

A local restart procedure for iterative projection methods for nonlinear symmetric eigenproblems

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Joint work with Marta Betcke (London) and Vera Lochmann (Hamburg)



- Nonlinear eigenvalue problem
- Iterative projection methods
- Nonlinear minmax characterization
- A local restart procedure
- Numerical example
- Conclusions

Nonlinear eigenvalue problem

Let $J \subset \mathbb{R}$ be an open interval (maybe unbounded), and let $T(\lambda) \in \mathbb{C}^{n \times n}$, $\lambda \in J$ be a family of Hermitian matrices.

Find $\lambda \in J$ and $x \neq 0$ such that

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Then λ is called an eigenvalue of $T(\cdot)$, and x a corresponding eigenvector.

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In this talk we assume the matrices to be large and sparse.

Iterative projection methods

For linear sparse eigenproblems

$$T(\lambda) = \lambda B - A$$

very efficient methods are iterative projection methods (Lanczos, Arnoldi, Jacobi–Davidson method, e.g.), where approximations to the wanted eigenvalues and eigenvectors are obtained from projections of the eigenproblem to subspaces of small dimension which are expanded in the course of the algorithm.

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general problems: V. (2003,2004); Liao, Bai, Lee, Ko (2006), Liao (2007)
- Jacobi-Davidson:
polynomial problems: Sleijpen, Boten, Fokkema, van der Vorst (1996)
Hwang, Lin, Wang, Wang (2004,2005)
general problems: T. Betcke, V. (2004), V. (2004,2007), Schwetlick,
Schreiber (2006), Schreiber (2008)

Expanding the subspace

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BUT: In each step have to solve large linear system with varying matrix

Ways out

- **Jacobi–Davidson type method**

Expand by (approximate) solution of the correction equation

$$\left(I - \frac{T'(\theta)xx^H}{x^HT'(\theta)x}\right)T(\theta)(I - xx^H)t = -r, \quad t \perp x$$

where (x, θ) is the current Ritz pair and $r = T(\theta)x$.

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- **Arnoldi type method**

Expand by

$$v = T(\sigma)^{-1}T(\theta)x, \quad \sigma \text{ fixed for several steps}$$

motivated by the residual inverse iteration (Neumaier 1985).

Nonlinear Arnoldi Method

- 1: start with initial basis V , $V^H V = I$; set $k = m = 1$
- 2: determine preconditioner $M \approx T(\sigma)^{-1}$, σ close to first wanted eigenvalue
- 3: **while** $m \leq$ number of wanted eigenvalues **do**
- 4: solve $V^H T(\mu) V y = 0$ for (μ, y) and set $u = Vy$, $r_k = T(\mu)u$
- 5: **if** $\|r_k\|/\|u\| < \epsilon$ **then**
- 6: Accept eigenpair $\lambda_m = \mu$, $x_m = u$,
- 7: **if** $m ==$ number of wanted eigenvalues **then STOP end if**
- 8: $m = m + 1$
- 9: **if** $(k > 1)$ & $(\|r_{k-1}\|/\|r_k\| > \text{tol})$ **then**
- 10: choose new pole σ , determine preconditioner $M \approx T(\sigma)^{-1}$
- 11: **end if**
- 12: restart if necessary
- 13: Choose approximations μ and u to next eigenvalue and eigenvector
- 14: determine $r = T(\mu)u$ and set $k = 0$
- 15: **end if**
- 16: $v = Mr$, $k = k + 1$
- 17: $v = v - VV^H v$, $\tilde{v} = v/\|v\|$, $V = [V, \tilde{v}]$ and reorthogonalize if necessary
- 18: **end while**

Solving projected problem

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For Hermitian problems one can often take advantage of a variational characterization of eigenvalues

Nonlinear minmax theory

Let $T(\lambda) \in \mathbb{C}^{n \times n}$, $T(\lambda) = T(\lambda)^H$, $\lambda \in J \subset \mathbb{R}$ an open interval, and assume that the entries of T depend continuously on λ .

