Numerical behavior of inexact linear solvers

Miro Rozložník
joint results with Zhong-zhi Bai and Pavel Jiránek

Institute of Computer Science, Czech Academy of Sciences,
Prague, Czech Republic

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Iterative solution of linear systems

Iterative methods in exact arithmetic

generate approximate solutions to the solution of $Ax = b$
$x_0, x_1, \ldots, x_n \to x$
with residual vectors $r_0 = b - Ax_0, \ldots, r_n = b - Ax_n \to 0$

Iterative methods in finite precision arithmetic

compute approximations $x_0, \bar{x}_1, \ldots, \bar{x}_n$ and updated residual vectors $\bar{r}_0, \bar{r}_1, \ldots, \bar{r}_n$ which are usually close to (but different from) the true residuals $b - A\bar{x}_n$

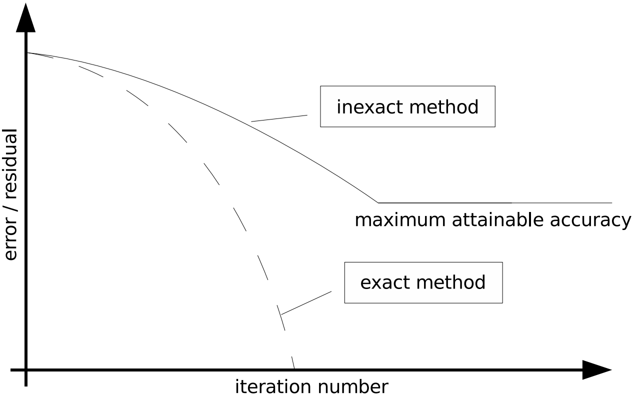
Two main questions and two main effects

- How good is the computed approximate solution $\bar{x}_n$? How many (extra) steps do we need to reach the same accuracy as one can get in the exact method?
- How well the computed vector $\bar{r}_n$ approximates the (true) residual $b - A\bar{x}_n$? Is there a limitation on the accuracy of the computed approximate solution?

Two main effects of rounding errors:

DELAY OF CONVERGENCE AND LIMIT ON THE FINAL (MAXIMUM ATTAINABLE) ACCURACY

Delay of convergence and maximum attainable accuracy



The concept of backward stability

A backward stable algorithm eventually computes the exact answer to a nearby problem, i.e. the approximate solution $\bar{x}_n$ satisfying

$$(A + \Delta A_n)\bar{x}_n = b + \Delta b_n$$
$$\|\Delta A_n\|/\|A\| \leq O(u), \ \|\Delta b_n\|/\|b\| \leq O(u)$$

$\iff$ The normwise backward error associated with the approximate solution $\bar{x}_n$ satisfies

$$\frac{\|b - A\bar{x}_n\|}{\|b\| + \|A\|\|\bar{x}_n\|} \leq O(u)$$

A forward stable algorithm eventually computes the approximate solution $\bar{x}_n$ with the error that satisfies

$$\|\bar{x}_n - x\| \leq O(u)\|A^{-1}\|\|A\|\|x\|$$

Prager, Oettli, 1964; Rigal, Gaches, 1967

see also Higham, 2nd ed. 2002; Stewart, Sun, 1990; Meurant 1999

The level of maximum attainable accuracy

We are looking for the difference between the updated $\bar{r}_n$ and true residual $b - A\bar{x}_n$ (divided by $\|b\| + \|A\|\|\bar{x}_n\|$)

$$\frac{\|b - A\bar{x}_n - \bar{r}_n\|}{\|b\| + \|A\|\|\bar{x}_n\|} \leq ?$$

$$\|\bar{r}_n\| \longrightarrow 0 \Longrightarrow \lim_{n\to\infty} \frac{\|b - A\bar{x}_n\|}{\|b\| + \|A\|\|\bar{x}_n\|} \leq ?$$

In the optimal case the bound is of $O(u)$; then we have a backward stable solution. The backward stability implies the forward stability.

