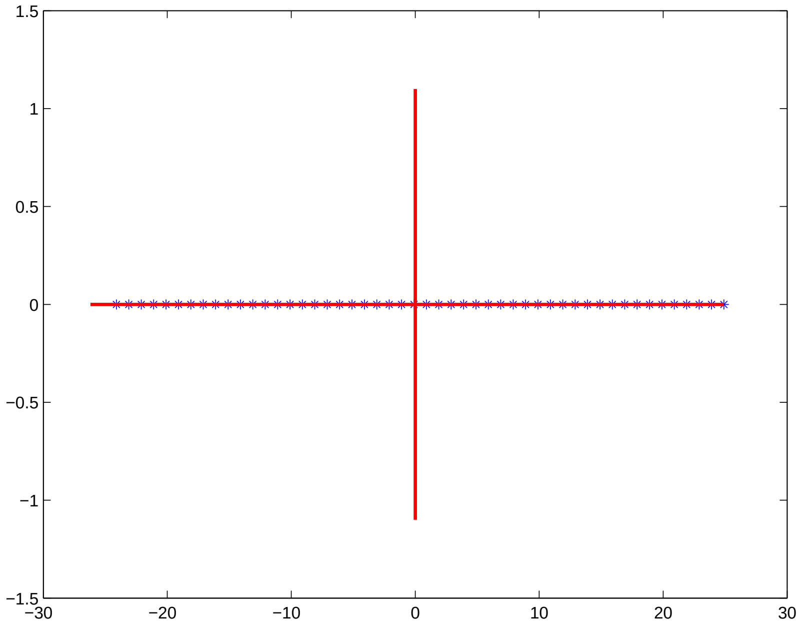
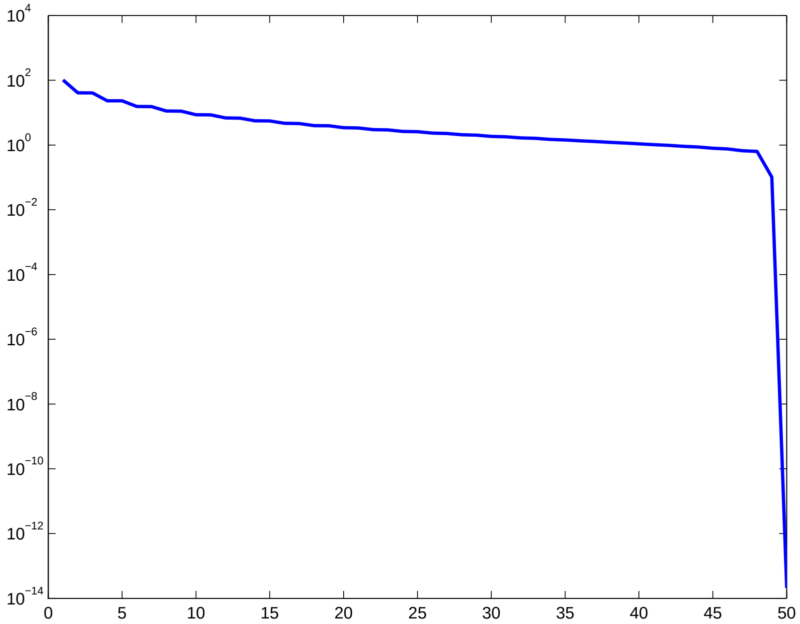
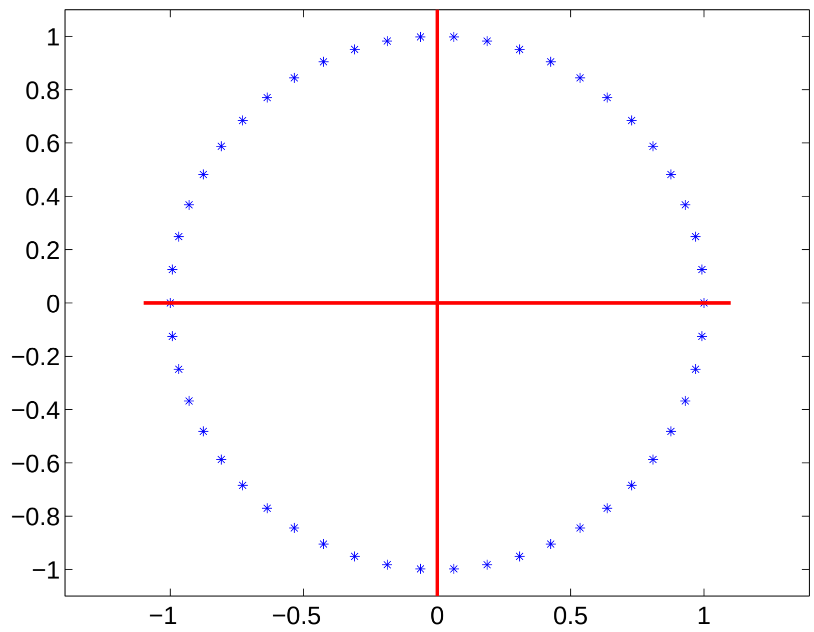
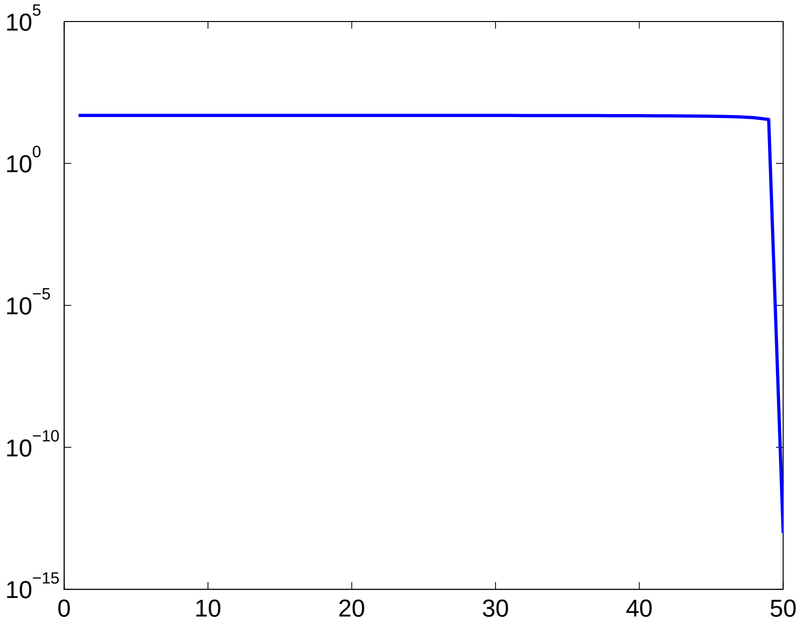




