Preconditioning Techniques for Large Eigenvalue Problems

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Outline

- Introduction
- Comparison of different preconditioned eigenvalue methods
- Preconditioners developed from the Newton recurrences
- Summary

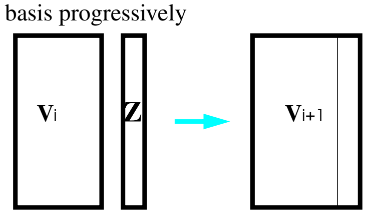
Eigenvalue Problem

$$Ax = \lambda x$$

- matrix size is small: QR methods (LAPACK, EISPACK)
- dominant eigenvalue/eigenvector: power method, subspace iterations, trace minimization...
- a few extreme eigenvalues/eigenvectors: the Lanczos method, the Arnoldi method...

Schematics of Preconditioned Eigenvalue Methods

1. Build a basis progressively



2. Rayleigh-Ritz projection

Preconditioning is solving

$$Mz = s$$

where s is computed from V_i, A, etc.

Preconditioning

The matrix: $M \approx A - \lambda_i I$

	RHS(s)
Arnoldi	Av_i
Davidson	r_i
Orthogonalized Arnoldi	$(I - V_i V_i^T) A v_i$
Approximate Cayley	$(A - \lambda_i I) v_i$
Approximate RQI	x_i

Number of eigenvalue problems solved

preconditioner	Arnoldi	App Cayley	Orth Arnoldi	Davidson
(NONE)	18	18	18	18
diagonal	9	9	10	28
SOR	6	5	15	34
ILU0	5	3	13	29
ILUTP	4	2	15	27

5 smallest eigenvalues and corresponding eigenvectors

45 RSA matrices from Harwell-Boeing collection

basis size 25

tolerance on residual norm $10^{-12}\|A\|_F$

restart, 12 Ritz vectors

starting vector $[1\ \ldots\ 1]^T$

Comparison of Execution Time

preconditioner	Arnoldi	App Cayley	Orth Arnoldi	Davidson
(NONE)	16	0	2	0
diagonal	0	0	0	28
SOR	0	0	0	34
ILU0	1	0	1	27
ILUTP	0	0	2	26

Number of cases where the method converged in the least amount of time.

Davidson vs. App. RQI

	Davidson	RQI prec
BCSSTM21	12	25
BCSSTM24	28	78
BCSSTM25	31	107

MATVEC used to solve the eigenvalue problems

5 smallest eigenvalues and corresponding eigenvectors

3 Largest diagonal matrices from Harwell-Boeing collection

basis size 25

tolerance on residual norm $10^{-12}\|A\|_F$

restart, 12 Ritz vectors

starting vector $[1\ \ldots\ 1]^T$

Davidson Preconditioning is Flawed

Si_6 solved with various preconditioners

	MATVEC	time (sec)
(NONE)	3758	414.9
Diagonal	5067	551.8
ILU0	-36	-
ILUTP	-17	-

Good preconditioners for linear systems are not effective preconditioners for eigenvalue problems

Eigenpair wanted 60 (smallest)

Basis size 20

Maximum MATVEC 6000

SGI R10000 190MHz

Flaws in the Davidson Preconditioner

Difficulties in approximating $(A-\lambda I)^{-1}$

1. When $(A-\lambda I)^{-1}$ is approximated well, the result is bad.

$$z = (A-\lambda I)^{-1} r \equiv (A-\lambda I)^{-1}(A-\lambda I)x = x$$

2. If λ is close to an exact eigenvalue, $(A-\lambda I)$ is ill-conditioned.
3. $(A-\lambda I)$ is indefinite if λ is not an extreme eigenvalue.
4. misconvergence.
5. complex eigenvalue for real matrices -- complex preconditioner.

Davidson Preconditioning is Inexact Newton

If the exact eigenvalue μ is known, the Newton recurrence for finding a solution of

$$(A-\mu I)x = 0$$

is

$$x_{i+1} = x_i - J^{-1} r_i$$

$$J = (A-\mu I),\ r_i = (A-\mu I)x_i$$

The Davidson preconditioner is an approximate form of the above Newton recurrence

$$z = M^{-1} r_i \approx (A-\mu I)^{-1} r_i$$

Newton Methods

The preconditioning equations used in various Newton methods.

1. Davidson (J_R)

$$(A-\delta_i I)z = r_i$$

2. Augmented Newton (J_A)

$$\begin{bmatrix} (A-\delta_i I) & -x_i \\ -x_i^T & 0 \end{bmatrix} \begin{bmatrix} z \\ \varsigma \end{bmatrix} = \begin{bmatrix} r_i \\ 0 \end{bmatrix}$$

3. Constrained Newton (J_C)

$$(A-\delta_i I - x_i x_i^T (A+A^T))z = r_i$$

$$x_{i+1} = \frac{x_i - z}{\|x_i - z\|}$$

4. Newton-Olsen

$$z = (A - \delta_i I)^{-1}\left(I - \frac{x_i x_i^T (A - \delta_i I)^{-1}}{x_i^T (A - \delta_i I)^{-1} x_i}\right) r_i$$

5. Deflated Newton (J_D)

$$(A - \delta_i I + \alpha x_i x_i^T) z = r_i$$

6. Jacobi-Davidson (J_J)

$$(I - x_i x_i^T)(A - \delta_i I)(I - x_i x_i^T) z = r_i$$

Newton Preconditioners

1. the Davidson preconditioner which approximates $(A - \delta I)$
2. Incomplete factorization of J_A
3. Olsen preconditioning -- run a Davidson preconditioner twice
4. Krylov subspace methods on J_C, J_D, J_J, J_R
5. Approximate Inverse on J_C, J_D, J_J, J_R

Si_6 --- CG preconditioning

	its	MATVEC	time (sec)
$A - \delta I$	307	51648	1286
$A - \delta I + xx^T$	254	44054	1133
$A - \delta I - 2xx^T A$	266	46610	1213
$(I - xx^T)(A - \delta I)(I - xx^T)$	-	-	-

Fixed number of CG steps to solve the preconditioning equation

Execution time

	GR3030	BCSSTM13
$A - \delta I$	1.0	10.0
$A - \delta I + xx^T$	0.7	9.9
$A - \delta I - 2xx^T A$	1.2	14.1
$(I - xx^T)(A - \delta I)(I - xx^T)$	111	12.7

Summary

- Inexact Newton methods are good preconditioners for eigenvalue problems
- CG($A - \delta I + xx^T$) offers an alternative to Jacobi-Davidson and the original Davidson preconditioning scheme