A fast and well-conditioned spectral method for singular integral equations

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Outline

- Singular integral equations:
  \[ \int_{\Gamma} K(x, y)u(y) \, dy = f(x), \quad Bu = c, \]

  Classical collocation method [Elliott 1982], hybrid quadrature rules [Alpert 1999], etc,...

- Classical applications
  - Boundary integral equations for Laplace & Helmholtz equations
  - Fracture mechanics

- Contemporary applications
  - Korteweg-de Vries (KdV) and nonlinear Schrödinger (NLS) equation via inverse scattering transform
  - Random matrix theory and orthogonal polynomials by reformulating as a matrix-valued Riemann–Hilbert problem.

- New combination of three key ingredients:
  - use a basis in which singularities are integrated exactly
  - The basis allows for banded linear algebra
  - and low rank bivariate approximants for integral kernels
2D Elliptic PDEs

In this work, we will consider:

- the Laplace equation:
  \[-\Delta u(x) = 0, \quad \Phi(x, y) = \frac{1}{2\pi} \log |x - y|,\]

- the Helmholtz equation:
  \[-(\Delta + k^2)u(x) = 0, \quad \Phi(x, y) = \frac{i}{4} H_0^{(1)}(k|x - y|),\]

- the gravity Helmholtz equation:
  \[-(\Delta + E + x_2^2)u(x) = 0, \quad \Phi(x, y) = \frac{1}{4\pi} \int_0^\infty \exp\left[\frac{|x - y|^2}{4t} + \left(E + \frac{x_2^2 + y_2^2}{2}\right)t - \frac{1}{12}t^3\right] \frac{dt}{t},\]

where the fundamental solution is derived in [Bracher et al 1998]. Numerical evaluation via the trapezoidal rule [Trefethen and Weideman 2014] on path of steepest descent. Timings of $10^5/s$ are reported in [Barnett et al. 2014].
Theorem [Vekua 1967] where for analytic coefficients of an elliptic PDO (accomplished with Riemann function):

\[ \Phi(x, y) = A(x, y) \log |x - y| + B(x, y), \quad \text{where} \quad A(x, x) = -(2\pi)^{-1}. \]

For any continuous density [Kress 2010] \( u \), let \( S_\Gamma \) and \( D_\Gamma \) define the single- and double-layer potentials:

\[ S_\Gamma u(x) = \int_{\Gamma} \Phi(x, y)u(y) \, d\Gamma(y), \quad \text{for} \quad x \in D, \]

\[ D_\Gamma u(x) = \int_{\Gamma} \frac{\partial \Phi(x, y)}{\partial n(y)} u(y) \, d\Gamma(y), \quad \text{for} \quad x \in D. \]

For homogeneous equations \( L[u] = 0 \), Green’s representation theorem allows for the determination of the exterior solutions given data on the boundary \( \Gamma \):

\[ u(x) = -S_\Gamma [\partial u/\partial n](x) + D_\Gamma [u](x), \quad \text{for} \quad x \in D. \]
Definition (Dirichlet Problem, Kress 2010)
Given \( u^i(x) \in C^2(\mathbb{R}^2) \) satisfying \( L[u^i] = 0 \), find \( u^s(x) \in C^2(D) \cap C^{0,\alpha}(\Gamma) \) satisfying \( L[u^s] = 0 \) and the radiation condition at infinity, and:

\[
u^i(x) + u^s(x) = 0, \quad \text{for} \quad x \in \Gamma.\]

Theorem (Dirichlet Solution, Kress 2010)
The scattered solution to the Dirichlet problem is represented everywhere by the single-layer potential. The density \([\partial u/\partial n]\) satisfies:

\[
\int_{\Gamma} \Phi(x, y) \left[ \frac{\partial u}{\partial n} \right] d\Gamma(y) = u^i(x), \quad x \in \Gamma.
\]
Practical approximation theory: Chebyshev polynomials

- Chebyshev polynomials:
  \[ T_n(x) = \cos(n \cos^{-1}(x)), \quad \text{for} \quad n \in \mathbb{N}_0, \quad \text{and} \quad x \in [-1, 1]. \]

- Interpolants: \( p_N(x) = \sum_{n=0}^{N} c_n T_n(x), \quad x \in [-1, 1], \)

- Interpolation condition:
  \[ p_N(x_n) = f(x_n) \quad \text{where} \quad x_n = \cos\left(\frac{2n + 1}{2N + 2}\pi\right), \quad \text{for} \quad n = 0, \ldots, N. \]

