Subspace Iterations for Rank-Structured Matrices

Some open problems, research directions (and disappointments) in designing fast eigensolvers for rank structured matrices

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The Perspective

- As has been the case for linear systems with structured matrices for a long time, the moment has now come to recognize the need for specialized eigenvalue algorithms for matrices with structure.
  As for linear systems with structure this will undoubtedly hinge on our ability to compute eigenvalues of structured matrices within the structure.

Rank-Structured Eigenvalue Problems

Let $A \in \mathbb{C}^{n\times n}$ satisfy
-) (rank-structured property)

$$\max_{1\le k\le n-1}\{\text{rank } A(k+1\colon n, 1\colon k), \text{rank } A(1\colon k, k+1\colon n)\} \le p$$

-) (small rank perturbation property)

$$A = B + U \cdot V^T, B = B^H \text{ and/or } B^H \cdot B = I_n, U, V \in \mathbb{C}^{n\times q}$$

where p and q are small constants independent of n

- **Input:** Given some condensed representation of A in terms of $O(n)$ parameters
- **Output:** Compute numerical approximations of (some) eigenvalues of A

Our Numerical Linear Algebra for Rank-Structured Matrices

- A can be reduced to tridiagonal or Hessenberg form B by unitary transformations at the cost of $O(n^2)$ flops (Eidelman & G. & Gohberg, LAA 2007)
- The Schur form of B can be computed by using a fast adaptation of the QR method applied to B at the cost of $O(n^2)$ flops (Eidelman & G. & Gohberg, NUMA 2008)
- The Schur form of A can directly be computed by using a fast adaptation of the QR method applied to A at the cost of $O(n^2)$ flops (Bini & Eidelman & G. & Pan , Numer. Math. 2005), (Bini & Eidelman & G. & Gohberg, SIMAX 2007), (Bini & Eidelman & G. & Gohberg, Math. Comp. 2008)

Some Challenging Problems

- Proving the backward stability of fast algorithms theoretically
- Extending the fast algorithms to rank-structured matrices where the property II is relaxed
- Extending the fast algorithms to generalized rank-structured eigenproblems
- Designing fast subspace iteration methods for large rank-structured eigenproblems

Stability for Almost Hermitian Eigenproblems

Theorem 1 *(Eidelman & G. & Gohberg, NUMA 2008) The matrix A_1 reconstructed by the generators computed by the fast QR iteration applied to the generators of A_0 is unitarily similar to a small perturbation of A_0.*

- More involved for Almost Unitary Eigenproblems. Looking for new simplified parametrizations (joint work with P. Boito)
- Specialized balancing techniques for the generators
- High relative accuracy for some subclasses (G., LAA 2008)

A Numerical Example

$$\widehat{T}_N = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & \ddots & & \\ & \ddots & \ddots & 1 & \\ & & 1 & 0 & 1 \\ & & & \alpha & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & \ddots & & \\ & \ddots & \ddots & 1 & \\ & & 1 & 0 & \alpha \\ & & & \alpha & 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1-\alpha \\ 0 \end{bmatrix} \cdot \boldsymbol{e}_N^T$$

α	10^2	10^4	10^8	10^{15}
max_err_abs	0.18e-12	0.16e-09	0.1e-03	0.86e+06
max_err_rel	0.18-13	0.16e-11	0.12e-7	0.26e-01
max_err_abs1	0.11e-13	0.13e-12	0.18e-08	0.57e-02

Complex Symmetric Eigenproblems

"Polynomial Algebra by Values" (Corless & Gonzalez- Vega & al.)

$$\left[\begin{array}{c|ccc} \alpha & c_1 & \dots & c_n \\ \hline b_1 & \lambda_1 & & \\ \vdots & & \ddots & \\ b_n & & & \lambda_n \end{array}\right] \boldsymbol{u} = \lambda \left[\begin{array}{c|ccc} \beta & & & \\ \hline & 1 & & \\ & & \ddots & \\ & & & 1 \end{array}\right] \boldsymbol{u}, \ \beta \in \{0, 1\}$$

- $\beta = 0 \rightarrow$ Eigenvalue Problem for complex diagonal plus rank-one matrices
- $\beta = 1 \rightarrow$ Eigenvalue Problem for complex arrowhead matrices

