A Constant 3-fold Autoconvolution

An experimental approach to numerically estimating the supremum of the 3-fold autoconvolution for functions $\|f\|_1 = 1$.

Richard Mikael Slevinsky[†]

[†]Mathematical Institute, University of Oxford
Andrew Wiles Building, Radcliffe Observatory Quarter
Woodstock Road, Oxford OX2 6GG
Richard.Slevinsky@maths.ox.ac.uk

February 17, 2015

Continuous Ramsey Theory & $B^*[g]$ Sets

- "A symmetric subset of the reals is one that remains invariant under some reflection $x \to c - x$. We consider, for any $0 < \epsilon \leq 1$, the largest real number $\Delta(\epsilon)$ such that every subset of $[0, 1]$ with measure greater than ϵ contains a symmetric subset with measure $\Delta(\epsilon)$." [Martin & O'Bryant 2007]
- Discrete problem [Green 2001]: a set S of integers is called a $B^*[g]$ set if for any given m there are at most g ordered pairs $(s_1, s_2) \in S \times S$ with $s_1 + s_2 = m$.
- Interest: estimating $\Delta(\epsilon)$ or the cardinality of $B^*[g]$ sets
- $\inf_{f \in C^0(-1,1)} \|f * f * f\|_\infty$, subject to $\|f\|_1 = 1$

Problem

- $\inf_{f \in C^0(-1,1)} \|f * f * f\|_\infty$, subject to $\|f\|_1 = 1$.
- In [Martin & O'Bryant 2007], a bound is obtained:

$$\inf_{f \in C^0(-1,1)} \frac{\|f * f * f\|_\infty}{\|f\|_1} \approx 0.287\,3\ldots$$

- Since a constant function has minimal infinity-norm, this is equivalent to calculating:
- Find $f \in C^0(-1,1)$ such that $f * f * f = 1$ on $[-1,1]$.
- Previous work's estimate is based on:

$$K_3(x) = \begin{cases} 1, & 0 \le |x| \le 1, \\ 0.6644 + 0.3356 \left(\frac{2}{\pi} \tan^{-1} \left(\frac{1 - x/2}{\sqrt{x-1}} \right) \right)^{1.2015}, & 1 \le |x| \le 2. \end{cases}$$

- Where is the intuition? How can we systematically improve?

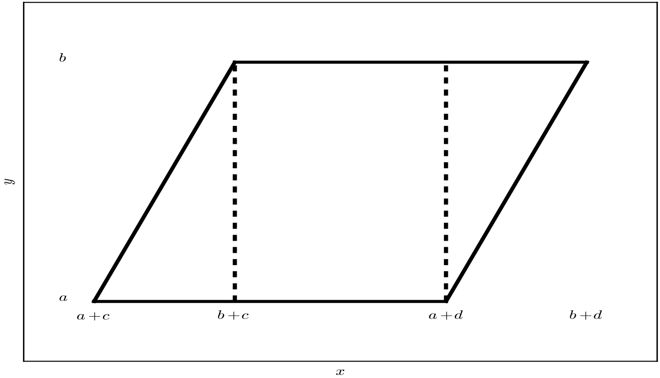
Approach

- Experimental mathematics: use principles of numerical analysis to guide the construction of a good algorithm
  - Systematic & general
  - Symmetry and convolution properties to reduce complexity
  - Exponential convergence $\leftrightarrow$ geometric decay in approximation's coefficients
- To build intuition
  - Use a general & universal software package for computing with functions. Chebfun!
  - Since f is defined on an interval, a Chebyshev interpolant is a good place to begin
- Outcome
  - Convincing numerical evidence for convergence
  - Optimized Julia code using DEQuadrature.jl and ApproxFun.jl
  - High accuracy approximation

Convolution

For integrable f compactly supported on $[a, b]$ and integrable g on $[c, d]$, convolution is defined as:

$$(f * g)(x) = \int_{\max(a,x-d)}^{\min(b,x-c)} f(y)g(x-y)\,\mathrm{d}y.$$



Convolution

For integrable f compactly supported on $[a, b]$ and integrable g on $[c, d]$, convolution is defined as:

$$(f * g)(x) = \int_{\max(a, x-d)}^{\min(b, x-c)} f(y)g(x-y)\,\mathrm{d}y.$$

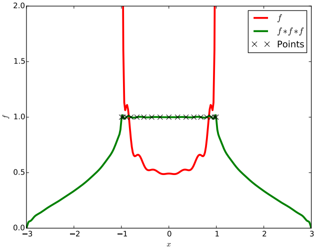
The parallelogram of the convolution domain can be explicitly written:

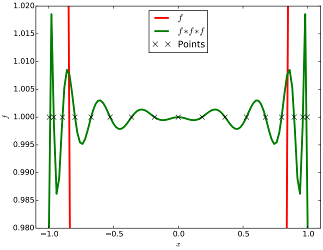
$$(f * g)(x) = \begin{cases} \displaystyle\int_a^{x-c} f(y)g(x-y)\,\mathrm{d}y, & x \in [a+c, b+c], \\ \displaystyle\int_a^b f(y)g(x-y)\,\mathrm{d}y, & x \in [b+c, a+d], \\ \displaystyle\int_{x-d}^b f(y)g(x-y)\,\mathrm{d}y, & x \in [a+d, b+d]. \end{cases}$$

Straightforward modifications for functions on open intervals.