Higham 2002, Higham, Knight 1993, Greenbaum, R, Strakoš, 1997

Stationary iterative methods

- $\mathcal{A}x = b$, $\mathcal{A} = \mathcal{M} - \mathcal{N}$
- A: $\mathcal{M}x_{k+1} = \mathcal{N}x_k + b$

  B: $x_{k+1} = x_k + \mathcal{M}^{-1}(b - \mathcal{A}x_k)$
- Inexact solution of systems with $\mathcal{M}$: **every computed solution $\overline{y}$ of $\mathcal{M}y = z$ is interpreted as an exact solution of a system with perturbed data and relative perturbation bounded by parameter** τ such that

$$(\mathcal{M} + \Delta\mathcal{M})\overline{y} = z, \quad \|\Delta\mathcal{M}\| \leq \tau\|\mathcal{M}\|, \quad \tau k(\mathcal{M}) \ll 1$$

Accuracy of the computed approximate solution

A: $\mathcal{M}x_{k+1} = \mathcal{N}x_k + b$

$$\frac{\|\hat{x}_{k+1} - x\|}{\|x\|} \leq \tau \|\mathcal{M}^{-1}\| (\|\mathcal{M}\| + \|\mathcal{N}\|) \left(1 + \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}\right)$$

$$\frac{\|b - \mathcal{A}\hat{x}_{k+1}\|}{\|b\| + \|\mathcal{A}\|\|\hat{x}_{k+1}\|} \leq \tau \frac{\|\mathcal{M}\| + \|\mathcal{N}\|}{\|\mathcal{A}\|} \left(1 + \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}\right)$$

B: $x_{k+1} = x_k + \mathcal{M}^{-1}(b - \mathcal{A}x_k)$

$$\frac{\|\hat{x}_{k+1} - x\|}{\|x\|} \leq O(u) \|\mathcal{M}^{-1}\| \, \|\mathcal{A}\| \left(1 + \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}\right)$$

$$\frac{\|b - \mathcal{A}\hat{x}_{k+1}\|}{\|b\| + \|\mathcal{A}\|\|\hat{x}_{k+1}\|} \leq O(u) \left(1 + \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}\right)$$

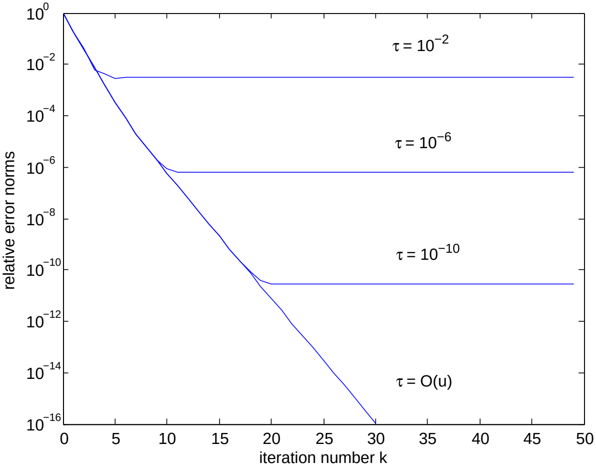
Higham, Knight 1993, Bai, R, 2012

Numerical experiments: small model example

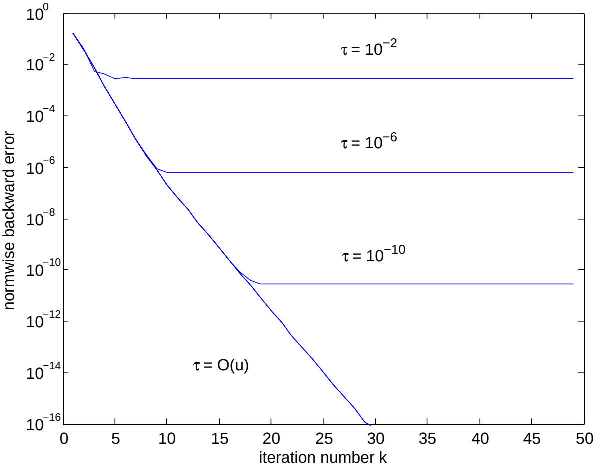
$$\mathcal{A} = \mathrm{tridiag}(1, 4, 1) \in \mathbb{R}^{100\times 100},\ b = \mathcal{A}\cdot \mathrm{ones}(100, 1),$$