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Then equation $f(\lambda, x) = 0$ implicitly defines a functional p on some subset D of \mathbb{C}^n which we call the **Rayleigh functional**.

If $D = \mathbb{C}^n \setminus \{0\}$ then $T(\lambda)x = 0$ is called **overdamped**.

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Let

$$(\lambda - p(x))f(\lambda, x) > 0 \quad \text{for every } \lambda \neq p(x) \text{ and every } x \in D.$$

Enumeration of eigenvalues

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If $\lambda \in J$ is an eigenvalue of $T(\cdot)$ then $\mu = 0$ is an eigenvalue of the linear problem $T(\lambda)y = \mu y$, and therefore there exists $\ell \in \mathbb{N}$ such that

$$0 = \max_{V \in H_\ell} \min_{v \in V \setminus \{0\}} \frac{v^H T(\lambda) v}{\|v\|^2}$$

where H_ℓ denotes the set of all ℓ -dimensional subspaces of \mathbb{C}^n .

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In this case λ is called an **ℓ -th eigenvalue of $T(\cdot)$** .

Minmax characterization; V., Werner 1982

Under the conditions given above it holds:

- (i) For every $\ell \in \mathbb{N}$ there is at most one ℓ -th eigenvalue of $T(\cdot)$ which can be characterized by

$$\lambda_\ell = \min_{\substack{V \in H_\ell \\ V \cap D \neq \emptyset}} \sup_{V \in V \cap D} \rho(V). \quad (*)$$

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- (ii) If

$$\lambda_\ell := \inf_{\substack{v \in H_\ell \\ v \cap D \neq \emptyset}} \sup_{v \in V \cap D} \rho(v) \in J$$

for some $\ell \in \mathbb{N}$ then λ_ℓ is the ℓ -th eigenvalue of $T(\cdot)$ in J , and $(*)$ holds.

Safeguarded iteration

The minimum in

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- 2: **for** $k = 1, 2, \dots$ until convergence **do**
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Converges globally to a first eigenvalue, and convergence is quadratic for simple eigenvalues

Computing several eigenvalues

If $T(\lambda)$ is a family of Hermitian matrices allowing a minmax characterization of its eigenvalues in an open interval J , and if the columns of $V \in \mathbb{C}^{n \times k}$ form a basis of the current search space \mathcal{V} , then the projected problem

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Usually, while computing the m -th eigenvalue λ_m the algorithm gathers enough information in the search space \mathcal{V} about the next eigenvector to compute λ_{m+1} safely, and the eigenvalues in J can be computed one after the other without determining the same eigenvalue repeatedly.

Global restarts

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Restarting with a subspace \mathcal{V} which contains the already converged eigenvectors x_1, \dots, x_k then obviously keeps the numeration of the eigenvalues, and we can continue as above to determine the subsequent eigenpairs.

Global restarts ct.

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Therefore the size of the projected problem is growing with the number of the wanted eigenvalue, which results in increasing time consumed by the nonlinear solver and increasing storage requirement.

A local restart technique

Let $\hat{\lambda} \in J$ (called **anchor**) be an eigenvalue of $T(\lambda)x = 0$, \hat{x} be a corresponding eigenvector, and let \mathcal{V} be a subspace of \mathbb{C}^n that contains \hat{x} .

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Then $\hat{\lambda}$ is also an eigenvalue of the projected problem

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Starting with $\mathcal{V} =: \mathcal{V}_0$ we determine approximations to the eigenvalue subsequent to the anchor $\hat{\lambda}$ projecting problem $T(\lambda)x = 0$ to a sequence of subspaces $\mathcal{V}_0 \subset \mathcal{V}_1 \subset \mathcal{V}_2 \subset \dots$ which are expanded in the same way as in the Nonlinear Arnoldi algorithm aiming at the $(\ell(\mathcal{V}_k) + 1)$ -th eigenvalue in the k -th iteration step.

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Notice that the number $\ell(\mathcal{V}_k)$ of the anchor may change in the course of the algorithm.

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After convergence we may continue the Nonlinear Arnoldi method aiming at the $(\ell(\mathcal{V}_k) + 2)$ -th eigenvalue or we may replace the anchor by the newly converged eigenpair.

