Spectral considerations in the solution of parameterized linear systems

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The problem

$$(\sigma_j^2 A + \sigma_j B + C)x = b \qquad j = 1, \ldots, s$$

$A, B, C \in \mathbb{C}^{n\times n} \quad b \in \mathbb{C}^n \quad \sigma_j \in \mathbb{C} \quad j = 1, \ldots, s \quad s \gg 1 \quad x = x(\sigma_j)$

Applications

- Frequency analysis of dynamical systems
  A, B, C complex symmetric $\quad \sigma_j$ in large interval
- Electromagnetic radiation scattering (also higher order in σ)
  A, B, C complex symmetric $\quad \sigma_j \in [\sigma_0 - \delta, \sigma_0 + \delta]$
- Wave propagation in porous media
- Quadratic eigenvalue problems/solvers (false friend)

Focus on: A, B, C complex symmetric

Solution methods

$$(\sigma_j^2 A + \sigma_j B + C)x_j = b \qquad j = 1, \ldots, s$$

- ⋆ Solution of each system separately
- ⋆ Matrix polynomial theory (for very small problems)
- ⋆ Newton-type methods (from non-linear equation theory)
- ⋆ Padè approximation (Kuzuoglu & Mittra, 1998)
- ⋆ Double–size matrix formulation (Feriani, Perotti & S. 1998, Perotti & S. 2002, Meerbergen 2003)
- ⋆ Second–order Arnoldi-type methods (T.J.Su & Craig '91, Bai, Freund '00-'06, ...)

Matrix formulation

$$(\sigma^2 A + \sigma B + C)x = b$$

Several (math. equiv.) formulations. We consider

$$\left[\begin{pmatrix} B & C \\ C^T & 0 \end{pmatrix} + \sigma \begin{pmatrix} A & \\ & -C^T \end{pmatrix}\right] \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix} \qquad y = \sigma x$$

$$(T + \sigma S)z = d \qquad T, S \quad \text{complex sym}$$

- ◇ S nonsingular $\Leftrightarrow$ A, C nonsingular
- ◇ C^T transpose of C (no conjugation)
- ◇ case of C singular can be handled!

Matrix formulation. Singular C

Let P be such that CP has full column rank. Then

$$\left[\begin{pmatrix} B & CP \\ P^TC^T & 0 \end{pmatrix} + \sigma \begin{pmatrix} A & \\ & -P^TC^TP \end{pmatrix}\right] \begin{bmatrix} \hat{y} \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

(Simoncini, '99)

Linearized problem

Solve

$$(T + \sigma_j S)z = d$$

$T + \sigma_j S$ (complex) symmetric $j = 1, \ldots, s$

T, S symmetric S nonsingular

Ideal Solver:

(a) Preserve symmetry

(b) Efficiently handle several σ_j's simultaneously

(a) Obtain fast convergence

System arises in other contexts: e.g. generalized eigenvalue pbs

Various approaches

(A) Solve

$$(TS^{-1} + \sigma_j I)\hat{z} = d \qquad z = S^{-1}\hat{z} \qquad j = 1, \ldots, s$$

- Give up symmetry
- Solve for multiple shifts with Krylov methods
- Mathematically equivalent to second-order Arnoldi methods

(B) If $S = LL^*$ is (Hermitian) positive definite, solve

$$(L^{-1}TL^{-*} + \sigma_j I)\hat{z} = d \qquad z = L^{-*}\hat{z}$$

- Maintain symmetry
- Solve multiple shifts with Krylov methods

Remark: Krylov subspace methods are invariant w.r.t shift:

$$K_m(M) = K_m(M + \sigma I)$$

S–symmetry

Given S symmetric, a matrix X is S–symmetric if $\quad XS = SX^T$

Set $X = TS^{-1} + \sigma_j I \qquad \Rightarrow \qquad X$ is S-symmetric

Solve

$$(TS^{-1} + \sigma_j I)\hat{z} = d \qquad z = S^{-1}\hat{z}$$

$$\Downarrow$$

$S -$ symmetric Lanczos process $\quad + \quad$ shift

(cost per iteration $\approx$ symmetric solver) $\quad$ invariance

(e.g. Parlett & Chen (1990), Young & Jea (1990), Freund & Nachtigal (1994), Perotti & S. (2002), Meerbergen (2003))

S–symmetric Lanczos

Solve $\qquad (TS^{-1} + \sigma_j I)\hat{z} = d \qquad z = S^{-1}\hat{z}$

using any Lanczos approach (BiCG, QMR, ...)