Building Intuition

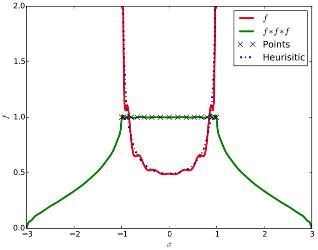
Using Chebfun, we collocate at Chebyshev roots to remove possibility of Runge's phenomenon:



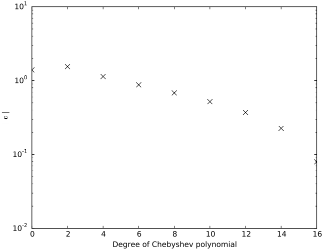


- Oscillations on the order of 2% $\Rightarrow$ a generalized Gibbs phenomenon
- This could imply the function is singular at the endpoints

Building Intuition



Conjecture



Coefficients

- We see an algebraic decay in the coefficients $\Rightarrow$ a poor approximation
- Since convolution is smoothing, f can have endpoint exponents as low as $-2/3$ for $f * f * f \in C^0[-3, 3]$
- Conjecture: $f(x) = \dfrac{g(x)}{\sqrt{1 - x^2}}$ for some analytic g.

Convolving with Singularities

- Chebfun has a very efficient algorithm for convolution of Chebyshev series [Hale & Townsend 2014]
  - Convert Chebyshev to Legendre coefficients with $\mathcal{O}\left(N \log^2 N / \log\log N\right)$ complexity
  - Use recurrences derived from spherical Bessel functions to convolve with $\mathcal{O}((M+N)^2)$ complexity
  - Revert to Chebyshev coefficients
- Significantly cheaper than quadrature with $\mathcal{O}((M+N)^3)$ complexity
- However, the algorithm is not applicable to functions with endpoint singularities
- Challenge comes from Jacobi elliptic integral of the first kind:

$$\left(\frac{1}{\sqrt{1-x^2}} * \frac{1}{\sqrt{1-x^2}}\right)(x) = \Re \frac{2F(\mathrm{i}\sqrt{4-x^2}/x, \mathrm{i}x/\sqrt{4-x^2})}{\mathrm{i}\sqrt{4-x^2}}$$
$$\sim \log|8/x|, \quad \text{as} \quad x \to 0.$$

Trapezoidal Rule

- The trapezoidal rule $\displaystyle\int_a^b f(x)\,\mathrm{d}x \approx (b-a)\left[\frac{f(a)+f(b)}{2}\right]$.
- The composite version $\displaystyle T(h) = h\sum_{k=1}^{n-1}\frac{f(x_{k-1})+f(x_k)}{2}$, where $h = \dfrac{b-a}{n}$ 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 is periodic, or if $f^{(n)}(\cdot) \to 0$ at endpoints, the convergence is faster than any power of h.
- Variable transformations $\phi : \mathbb{R} \to (a, b)$ with exponential decay [Stenger 1973] and [Takahasi & Mori 1974].

Quadrature by Variable Transformation

Consider the integral:

$$\int_a^b f(x)\,\mathrm{d}x = \int_{-\infty}^{+\infty} f(\phi(t))\phi'(t)\,\mathrm{d}t.$$

Variable transformations which induce single exponential endpoint decay are:

$$x = \phi_{\mathrm{SE}}(t) = \frac{a+b}{2} + \left(\frac{b-a}{2}\right)\tanh(t/2),$$

$$\mathrm{d}x = \phi'_{\mathrm{SE}}(t)\,\mathrm{d}t = \left(\frac{b-a}{4}\right)\mathrm{sech}^2(t/2)\,\mathrm{d}t,$$

Double exponential endpoint decay are:

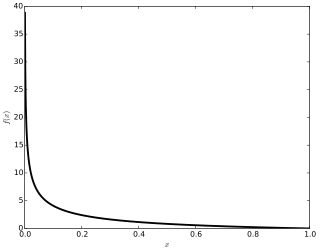
$$x = \phi_{\mathrm{DE}}(t) = \frac{a+b}{2} + \left(\frac{b-a}{2}\right)\tanh\left(\frac{\pi}{2}\sinh t\right),$$

$$\mathrm{d}x = \phi'_{\mathrm{DE}}(t)\,\mathrm{d}t = \left(\frac{b-a}{2}\right)\mathrm{sech}^2\left(\frac{\pi}{2}\sinh t\right)\frac{\pi}{2}\cosh t\,\mathrm{d}t.$$

