An Iterative Method for Contour Based Nonlinear Eigensolvers

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Beyn's Method

Use Keldysh theorem to probe Jordan decomposition for spectral information, giving a linearization of $T(\lambda)$.

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

Taking the SVD $A_0 = V_0 \Sigma_0 W_0^H$ we can derive the following (computable) similarity.

$$\Lambda \sim V_0^H A_1 W_0 \Sigma_0^{-1} \tag{2}$$

This gives a standard problem $V_0^H A_1 W_0 \Sigma_0^{-1} Y = Y \Lambda$, taking $X = V_0 Y$ recovers eigenvectors.

NLFEAST

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

$$Q_0 = \frac{1}{2\pi i}\int_\Gamma \Big(X - T(z)^{-1}T(X,\Lambda)\Big)(zI-\Lambda)^{-1}\,dz \tag{3}$$

Each iteration solve the projected problem.

$$Q_0^H T(\lambda) Q_0 y = 0 \tag{4}$$

Recover eigenvectors by taking $X = Q_0 Y$.

Problems

- How to share contour nodes (and thus linear system solves) when using NLFEAST with Beyn?
- How can Beyn's method be iteratively refined? Doing so would address drawbacks of using many quadrature points.

NLFEAST-Beyn Hybrid Algorithm

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

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

Then apply the linearization of Beyn's method to these moments.

NLFEAST-Beyn Hybrid Algorithm

$Q_0 = \sum_{j=1}^{N} \omega_j T(z_j)^{-1} X$

$Q_1 = \sum_{j=1}^{N} \omega_j z_j T(z_j)^{-1} X$

Compute the QR Decomposition $qr \leftarrow Q_0$

$B = q^H Q_1 r^{-1}$

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 linearization (from Keldysh) of Beyn's method directly.
- 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.

Higher Moments

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

General way of considering most higher moment algorithms by considering "left probing matrix" $\widehat{X} \in \mathbb{C}^{n\times\ell}$ in addition to "right probing matrix" $X \in \mathbb{C}^{n\times m}$ and defining

$$\widehat{A}_k = \widehat{X}^H A_k = \frac{1}{2\pi i} \int_\Gamma z^k \widehat{X}^H T(z)^{-1} X \, dz. \tag{6}$$

Higher Moment Matrix

Choosing $K \in \mathbb{N}$ as the number of computed moments, form the $K\ell \times Km$ block Hankel matrices

$$H_0 = \begin{bmatrix} \widehat{A}_0 & \cdots & \widehat{A}_{K-1} \\ \vdots & & \vdots \\ \widehat{A}_{K-1} & \cdots & \widehat{A}_{2K-2} \end{bmatrix}, H_1 = \begin{bmatrix} \widehat{A}_1 & \cdots & \widehat{A}_K \\ \vdots & & \vdots \\ \widehat{A}_K & \cdots & \widehat{A}_{2K-1} \end{bmatrix}. \quad (7)$$

From the Keldysh theorem we have $\widehat{A}_k = \widehat{X} V \Lambda^k W^H X$, letting

$$V_{[K]} = \begin{bmatrix} \widehat{X} V \\ \vdots \\ \widehat{X} V \Lambda^{K-1} \end{bmatrix}, \quad W_{[K]}^H = \left[W^H X, \ldots, \Lambda^{K-1} W^H X \right] \quad (8)$$

we have, similarly to before with A_0 and A_1, that

$$H_0 = V_{[K]} W_{[K]}^H, \quad H_1 = V_{[K]} \Lambda W_{[K]}^H. \quad (9)$$

Higher Moment Methods

Using the same similarity as Beyn's method, taking the SVD $H_0 = V_0 \Sigma_0 W_0^H$, we can diagonalize $V_0^H H_1 W_0 \Sigma_0^{-1}$ to find Λ. Recovering the eigenvectors depends on the form of $\widehat{X}$.

- Taking $\widehat{X} = I \in \mathbb{C}^{n \times n}$ gives Beyn's method.
- Taking $\widehat{X} = X$ gives the SS-Hankel method. Here H_0, H_1 are square and another approach is need to recover eigenvectors.

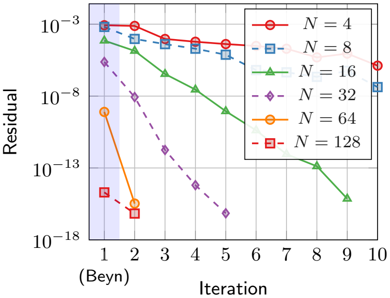
For $\widehat{X} = I$ (thus $\widehat{A}_k = A_k$) we have applied the RII method. This requires deflating the subspace after every iteration.

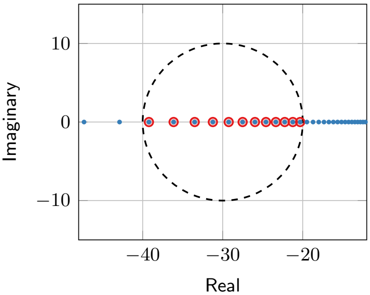
Problems with Higher Moments

- Eigenvectors (potentially) only recoverable in special cases, limiting iteration to Beyn and SS type methods.
- 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.
- No way to determine when there are deficient eigenvectors without computing many higher moments.

Numerical Experiments

Hadeler Problem





Butterfly Problem