

Scientific Computing WS 2019/2020

Lecture 11

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Recap

Regular splittings

- ▶ $A = M - N$ is a regular splitting if
 - ▶ M is nonsingular
 - ▶ M^{-1} , N are nonnegative, i.e. have nonnegative entries
- ▶ Regard the iteration $u_{k+1} = M^{-1}Nu_k + M^{-1}b$.
- ▶ $B = I - M^{-1}A = M^{-1}N$ is a nonnegative matrix.

Convergence theorem for regular splitting

Theorem: Assume A is nonsingular, $A^{-1} \geq 0$, and $A = M - N$ is a regular splitting. Then $\rho(M^{-1}N) < 1$.

Proof: Let $B = M^{-1}N$. Then $A = M(I - B)$, therefore $I - B$ is nonsingular.

In addition

$$A^{-1}N = (M(I - M^{-1}N))^{-1}N = (I - M^{-1}N)^{-1}M^{-1}N = (I - B)^{-1}B$$

By Perron-Frobenius (for general matrices), $\rho(B)$ is an eigenvalue with a nonnegative eigenvector \mathbf{x} . Thus,

$$0 \leq A^{-1}N\mathbf{x} = \frac{\rho(B)}{1 - \rho(B)}\mathbf{x}$$

Therefore $0 \leq \rho(B) \leq 1$.

Assume that $\rho(B) = 1$. Then there exists $\mathbf{x} \neq \mathbf{0}$ such that $B\mathbf{x} = \mathbf{x}$.

Consequently, $(I - B)\mathbf{x} = \mathbf{0}$, contradicting the nonsingularity of $I - B$.

Therefore, $\rho(B) < 1$. □

M-Matrix definition

Definition Let A be an $n \times n$ real matrix. A is called M-Matrix if

- (i) $a_{ij} \leq 0$ for $i \neq j$
- (ii) A is nonsingular
- (iii) $A^{-1} \geq 0$

Corollary: If A is an M-Matrix, then $A^{-1} > 0 \Leftrightarrow A$ is irreducible.

Proof: See Varga. □

Main practical M-Matrix criterion

Corollary: Let A be sdd or idd. Assume that $a_{ii} > 0$ and $a_{ij} \leq 0$ for $i \neq j$. Then A is an M-Matrix.

Proof: We know that A is nonsingular, but we have to show $A^{-1} \geq 0$.

- ▶ Let $B = I - D^{-1}A$. Then $\rho(B) < 1$, therefore $I - B$ is nonsingular.
- ▶ We have for $k > 0$:

$$\begin{aligned}I - B^{k+1} &= (I - B)(I + B + B^2 + \dots + B^k) \\(I - B)^{-1}(I - B^{k+1}) &= (I + B + B^2 + \dots + B^k)\end{aligned}$$

The left hand side for $k \rightarrow \infty$ converges to $(I - B)^{-1}$, therefore

$$(I - B)^{-1} = \sum_{k=0}^{\infty} B^k$$

As $B \geq 0$, we have $(I - B)^{-1} = A^{-1}D \geq 0$. As $D > 0$ we must have $A^{-1} \geq 0$. □

Incomplete LU factorizations (ILU)

Idea (Varga, Buleev, 1960):

- ▶ fix a predefined zero pattern
- ▶ apply the standard LU factorization method, but calculate only those elements, which do not correspond to the given zero pattern
- ▶ Result: incomplete LU factors L , U , remainder R :

$$A = LU - R$$

- ▶ Problem: with complete LU factorization procedure, for any nonsingular matrix, the method is stable, i.e. zero pivots never occur. Is this true for the incomplete LU Factorization as well ?

Intermediate Summary

- ▶ Given some matrix, we now have some nice recipes to establish nonsingularity and iterative method convergence:
- ▶ **Check if the matrix is irreducible.**
This is mostly the case for elliptic and parabolic PDEs.
- ▶ **Check if the matrix is strictly or irreducibly diagonally dominant.**
If yes, it is in addition nonsingular.
- ▶ **Check if main diagonal entries are positive and off-diagonal entries are nonpositive.**
If yes, in addition, the matrix is an M-Matrix, its inverse is nonnegative, and elementary iterative methods converge.
- ▶ These criteria do not depend on the symmetry of the matrix!

