A Contour Integral-based Parallel Eigensolver for Nonlinear Eigenvalue Problems

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Introduction

- Nonlinear Eigenvalue Problem (NEP)

$$T(\lambda)\boldsymbol{x} = \mathbf{0},$$

where $T(\lambda)$ is a matrix-valued function.

- We find eigenvalues in a given domain on the complex plane
  - Interior eigenvalue problem
  - Large-scale sparse matrices

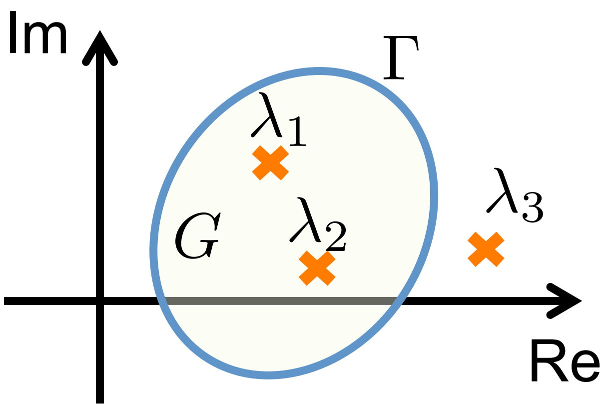
Large and sparse NEP

$\Downarrow$ Projection

Small size NEP

Introduction

- Contour Integral-based Methods
  - GEPs
    - SS-Hankel (S and Sugiura, 2003)
    - SS-RR (S and Tadano, 2007)
    - FEAST (Polizzi, 2009)
    - SS-Arnoldi (Imakura, Du and S, 2013)
  - NEPs
    - SS-Hankel (Asakura, S, et al. 2009)
    - Beyn's method (Beyn, 2012)
    - SS-RR (Yokota and S, 2013)



Map of CI-based eigensolvers (under investigation)

Target eigenproblem in Γ

$$T(\lambda_i)\boldsymbol{x}_i = \boldsymbol{0}$$

Rayleigh-Ritz procedure with filtered subspace

$$V^{\mathrm{H}}T(\theta_i)V\boldsymbol{y}_i = \boldsymbol{0}$$

SS-RR (GEP: 2007, NEP: 2013)
FEAST (GEP: 2009)

(Implicit) Linear EP

Petrov-Galerkin condition with filtered subspace

$$W^{\mathrm{H}}AV\boldsymbol{y}_i = \theta_i W^{\mathrm{H}}V\boldsymbol{y}_i$$

SS-Hankel (GEP:2003, NEP:2009)

Corresponding linear eigenproblem

$$A\boldsymbol{x}_i = \lambda_i\boldsymbol{x}_i$$

Rayleigh-Ritz procedure with filtered subspace

$$V^{\mathrm{H}}AV\boldsymbol{y}_i = \theta_i\boldsymbol{y}_i$$

Beyn's method (NEP:2012)

Arnoldi method with filtered subspace

$$V^{\mathrm{H}}AV\boldsymbol{y}_i = \theta_i\boldsymbol{y}_i$$

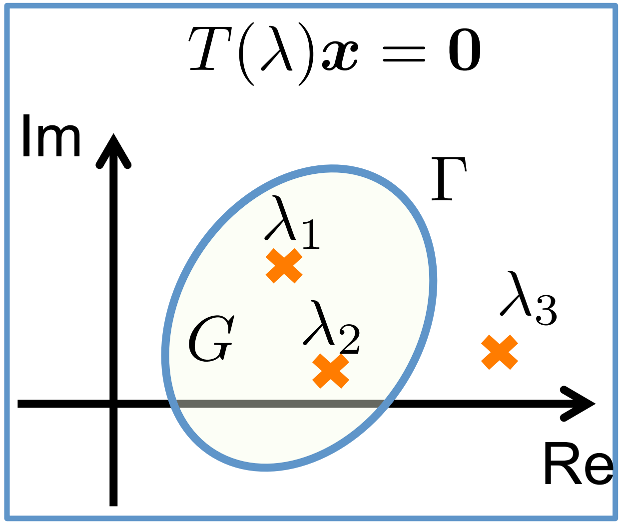
SS-Arnoldi (GEP:2013)
Improvement is now under investigation

Spectral Projection using Contour Integral

Contour Integral-based Eigensolver

- Contour integral for a rational function

$$\frac{1}{2\pi\mathrm{i}}\oint_\Gamma \sum_{i=1}^{n} \frac{\nu_i}{z-\lambda_i}\mathrm{d}z = \sum_{\lambda_i \in G} \nu_i$$



- Spectral decomposition of $T^{-1}(z)$ (Keldish 1951, Beyn 2012)

$$T^{-1}(z) = \sum_{i=1}^{k} \frac{P_i}{z-\lambda_i} + R(z)$$

λ_i : eigenvalue, P_i : spectral projection with respect to λ_i , k : #eigs in Γ
(for simplicity, we consider the case that λ_i is simple)

Localization of spectral projection using contour integral

$$P_\Gamma = \frac{1}{2\pi\mathrm{i}}\oint_\Gamma T^{-1}(z)\mathrm{d}z = \sum_{\lambda_i \in G} P_i$$