- Clenshaw’s algorithm for \( O(n) \) evaluation of interpolants,
- DCT for \( O(n \log n) \) transformation of the interpolation condition into approximate projections,
- Convergence depends on regularity.
The ultraspherical spectral method of [Olver and Townsend 2013] represents solutions of linear ordinary differential equations of the form:

\[ \mathcal{L}u = f, \quad Bu = c, \]

where \( \mathcal{L} \) is a linear operator of the form:

\[ \mathcal{L} = a_N(x) \frac{d^N}{dx^N} + \cdots + a_1(x) \frac{d}{dx} + a_0(x), \]

and \( B \) contains \( N \) linear functionals satisfied by \( u(x) \) in Chebyshev expansions:

\[ u(x) = \sum_{n=0}^{\infty} u_n T_n(x), \]

where \( T_n(x) \) is the Chebyshev polynomial of the first kind of degree \( n \), and \( u = (u_0, u_1, \ldots)^\top \) is a vector of coefficients. Three ingredients we need are:

- Differentiation
- Conversion
- Multiplication
Differentiation

- Differentiation is banded if we change bases:

\[
\frac{d^\lambda T_n(x)}{dx^\lambda} = \begin{cases} 
0, & 0 \leq n \leq \lambda - 1, \\
2^{\lambda-1}(\lambda - 1)! \ n \ C_{n-\lambda}^{(\lambda)}(x), & n \geq \lambda,
\end{cases}
\]

where \( C_n^{(\lambda)} \) represents the ultraspherical polynomial of integral order \( \lambda \) and of degree \( n \).

- This sparse differentiation has the operator representation:

\[
\mathcal{D}_\lambda = 2^{\lambda-1}(\lambda - 1)! \begin{pmatrix} 
\lambda \text{ times} \\
0 & \cdots & 0 & \lambda \\
\lambda + 1 \\
\lambda + 2 \\
\ddots
\end{pmatrix},
\]

mapping \( T_n \) to \( C_n^{(\lambda)} \).
Conversion & Multiplication

- Conversion from $T_n$ to $C^{(1)}_n$ and from $C^{(\lambda)}_n$ to $C^{(\lambda+1)}_n$ is banded:

\[
S_0 = \begin{pmatrix}
1 & 0 & -\frac{1}{2} \\
\frac{1}{2} & 0 & -\frac{1}{2} \\
\frac{1}{2} & 0 & \ddots \\
\ddots & \ddots & \ddots
\end{pmatrix}, \quad S_\lambda = \begin{pmatrix}
1 & 0 & -\frac{\lambda}{\lambda+2} \\
\frac{\lambda}{\lambda+1} & 0 & -\frac{\lambda}{\lambda+3} \\
\frac{\lambda}{\lambda+2} & 0 & \ddots \\
\ddots & \ddots & \ddots
\end{pmatrix}.
\]

- Multiplication is banded:

\[
M_0[a] = \frac{1}{2} \begin{bmatrix}
2a_0 & a_1 & a_2 & \cdots \\
a_1 & 2a_0 & a_1 & \ddots \\
a_2 & a_1 & 2a_0 & \ddots \\
\vdots & \ddots & \ddots & \ddots
\end{bmatrix} + \begin{bmatrix}
a_1 & a_2 & a_3 & \cdots \\
a_2 & a_3 & a_4 & \ddots \\
a_3 & a_4 & a_5 & \ddots \\
\vdots & \ddots & \ddots & \ddots
\end{bmatrix}.
\]

Using the recurrence relation for the ultraspherical polynomials, multiplication operators are built in higher order bases as needed.
Ultraspherical spectral method: Example

We solve $\epsilon (\epsilon + x^2) u''(x) = x u(x)$, $u(-1) = 1$, $u(1) = 0$ in as little as $\sim 0.0057$ s in Chebfun or ApproxFun.jl.

Left: the structure of the system. Right: a plot of the solution for $\epsilon = 10^{-4}$. In this case, a Chebyshev expansion of degree 3,276 is required to approximate the solution to double precision.
Singular integral equations

Consider the SIE:

\[
\frac{1}{\pi} \int_{-1}^{1} \left( \frac{K_1(x, y)}{(y - x)^2} + \frac{K_2(x, y)}{y - x} + \log |y - x| K_3(x, y) + K_4(x, y) \right) u(y) \, dy = f(x),
\]

- where \( K_1, K_2, K_3 \) and \( K_4 \) are continuous bivariate kernels,
- \( f \) is a known continuous function,
- and integration is interpreted by the Cauchy principal value or Hadamard finite-part.