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Since the current search space contains useful information about further eigenvalues it is advisable to continue expanding the search spaces until the convergence has become too slow or the dimension exceeds a given bound.

A local restart technique ct.

It may happen that the algorithm converges to an eigenvalue twice, i.e. it returns $\lambda_j < \lambda_{j+1} < \dots < \lambda_{i+k} \approx \lambda_{i+k+1}$ for some $k \geq 1$.

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If λ_{i+k} is not a multiple eigenvalue, then for the current search space \mathcal{V} the projected problem (*) possesses an additional eigenvalue $\theta \in (\lambda_i, \lambda_{i+k})$ such that $\theta \neq \lambda_{i+j}$ for $j = 0, \dots, k$.

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Therefore the local number of λ_{i+k} is raised by 1, and λ_{i+k} is accepted as an $(i + k + 1)$ -th eigenvalue. This may have happened for one of the following two reasons:

A local restart technique ct.

First, an eigenvalue of $T(\lambda)x = 0$ in the interval $(\lambda_i, \lambda_{i+k})$ might have been missed out because the corresponding eigenvector \hat{x} were not sufficiently present in the initial search space and might have not been amplified sufficiently in the course of the expansions of \mathcal{V} until computing λ_{i+k} .

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Secondly, it might be the case that no eigenvalue of $T(\lambda)x = 0$ is missing in $(\lambda_i, \lambda_{i+k})$ but the newly produced eigenvector of the projected problem is a linear combination of eigenvectors of $T(\lambda)x = 0$ corresponding to eigenvalues less than λ_i and of eigenvectors corresponding to eigenvalues greater than λ_{i+k} .

A local restart technique ct.

In both cases we determine the additional eigenvalue θ and its local number $\ell + j$, and expand the search space $\hat{\mathcal{V}} = \text{span}\{\mathcal{V}, MT(\theta)x_\theta\}$ by residual inverse iteration at (θ, x_θ) , where x_θ denotes the Ritz vector corresponding to θ .

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Then by the minmax principle all eigenvalues of the projected problem

$$T_{\hat{\mathcal{V}}}(\lambda)\hat{y} = 0 \quad (**)$$

are less than or equal to the corresponding ones of $T_{\mathcal{V}}(\lambda)y = 0$, and either problem (**) has exactly $k + 1$ eigenvalues $\lambda_i, \dots, \lambda_{i+k} \in [\lambda_i, \lambda_{i+k}]$ (i.e. the additional eigenvalue has left the interval of interest) or there are $k + 2$ eigenvalues $\lambda_i, \dots, \lambda_{i+k}, \hat{\theta} \in [\lambda_i, \lambda_{i+k}]$, and it holds $\hat{\theta} \leq \theta$.

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In the latter case we repeat the expansion by residual inverse iteration until the additional eigenvalue has been moved out of the interval or has converged to an additional eigenvalues. We then adjust the numeration of the eigenvalues and continue the Arnoldi method.

Numerical Example: Rotating Wheel

Consider the gyroscopic eigenproblem

$$Kx + i\lambda Gx - \lambda^2 Mx = 0, \quad K = K^T > 0, \quad M = M^T > 0, \quad G = -G^T$$

which corresponds to a FE model of a tire with 124992 DoFs, which rotates corresponding to 50 km/h vehicle speed.

To demonstrate the efficiency of the local restart procedure we compute the eigenvalues $\lambda_{101}, \dots, \lambda_{200}$, i.e. all eigenvalues in [8250, 133367].

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To demonstrate the efficiency of the local restart procedure we compute the eigenvalues $\lambda_{101}, \dots, \lambda_{200}$, i.e. all eigenvalues in $[8250, 133367]$.

All tests were run on an SGI Altix machine with one Itanium 2 Madison 9M processor (1.6 GHz, 6MB L3, single core) with 448 GRAM.

