Reduction of nonlinear eigenproblems with JD

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Outline

Polynomial Eigenproblems

$$(\lambda^\ell C_\ell + \cdots \lambda C_1 + C_0)x = 0)$$

or $\psi(\lambda)x = 0$

For examples: quadratic eigenproblems

- Reduction to standard problem

- Newton for Rayleigh quotient

Jacobi Davidson approach

Alternatives for Rayleigh quotient

Classical: Reduction

From $(\lambda^2 M + \lambda C + K)x = 0$

To $Az = \lambda Bz$

with $A = \begin{pmatrix} 0 & I \\ -K & -C \end{pmatrix} \quad B = \begin{pmatrix} I & 0 \\ 0 & M \end{pmatrix} \quad z = \begin{pmatrix} x \\ \lambda x \end{pmatrix}$

and then $B^{-1}Az = \lambda z$

Problems:

- matrices twice as big

- how to select wanted solutions?

- inversion of B

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Classical: Newton for RQ

$$x^*\psi(\lambda)x = 0$$

$$\lambda^2(x^*Mx) + \lambda(x^*Cx) + x^*Kx = 0$$

Two roots; one useful, one spurious

In subspace methods: approximations

How to select?

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Jacobi-Davidson

the basic ideas for $Ax = \lambda x$:

Given some subspace $V_m = \{v_1, ..., v_m\}$ (orthonormal)

Determine approximations $z = V_m s$, θ such that

$AV_m s - \theta V_m s \perp \{v_1, ..., v_m\}$

or $V_m^* A V_m s = \theta s$

θ is Rayleigh quotient for $V_m s$

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Jacobi-Davidson (2)

θ, s eigenpair of $V_m^* A V_m$

Select proper eigenpair

Determine $t \perp s$ such that

$$A(s+t) = \lambda(s+t)$$

t satisfies:

$$(1 - ss^*)(A - \lambda I)(I - ss^*)t = -(AV_m s - \theta V_m s)$$

Replace λ by θ

Solve (approximately) for t and expand V_m with t

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Other viewpoint

$Ax = \lambda x$, **Let** $\theta = y^* Ay$ **with** $y^* y = 1$

write $x = y + \Delta y$, $\Delta y \perp y$, $\lambda = \theta + \Delta\theta$

Ignore quadratic terms

Then

$$(I - yy^*)(A - \theta I)(I - yy^*)\Delta y = -r$$

with $r = Ay - \theta y$

Newton method; quadratic convergence

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Nonlinear eigenproblems

Similar Newton approach for Rayleigh quotient:

$x^*\psi(\lambda)x = 0$

leads to the projected problem:

$V_m^*\psi(\theta)V_m s = 0$

V_m **is expanded with approximate** $t \perp y = V_m s$ **from**

$(I - \frac{py^*}{y^*p})\psi(\theta)(I - yy^*)t = -\psi(\theta)y$

with $p = \psi'(\theta)y$

for this choice of p**: quadratic convergence**

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QEP

Expansion of subspace with

$$(I - \frac{py^*}{y^*p})(A + \theta B + \theta^2 C)(I - yy^*)t = -(Ay + \theta By + \theta^2 Cy)$$

V_m **is expanded with** t

New s **and** θ **from:**

$$W_m^* AV_m s + \theta V_m^* BV_m s + \theta^2 V_m^* CV_m s = 0$$

Problem: selection of proper θ **and** s

Rayleigh quotient has two solutions for θ

Example from acoustics

$Ax + \lambda Bx + \lambda^2 Cx = 0$

A, C **19 nonzero's per row,** B **complex,** $n = 136161$

Results for interior isolated eigenvalue on CRAY T3D

Processors	**Elapsed time**
16	206.4
32	101.3
64	52.1

one (sparse) matrix inversion takes about 5 **minutes**

on 64 **processors when at peak performance**

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Rayleigh Quotient for QEP

Work with Hochstenbach

With y an approximation for eigenvector:

$(A + \theta B + \theta^2 C)y \perp y$

Hence $\alpha\theta^2 + \beta\theta + \gamma = 0$

$\alpha = y^* C y$, $\beta = y^* B y$, $\gamma = y^* A y$

For y close to eigenvector: One θ meaningful

Decision based on value of $||(A + \theta B + \theta^2 C)y||_2$

If y not accurate: difficult to decide

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Inaccurate approximations

Situation occurs in subspace methods

Rayleigh quotient for standard eigenproblem is accurate:

First order perturbation in eigenvector gives second

order perturbation in Rayleigh quotient

For QEP: if $\beta^2 - 4\alpha\gamma$ is small then both solutions for θ

are very sensitive for perturbations in y

QEP (and higher order) offer more possibilities for eigenvalue approximations

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Alternatives for RQ

For standard problem Ay and y

θ follows from projecting Ay onto y

For QEP three vectors: Ay, By, and Cy

Form asymptotically one plane

Consider projection of these vectors on plane $\{p, q\}$

with p, q combinations of the three vectors

Consider generalized residual $r = (\mu C + \nu B + A)y$

$\mu \approx \lambda^2$, $\nu \approx \lambda$

Hence μ/ν and ν both approximations for λ

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Alternatives for RQ (2)

Galerkin conditions for $\{p, q\}$: $r \perp p$ and $r \perp q$

$$[p \ \ q]^*[Ay \ \ By] \begin{pmatrix} \mu \\ \nu \end{pmatrix} = -[p \ \ q]^* Cy$$

Good choices for p, q: two largest left singular vectors of $[Cy \ \ By \ \ Ay]$

$$\frac{\delta\mu/\nu}{\delta y}(x) = \frac{1}{\lambda}\frac{\delta\mu}{\delta y}(x) - \frac{\delta\nu}{\delta y}(x)$$

This suggests:

If θ is small then ν may be better

otherwise μ/nu also good candidate

quality judged by residual

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Example

Results for randomly generated A, B, c, $n = 100$

Method	Approx	error	$\|\|r\|\|$
1-dim Gal	$7.218 + 2.738i$	0.0428	0.307
2-dim Gal	$7.230 + 2.769i$	0.0110	0.290
2-dim ν	$7.189 + 2.800i$	0.0445	0.329

for situation with small discriminant

Method	Approx	error	$\|\|r\|\|$
1-dim Gal	$1.0117 - 0.0444i$	0.0444	0.0431
2-dim Gal	$1.0076 - 0.0025i$	0.0034	0.0034
2-dim ν	$1.0095 - 0.0014i$	0.0015	0.0027

Relevant references

SIAM Templates for Eigenproblems

Hochstenbach and VDV

SIAM J. Sci. Comput., 25(2), p. 591-603, 2003

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