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Recursive Monte Carlo for linear ODEs

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Abstract

This thesis explores applying recursive Monte Carlo for solving linear ordinary differential equations with a vision towards partial differential equations. The proposed algorithms capitalize on the appropriate combination of Monte Carlo techniques. These Monte Carlo techniques get introduced with examples and code.

1 Introduction

1.1 Notation

Notations utilized include:

- $B(p) \sim \text{Bernoulli}(p) = \begin{cases} 1 & \text{if } U < p \\ 0 & \text{else} \end{cases}$
- BVP = Boundary Value Problem
- FP = First Passage
- $H(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{else} \end{cases}$
- i.i.d. = independent identically distributed
- $U \sim \text{Uniform}(0, 1)$
- IVP = Initial Value Problem
- MC = Monte Carlo
- ODE = Ordinary Differential Equation
- PDE = Partial Differential Equation
- RMC = Recursive Monte Carlo
- RRMC = Recursion in Recursion Monte Carlo
- RRVE (Recursive Random Variable Equation): An equation that defines a family of random variables in terms of itself
- RV = Random Variable
- Random variables will be denoted with capital letters, e.g., X , Y or Z .

1.2 Related Work

The primary motivating paper for this work is the work by Sawhney et al. (2022) [Saw+22], which introduces the walk-on-sphere method for solving second-order elliptic PDEs with varying coefficients and Dirichlet boundary conditions. Their techniques have shown high accuracy even in the presence of geometrically complex boundary conditions. We were inspired to apply the underlying mechanics of these Monte Carlo techniques to ODEs to explore parallel in time and the possibility to extend their techniques to other types of PDEs.

We made an interactive data map of the literature read mainly in function of this thesis available at https://huggingface.co/spaces/ISIPINK/zotero_map. It may take 10 seconds to load.

The latest paper that we found on an unbiased IVP solver is by Ermakov and Smilovitskiy’s 2021 [ES21] that study an unbiased method for a Cauchy problem for large systems of linear differential equations for describing queuing systems. Similarly to us they base their solver on Volterra integral equations.

Other literature is a bit further away. The most important fields we draw from are:

- rendering and walk-on-sphere/first passage literature which contain many practical recursive Monte Carlo techniques,
- Stochastic Gradient Descent literature that is connected through continuous gradient descent/Newton which we first encountered in [Hua+17],
- information complexity literature which was unexpected to us, there are some interesting biased algorithms applied on ODEs that achieve optimal information complexity rates in the randomized case, similar to us Daun’s 2011 [Dau11] uses control variates to achieve optimal order of convergence.

A recurrent theme in these fields is that informational optimal algorithms and unbiased algorithms are of theoretical importance and lead to more efficient algorithms in the long run.

1.3 Contributions

TODO: add intuition and motivations to the beginning of sections and do section descriptions here.

A significant part of this thesis is dedicated to informally introducing recursive Monte Carlo and applying variance reduction techniques for ODEs.

The key contribution is an unbiased Monte Carlo method (3.3.3) for linear initial value problems for systems of ordinary differential equations by using recursion in recursion and variance reduction techniques. We conjecture that this method achieves optimal information complexity.

2 Background

2.1 Monte Carlo Integration

TODO:

- add information theory
- add curse of dimensionality

In this subsection, we review basic Monte Carlo theory.

Monte Carlo integration is an algorithm that uses random sampling to estimate an integral.

Definition 2.1.1 (Uniform Monte Carlo Integration)

We define uniform Monte Carlo integration of $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ over $\Omega \subset \mathbb{R}^n$ as an estimation of the average of $f(U)$, with $U \sim \text{Uniform}(\Omega)$. Combined with the Best Linear Unbiased Estimators (BLUEs) for the average, Monte Carlo Integration in that case can be summarized in the following formula:

$$\int_{\Omega} f(s) ds \approx \frac{1}{n} \sum_{i=1}^n f(U_i), \quad (1)$$

where n is the amount of samples used.

Because estimators are Random Variables (RV) the cost and error also are RVs. In most cases these RVs are hard to impossible to get. Directly making comparisons between estimators based on these RVs is hard, there is no Pareto front we can draw. Instead statistics of these variables are used to do comparisons.

Accuracy comparisons between estimators are usually done with (root) mean square error.

Definition 2.1.2 (Root Mean Square Error (RMSE))

We define the RMSE of an estimator $\tilde{\theta}$ for θ as follows:

$$\text{RMSE}(\tilde{\theta}) = \sqrt{E[||\tilde{\theta} - \theta||_2^2]}. \quad (2)$$

Even comparisons based on RMSE can be counterintuitive look at Stein's paradox for example. We will limit us to 1 dimensional unbiased estimators, so that RMSE becomes the variance. It is easy to estimate the variance wich we use to get confidence intervals via Chebyshev's inequality or in the case of the BLUE via approximate normal distribution.

Average (FLOPs or time)/simulation are very common cost statistics. We can imagine (memory or wall time) at risk (similar to value at risk) to be useful to keep track of. The statistics are problem dependent. If we limit ourselves to BLUEs with big sample size and finite variance assumption on error and simulation time. Memory needs to be just enough to evaluate f and to keep an accumulation of the sum which is negligible. Computation across simulations is embarrassingly parallel

which make them well suited to a GPU implementation. These assumptions get you pretty close to optimal solutions and are very practical for high dimensions or complex domains. There is a linear trade off between average simulation time and variance which allows us to define a relative efficiency statistic.

Definition 2.1.3 (Relative Monte Carlo Efficiency)

Define relative Monte Carlo efficiency of an estimator F as follows:

$$\epsilon[F] = \frac{1}{\text{Var}[F]T[F]}, \quad (3)$$

with T the average simulation time.

Related Work 2.1.4 (Relative Monte Carlo Efficiency)

For a reference see [Vea97].