Numerical Quadrature

- Contour integral is approximated by numerical quadrature

$$\sum_{\lambda_i \in G} P_i = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma T^{-1}(z) \mathrm{d}z \approx \sum_{j=1}^{N} w_j T^{-1}(z_j), \quad (N \gg 1)$$

z_j : quadrature point, w_j : quadrature weight

- Apply for an arbitrary vector $\boldsymbol{v}$

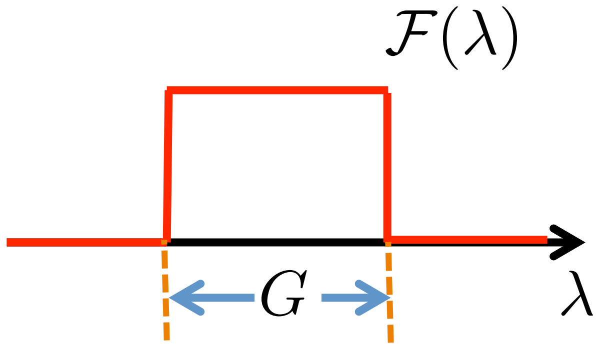
$$\sum_{\lambda_i \in G} P_i \boldsymbol{v} \approx \sum_{j=1}^{N} w_j T^{-1}(z_j) \boldsymbol{v}$$

Systems of linear equations at z_j

$$T(z_j)\boldsymbol{y}_j = \boldsymbol{v}, \ j = 1, \ldots, N$$

Filter for a Subspace

- Define a filter function

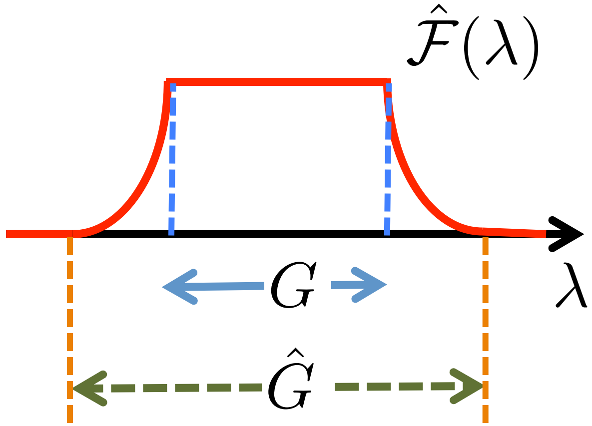


$$\mathcal{F}(\lambda) = \frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} \frac{1}{z-\lambda} \mathrm{d}z$$

- A projection is represented by

$$\frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} T^{-1}(z) \mathrm{d}z = \sum_{i} \mathcal{F}(\lambda_i) P_i + \tilde{R}(z)$$

- For numerical quadrature, the filter function is given by



$$\hat{\mathcal{F}}(\lambda) = \sum_{j=1}^{N} \frac{w_j}{z_j - \lambda}$$

By taking larger size of subspace, contamination is avoided.

(Ikegam, S and Nagashima, 2010)

Quadrature Rule and Filter

- Trapezoidal Rule: Ellipse
  - Quadrature points

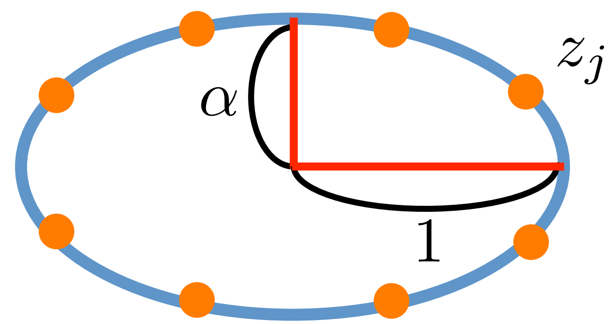
$$z_j = \cos\theta_j + \mathrm{i}\alpha\sin\theta_j$$

