Iteration for Contour-Based Nonlinear Eigensolvers

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The Nonlinear Eigenvalue Problem

Working towards a "black box" solver for the nonlinear eigenvalue problem for matrix valued functions $T \in H(\Omega, \mathbb{C}^{n\times n})$.

$$T(\lambda)x = 0, \qquad x \in \mathbb{C}^n, \qquad \lambda \in \mathbb{C} \tag{1}$$

Here $T(\lambda) = A - \lambda I$ recovers the standard eigenvalue problem.

See the review paper by Güttel and Tisseur [4] for an overview.

Previous Techniques

Contour based methods:

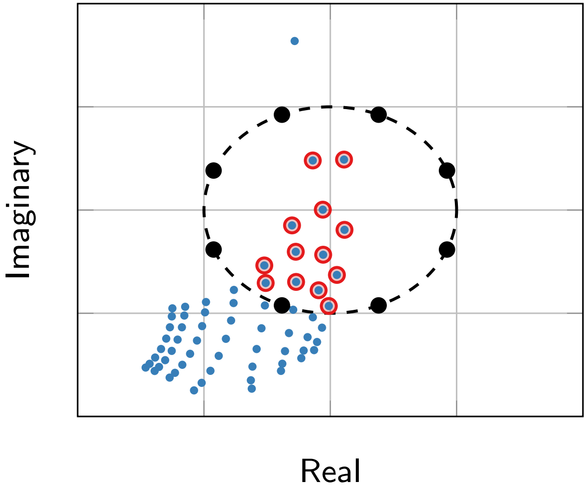
- Beyn's method
- SS methods of Yokota, Sakurai, Asakura, et al.
- NLFEAST

Newton and Approximation based methods:

- Newton methods, such as residual inverse iteration (RII)
- Infinite Arnoldi, Krylov methods
- NLEIGS, CORK
- Many others

Contour

Example contour for Butterfly problem (quartic).



Beyn's Method

$$\frac{1}{2\pi i}\int_\Gamma f(z)T(z)^{-1}\,dz = Vf(J)W^H \tag{2}$$

Use the Keldysh theorem to probe Jordan decomposition of $T(\lambda)$ locally in a contour for spectral information. Approximate moments

$$A_k = \frac{1}{2\pi i}\int_\Gamma z^k T(z)^{-1}X\,dz = V\Lambda^k W^H X. \tag{3}$$

With "probing matrix" X. In particular,

$$A_0 = VW^H X, \qquad A_1 = V\Lambda W^H X. \tag{4}$$

Computing a decomposition of A_0 and applying a similarity transform, we can compute V, Λ from A_0 and A_1.

Beyn's Method

Pros

- Any type of nonlinearity in $T(\lambda)$ (no need for approximation).
- Highly parallel.
- Spectral slicing.
- Generalizes to higher moments.
- Converges in number of quadrature nodes.

Cons

- Many linear system solves needed (main computational cost).
- Linear systems need to be solved accurately.
- No way to iterate (other than adaptive quadrature).
- For many contour nodes, can be difficult to position away from eigenvalues.

NLFEAST

Applying a Residual Inverse Iteration with contour points as fixed shifts gives a Newton-type iteration.

$$Q_0 = \frac{1}{2\pi i} \int_\Gamma \Big(X - T(z)^{-1} T(X, \Lambda) \Big) (zI - \Lambda)^{-1} \, dz \qquad (5)$$

Each iteration we solve the projected nonlinear reduced problem.

$$Q_0^H T(\lambda) Q_0 y = 0 \qquad (6)$$

NLFEAST

Pros

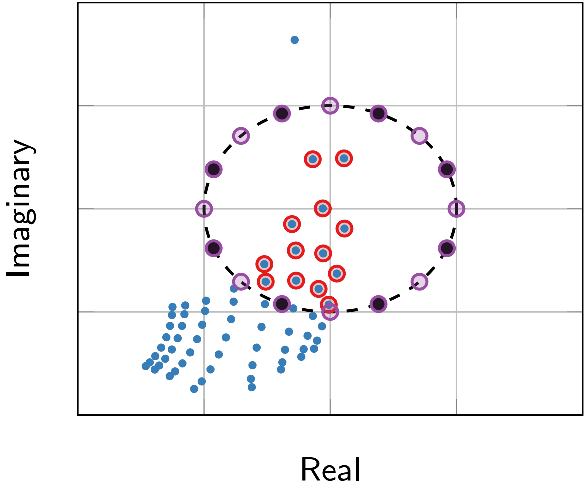
- Iterative convergence properties of (linear) FEAST.
- Highly parallel.
- Linear systems can be solved to relatively low accuracy.
- Implementation for polynomial available in FEAST 4.0.

Cons

- Only a projection method (for non-polynomial).
- Internal solver must be used.

Contour

When using Beyn as the internal solver for NLFEAST, some practical difficulties arise in the choice of internal contour.



Problems

- How to share contour nodes (and thus linear system solves) when using NLFEAST with Beyn as an internal solver?

- How can Beyn's method be effectively iterated? Doing so would address drawbacks of using many quadrature points.

Motivated by these questions, we combine the algorithms to get the benefits of both.

NLFEAST-Beyn Hybrid Algorithm

We can generalize the RII moment Q_0 of NLFEAST to Q_k.

$$Q_k = \frac{1}{2\pi i} \int_\Gamma z^k \Big(X - T(z)^{-1} T(X, \Lambda) \Big) (zI - \Lambda)^{-1} \, dz \tag{7}$$

Then apply the similarity transform approach of Beyn's method to probe the Jordan matrix.

