Shift optimization for solution of large scale evolutionary problems by means of Galerkin approach on rational Krylov subspaces

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1 Objective:

Economical computation of

$$\mathbf{exp}(-tA)\varphi, \qquad t \geq \mathbf{0}, \tag{1}$$

for

$$A^* = A, \quad \mathbf{0} < \lambda_{\mathbf{min}} I \leq A \leq \lambda_{\mathbf{max}} I. \tag{2}$$

This problem is related with computation of

$$(A + i\omega I)^{-\mathbf{1}}\varphi, \quad \omega \in \mathbf{R}, \tag{3}$$

via Fourier transform. Both the problems contain a parameter (ω or t).

2 Outline:

1. Galerkin approach on Rational Krylov Subspace. 2. Skeleton approximation. 3. Problem (1–2).

3 Galerkin approach on Rational Krylov Subspace

Rational Krylov subspace (A. Ruhe):

$$U = \mathbf{span}\{(A + s_1 I)^{-1}\varphi, \ldots, (A + s_n I)^{-1}\varphi\}, \quad s_j \notin -\mathbf{Co\,Sp}\, A. \quad (4)$$

Our solution method: Galerkin projection with **good choice of** s_j.

RKSR approximant:

$$f(A)\varphi = u \approx u_n = G f(V) G^* \varphi, \qquad f(\lambda) = (\lambda + i\omega)^{-1}, \quad (5)$$

where the columns of G form an orthonormal basis of U, $V = G^* A G$.

Good approximation with poles $-s_j$ implies a good error estimate:

Proposition 1 *Let p be a polynomial of degree not exceeding $n-1$. Then the estimate*

$$\|u - u_n\| \le 2 \max_{\lambda \in \mathbf{Co\,Sp}\, A} \left| f(\lambda) - \frac{p(\lambda)}{q(\lambda)} \right| \quad (6)$$

takes place with

$$q(\lambda) = \prod_{j=1}^{n} (\lambda + s_j). \quad (7)$$

Remark 1 *A similar result was independently presented by B. Beckermann and L. Reichel 2008.*

4 Skeleton approximation

Motivation of use: presence of a parameter. Standard RA is not enough. SA was introduced in [Tyrtyshnikov96] and exploited in [Goreinov99, HackbuschKhoromskiiTyrtyshnikov05]. For the function $\mathbf{1}/(\lambda + s)$ it was investigated in [Oseledets07]. The definition:

$$f_{\mathbf{skel}}(\lambda, s) = \left(\tfrac{\mathbf{1}}{\lambda+s_{\mathbf{1}}}, \ \ldots, \ \tfrac{\mathbf{1}}{\lambda+s_n}\right) M^{-\mathbf{1}} \left(\tfrac{\mathbf{1}}{s+\lambda_{\mathbf{1}}}, \ldots \tfrac{\mathbf{1}}{s+\lambda_n}\right)^T, \tag{8}$$

where

$$M = (M_{kl}), \quad M_{kl} = \mathbf{1}/(\lambda_k + s_l), \quad \mathbf{1} \le k, l \le n. \tag{9}$$

Theorem 3 from [Oseledets07] gives an expression for the relative error:

$$\eta = \left[\frac{\mathbf{1}}{\lambda + s} - f_{\mathbf{skel}}(\lambda, s)\right] \Big/ \frac{\mathbf{1}}{\lambda + s} = \prod_{j=\mathbf{1}}^{n} \frac{\lambda - \lambda_j}{\lambda + s_j} \cdot \prod_{j=\mathbf{1}}^{n} \frac{s - s_j}{s + \lambda_j}. \tag{10}$$

A convenient error representation (leading to **Zolotaryov's problem**):

$$\eta(\lambda, s) = \frac{r(\lambda)}{r(-s)}, \qquad r(z) = \prod_{j=\mathbf{1}}^{n} \frac{z - \lambda_j}{z + s_j}. \tag{11}$$

Keep in mind: $\lambda \hookrightarrow A, \ s \hookrightarrow i\omega I.$

5 Evolutionary problem

[Quadrature approach: a number of papers by L. N. Trefethen with collaborators; designed for moderate $t_{\mathbf{max}}/t_{\mathbf{min}}$.]