Not Unitary Methods

This in an ongoing research with F. Uhlig

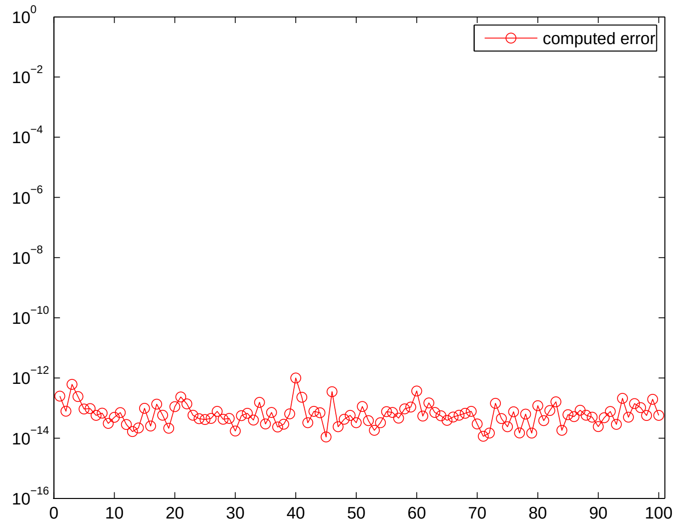
1. Transform A by diagonal similarity into complex symmetric form B.
2. Reduce B by similarity into tridiagonal form

   Theorem 2 *Under the assumption that all the transformations involved are well-defined, the matrix B can be converted into tridiagonal form T by similarity using complex-orthogonal transformations at an overall cost of $O(n^2)$ operations and in $O(n)$ storage.*

3. Compute the eigenvalues of T by using the DQR method (Uhlig, Numer. Math. 1997)

Experimental Evidence

- The step 2 is numerically robust (with some randomization)



Errors for random arrowhead matrices of size $n = 512$

- Problems are encountered when using the DQR method: Deflation can lead to ill-conditioned subproblems

Hermitian Generalized Eigenproblems

$$A\boldsymbol{x} = \lambda B\boldsymbol{x}$$

–A, B rank-structured
–$A^H B = B^H A +$ small rank

- ORF (Fasino& G. & Mastronardi & Van Barel, SIMAX 2005), RQF (Fasino& G., NUMA 2007)

$$\Sigma = \gamma A + \delta B, \quad \Delta = \gamma A - \delta B$$
$$\Sigma^H \Sigma = \Delta^H \Delta + \text{small rank}$$
$$\Sigma \boldsymbol{x} = \mu \Delta \boldsymbol{x}$$

- $(\Sigma\Delta^{-1})^H \cdot (\Sigma\Delta^{-1}) = I +$ small rank $\Rightarrow$ transformation into a unitary generalized eigenproblem

Computing the Eigenvalues of Rational Toeplitz Matrices

This in an ongoing research with M. Van Barel & K. Frederix

The Problem: Let us given two real polynomials

$$a(z) = a_0 + \ldots + a_q z^q,\ c(z) = c_p z^{-p} + \ldots + c_1 z^{-1} + c_0 + c_1 z + \ldots + c_p z^p,$$

where $p \leq q$ and $a(z)$ has no zeros in $|z| \leq 1$. The task is to compute the eigenvalues of the symmetric rationally generated Toeplitz matrices defined by

$$T_n = \begin{bmatrix} t_0 & t_1 & \ldots & t_{n-1} \\ t_1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & t_1 \\ t_{n-1} & \ldots & t_1 & t_0 \end{bmatrix}, t(z) = \frac{c(z)}{a(z)a(1/z)} = \sum_{j=-\infty}^{\infty} t_{|j|} z^j$$

Where is the Generalized Eigenproblem?

- Embedding in Matrix Algebras (Arbenz; Di Benedetto)

$$(C_1 + U_1 \cdot V_1^T)\boldsymbol{x} = \lambda(C_2 + U_2 \cdot V_2^T)\boldsymbol{x}$$

–C_1, C_2 are simultaneously diagonalizable

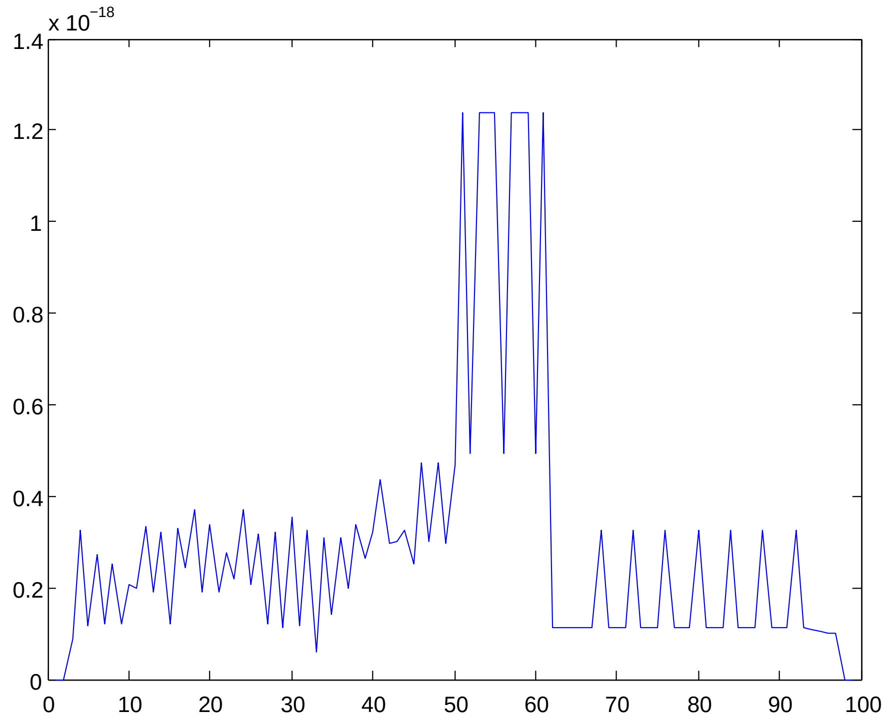
$$(\Sigma_1 + Z_1 \cdot W_1^T)\boldsymbol{x} = \lambda(\Sigma_2 + Z_2 \cdot W_2^T)\boldsymbol{x}$$

