Numerical behavior of iterative methods and iterative refinement

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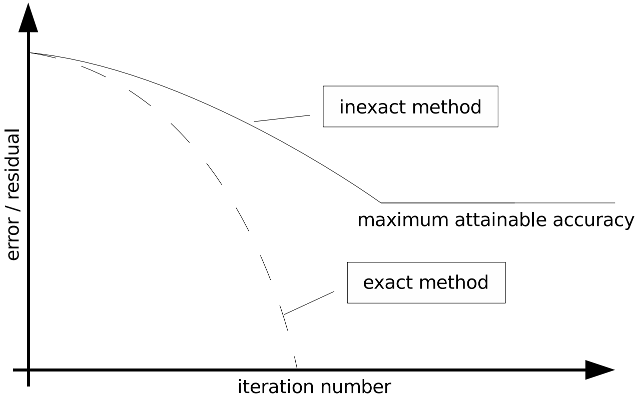
Delay of convergence and maximum attainable accuracy



Stationary iterative methods

- $\mathcal{A}x = b$, $\mathcal{A} = \mathcal{M} - \mathcal{N}$, $\mathcal{G} = \mathcal{M}^{-1}\mathcal{N}$, $\mathcal{F} = \mathcal{N}\mathcal{M}^{-1}$
- 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

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

- Higham, Knight 1993: $\mathcal{M}$ triangular, $\tau = O(u)$

Accuracy of the computed approximate solution

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

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

$$\frac{\|b - \mathcal{A}\hat{x}_{k+1}\|}{\|b\| + \|\mathcal{A}\|\|\hat{x}_{k+1}\|} \le \tau \frac{\|\mathcal{M}\|}{\|\mathcal{A}\|} \frac{\|I - \mathcal{F}\|}{1 - \|\mathcal{F}\|} \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}$$

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

$$\frac{\|\hat{x}_{k+1} - x\|}{\|x\|} \le O(u) \frac{\|\mathcal{M}^{-1}\| \, (\|\mathcal{M}\| + \|\mathcal{N}\|)}{1 - \|\mathcal{G}\| - 2\tau\|\mathcal{M}^{-1}\|\|\mathcal{M}\|} \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}$$

$$\frac{\|b - \mathcal{A}\hat{x}_{k+1}\|}{\|b\| + \|\mathcal{A}\|\|\hat{x}_{k+1}\|} \le O(u) \frac{\|\mathcal{M}\| + \|\mathcal{N}\|}{\|\mathcal{A}\|} \frac{\|I - \mathcal{F}\|}{1 - \|\mathcal{F}\| - 2\tau\|\mathcal{M}^{-1}\|\|\mathcal{M}\|} \frac{\max_{i=0,\dots,k}\{\|\hat{x}_i\|\}}{\|x\|}$$

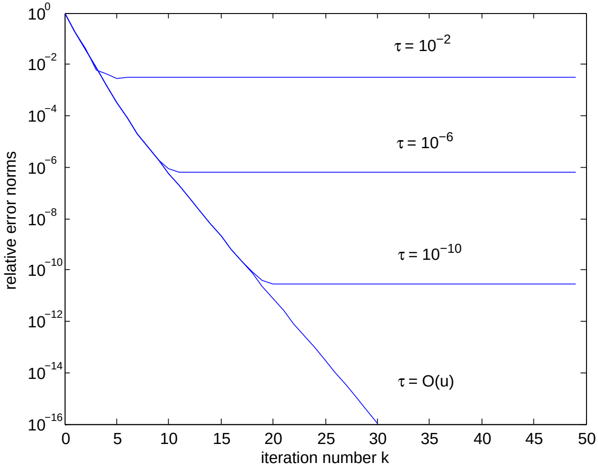
Higham, Knight 1993, Bai, R, 2012

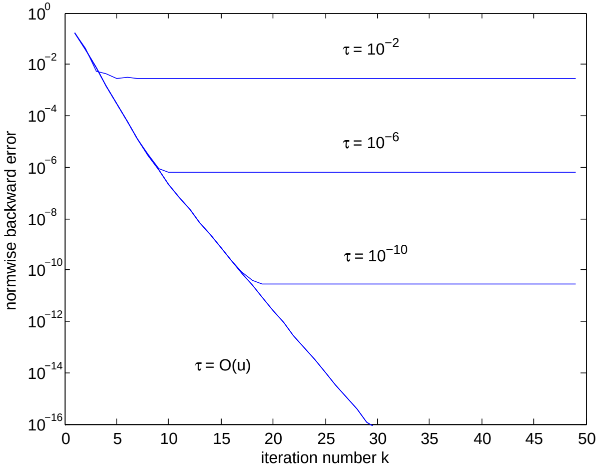
Numerical experiments: small model example