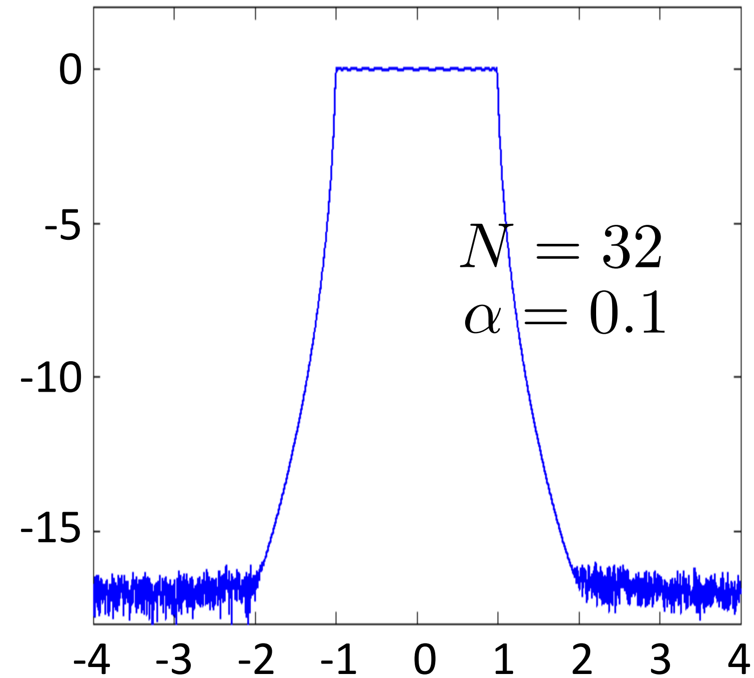
  - Quadrature weights

$$w_j = \alpha\cos\theta_j + \mathrm{i}\sin\theta_j$$

  - Filter function

$$\hat{\mathcal{F}}(\lambda) = \sum_{j=1}^{N} \frac{w_j}{z_j - \lambda}$$



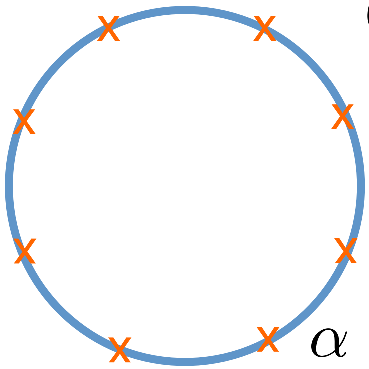


Filter for a Subspace

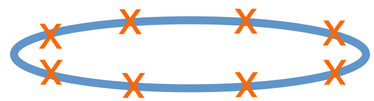
- Selection of α

$$z_j = \cos\theta_j + \mathrm{i}\alpha\sin\theta_j$$

$$\theta_j = \frac{2\pi}{N}\left(j - \frac{1}{2}\right)$$



$\alpha = 1$

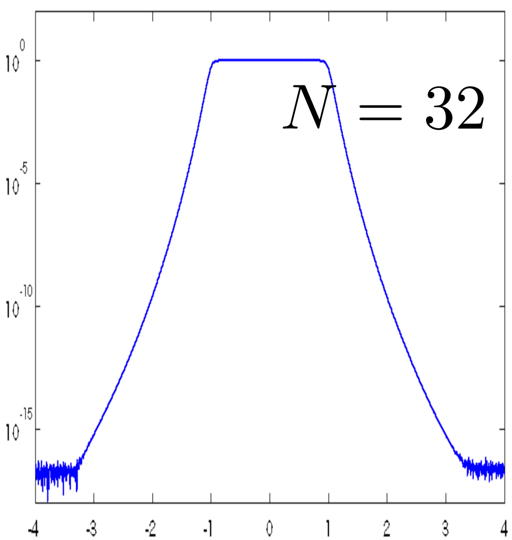


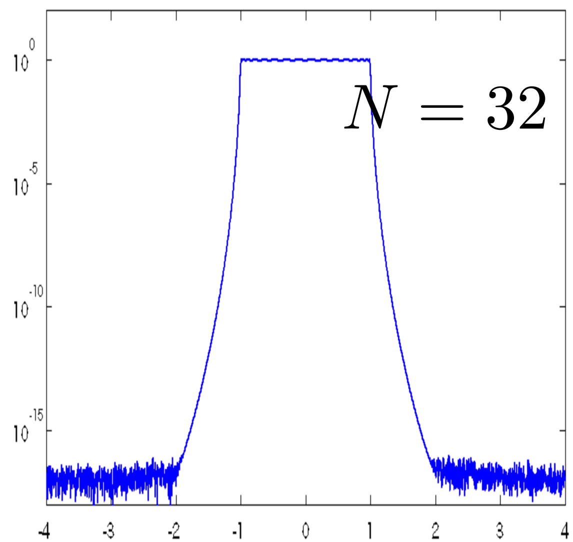
$\alpha = 0.1$

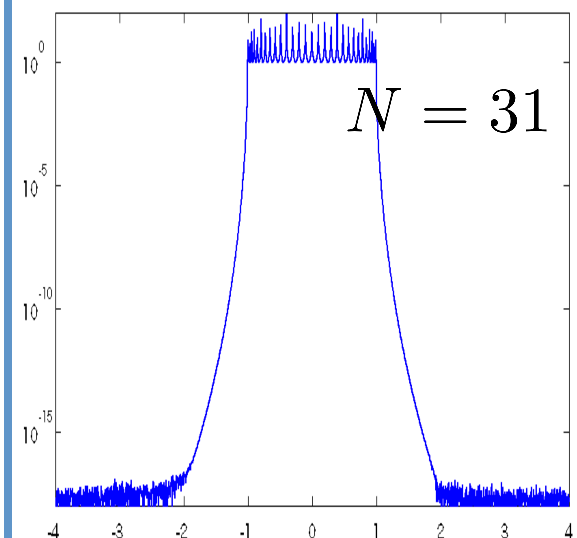
$$\theta_j = \frac{2\pi}{N}\left(j - \frac{1}{4}\right)$$

Equivalent to rational interpolation with Chebyshev points (Austin and Trefethen 2013)

$\alpha = 0$







SS-Hankel

- Consider a scalar function

$$f(z) := \boldsymbol{w}^{\mathrm{H}} T^{-1}(z) \boldsymbol{v}$$

where $\boldsymbol{w}$ and $\boldsymbol{v}$ are nonzero vectors.

