An Implementation and Analysis of the Refined Projection Method For (Jacobi-)Davidson Type Methods

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Standard eigenvalue problem

Find *k* eigenvalues and associated eigenvectors of a large, sparse symmetric matrix $A \in \Re^{n \times n}$:

$$Ax_i = \lambda_i x_i, \ \lambda_1 \leq \ldots \leq \lambda_k$$

Our problem: compute a few λ_i closest to a shift τ or multiple shifts $\tau_1, \tau_2, \ldots, \tau_k$

Our focus: efficiency and accuracy in general subspace (not Krylov subspace)

Problem of standard Rayleigh-Ritz

Standard Rayleigh-Ritz extracts Ritz pairs (θ, u) where $u \in V$ by imposing Galerkin condition

$$Au - \theta u \perp V$$

Best convergence for extreme eigenvalues, but not for interior eigenvalues due to spurious Ritz values

Reason for spurious Ritz values: the associated Ritz vector is a combination of nearby eigenvectors $\rightarrow$ meaningless vector

Trouble and effect causing by spurious Ritz values: difficult to select appropriate vectors and cause irregular convergence

Harmonic and refined Rayleigh-Ritz

Harmonic Rayleigh-Ritz extracts harmonic Ritz pairs $(\widetilde{\theta}_i, \widetilde{u}_i)$ by imposing Petrov-Galerkin condition

$$(A - \widetilde{\theta}_i I)\widetilde{u}_i \perp (A - \tau I)V$$

Refined Rayleigh-Ritz replaces Ritz vector with a vector $\hat{u} \in V$

$$\text{minimize} \quad \|A\hat{u}_i - \theta_i \hat{u}_i\|, \; i = 1, 2, \ldots, k.$$

Refined Rayleigh-Ritz achieves monotonic convergence while computational costs are much more expensive

Our goal: develop an efficient approach with similar costs to Rayleigh-Ritz

Computation and accuracy of refined projection

Approach I: Solve a set of skinny tall SVD problems

1. compute $(A - \theta_i I)V = Q_i R_i, i = 1, 2, \ldots, k$.
2. solve a set of small SVD problems on each R_i.

Merits: numerically stable; Drawbacks: $O(knm^3)$ per restart

Approach II: Solve a set of small eigenvalue problems

1. compute $\lambda_{min}(V^T A^T AV - 2\theta_i V^T AV + \theta_i^2 I)$

Merits: $O(km^4)$ per restart; Drawbacks: numerically unstable

Approach III: Solve one skinny tall SVD problem

1. Compute a set of the smallest singular triplets of R_1.

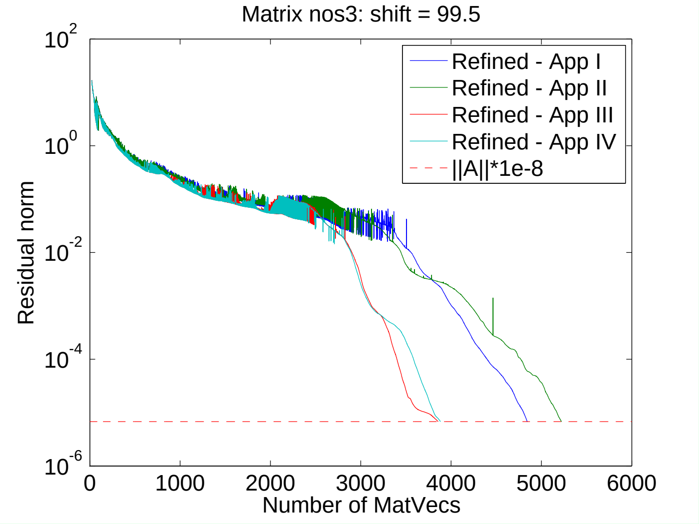
Merits: numerically stable; Drawbacks: $O(nm^3)$ per restart and effectiveness of $\hat{u}_i, i = 2, \ldots, k$ may reduce

Computation and accuracy of refined projection

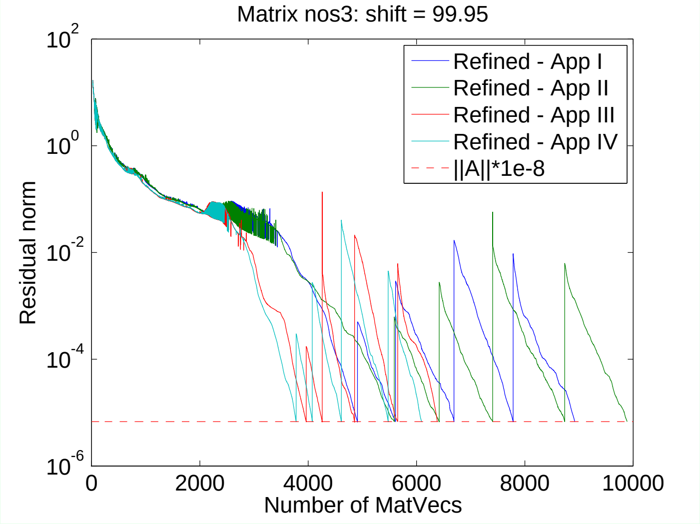
Approach IV: Solve one small eigenvalue problem

