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

Richard Mikael Slevinsky† and Sheehan Olver‡

†Mathematical Institute, University of Oxford
‡School of Mathematics and Statistics, The University of Sydney

Numerical Analysis Seminar, The University of Tokyo

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- **Trapezoidal Rule**
  - 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
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- Examples & Applications
Trapezoidal Rule

- The trapezoidal rule \( \int_a^b f(x) \, dx \approx (b - a) \left[ \frac{f(a) + f(b)}{2} \right] \).

- 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 \( T(h) - \int_a^b f(x) \, dx \sim \sum_{l=1}^{\infty} h^{2l} \frac{B_{2l}}{(2l)!} \left( f^{(2l-1)}(b) - f^{(2l-1)}(a) \right) \), as \( h \to 0 \).

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

Variable transformations which induce endpoint decay are:

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

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

Integrand $\epsilon = 1$  
SE transformation  
DE transformation
$\epsilon = 1$

A total failure in the quadrature rules with nearby singularities.

Is there an optimal variable transformation?

$\epsilon = 0.001$
\[ \epsilon = 1 \]

\[ x = \phi_{DEopt}(t) = \tanh(\tan^{-1}(\epsilon) \sinh(t)), \]

\[ \phi'_{DEopt}(t) = \text{sech}^2(\tan^{-1}(\epsilon) \sinh(t)) \tan^{-1}(\epsilon) \cosh(t). \]
Quadrature by Variable Transformation

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

$$\mathcal{D}_d = \{z \in \mathbb{C} : |\text{Im } z| < d\}.$$ 

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

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

Let $\mathcal{E}^T_{N,h}(H^\infty(\mathcal{D}_d, \omega))$ denote the error norm in $H^\infty(\mathcal{D}_d, \omega)$:

$$\mathcal{E}^T_{N,h}(H^\infty(\mathcal{D}_d, \omega)) = \sup_{||f|| \leq 1} \left| \int_{-\infty}^{+\infty} f(x) \, dx - h \sum_{k=-n}^{+n} f(kh) \right|.$$ 

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

$$\mathcal{N}_1(f, \mathcal{D}_d) = \int_{\partial \mathcal{D}_d} |f(z)| \, dz < +\infty.$$
Thm 1 [Sugihara 1997] Suppose:

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

Then:

\[
\mathcal{E}_{N,h}^{T}(\mathcal{H}^{\infty}(\mathcal{D}_d,\omega)) \leq C_{d,\omega} \exp \left( -(\pi d \beta N)^{\frac{\rho}{\rho+1}} \right),
\]

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 \( \omega \).
Theorem [Sugihara 1997] Suppose:

1. \( \omega(z) \in B(D_d); \)
2. \( \omega(z) \) does not vanish at any point in \( D_d \) and takes real values on the real axis;
3. \( \alpha_1 \exp\left(-\beta_1 e^{\gamma|x|}\right) \leq |\omega(x)| \leq \alpha_2 \exp\left(-\beta_2 e^{\gamma|x|}\right), \quad x \in \mathbb{R}, \)

where \( \alpha_1, \alpha_2, \beta_1, \beta_2, \gamma > 0. \)

Then:

\[
\mathcal{E}_N^T(H^\infty(D_d, \omega)) \leq C_{d,\omega} \exp\left(-\frac{\pi d \gamma N}{\log(\pi d \gamma N/\beta_2)}\right),
\]

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 \( \omega. \)
Sinc Numerical Methods

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

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

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 $\mathcal{E}_{N,h}^{\text{Sinc}}(H^\infty(\mathcal{D}_d, \omega))$ denote the error norm in $H^\infty(\mathcal{D}_d, \omega)$:

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

**Theorem** [Sugihara 2003] Suppose:

1. $\omega(z) \in B(\mathcal{D}_d)$;
2. $\omega(z)$ does not vanish at any point in $\mathcal{D}_d$ 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:

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

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 $\omega$. 
Sinc Numerical Methods

**Theorem** [Sugihara 2003] Suppose:

1. \( \omega(z) \in B(\mathcal{D}_d); \)
2. \( \omega(z) \) does not vanish at any point in \( \mathcal{D}_d \) and takes real values on the real axis;
3. \( \alpha_1 \exp\left(-\beta_1 e^{\gamma|x|}\right) \leq |\omega(x)| \leq \alpha_2 \exp\left(-\beta_2 e^{\gamma|x|}\right), \quad x \in \mathbb{R}, \)
   where \( \alpha_1, \alpha_2, \beta_1, \beta_2, \gamma > 0. \)