$$\kappa(A) = \|A\| \cdot \|A^{-1}\| = 5.9990 \cdot 0.4998 \approx 2.9983$$

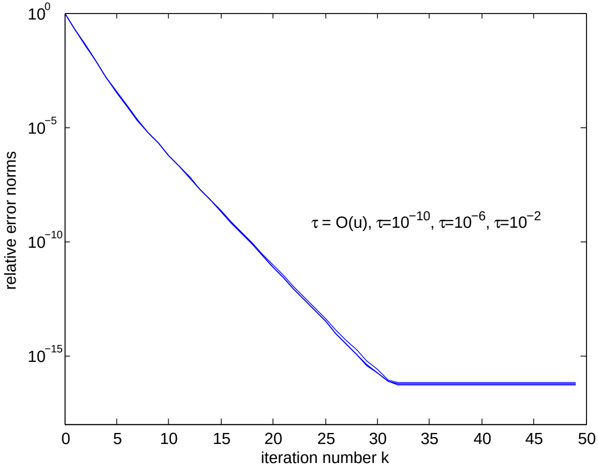
$$\mathcal{A} = \mathcal{M} - \mathcal{N},\ \mathcal{M} = D - L,\ \mathcal{N} = U$$



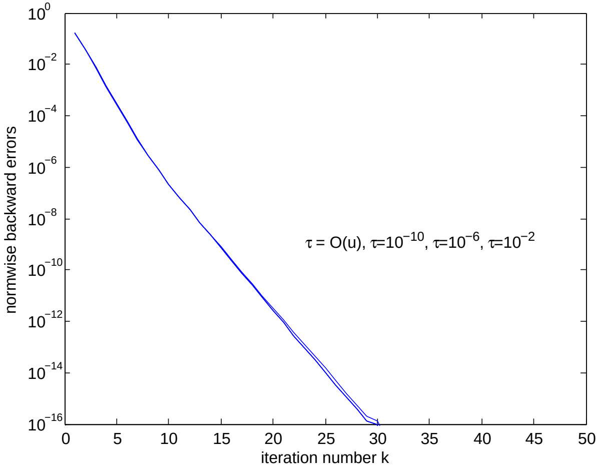
relative error norms
iteration number k
$\tau = 10^{-2}$
$\tau = 10^{-6}$
$\tau = 10^{-10}$
$\tau = O(u)$



10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
normwise backward error
0 5 10 15 20 25 30 35 40 45 50
iteration number k
$\tau = 10^{-2}$
$\tau = 10^{-6}$
$\tau = 10^{-10}$
$\tau = O(u)$



10^{0}
10^{-5}
10^{-10}
10^{-15}
relative error norms
$\tau = O(u)$, $\tau=10^{-10}$, $\tau=10^{-6}$, $\tau=10^{-2}$
0 5 10 15 20 25 30 35 40 45 50
iteration number k


normwise backward errors
iteration number k
τ = O(u), τ=10^−10, τ=10^−6, τ=10^−2
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
10^−16
0 5 10 15 20 25 30 35 40 45 50

Two-step splitting iteration methods

$$\begin{aligned} \mathcal{M}_1 x_{k+1/2} &= \mathcal{N}_1 x_k + b, & \mathcal{A} &= \mathcal{M}_1 - \mathcal{N}_1 \\ \mathcal{M}_2 x_{k+1} &= \mathcal{N}_2 x_{k+1/2} + b, & \mathcal{A} &= \mathcal{M}_2 - \mathcal{N}_2 \end{aligned}$$

Numerous solution schemes: Hermitian/skew-Hermitian (HSS) splitting, modified Hermitian/skew-Hermitian (MHSS) splitting, normal Hermitian/skew-Hermitian (NSS) splitting, preconditioned variant of modified Hermitian/skew-Hermitian (PMHSS) splitting and other splittings, ...

Bai, Golub, Ng 2003, 2007, 2008; Bai 2009
Bai, Benzi, Chen 2010, 2011; Bai, Benzi, Chen, Wang 2012

$$\frac{\|\hat{x}_{k+1} - x\|}{\|x\|} \leq \left[\tau_1 \|\mathcal{M}_2^{-1}\mathcal{N}_2\| \|\mathcal{M}_1^{-1}\| (\|\mathcal{M}_1\| + \|\mathcal{N}_1\|) + \tau_2 \|\mathcal{M}_2^{-1}\| (\|\mathcal{M}_2\| + \|\mathcal{N}_2\|)\right] \left(1 + \frac{\max_{i=0,1/2,\dots,k+1/2}\{\|\hat{x}_i\|\}}{\|x\|}\right)$$