For smooth 1 dimensional integration is the linear trade off between variance and average simulation time is not even close to optimal.

Explain how information complexity was used in devolving quantum algorithms.

Definition 2.1.5 (Information Complexity)

Define information complexity. Rough measure of how many function calls are used.

Intuition behind the curse of dimensionality.

Theorem 2.1.6 (Curse of Dimensionality)

State the information curse of dimensionality for integration for deterministic errors.

Related Work 2.1.7 (Curse of Dimensionality)

[Fou22] chapter on the curse of dimensionality.

Explain why the underlying assumptions of information are relevant. And give realistic examples with them.

Explain the limitations using information complexity.

calculate the information complexity of Monte Carlo

2.2 Recursive Monte Carlo

In this subsection, we introduce recursive Monte Carlo with the following initial value problem:

$$y' = y, \quad y(0) = 1. \quad (4)$$

By integrating both sides of equation (4), we obtain:

$$y(t) = 1 + \int_0^t y(s)ds. \quad (5)$$

Equation (5) represents a recursive integral equation, specifically a linear Volterra integral equation of the second type. By estimating the recursive integral in equation (5) using Monte Carlo, we derive the following estimator:

$$Y(t) = 1 + ty(Ut), \quad (6)$$

where $U \sim \text{Uniform}(0, 1)$. If y is well-behaved, then $E[Y(t)] = y(t)$, but we cannot directly simulate $Y(t)$ without access to $y(s)$ for $s < t$. However, we can replace y with an unbiased estimator without affecting $E[Y(t)] = y(t)$, by the law of total expectation ($E[X] = E[E[X|Z]]$). By replacing y with Y itself, we obtain a recursive expression for Y :

$$Y(t) = 1 + tY(Ut). \quad (7)$$

Equation (7) is a recursive random variable equation. If one were to try to simulate Y with equation (7), it would recurse indefinitely. To overcome this, approximate $Y(t) \approx 1$ near $t = 0$ introducing minimal bias. Later, we will discuss Russian roulette (2.3.2), which can be used as an unbiased stopping mechanism.

Python Code 2.2.1 (implementation of (7))

```
1 from random import random as U
2 def Y(t, eps): return 1 + t*Y(U()*t, eps) if t > eps else 1
3 def y(t, eps, nsim):
4     return sum(Y(t, eps) for _ in range(nsim))/nsim
5 print(f"y(1) approx {y(1,0.01,10**3)}")
6 # y(1) approx 2.710602603240193
```

To gain insight into realizations of recursive random variable equations, it can be helpful to plot all recursive calls $(t, Y(t))$, as shown in Figure 1 for this implementation.

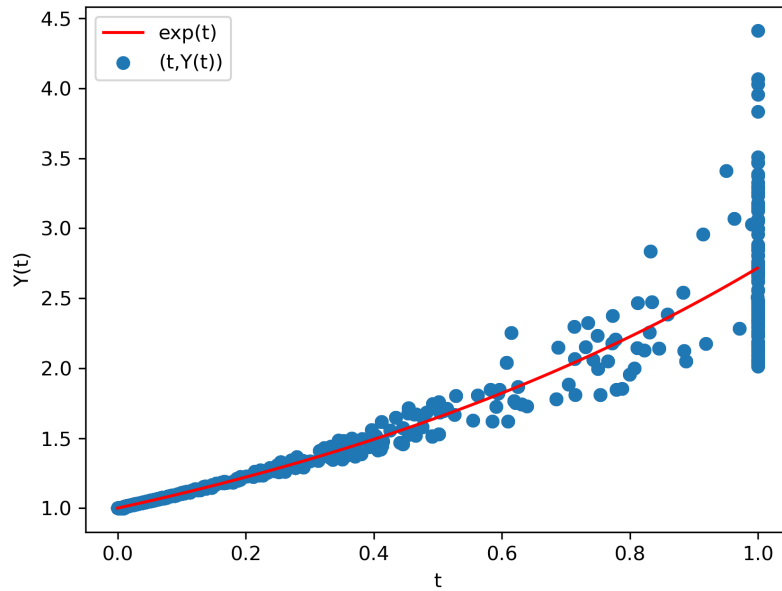


Figure 1: Recursive calls of (2.2.1)

One issue with (2.2.1) is that the variance increases rapidly as t increases. This issue gets resolved later (see (3.3.1)). It is important to note that (2.2.1) retains desirable

properties of unbiased Monte Carlo methods, such as being embarrassingly parallel and having simple error estimates.

2.3 Modifying Monte Carlo

In this subsection, we discuss techniques for modifying RRVEs in a way that preserves the expected value of the solution while acquiring more desirable properties.

Motivate why switching between similar is allowed and it is frequent.

Notation 2.3.1 (\cong)

$$X \cong Y \iff E[X] = E[Y].$$

Russian roulette is a MC technique commonly employed in rendering algorithms. The concept behind Russian roulette is to replace a RV with a less computationally expensive approximation sometimes.

Definition 2.3.2 (Russian roulette)

We define Russian roulette on X with free parameters Y_1, Y_2 ($E[Y_1] = E[Y_2]$), $p \in [0, 1]$ and U independent of Y_1, Y_2, X as follows:

$$X \cong \begin{cases} \frac{1}{p}(X - (1-p)Y_1) & \text{if } U < p \\ Y_2 & \text{else} \end{cases}. \quad (8)$$

Example 2.3.3 (Russian roulette)

Let us consider the estimation of $E[Z]$, where Z is defined as follows:

$$Z = U + \frac{f(U)}{1000}. \quad (9)$$

Here, $f : \mathbb{R} \rightarrow [0, 1]$ is an expensive function to compute. Directly estimating $E[Z]$ would involve evaluating f in each simulation, which can be computationally costly. To address this, we can modify Z to:

$$Z \cong U + B\left(\frac{1}{100}\right) \frac{f(U)}{10}. \quad (10)$$

This RV requires calling f on average once every 100 simulations. This significantly reduces the computational burden while increasing the variance slightly thereby increasing the MC efficiency.