Then:

\[
\|Sinc_N, h(H^\infty(\mathcal{D}_d, \omega))\| \leq C_{d, \omega} \exp\left(-\frac{\pi d \gamma N}{2 \log(\pi d \gamma N/(2\beta_2))}\right),
\]

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

1. $\omega(z) \in B(D_d)$;
2. $\omega(z)$ does not vanish at any point in $D_d$ and takes real values on the real axis;
3. $\omega(x) = O\left(\exp(-\beta e^{\gamma|x|})\right)$ 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:

\[
\int_{-\infty}^{\infty} f(\phi(t))\phi'(t) \, dt \approx h \sum_{k=-n}^{+n} f(\phi(kh))\phi'(kh),
\]

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

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

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

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

$$\arg\max_{\phi \in \Phi_{\text{ad}}} \left( \frac{\pi d \gamma N}{\log(\pi d \gamma N / \beta_2)} \right)$$

subject to

$$d \gamma \leq \frac{\pi}{2}$$

Trapezoidal Convergence Theorem

Result: an infinite-dimensional optimization problem for $\phi$.

$$\arg\max_{\phi \in \Phi_{\text{ad}}} \left( \frac{\pi d \gamma N}{2 \log(\pi d \gamma N / (2\beta_2))} \right)$$

subject to

$$d \gamma \leq \frac{\pi}{2}$$

Sinc Convergence Theorem
Maximizing the Convergence Rates

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

$$\frac{\pi d\gamma N}{\log(\pi d\gamma N/\beta_2)} = \frac{\pi d\gamma N}{\log N + \log(\pi d\gamma/\beta_2)},$$

$$\sim \frac{\pi d\gamma N}{\log N}, \quad \text{as} \quad N \to \infty,$$

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

$$\sim \frac{\pi d\gamma N}{2 \log N}, \quad \text{as} \quad N \to \infty.$$

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

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

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 $\omega$. This same $\phi_{as}$ ensures that:

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

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 $\omega$. 
## Practical Application

<table>
<thead>
<tr>
<th>Interval</th>
<th>Single Exponential</th>
<th>Double Exponential</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[-1, 1]$</td>
<td>$\tanh(t/2)$</td>
<td>$\tanh(\frac{\pi}{2} \sinh t)$</td>
</tr>
<tr>
<td>$(-\infty, +\infty)$</td>
<td>$\sinh(t)$</td>
<td>$\sinh(\frac{\pi}{2} \sinh t)$</td>
</tr>
<tr>
<td>$[0, +\infty)$</td>
<td>$\log(\exp(t) + 1)$</td>
<td>$\log(\exp(\frac{\pi}{2} \sinh t) + 1)$</td>
</tr>
<tr>
<td>$[0, +\infty)$</td>
<td>$\exp(t)$</td>
<td>$\exp(\frac{\pi}{2} \sinh t)$</td>
</tr>
</tbody>
</table>

The four maps can be written as compositions:

$$
\psi(z) = \tanh(z), \quad \psi^{-1}(z) = \tanh^{-1}(z),
$$

$$
\psi(z) = \sinh(z), \quad \psi^{-1}(z) = \sinh^{-1}(z),
$$

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

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

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

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Schwarz-Christoffel Formula

- sinh maps $\mathbb{D}_{\frac{\pi}{2}} \to \mathbb{C}$ with two branches at $\pm i$.
- Let $g$ map the strip $\mathbb{D}_{\frac{\pi}{2}}$ to the polygonally bounded region $P$ having vertices $\{w_k\}_{k=1}^n = \{\tilde{\delta}_1 + i\tilde{\epsilon}_1, \ldots, \tilde{\delta}_n + i\tilde{\epsilon}_n\}$ 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 $\mathbb{D}_{\frac{\pi}{2}}$. Then the function:

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

where $z_k = g(w_k)$ and for some $A$ and $C$ maps the interior of the top half of the strip $\mathbb{D}_{\frac{\pi}{2}}$ 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.
For any real values of the $n + 1$ parameters $\{u_k\}_{k=0}^{n}$, the function:

