contFEAST+: Conformal Mapping and Divide and Conquer for Differential Eigenvalue Problems

Anna Dietrich
Amherst College

Ziyu Huang
Boston College

Qingxuan Jiang
Cornell University

Kelly Robinett
University of Vermont

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Introduction

Problem Introduction

Problem: We are looking at the eigenvalue problem

$$\mathcal{L}u = \lambda u,$$

where $\mathcal{L}$ is an elliptic self-adjoint operator, which means all of its eigenvalues are on the positive real axis.

Goal: Find all the eigenvalues on an interval $[a, b]$.

Idea of contFEAST

- **Input**: Operator $\mathcal{L}$, contour $\Omega \subseteq \mathbb{C}$, and a function F (initial condition)
- **Step 1:** Compute the spectral projector

$$V = \mathcal{P}_{\mathcal{V}} F = \frac{1}{2\pi i} \int_{\partial\Omega} (zI - \mathcal{L})^{-1} dz.$$

  which projects F onto the span of the eigenvectors located in Ω.
- **Step 2:** Orthonormalize $V = QR$, where Q has orthonormal columns and R is upper-triangular.
- **Step 3:** Perform a Rayleigh-Ritz step, which will get us our eigenvalues and eigenfunctions.

Spectral Projector

The integral from the spectral projector can be approximated by a quadrature rule:

$$\mathcal{P}_{\mathcal{V}} = \frac{1}{2\pi i}\int_{\partial\Omega}(zI - \mathcal{L})^{-1}dz \approx \frac{1}{2\pi i}\sum_{k=1}^{q} w_k(z_kI - \mathcal{L})^{-1}.$$

Parameters for contFEAST

In general, we use the trapezoidal quadrature rule, where two parameters need to be chosen:

- **Shape of the contour**
- **Number of quadrature nodes** q

Additionally, to discretize this problem on operators into a matrix problem, we also need to choose:

- **Discretization size** N

Example Operator

Consider the operator

$$\mathcal{L}(v) = -\frac{1}{\cosh(x)}v'' + \frac{x^2}{\cosh(x)}v, v(-1) = v(1) = 0.$$

From Sturm-Liouville theory, its eigenvalues are given by the asymptotic formula [1, Eq. 4.7]

$$\lambda_n = \frac{n^2\pi^2}{\left(\int\limits_{-1}^{1} \sqrt{\cosh(x)}dx\right)^2} + a_0 + O(\frac{1}{n^2}), \tag{1}$$

where $a_0 \approx 0.4235$ is a constant.

Parameters for applying contFEAST

To find eigenvalues in the range $[a, b]$ of the above operator, we will use the following parameters:

- **Shape of contour**: A circle with the interval $[a, b]$ being the diameter.
- **Number of quadrature nodes**:

$$q \geq \left(C + \log\left(\frac{1}{\epsilon}\right)\right)\left(\frac{b-a}{\delta}\right)$$

  for δ being the smallest distance from either a or b to any eigenvalue, $C > 0$ being a small constant, and $\epsilon > 0$ being the error threshold (e.g. $\epsilon \approx 10^{-16}$ for machine precision)
- **Discretization size**: $N \approx \pi n$, for n being the largest index of eigenvalue in the range.

Advantage and Disadvantages of contFEAST

Advantage:

- contFEAST is very accurate if we compute one eigenvalue using a small circle contour.

Disadvantage:

- The number quadrature nodes needed for contFEAST scales linearly with $\frac{b-a}{\delta}$.
- If we want to compute eigenvalues on a long interval, the number of quadrature nodes needed would be huge.
  - Takes long time to compute
  - Introduce numerical instability as we are doing more operations

Conformal Mapping

Theory

Finding the Optimal Contour

Goal: Develop a better contour that reduces the number of quadrature nodes q needed to approximate eigenvalues.

General Idea: Apply node clustering, where more quadrature nodes are used in places closer to the singularity.

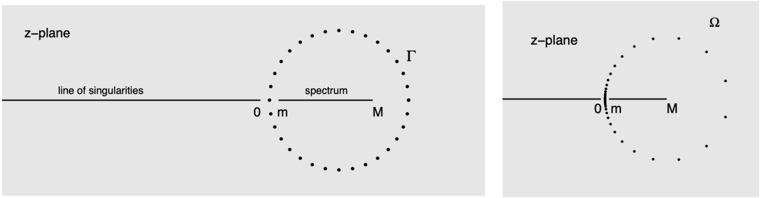


Figure: Illustration of node clustering around the singularity of the function [2].