Alternatively it is possible to estimate the expectance of the 2 terms of Z separately. Given the variances and computational complexity of both terms, you can calculate the asymptotic optimal division of samples for each term.

Example 2.3.4 (Russian roulette on (7))

To address the issue of indefinite recursion in equation (7), Russian roulette can be employed by approximating the value of Y near $t = 0$ with 1 sometimes. Specifically, we replace the coefficient t in front of the recursive term with $B(t)$ when $t < 1$. The modified recursive expression for $Y(t)$ becomes:

$$y(t) \cong Y(t) = \begin{cases} 1 + B(t)Y(Ut) & \text{if } t < 1 \\ 1 + tY(Ut) & \text{else} \end{cases}. \quad (11)$$

Python Code 2.3.5 (implementation of (11))

```

1 from random import random as U
2 def Y(t):
3     if t>1: return 1 + t*Y(U()*t)
4     return 1 + Y(U()*t) if U() < t else 1
5 def y(t, nsim): return sum(Y(t) for _ in range(nsim))/nsim
6 print(f"y(1) approx {y(1,10**3)}")
7 # y(1) approx 2.698

```

Interestingly, $\forall t \leq 1 : Y(t)$ is constrained to take on only integer values. This is visually clear in Figure 2.

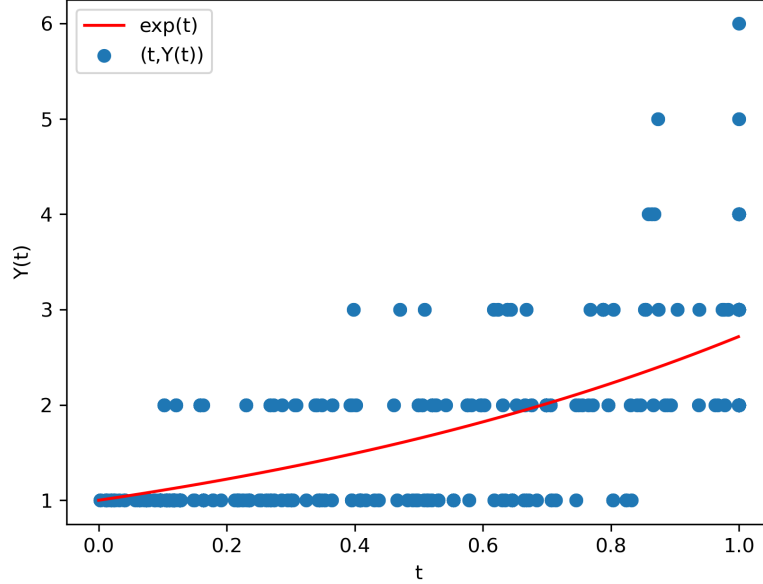


Figure 2: Recursive calls $(t, Y(t))$ of (2.3.5)

Splitting is a technique that has almost the reverse effect of Russian roulette. Instead of reducing the number of simulations of a RV as Russian roulette does, we increase it by using more samples (i.e., splitting the sample) which reduces the variance.

Definition 2.3.6 (splitting)

Splitting X refers to utilizing multiple $X_j \sim X$ (not necessarily independent) to reduce variance by taking their average:

$$X \cong \frac{1}{N} \sum_{j=1}^N X_j. \quad (12)$$

Splitting the recursive term in a RRVE can result in additive branching recursion, necessitating cautious management of terminating the branches promptly to prevent exponential growth in computational complexity. To accomplish this, termination strategies that have been previously discussed can be employed. Subsequently, we will explore the utilization of coupled recursion as a technique to mitigate additive branching recursion in RRVEs (refer to (3.2.3)).

Example 2.3.7 (splitting on (7))

We can "split" the recursive term of Equation (7) into two parts as follows:

$$y(t) \cong Y(t) = 1 + \frac{t}{2}(Y_1(Ut) + Y_2(Ut)), \quad (13)$$

where $Y_1(t)$ and $Y_2(t)$ are i.i.d. with $Y(t)$.

Python Code 2.3.8 (implementation of (2.3.7))

```
1 from random import random as U
2 def Y(t):
3     u = U()
4     if t > 1: return 1 + t*(Y(u*t)+Y(u*t))/2
5     return 1 + (Y(u*t)+Y(u*t))/2 if U() < t else 1
6 def y(t, nsim): return sum(Y(t) for _ in range(nsim))/nsim
7 print(f"y(1) approx {y(1,10**3)}")
8 # y(1) approx 2.73747265625
```

Definition 2.3.9 (control variates)

Define control variating $f(X)$ with \tilde{f} an approximation of f as:

$$f(X) \cong (f - \tilde{f})(X) + E[\tilde{f}(X)]. \quad (14)$$

Note that control variating requires the evaluation of $E[\tilde{f}(X)]$. When this is estimated instead of evaluated exactly, we refer to it as 2-level MC.

Example 2.3.10 (control variate on (7))

To create a control variate for Equation (7) that effectively reduces variance, we employ the approximation $y(t) \approx \tilde{y} = 1 + t$ and define the modified recursive term as follows:

$$Y(t) = 1 + E[\tilde{y}(Ut)] + t(Y(Ut) - \tilde{y}(Ut)) \quad (15)$$

$$= 1 + t + \frac{t^2}{2} + t(Y(Ut) - 1 - Ut). \quad (16)$$

It is important to note that while we could cancel out the constant term of the control variate, doing so would have a negative impact on the Russian roulette implemented later.

