Analytical and Experimental Results for Inexact Methods for Linear and Nonlinear Eigenvalue Problems

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1. OUTLINE

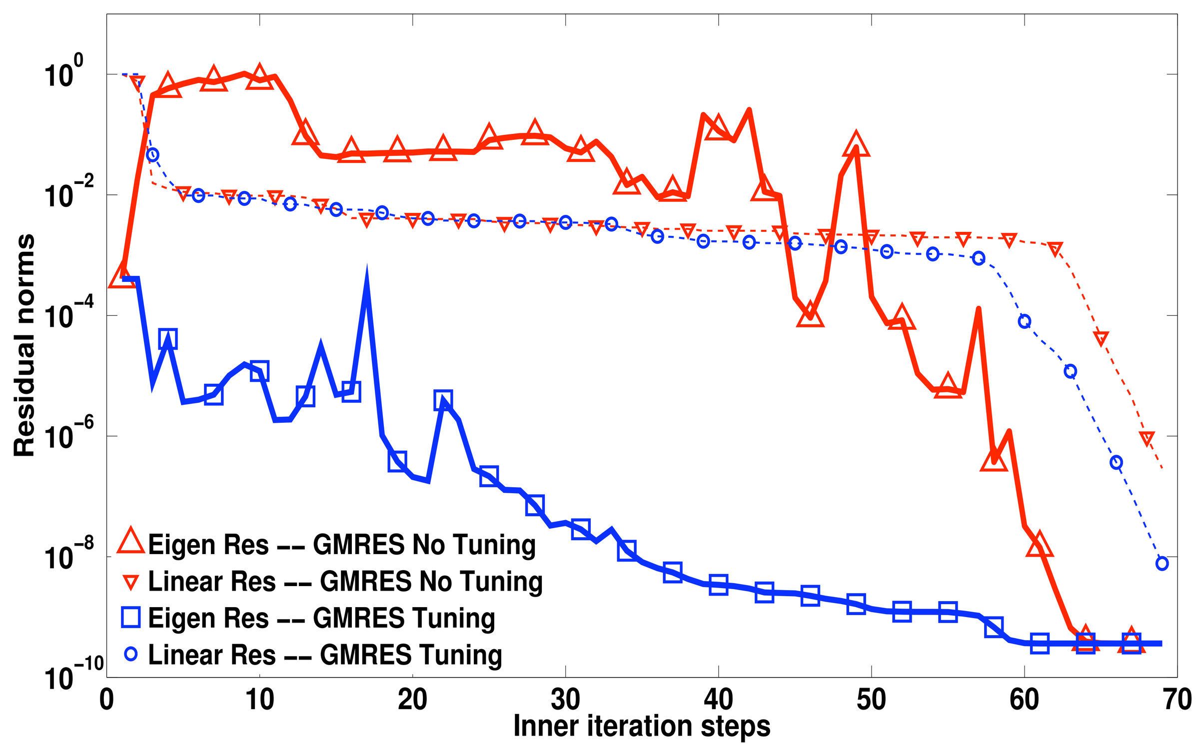
Single/multiple-vector iterations (inverse iteration, RQI, subspace iteration, etc) are widely used by engineers in a variety of applications. A special type of preconditioner with "tuning" is important for fast iterative solution of linear systems arising in inexact Rayleigh quotient iteration (IRQI).

We provide a better understanding of tuning in following aspects:

- An improved local convergence analysis of IRQI
- A new result on the equivalence of the inner solves of IRQI and single-vector Jacobi-Davidson (JD) method
- Flexible GMRES with a special initial step competitive with GMRES with tuning
- IRQI with tuning competitive with shift-invert Arnoldi
- Tuning also applicable to IRQI for general nonlinear eigenvalue problems

2. MOTIVATION

- RQI converges to (λ, v) quadratically (non-Hermitian) or cubically (Hermitian).
- Consider the iterative solution of $(A - \rho^{(i)} B)y = Bx^{(i)}$ in the ith RQI iteration $x^{(i)}$ — current eigenvector approximation $\rho^{(i)} = \frac{w^{(i)}Ax^{(i)}}{w^{(i)}Bx^{(i)}}$ — RQ.
  1. iterative solution of this linear system mandatory for very large applications
  2. preconditioned Krylov subspace solve $(A - \rho^{(i)} B)Q^{-1}\tilde{y} = Bx^{(i)}$ often leads to slow progress in eigenvector approximation for a large number of iterations
- Tuning resolves this difficulty
  1. $\mathbb{Q}$ is a low-rank modification of Q that satisfies $\mathbb{Q}x = Bx$; MVP involving $\mathbb{Q}^{-1}$ by Sherman-Morrison-Woodbury formula at minimal extra cost
  2. Steady progress in eigenvector approximation as the inner iteration proceeds