We use skeleton approximation. Put

$$\epsilon(\lambda, t) \equiv \mathcal{F}_{\omega}^{-1}\left[\frac{1}{\lambda + i\omega} - f_{\mathbf{skel}}(\lambda, i\omega)\right](t) \tag{12}$$

— approximation error for $e^{-t\lambda}$. Plancherel's theorem implies:

Proposition 2 *The approximation error satisfies the inequality*

$$\max_{\lambda\in[\lambda_{\mathbf{min}},\lambda_{\mathbf{max}}]} \|\epsilon(\lambda, \cdot)\|_{L_2[0,+\infty[} \tag{13}$$
$$\leq \pi\sqrt{\frac{2}{\lambda_{\mathbf{min}}}} \max_{\lambda\in[\lambda_{\mathbf{min}},\lambda_{\mathbf{max}}]} |r(\lambda)| \max_{s\in i\mathbf{R}\cup\{\infty\}} |r(s)|^{-1}.$$

Parameter optimization: **the third Zolotaryov problem** with the condenser (E, D) whose compact (in $\overline{\mathbf{C}}$) plates are

$$E = [\lambda_{\mathbf{min}}, \lambda_{\mathbf{max}}] \qquad \text{and} \qquad D = \{z \in \mathbf{C} \mid \Re z \leq \mathbf{0}\}. \tag{14}$$

Introduce the quantity

$$\sigma_n(E, D) = \min_{\lambda_1,\ldots,\lambda_n,s_1,\ldots,s_n} \frac{\max_{\lambda\in[\lambda_{\mathbf{min}},\lambda_{\mathbf{max}}]} |r(\lambda)|}{\min_{s\in i\mathbf{R}\cup\{\infty\}} |r(s)|}; \tag{15}$$

$$\delta = \lambda_{\mathbf{min}}/\lambda_{\mathbf{max}}, \qquad \mu = \left(\frac{\mathbf{1}-\sqrt{\delta}}{\mathbf{1}+\sqrt{\delta}}\right)^{\mathbf{2}}, \tag{16}$$

$$\rho = \exp\left(-\frac{\pi}{\mathbf{4}}\cdot\frac{K'(\mu)}{K(\mu)}\right) \overset{\text{large } \lambda_{\mathbf{max}}/\lambda_{\mathbf{min}}}{\approx} \exp\left(-\frac{\pi^{\mathbf{2}}}{\mathbf{2}} \Big/ \log\frac{\mathbf{4}\lambda_{\mathbf{max}}}{\lambda_{\mathbf{min}}}\right). \tag{17}$$

Theorem 1 *The assertion*

$$\rho^n \leq \sigma_n(E, D) \leq \mathbf{2}\rho^n \tag{18}$$

holds.

The lower bound: computation of the Riemann modulus of the condenser (E, D) and application of Gonchar's theorem from [Gonchar69]. The upper bound is provided with the parameter set obtained by means of minimization under the additional condition $s_j = \lambda_j$:

$$s_j = \lambda_j = \lambda_{\mathbf{max}} \,\mathbf{dn}\left(\frac{\mathbf{2}(n - j) + \mathbf{1}}{\mathbf{2}n} K'(\delta), \sqrt{\mathbf{1} - \delta^2}\right), \quad j = \mathbf{1}, \ldots, n. \tag{19}$$

It was shown in [BaillyThiran00] that (19) satisfy some local optimality condition.

Remark 2 *All the parameters in (19) are real which enables us to exploit real arithmetic in industrial Fortran programs.*

Remark 3 *If we take (again real) infinite sequence of parameters $s_j = \lambda_j$, having the same limit (as $n \to \infty$) distribution as in (19), we shall obtain the same asymtotical (in the Cauchy–Hadamard sense) convergence factor ρ. This allows us to extend the parameter set when moving from n to $n + \mathbf{1}$ (in the style of [Gonchar78, SaffTotik97, Leja57, BaglamaCalvettiReichel98]).*