Python Code 2.3.11 (implementation of (2.3.10))

```
1 from random import random as U
2 def Y(t):
```

```

3     u = U()
4     if t > 1: return 1+t**2/2 + t*(Y(u*t)-u*t)
5     return 1 + t + t**2/2 + (Y(u*t)-1-u*t if U() < t else 0)
6 def y(t, nsim): return sum(Y(t) for _ in range(nsim))/nsim
7 print(f"y(1) approx {y(1,10**3)}")
8 # y(1) approx 2.734827303480301

```

Related Work 2.3.12 (MC modification)

For further reference on these techniques see [Vea97].

2.4 Monte Carlo Trapezoidal Rule

TODO:

- explain info complexity composite MC
- add results and references of optimal info complexity

In this subsection, we introduce a MC trapezoidal rule that exhibits similar convergence behavior to the methods discussed later. The MC trapezoidal rule is essentially a regular Monte Carlo method enhanced with control variates based on the trapezoidal rule.

Definition 2.4.1 (MC trapezoidal rule)

We define the MC trapezoidal rule for approximating the integral of function f over the interval $[x, x + \Delta x]$ with a Russian roulette rate l and \tilde{f} the linear approximation of f corresponding to the trapezoidal rule as follows:

$$\int_x^{x+\Delta x} f(s) ds \quad (17)$$

$$= \int_x^{x+\Delta x} \tilde{f}(s) ds + \int_x^{x+\Delta x} f(s) - \tilde{f}(s) ds \quad (18)$$

$$= \Delta x \frac{f(x) + f(x + \Delta x)}{2} + E \left[f(S_x) - \tilde{f}(S_x) \right] \quad (19)$$

$$\cong \Delta x \frac{f(x) + f(x + \Delta x)}{2} \quad (20)$$

$$+ \Delta x l B \left(\frac{1}{l} \right) \left(f(S_x) - f(x) - \frac{S_x - x}{\Delta x} (f(x + \Delta x) - f(x)) \right), \quad (21)$$

where $S_x \sim \text{Uniform}(x, x + \Delta x)$.

This MC trapezoidal rule has on average $\frac{1}{l}$ more function calls than the normal trapezoidal rule. For the composite rule with n intervals, there are $\text{Binomial}(n, \frac{1}{l})$ additional function calls (repeated Bernoulli experiments).

Definition 2.4.2 (composite MC trapezoidal rule)

Define the composite MC trapezoidal rule for approximating the integral of function f over the interval $[a, b]$ with n intervals and a Russian roulette rate l as follows:

$$\int_a^b f(s)ds \cong \Delta x \sum_x \frac{f(x) + f(x + \Delta x)}{2} \quad (22)$$

$$+ lB \left(\frac{1}{l} \right) \left(f(S_x) - f(x) - \frac{S_x - x}{\Delta x} (f(x + \Delta x) - f(x)) \right), \quad (23)$$

where $S_x \sim \text{Uniform}(x, x + \Delta x)$.

Python Code 2.4.3 (implementation of (2.4.2))

We implement (2.4.2) for $\int_0^1 e^s ds$.

```

1 from random import random as U
2 from math import exp
3 import numpy as np
4 def f(x): return exp(x)
5 def trapezium(n): return sum((f(j/n)+f((j+1)/n))/2
6     for j in range(n))/n
7 def MCTrapezium(n, l=100):
8     sol = 0
9     for j in range(n):
10         if U()*l < 1:
11             x, xx = j/n, (j+1)/n
12             S = x + U()*(xx-x) # \sim Uniform(x,xx)
13             sol += l*(f(S)-f(x)-(S-x)*(f(xx)-f(x))*n)/n
14     return sol+trapezium(n)
15 def exact(a, b): return exp(b)-exp(a)
16 def error(s): return (s-exact(0, 1))/exact(0, 1)
17 print(f" error:{error(trapezium(10000))}")
18 print(f"MCerror:{error(MCTrapezium(10000,100))}")
19 # error:8.333344745642098e-10
20 # MCerror:-1.5216231703870405e-10

```

For the sake of simplicity, we reduce the study of the local truncation error to the following expression:

$$\int_0^h s^2 ds = O(h^3). \quad (24)$$

In the standard composite rule, we would drop this term, but in the MC version, we eliminate the bias. As a result, the local truncation error behaves similarly to:

$$\int_0^h s^2 ds - h(hU)^2 = \int_0^h s^2 ds - h^3 U^2 = O(h^3). \quad (25)$$

The main distinction between the standard and MC rule lies in how they accumulate local truncation errors into global truncation error. In the standard case, there is a loss of one order. When measuring the error of randomized algorithms, the root-mean-square error is typically used, which, in the unbiased case, is equivalent to the standard deviation:

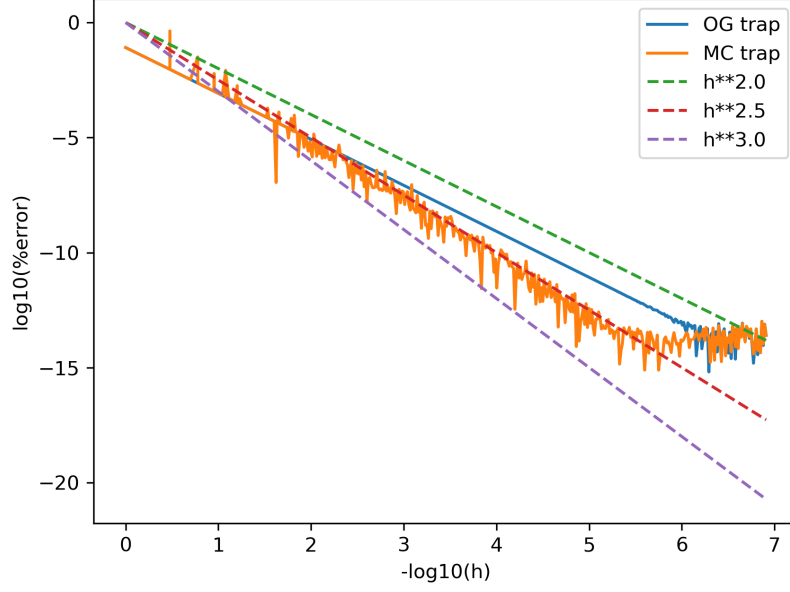


Figure 3: Log-log plot of the error of (2.4.2) for $\int_0^1 e^s ds$ with $l = 100$ at which the additional function calls are negligible. At floating point accuracy, the convergence ceases.