3. A NEW LOCAL CONVERGENCE ANALYSIS OF IRQI

- Known: a **fixed** inner solve tolerance → **at least linear or quadratic** local convergence; some **decreasing** tolerance → **quadratic or cubic** convergence.
- New: under some assumptions, a small **fixed** tolerance + Krylov subspace method with a tuned preconditioner → **quadratic or cubic** convergence.

problem	inner tol	initial err angle	iter 1 err angle	iter 2 err angle	iter 3 err angle	iter 4 err angle
$k(m)3plates$	$7.5e{-2}$	$2.553e{-3}$	$1.840e{-1}$	$3.437e{-3}$	$1.265e{-5}$	$8.149e{-9}$
	$5e{-3}$		$3.560e{-2}$	$1.913e{-5}$	$7.035e{-10}$	-
	exact		$6.845e{-2}$	$6.523e{-5}$	$1.659e{-10}$	-
$thermo\_dk(m)$	$2.5e{-2}$	$1.165e{-2}$	$9.874e{-3}$	$3.782e{-3}$	$8.426e{-6}$	$1.632e{-10}$
	$1e{-3}$		$3.008e{-3}$	$1.272e{-6}$	$1.825e{-11}$	-
	exact		$1.443e{-3}$	$3.336e{-6}$	$2.037e{-11}$	-
$IFISS\_1$	$1e{-1}$	$5.837e{-2}$	$1.211e{-1}$	$1.346e{-2}$	$1.307e{-4}$	$2.292e{-7}$
	$1e{-3}$		$6.148e{-3}$	$2.851e{-5}$	$7.633e{-10}$	-
	exact		$6.698e{-3}$	$3.353e{-5}$	$7.290e{-10}$	-

Table 1: *Eigenvalue residual norms of outer iterates for non-Hermitian problems*

problem	inner tol	initial err angle	iter 1 err angle	iter 2 err angle	iter 3 err angle
$bcsstk(m)13$	$5e{-4}$	$1.403e{-4}$	$2.368e{-2}$	$1.690e{-5}$	$3.274e{-12}$
	$1e{-6}$		$2.993e{-4}$	$6.818e{-11}$	-
	exact		$2.400e{-4}$	$1.005e{-11}$	-
$bcsstk(m)39$	$1e{-3}$	$1.1626e{-3}$	$2.0426e{-2}$	$1.5086e{-5}$	$4.2022e{-12}$
	$2.5e{-6}$		$1.3547e{-3}$	$2.0753e{-9}$	-
	exact		$1.8604e{-4}$	$8.8151e{-12}$	-
$thermo\_tk(c)$	$1.25e{-2}$	$8.8808e{-3}$	$1.3759e{-2}$	$3.7919e{-5}$	$4.5113e{-12}$
	$1.25e{-4}$		$2.6774e{-3}$	$1.8239e{-8}$	-
	exact		$4.4756e{-4}$	$1.2356e{-10}$	-

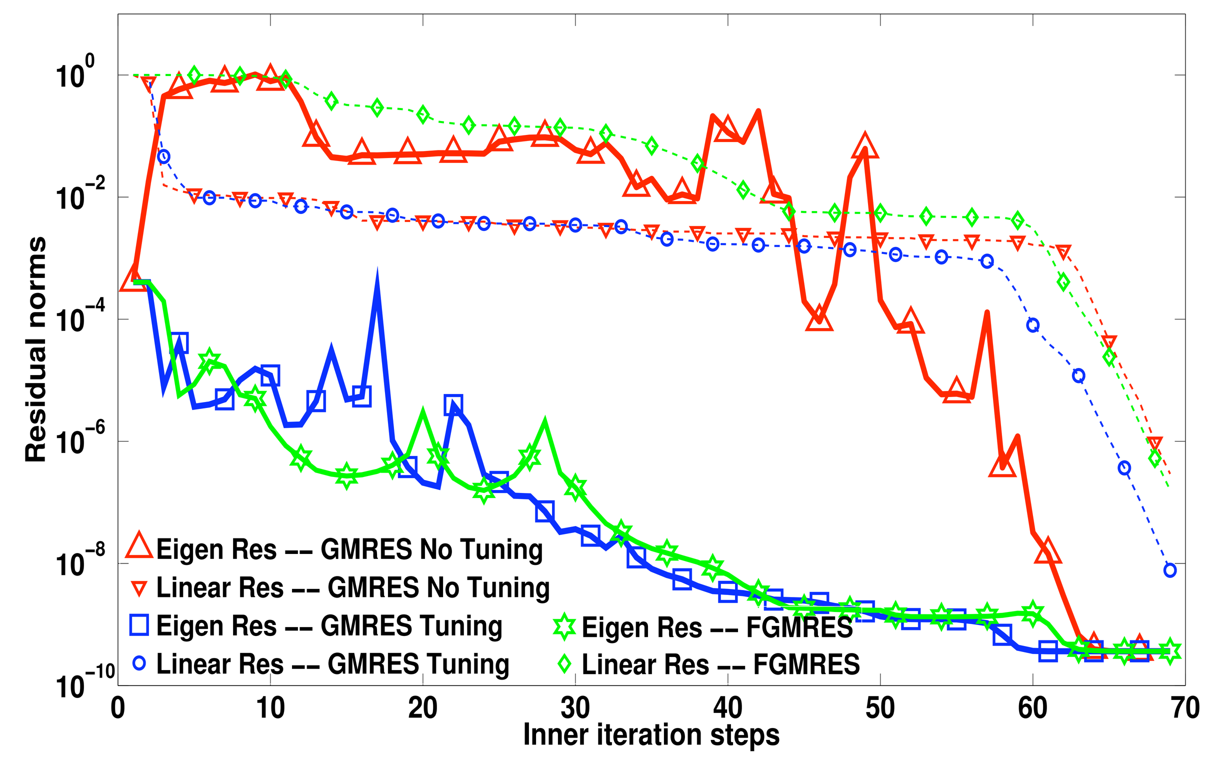
Table 2: *Eigenvalue residual norms of outer iterates for Hermitian problems*