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

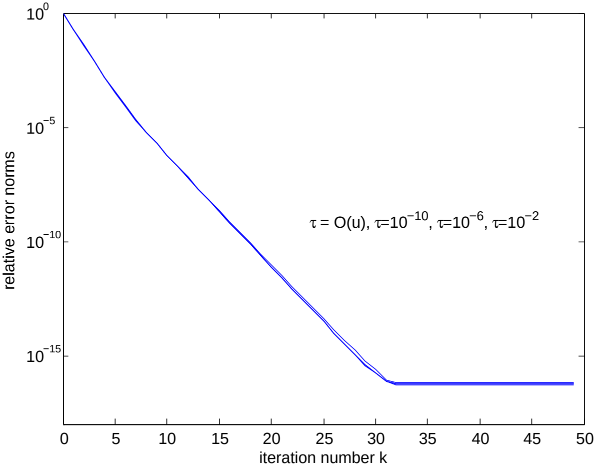
$$\kappa(A) = \|A\| \cdot \|A^{-1}\| = 5.9990 \cdot 0.4998 \approx 2.9983$$

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

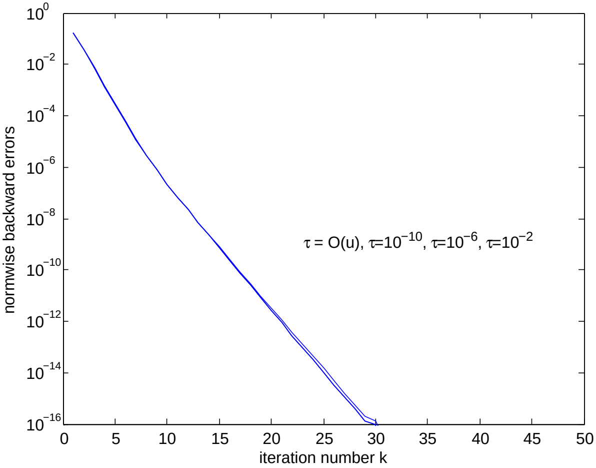

$\tau = 10^{-2}$
$\tau = 10^{-6}$
$\tau = 10^{-10}$
$\tau = O(u)$
relative error norms
iteration number k
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
0
5
10
15
20
25
30
35
40
45
50



normwise backward error
iteration number k
τ = 10^−2
τ = 10^−6
τ = 10^−10
τ = O(u)
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



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



normwise backward errors
iteration number k
τ = O(u), τ=10^−10, τ=10^−6, τ=10^−2

Two-step splitting iteration methods

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

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

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

Two-step splitting iteration methods

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

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

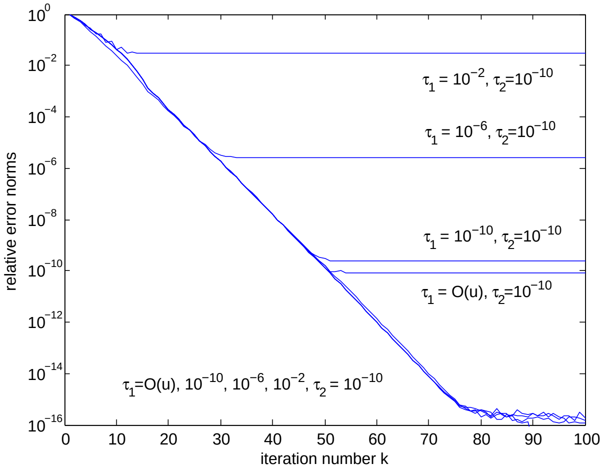
Numerical experiments: small model example