For the ultraspherical spectral method, we require singular integral operators and bivariate kernels.
Hilbert transform

- We have the finite Hilbert transform [King 2009]:

\[
\mathcal{H}_{(-1,1)} \left[ \frac{T_n(x)}{\sqrt{1-x^2}} \right] = \begin{cases} 
0, & n = 0, \\
C_n^{(1)}(x), & n \geq 1,
\end{cases}
\]

- Integrating with respect to \( x \), we obtain the log transform:

\[
\mathcal{L}_{(-1,1)} \left[ \frac{T_n(x)}{\sqrt{1-x^2}} \right] = \begin{cases} 
-\log 2, & n = 0, \\
-\frac{T_n(x)}{n}, & n \geq 1,
\end{cases}
\]

- Differentiating:

\[
\mathcal{H}'_{(-1,1)} \left[ \frac{T_n(x)}{\sqrt{1-x^2}} \right] = \begin{cases} 
0, & n = 0,1, \\
C_n^{(2)}(x), & n \geq 2,
\end{cases}
\]

- Integration (divided by \( \pi \)):

\[
\Sigma_{(-1,1)} \left[ \frac{T_n(x)}{\sqrt{1-x^2}} \right] = \begin{cases} 
1, & n = 0, \\
0, & n \geq 1.
\end{cases}
\]
2D: Tensor and SVD

- In 2D, we scale with $O(mn)$ function samples and $O(\min(mn \log n, nm \log m))$ arithmetic via fast 2D transforms.
- Consider the function $f \in C([-1, 1]^2)$, then the two dimensional interpolant takes the form:

$$p_{m,n}(x, y) = \sum_{i=0}^{m-1} \sum_{j=0}^{n-1} A_{i,j} T_i(x) T_j(y).$$

- Using the SVD: $A = U\Sigma V^*$, we reveal the rank of $A$:

$$p_{\text{SVD}}(x, y) = \sum_{i=1}^{k} \sigma_i u_i(x) v_i^*(y),$$

where $\sigma_i$ are the singular values, and $u_i(x)$ and $v_i^*(y)$ are univariate approximations and $A$ the optimal rank-$k$ approximant in $L^2([-1, 1]^2)$.
- Can we get a low rank form without computing the 2D matrix of coefficients or the SVD?
Given $f(x, y) \in C([-1, 1]^2)$ and a tol, we find $f_k$ such that $\|f - f_k\| < \text{tol}$.

Set $e_0(x, y) = f(x, y)$, $f_0(x, y) = 0$, $k = 0$.

while $|e_k(x_k, y_k)| = \max(|e_k(x, y)|) > \text{tol}$

$$e_{k+1}(x, y) = e_k(x, y) - \frac{e_k(x_k, y) e_k(x, y_k)}{e_k(x_k, y_k)}$$

$$f_{k+1}(x, y) = f_k(x, y) + \frac{e_k(x_k, y) e_k(x, y_k)}{e_k(x_k, y_k)}$$

$k = k + 1$

end

Result: $p_{GE}(x, y) = \sum_{i=1}^{k} A_i(x) B_i(y)$,

Scales with a search over $O(mn)$ function samples and $O(k (m \log m + n \log n))$ arithmetic via fast one-dimensional transforms.
Low rank approximations are separable models:

\[ K_\lambda(x, y) = \sum_{i=1}^{k_\lambda} A_{\lambda,i}(x) B_{\lambda,i}(y), \quad \text{for} \quad \lambda = 1, 2, 3, 4, \]

then:

\[ \mathcal{H}_{(-1,1)}'[K_1] = \sum_{i=1}^{k_1} \mathcal{M}_2[A_{1,i}(x)] \mathcal{H}_{(-1,1)}'[\mathcal{M}_0[B_{1,i}(y)]], \quad \mathcal{H}_{(-1,1)}[K_2] = \sum_{i=1}^{k_2} \mathcal{M}_1[A_{2,i}(x)] \mathcal{H}_{(-1,1)}[\mathcal{M}_0[B_{2,i}(y)]], \]

\[ \mathcal{L}_{(-1,1)}'[K_3] = \sum_{i=1}^{k_3} \mathcal{M}_0[A_{3,i}(x)] \mathcal{L}_{(-1,1)}[\mathcal{M}_0[B_{3,i}(y)]], \quad \Sigma_{(-1,1)}[K_4] = \sum_{i=1}^{k_4} \mathcal{M}_0[A_{4,i}(x)] \Sigma_{(-1,1)}[\mathcal{M}_0[B_{4,i}(y)]], \]

and ultimately:

\[ (\mathcal{H}_{(-1,1)}'[K_1] + S_1 \mathcal{H}_{(-1,1)}[K_2] + S_1 S_0 (\mathcal{L}_{(-1,1)}'[K_3] + \Sigma_{(-1,1)}[K_4])) u = S_1 S_0 f. \]

