Numerical solution of delayed differential equations using QMC methods

Quasi-randomized schemes for heavily varying equations

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Overview

1. Sketch of the numerical solution
2. Historic background
3. The RKQMC solution methods (Hermite Interpolation, QMC methods)
4. Convergence proofs
5. Numerical examples

The problem

Heavily varying delay differential equations (DDE) or DDE with heavily varying solutions.

$$\begin{aligned} y'(t) &= f\left(t, y(t), y(t-\tau_1(t)), \ldots, y(t-\tau_k(t))\right), && \text{for } t \geq t_0,\ k \geq 1, \\ y(t) &= \phi(t), && \text{for } t \leq t_0\ , \end{aligned}$$

with

$f(t, y(t), y_{ret}(t))$ ...piecewise smooth in y and y_{ret}, bounded and Borel measurable in t

$y(t)$ ...solution, d-dimensional real-valued function

$\tau_1(t), ..., \tau_k(t)$ ...cont. delay functions, bounded from below by $\tau_0 > 0$, satisfy $t_1 - \tau_j(t_1) \leq t_2 - \tau_j(t_2)$ for $t_1 \leq t_2$

$\phi(t)$ ...initial function, cont. on $\left[\inf_{t_0 \leq t, 1 \leq j \leq k} \left(t - \tau_j(t)\right), t_0\right]$.

Sketch of the numerical solution

For heavily oscillating DDE: conventional Runge-Kutta methods unstable.

- Hermite interpolation for retarded argument $\Rightarrow$ ODE
- use RKQMC methods for ODE:
  Large Runge-Kutta error for heavily oscillating DE
  Idea (Stengle, Lécot): integrate over whole step size
  - Runge Kutta: Integration over y and t discretized
  - RK(Q)MC: Integration over y discretized, numerical Integration in t (using MC or QMC integration to minimize the error)

Historical background

Halton (1960), **Sobol** (1960/67), **Niederreiter** (1978), **Faure** (1981/82):
Low-discrepancy sequences

Oppelstrup (1976), **Oberle and Pesch** (1981), ...:
Treatment of DDE with Hermite interpolation for retarded arguments

Stengle (1990, 1995):
Randomized Runge Kutta schemes for (heavily oscillating) ordinary differential equations

Coulibaly and Lécot (1999), **Lécot** (2001), **Lécot and Koudiraty** (2002):
Quasi-Monte Carlo Runge Kutta schemes (using low-discrepancy sequences) for ODE

Kainhofer and Tichy (2001/02):
RKQMC methods for delayed differential equations, combining the Hermite interpolation with RKQMC methods.

Hermite interpolation

Use hermite interpolation for the retarded arguments:

$$z_j(t) := y(t - \tau_j(t)) = \begin{cases} \phi(t - \tau_j(t)), & \text{if } t - \tau_j(t) \leq t_0 \\ P_q(t - \tau_j(t); (y_i); (y_i')) & \text{otherwise} \end{cases}$$

DDE transforms to a ODE:

$$y'(t) = f(t, y(t), y(t - \tau_1(t)), \dots, y(t - \tau_k(t))) \approx$$
$$\approx f(t, y(t), z_1(t), \dots, z_k(t)) =: g(t, y(t)) \; .$$

Solution has to be piecewise $r/2$-times continuously differentiable in t. Resulting ODE has to fulfill requirements for RKQMC methods (Borel-measurable in t, continously differentiable in $y(t)$).

Runge Kutta QMC methods for ODE

G. Stengle, Ch. Lécot, I. Coulibaly, A. Koudiraty

$$y'(t) = f(t, y(t)), \qquad 0 < t < T,$$
$$y(0) = y_0$$

f smooth in y, bounded and Borel measurable in t.

f is Taylor-expanded only in $y \Rightarrow$ integral equation in t.

e.g. 2$^{\text{nd}}$ order:

$$y(t_{n+1}) = y(t_n) + \frac{1}{2h_n} \int_{t_n}^{t_{n+1}} \int_{t_n}^{t_{n+1}} \left(f(\underline{u}, y(t_n)) + \frac{1}{\beta} f(\bar{u}, y(t_n)) + \frac{1}{\alpha} f(\bar{u}, y(t_n) + \alpha h_n f(\underline{u}, y(t_n))) \right) du$$