Example: 1D finite difference matrix:

$$A\mathbf{u} = \begin{pmatrix} \alpha + \frac{1}{h} & -\frac{1}{h} & & & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\ & & & & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\ & & & & & -\frac{1}{h} & \frac{1}{h} + \alpha \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \\ u_N \end{pmatrix} = \mathbf{f} = \begin{pmatrix} \alpha v_1 \\ hf_2 \\ hf_3 \\ \vdots \\ hf_{N-2} \\ hf_{N-1} \\ \alpha v_n \end{pmatrix}$$

- ▶ idd
- ▶ positive main diagonal entries, nonpositive off-diagonal entries

⇒ A is nonsingular, has the M-property, and we can e.g. apply the Jacobi and Gauss-Seidel iterative method to solve it (ok, in 1D we already know this is a bad idea ...).

⇒ for $f \geq 0$ and $v \geq 0$ it follows that $u \geq 0$.

≡ heating and positive environment temperatures cannot lead to negative temperatures in the interior.

Iterative solver complexity I

- ▶ Solve linear system iteratively until $\|e_k\| = \|(I - M^{-1}A)^k e_0\| \leq \epsilon$

$$\rho^k e_0 \leq \epsilon$$

$$k \ln \rho < \ln \epsilon - \ln e_0$$

$$k \geq k_\rho = \left\lceil \frac{\ln e_0 - \ln \epsilon}{\ln \rho} \right\rceil$$

- ▶ \Rightarrow we need at least k_ρ iteration steps to reach accuracy ϵ
- ▶ Optimal iterative solver complexity - assume:
 - ▶ $\rho < \rho_0 < 1$ independent of h resp. N
 - ▶ A sparse ($A \cdot u$ has complexity $O(N)$)
 - ▶ Solution of $Mv = r$ has complexity $O(N)$.

\Rightarrow Number of iteration steps k_ρ independent of N

\Rightarrow Overall complexity $O(N)$

Iterative solver complexity II

▶ Assume

▶ $\rho = 1 - h^\delta \Rightarrow \ln \rho \approx -h^\delta \rightarrow k_\rho = O(h^{-\delta})$

▶ d : space dimension $\Rightarrow h \approx N^{-\frac{1}{d}} \Rightarrow k_\rho = O(N^{\frac{\delta}{d}})$

▶ $O(N)$ complexity of one iteration step (e.g. Jacobi, Gauss-Seidel)

\Rightarrow Overall complexity $O(N^{1+\frac{\delta}{d}}) = O(N^{\frac{d+\delta}{d}})$

▶ Jacobi: $\delta = 2$

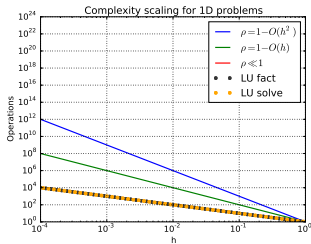
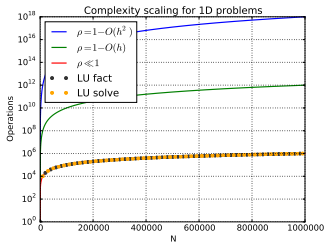
▶ Hypothetical “Improved iterative solver” with $\delta = 1$?

▶ Overview on complexity estimates

dim	$\rho = 1 - O(h^2)$	$\rho = 1 - O(h)$	LU fact.	LU solve
1	$O(N^3)$	$O(N^2)$	$O(N)$	$O(N)$
2	$O(N^2)$	$O(N^{\frac{3}{2}})$	$O(N^{\frac{3}{2}})$	$O(N \log N)$
3	$O(N^{\frac{5}{3}})$	$O(N^{\frac{4}{3}})$	$O(N^2)$	$O(N^{\frac{4}{3}})$