- Affine maps from \((-1, 1)\) to \((a, b)\) allow general intervals in \(\mathbb{C}\).
- Union of disjoint intervals by interlacing operators & coefficients.
Applications: the Faraday cage

Consider $n$ infinitesimally thin plates located at the $n$ roots of unity [Chapman, Hewett and Trefethen 2015]. We seek to find the solution to the Laplace equation such that:

$$u(x) = u_0 \quad \text{for} \quad x \in D,$$
$$u(x) = \log |x - x_0| + O(1), \quad \text{as} \quad |x - x_0| \to 0,$$
$$u(x) = \log |x| + o(1), \quad \text{as} \quad |x| \to \infty.$$

We can split the solution $u = u^i + u^s$ as in a scattering problem, where:

$$u^i(x) = \log |x - (2, 0)|,$$

is the source term with strength $2\pi$ located at $(2, 0)$.

Dirichlet boundary conditions on $\Gamma$. We augment our system with the zero sum condition on the total charge:

$$\int_{\Gamma} \left[ \frac{\partial u(y)}{\partial n} \right] \, d\Gamma(y) = 0,$$

and the unknown constant $u_0$ to accommodate this condition.
Applications: the Faraday cage

Left: a plot of the solution $u(x)$ with 10 normal plates with radial parameter $r = 10^{-1}$. Right: a plot of the solution $u(x)$ with 40 tangential plates with the same radial parameter.
Applications: acoustic scattering

Acoustic scattering with Neumann boundary conditions from an incident wave with $k = 50$ and $\mathbf{d} = (1/\sqrt{2}, -1/\sqrt{2})$. 
Acoustic scattering with Neumann boundary conditions from an incident wave with $k = 50$ and $d = (1/\sqrt{2}, -1/\sqrt{2})$. 
Scattering in a linearly stratified medium \(- (\Delta + E + x_2) u(x) = 0\).

- Fourier transform from time-energy \(\Rightarrow\) an interpretation as the Schrödinger equation with linear potential
- Models quantum particles of fixed energy in a uniform gravitational field [Barnett et al. 2014]
- Classical Hamiltonian \(\Rightarrow\) rays are \textit{parabolic} instead of linear
- Every point in the “classically allowed” region is illuminated twice
Applications: gravity Helmholtz

In the figure $E = 20$ and source located at $(0, -5)$. 
Diagonal preconditioner for compactness

The space $\ell^2_\lambda \subset \mathbb{C}^\infty$ is defined as the Banach space with norm:

$$\|u\|_{\ell^2_\lambda} = \sqrt{\sum_{k=0}^{\infty} |u_k|^2 (k + 1)^{2\lambda}} < \infty.$$ 

**Lemma**

If $\Phi = A(x, y) \log |x - y| + B(x, y)$ and if:

$$R = \begin{pmatrix} \frac{1}{2 \log 2} & 2 \\ 2 & 4 \\ \vdots & \vdots \end{pmatrix} : \ell^2_\lambda \to \ell^2_{\lambda - 1},$$

then:

$$\left( \mathcal{L}_{(-1,1)}[\pi A] + \Sigma_{(-1,1)}[\pi B] \right) R = I + \mathcal{K},$$

where $\mathcal{K} : \ell^2_\lambda \to \ell^2_\lambda$ is compact for $\lambda = 1, 2, \ldots$. 
Fast Chebyshev multiplication + banded operators = fast operator-function products ⇒ continuous Krylov methods.
Conclusion & Outlook

- SingularIntegralEquations.jl is an open-source framework for solving singular integral equations. It requires open-source ApproxFun.jl and is written in free & open-source JULIA.
- Polynomially mapped domains can be treated via the spectral mapping theorem.
- Fundamental solution is known for Helmholtz equation with a parabolic refractive index. Models Gaussian beams in optical fibres.
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References