On the Use of Conformal Maps for the Acceleration of Convergence of the Trapezoidal Rule and Sinc Numerical Methods

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Outline

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  - Review trapezoidal rule
  - Introduce variable transformations
  - Error analysis
- Sinc Numerical Methods
  - Review Sinc numerical methods
  - Error analysis
- Maximize convergence rates despite nearby complex singularities
  - Existence of variable transformations
  - Schwarz-Christoffel formula
  - Practical alternative
  - Locations of singularities unknown
- Examples & Applications

Trapezoidal Rule

- The trapezoidal rule $\int_a^b f(x)\,\mathrm{d}x \approx (b-a)\left[\frac{f(a)+f(b)}{2}\right]$.
- The composite version $T(h) = h\sum_{k=1}^{n-1}\frac{f(x_{k-1})+f(x_k)}{2}$, where $h = \frac{b-a}{n}$ and $x_k = a + k\,h$.
- Euler-Maclaurin summation formula $T(h) - \int_a^b f(x)\,\mathrm{d}x \sim$ $\sum_{l=1}^{\infty} h^{2l}\frac{B_{2l}}{(2l)!}\left(f^{(2l-1)}(b) - f^{(2l-1)}(a)\right), \quad \text{as} \quad h \to 0.$
- If $f^{(n)}(\cdot) \to 0$ at endpoints, the convergence is faster than any power of h [Trefethen and Weidemann 2015].
- Variable transformations $\phi : \mathbb{R} \to (a, b)$ with exponential decay [Stenger 1970] and [Takahasi and Mori 1974].

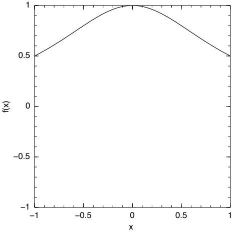
Preview of Optimization

Consider the integral for $\epsilon > 0$: $\int_{-1}^{1} \frac{\epsilon^2}{x^2 + \epsilon^2}\,\mathrm{d}x = \epsilon \tan^{-1}(\epsilon^{-1})$.

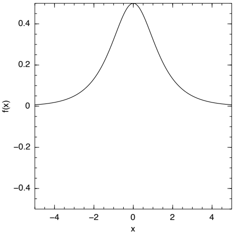
Variable transformations which induce endpoint decay are:

$$x = \phi_{SE}(t) = \tanh(t/2), \qquad x = \phi_{DE}(t) = \tanh(\pi/2 \sinh(t)).$$

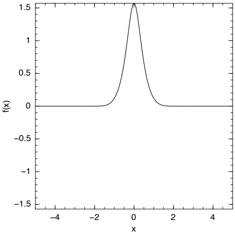
$$\phi'_{SE}(t) = \operatorname{sech}^2(t/2)/2, \qquad \phi'_{DE}(t) = \operatorname{sech}^2(\pi/2 \sinh(t))\pi/2 \cosh(t).$$



Integrand $\epsilon = 1$

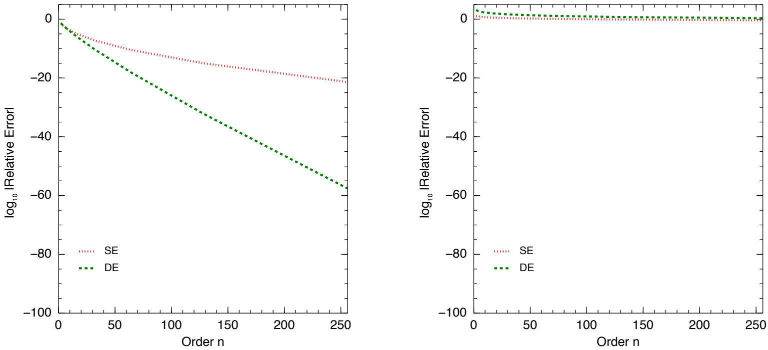


SE transformation



DE transformation

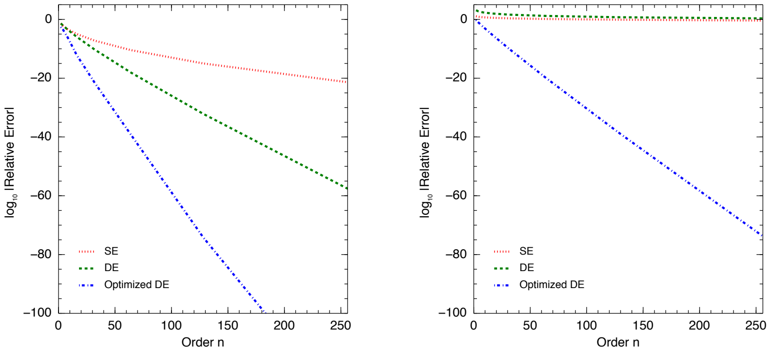
Preview of Optimization



$\epsilon = 1$ $\epsilon = 0.001$

A total failure in the quadrature rules with nearby singularities.
Is there an optimal variable transformation?