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

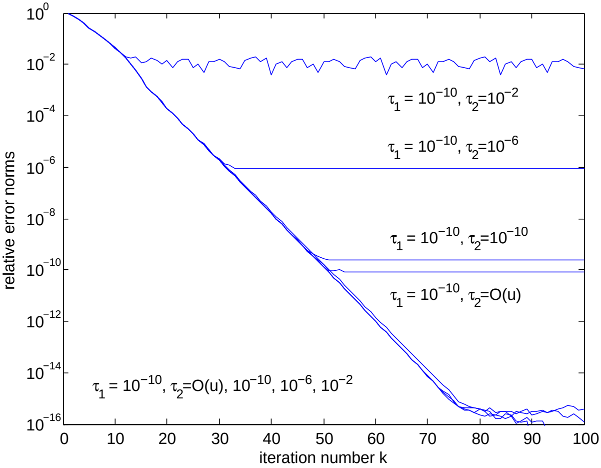
$$\kappa(A) = \|A\|\cdot\|A^{-1}\| = 5.9990\cdot 0.4998 \approx 2.9983$$

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

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



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



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

Schur complement reduction method

- Compute y as a solution of the Schur complement system

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

- 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

$$\left.\begin{array}{l}
\text{choose } y_0,\ \text{solve } Ax_0 = f - By_0 \\
\text{compute } \alpha_k \text{ and } p_k^{(y)} \\
y_{k+1} = y_k + \alpha_k p_k^{(y)} \\
\quad \left|\begin{array}{l}
\text{solve } Ap_k^{(x)} = -Bp_k^{(y)} \\
\text{back-substitution:} \\
\textbf{A: } x_{k+1} = x_k + \alpha_k p_k^{(x)}, \\
\textbf{B: } \text{solve } Ax_{k+1} = f - By_{k+1}, \\
\textbf{C: } \text{solve } Au_k = f - Ax_k - By_{k+1}, \\
\qquad x_{k+1} = x_k + u_k.
\end{array}\right\} \text{inner iteration} \\
r_{k+1}^{(y)} = r_k^{(y)} - \alpha_k B^T p_k^{(x)}
\end{array}\right\} \text{outer iteration}$$

Accuracy in the saddle point system

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

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

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

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	additional system with A
C: Corrected dir. subst. $x_{k+1} = x_k + A^{-1}(f - Ax_k - By_{k+1})$	u	τ	

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

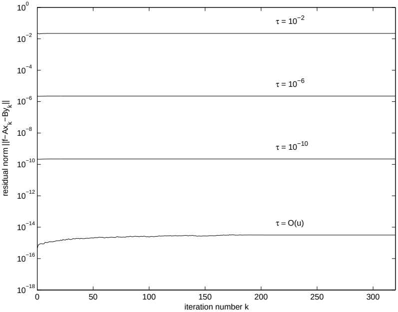
Numerical experiments: a small model example

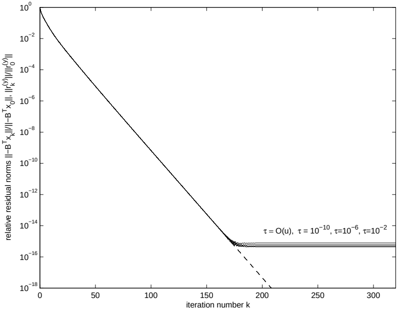
$$A = \mathrm{tridiag}(1,4,1) \in \mathbb{R}^{100\times 100},\ B = \mathrm{rand}(100,20),\ f = \mathrm{rand}(100,1),$$

$$\kappa(A) = \|A\| \cdot \|A^{-1}\| = 5.9990 \cdot 0.4998 \approx 2.9983,$$
$$\kappa(B) = \|B\| \cdot \|B^{\dagger}\| = 7.1695 \cdot 0.4603 \approx 3.3001.$$

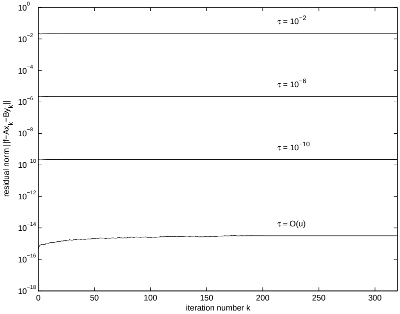
[R, Simoncini, 2002]