1. Compute a set of the smallest eigenpairs of $\lambda_{min}(V^T A^T AV - 2\theta_1 V^T AV + \theta_1^2 I)$.

Merits: $O(m^4)$ per restart; Drawbacks: numerically unstable



(a) Seeking one

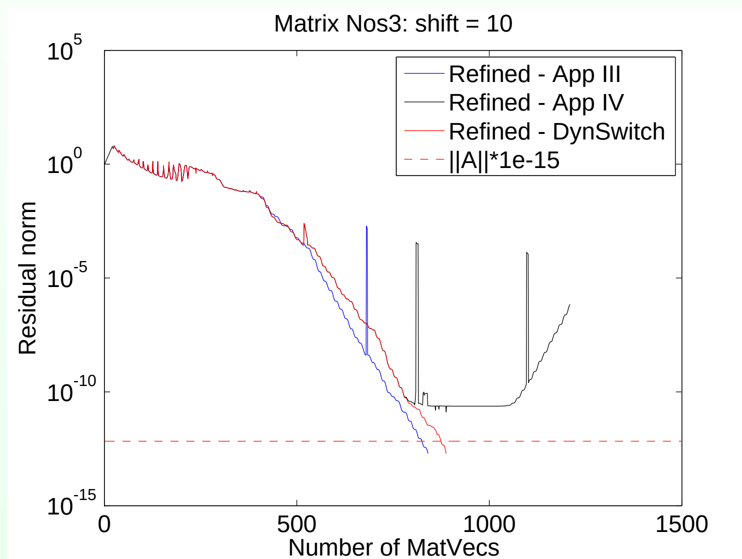


(b) Seeking a few

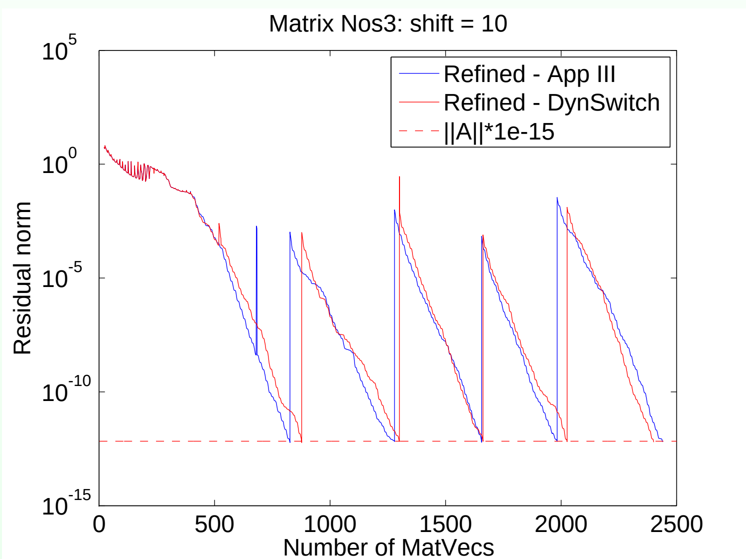
Approaches III and IV converge faster than approaches I and II

An efficient and accurate hybrid method

Hybrid Approach: combining Approach III and IV



(a) Seeking one



(b) Seeking a few

Advantages of hybrid approach:

1) converges similarly with approach III

2) needs much less computation cost

Evaluation: Test matrices

Table 1: Properties of the test matrices

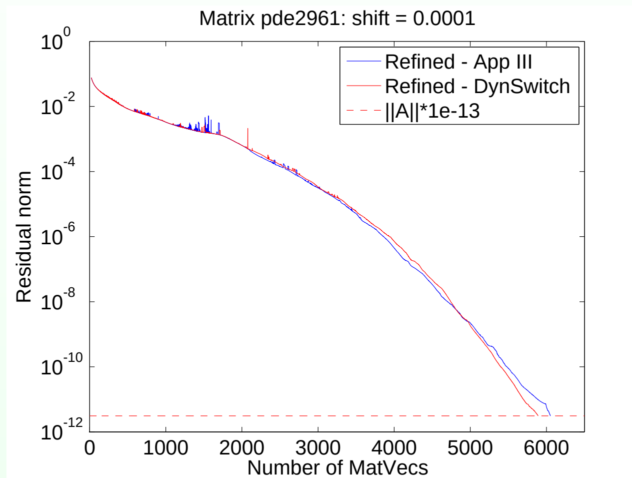
Matrix	pde2961	dw2048	SiNa	Kuu
order	2961	2048	5743	7102
nnz(A)	14585	10114	198787	340200
$\kappa(A)$	9.5E+2	5.3E+3	5.0E+2	1.6E+4
$\|A\|_2$	1.0E+1	1.0E+0	2.6E+1	5.4E+1
Application	Model PDE	Dielectric waveguide	Quantum chemistry	Structural problem