Preview of Optimization



$\epsilon = 1$ $\epsilon = 0.001$

$$x = \phi_{DEopt}(t) = \tanh(\tan^{-1}(\epsilon)\sinh(t)),$$
$$\phi'_{DEopt}(t) = \operatorname{sech}^2(\tan^{-1}(\epsilon)\sinh(t))\tan^{-1}(\epsilon)\cosh(t).$$

Quadrature by Variable Transformation

Let d be a positive number and let $\mathscr{D}_d$ denote the strip region of width $2d$ about the real axis:

$$\mathscr{D}_d = \{z \in \mathbb{C} : |\mathrm{Im}\, z| < d\}.$$

Let $\omega(z)$ be a non-vanishing function defined on $\mathscr{D}_d$, and let:

$$H^\infty(\mathscr{D}_d, \omega) = \{f : \mathscr{D}_d \to \mathbb{C} |\, f(z) \text{ is analytic in } \mathscr{D}_d, \text{ and } ||f|| < +\infty\}.$$

Let $\mathscr{E}^{\mathrm{T}}_{N,h}(H^\infty(\mathscr{D}_d, \omega))$ denote the error norm in $H^\infty(\mathscr{D}_d, \omega)$:

$$\mathscr{E}^{\mathrm{T}}_{N,h}(H^\infty(\mathscr{D}_d, \omega)) = \sup_{||f|| \le 1} \left| \int_{-\infty}^{+\infty} f(x)\,\mathrm{d}x - h \sum_{k=-n}^{+n} f(kh) \right|.$$

Let $B(\mathscr{D}_d)$ be the family of functions f such that:

$$\mathcal{N}_1(f, \mathscr{D}_d) = \int_{\partial \mathscr{D}_d} |f(z)|\,\mathrm{d}z < +\infty.$$

Quadrature by Variable Transformation

Theorem [Sugihara 1997] Suppose:

1. $\omega(z) \in B(\mathscr{D}_d)$;
2. $\omega(z)$ does not vanish at any point in $\mathscr{D}_d$ and takes real values on the real axis;
3. $\alpha_1 \exp\left(-(\beta|x|^\rho)\right) \le |\omega(x)| \le \alpha_2 \exp\left(-(\beta|x|^\rho)\right), \quad x \in \mathbb{R}$,
   where $\alpha_1, \alpha_2, \beta > 0$ and $\rho \ge 1$.

Then:

$$\mathscr{E}^{\mathrm{T}}_{N,h}(H^\infty(\mathscr{D}_d, \omega)) \le C_{d,\omega} \exp\left(-(\pi d \beta N)^{\frac{\rho}{\rho+1}}\right),$$

where $N = 2n+1$, the mesh size h is chosen optimally as:

$$h = (2\pi d)^{\frac{1}{\rho+1}} (\beta n)^{-\frac{\rho}{\rho+1}},$$

and $C_{d,\omega}$ is a constant depending on d and ω.

Quadrature by Variable Transformation

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   where $\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma > 0$.

Then:

$$\mathscr{E}^{\mathrm{T}}_{N,h}(H^\infty(\mathscr{D}_d, \omega)) \le C_{d,\omega} \exp\left(-\frac{\pi d \gamma N}{\log(\pi d \gamma N / \beta_2)}\right),$$

where $N = 2n + 1$, the mesh size h is chosen optimally as:

$$h = \frac{\log(2\pi d \gamma n / \beta_2)}{\gamma n},$$

and $C_{d,\omega}$ is a constant depending on d and ω.

Sinc Numerical Methods

Let us consider the $N(= 2n + 1)$-point Sinc approximation of a function on the real line:

$$f(x) \approx \sum_{j=-n}^{+n} f(j\,h) S(j,h)(x),$$

where $S(j,h)(x)$ is the so-called Sinc function:

$$S(j,h)(x) = \frac{\sin[\pi(x/h - j)]}{\pi(x/h - j)},$$

and where the step size h is suitably chosen for a given positive integer n. Let $\mathscr{E}_{N,h}^{\mathrm{Sinc}}(H^\infty(\mathscr{D}_d,\omega))$ denote the error norm in $H^\infty(\mathscr{D}_d,\omega)$:

$$\mathscr{E}_{N,h}^{\mathrm{Sinc}}(H^\infty(\mathscr{D}_d,\omega)) = \sup_{||f||\leq 1} \left\{ \sup_{x\in\mathbb{R}} \left| f(x) - \sum_{j=-n}^{+n} f(j\,h)\,S(j,h)(x) \right| \right\}.$$

Sinc Numerical Methods

Theorem [Sugihara 2003] Suppose:

1. $\omega(z) \in B(\mathscr{D}_d)$;
2. $\omega(z)$ does not vanish at any point in $\mathscr{D}_d$ and takes real values on the real axis;
3. $\alpha_1 \exp\left(-(\beta|x|^\rho)\right) \leq |\omega(x)| \leq \alpha_2 \exp\left(-(\beta|x|^\rho)\right), \quad x \in \mathbb{R}$,
   where $\alpha_1, \alpha_2, \beta > 0$ and $\rho \geq 1$.

Then:

$$\mathscr{E}_{N,h}^{\mathrm{Sinc}}(H^\infty(\mathscr{D}_d, \omega)) \leq C_{d,\omega} N^{\frac{1}{\rho+1}} \exp\left(-\left(\frac{\pi d \beta N}{2}\right)^{\frac{\rho}{\rho+1}}\right),$$

where $N = 2n+1$, the mesh size h is chosen optimally as:

$$h = (\pi d)^{\frac{1}{\rho+1}} (\beta n)^{-\frac{\rho}{\rho+1}},$$

and $C_{d,\omega}$ is a constant depending on d and ω.