natural inner product for complex sym matrices:

$$(x, y) = x^T y \qquad x, y \in \mathbb{C}^n$$

with auxiliary vector $\tilde{r}_0 = S^{-1} r_0$ (e.g. Freund & Friedman 1995-'97)

$$\Downarrow$$

Left Krylov subspace $= S^{-1}\times$ Right Krylov subspace

Real application: Soil-structure interaction

$$\left(\frac{1}{\omega^2}K + \frac{1}{\omega}C_V - M\right)\hat{x} = b$$

K	sparse complex sym. (stiffness+hyst. dumping)
C_V	diagonal only imag. part (viscous damping)
M	real diagonal (inertia matrix)
$\omega \in 2\pi[10, 50]$	up to a few hundreds $\Rightarrow$ $\sigma = \frac{1}{\omega}$

$$\left[\begin{pmatrix} C_V & MP \\ P^T M^T & 0 \end{pmatrix} + \sigma \begin{pmatrix} K & \\ & P^T M^T P \end{pmatrix}\right] \begin{bmatrix} \widetilde{y} \\ \widetilde{x} \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

Typical setting

$$\left(\frac{1}{\omega^2}K + \frac{1}{\omega}C_V - M\right)\hat{x} = b$$

Pb.	Pb. size	$\#(K)$	condest(K)	$\#(C_V)$	$\|C_V\|$	$\#(M)$	$\|M\|$
B	3 627	102 378	$9.7 \cdot 10^4$	211	381	3 627	0.3
C	2 472	24 340	$3.6 \cdot 10^7$	36	20243	1475	48
F	11 957	419 160	$2.6 \cdot 10^{12}$	3 243	212	11 907	0.4
F1	11 907	416 855	$2.0 \cdot 10^7$	3 243	212	11 857	0.4

Case **F**: $\|K\|_1 = 1.6 \cdot 10^9$

Case **F1**: $\|K\|_1 = 1.6 \cdot 10^8$

...Obtain fast convergence

$$\left[\begin{pmatrix} C_V & MP \\ P^T M^T & 0 \end{pmatrix} + \sigma \begin{pmatrix} K & \\ & P^T M^T P \end{pmatrix}\right] \begin{bmatrix} \widetilde{y} \\ \widetilde{x} \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

$$(T + \sigma S)z = d \qquad \Rightarrow \begin{cases} (TS^{-1} + \sigma I)\widehat{z} = d \\ \text{or} \\ (I + \sigma ST^{-1})\widetilde{z} = d \end{cases} \qquad ??$$

T, S, complex sym

Spectral properties of TS^{-1} or of ST^{-1}

Problem: Singularity of T in Structural Dynamics!

Spectral properties $\qquad \mu \in \mathrm{spec}(TS^{-1})$ then

$$\mathrm{spec}(TS^{-1} + \sigma I): \qquad \mu + \sigma$$

$$\mathrm{spec}(I + \sigma S T^{-1}): \qquad 1 + \sigma \frac{1}{\mu}$$

$$Tz = \mu S z, \qquad \Rightarrow \quad (\mu^2 K - \mu C_V - M) z = 0$$

Extension of Cauchy's Theorem (Higham & Tisseur, '03):

$$\rho_1 \le |\mu| \le \rho_2$$

$$\rho_1 = \frac{1}{2\|K\|} \left(-\|C_V\| + \sqrt{\|C_V\|^2 + 4 \frac{\|K\|}{\|M^{-1}\|}} \right)$$

$$\rho_2 = \frac{\|K^{-1}\|}{2} \left(\|C_V\| + \sqrt{\|C_V\|^2 + 4 \frac{\|M\|}{\|K^{-1}\|}} \right)$$

The new Frontier: two parameters

$$\left(\frac{1}{\omega^2}K + \frac{1}{\omega}C_V - M\right)\hat{x} = b$$

$K = K_s + \beta K_g$, $\beta = \{0.1, ..., 2\}$, rank$(K_g) <$ rank(K_s)

$$\left(\frac{1}{\omega^2}K_s + \frac{\beta}{\omega^2}K_g + \frac{1}{\omega}C_V - M\right)\hat{x} = b$$

Some strategies using subspace projection:

- Two-sided Arnoldi
- Solve for each β with solution recycling
- "Rational Interpolant Reduced order Model" (Gallivan et al, '99)
- ...

Other related issues

- $(\sigma^2 K + \sigma C_V - M)x = f(\sigma)$ (Gu & S., '05)
- $\widehat{K} = K + UV^T$, Modified (nonsym.) stiffness matrix
- Model order reduction...
- ...