Solver complexity scaling for 1D problems

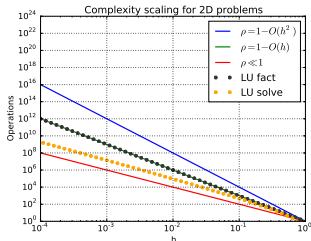
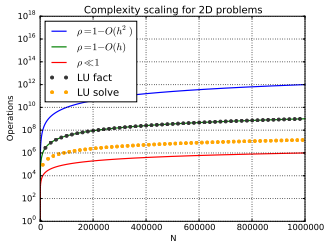
dim	$\rho = 1 - O(h^2)$	$\rho = 1 - O(h)$	LU fact.	LU solve
1	$O(N^3)$	$O(N^2)$	$O(N)$	$O(N)$



- Direct solvers significantly better than iterative ones

Solver complexity scaling for 2D problems

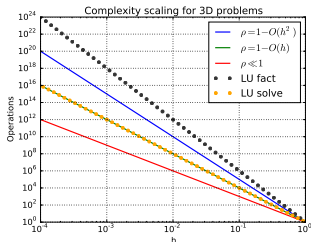
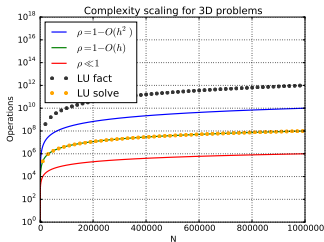
dim	$\rho = 1 - O(h^2)$	$\rho = 1 - O(h)$	LU fact.	LU solve
2	$O(N^2)$	$O(N^{\frac{3}{2}})$	$O(N^{\frac{3}{2}})$	$O(N \log N)$



- ▶ Direct solvers better than simple iterative solvers (Jacobi etc.)
- ▶ Direct solves on par with improved iterative solvers

Solver complexity scaling for 3D problems

dim	$\rho = 1 - O(h^2)$	$\rho = 1 - O(h)$	LU fact.	LU solve
3	$O(N^{\frac{5}{3}})$	$O(N^{\frac{4}{3}})$	$O(N^2)$	$O(N^{\frac{4}{3}})$



- ▶ LU factorization is expensive
- ▶ LU solve on par with improved iterative solvers

What could be done ?

- ▶ Find optimal iterative solver with $O(N)$ complexity
- ▶ Find “improved preconditioner” with $\kappa(M^{-1}A) = O(h^{-1}) \Rightarrow \delta = 1$
- ▶ Find “improved iterative scheme”: with $\rho = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$:

For Jacobi, we had $\kappa = X^2 - 1$ where $X = \frac{2(1+2h)}{\pi h} = O(h^{-1})$.

$$\begin{aligned}\rho &= 1 + \frac{\sqrt{X^2 - 1} - 1}{\sqrt{X^2 - 1} + 1} - 1 \\ &= 1 + \frac{\sqrt{X^2 - 1} - 1 - \sqrt{X^2 - 1} - 1}{\sqrt{X^2 - 1} + 1} \\ &= 1 - \frac{1}{\sqrt{X^2 - 1} + 1} \\ &= 1 - \frac{1}{X \left(\sqrt{1 - \frac{1}{X^2}} + \frac{1}{X} \right)} \\ &= 1 - O(h)\end{aligned}$$

$$\Rightarrow \delta = 1$$

Krylov subspace methods

Generalization of iteration schemes

- ▶ So far we considered simple iterative schemes, perhaps with preconditioners
- ▶ Here, we introduce Krylov subspace methods which indeed in many cases yield faster convergence than simple iterative schemes
- ▶ Material after
 - ▶ M. Gutknecht [A Brief Introduction to Krylov Space Methods for Solving Linear Systems](#)
 - ▶ J. Shewchuk: [An Introduction to the Conjugate Gradient Method Without the Agonizing Pain](#)
- ▶ Extended reading: J. Liesen, Z. Strakoš: [Krylov Subspace Methods: Principles and Analysis](#)
- ▶ Extended coverage of the topic available at TU: Prof. Jörg Liesen, Prof. Reinhard Nabben are active researchers in the field.