Sinc Numerical Methods

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   where $\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma > 0$.

Then:

$$\mathscr{E}^{\mathrm{Sinc}}_{N,h}(H^\infty(\mathscr{D}_d, \omega)) \leq C_{d,\omega} \exp\left(-\frac{\pi d \gamma N}{2\log(\pi d \gamma N/(2\beta_2))}\right),$$

where $N = 2n + 1$, the mesh size h is chosen optimally as:

$$h = \frac{\log(\pi d \gamma n/\beta_2)}{\gamma n},$$

and $C_{d,\omega}$ is a constant depending on d and ω.

An Upper Bound

Nonexistence Theorem [Sugihara 1997] There exists no function $\omega(z)$ that satisfies at once:

1. $\omega(z) \in B(\mathscr{D}_d)$;
2. $\omega(z)$ does not vanish at any point in $\mathscr{D}_d$ and takes real values on the real axis;
3. $\omega(x) = \mathcal{O}\left(\exp(-\beta e^{\gamma|x|})\right)$ as $|x| \to \infty$, where $\beta > 0$, and $d\gamma > \pi/2$.

Conclusion:

- Based essentially on the celebrated Pragmén-Lindelöf principle, Sugihara excludes utility of further decay.
- Optimality of the DE transformation for the trapezoidal rule and Sinc numerical methods.

Maximizing the Convergence Rates

Problem: How can we maximize the convergence rate of the trapezoidal rule or the Sinc approximation:

$$\int_{-\infty}^{\infty} f(\phi(t))\phi'(t)\,\mathrm{d}t \approx h \sum_{k=-n}^{+n} f(\phi(k\,h))\phi'(k\,h),$$

$$f(x) \approx \sum_{j=-n}^{+n} f(\phi(j\,h))S(j,h)(\phi^{-1}(x)),$$

despite the singularities of $f \in \mathbb{C}$? Let

$$\Phi_{\rm ad} = \left\{ \begin{array}{lll} \phi & : & f(\phi(t))\phi'(t) \in H^{\infty}(\mathscr{D}_d,\omega) \text{ for some } d>0, \\ & & \text{and for some } \omega \text{ such that:} \\ & 1. & \omega(z) \in B(\mathscr{D}_d); \\ & 2. & \omega(z) \text{ does not vanish at any point in } \mathscr{D}_d \\ & & \text{ and takes real values on the real axis;} \\ & 3. & \alpha_1 \exp\left(-\beta_1 e^{\gamma|x|}\right) \le |\omega(x)| \le \alpha_2 \exp\left(-\beta_2 e^{\gamma|x|}\right), \\ & & x \in \mathbb{R}, \quad \text{where } \alpha_1,\alpha_2,\beta_1,\beta_2,\gamma > 0. \end{array} \right\}$$

Maximizing the Convergence Rates

Then we wish to find $\phi \in \Phi_{\mathrm{ad}}$ such that the convergence rates are maximized:

$$\underbrace{\operatorname*{argmax}_{\phi \in \Phi_{\mathrm{ad}}} \left(\frac{\pi d \gamma N}{\log(\pi d \gamma N / \beta_2)} \right)}_{\text{Trapezoidal Convergence Theorem}} \qquad \text{subject to} \qquad \underbrace{d\gamma \leq \frac{\pi}{2}}_{\text{Nonexistence Theorem}}$$

$$\underbrace{\operatorname*{argmax}_{\phi \in \Phi_{\mathrm{ad}}} \left(\frac{\pi d \gamma N}{2\log(\pi d \gamma N / (2\beta_2))} \right)}_{\text{Sinc Convergence Theorem}} \qquad \text{subject to} \qquad \underbrace{d\gamma \leq \frac{\pi}{2}}_{\text{Nonexistence Theorem}}$$

Result: an infinite-dimensional optimization problem for ϕ.

Maximizing the Convergence Rates

Consider the asymptotic problems as $N \to \infty$:

$$
\begin{aligned}
\frac{\pi d\gamma N}{\log(\pi d\gamma N/\beta_2)} &= \frac{\pi d\gamma N}{\log N + \log(\pi d\gamma/\beta_2)}, \\
&\sim \frac{\pi d\gamma N}{\log N}, \quad \text{as} \quad N \to \infty, \\
\frac{\pi d\gamma N}{2\log(\pi d\gamma N/(2\beta_2))} &= \frac{\pi d\gamma N}{2\log N + 2\log(\pi d\gamma/(2\beta_2))}, \\
&\sim \frac{\pi d\gamma N}{2\log N}, \quad \text{as} \quad N \to \infty.
\end{aligned}
$$

Then, the linearity of $d\gamma$ leads directly to the following result. We maximize the convergence rates when $d\gamma = \pi/2$.