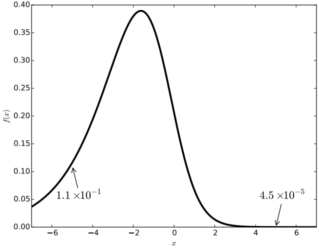
Quadrature by Variable Transformation

Example [Mori & Sugihara 2001]:

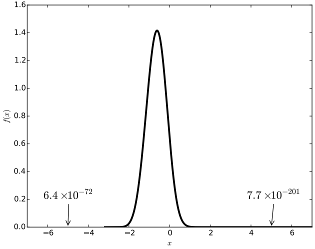
$$\int_0^1 x^{-1/4} \log(1/x)\,\mathrm{d}x = 16/9.$$



Integrand

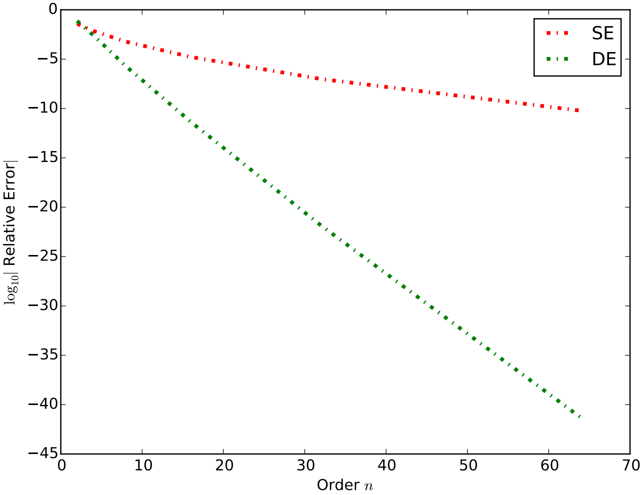


SE transformation



DE transformation

Quadrature by Variable Transformation



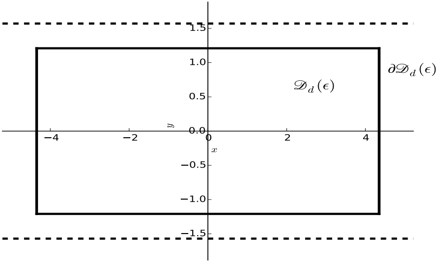
How to determine step size h for composite rule on $\mathbb{R}$?

Let d be a positive number and let $\mathscr{D}_d = \lim_{\epsilon \to 0} \mathscr{D}_d(\epsilon)$ denote the strip region of width $2d$ about the real axis:

$$\mathscr{D}_d(\epsilon) = \{z \in \mathbb{C} : |\mathrm{Re}\, z| < \epsilon^{-1}, \quad |\mathrm{Im}\, z| < d(1-\epsilon)\}.$$

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

$$\mathcal{N}_1(f, \mathscr{D}_d) = \lim_{\epsilon \to 0} \int_{\partial \mathscr{D}_d(\epsilon)} |f(z)|\, \mathrm{d}z < +\infty.$$



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

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

where the norm is given by:

$$\|f\| = \sup_{z\in\mathscr{D}_d} \left|\frac{f(z)}{\omega(z)}\right|.$$

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

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

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. $\alpha_1 \exp\left(-\beta|x|\right) \leq |\omega(x)| \leq \alpha_2 \exp\left(-\beta|x|\right), \quad x \in \mathbb{R}$, where α_1, α_2, and $\beta > 0$.

Then:

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

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

$$h = \sqrt{\frac{2\pi d}{\beta n}},$$

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

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. $\alpha_1 \exp\left(-\beta_1 e^{\gamma|x|}\right) \leq |\omega(x)| \leq \alpha_2 \exp\left(-\beta_2 e^{\gamma|x|}\right), \quad x \in \mathbb{R}$, where $\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma > 0$.

Then:

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

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 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 $d\gamma > \pi/2$.

Outcome:

- Optimality of the DE transformation for the trapezoidal rule.

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 $d\gamma > \pi/2$.

Outcome:

- Optimality of the DE transformation for the trapezoidal rule.
- What happens when complex singularities are present?