Note: In general $Q_k = A_k$ for linear problems only.

NLFEAST-Beyn Hybrid Algorithm

$A_0 = \sum_{j=1}^{N} \omega_j T(z_j)^{-1} X$
$A_1 = \sum_{j=1}^{N} \omega_j z_j T(z_j)^{-1} X$
Compute the QR Decomposition $qr \leftarrow A_0$
$B = q^H A_1 r^{-1}$
Solve $BY = Y\Lambda$
$X \leftarrow qY$

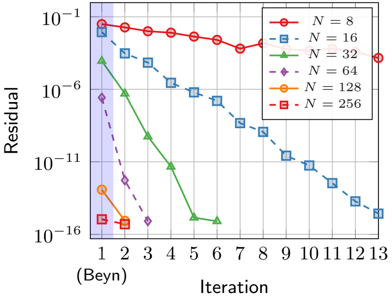
while not converged **do**
  $Q_0 \leftarrow \sum_{j=1}^{N} \omega_j [X - T(z_j)^{-1} T(X, \Lambda)](z_j I - \Lambda)^{-1}$
  $Q_1 \leftarrow \sum_{j=1}^{N} \omega_j z_j [X - T(z_j)^{-1} T(X, \Lambda)](z_j I - \Lambda)^{-1}$
  Compute the QR Decomposition $qr \leftarrow Q_0$
  $B \leftarrow q^H Q_1 r^{-1}$
  Solve $BY = Y\Lambda$
  $X \leftarrow qY$
end while
return X, Λ

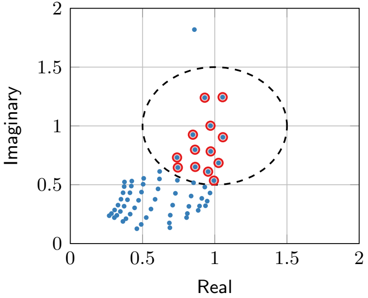
NLFEAST-Beyn Hybrid Algorithm

- From one perspective, this can be viewed as NLFEAST using the decomposition of Beyn's method directly.
  No reduced system needs to be solved.
- From the other, it can be viewed as Beyn's method using the RII (from Neumaier) approach of NLFEAST.
- Can be reduced to standard FEAST for linear problems.

Numerical Experiments

Butterfly Problem (quartic)

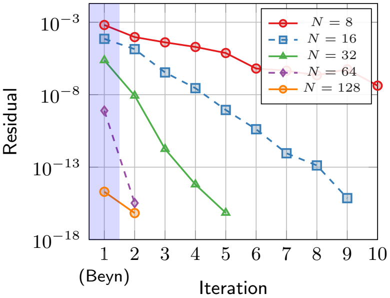


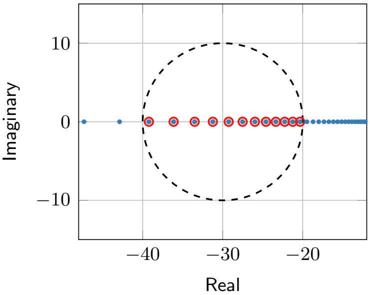


	Linear System Solves	Factorizations
$N = 16$	208	16
$N = 32$	160	32
$N = 64$	192	64
Beyn	256	256

Numerical Experiments

Hadeler Problem $\quad T(\lambda) = (e^{\lambda} - I)T_2 + \lambda^2 T_1 - \alpha T_0$





	Linear System Solves	Factorizations
$N = 16$	144	16
$N = 32$	160	32
$N = 64$	128	64
Beyn	≥ 128	≥ 128

Higher Moments

Necessary to use higher moments for eigenvector defects or many eigenvalues in a contour.

$$H_0 = \begin{bmatrix} A_0 & \cdots & A_{K-1} \\ \vdots & & \vdots \\ A_{K-1} & \cdots & A_{2K-2} \end{bmatrix}, H_1 = \begin{bmatrix} A_1 & \cdots & A_K \\ \vdots & & \vdots \\ A_K & \cdots & A_{2K-1} \end{bmatrix}. \quad (8)$$

$$V_{[K]} = \begin{bmatrix} V \\ \vdots \\ V\Lambda^{K-1} \end{bmatrix}, \quad W_{[K]}^H = \left[W^H X, \ldots, \Lambda^{K-1} W^H X\right] \quad (9)$$

Similar to the relation between A_0 and A_1 before

$$H_0 = V_{[K]} W_{[K]}^H, \quad H_1 = V_{[K]} \Lambda W_{[K]}^H. \quad (10)$$

Problems with Higher Moments

- SS-Hankel approach has benefits, but not yet explored.
- Deflation after every iteration limits number of eigenvalues. Unclear how RII can be modified to reuse all spectral information after iteration (work in progress).

Future Work

- Higher moments.
- Analysis of contour shifted RII.
- Theoretical relation to other algorithms.

Software

- The FEAST library
  - Polynomial solver in FEAST 4.0 (current release).
  - Hybrid (fully nonlinear) solver in FEAST 5.0 (upcoming).
- FEASTSolver.jl (used in numerical results)
  - Julia implementation.
  - Less optimized, very extensible, fully nonlinear.
  - Will (eventually) be compatible with NEP-PACK.
- FEAST.jl Julia bindings (work in progress!)

Citations

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