$$\sqrt{\text{Var} \left(\sum_{j=1}^n \int_0^h s^2 ds - h^3 U_j^2 \right)} = \sqrt{\text{Var} \left(\sum_{j=1}^n h^3 U_j^2 \right)} \quad (26)$$

$$= h^3 \sqrt{\text{Var} \left(\sum_{j=1}^n U_j^2 \right)} \quad (27)$$

$$= h^3 \sqrt{\sum_{j=1}^n \text{Var}(U_j^2)} \quad (28)$$

$$= h^3 \sqrt{n \text{Var}(U^2)} \quad (29)$$

$$= h^3 \sqrt{n} \sqrt{\text{Var}(U^2)} \quad (30)$$

$$= O(h^{2.5}). \quad (31)$$

Note that the meaning of a bound on the error that behaves as $O(h^2)$ and a bound on the root-mean-square error that behaves as $O(h^2)$ is different. A bound on the error implies a bound on the root-mean-square error, but the reverse is not true.

Related Work 2.4.4 (Monte Carlo Trapezoidal Rule)

The optimal information complexity for integration in the randomized setting is known see [HN01].

2.5 Unbiased Non-Linearity

In this subsection, we present techniques for handling polynomial non-linearity. The backbone for this is using independent samples $y^2 \cong Y_1 Y_2$ with Y_1 independent of Y_2 and $Y_1 \cong Y_2 \cong y$.

Example 2.5.1 ($y' = y^2$)

Consider the following ODE:

$$y' = y^2, \quad y(1) = -1. \quad (32)$$

The solution to this equation is given by $y(t) = -\frac{1}{t}$. By integrating both sides of equation (32), we obtain the following integral equation:

$$y(t) = -1 + \int_1^t y(s)y(s)ds. \quad (33)$$

To estimate the recursive integral in equation (32), we use i.i.d. $Y_1, Y_2 \sim Y$ in following RRVE:

$$y(t) \cong Y(t) = -1 + (t-1)Y_1(S)Y_2(S), \quad (34)$$

where $S \sim \text{Uniform}(1, t)$. Branching RRVEs are typical when dealing with non-linearity.

Python Code 2.5.2 (implementation (2.5.1))

```
1 from random import random as U
2 def Y(t):
3     if t>2: raise Exception("doesn't support t>2")
4     S = U()*(t-1)+1
5     # Y(u)**2 != Y(u)*Y(u) !!!
6     return -1 + Y(S)*Y(S) if U()<t-1 else -1
7 def y(t, nsim): return sum(Y(t) for _ in range(nsim))/nsim
8 print(f"y(2) approx {y(2,10**3)}")
9 # y(2) approx -0.488
```

In this implementation $Y(t)$ only takes values $\{-1, 0\}$.

Example 2.5.3 ($e^{E[X]}$)

$e^{\int x(s)ds}$ is a common expression encountered when studying ODEs. In this example, we demonstrate how you can generate unbiased estimates of $e^{E[X]}$ with simulations of X . The Taylor series of e^x is:

$$e^{E[X]} = \sum_{n=0}^{\infty} \frac{E^n[X]}{n!} \quad (35)$$

$$= 1 + \frac{1}{1}E[X] \left(1 + \frac{1}{2}E[X] \left(1 + \frac{1}{3}E[X] (1 + \dots) \right) \right). \quad (36)$$

Change the fractions of equation (36) to Bernoulli processes and replace all X with

independent X_j with $E[X] = E[X_i]$.

$$e^{E[X]} = E \left[1 + B \left(\frac{1}{1} \right) E[X_1] \left(1 + B \left(\frac{1}{2} \right) E[X_2] \left(1 + B \left(\frac{1}{3} \right) E[X_3] (1 + \dots) \right) \right) \right] \quad (37)$$

$$= E \left[1 + B \left(\frac{1}{1} \right) X_1 \left(1 + B \left(\frac{1}{2} \right) X_2 \left(1 + B \left(\frac{1}{3} \right) X_3 (1 + \dots) \right) \right) \right] \quad (38)$$

What is inside the expectation is something that we can simulate with simulations of X_j .

Related Work 2.5.4 (example 2.5.3)

NVIDIA has a great paper on optimizing example 2.5.3 [Ket+21].

2.6 Recursion

TODO:

- add forward implementation of recursion using a stack

In this subsection, we discuss recursion-related techniques.

Technique 2.6.1 (coupled recursion)

The idea behind coupled recursion is sharing recursion calls of multiple RRVes for simulation. This does make them dependent.

Example 2.6.2 (coupled recursion)

Consider calculating the sensitivity of following ODE to a parameter a :

$$y' = ay, y(0) = 1 \Rightarrow \quad (39)$$

$$\partial_a y' = y + a \partial_a y \quad (40)$$

Turn (39) and (40) into RRVes. To emphasize that they are coupled, that they should recurse together we write them in a matrix equation:

$$\begin{bmatrix} Y(t) \\ \partial_a Y(t) \end{bmatrix} = X(t) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} + t \begin{bmatrix} a & 0 \\ 1 & a \end{bmatrix} X(Ut). \quad (41)$$

Observe how this eliminates the additive branching recursion present in equation (40).