Maximizing the Convergence Rates

Theorem Let $\Phi_{\mathrm{as,ad}} = \{\Phi_{\mathrm{ad}} : d\gamma = \pi/2\}$. Then for every $\phi_{\mathrm{as}} \in \Phi_{\mathrm{as,ad}}$ such that:

$$\mathscr{E}^{\mathrm{T}}_{N,h}(H^\infty(\mathscr{D}_d,\omega)) \leq C_{d,\omega} \exp\left(-\frac{\pi^2 N}{2\log(\pi^2 N/2\beta_2)}\right),$$

where $N = 2n+1$, the mesh size h is chosen optimally as:

$$h = \frac{\log(\pi^2 n/\beta_2)}{\gamma n},$$

and $C_{d,\omega}$ is a constant depending on d and ω. This same ϕ_{as} ensures that:

$$\mathscr{E}^{\mathrm{Sinc}}_{N,h}(H^\infty(\mathscr{D}_d,\omega)) \leq C_{d,\omega} \exp\left(-\frac{\pi^2 N}{4\log(\pi^2 N/4\beta_2)}\right),$$

where $N = 2n+1$, the mesh size h is chosen optimally as:

$$h = \frac{\log(\pi^2 n/2\beta_2)}{\gamma n},$$

and $C_{d,\omega}$ is a constant depending on d and ω.

Practical Application

Interval	Single Exponential	Double Exponential
$[-1, 1]$	$\tanh(t/2)$	$\tanh(\frac{\pi}{2}\sinh t)$
$(-\infty, +\infty)$	$\sinh(t)$	$\sinh(\frac{\pi}{2}\sinh t)$
$[0, +\infty)$	$\log(\exp(t) + 1)$	$\log(\exp(\frac{\pi}{2}\sinh t) + 1)$
$[0, +\infty)$	$\exp(t)$	$\exp(\frac{\pi}{2}\sinh t)$

The four maps can be written as compositions:

$$\psi(z) = \tanh(z), \quad \psi^{-1}(z) = \tanh^{-1}(z),$$
$$\psi(z) = \sinh(z), \quad \psi^{-1}(z) = \sinh^{-1}(z),$$
$$\psi(z) = \log(e^z + 1), \quad \psi^{-1}(z) = \log(e^z - 1),$$
$$\psi(z) = \exp(z), \quad \psi^{-1}(z) = \log(z).$$

with the $\frac{\pi}{2}\sinh$ function. Let f have singularities at the points $\{\delta_k \pm \mathrm{i}\epsilon_k\}_{k=1}^n$. Let $\{\tilde{\delta}_k \pm \mathrm{i}\tilde{\epsilon}_k\}_{k=1}^n = \{\psi^{-1}(\delta_k \pm \mathrm{i}\epsilon_k)\}_{k=1}^n$.

Schwarz-Christoffel Formula

- sinh maps $\mathscr{D}_{\frac{\pi}{2}} \to \mathbb{C}$ with two branches at $\pm \mathrm{i}$.
- Let g map the strip $\mathscr{D}_{\frac{\pi}{2}}$ to the polygonally bounded region P having vertices $\{w_k\}_{k=1}^n = \{\tilde{\delta}_1 + \mathrm{i}\tilde{\epsilon}_1, \ldots, \tilde{\delta}_n + \mathrm{i}\tilde{\epsilon}_n\}$ and interior angles $\{\pi\alpha_k\}_{k=1}^n$. Let also $\frac{\pi}{2}\alpha_\pm$ be the divergence angles at the left and right ends of the strip $\mathscr{D}_{\frac{\pi}{2}}$. Then the function:

$$g(z) = A + C \int^z e^{(\alpha_- - \alpha_+)\zeta} \prod_{k=1}^n [\sinh(\zeta - z_k)]^{\alpha_k - 1} \, \mathrm{d}\zeta,$$

  where $z_k = g(w_k)$ and for some A and C maps the interior of the top half of the strip $\mathscr{D}_{\frac{\pi}{2}}$ to the interior of the polygon P.
- [Hale and Tee 2008] use the Schwarz-Christoffel formula from the unit circle to maximize convergence rate of Chebyshev methods.

Practical Alternative

For any real values of the $n+1$ parameters $\{u_k\}_{k=0}^n$, the function:

$$h(t) = u_0 \sinh(t) + \sum_{j=1}^{n} u_j t^{j-1}, \qquad u_0 > 0,$$

still grows single exponentially. The composition $\psi(h(t))$ still induces a double exponential variable transformation.

$$\begin{aligned} &\text{maximize } u_0 && \left(= \frac{\displaystyle\sum_{k=1}^{n} \left\{ \tilde{\epsilon}_k - \Im \sum_{j=1}^{n} u_j (x_k + \mathrm{i}\pi/2)^{j-1} \right\}}{\displaystyle\sum_{k=1}^{n} \cosh(x_k)} \right), \\ &\text{subject to} && h(x_k + \mathrm{i}\pi/2) = \tilde{\delta}_k + \mathrm{i}\tilde{\epsilon}_k, \quad \text{for} \quad k = 1, \ldots, n. \end{aligned}$$

Example: Endpoint and Complex Singularities

$$\int_{-1}^{1} \frac{\exp\left((\epsilon_1^2+(x-\delta_1)^2)^{-1}\right)\log(1-x)}{(\epsilon_2^2+(x-\delta_2)^2)\sqrt{1+x}}\,\mathrm{d}x = -2.04645\ldots,$$

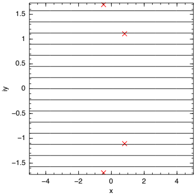
for the values $\delta_1 + \mathrm{i}\epsilon_1 = -1/2 + \mathrm{i}$ and $\delta_2 + \mathrm{i}\epsilon_2 = 1/2 + \mathrm{i}/2$. This integral has two different endpoint singularities and two pairs of complex conjugate singularities of different types near the integration axis.

