New Tricks for an Old Dog: Archimedes, Gauss, and the Fast Computation of Stochastic Inverse Transcendentals

Kevin Long and Kaleb D. McKale

Department of Mathematics and Statistics
Texas Tech University

DOE Applied Math Meeting
Oct 2011

Problem: compute inverse transcendental functions of polynomial chaos expansion (PCE)

Most classical methods for computing transcendentals are not useable with PCE

- Computation of double-precision transcendentals usually involves piecewise functions
- Example: computation of arctangent
  - $0 < x \leq 1$: do something fast and accurate (*e.g.* Pade approximant, Chebyshev fit)
  - $x > 1$: map into $[0, 1]$ using $\arctan(x^{-1}) = \frac{\pi}{2} - \arctan x$
  - $x < 0$: use odd symmetry to map to $[0, \infty)$
- Piecewise approximations not suitable in PCE work

Workarounds

- NISP
- Line integration (reduction to 1D quadrature or ODE)

Why are stochastic inverse transcendentals challenging?

- Taylor series approximations not convergent
  - Support of PDF can extend beyond radius of convergence
- Non-polynomial integrands make line integration expensive
  - Line integration requires linear solve (or worse) at each quadrature point
  - Convergence of quadrature can be slow
- Non-polynomial behavior requires high order PCE with accurate coefficients
  - $\tan^{-1}$ is bounded
  - log is singular at zero
  - $\sin^{-1}$ non-differentiable at ± 1

Inverse transcendentals through line integration

Line integration method (Debusschere *et al.*) reduces computation of stochastic transcendentals to 1D quadrature

- Arctangent

$$\tan^{-1} u(\xi) = u(\xi) \int_0^1 \frac{dt}{1 + u(\xi)^2 t^2}$$

- Arcsine

$$\sin^{-1} u(\xi) = u(\xi) \int_0^1 \frac{dt}{\sqrt{1 - u(\xi)^2 t^2}}$$

- Logarithm

$$\log u(\xi) = (u(\xi) - 1) \int_0^1 \frac{dt}{1 + (u(\xi) - 1) t}$$

A different approach to computing inverse transcendentals: Borchardt-Gauss (BG) iterated means

Example: BG computation of arctangent

Initialize:

$$a_0 = 1 \quad g_0 = \left(1 + x^2\right)^{1/2}$$

Loop: syncopated arithmetic-geometric mean

$$a_{n+1} = \frac{1}{2}\left(a_n + g_n\right), \qquad g_{n+1} = \sqrt{g_n a_{n+1}}$$

$$B(a_0, g_0) = lim_{n\to\infty} g_n$$

Postprocess:

$$\arctan x = \frac{x}{B(a_0, g_0)}$$

- Requires only addition/subtraction, multiplication/division, square root
- This is a *very* old idea: Archimedes developed a similar algorithm using harmonic means instead of geometric means.

Why it works: half-angle identities

BG computation of arctangent

- If $\theta = \arctan(x)$ then $\sin(\theta) = \frac{x}{\sqrt{1+x^2}}$, $\cos(\theta) = \frac{1}{\sqrt{1+x^2}}$
- $\theta = \lim_{n\to\infty} 2^n \sin\left(\frac{\theta}{2^n}\right)$
- Iterated half-angle identity:

$$2^n \sin\left(\frac{\theta}{2^n}\right) = \frac{\sin(\theta)}{\prod_{k=1}^{n} \cos\left(\frac{\theta}{2^k}\right)}$$

- Sequence of geometric means g_n goes to

$$\prod_{k=1}^{\infty} \cos\left(\frac{\theta}{2^k}\right)$$

  from below
- $a_n \to$ same limit from above
- $\arctan(x) = \theta = \frac{\sin(\theta)}{\prod_{k=1}^{\infty} \cos\left(\frac{\theta}{2^k}\right)} = \frac{x}{B(a_0, g_0)\sqrt{1+x^2}}$

The Borchardt-Gauss-Carlson algorithm (BGC)

BG computation of other inverse transcendentals is similar

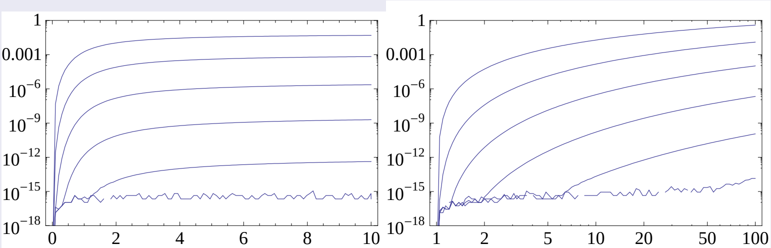
- same AGM recurrence as arctangent
- different initialization and postprocessing

Convergence is linear or better

- Original BG: contraction factor $\to \frac{1}{4}$ per iteration
- Carlson: Accelerate via Richardson extrapolation (BGC)
  - Contraction factor $\approx \frac{1}{1000}$ per iteration
  - Mildly superlinear: contraction factor improves per step
  - Some overhead, but no additional square roots
- Bottleneck is square root calculation
  - Use weak square root: compute $u = \sqrt{f}$ by solving $(v, u^2 - f) = 0$

Numerical results on the reals

Convergence of BGC arctangent and logarithm



- Very fast convergence over a large dynamic range

BGC has the features we'd like for PCE computation

Good features

- Single algorithm applicable throughout domain of function
- Needs only arithmetic plus square root

Also

- Cost determined by square root cost
- Needs ~ 5 square roots per computation
- Scales well with dimension (equivalent to scaling of reciprocal)

All elementary inverse transcendentals can be expressed in terms of the Borchardt-Gauss mean