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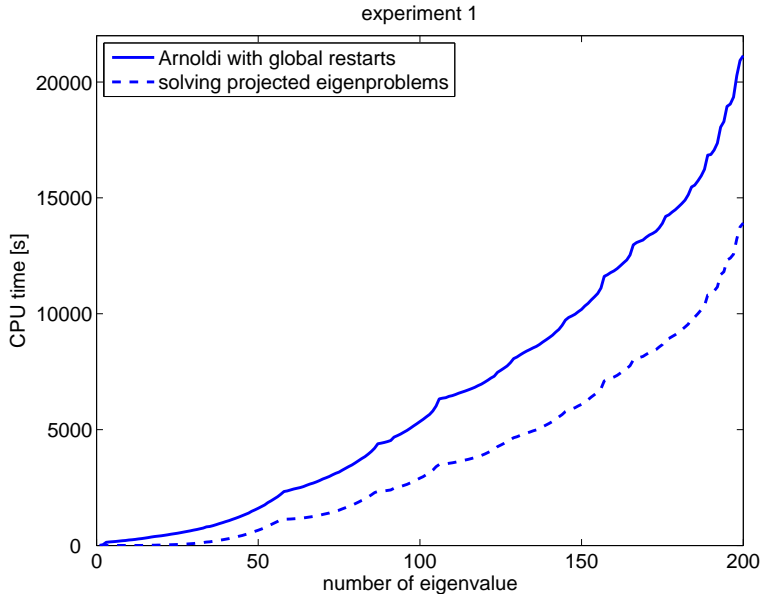
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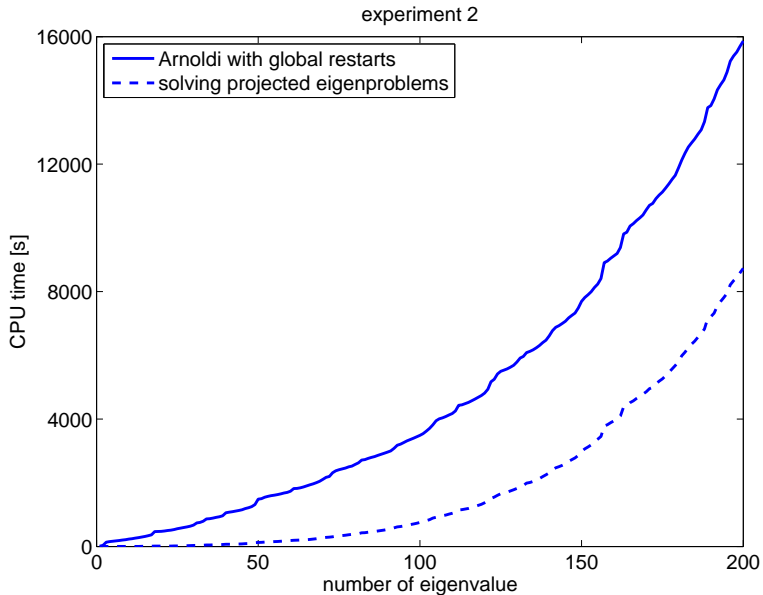
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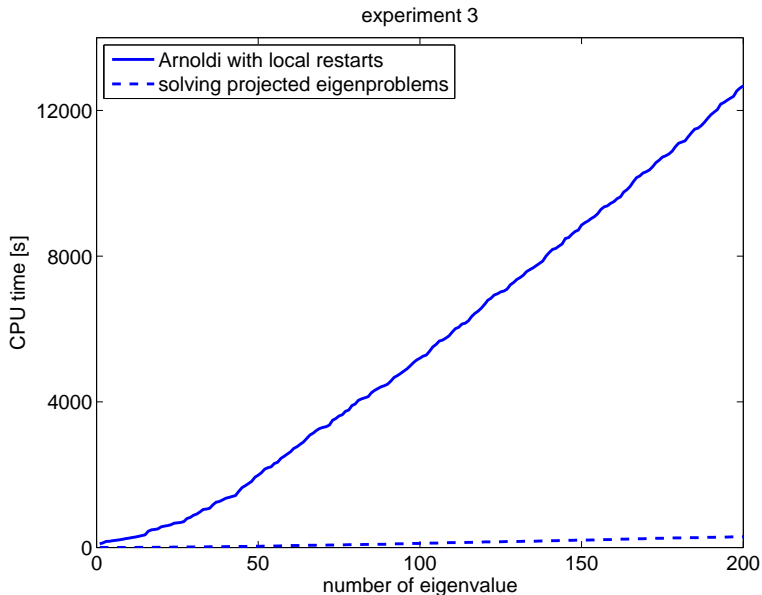
The projected problems were solved by linearization.