Hale, Higham, and Trefethen's method

In [2], the authors evaluate $f(A)$ with the contour integral

$$f(A) = \frac{1}{2\pi i} \int_{\Omega} f(z)(zI - A)^{-1} dz,$$

for a closed contour Ω in the region of analyticity of f, winding around the spectrum of the matrix A.

Applying to our problem

Let $f(z) \equiv 1$. If we discretize $\mathcal{L}$ into a matrix $A \in \mathbb{C}^{N \times N}$, then we recover the spectral projector

$$P_\Omega = \frac{1}{2\pi i} \int_\Omega (zI - A)^{-1} dz.$$

and we take Ω to be a circular contour that winds around the interval $[a, b]$.

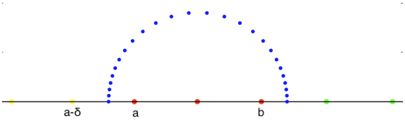
Symmetry of the Integral

Since the contour Ω is symmetric to the real axis, we have

$$P_\Omega = \frac{1}{2\pi i}\int_\Omega f(z)(zI-A)^{-1}dz = \frac{1}{\pi}\mathrm{Im}\int_{\Omega_1}(zI-A)^{-1}\,dz,$$

where Ω_1 is Ω on the upper half plane with same orientation.

Thus, we only need to consider the part of contour above the real axis.



Conformal Mapping

Conformal Mapping: A function $\mathbb{C} \to \mathbb{C}$ that locally preserves angles;

- **Jacobi elliptic function**: $u = \int\limits_0^{\phi} \frac{d\theta}{\sqrt{1-m\sin^2(\theta)}}$,

  $\mathrm{sn}(u) = \sin(\phi),\ \mathrm{cn}(u) = \cos(\phi),\ \mathrm{dn}(u) = \sqrt{1-m\sin^2(\phi)}$;

  The Schwarz-Christoffel Toolbox: [sn cn dn] = ellipjc(u,m);
- **Möbius transformation**: transformation combining translations, rations, magnifications, and inverses.

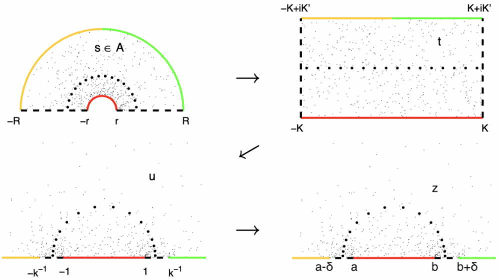
Building the New Contour

Spectrum: $[a, b]$;
Eigenvalue-free Region:
$(a-\delta, a) \cup (b, b+\delta)$

Steps:

1. $t(s) = \frac{2Ki}{\pi} \log(-\frac{si}{r})$
2. $u(t) = \mathrm{sn}(t \mid k^2)$
3. $z(u) = \frac{b-a}{2} u + \frac{a+b}{2}$

r, R, k, K are determined by reversed mapping.



Building the New Contour

Ω_1 is parameterized by $z(t)$ where $t \in [-K + iK'/2, K + iK'/2]$.

After the change of variable,

$$P_\Omega = -\frac{b-a}{2\pi}\mathrm{Im}\int_{-K+iK'/2}^{K+iK'/2}(z(t)I - A)^{-1}\mathrm{cn}(t)\mathrm{dn}(t)dt.$$

Then the equally-spaced trapezoidal quadrature rule $t_j = -K + \frac{iK'}{2} + \frac{2jK}{q}$ for $0 \le j \le q$; $w_0 = w_q = \frac{1}{2}$, $w_k = 1$ for $1 \le k \le q-1$ gives

$$P_\Omega \approx -\frac{K(b-a)}{q\pi}\mathrm{Im}\left(\sum_{j=0}^{q} w_j(z(t_j)I - A)^{-1}\mathrm{cn}(t_j)\mathrm{dn}(t_j)\right).$$

Building the New Contour

In coding, we want to simplify the calculation of P_Ω and store the extra coefficients into the weights. We have

$$P_\Omega \approx \operatorname{Im}\left(\sum_{j=0}^{q} w_j'(z(t_j)I - A)^{-1}\right),$$

where $w_j' = -\dfrac{K(b-a)}{q\pi}\operatorname{cn}(t_j)\operatorname{dn}(t_j)$ for $1 \le j \le q-1$,
and $w_j' = -\dfrac{K(b-a)}{2q\pi}\operatorname{cn}(t_j)\operatorname{dn}(t_j)$ for $j = 0, q$.