Two-step splitting iteration methods

$$
\begin{aligned}
x_{k+1/2} &= x_k + \mathcal{M}_1^{-1}(b - \mathcal{A}x_k) \\
x_{k+1} &= x_{k+1/2} + \mathcal{M}_2^{-1}(b - \mathcal{A}x_{k+1/2}) \\
&\Leftrightarrow \\
x_{k+1} &= x_k + (\mathcal{M}_1^{-1} + \mathcal{M}_2^{-1} - \mathcal{M}_2^{-1}\mathcal{A}\mathcal{M}_1^{-1})(b - \mathcal{A}x_k) \\
&= x_k + (\mathcal{I} + \mathcal{M}_2^{-1}\mathcal{N}_1)\mathcal{M}_1^{-1}(b - \mathcal{A}x_k) \\
&= x_k + \mathcal{M}_2^{-1}(\mathcal{I} + \mathcal{N}_2\mathcal{M}_1^{-1})(b - \mathcal{A}x_k)
\end{aligned}
$$

$$
\frac{\|\hat{x}_{k+1} - x\|}{\|x\|} \leq O(u)\|\mathcal{M}_2^{-1}(\mathcal{I} + \mathcal{N}_2\mathcal{M}_1^{-1})\|\|\mathcal{A}\| \left(1 + \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}\right)
$$

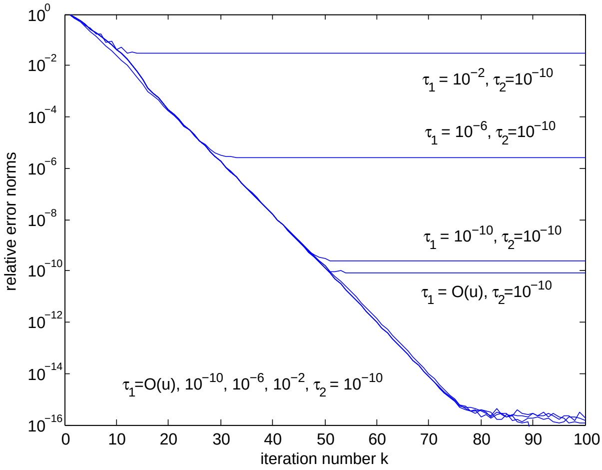
Numerical experiments: small model example

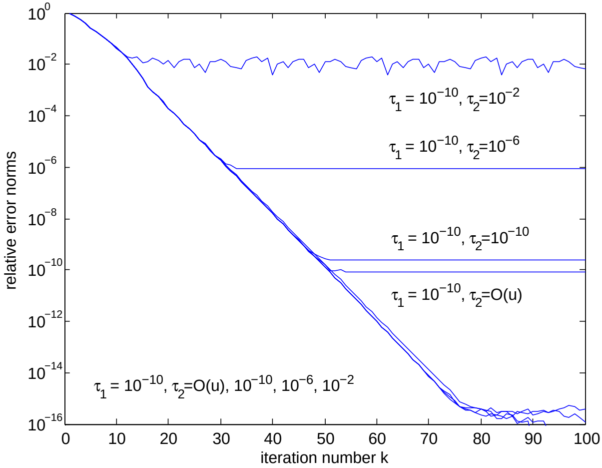
$$\mathcal{A} = \mathrm{tridiag}(2,4,1) \in \mathbb{R}^{100\times 100},\ b = \mathcal{A}\cdot \mathrm{ones}(100,1),$$

$$\kappa(A) = \|A\|\cdot\|A^{-1}\| = 5.9990\cdot 0.4998 \approx 2.9983$$

$$\mathcal{A} = \mathcal{H}+\mathcal{S},\quad \mathcal{H} = \frac{1}{2}(\mathcal{A}+\mathcal{A}^T),\quad \mathcal{S} = \frac{1}{2}(\mathcal{A}-\mathcal{A}^T)$$

$$\mathcal{H} = \mathrm{tridiag}(\frac{3}{2},4,\frac{3}{2}),\ \mathcal{S} = \mathrm{tridiag}(\frac{1}{2},0,-\frac{1}{2})$$