–generalized rank-k change

1. iterative diagonalization of a sequence of matrix pencils obtained by successive rank one updates
2. computation of eigenvectors $\rightarrow$ numerical difficulties

A Numerical Example

$$t(z) = \frac{-z^{-1} + 2 + z}{(z-2)(z-3)(z^{-1}-2)(z^{-1}-3)}.$$



For each submatrix $T_{100}(k+2\colon 100, 1\colon k)$, $1 \le k \le 99$, the third singular value returned by the Matlab function svd is plotted.

The Rank Structure of T_n

Theorem : The symmetric Toeplitz matrix T_n, $n = m \cdot q$, can be partitioned in a block form $T_n = (T_{i,j}^{(n)})_{i,j=1}^{m}$, where $T_{i,j}^{(n)} \in \mathbb{R}^{q \times q}$ and

$$T_{i,j} = A_0^{-1} \cdot F_a^{q(i-j-1)} \cdot \Gamma_1 \ \text{ if } i - j \geq 1,$$

where F_a is the companion matrix associated with $a(z)$ and A_0 and Γ_1 are suitable $q \times q$ matrices. Moreover, if

$$B_n = \begin{bmatrix} I_q & & \\ -\Sigma & I_q & \\ & \ddots & \ddots \end{bmatrix}, \quad \Sigma = A_0^{-1} F_a^q A_0$$

then $P_n = B_n \cdot T_n \cdot B_n^T$ is symmetric block tridiagonal

A Fast Tridiagonalization Procedure

- Exploit the representation $T_n = B_n^{-1} \cdot P_n \cdot B_n^{-T}$. Let $R_m = \Sigma$. For $k = m : -1 : 2$ repeat
  1. Determine $U \in \mathbb{R}^{2q \times 2q}$ orthogonal such that

$$U^T \left[\begin{array}{c} I_q \\ R_k \end{array} \right] = \left[\begin{array}{c} R_{k-1} \\ 0 \end{array} \right], \; R_{k_1} \text{ triangular}$$

  2. Perform the similarity transformation driven by U;
  3. Chase the possible bulge in the transformed matrix
- Overall cost $O(n^2)$ flops.
- Numerical results soon !!!

Some Subspace Iteration Problems

- The matrix eigenvalue tracking algorithm used by my students in engineering
  For t=1,2, . . . , for each time step compute:

$$\left[\begin{array}{c} D(t) = A(t)Q(t-1) \\ D(t) = Q(t)R(t) \\ H(t) = Q^T(t)A(t)Q(t) \end{array}\right.$$

- It follows from the simultaneous orthogonal iteration:
  For t=1,2, . . . , for each time step compute:

$$\left[\begin{array}{c} D(t) = AQ(t-1) \\ D(t) = Q(t)R(t) \end{array}\right.$$

- Complexity: It depends on $Q(0)$ and on the structure of $A(t)$

More on Subspace Iteration Problems

- Continuation of Invariant Subspaces
  1. $A(t)$ companion matrix associated with a time varying polynomial;
  2. $A(t_0) = Q(t_0)^T R(t_0) Q(T_0)$ Schur form at time t_0;
  3. $R(t_0) = \begin{bmatrix} R_{11}(t_0) & R_{12}(t_0) \\ 0 & R_{22}(t_0) \end{bmatrix}$,
     spec$(R_{11}(t_0)) \cap$ spec$(R_{22}(t_0)) = \emptyset$
  4. $B(t) = Q(t_0)A(t)Q(t_0)^T = \begin{bmatrix} B_{11}(t) & B_{12}(t) \\ B_{21}(t) & B_{22}(t) \end{bmatrix}$
  5. Rank-Structured Riccati Equation

$$XB_{11}(t) - B_{22}(t)X - XB_{12}(t)X + B_{21}(t) = 0$$