- Apply a root-finding method with contour integral (*cf.* Kravanja, S and Van Barel, 1999)

- The problem is reduced to the GEP with Hankel matrices.

$$\mu_k = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma z^k f(z) \mathrm{d}z, \;\; k = 0, 1, \ldots, 2m-1$$

$$H_m = (\mu_{i+j-2})_{i,j=1,m} \qquad H_m^< = (\mu_{i+j-1})_{i,j=1,m}$$

$$\Downarrow$$

$$H_m^< \boldsymbol{y} = \lambda H_m \boldsymbol{y}$$

SS-RR

- Filter by Contour Integral:

$$S_k = \frac{1}{2\pi \mathrm{i}} \oint_\Gamma z^k T^{-1}(z) \mathrm{d}z V, \ \ k = 0, 1, \ldots, M-1$$

  - Rayleigh-Ritz procedure:

$$S = [S_0, S_1, \ldots, S_{M-1}] \qquad S = Q \Sigma U^{\mathrm{H}}$$

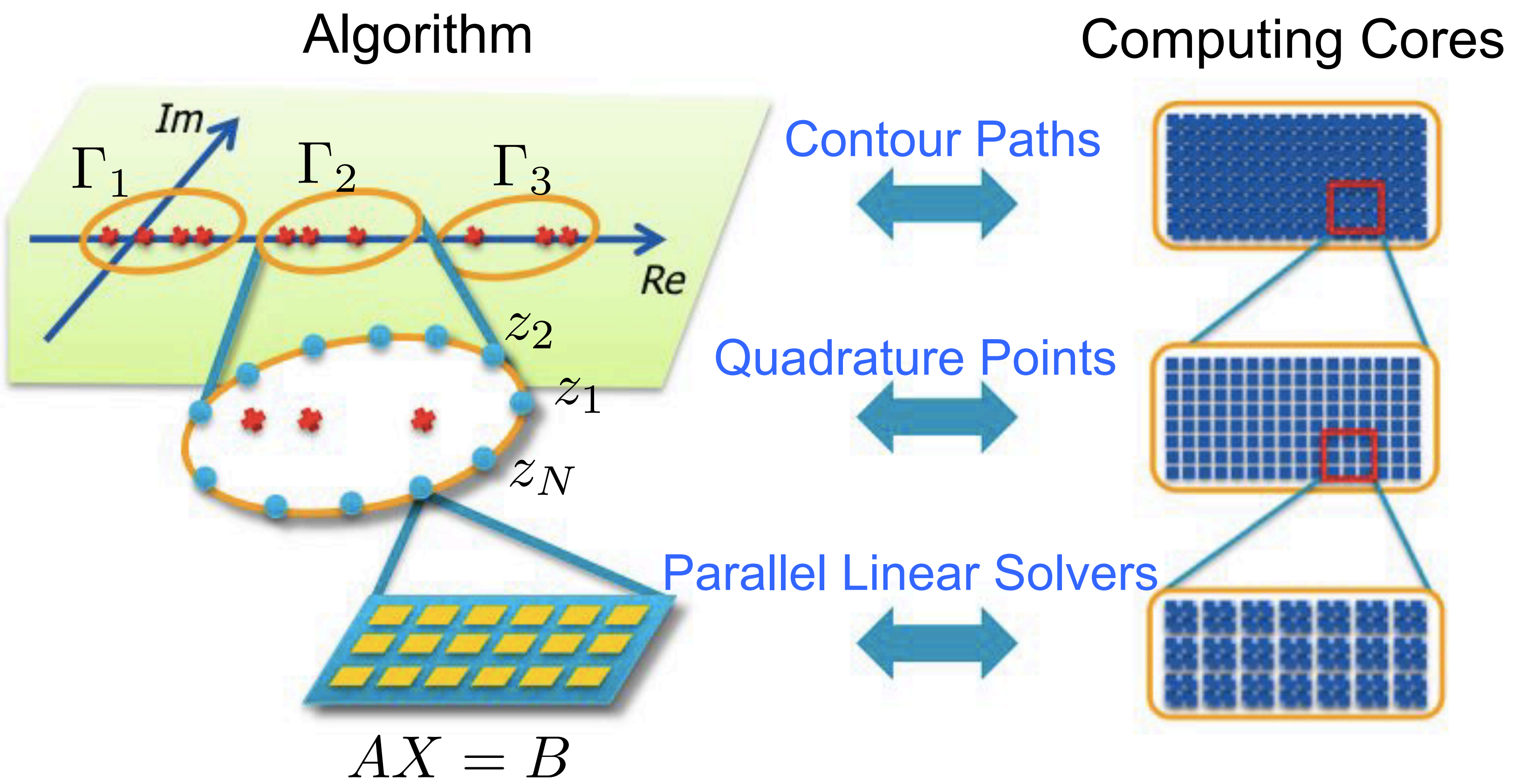
$$T(z) \xrightarrow{Q^{\mathrm{H}} T(z) Q} \boxed{\tilde{T}(z)}$$

Linearization(companion), SS-Hankel, Beyn, NL-JD, TDS-Arnoldi, etc.