Two types of problems:

1) Seek smallest magnitude eigenvalue of $B = \begin{pmatrix} 0 & A^T \\ A & 0 \end{pmatrix}$

2) Seek interior eigenvalue of real symmetric A

Seek smallest magnitude eigenvalue of B



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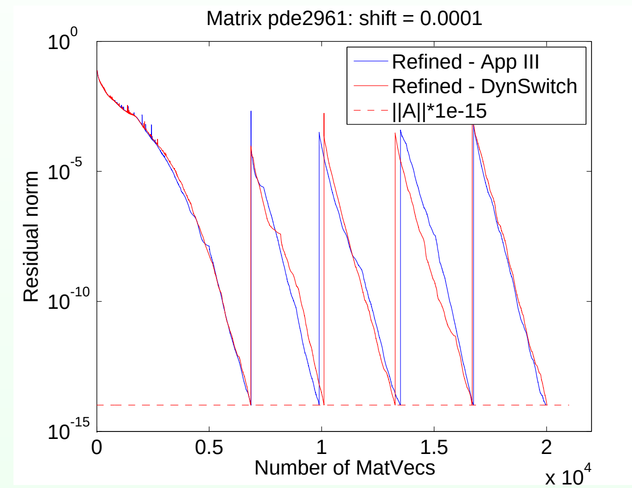
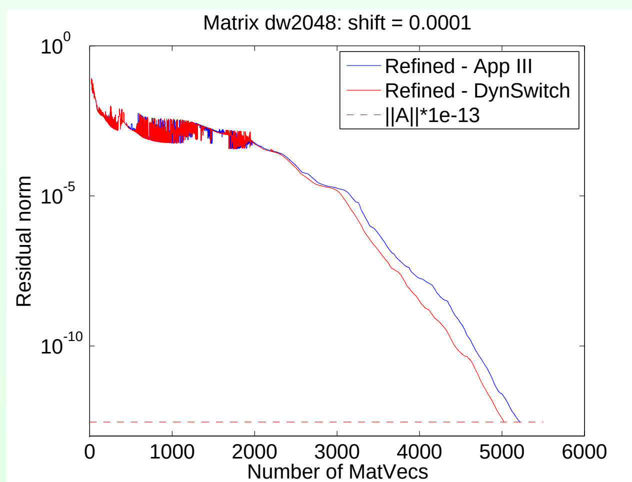
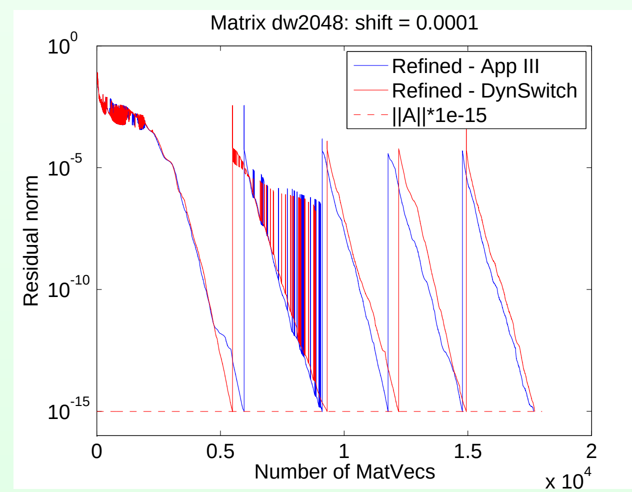