Python Code 2.6.3 (implementation of (41))

```
1 from random import random as U
2 import numpy as np
3 def X(t, a): # only supports t<1
4     q, A = np.array([1, 0]), np.array([[a, 0], [1, a]])
5     return q + A @ X(U()*t, a) if U() < t else q
6 def sol(t, a, nsim): return sum(X(t, a) for _ in
7     range(nsim))/nsim
8 print(f"x(1,1) = {sol(1,1,10**3)}")
# x(1,1) = [2.7179 2.7104]
```

Related Work 2.6.4 (coupled recursion)

Example (2.6.2) is inspired by [VSJ21]. [VSJ21] propose an efficient unbiased back-propagation algorithm for rendering.

Technique 2.6.5 (recursion in recursion)

Recursion in recursion is like proving an induction step of an induction proof with induction. Recursion in recursion uses an inner recursion in the outer recursion.

Related Work 2.6.6 (recursion in recursion)

Beautiful examples of recursion in recursion are the next flight variant of WoS in [Saw+22] and epoch-based algorithms in optimization [GH21].

Most programming languages do support recursion, but it often comes with certain limitations such as maximum recursion depth and potential performance issues. When applicable, tail recursion can be used to implement recursion that addresses these concerns in some cases.

Technique 2.6.7 (non-branching tail recursion)

Tail recursion involves reordering all operations so that almost no operation needs to happen after the recursion call. This allows us to return the answer without retracing all steps when we reach the last recursion call and it can achieve similar speeds to a forward implementation.

The non-branching recursion presented in the RRVEs can be implemented with tail recursion due to the associativity of all operations ($(xy)z = x(yz)$) involved. However, tail recursion may not always be desirable as it discards intermediate values of the recursion calls which may be of interest or can increase computational cost. To retain some of these intermediate values, it is possible to combine tail recursion with normal recursion.

Python Code 2.6.8 (tail recursion on (41))

We implement (41) but this time with tail recursion. We collect addition operations in a vector sol and multiplication in a matrix W . W may be referred to as accumulated weight or throughput.

```
1 from random import random as U
2 import numpy as np
3 def X(t, a) -> np.array:
4     q, A = np.array([1.0, 0.0]), np.array([[a, 0.0], [1.0, a]])
5     sol, W = np.array([1.0, 0.0]), np.identity(2)
6     while U() < t:
7         W = W @ A if t < 1 else t * W @ A
8         sol += W @ q
9         t *= U()
10    return sol
11 def sol(t, a, nsim): return sum(X(t, a) for _ in
12     range(nsim))/nsim
13 print(f"x(1,1) = {sol(1,1,10**3)}")
# x(1,1) = [2.7198 2.7163]
```


3 Ordinary Differential Equations

3.1 Green Functions

In this subsection, we discuss informally how to turn ODEs into integral equations mainly by example. Our main tool for this are green functions. Prior to discussing green functions, we offer several examples.

Example 3.1.1 ($y' = y$ average condition)

We will solve the equation:

$$y' = y, \quad (42)$$

but this time with a different condition:

$$\int_0^1 y(s)ds = e - 1. \quad (43)$$

The solution to this equation remains the same: $y(t) = e^t$. We define the corresponding source green function $G(t, x)$ for y' and this type of condition as follows:

$$G' = \delta(x - t), \quad \int_0^1 G(s, x)ds = 0. \quad (44)$$

Solving this equation yields:

$$G(t, x) = H(t - x) + x - 1. \quad (45)$$

It is worth noting that we could have chosen a different green function corresponding to a different linear differential operator.

At this point, it may not be clear, but using this green function, we can form the following integral equation for (42):

$$y(t) = e - 1 + \int_0^1 G(t, s)y(s)ds. \quad (46)$$

Converting equation (46) into a RRVE using RMC, we obtain:

$$Y(t) = e - 1 + 2B\left(\frac{1}{2}\right)Y(S)(H(t - S) + S - 1), \quad (47)$$

where $S \sim U$. We will skip the Python implementation of equation (47) as it does not provide any new information. Instead, we will plot realizations of equation (47) in Figure 4.

Definition 3.1.2 (green function)

Vaguely speaking, we define the green function as a type of kernel function used to solve linear problems with linear conditions. The green function is the kernel that we place in front of the linear conditions or the source term, which we integrate over to obtain the solution. The green function possesses the property of satisfying either null linear conditions and a Dirac delta source term, or vice versa.

Related Work 3.1.3 (green function)

Our notion of green function is similar to that in [HGM01].

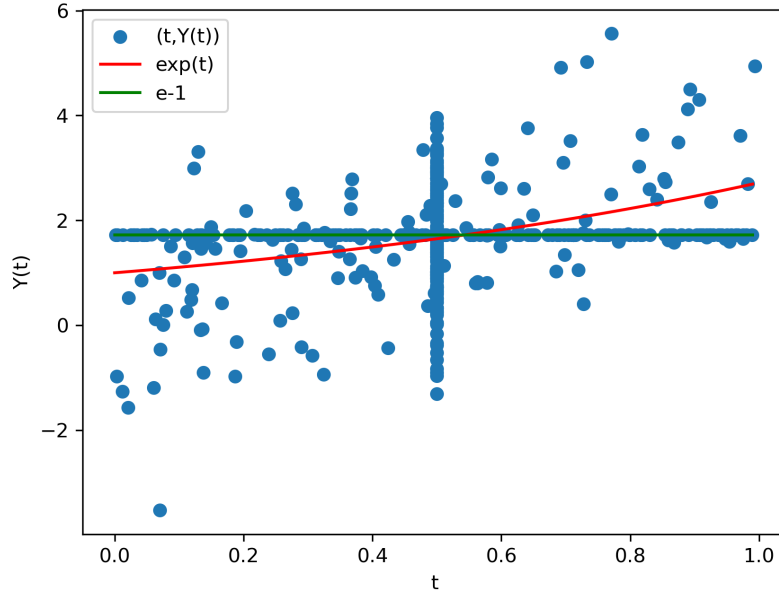


Figure 4: Recursive calls of (47) when calling $Y(0.5)$ 300 times. Points accumulate on the green line due to the Russian roulette, and at $t = 0.5$ because it is the starting value of the simulation.