The projected problem is solved by an appropriate nonlinear eigensolver

Parallel Implementation

- Computing cores are assigned according to a hierarchical structure of the algorithm



Stochastic Estimation of Eigenvalue Count

Stochastic Estimation of Eigenvalue Count

- To find good parameters in the method:
  - Number of eigenvalues in Γ is given by

$$m = \frac{1}{2\pi \mathrm{i}} \oint_{\Gamma} \mathrm{tr}(T^{-1}(z)T'(z))\mathrm{d}z$$

  - Approximate the trace of inverse matrix by

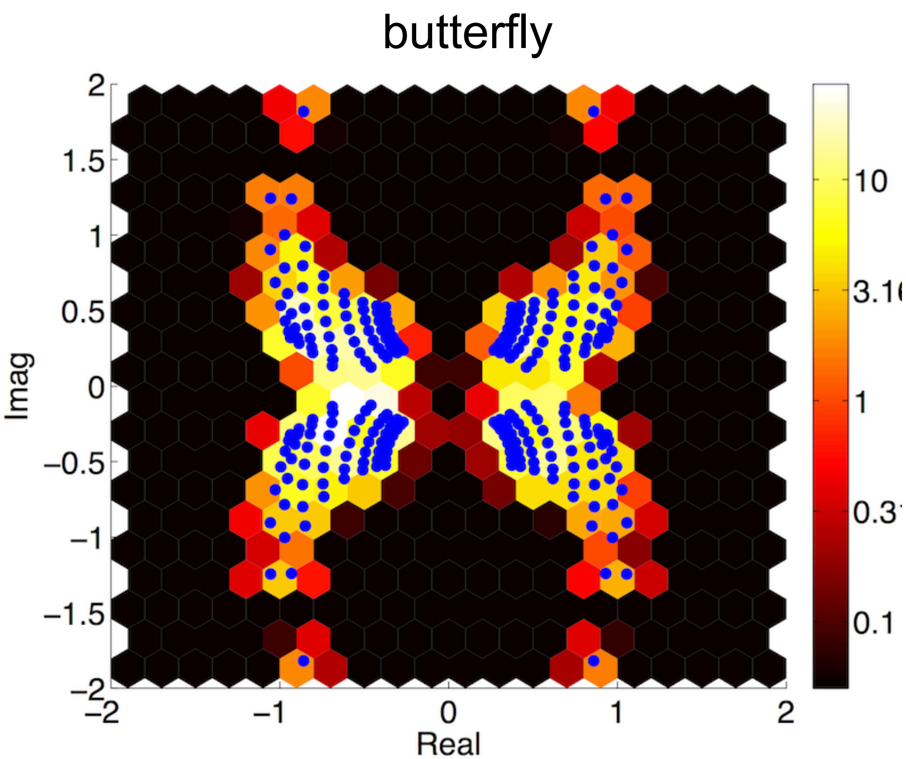
$$\mathrm{tr}(T^{-1}(z)T'(z)) \approx \frac{1}{L} \sum_{\ell=1}^{L} \boldsymbol{v}_\ell^{\mathrm{T}} T^{-1}(z)T'(z)\boldsymbol{v}_\ell$$

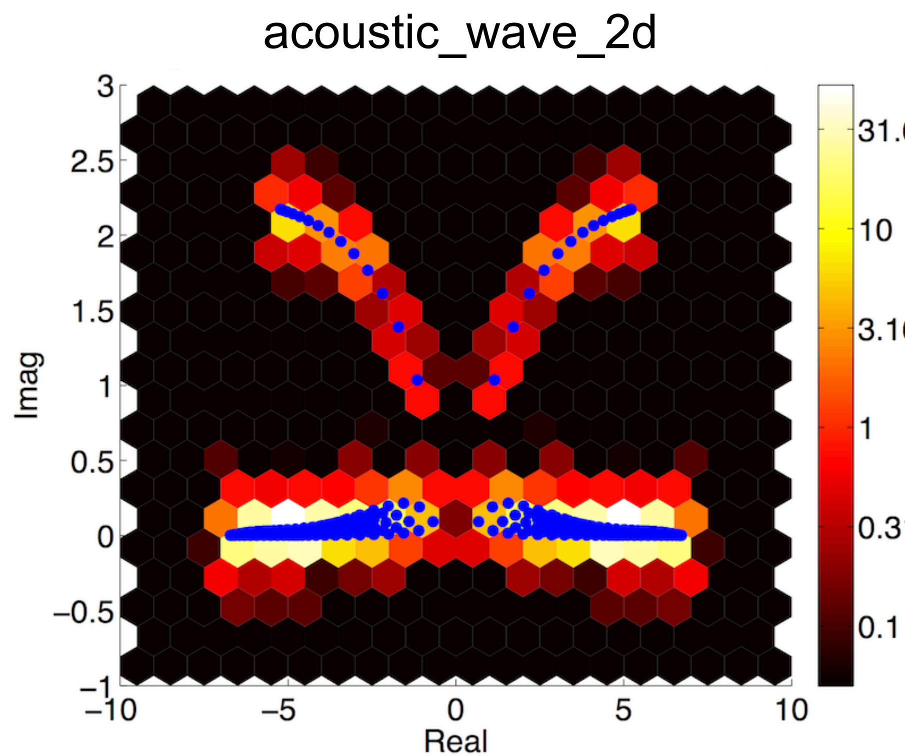
  where $\boldsymbol{v}_l$ is a vector of which elements are taken as 1 or -1 with equal probability.