The inverse transcendentals through the BG mean

Function	Relation to BG mean	Domain of applicability
$\tan^{-1}(x)$	$\frac{x}{B\left(1,\sqrt{1+x^2}\right)}$	$-\infty < x < \infty$
$\sin^{-1}(x)$	$\frac{x}{B\left(\sqrt{1-x^2},1\right)}$	$-1 \leq x \leq 1$
$\cos^{-1}(x)$	$\frac{\sqrt{1-x^2}}{B(x,1)}$	$0 \leq x \leq 1$
$\tanh^{-1}(x)$	$\frac{x}{B\left(1,\sqrt{1-x^2}\right)}$	$-1 < x < 1$
$\sinh^{-1}(x)$	$\frac{x}{B\left(\sqrt{1+x^2},1\right)}$	$-\infty < x < \infty$
$\cosh^{-1}(x)$	$\frac{\sqrt{x^2-1}}{B(x,1)}$	$x \geq 1$
$\log(x)$	$\frac{x-1}{B\left(\frac{x+1}{2},x\right)}$	$x > 0$

Some theory

Assuming no truncation of PCE

- Neglecting truncation of PCE, convergence theory for BG is simple on any Banach space
- On compact domain, $B(a_n, g_n)$ converges uniformly for any bounded a_0, g_0.
- As on $\mathbb{R}$, convergence is linear (factor 0.25, factor $\sim 10^{-3}$ with Carlson)

Including truncation of PCE

- Assuming truncation of PCE in square root, have proved weak convergence of $B(a_n, g_n)$

Cost metrics for BGC iteration and line integration

Definitions

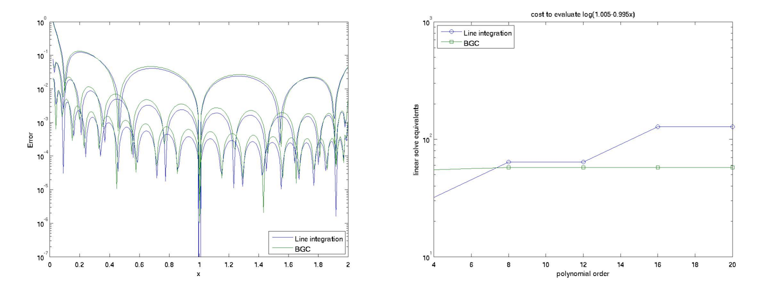
- N_Q is number of quadrature points in line integration
- N_{Newt} is number of Newton steps to compute square root
- N_{BGC} is number of outer iterations in BGC method
- Cost of Newton step for a square root is 1 linear solve plus 1 symmetric matrix-matrix multiply ($\frac{5}{2}$ linear solve equivalents)

Cost required for each function (linear solve equivalents)

- Arctangent
  - Line integration: N_Q
  - BGC: $\frac{5}{2}(N_{BGC}+1)N_{Newt}+1$
- Arcsine
  - Line integration: $N_Q\left(\frac{5}{2}N_{Newt}+1\right)$
  - BGC: $\frac{5}{2}(N_{BGC}+1)N_{Newt}+1$
- Logarithm
  - Line integration: N_Q
  - BGC: $\frac{5}{2}N_{BGC}N_{Newt}+1$

Numerical results: $\log(x)$ on $[10^{-2}, 2]$

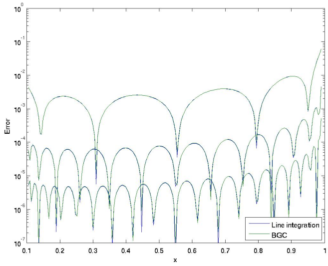
Error and cost for stochastic logarithm

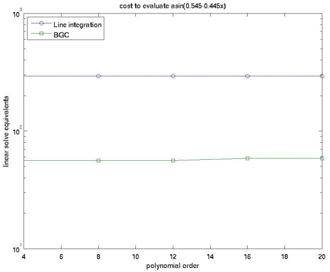


- Errors shown for $p = 4, 12, 20$
- Line integration: number of linear solves grows with polynomial order
- BGC: number of linear solves independent of polynomial order

Numerical results: $\sin^{-1}(x)$ on $[0.1, 0.99]$

Error and cost for stochastic arcsine

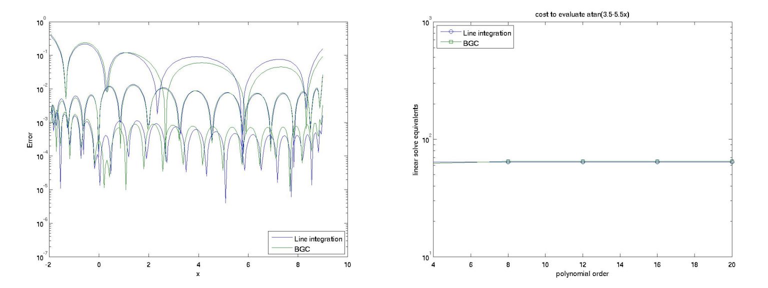




- Errors shown for $p = 4, 12, 20$
- Line integration and BGC have nearly identical accuracy
- BGC significantly less expensive than line integration

Numerical results: $\tan^{-1}(x)$ on $[-2, 9]$

Error and cost for stochastic arctangent



- Errors shown for $p = 4, 12, 20$
- Cost nearly identical for BGC and line integration

Conclusions

The BGC algorithm is a promising approach to the fast and robust calculation of stochastic inverse transcendental functions

- Rapid convergence
- Accuracy comparable to line integration
- Efficiency comparable to line integration for arctangent
- Efficiency superior to line integration for logarithm and arcsine

Implemented using Stokhos package of Trilinos library