Convergence of GMRES for a complex spectrum





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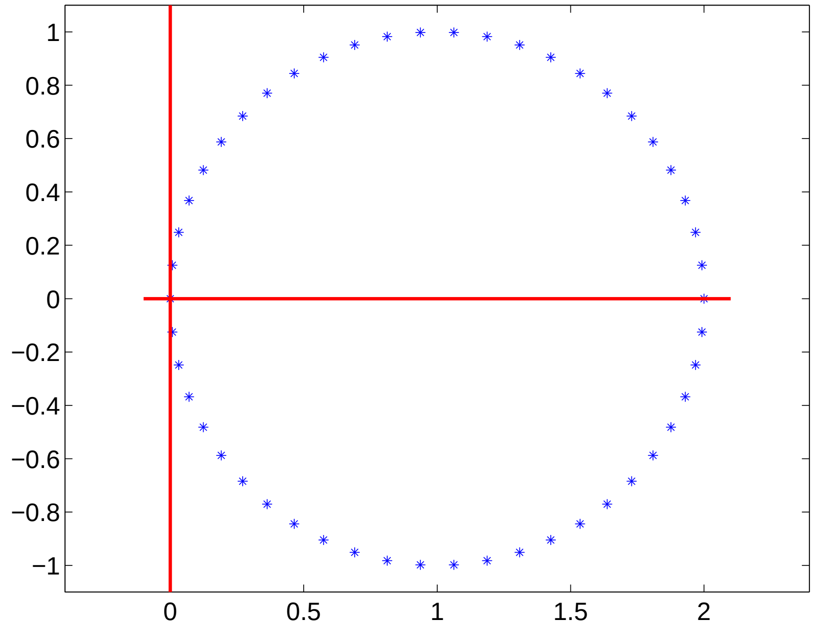