Experiments

Experiment 1: Plotting the Contours

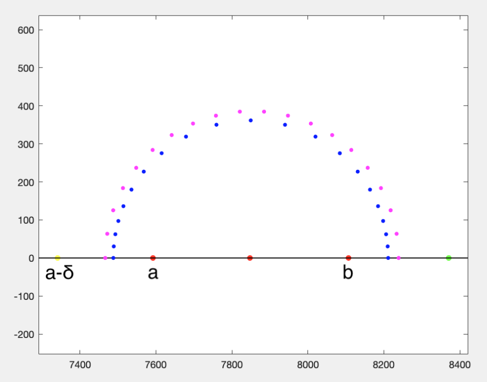


Figure: The contour generated by the conformal mapping (blue) versus the equally spaced circular contour (pink)

Experiment 2: Comparing to contFEAST

We tested on the minimum number of nodes needed under the accuracy of 10^{-11} respectively for the conformal mapping contour and the equally spaced circular contour. The set of eigenvalues being estimated is $\{\lambda_{1000}, \ldots, \lambda_{1000+e}\}$

	contFEAST+		contFEAST	
e	nodes	accuracy	nodes	accuracy
11	18	10^{-11}	180	10^{-11}
21	21	10^{-11}	390	10^{-11}
51	25	10^{-11}	600	10^{-11}
101	28	10^{-11}	1700	10^{-11}
201	32	10^{-11}	3500	10^{-11}

Clustering the nodes improves the approximation.

Analysis on the Number of Nodes

In [2, Thm 2.1, Eqn 2.9], for an interval $[m, M]$ and q quadrature nodes, the rate of convergence is

$$\|f(A) - f_q(A)\| = O(e^{-\pi^2 q/(\log(M/m)+3)}).$$

In our case, the ratio is $\dfrac{M}{m} = \dfrac{b-(a-\delta)}{a-(a-\delta)} = \dfrac{b-a}{\delta} + 1.$
Fixing the accuracy $\epsilon > \|f(A) - f_q(A)\|$, we have

$$q \geq \frac{1}{\pi^2} \log(\frac{1}{\epsilon}) \left(\log(\frac{b-a}{\delta} + 1) + 3 \right),$$

so the minimum of q grows linearly with $\log(\frac{b-a}{\delta})$.

Experiment 3: Number of Nodes versus the Ratio $\frac{b-a}{\delta}$

Using the asymptotic formula to pick the eigenvalues, we have

trial	ratio	λ	# of λ	nodes	relative error
1	10	λ_8	4	15	10^{-11}
2	10^2	λ_{80}	40	25	10^{-11}
3	10^2	λ_{203}	45	24	10^{-12}
4	10^2	λ_{1201}	49	20	10^{-11}
5	10^3	λ_{67}	200	33	10^{-11}
6	10^3	λ_{225}	300	34	10^{-10}
7	10^3	λ_{800}	400	33	10^{-12}
8	10^4	λ_{17}	400	43	10^{-11}
9	10^4	λ_{28}	500	46	10^{-10}
10	10^4	λ_{125}	1000	46	10^{-10}
11	10^5	λ_{42}	2000	190	10^{-13}

Divide and Conquer

Divide and Conquer Method

- **How it works**: Split up the interval into smaller regions with a constant number of eigenvalues and quadrature nodes, but variable discretization size.
- **Why it matters**: The total cost of these computations will be less because they are split into smaller, easier to manage subsections which will subsequently make the program faster and more efficient to run.