3.2 Fredholm Integral Equations

TODO:

- explain better the graph for coupled splitting
- add better explanation to coupled splitting

The integral equations obtained in the previous subsection are Fredholm integral equations of the second kind. In this subsection, we introduce a technique called coupled splitting.

Definition 3.2.1 (Fredholm equation of the second kind)

A Fredholm equation of the second kind for φ is of the following form:

$$\varphi(t) = f(t) + \lambda \int_a^b K(t, s) \varphi(s) ds. \quad (48)$$

Given the kernel $K(t, s)$ and $f(t)$.

If both K and f satisfy certain regularity conditions, then for sufficiently small λ , it is relatively straightforward to establish the existence and uniqueness of solutions using a fixed-point argument.

Example 3.2.2 (Dirichlet $y'' = y$)

The following ODE will be the main testing example for boundary value problems:

$$y'' = y, \quad y(b_0), y(b_1). \quad (49)$$

The green functions corresponding to y'' and Dirichlet conditions are:

$$P(t, x) = \begin{cases} \frac{b_1-t}{b_1-b_0} & \text{if } x = b_0 \\ \frac{t-b_0}{b_1-b_0} & \text{if } x = b_1 \end{cases}, \quad (50)$$

$$G(t, s) = \begin{cases} -\frac{(b_1-t)(s-b_0)}{b_1-b_0} & \text{if } s < t \\ -\frac{(b_1-s)(t-b_0)}{b_1-b_0} & \text{if } t < s \end{cases}. \quad (51)$$

Straight from these green functions you get the following integral equation and RRVE:

$$y(t) = P(t, b_0)y(b_0) + P(t, b_1)y(b_1) + \int_{b_0}^{b_1} G(t, s)y(s)ds, \quad (52)$$

$$Y(t) = P(t, b_0)y(b_0) + P(t, b_1)y(b_1) + lB\left(\frac{1}{l}\right)(b_1 - b_0)G(t, S)y(S), \quad (53)$$

where $l \in \mathbb{R}$ the Russian roulette rate is and $S \sim \text{Uniform}(b_1, b_0)$.

Example 3.2.3 (coupled splitting on (3.2.2))

In addition to normal splitting (see Definition 2.3.6), we can also split the domain in Equation (52) as follows:

$$y(t) = P(t, b_0)y(b_0) + P(t, b_1)y(b_1) + \frac{1}{2} \int_{b_0}^{b_1} G(t, s)y(s)ds + \frac{1}{2} \int_{b_0}^{b_1} G(t, s)y(s)ds, \quad (54)$$

$$y(t) = P(t, b_0)y(b_0) + P(t, b_1)y(b_1) + \int_{b_0}^{\frac{b_1+b_0}{2}} G(t, s)y(s)ds + \int_{\frac{b_1+b_0}{2}}^{b_1} G(t, s)y(s)ds. \quad (55)$$

By coupling, we can eliminate the additive branching recursion in the RRVEs corresponding to Equations (54) and (55). This results in the following RRVE:

$$X(t_1, t_2) = \begin{bmatrix} P(t_1, b_0) & P(t_1, b_1) \\ P(t_2, b_0) & P(t_2, b_1) \end{bmatrix} \begin{bmatrix} y(b_0) \\ y(b_1) \end{bmatrix} + W \begin{bmatrix} G(t_1, S_1) & G(t_1, S_2) \\ G(t_2, S_1) & G(t_2, S_2) \end{bmatrix} X(S_1, S_2), \quad (56)$$

where W the right weighting matrix is (see code (3.2.4)), and S_1 and S_2 can be chosen in various ways.

Python Code 3.2.4 (implementation of (56))

We implemented equation (56) in example (3.2.3) with recursion but in this case, it is also possible to implement it forwardly.

```
1 from random import random as U
2 from math import exp
3 import numpy as np
4 def Pb0(t, b0, b1): return (b1-t)/(b1-b0)
5 def Pb1(t, b0, b1): return (t-b0)/(b1-b0)
```

```

6 def G(t, s, b0, b1): return - (b1-s)*(t-b0)/(b1-b0) if t < s
  else - (b1-t)*(s-b0)/(b1-b0)
7 def X(T, y0, y1, b0, b1):
8   yy = np.array([y0, y1])
9   bb = np.diag([(b1-b0)/len(T)]*len(T))
10  PP = np.array([[Pb0(t, b0, b1), Pb1(t, b0, b1)] for t in T])
11  sol = PP @ yy
12  l = 1.2 # russian roulette rate
13  if U()*l < 1:
14    u = U()
15    SS = [b0+(u+j)*(b1-b0)/len(T) for j in range(len(T))]
16    GG = np.array([[G(t,S,b0,b1) for S in SS] for t in T])
17    sol += l*GG @ bb @ X(SS, y0, y1, b0, b1)
18  return sol