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

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

$$\maximize u_0 \left( \sum_{k=1}^{n} \left\{ \tilde{\epsilon}_k - \Im \sum_{j=1}^{n} u_j (x_k + i \pi / 2)^{j-1} \right\} \right),$$

subject to $h(x_k + i \pi / 2) = \tilde{\delta}_k + i \tilde{\epsilon}_k$, for $k = 1, \ldots, n.$
Example: Endpoint and Complex Singularities

\[
\int_{-1}^{1} \frac{\exp \left( (\epsilon_1^2 + (x - \delta_1)^2)^{-1} \right) \log(1 - x)}{(\epsilon_2^2 + (x - \delta_2)^2)^{1/2} \sqrt{1 + x}} \, dx = -2.04645 \ldots ,
\]

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

<table>
<thead>
<tr>
<th></th>
<th>Single</th>
<th>Double</th>
<th>Optimized Double</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \phi(t) )</td>
<td>( \tanh(t/2) )</td>
<td>( \tanh \left( \frac{\pi}{2} \sinh(t) \right) )</td>
<td>( \tanh(h(t)) )</td>
</tr>
<tr>
<td>( \rho ) or ( \gamma )</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \beta ) or ( \beta_2 )</td>
<td>1/2</td>
<td>( \pi/4 )</td>
<td>0.06956</td>
</tr>
<tr>
<td>( d )</td>
<td>1.10715</td>
<td>0.34695</td>
<td>( \pi/2 )</td>
</tr>
</tbody>
</table>

The optimized transformation is given by:

\[
h(t) \approx 0.13912 \sinh(t) + 0.19081 + 0.21938 \, t.
\]
Example: Endpoint and Complex Singularities

\[ D \frac{\pi}{2} \quad \text{tanh}\left(\frac{1}{2} D \frac{\pi}{2}\right) \]

\[ D \frac{\pi}{2} \quad \frac{\pi}{2} \sinh(D \frac{\pi}{2}) \quad \text{tanh}\left(\frac{\pi}{2} \sinh(D \frac{\pi}{2})\right) \]
Example: Endpoint and Complex Singularities

\[ \mathcal{D}_{\frac{\pi}{2}} \]

\[ g(\mathcal{D}_{\frac{\pi}{2}}) \]

\[ \tanh(g(\mathcal{D}_{\frac{\pi}{2}})) \]

\[ \mathcal{D}_{\frac{\pi}{2}} \]

\[ h(\mathcal{D}_{\frac{\pi}{2}}) \]

\[ \tanh(h(\mathcal{D}_{\frac{\pi}{2}})) \]
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 \( \{ \bar{\delta} + i\tilde{\epsilon}_k \}_{k=1}^n \) is exactly solved by:

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

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

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

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 $k = -\left\lfloor \frac{r+s}{2} \right\rfloor, \ldots, \left\lceil \frac{r+s}{2} \right\rceil$. 
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 $|\text{RelativeError}| \geq 10^{-3}$ do
    Double $n$ and naively compute the $n^{th}$ double exponential approximation;
end;

while $|\text{RelativeError}| \geq \epsilon$ 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

\[ \int_{0}^{\infty} \frac{x \, dx}{\sqrt{\epsilon_1^2 + (x - \delta_1)^2(\epsilon_2^2 + (x - \delta_2)^2)(\epsilon_3^2 + (x - \delta_3)^2)}}, \]

for the values \( \delta_1 + i\epsilon_1 = 1 + i \), \( \delta_2 + i\epsilon_2 = 2 + i/2 \), and \( \delta_3 + i\epsilon_3 = 3 + i/3 \).
Adaptive Optimization via Sinc-Padé

\[ D_{\frac{\pi}{2}} \]

\[ h(D_{\frac{\pi}{2}}) \]

\[ \exp(h(D_{\frac{\pi}{2}})) \]
Molecular Integrals

- Many molecular properties are based on the electronic density.
- Molecular structure ⇒ 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:

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

includes kinetic energy, nuclear attraction, and electron repulsion.
- The Born-Oppenheimer approximation ⇒ atoms do not move.
- The Pauli exclusion principle ⇒ Slater determinant for wavefunction.
Using a LCAO-MO (Rayleigh-Ritz) approach:

\[ \Psi_i = \sum_{k=1}^{\infty} c_{ki} \varphi_k, \quad i = 1, 2, \ldots, n. \]