Simple iterative method I

Solve $Au = b$, assume exact solution \hat{u} .

$$u_{k+1} = u_k - \alpha(Au_k - b) \quad (k = 0, 1 \dots)$$

1. Choose initial value u_0 , tolerance ε , set $k = 0$
2. Calculate *residuum* $r_k = Au_k - b$
3. Test convergence: if $\|r_k\| < \varepsilon$ set $u = u_k$, finish
4. Update solution: $u_{k+1} = u_k - \alpha r_k$, set $k = k + 1$, repeat with step 2.

Simple iterative method II

- ▶ From step 4:

$$\begin{aligned}Au_{k+1} &= Au_k - \alpha Ar_k \\ Au_{k+1} - b &= Au_k - b - \alpha Ar_k \\ r_{k+1} &= r_k - \alpha Ar_k\end{aligned}$$

- ▶ Therefore $r_k = p_k(A)r_0 \in \text{span}\{r_0, Ar_0, \dots, A^k r_0\}$ where $p(\xi) = (1 - \alpha\xi)^k$ is a polynomial of degree k

- ▶ For the iterate u_k , we have

$$\begin{aligned}u_k &= u_{k-1} - \alpha r_{k-1} = u_{k-2} - \alpha r_{k-2} - \alpha r_{k-1} \\ &= u_0 - \alpha(r_0 + r_1 + \dots + r_{k-1}) \\ &= u_0 + q_{k-1}(A)r_0\end{aligned}$$

where q_{k-1} is a polynomial of degree $n - 1$.

- ▶ From $r_k = Au_k - b = Au_0 - b + Aq_{k-1}(A)r_0 = (I + Aq_{k-1}(A))r_0$ one obtains $p_k(\xi) = 1 + \xi q_{k-1}(\xi)$.
- ▶ Consequently, $x_k \in x_0 + \text{span}\{r_0, Ar_0, \dots, A^{k-1}r_0\}$

The Krylov subspace

Definition: Let $A \in \mathbb{R}^{N \times N}$ be nonsingular, let $0 \neq y \in \mathbb{R}^n$. The k -th *Krylov subspace* generated from A by y is defined as $\mathcal{K}_k(A, y) = \text{span}\{y, Ay, \dots, A^{k-1}y\}$.

- ▶ For the simple iteration,

$$u_k = u_0 + q_{k-1}(A)r_0 \in \mathcal{K}_k(A, r_0)$$

$$r_k = p_k(A)r_0 \in \mathcal{K}_{k+1}(A, r_0)$$

$$p_k(\xi) = 1 + \xi q_k(\xi)$$

$$p_k(0) = 1$$

with particular polynomials p, q .

- ▶ Are these the best ones ?

Krylov subspace

- ▶ $\mathcal{K}_1 \subseteq \mathcal{K}_2 \subseteq \dots \subseteq \mathcal{K}_k$
- ▶ $\dim \mathcal{K}_i \leq \dim \mathcal{K}_{i-1} + 1$

When does the exact solution lie in \mathcal{K}_k ?

Definition: The grade of y is a positive integer $\nu = \nu(y, A)$ such that

$$\dim \mathcal{K}_k(A, y) = \begin{cases} k & \text{if } k \leq \nu \\ \nu & \text{if } k \geq \nu \end{cases}$$

- ▶ $\mathcal{K}_\nu(A, y)$ is the smallest A -invariant subspace which contains y .
- ▶ $\nu = \min\{k \mid A^{-1}y \in \mathcal{K}_k(A, y)\}$
- ▶ For any initial iterate u_0 and initial residual $r_0 = Au_0 - b$, the exact solution $\hat{u} \in \mathcal{K}_{\nu(r_0, A)}(A, r_0)$ lies in the Krylov subspace corresponding to the grade of r_0 .

Krylov subspace methods

Definition: Let $A \in \mathbb{R}^{N \times N}$ be nonsingular, let $0 \neq y \in \mathbb{R}^N$. An iterative method such that

$$u_k = u_0 + q_{k-1}(A)r_0 \in \mathcal{K}_k(A, r_0)$$

where q_{k-1} is a polynomial of degree k is called *Krylov subspace method*.