10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
relative error norms
0 10 20 30 40 50 60 70 80 90 100
iteration number k
$\tau_1 = 10^{-2}$, $\tau_2=10^{-10}$
$\tau_1 = 10^{-6}$, $\tau_2=10^{-10}$
$\tau_1 = 10^{-10}$, $\tau_2=10^{-10}$
$\tau_1 = O(u)$, $\tau_2=10^{-10}$
$\tau_1=O(u)$, 10^{-10}, 10^{-6}, 10^{-2}, $\tau_2 = 10^{-10}$



10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
relative error norms
0 10 20 30 40 50 60 70 80 90 100
iteration number k
$\tau_1 = 10^{-10}$, $\tau_2=10^{-2}$
$\tau_1 = 10^{-10}$, $\tau_2=10^{-6}$
$\tau_1 = 10^{-10}$, $\tau_2=10^{-10}$
$\tau_1 = 10^{-10}$, $\tau_2=O(u)$
$\tau_1 = 10^{-10}$, $\tau_2=O(u)$, 10^{-10}, 10^{-6}, 10^{-2}

Saddle point problems

We consider a saddle point problem with the symmetric 2×2 block form

$$\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}.$$

- A is a square $n \times n$ nonsingular (symmetric positive definite) matrix,
- B is a rectangular $n \times m$ matrix of (full column) rank m.

Applications: mixed finite element approximations, weighted least squares, constrained optimization, computational fluid dynamics, electromagnetism etc. [Benzi, Golub and Liesen, 2005], [Elman, Silvester, Wathen, 2005]. For the updated list of applications leading to saddle point problems contact [Benzi].

Iterative solution of saddle point problems

Numerous solution schemes: inexact Uzawa algorithms, inexact null-space methods, inner-outer iteration methods, two-stage iteration processes, multilevel or multigrid methods, domain decomposition methods

Numerous preconditioning techniques and schemes: block diagonal preconditioners, block triangular preconditioners, constraint preconditioning, Hermitian/skew-Hermitian preconditioning and other splittings, combination preconditioning

Numerous iterative solvers: conjugate gradient (CG) method, MINRES, GMRES, flexible GMRES, GCR, BiCG, BiCGSTAB, ...

Schur complement reduction method

- Compute y as a solution of the Schur complement system

$$B^T A^{-1} B y = B^T A^{-1} f,$$

- compute x as a solution of

$$Ax = f - By.$$

- Segregated vs. coupled approach: x_k and y_k approximate solutions to x and y, respectively.
- Inexact solution of systems with A: **every computed solution $\hat{u}$ of $Au = b$ is interpreted as an exact solution of a perturbed system**

$$(A + \Delta A)\hat{u} = b + \Delta b, \ \|\Delta A\| \leq \tau \|A\|, \ \|\Delta b\| \leq \tau \|b\|, \ \tau\kappa(A) \ll 1.$$

Iterative solution of the Schur complement system

choose y_0, solve $Ax_0 = f - By_0$

compute α_k and $p_k^{(y)}$

$y_{k+1} = y_k + \alpha_k p_k^{(y)}$

solve $Ap_k^{(x)} = -Bp_k^{(y)}$

back-substitution:

A: $x_{k+1} = x_k + \alpha_k p_k^{(x)}$,

B: solve $Ax_{k+1} = f - By_{k+1}$,

C: solve $Au_k = f - Ax_k - By_{k+1}$,

$x_{k+1} = x_k + u_k$.

inner iteration

$r_{k+1}^{(y)} = r_k^{(y)} - \alpha_k B^T p_k^{(x)}$

outer iteration

Accuracy in the saddle point system

$$\|f - Ax_k - By_k\| \leq \frac{O(\alpha_1)\kappa(A)}{1 - \tau\kappa(A)}(\|f\| + \|B\|Y_k),$$

$$\| - B^T x_k - r_k^{(y)}\| \leq \frac{O(\alpha_2)\kappa(A)}{1 - \tau\kappa(A)}\|A^{-1}\|\|B\|(\|f\| + \|B\|Y_k),$$