Remark 4 *Adaptive change of parameters: a work by D and Z under preparation.*

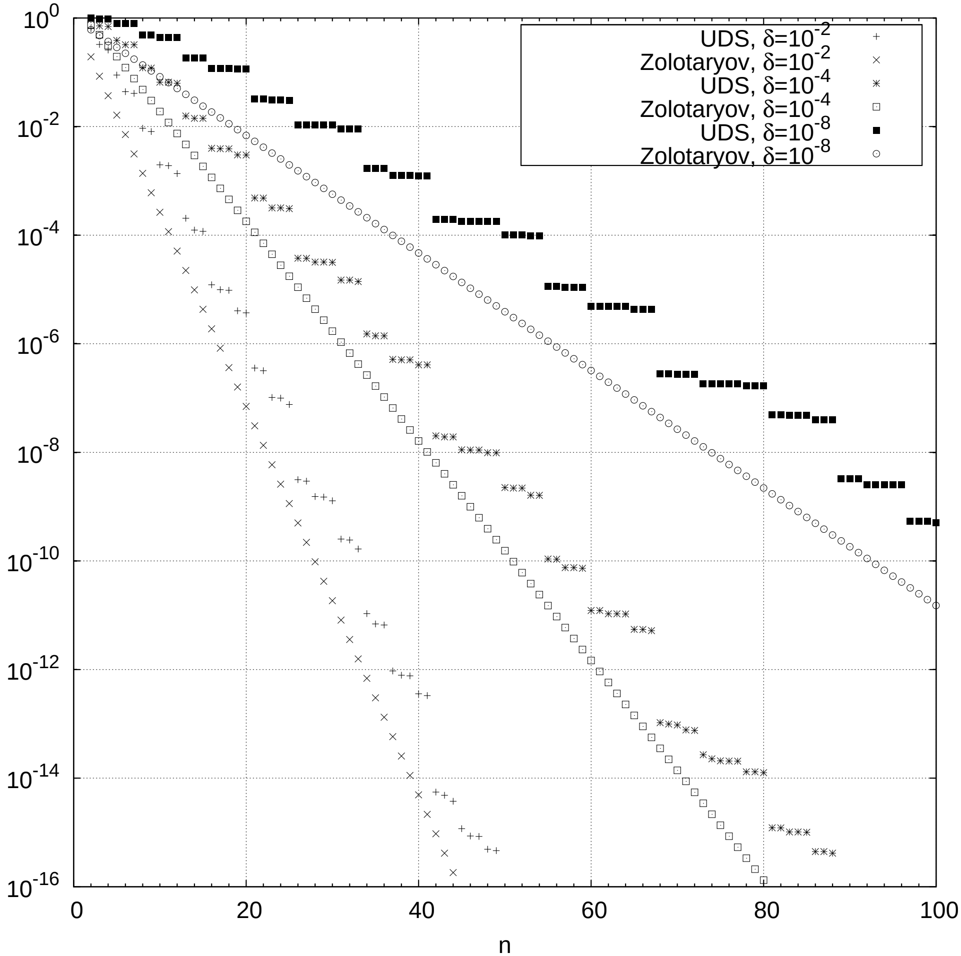

Figure 1: Comparison of Zolotaryov fractions with ones based on uniformly distributed sequences (UDS). The error $\max_{z\in[\lambda_{\min},\lambda_{\max}]}\left|\prod_{l=1}^{n}\frac{z-s_l}{z+s_l}\right|$ as a function of n for the two families of parameter sets; $\lambda_{\min}=10^{-4}$, $\lambda_{\max}=1$; three values of $\delta=\lambda_{\min}/^{8}\lambda_{\max}$.

Numerical experiments. Maxwell's system. Comparison with the version of the Restricted Denominator Method from [vdEshofHochbruck06] designed for a particular t (parameter choice from [Andersson81]).

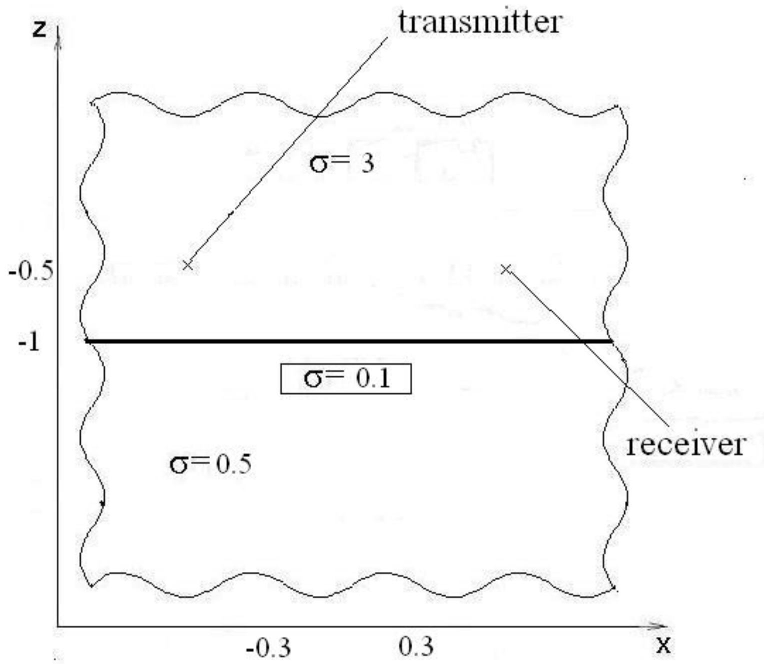

Figure 2: Model medium.