	Single	Double	Optimized Double
$\phi(t)$	$\tanh(t/2)$	$\tanh\left(\frac{\pi}{2}\sinh(t)\right)$	$\tanh(h(t))$
ρ or γ	1	1	1
β or β_2	$1/2$	$\pi/4$	0.06956
d	1.10715	0.34695	$\pi/2$

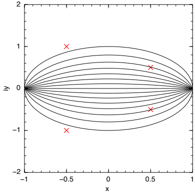
The optimized transformation is given by:

$$h(t) \approx 0.13912\sinh(t) + 0.19081 + 0.21938\,t.$$

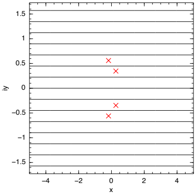
Example: Endpoint and Complex Singularities



$\mathscr{D}_{\frac{\pi}{2}}$



$\tanh(\frac{1}{2}\mathscr{D}_{\frac{\pi}{2}})$



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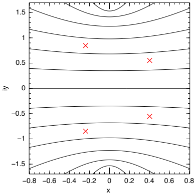
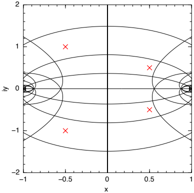
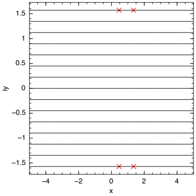


$\frac{\pi}{2}\sinh(\mathscr{D}_{\frac{\pi}{2}})$

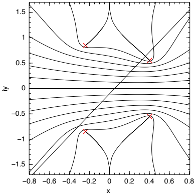


$\tanh(\frac{\pi}{2}\sinh(\mathscr{D}_{\frac{\pi}{2}}))$

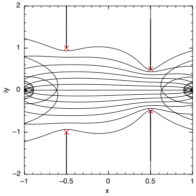
Example: Endpoint and Complex Singularities



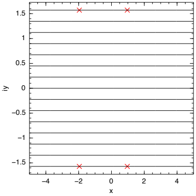
$\mathscr{D}_{\frac{\pi}{2}}$



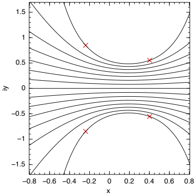
$g(\mathscr{D}_{\frac{\pi}{2}})$



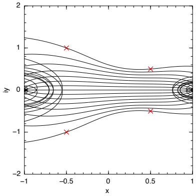
$\tanh(g(\mathscr{D}_{\frac{\pi}{2}}))$



$\mathscr{D}_{\frac{\pi}{2}}$

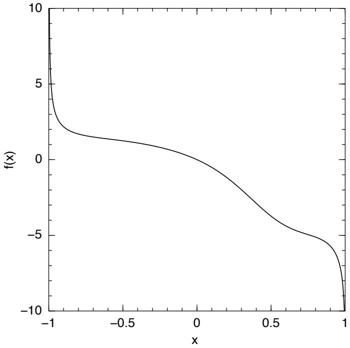


$h(\mathscr{D}_{\frac{\pi}{2}})$

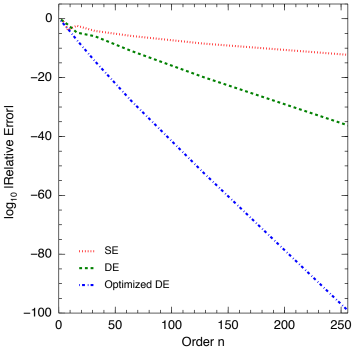


$\tanh(h(\mathscr{D}_{\frac{\pi}{2}}))$

Example: Endpoint and Complex Singularities



Integrand



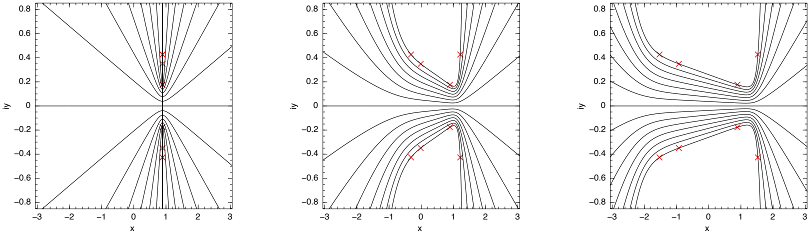
Error

Obtaining an Initial Guess

Let $\bar{\epsilon}$ be the smallest of $\{\tilde{\epsilon}_k\}_{k=1}^n$ and $\bar{\delta}$ be the $\tilde{\delta}_k$ of the same index. Then the nonlinear program with singularities $\{\bar{\delta} + \mathrm{i}\tilde{\epsilon}_k\}_{k=1}^n$ is exactly solved by:

$$h(t) = \bar{\epsilon} \sinh t + \bar{\delta}.$$

A homotopy $\mathscr{H}(t)$ is then constructed between $\{\bar{\delta} + \mathrm{i}\tilde{\epsilon}_k\}_{k=1}^n$ at $t = 0$ and $\{\tilde{\delta}_k + \mathrm{i}\tilde{\epsilon}_k\}_{k=1}^n$ at $t = 1$.