- ▶ For the residuals of the method, we have $r_k = p_k(A)r_0 \in \mathcal{K}_{k+1}(A, r_0)$ with $p_k(\xi) = 1 + \xi q_k(\xi)$
- ▶ Preconditioned form: use the same ansatz for $M^{-1}Ax = M^{-1}b$ and define Krylov subspace for $M^{-1}A$

The case of symmetric positive definite matrices

Assume A is spd (symmetric, positive definite)

$$a(u, v) = (Au, v) = v^T Au = \sum_{i=1}^n \sum_{j=1}^n a_{ij} v_i u_j$$

As A is SPD, for all $u \neq 0$ we have $(Au, u) > 0$.

For a given vector b , regard the function

$$f(u) = \frac{1}{2} a(u, u) - b^T u$$

What is the minimizer of f ?

$$f'(u) = Au - b = 0$$

- ▶ Solution of SPD system \equiv minimization of f .

Method of steepest descent

- ▶ Given some vector u_i , look for a new iterate u_{i+1} .
- ▶ The direction of steepest descent is given by $-f'(u_i)$.
- ▶ So look for u_{i+1} in the direction of $-f'(u_i) = r_i = b - Au_i$ such that it minimizes f in this direction, i.e. set $u_{i+1} = u_i + \alpha r_i$ with α chosen from

$$\begin{aligned}0 &= \frac{d}{d\alpha} f(u_i + \alpha r_i) = f'(u_i + \alpha r_i) \cdot r_i \\ &= (b - A(u_i + \alpha r_i), r_i) \\ &= (b - Au_i, r_i) - \alpha(Ar_i, r_i) \\ &= (r_i, r_i) - \alpha(Ar_i, r_i) \\ \alpha &= \frac{(r_i, r_i)}{(Ar_i, r_i)}\end{aligned}$$

Method of steepest descent: iteration scheme

$$r_i = b - Au_i$$

$$\alpha_i = \frac{(r_i, r_i)}{(Ar_i, r_i)}$$

$$u_{i+1} = u_i + \alpha_i r_i$$

Let \hat{u} the exact solution. Define $e_i = u_i - \hat{u}$, then $r_i = -Ae_i$

Let $\|u\|_A = (Au, u)^{\frac{1}{2}}$ be the *energy norm* wrt. A .

Theorem The convergence rate of the method is

$$\|e_i\|_A \leq \left(\frac{\kappa - 1}{\kappa + 1} \right)^i \|e_0\|_A$$

where $\kappa = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$ is the spectral condition number.

Method of steepest descent: advantages

- ▶ Simple Richardson iteration $u_{k+1} = u_k - \alpha(Au_k - f)$ needs good eigenvalue estimate to be optimal with $\alpha = \frac{2}{\lambda_{max} + \lambda_{min}}$
- ▶ In this case, asymptotic convergence rate is $\rho = \frac{\kappa - 1}{\kappa + 1}$
- ▶ Steepest descent has the same rate without need for spectral estimate

Conjugate directions

For steepest descent, there is no guarantee that a search direction $d_i = r_i = -Ae_i$ is not used several times. If all search directions would be orthogonal, or, indeed, A -orthogonal, one could control this situation.

So, let $d_0, d_1 \dots d_{n-1}$ be a series of A -orthogonal (or conjugate) search directions, i.e. $(Ad_i, d_j) = 0, i \neq j$.

- ▶ Look for u_{i+1} in the direction of d_i such that it minimizes f in this direction, i.e. set $u_{i+1} = u_i + \alpha_i d_i$ with α chosen from

$$\begin{aligned} 0 &= \frac{d}{d\alpha} f(u_i + \alpha d_i) = f'(u_i + \alpha d_i) \cdot d_i \\ &= (b - A(u_i + \alpha d_i), d_i) \\ &= (b - Au_i, d_i) - \alpha(Ad_i, d_i) \\ &= (r_i, d_i) - \alpha(Ad_i, d_i) \\ \alpha_i &= \frac{(r_i, d_i)}{(Ad_i, d_i)} \end{aligned}$$