Solved by (Quasi-)Monte Carlo integration

Quasi-Monte Carlo methods

Integrals replaced by a discrete sum over N (quasi-)random points:

$$\int_{[0,1]^s} f(x)dx = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

MC methods: x_i random points

QMC methods: x_i low-discrepancy sequences

Low discrepancy sequences: deterministic point sequences $\{x_i\}_{1\leq n\leq N} \in [0,1)^s$, good uniform distribution

star-discrepancy of the point set S

$$D_N^*(S) = \sup_{a,b\in[0,1]^s}\left|\frac{A([0,1)\,,S)}{N} - \lambda_s([a,b))\right|$$

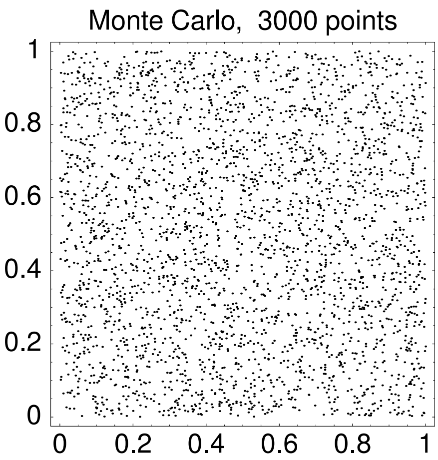
Koksma-Hlawka inequality:

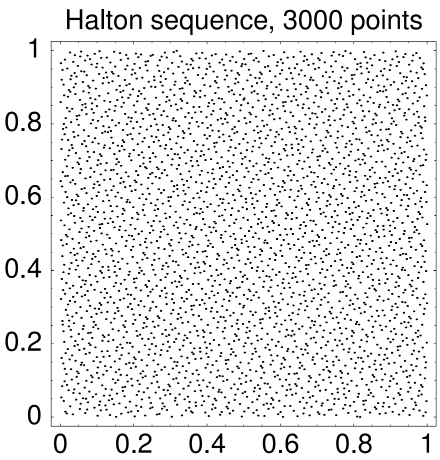
$$\left|\frac{1}{N}\sum_{n=1}^{N} f(x_n) - \int_{[0,1)^s} f(u)du\right| \leq V([0,1)^s, f)D_N^*\left(x_1,\ldots,x_N\right)\ .$$

Low-Discrepancy sequences

$$D_N^*(S) \leq \mathcal{O}\left(\frac{(\log N)^s}{N}\right)$$

- Halton-sequence in bases $(b_1, \ldots b_s)$: inversion of digit expansion of n in base b_i at the comma
- (t, s) nets in base b (Niederreiter, Sobol, Faure): net-like structure $\rightarrow$ best possible uniform distribution on elementary intervals





Problem: correlations between elements

General form of RKQMC method

$$y_{n+1} = y_n + \frac{h_n}{s!N} \sum_{0 \le j < N} G_s\left(\bar{t}_{j,n}; y\right)$$

$G_s\left(\bar{t}_{j,n}; y\right) \ldots$ differential increment function of scheme

$$G_1(u; y) = f(u, y)$$

$$G_2(\bar{u}; y) = f(\bar{u}_1, y) + \frac{1}{\beta} f(\bar{u}_2, y)) + \frac{1}{\alpha} f(\bar{u}_2, y + \alpha h_n f(\bar{u}_1, y)))$$

$$G_3(\bar{u}; y) = a_1 f(\bar{u}_1, y) + \sum_{l=1}^{L_2} a_{2,l} f\left(\bar{u}_2, y + b_{2,l} h_n f(\bar{u}_1, y)\right) + $$

$$+ \sum_{l=1}^{L_3} a_{3,l} \left(\bar{u}_3, y + b_{3,l}^{(1)} h_n f(\bar{u}_1, y) + b_{3,l}^{(2)} h_n f\left(\bar{u}_2, y_n + c_{3,l} h_n(\bar{u}_1, y_n)\right)\right)$$

Convergence proof by Koudiraty and Lécot:
If initial error $\|e_0\|$, the step size H, the discrepancy $D_N^*(X)$ and $\|f\|_E$ are small enough,

$$\|e_n\| \le e^{c_2 t_n} \|e_0\| + \frac{e^{c_2 t_n} - 1}{c_2} \left(c_1 H^3 + c_3 D_N^*(X)\right)$$

RKQMC for Volterra functional equations

$$\begin{aligned} y'(t) &= f(t, y(t), z(t)) && t \geq t_0 \\ z(t) &= (Fy)(t) \\ y(s) &= \phi(s) && s \leq t_0 \end{aligned}$$

- $(Fy)(t)$ contains dependence on retarded values.
- F and f are Lipschitz continuous in all arguments except t.