$\mathscr{H}(0)$ $\mathscr{H}(1/2)$ $\mathscr{H}(1)$

Singularities Unknown

Definition Let $x_k = kh$ be the Sinc points and let $f(x_k)$ be the $N(= 2n+1)$ Sinc sampling of f. Then for $r + s \leq 2n$, the Sinc-Padé approximants $\{r/s\}_f(x)$ are given by:

$$\{r/s\}_f(x) = \frac{\displaystyle\sum_{i=0}^{r} p_i\, x^i}{1 + \displaystyle\sum_{j=1}^{s} q_j\, x^j},$$

where the $r + s + 1$ coefficients solve the system:

$$\sum_{i=0}^{r} p_i\, x_k^i - f(x_k) \sum_{j=1}^{s} q_j\, x_k^j = f(x_k),$$

for $k = -\lfloor \frac{r+s}{2} \rfloor, \ldots, \lceil \frac{r+s}{2} \rceil$.

Singularities Unknown

Our adaptive algorithm is based on the following principles:

1. Sinc-Padé approximants are useful only when the Sinc approximation obtains some degree of accuracy,
2. Sinc-Padé approximants are useful for $r, s = \mathcal{O}(\log n)$ as $n \to \infty$.

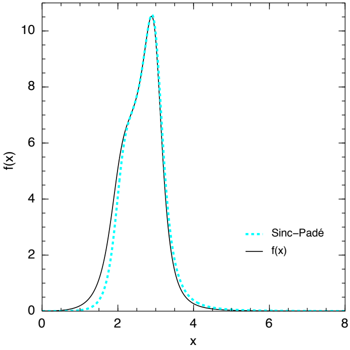
Algorithm

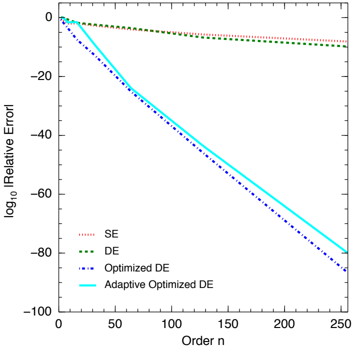
Set $n = 1$;
while $|\mathrm{RelativeError}| \geq 10^{-3}$ **do**
  Double n and naïvely compute the n^{th} double exponential approximation;
end;
while $|\mathrm{RelativeError}| \geq \epsilon$ **do**
  Compute the poles of the Sinc-Padé approximant;
  Solve the nonlinear program for $h(t)$;
  Double n and compute the n^{th} adapted optimized approximation;
end.

Adaptive Optimization via Sinc-Padé

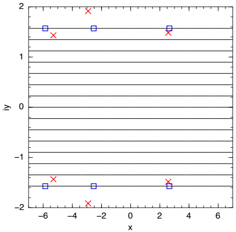
$$\int_0^\infty \frac{x\,\mathrm{d}x}{\sqrt{\epsilon_1^2+(x-\delta_1)^2}(\epsilon_2^2+(x-\delta_2)^2)(\epsilon_3^2+(x-\delta_3)^2)},$$

for the values $\delta_1+\mathrm{i}\epsilon_1 = 1+\mathrm{i}$, $\delta_2+\mathrm{i}\epsilon_2 = 2+\mathrm{i}/2$, and $\delta_3+\mathrm{i}\epsilon_3 = 3+\mathrm{i}/3$.

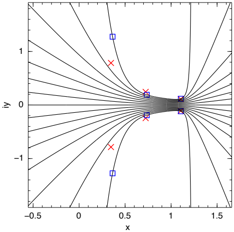




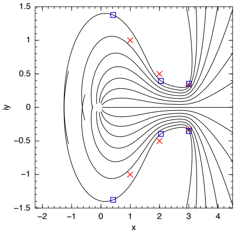
Adaptive Optimization via Sinc-Padé



$\mathscr{D}_{\frac{\pi}{2}}$



$h(\mathscr{D}_{\frac{\pi}{2}})$



$\exp(h(\mathscr{D}_{\frac{\pi}{2}}))$

Molecular Integrals

- Many molecular properties are based on the electronic density.
- Molecular structure $\Rightarrow$ ability to interact with other molecules.
- Applications in pharmaceutical industry, efficiency of combustion engines.
- The N atom and n electron Schrödinger equation:

$$\mathcal{H}\psi = E\psi,$$

where:

$$\mathcal{H} = \sum_{i=1}^{n} \left\{ -\frac{\nabla_i^2}{2} + \sum_{A=1}^{N} \frac{Z_A}{r_{iA}} + \sum_{i<j}^{n} \frac{1}{r_{ij}} \right\}.$$

includes kinetic energy, nuclear attraction, and electron repulsion.

- The Born-Oppenheimer approximation $\Rightarrow$ atoms do not move.
- The Pauli exclusion principle $\Rightarrow$ Slater determinant for wavefunction.