$$Y_k \equiv \max\{\|y_i\| \mid i = 0, 1, \ldots, k\}.$$

Back-substitution scheme	α_1	α_2
A: Generic update $x_{k+1} = x_k + \alpha_k p_k^{(x)}$	τ	u
B: Direct substitution $x_{k+1} = A^{-1}(f - By_{k+1})$	τ	τ
C: Corrected dir. subst. $x_{k+1} = x_k + A^{-1}(f - Ax_k - By_{k+1})$	u	τ

additional system with A

$$-B^T A^{-1} f + B^T A^{-1} B y_k = -B^T x_k - B^T A^{-1}(f - Ax_k - By_k)$$

Numerical experiments: a small model example

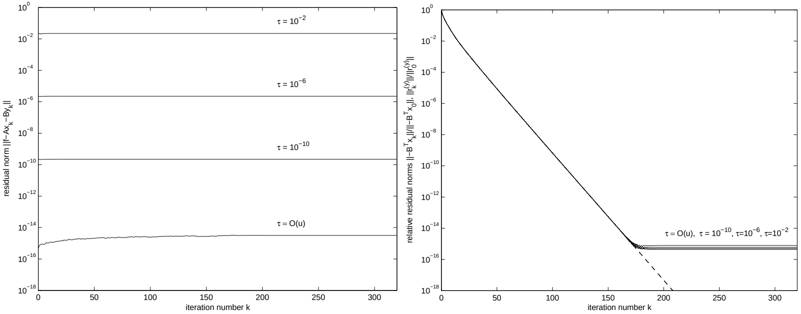
$$A = \mathrm{tridiag}(1,4,1) \in \mathbb{R}^{100\times 100},\ B = \mathrm{rand}(100,20),\ f = \mathrm{rand}(100,1),$$

$$\kappa(A) = \|A\| \cdot \|A^{-1}\| = 5.9990 \cdot 0.4998 \approx 2.9983,$$

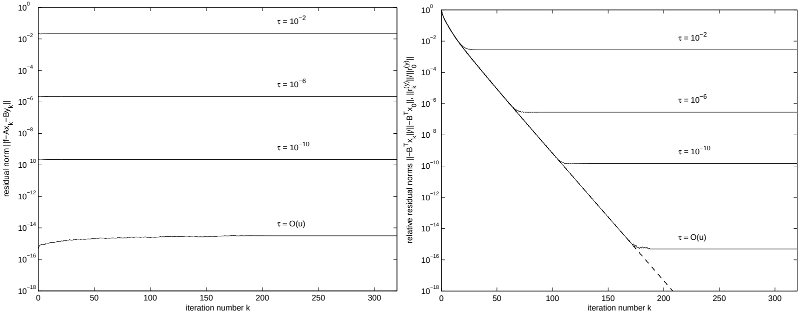
$$\kappa(B) = \|B\| \cdot \|B^{\dagger}\| = 7.1695 \cdot 0.4603 \approx 3.3001.$$

[R, Simoncini, 2002]

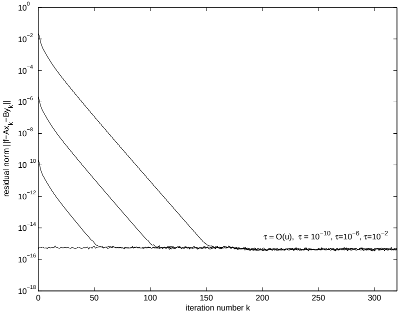
Generic update: $x_{k+1} = x_k + \alpha_k p_k^{(x)}$

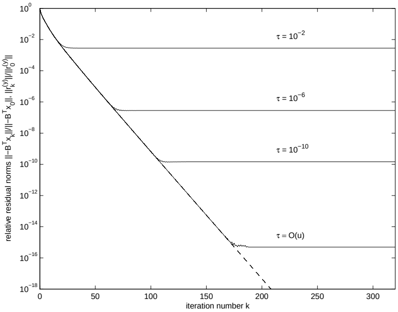


Direct substitution: $x_{k+1} = A^{-1}(f - By_{k+1})$



Corrected direct substitution: $x_{k+1} = x_k + A^{-1}(f - Ax_k - By_{k+1})$





Null-space projection method

- compute $x \in N(B^T)$ as a solution of the projected system

$$(I - \Pi)A(I - \Pi)x = (I - \Pi)f,$$

- compute y as a solution of the least squares problem

$$By \approx f - Ax,$$

$\Pi = B(B^T B)^{-1} B^T$ is the orthogonal projector onto $R(B)$.