- ▶ $u_{i+1} \in \text{span}\{d_0 \dots d_i\}$

Conjugate gradients

- ▶ Choose $d_0 \dots d_i$ such that $\text{span}\{d_0 \dots d_i\} = \mathcal{K}_i(A, r_0)$.
- ▶ Orthogonalize by Gram-Schmidt
- ▶ Result: short recursions!
- ▶ $u_i \in u_0 + \mathcal{K}_i(A, r_0)$ minimizes the energy norm of the error e_i :
 $\|e_i\|_A = (Ae_i, e_i)$.
- ▶ $r_{i+1} \perp \mathcal{K}_i(A, r_0)$
- ▶ There are at most N directions, so the method yields the exact solution after at most N iteration steps.

Conjugate gradients - the algorithm

Given initial value u_0 , spd matrix A , right hand side b .

$$d_0 = r_0 = b - Au_0$$

$$\alpha_i = \frac{(r_i, r_i)}{(Ad_i, d_i)}$$

$$u_{i+1} = u_i + \alpha_i d_i$$

$$r_{i+1} = r_i - \alpha_i Ad_i$$

$$\beta_{i+1} = \frac{(r_{i+1}, r_{i+1})}{(r_i, r_i)}$$

$$d_{i+1} = r_{i+1} + \beta_{i+1} d_i$$

At the i -th step, the algorithm yields the element from $e_0 + \mathcal{K}_i$ with the minimum energy error.

Theorem The convergence rate of the method is

$$\|e_i\|_A \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^i \|e_0\|_A$$

where $\kappa = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$ is the spectral condition number of A .

Preconditioning

Let M be spd, and spectrally equivalent to A , and assume that $\kappa(M^{-1}A) \ll \kappa(A)$.

Let E be such that $M = EE^T$, e.g. its Cholesky factorization. Then, $\sigma(M^{-1}A) = \sigma(E^{-1}AE^{-T})$:

Assume $M^{-1}Au = \lambda u$. We have

$$(E^{-1}AE^{-T})(E^T u) = (E^T E^{-T})E^{-1}Au = E^T M^{-1}Au = \lambda E^T u$$

$\Leftrightarrow E^T u$ is an eigenvector of $E^{-1}AE^{-T}$ with eigenvalue λ .

Preconditioned CG I

Now we can use the CG algorithm for the preconditioned system

$$E^{-1}AE^{-T}\tilde{x} = E^{-1}b$$

with $\tilde{u} = E^T u$

$$\tilde{d}_0 = \tilde{r}_0 = E^{-1}b - E^{-1}AE^{-T}u_0$$

$$\alpha_i = \frac{(\tilde{r}_i, \tilde{r}_i)}{(E^{-1}AE^{-T}\tilde{d}_i, \tilde{d}_i)}$$

$$\tilde{u}_{i+1} = \tilde{u}_i + \alpha_i \tilde{d}_i$$

$$\tilde{r}_{i+1} = \tilde{r}_i - \alpha_i E^{-1}AE^{-T}\tilde{d}_i$$

$$\beta_{i+1} = \frac{(\tilde{r}_{i+1}, \tilde{r}_{i+1})}{(\tilde{r}_i, \tilde{r}_i)}$$

$$\tilde{d}_{i+1} = \tilde{r}_{i+1} + \beta_{i+1}\tilde{d}_i$$

Not very practical as we need E

Preconditioned CG II

Assume $\tilde{r}_i = E^{-1}r_i$, $\tilde{d}_i = E^T d_i$, we get the equivalent algorithm

$$r_0 = b - Au_0$$

$$d_0 = M^{-1}r_0$$

$$\alpha_i = \frac{(M^{-1}r_i, r_i)}{(Ad_i, d_i)}$$

$$u_{i+1} = u_i + \alpha_i d_i$$

$$r_{i+1} = r_i - \alpha_i Ad_i$$

$$\beta_{i+1} = \frac{(M^{-1}r_{i+1}, r_{i+1})}{(r_i, r_i)}$$

$$d_{i+1} = M^{-1}r_{i+1} + \beta_{i+1}d_i$$

It relies on the solution of the preconditioning system, the calculation of the matrix vector product and the calculation of the scalar product.