GEP: Futamura, Tadano and S (2010), NEP: Maeda, Futamura and S (2011)

Stochastic Estimation of Eigenvalue Counts

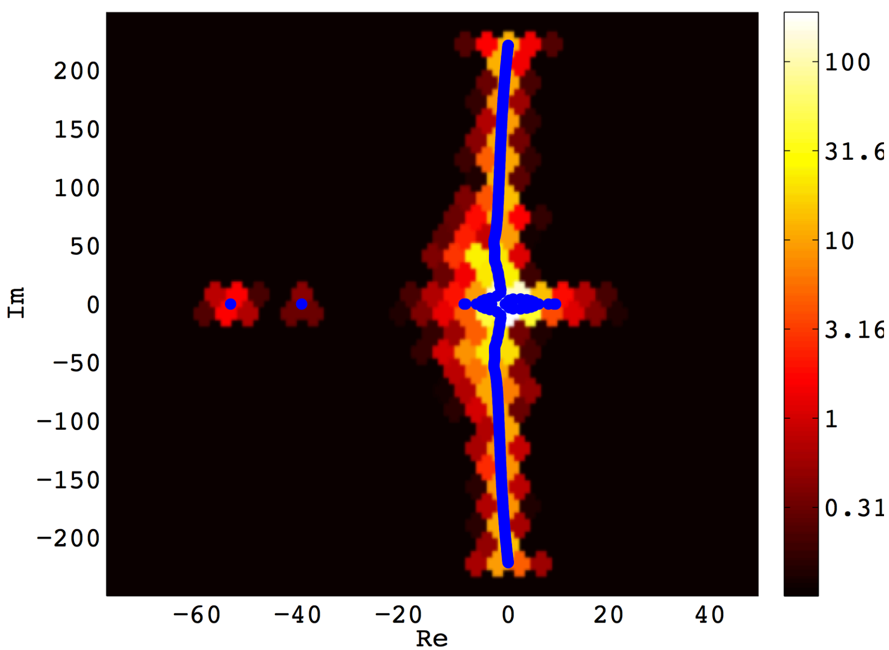
- Find areas that include eigenvalues
  - Estimate eigenvalue density
    Put many circles on the complex plane
  - Examples form NLEVP