4. EQUIVALENCE OF THE INNER SOLVES OF IRQI AND JD

- If both inner solves are done by the full orthogonalization method (FOM) with a tuned preconditioner $\mathbb{Q}$, they generate the same sequence of inner iterates.
- Tuning for the inner solves of IRQI implicitly achieves the way JD solves for a correction to obtain a better eigenvector approximation.

5. A SPECIAL FLEXIBLE GMRES INNER SOLVER FOR IRQI

- With an untuned Q, the initial inner iterate $y_1 = Q^{-1}Bx$ is usually a poor eigenvector approximation (much worse than x).
  With a tuned $\mathbb{Q}$, $y_1 = \mathbb{Q}^{-1}Bx = x \approx v$; tuning has no further impact afterwards.
- A flexible GMRES with tuning in the 1st iteration and no tuning in subsequent iterations: performance similar to GMRES with tuning in every inner iteration; only one extra vector storage.
- Also closely connected to single-vector JD



6. PERFORMANCE COMPARISON WITH SHIFT-INVERT ARNOLDI

- For non-Hermitian problems, given the same initial eigenvector approximation $x^{(0)}$, our IRQI converges to (λ, v) at least twice as quickly as shift-invert Arnoldi, in terms of total inner iteration counts.

problem	$utm1700a(b)$		$mhd4800a(b)$		$k(m)3plates$	
method	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES
eigres	$1.567e{-10}$	$5.357e{-10}$	$5.115e{-11}$	$6.024e{-12}$	$3.285e{-8}$	$2.109e{-8}$
outer	5	3	8	3	7	2
inner	296	177	765	237	425	143
method	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR
eigres	$1.735e{-10}$	$1.111e{-10}$	$3.085e{-11}$	$2.155e{-12}$	$8.913e{-8}$	$2.536e{-7}$
outer	5	3	8	3	6	3
inner	552	320	1474	639	1047	569
problem	$thermo\_dk(m)$		$IFISS\_1$		$IFISS\_2$	
method	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES	AR/GCRO	RQ/GMRES
eigres	$1.251e{-8}$	$7.839e{-9}$	$7.859e{-10}$	$7.945e{-10}$	$1.182e{-09}$	$1.845e{-10}$
outer	6	2	12	3	19	3
inner	992	251	965	174	3164	409
method	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR	AR/IDR	RQ/IDR
eigres	$3.148e{-5}$	–*	$7.699e{-10}$	$7.659e{-10}$	$1.669e{-09}$	$1.511e{-10}$
outer	4	–	12	3	19	3
inner	943	–	1705	253	8820	954

Table 3: *IRQI vs. shift-invert Arnoldi for computing one interior eigenpair*

* IDR(4) with a tuned preconditioner fails to converge to $\tau = 0.1$ for $thermo\_dk(m)$.

References

[1] DANIEL B. SZYLD AND FEI XUE, *Efficient preconditioned inner solves for inexact Rayleigh quotient iteration and their connections to the single-vector Jacobi-Davidson method*, SIAM Journal on Matrix Analysis and Applications. vol. 32 (2011) pp. 993–1018.

7. NONLINEAR EIGENVALUE PROBLEMS

- Solve $T(\lambda)v = 0$ for (λ, v), where $T(\cdot) : \Omega \to \mathbb{C}^{n\times n}$ is a nonlinear matrix-valued function; a very recent active research area, with a large variety of applications.
- Tuning also applicable to IRQI for nonlinear eigenvalue problems.
- Local convergence analysis of inexact inverse iteration, IRQI, single-vector JD and generalized Davidson (GD) method with several different sequences of inner solve tolerances.
- Possible improved local convergence analysis of IRQI and JD, inspired by the work shown above for linear problems.
- Study of deflation and restarting techniques for inexact algorithms with subspace acceleration, e.g., full JD or the nonlinear Arnoldi method, for computing several eigenpairs; more robust convergence with random starting vector.