Time Complexity Analysis

- **Problem**: Compute all eigenvalues from λ_{n+1} to λ_{n+m}.
- **Original Method Time Complexity**:

$$O\left(m^3 + m^2 n + (m^2 + mn)\log(m+n)\right)$$

- **Divide and Conquer Time complexity**: Say we split the interval into k parts, each containing $\frac{m}{k}$ eigenvalues, and apply above method to each interval. Time complexity becomes

$$O\left(\frac{m^3}{k} + m^2 n + (m^2 + mn)\log(m+n)\right)$$

Interpretation of Time Complexity Analysis

- **Balancing**: In practice, we need to pick the number of intervals k to balance the overhead and computation times.
- **Parallelization**: Divide and conquer allows the problem to be run on multiple machines, significantly reducing the running time.

Load Balancing

We begin with (10) intervals of equal size:

200	**200**	**200**	**200**	**200**	**200**	**200**	**200**	**200**	**200**

And end up with (9) intervals balanced for anticipated cost:

350	**280**	**244**	**220**	**204**	**191**	**181**	**173**	**157**

Experimental Results

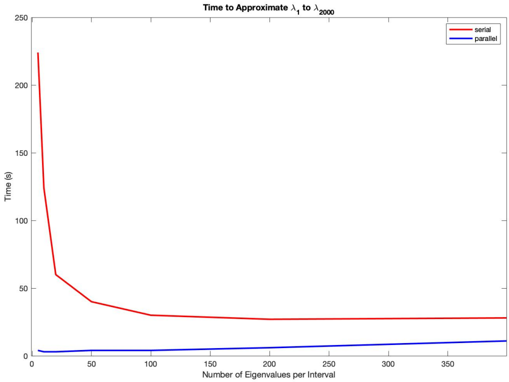
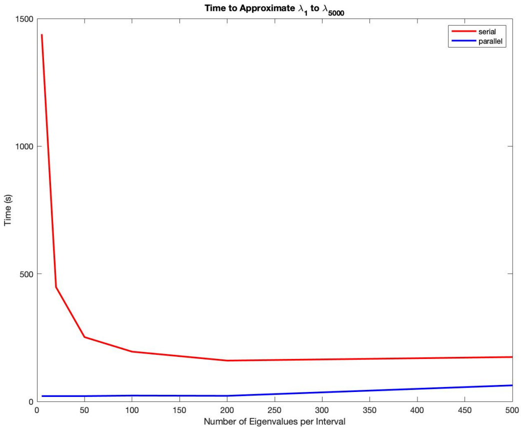


Figure: Comparing serial and parallel computation for $\lambda_1 \ldots \lambda_{2000}$

Experimental Results Cont.



Future Work

Next Steps

We want to see if the conformal mapping design of contour can be applied to the sectorial operators.

Self-adjoint Operator: eigenvalues on the positive real axis; e.g

$$\mathcal{L}(v) = (v'' + x^2 v)/\cosh(x).$$

Sectorial Operator: eigenvalues contained in a sector in the right half of the complex plane; e.g

$$\mathcal{L}(v) = -e^{-x^2/\epsilon^2} v'' + \cos(\pi x/2) v'.$$

Next Steps

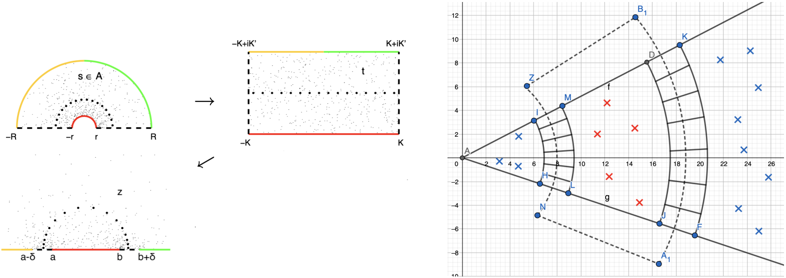


Figure: conformal mapping of the self-adjoint operator (left); eigenvalue distribution of the sectorial operator (right)

References

[1] C. T. Fulton and S. A. Pruess. Eigenvalue and eigenfunction asymptotics for regular sturm-liouville problems. *Journal of Mathematical Analysis and Applications*, 188(1):297–340, 1994.

[2] N. Hale, N. J. Higham, and L. N. Trefethen. Computing A^{α}, log(A), and related matrix functions by contour integrals. *SIAM J. Numer. Anal.*, 46(5):2505–2523, 2008.