RKQMC method ($n \geq 0$):

$$\begin{aligned} y_{n+1} &= y_n + h_n \sum_{i=1}^{N} G_s\left(t_{n,i}; y_n, \tilde{z}(t)\right) \\ \tilde{z}(t) &= (\tilde{F} y_j)(t) \end{aligned}$$

Convergence: RKQMC for DDE

Theorem[K., 2002] If

(i) RKQMC method converges for ordinary differential equations with order p

(ii) the increment function G_s of the method and F are Lipschitz

(iii) the interpolation fulfills a Lipschitz condition

(iv) Hermite interpolation is used with order r

(v) the initial error $\|e_0\|$ vanishes

then the method converges. If at least ii and iii hold, the error is bounded by

$$\|e_{j+1}\| \leq \|e_0\| \, e^{\mathcal{L}t_j} + \frac{(e^{t_j\mathcal{L}} - 1)}{\mathcal{L}} \left(\left\| E_G^{\mathrm{ODE}} \right\| + \mathcal{L}_1 \mathcal{L}_2 \left\| E_r^{\mathrm{interpol}} \right\| \right) \; .$$

Special case: one retarded argument

Choose the RKQMC method:

- G_s Lipschitz ($\mathcal{L}_2$) in 2^{nd} and 3^{rd} argument, bounded variation (in the sense of Hardy and Krause).
- $\exists\ c_1,\ c_2,\ c_3$ such that for a $p > 0$

$$\begin{aligned} \text{loc. trunc. error } \|\epsilon_n\| &\leq c_1(h_n)h_n^p \\ \text{RK error } \|\delta_n\| &\leq c_2(h_n)\,\|e_n\| \\ \text{QMC error } \|d_n\| &\leq c_3(h_n)D_N^*(S) \end{aligned}$$

- interpolation order p, fulfils a certain Lipschitz condition

Then the error $\|e_n\| = \|y_n - y(t_n)\|$ of the method is bounded from above by:

$$\|e_n\| \leq \|e_0\|\, e^{t_n\left(c_2+\frac{\mathcal{L}_2}{s!}\right)} + \frac{e^{t_n\left(c_2+\frac{\mathcal{L}_2}{s!}\right)} - 1}{c_2 + \frac{\mathcal{L}_2}{s!}} \cdot \left\{ c_3 D_N^*(X) + \frac{\mathcal{L}_2}{s!} M H^q + c_1 H^p \right\}$$

Numerical examples

$$y'(t) = 3y(t-1)\sin(\lambda t) + 2y(t-1.5)\cos(\lambda t), \quad t \geq 0$$
$$y(t) = 1, \quad t \leq 0\ ,$$

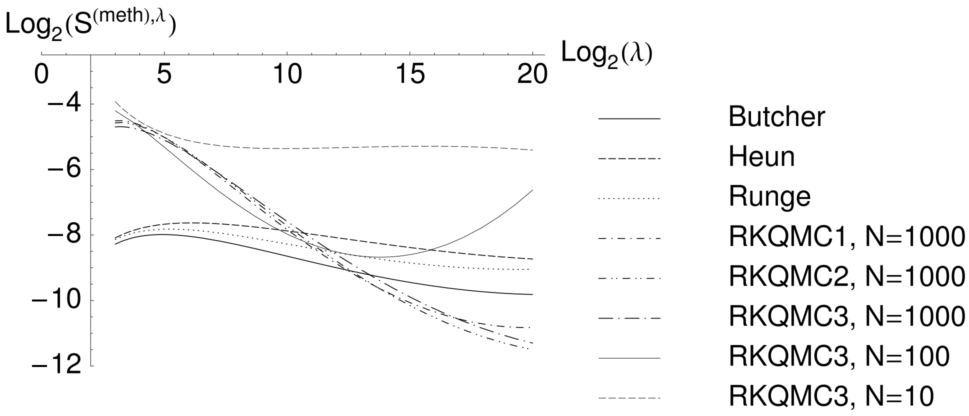


Fig: Error of the RK and RKQMC methods, $h_n = 0.001$ for RK, $h_n = 0.01$ for RKQMC