- Schemes with the inexact solution of least squares with B. Every computed approximate solution $\bar{v}$ of a least squares problem $Bv \approx c$ is interpreted as an exact solution of a perturbed least squares

$$(B + \Delta B)\bar{v} \approx c + \Delta c, \ \|\Delta B\| \leq \tau \|B\|, \ \|\Delta c\| \leq \tau \|c\|, \ \tau\kappa(B) \ll 1.$$

Null-space projection method

$$
\left.
\begin{array}{l}
\text{choose } x_0, \text{ solve } By_0 \approx f - Ax_0 \\
\text{compute } \alpha_k \text{ and } p_k^{(x)} \in N(B^T) \\
x_{k+1} = x_k + \alpha_k p_k^{(x)} \\
\quad \left|
\begin{array}{l}
\text{solve } Bp_k^{(y)} \approx r_k^{(x)} - \alpha_k A p_k^{(x)} \\
\color{red}{\text{back-substitution:}} \\
\textbf{A: } y_{k+1} = y_k + p_k^{(y)}, \\
\textbf{B: } \text{solve } By_{k+1} \approx f - Ax_{k+1}, \\
\textbf{C: } \text{solve } Bv_k \approx f - Ax_{k+1} - By_k, \\
\qquad y_{k+1} = y_k + v_k.
\end{array}
\right\} \begin{array}{l}\text{inner}\\ \text{iteration}\end{array} \\
r_{k+1}^{(x)} = r_k^{(x)} - \alpha_k A p_k^{(x)} - Bp_k^{(y)}
\end{array}
\right\} \begin{array}{l}\text{outer}\\ \text{iteration}\end{array}
$$

Accuracy in the saddle point system

$$\|f - Ax_k - By_k - r_k^{(x)}\| \leq \frac{O(\alpha_3)\kappa(B)}{1 - \tau\kappa(B)}(\|f\| + \|A\|X_k),$$

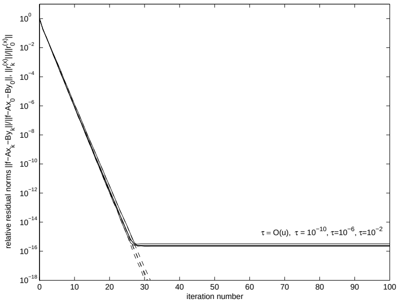
$$\|-B^T x_k\| \leq \frac{O(\tau)\kappa(B)}{1 - \tau\kappa(B)}\|B\|X_k,$$

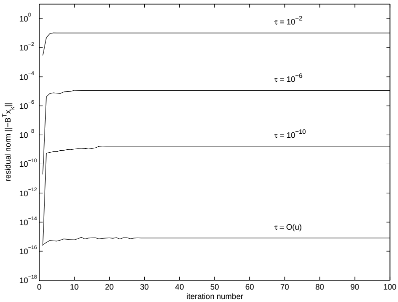
$$X_k \equiv \max\{\|x_i\| \,|\, i = 0, 1, \dots, k\}.$$

Back-substitution scheme		α_3
A:	Generic update $y_{k+1} = y_k + p_k^{(y)}$	u
B:	Direct substitution $y_{k+1} = B^\dagger(f - Ax_{k+1})$	τ
C:	Corrected dir. subst. $y_{k+1} = y_k + B^\dagger(f - Ax_{k+1} - By_k)$	u