We obtain an infinite system of linear equations, whose generalized eigenvalues approximate the eigenvalues of the \( i \)th electron’s Hamiltonian:

\[
\begin{bmatrix}
\langle \varphi_1 | H_e | \varphi_1 \rangle & \langle \varphi_1 | H_e | \varphi_2 \rangle & \cdots \\
\langle \varphi_2 | H_e | \varphi_1 \rangle & \langle \varphi_2 | H_e | \varphi_2 \rangle & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix}
\begin{bmatrix}
c_{1i} \\
c_{2i}
\end{bmatrix}
= E_i
\begin{bmatrix}
\langle \varphi_1 | \varphi_1 \rangle & \langle \varphi_1 | \varphi_2 \rangle & \cdots \\
\langle \varphi_2 | \varphi_1 \rangle & \langle \varphi_2 | \varphi_2 \rangle & \cdots \\
\vdots & \vdots & \ddots
\end{bmatrix}.
\]
Molecular Integrals

The $B$ functions of [Filter and Steinborn 1978]:

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

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:

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

The four-center two-electron Coulomb integrals:

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

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

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

allows expectations to be written as:

\[
\langle \frac{1}{|\vec{r} - \vec{s}|} \big| f(\vec{r}) \bigg| \bigg| g(\vec{r} - \vec{R}) \rangle_{\vec{r}} = \frac{1}{2\pi^2} \int_{\vec{\chi}} \frac{e^{i\vec{\chi} \cdot \vec{s}}}{\chi^2} \langle \frac{1}{|\vec{r} - \vec{s}|} \big| f(\vec{r}) \bigg| \bigg| e^{-i\vec{\chi} \cdot \vec{r}} \bigg| g(\vec{r} - \vec{R}) \rangle_{\vec{r}} \, d^3\vec{\chi}.
\]

Then, a generalized convolution:

\[
\langle f(\vec{r}) \bigg| e^{-i\vec{\chi} \cdot \vec{r}} \bigg| g(\vec{r} - \vec{R}) \rangle_{\vec{r}} = e^{-i\vec{\chi} \cdot \vec{R}} \langle \bar{f}(\vec{p}) \bigg| e^{-i\vec{p} \cdot \vec{R}} \bigg| \bar{g}(\vec{p} + \vec{\chi}) \rangle_{\vec{p}},
\]

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

The bottleneck in the Fourier transform method:

\[ \mathcal{I} = \int_{-\infty}^{\infty} J_\nu(\beta x) \frac{K_{\mu_1}(\alpha_1 \sqrt{x^2 + \gamma_1^2})}{\sqrt{(x^2 + \gamma_1^2)^n \gamma_1}} \frac{K_{\mu_2}(\alpha_2 \sqrt{x^2 + \gamma_2^2})}{\sqrt{(x^2 + \gamma_2^2)^n \gamma_2}} x^{n_x + 1} \, dx, \]

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

\[ \mathcal{I} = \Re \left\{ \int_C H_\nu^{(1)}(\beta z) \frac{K_{\mu_1}(\alpha_1 \sqrt{z^2 + \gamma_1^2})}{\sqrt{(z^2 + \gamma_1^2)^n \gamma_1}} \frac{K_{\mu_2}(\alpha_2 \sqrt{z^2 + \gamma_2^2})}{\sqrt{(z^2 + \gamma_2^2)^n \gamma_2}} z^{n_z + 1} \, dz \right\} . \]

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

\[ \zeta(x) = \frac{(\alpha_1 + \alpha_2)}{\beta^2 + (\alpha_1 + \alpha_2)^2} x + i \frac{\beta}{\beta^2 + (\alpha_1 + \alpha_2)^2} \left( \sqrt{x^2 + b^2} + c \right), \quad x \in \mathbb{R}, \]
Molecular Integrals
Consider the integral:

\[
\int_{-\infty}^{+\infty} \frac{e^{ibz-a_1\sqrt{z^2+c_1^2}-a_2\sqrt{z^2+c_2^2}}}{(z^2+c_1^2)^{\mu_1}(z^2+c_2^2)^{\mu_2}} \, dz,
\]

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:

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

for some values of the parameters \( \lambda \). 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:

\[ a_1 \sim U(0, 1), \quad a_2 \sim U(0, 1), \quad b \sim U(0, 20), \]
\[ c_1 \sim U(0, 1), \quad c_2 \sim U(0, 2), \quad \mu_1 \sim U(0, 1), \quad \mu_2 \sim U(0, 1). \]
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 + polynomial in a Chebyshev basis
- sinh + 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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