(b) Seeking a few

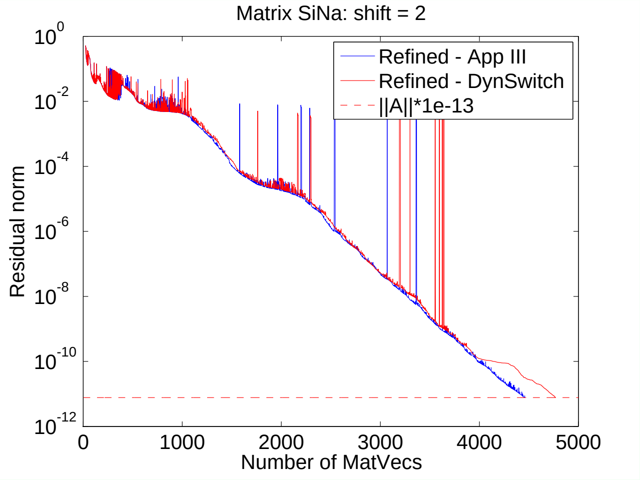


(c) Seeking one

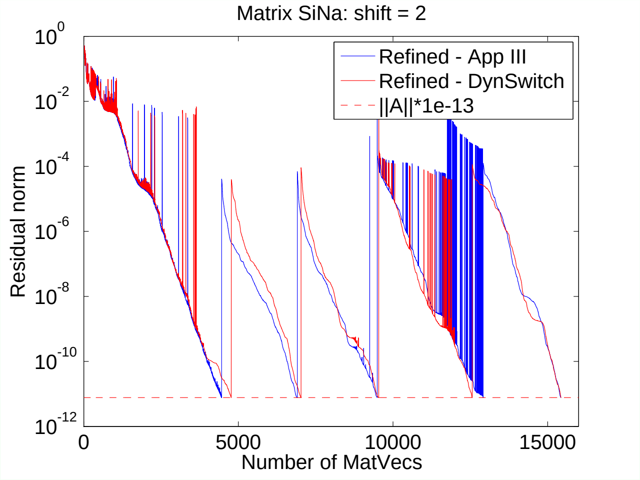


(d) Seeking a few

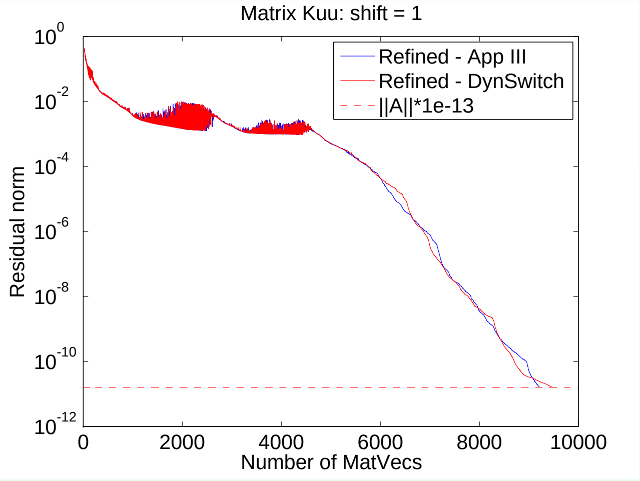
Seek interior eigenvalue of real symmetric A



(a) Seeking one



(b) Seeking a few



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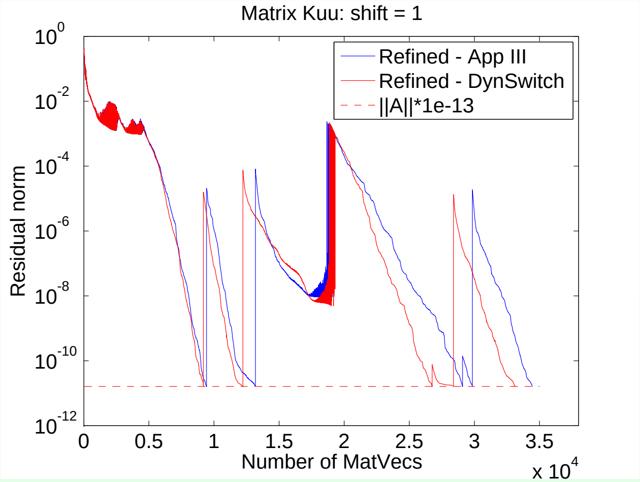

(d) Seeking a few

Comparing Matvecs and Time

Table 2: Seeking one

Mat:	pde2961		dw2048		SiNa		Kuu	
App	MV	Sec	MV	Sec	MV	Sec	MV	Sec
RR	7014	62	7536	56	4833	49	12774	292
III	6054	123	5215	85	4458	102	9215	412
Hyd	5892	78	5023	52	4771	65	9468	280

Table 3: Seeking a few

Mat:	pde2961		dw2048		SiNa		Kuu	
App	MV	Sec	MV	Sec	MV	Sec	MV	Sec
RR	17572	180	17602	135	12668	137	45325	577
III	17313	362	14399	227	15424	367	34451	888
Hyd	17862	249	14069	161	15433	228	33149	556

Conclusion and future work

Refined and Harmonic Rayleigh-Ritz methods are useful tools to tackle interior eigenvalue problems.

- Present a promising novel efficient approach for computing refined Ritz vectors
- A robust metric to monitor the error of the desired Ritz vector
- Study similar issues in the harmonic projection method
- Study an efficient approach for refined harmonic projection method

Thank you for your attention!

Any Question?