Maximizing the Convergence Rate

Problem [Slevinsky & Olver 2015]: How can we maximize the convergence rate of the trapezoidal rule:

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

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

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

Maximizing the Convergence Rate

Then we wish to find $\phi \in \Phi_{\rm ad}$ such that the convergence rate is maximized:

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

Result: an infinite-dimensional optimization problem for ϕ.
Consider the asymptotic problem as $N \to \infty$:

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

- We maximize the convergence rate when $d\gamma = \pi/2$
- Numerical algorithm is the subject of [Slevinsky & Olver 2015]

Return to Convolution

Let $\mathbf{c} = [c_1, c_2, \ldots, c_{\lceil N/2 \rceil}]^T$, $w(x) = (1 - x^2)^\lambda$, and x_i the $\lceil N/2 \rceil$ nonnegative roots of $T_N(x)$. Then:

$$g(\mathbf{c}, x_i) = \mathrm{conv}(\mathbf{c}^T T_{0:2:N} w, \mathrm{conv}(\mathbf{c}^T T_{0:2:N} w, \mathbf{c}^T T_{0:2:N} w))(x_i) - 1,$$

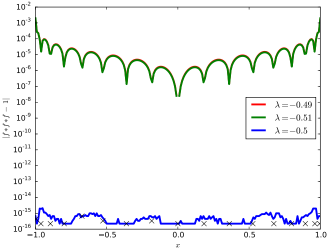
Newton iteration is the most efficient nonlinear solver.
By commutativity and associativity of convolution, we have:

$$[J(g)]_{i,j} = 3\mathrm{conv}(T_{2j-2} w, \mathrm{conv}(\mathbf{c}^T T_{0:2:N} w, \mathbf{c}^T T_{0:2:N} w))(x_i).$$

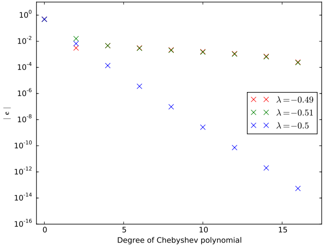
For each point x_i, we pre-compute the inner autoconvolution, and $[J(g)]_{i,j}$ can be computed in the cost of only 2 integrals (parallelogram overlap). By linearity of convolution, g is simply:

$$g(\mathbf{c}, x_i) = \frac{1}{3} J(g)\mathbf{c} - 1.$$

DE Convolution & Numerical Evidence for Conjecture



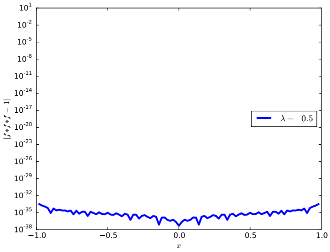
Convolution



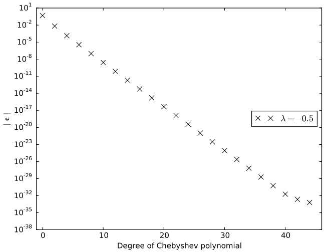
Coefficients

Algorithmic complexity scales as $\mathcal{O}(n^2 N^2)$ where:

- n is the number of quadrature nodes
- N is the number of coefficients
- 101 quadrature nodes and 9 coefficients takes ≈ 0.1 seconds per Newton iteration in double precision



Convolution



Coefficients

Algorithmic complexity scales as $\mathcal{O}(n^2 N^2)$ where:

- n is the number of quadrature nodes
- N is the number of coefficients
- 1001 quadrature nodes and 23 coefficients takes $\approx$ 3 hours per Newton iteration in extended precision

Outlook

- A simple & systematic representation is conjectured for the continuous function whose 3-fold autoconvolution is constant
- Geometric convergence is observed with inverse square root endpoint singularities with $\mathcal{O}(n^2 N^2)$ complexity
- Previous result [Martin & O'Bryant 2007]:
  $$\inf_{f \in C^0(-1,1)} \frac{\|f * f * f\|_\infty}{\|f\|_1} \approx 0.287\,3\ldots$$
- New result:
  $$\inf_{f \in C^0(-1,1)} \frac{\|f * f * f\|_\infty}{\|f\|_1} \approx 0.287\,319\,803\,575\,759\,796\,363\,627\,713\,763\,526\ldots$$
- Is the function simple or can we determine a closed-form for the coefficients?
  - The ratio of successive coefficients may offer some insight
  - PSLQ may detect a simple representation for the constants

Thank you all very much for your time!

References

1. B. Green. *Acta Arithmetica*, C.4:365–390, 2001.
2. N. Hale and A. Townsend. *SIAM SISC*, 36:A1207–A1220, 2014.
3. G. Martin and K. O'Bryant. *Exp. Math.*, 16:145–165, 2007.
4. M. Mori and M. Sugihara. *J. Comp. Appl. Math.*, 127:287–296, 2001.
5. R.M. Slevinsky and S. Olver. *to appear in SIAM SISC*, 2015.
6. F. Stenger. *J. Inst. Math. Appl.*, 12:103–114, 1973.
7. M. Sugihara. *Numerische Mathematik*, 75:379–395, 1997.
8. H. Takahasi and M. Mori. *RIMS*, 9:721–741, 1974.