Molecular Integrals

Using a LCAO-MO (Rayleigh-Ritz) approach:

$$\Psi_i = \sum_{k=1}^{\infty} c_{ki}\varphi_k, \qquad i = 1, 2, \ldots, n.$$

We obtain an infinite system of linear equations, whose generalized eigenvalues approximate the eigenvalues of the i^{th} electron's Hamiltonian:

$$\begin{bmatrix} \langle\varphi_1|\mathcal{H}_e|\varphi_1\rangle & \langle\varphi_1|\mathcal{H}_e|\varphi_2\rangle & \cdots \\ \langle\varphi_2|\mathcal{H}_e|\varphi_1\rangle & \langle\varphi_2|\mathcal{H}_e|\varphi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} c_{1i} \\ c_{2i} \\ \vdots \end{bmatrix} = E_i \begin{bmatrix} \langle\varphi_1|\varphi_1\rangle & \langle\varphi_1|\varphi_2\rangle & \cdots \\ \langle\varphi_2|\varphi_1\rangle & \langle\varphi_2|\varphi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}.$$

Molecular Integrals

The B functions of [Filter and Steinborn 1978]:

$$B_{n,l}^{m}(\zeta, \vec{r}) = \frac{(\zeta r)^l}{2^{n+l}(n+l)!} \hat{k}_{n-\frac{1}{2}}(\zeta r) Y_l^m(\theta_{\vec{r}}, \phi_{\vec{r}}),$$

where n, l, and m are the quantum numbers. Linear combination of Slater-type orbitals with compact Fourier transform.
The three-center nuclear attraction integrals:

$$\mathcal{I}_{n_1,l_1,m_1}^{n_2,l_2,m_2} = \int \left[B_{n_1,l_1}^{m_1}(\zeta_1, \vec{r}) \right]^* \frac{1}{|\vec{r} - \vec{R}_1|} B_{n_2,l_2}^{m_2}(\zeta_2, \vec{r} - \vec{R}_2) \, \mathrm{d}^3 \vec{r},$$

The four-center two-electron Coulomb integrals:

$$\mathcal{J}_{n_1,l_1,m_1,n_3,l_3,m_3}^{n_2,l_2,m_2,n_4,l_4,m_4} = \int \left[B_{n_1,l_1}^{m_1}(\zeta_1, \vec{r}) B_{n_3,l_3}^{m_3}(\zeta_3, \vec{r}' - \vec{R}_{34}) \right]^* \frac{1}{|\vec{r} - \vec{r}' - \vec{R}_{41}|} B_{n_2,l_2}^{m_2}(\zeta_2, \vec{r} - \vec{R}_{21}) B_{n_4,l_4}^{m_4}(\zeta_4, \vec{r}') \, \mathrm{d}^3 \vec{r} \, \mathrm{d}^3 \vec{r}',$$

Molecular Integrals

The Fourier transform of the Coulomb operator [Gel'fand and Shilov 1964]:

$$\frac{1}{|\vec{r}-\vec{s}|} = \frac{1}{2\pi^2}\int_{\vec{p}} \frac{e^{-\mathrm{i}\vec{p}\cdot(\vec{r}-\vec{s})}}{p^2}\,\mathrm{d}^3\vec{p},$$

allows expectations to be written as:

$$\left\langle f(\vec{r}) \left| \frac{1}{|\vec{r}-\vec{s}|} \right| g(\vec{r}-\vec{R}) \right\rangle_{\vec{r}} = \frac{1}{2\pi^2}\int_{\vec{x}} \frac{e^{\mathrm{i}\vec{x}\cdot\vec{s}}}{x^2} \left\langle f(\vec{r}) \middle| e^{-\mathrm{i}\vec{x}\cdot\vec{r}} \middle| g(\vec{r}-\vec{R}) \right\rangle_{\vec{r}} \mathrm{d}^3\vec{x}.$$

Then, a generalized convolution:

$$\left\langle f(\vec{r}) \middle| e^{-\mathrm{i}\vec{x}\cdot\vec{r}} \middle| g(\vec{r}-\vec{R}) \right\rangle_{\vec{r}} = e^{-\mathrm{i}\vec{x}\cdot\vec{R}} \left\langle \bar{f}(\vec{p}) \middle| e^{-\mathrm{i}\vec{p}\cdot\vec{R}} \middle| \bar{g}(\vec{p}+\vec{x}) \right\rangle_{\vec{p}},$$

allows us to consider integrals over the Fourier transforms instead. Purpose: reduction of dimensionality. $3 \to 2$ for three-center and $6 \to 3$ for four-center integrals.

Molecular Integrals

The bottleneck in the Fourier transform method:

$$\mathcal{I} = \int_{-\infty}^{\infty} J_\nu(\beta\, x) \frac{K_{\mu_1}(\alpha_1\sqrt{x^2+\gamma_1^2})}{\sqrt{(x^2+\gamma_1^2)^{n_{\gamma_1}}}} \frac{K_{\mu_2}(\alpha_2\sqrt{x^2+\gamma_2^2})}{\sqrt{(x^2+\gamma_2^2)^{n_{\gamma_2}}}} x^{n_x+1}\,\mathrm{d}x,$$

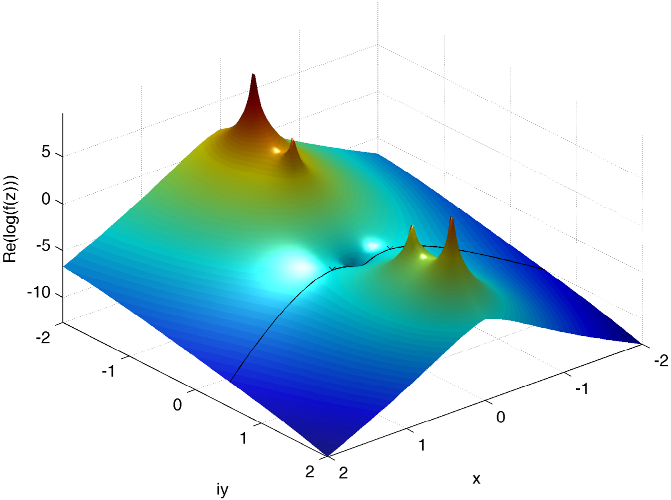
Characteristics: Oscillatory (from $J_\nu(\cdot)$), Exponentially decaying (from $K_\mu(\cdot)$'s), Heavily parameterized, and Singularities arbitrarily close to integration contour.