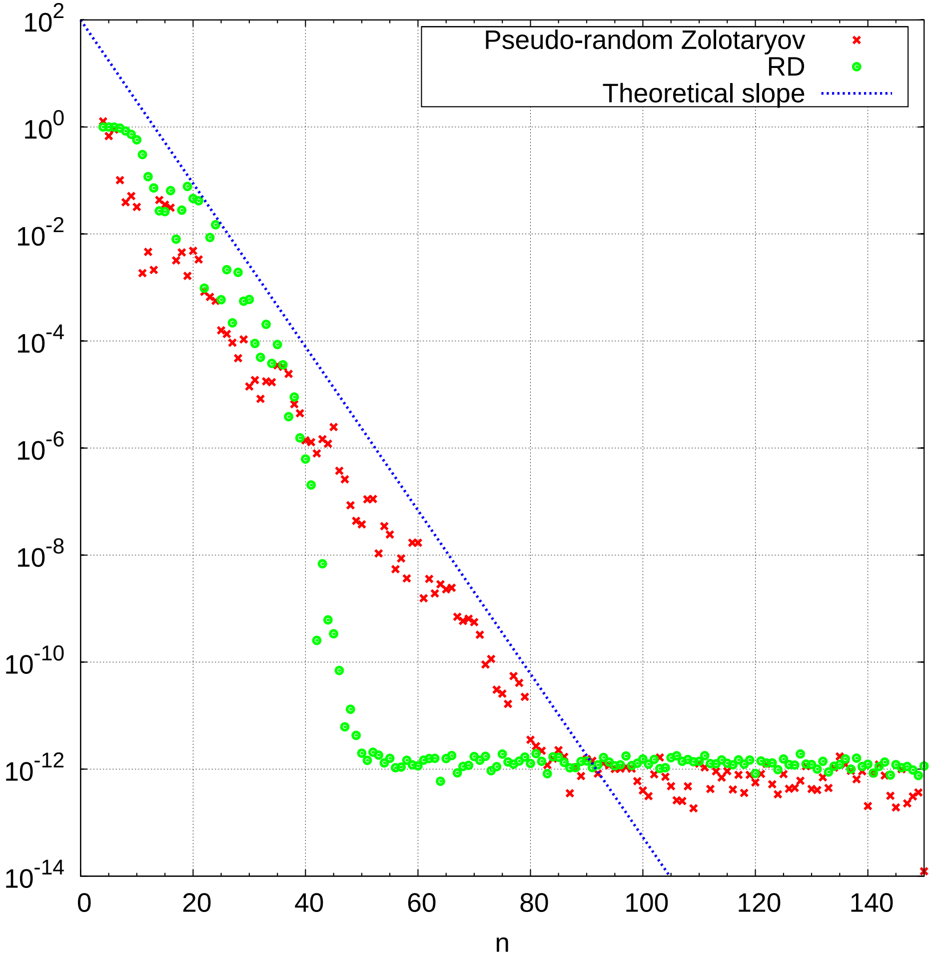

Figure 3: $t = \mathbf{1}$. RD approach converges significantly faster than our approach.