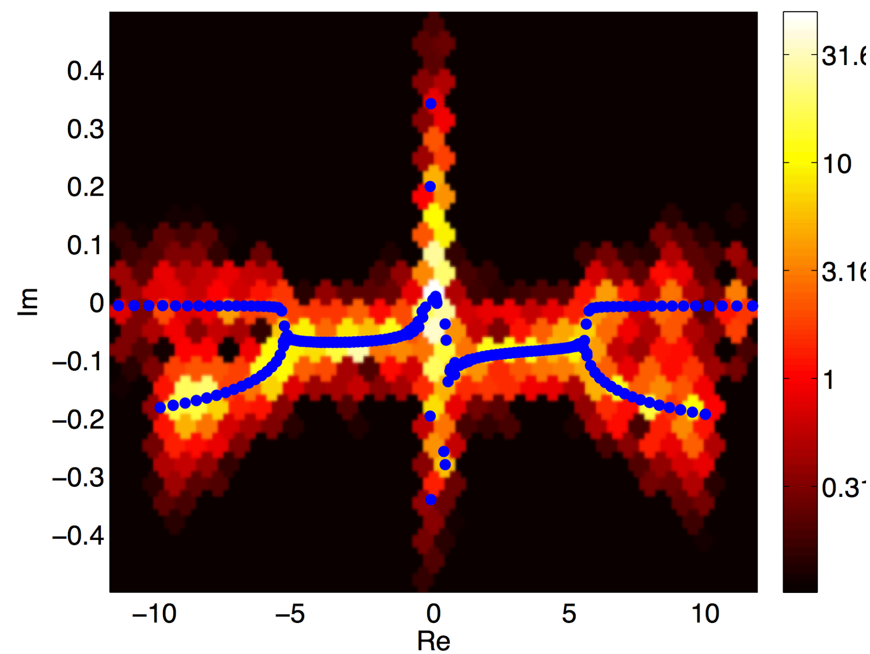


Stochastic Estimation of Eigenvalue Counts

planar_waveguide



plasma_drift

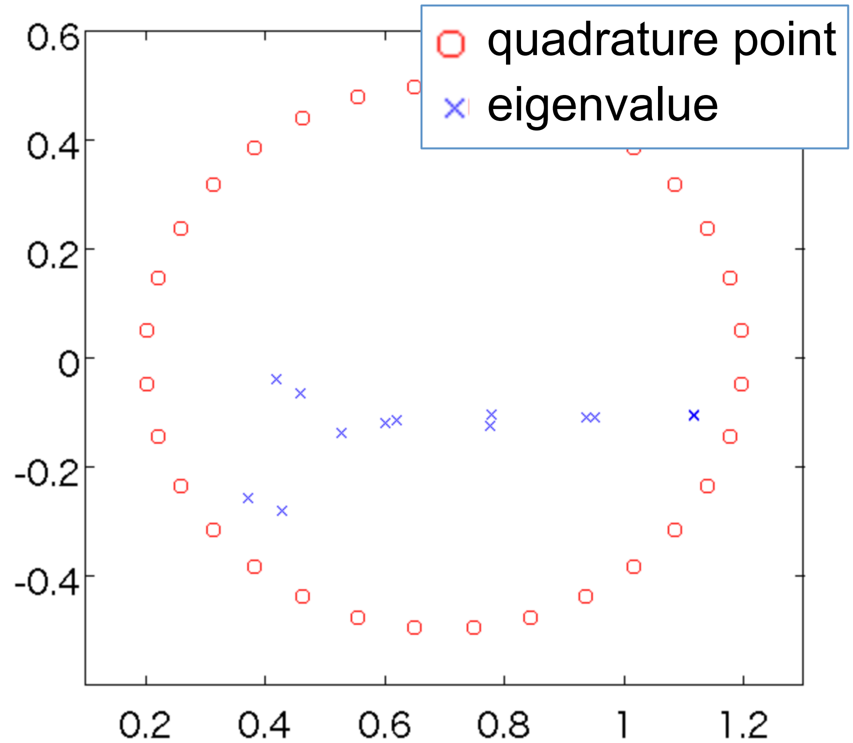


Numerical Examples

Numerical Example

- Test problem: NLEVP: plasma_drift
  - Cubic PEP, Matrix dim. = 512

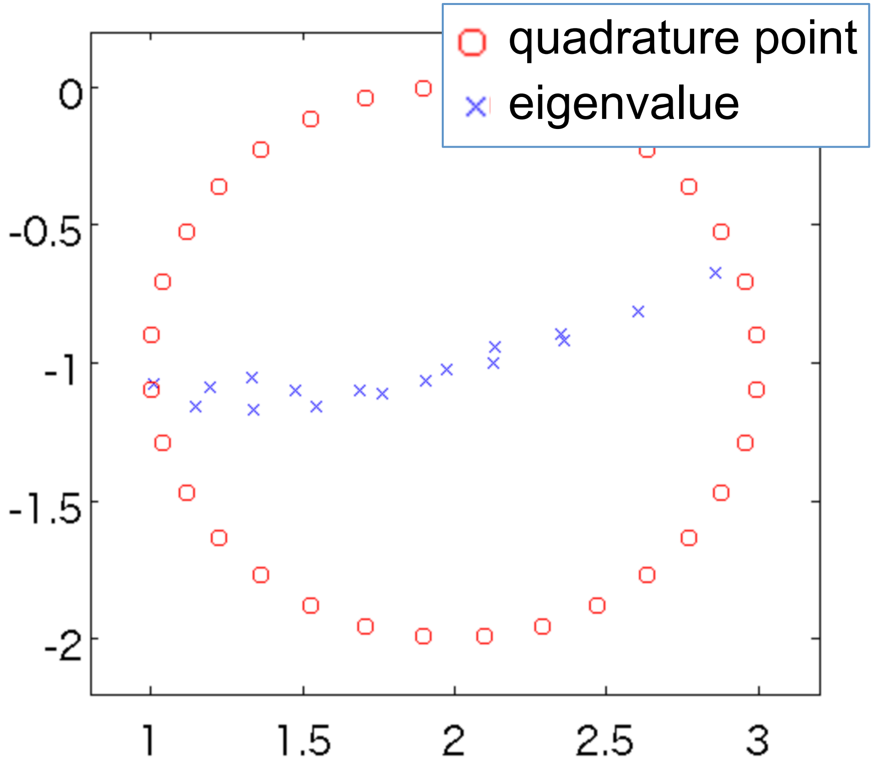
- Solver: SS-RR + polyeig
  - Domain: center = 1.5, radius = 0.8
    Parameters:
    N = 32 (#quad points)
    M = 8 (moment deg.)
    L = 16 (block size)
  - 19 eigs are found
    - Subspace size = 47
    - max(res) = 1.8e-12



Numerical Example

- Test problem: NLEVP: orr_sommerfeld
  - Quartic PEP, Matrix dim. = 5,000

- Solver: SS-RR + polyeig
  - Domain: center = 2 - i, radius = 1
    Parameters:
    N = 32 (#quad points)
    M = 8 (moment deg.)
    L = 16 (block size)
  - 17 eigs are found
    - Subspace size = 49
    - max(res) = 1.0e-15