The convergence rate of the method is

$$\|e_i\|_{E^{-1}AE^{-T}} \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^i \|e_0\|_{E^{-1}AE^{-T}}$$

where $\kappa = \frac{\gamma_{\max}}{\gamma_{\min}}$ comes from $\gamma_{\min}(Mu, u) \leq (Au, u) \leq \gamma_{\max}(Mu, u)$.

Issues and consequences

- ▶ Usually we stop the iteration when the residual r becomes small. However during the iteration, floating point errors occur which distort the calculations and lead to the fact that the accumulated residuals

$$r_{i+1} = r_i - \alpha_i A d_i$$

give a much more optimistic picture on the state of the iteration than the real residual

$$r_{i+1} = b - A u_{i+1}$$

- ▶ The convergence rate estimate in terms of $\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$ indeed provides a qualitatively better complexity estimate for the solution algorithm
- ▶ Always consider CG when solving symmetric positive definite linear systems iteratively

Unsymmetric problems

- ▶ By definition, CG is only applicable to symmetric problems.
- ▶ The biconjugate gradient (BICG) method provides a generalization:

Choose initial guess x_0 , perform

$$r_0 = b - Ax_0$$

$$\tilde{r}_0 \neq 0$$

$$p_0 = r_0$$

$$\tilde{p}_0 = \tilde{r}_0$$

$$\alpha_j = \frac{(\tilde{r}_j, r_j)}{(\tilde{p}_j, Ap_j)}$$

$$x_{i+1} = x_i + \alpha_i p_i$$

$$\tilde{x}_{i+1} = \tilde{x}_i + \alpha_i \tilde{p}_i$$

$$r_{i+1} = r_i - \alpha_i Ap_i$$

$$\tilde{r}_{i+1} = \tilde{r}_i - \alpha_i \tilde{p}_i A^T$$

$$\beta_j = \frac{(\tilde{r}_{j+1}, r_{j+1})}{(\tilde{r}_j, r_j)}$$

$$p_{i+1} = r_{i+1} + \beta_i p_i$$

$$\tilde{p}_{i+1} = \tilde{r}_{i+1} + \beta_i \tilde{p}_i$$

- ▶ The two sequences produced by the algorithm are biorthogonal, i.e., $(\tilde{p}_i, Ap_j) = (\tilde{r}_i, r_j) = 0$ for $i \neq j$.
- ▶ We have $r_i \in \mathcal{K}_i(A, r_0)$ and $\tilde{r}_i \in \mathcal{K}(A^T, \tilde{r}_0)$

Unsymmetric problems II

- ▶ BiCG is very unstable and additionally needs the transposed matrix vector product, it is seldomly used in practice
- ▶ There is as well a preconditioned variant of BiCG which also needs the transposed preconditioner.
- ▶ Main practical approaches to fix the situation:
 - ▶ “Conjugate gradients squared” (CGS, Sonneveld, 1989): Replace multiplication by A^T in BICG with multiplication by A , residual polynomial $p_{CGS} = p_{BICG}^2$.
 - ▶ “Stabilize” BiCG \rightarrow BiCGstab (H. Van der Vorst, 1992), BiCGstab(l) (Sleijpen/Fokkema 1993)
 - ▶ Error minimization in Krylov subspace \rightarrow “Generalized Minimum Residual” (GMRES, Saad/Schulz, 1986)
- ▶ Both CGS and BiCGstab can show erratic convergence behavior \Rightarrow always try to stop iteration after residual check
- ▶ For GMRES one has to keep the full Krylov subspace, which is not possible in practice \Rightarrow restart strategy.
- ▶ As in the case of CG, always combine preconditioners with Krylov subspace methods
- ▶ From my experience, BiCGstab is a good first guess

Krylov subspace methods in Julia

- ▶ Several packages available
- ▶ Seemingly most well maintained: [IterativeSolvers.jl](#)
 - ▶ CG, GMRES, BiCGStab and others.
 - ▶ We will explore these later when we go to 2D examples.