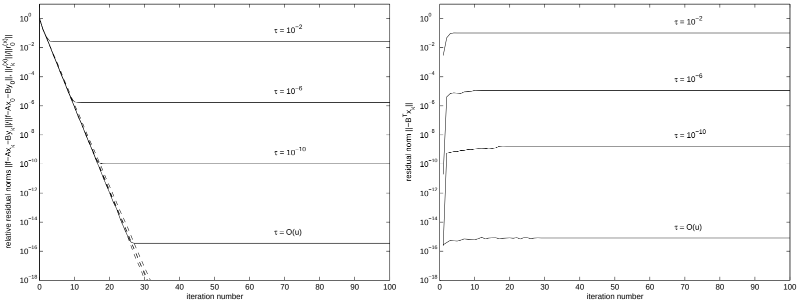
additional least square with B

Generic update: $y_{k+1} = y_k + p_k^{(y)}$

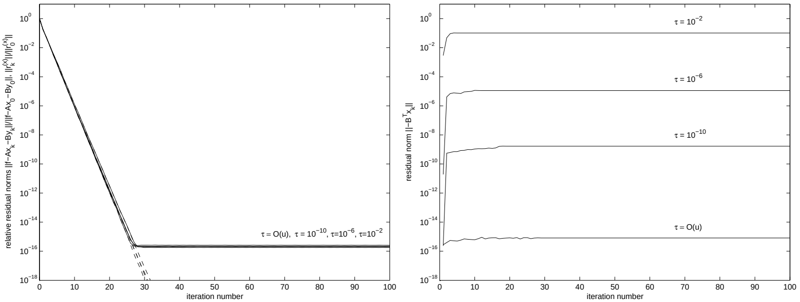




Direct substitution: $y_{k+1} = B^{\dagger}(f - Ax_{k+1})$

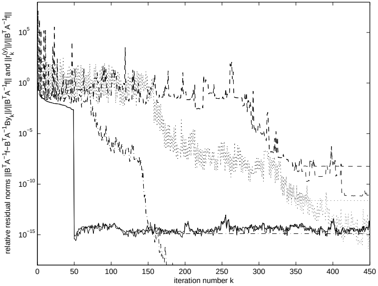


Corrected direct substitution: $y_{k+1} = y_k + B^\dagger(f - Ax_{k+1} - By_k)$



The maximum attainable accuracy of saddle point solvers

- The accuracy measured by the residuals of the saddle point problem depends on the choice of the back-substitution scheme [Jiránek, R, 2008]. The schemes with (generic or corrected substitution) updates deliver approximate solutions which satisfy either the first or second block equation to working accuracy.
- Care must be taken when solving nonsymmetric systems [Jiránek, R, 2008], all bounds of the limiting accuracy depend on the maximum norm of computed iterates, cf. [Greenbaum 1994,1997], [Sleijpen, et al. 1994].



Conclusions

"new_value = old_value + small_correction"

- Stationary iterative methods for $Ax = b$ and their maximum attainable accuracy [Higham and Knight, 1993]: assuming splitting $A = M - N$ and inexact solution of systems with M, use $x_{\mathrm{new}} = x_{\mathrm{old}} + M^{-1}(b - Ax_{\mathrm{old}})$ rather than $x_{\mathrm{new}} = M^{-1}(Nx_{\mathrm{old}} + b)$, [Higham, 2002; Bai, R].
- Two-step splitting iteration framework: $A = M_1 - N_1 = M_2 - N_2$ assuming inexact solution of systems with M_1 and M_2, reformulation of $M_1 x_{1/2} = N_1 x_{\mathrm{old}} + b$, $M_2 x_{\mathrm{new}} = N_2 x_{1/2} + b$, Hermitian/skew-Hermitian splitting (HSS) iteration [Bai, Golub and Ng 2003; Bai, R].
- Saddle point problems and inexact linear solvers: Schur complement and null-space approach [Jiránek, R 2008] Preconditioners for saddle point problems: SIMPLE and SIMPLE(R) type algorithms [Vuik and Saghir, 2002] and constraint preconditioners [R, Simoncini, 2002].
- Fixed-precision iterative refinement for improving the computed solution x_{old} to a system $Ax = b$: solving update equations $Az_{\mathrm{corr}} = r$ that have residual $r = b - Ay_{\mathrm{old}}$ as a right-hand side to obtain $x_{\mathrm{new}} = x_{\mathrm{old}} + z_{\mathrm{corr}}$, see [Wilkinson, 1963], [Higham, 2002].

Thank you for your attention.

`http://www.cs.cas.cz/~miro`

Zhong-Zhi Bai and M. Rozložník, On the behavior of two-step splitting iteration methods, *in preparation*.

P. Jiránek and M. Rozložník. Maximum attainable accuracy of inexact saddle point solvers. *SIAM J. Matrix Anal. Appl.*, 29(4):1297–1321, 2008.

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M. Rozložník and V. Simoncini, Krylov subspace methods for saddle point problems with indefinite preconditioning, *SIAM J. Matrix Anal. Appl., 24 (2002), pp. 368–391.*