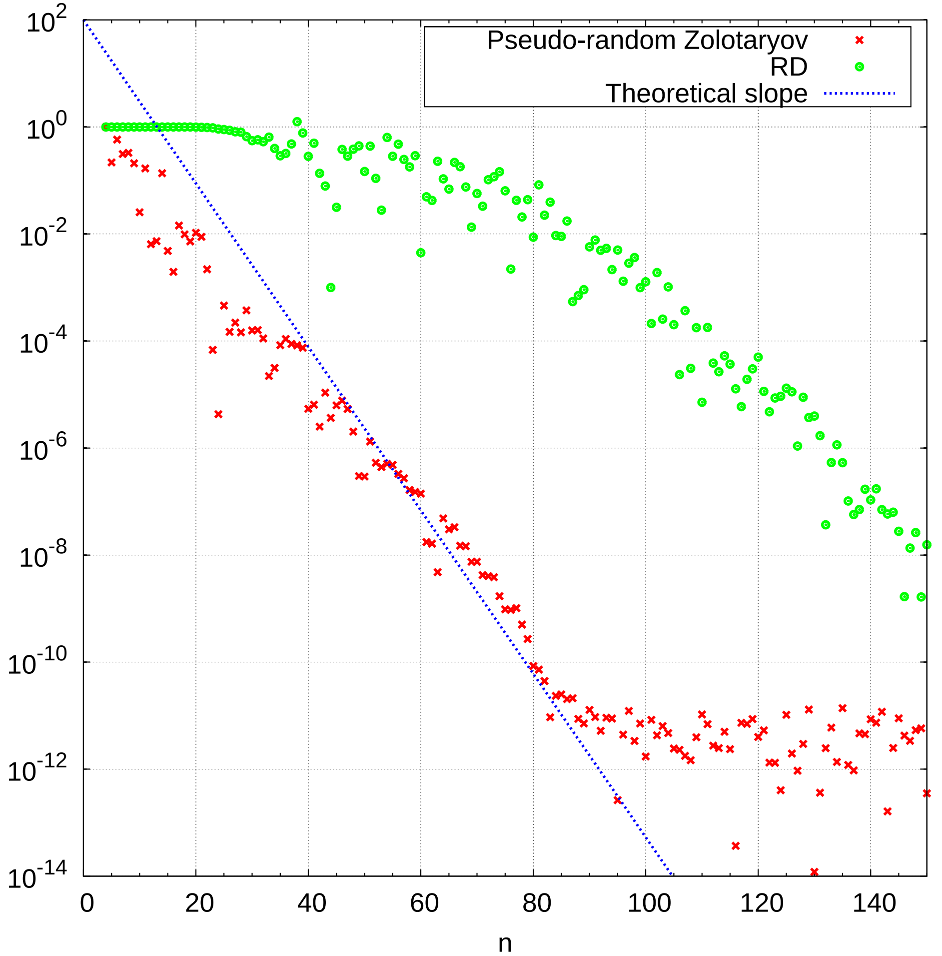

Figure 4: $t = \mathbf{10}$. Our approach becomes favorable for values of t not close to the one RD approach is targeted to.

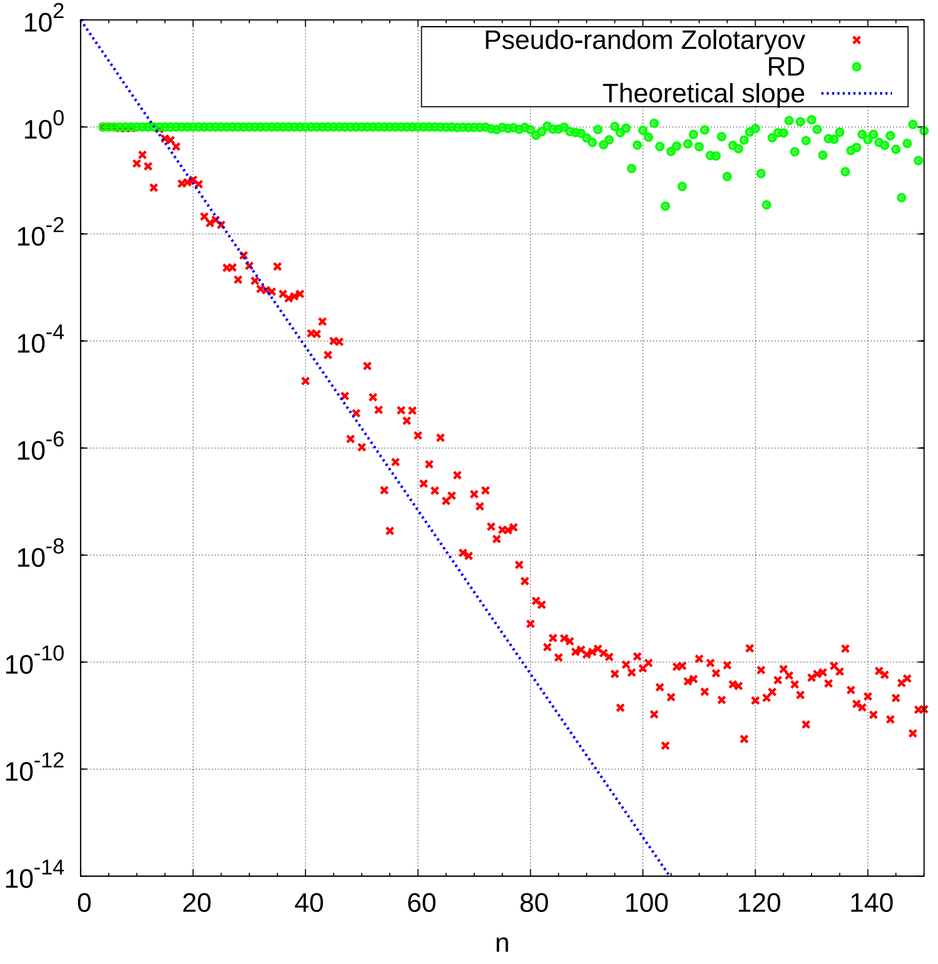

Figure 5: $t = \mathbf{100}$. RD approach almost stops converging while our approach shows almost the same convergence rate as for $t = \mathbf{1}$ and $t = \mathbf{10}$.

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