$$\mathcal{I} = \Re\left\{ \int_C H_\nu^{(1)}(\beta\, z) \frac{K_{\mu_1}(\alpha_1\sqrt{z^2+\gamma_1^2})}{\sqrt{(z^2+\gamma_1^2)^{n_{\gamma_1}}}} \frac{K_{\mu_2}(\alpha_2\sqrt{z^2+\gamma_2^2})}{\sqrt{(z^2+\gamma_2^2)^{n_{\gamma_2}}}} z^{n_x+1}\,\mathrm{d}z \right\}.$$

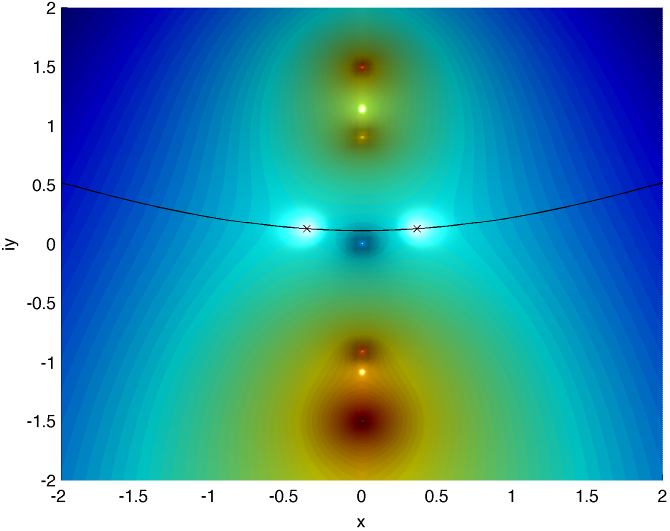
Take $z = \zeta(x)$ as an approximate steepest descent path through the saddle points:

$$\zeta(x) = \frac{(\alpha_1+\alpha_2)}{\beta^2+(\alpha_1+\alpha_2)^2}x + \mathrm{i}\frac{\beta}{\beta^2+(\alpha_1+\alpha_2)^2}\left(\sqrt{x^2+b^2}+c\right), \quad x\in\mathbb{R},$$

Molecular Integrals



Molecular Integrals



Molecular Integrals

Consider the integral:

$$\int_{-\infty}^{+\infty} \frac{e^{\mathrm{i}\, b\, z - a_1\sqrt{z^2+c_1^2} - a_2\sqrt{z^2+c_2^2}}}{(z^2+c_1^2)^{\mu_1}(z^2+c_2^2)^{\mu_2}}\,\mathrm{d}z,$$

for positive real parameter values. To remove oscillations, we deform the integration contour to a path of steepest descent. We use an asymptotic path of steepest descent parameterized by:

$$\zeta(x) = \lambda_1 x + \mathrm{i}\left(\sqrt{\lambda_2^2 x^2 + \lambda_3^2} + \lambda_4\right),$$

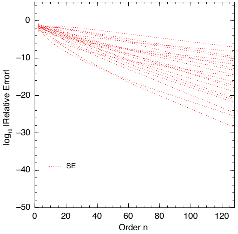
for some values of the parameters $\boldsymbol{\lambda}$. From horizontal and vertical symmetry, we can use:

$$h(t) = u_0 \sinh(t) + u_2\, t.$$

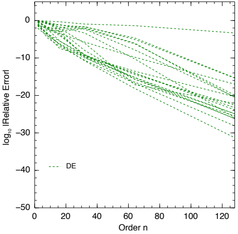
Molecular Integrals

20 runs with randomized values for the parameters distributed uniformly:

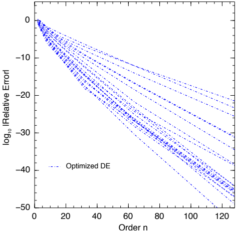
$$a_1 \sim U(0,1), \quad a_2 \sim U(0,1), \quad b \sim U(0,20),$$
$$c_1 \sim U(0,1), \quad c_2 \sim U(0,2), \quad \mu_1 \sim U(0,1), \quad \mu_2 \sim U(0,1).$$



SE



DE



Optimized DE

Conclusions & Outlook

- Conformal maps maximize the convergence rates of trapezoidal rule and Sinc numerical methods (subject to their very existence!)
- Practical & general solution as a polynomial adjustment to sinh map
- Sinc-Padé approximants for unknown singularities
- Free & open-source implementation available in the JULIA software package `DEQuadrature.jl`

Will polynomial adjustments (in the monomial basis) to the sinh map stand the test of time? There is lots to explore:

- $\sinh + \text{polynomial}$ in a Chebyshev basis
- $\sinh + \text{rational approximant}$
- Potential-theoretic approach to interpolatory nodes and weights on the whole real line
- shortest enclosing walks to find optimal contours for Cauchy integrals [Bornemann and Wechslberger 2012]

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