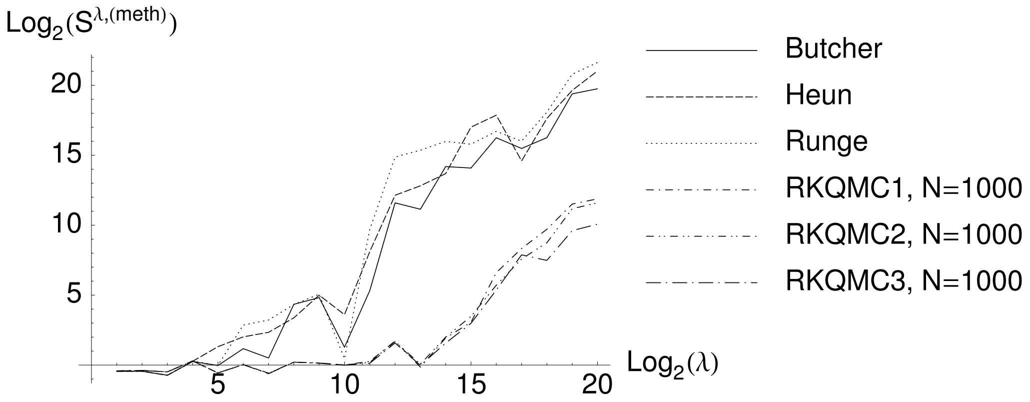
slowly varying (small λ): conventional RK better
rapidly varying (high λ): RKQMC outperform higher order RK

Advantage of RKQMC for unstable DDE

$$y'(t) = \pi\frac{\lambda}{2}\left(y\left(t-2-\frac{3}{2\lambda}\right) - y\left(t-2-\frac{1}{2\lambda}\right)\right), \quad t \geq 0$$
$$y(t) = sin(\lambda t \pi), \quad t < 0\ ,$$

Exact Solution: $y(t) = sin(\lambda t \pi)$

- No discontinuities in any derivative
- k-th derivative only bounded by $\lambda^k \rightarrow$ "exploding" error



RKQMC schemes can delay the instability of the solution for heavily oscillating delay differential equations.

Time-corrected error

QMC integration is more expensive than 1 evaluation (Runge-Kutta)
$\rightarrow$ Compare a time-corrected error

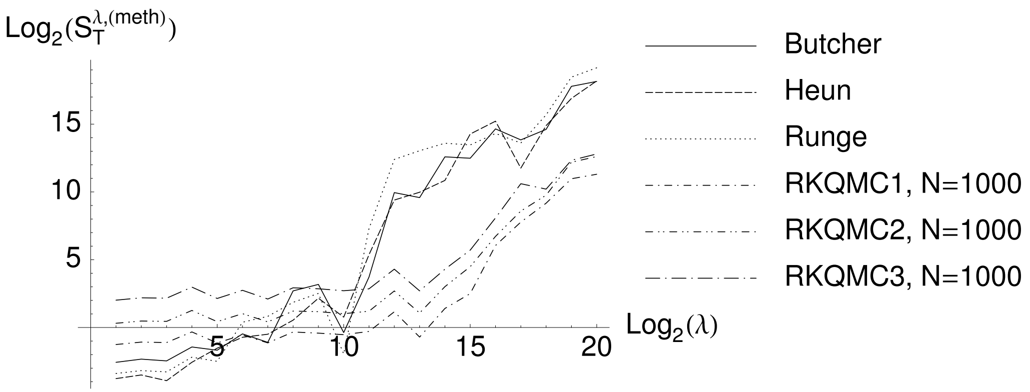


Fig: Time-corrected error of the RK and RKQMC methods

Result: RKQMC methods loose some advantage, but still better than Runge-Kutta for heavily oscillating DDE.

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