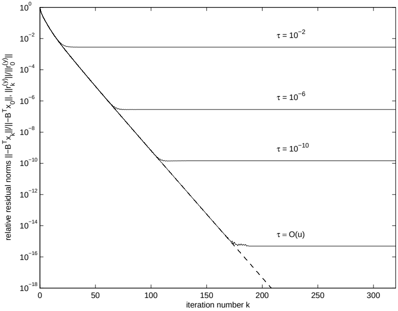
Generic update: $x_{k+1} = x_k + \alpha_k p_k^{(x)}$



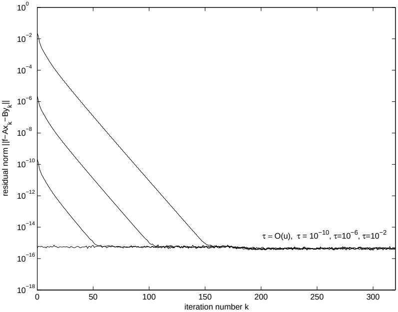


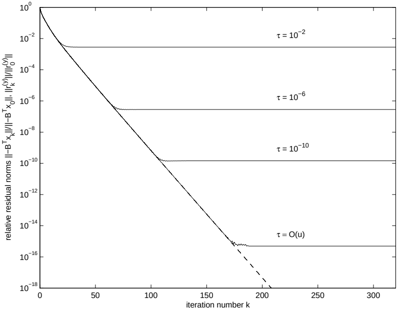
Direct substitution: $x_{k+1} = A^{-1}(f - By_{k+1})$





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





Conclusions

"new_value = old_value + small_correction"

- 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].
- 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]

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*.

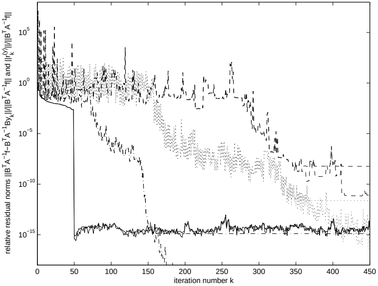
P. Jiránek and M. Rozložník. Maximum attainable accuracy of inexact saddle point solvers. *SIAM J. Matrix Anal. Appl.*, 29(4):1297–1321, 2008.

P. Jiránek and M. Rozložník. Limiting accuracy of segregated solution methods for nonsymmetric saddle point problems. *J. Comput. Appl. Math.* 215 (2008), pp. 28-37.

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.*

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].



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

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

Accuracy in the saddle point system

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

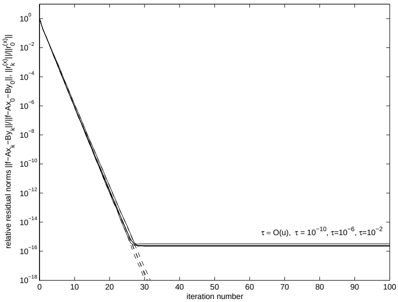
$$\|-B^T x_k\| \leq \frac{O(\tau)\kappa(B)}{1-\tau\kappa(B)}\|B\|X_k,$$

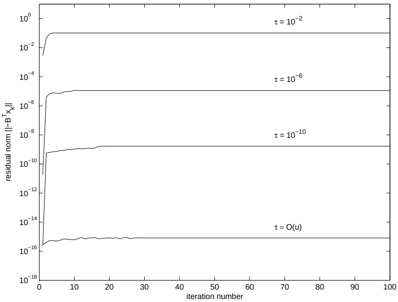
$$X_k \equiv \max\{\|x_i\| \,|\, i = 0, 1, \ldots, k\}.$$

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

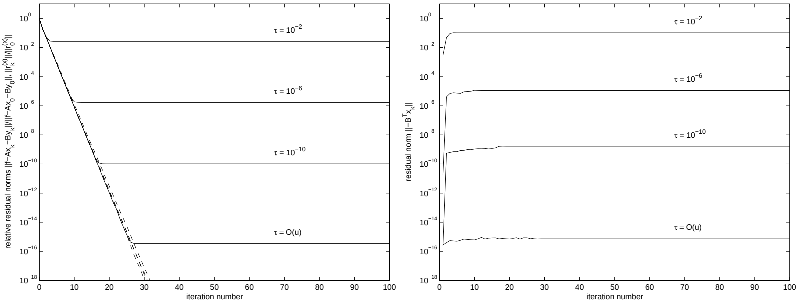
additional least square with B

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





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



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