All evs $\lambda_1, \dots, \lambda_{200}$; global restart if $\dim V \geq 230$ 

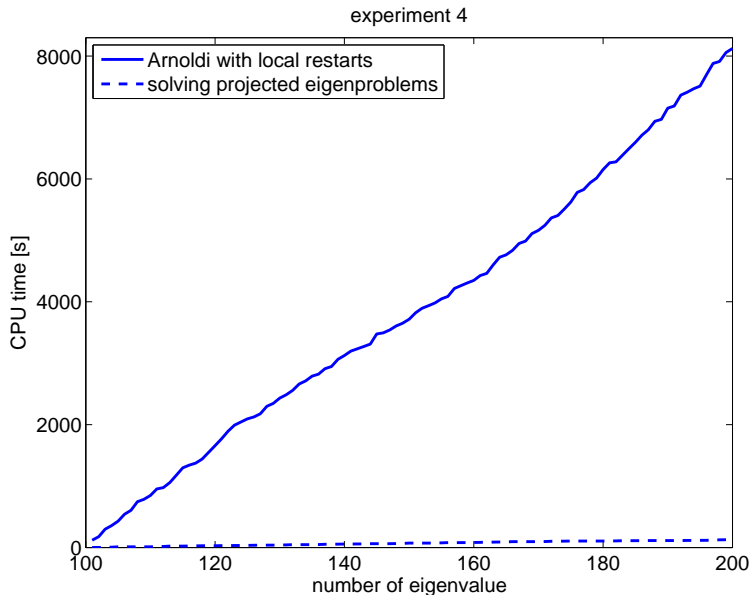
All evs $\lambda_j, j = 1, \dots, 200$; global restart if $\dim V \geq j + 60$

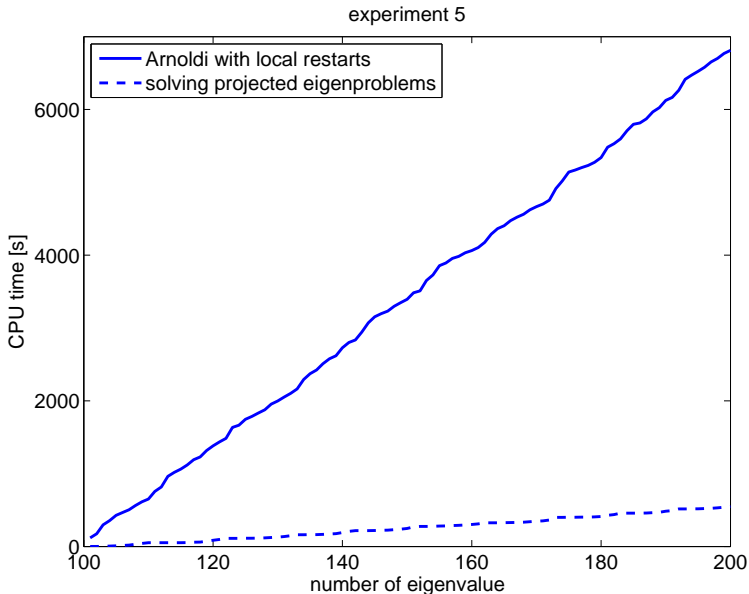


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eigs $\lambda_j, j = 101, \dots, 200$; improved local restarts

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Properly initialized, the method can be employed for computing eigenvalues in the interior of the spectrum.

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The efficiency of the method was demonstrated for a large gyroscopic eigenvalue problem modelling the dynamic behavior of a rotating tire.