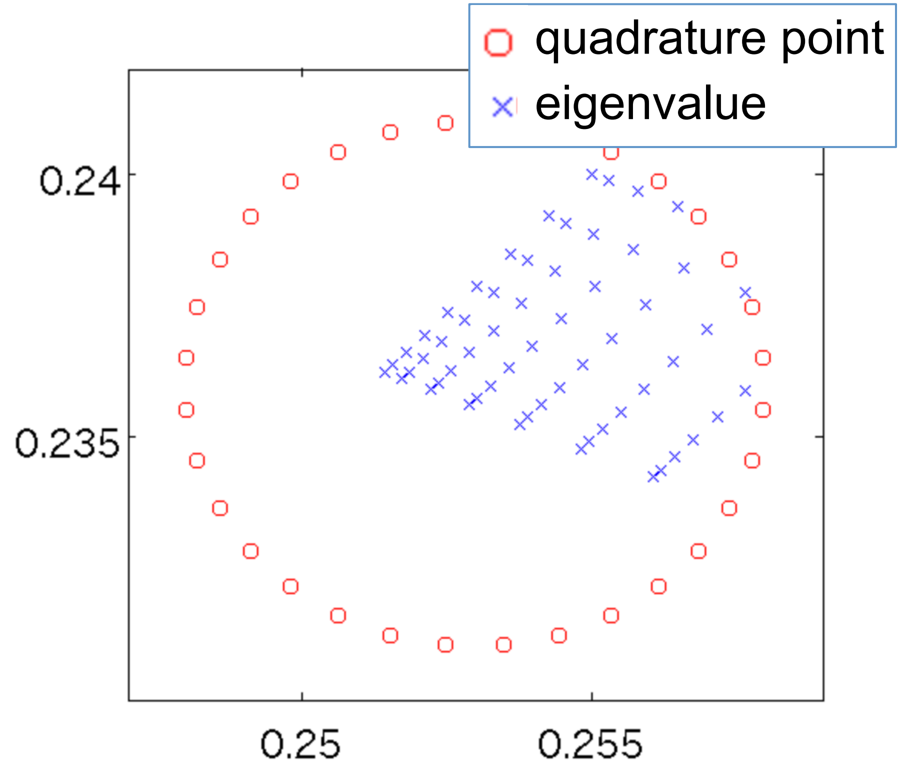


Numerical Example

- Test problem: NLEVP: butterfly
  - Quartic PEP, Matrix dim. = 10,000

- Solver: SS-RR + polyeig
  - Domain: center = 0.253 + 0.236i, radius = 0.005
    Parameters:
    N = 32 (#quad points)
    M = 8 (moment deg.)
    L = 32 (block size)

  - 58 eigs are found
    - Subspace size = 74
    - max(res) = 2.4e-12

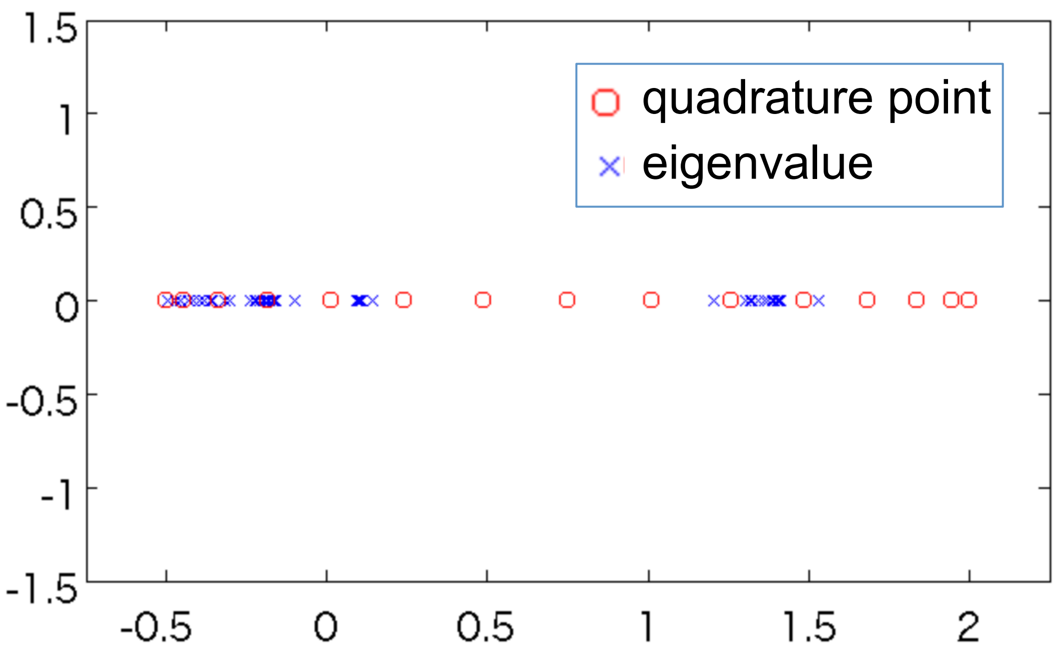


Numerical Example

- Test problem: NLEVP: schrodinger
  - QEP, Matrix dim. = 1,998

- Solver: SS-RR + polyeig
  - Interval: [-0.5, 2] (real quadrature points)
    Parameters:
    N = 15 (#quad points)
    M = 4 (moment deg.)
    L = 32 (block size)

  - 58 eigs are found
    - Subspace size = 96
    - max(res) = 1.0e-12



Numerical Example

- Test problem:
  Simulation of the international linear collider

$$T(z) = K - z^2 M + \mathrm{i} \sum_{j=1}^{t} \sqrt{z^2 - \sigma_j^2} W_j,$$

where $t = 1$, $\sigma_1 = 0$.

- Test environment: Cray-XT4 at NERSC @Berkeley
- Compiler: PGI Fortran
- Linear solver: SuperLU_DIST
- Eigensolver: SS-Hankel

Numerical Example 3 (NEP)

- Strong scalability for nonlinear (NEP) case
  - Matrix size: 2,738,556

- Two contour paths are used.
  - The number of quadrature points is $N = 32$.
  - 64 linear systems are solved in total.

#cores	256	512	1024	2048
time(sec.)	2513	1273	661	334
speedup	-	1.97	1.93	1.92

(Yamazaki et al., 2013)

Summary

- SS method: Contour integral-based method
  - Applicable for various problems, SEPs, GEPs and NEPs
  - SS-RR: Large sparse NEP is projected to a small size NEP

- Software
  - Fortran95+MPI: z-Pares (GEPs)
  - C: CISS in SLEPc (GEPs)
  - MATLAB: sseig_gep, sseig_pep, sseig_nep

- Future Work
  - Development of high performance software
    - Extension to NEPs
  - Prediction of appropriate parameters