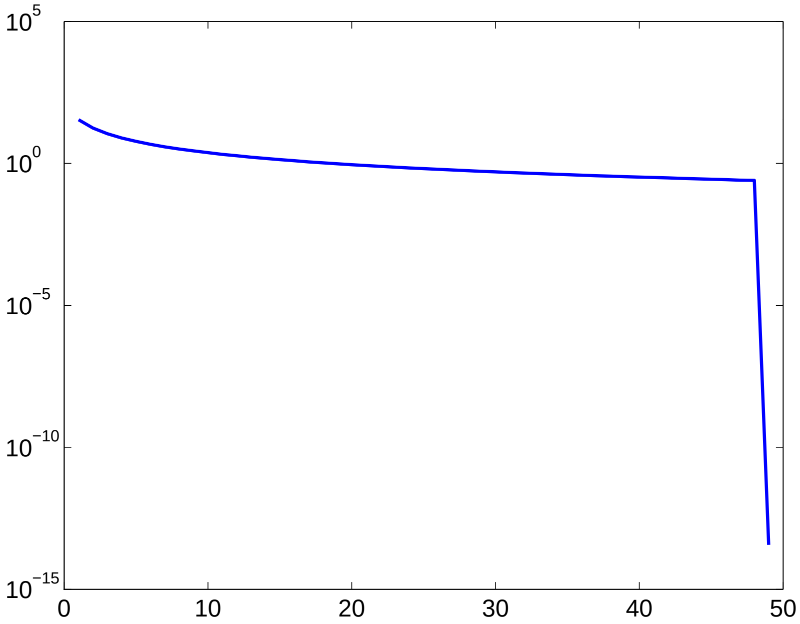

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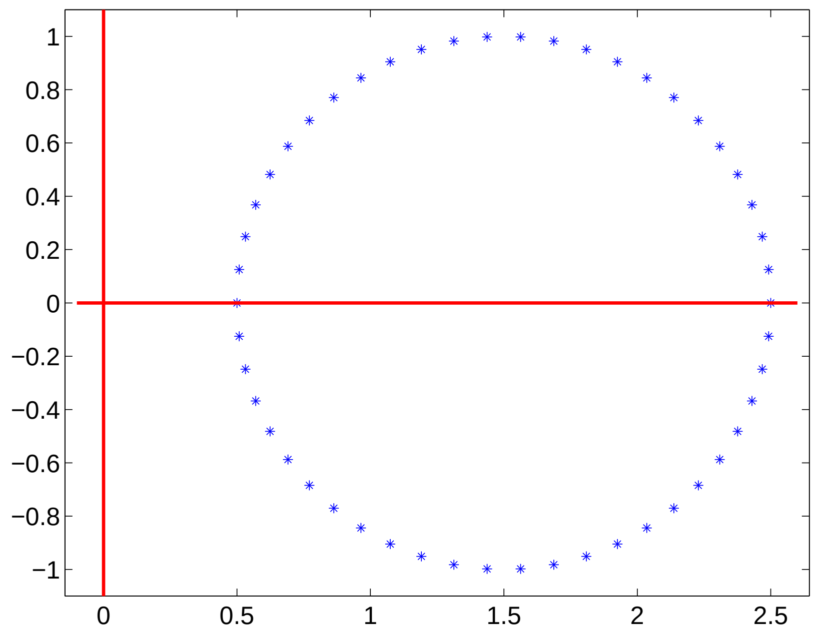

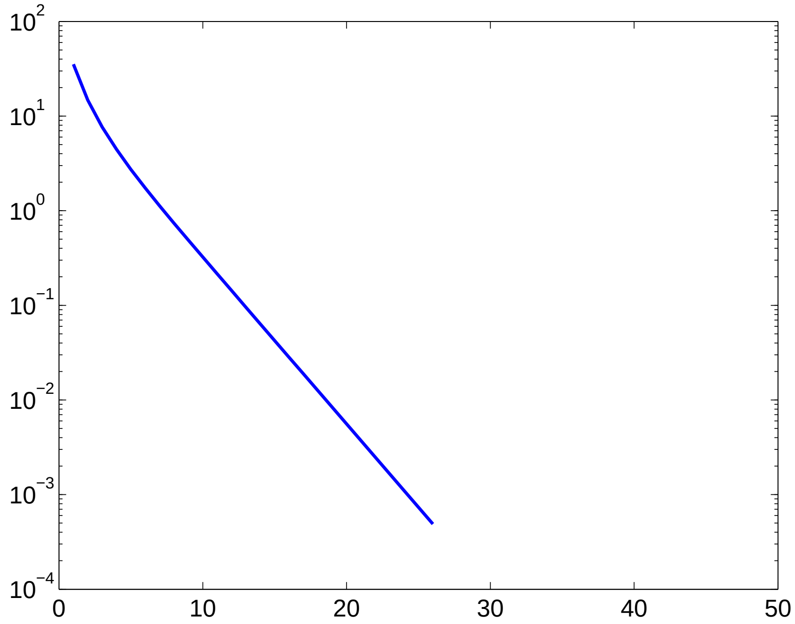

4. Conclusions

- Direct solution methods are not feasible for 3D problems
- The standard geometric Multigrid methods is not applicable
- The spectrum of the preconditioned matrix is important for the convergence of Krylov methods
- Negative and positive eigenvalues lead to slow convergence
- Eigenvalues clustered around 1 lead to fast convergence