```

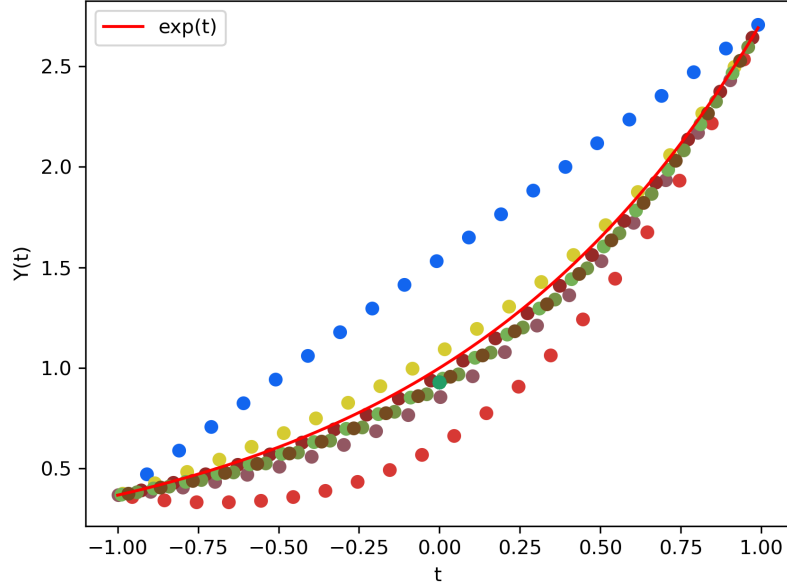


Figure 5: Recursive calls of equation (56) when calling $X(0)$ once, with a split size of 20, S_j are coupled such they are equally spaced and the coupling is colored. The initial conditions for this call are $y(-1) = e^{-1}$ and $y(1) = e^1$, with Russian roulette rate $l = 1.2$.

Example (3.2.3) does not exploit the locality and smoothness of the problem. We conjecture that coupled splitting can be particularly valuable when dealing with linear Fredholm equations of the second kind, especially in scenarios where MC integration surpasses traditional integration methods. This holds true for high-dimensional problems, non-smooth kernels, and challenging domains. We conjecture that employing coupled splitting in such cases can yield favorable results.

Related Work 3.2.5 (coupled splitting)

Coupled splitting is partly inspired by how [SM09] reduces variance by using bigger submatrices. Reusing samples for walk on sphere gets discussed in [Mil+23] and [BP23].

Figure 5 resembles fixed-point iterations, leading us to hypothesize that coupled splitting can achieve convergence in most cases where a fixed-point argument holds true and the convergence speed is very similar to fix-points methods until the accuracy of the stochastic approximation of the operator is reached (the approximate operator bottleneck). The approximation of the operator can be improved by increasing coupled splitting amount when approaching the bottleneck. Alternatively when reaching the bottleneck it is possible to rely on MC convergence.

Related Work 3.2.6 (convergence coupled splitting)

See [GH21] for a discussion on the convergence of recursive stochastic algorithms.

Coupled splitting was originally motivated to help with convergence. It didn't increase the convergence domain for the example shown in Figure 6.

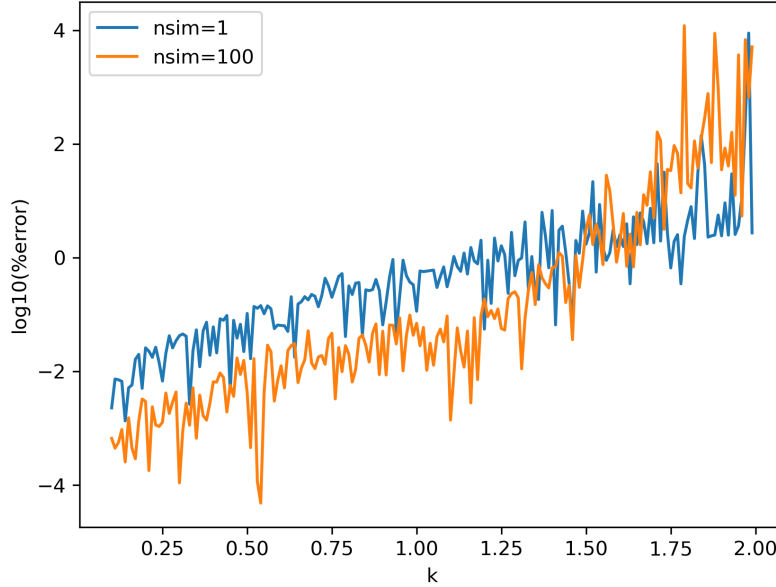


Figure 6: The logarithmic percentage error of $Y(0)$ for (53), with $l = 1.2$ and initial conditions $y(-k) = e^{-k}$ and $y(k) = e^k$, displays an exponential increase until approximately $k = 1.5$, beyond which additional simulations fail to reduce the error, indicating that the variance doesn't exist.

3.3 Initial Value Problems

Classic IVP solvers rely on shrinking the time steps for convergence. In this subsection we build up to Recursion in Recursion MC (RRMC) for IVPs that tries to emulate this behavior.

Example 3.3.1 (RRMC $y' = y$)

We demonstrate RRMC for IVPs with

$$y' = y, \quad y(0) = 1. \quad (57)$$

Imagine we have a time-stepping scheme $(t_n), \forall n : t_{n-1} < t_n$ then the following integral equations hold:

$$y(t) = y(t_n) + \int_{t_n}^t y(s)ds, \quad t > t_n. \quad (58)$$

Turn these in the following class of RRVEs:

$$Y_n(t) = y(t_n) + (t - t_n)Y_n((t - t_n)U + t_n), \quad t > t_n. \quad (59)$$

A problem with these RRVEs is that we do not know $y(t_n)$. Instead, we can replace it with an unbiased estimate y_n which we keep frozen in the inner recursion:

$$Y_n(t) = y_n + (t - t_n)Y_n((t - t_n)U + t_n), \quad t > t_n \quad (60)$$

$$y_n = \begin{cases} Y_{n-1}(t_n) & \text{if } n \neq 0 \\ y(t_0) & \text{if } n = 0 \end{cases}. \quad (61)$$

We refer to equation (60) as the inner recursion and equation (61) as the outer recursion of the recursion in recursion.

Python Code 3.3.2 (implementation of (3.3.1))

```
1 from random import random as U
2 def Y_in(t, tn, yn, h):
3     S = tn + U()*(t-tn) # \sim Uniform(T,t)
4     return yn + h*Y_in(S, tn, yn, h) if U() < (t-tn)/h else yn
5 def Y_out(tn, h): # h is out step size
6     TT = tn-h if tn-h > 0 else 0
7     return Y_in(tn, TT, Y_out(TT, h), h) if tn > 0 else 1
```

We measured the convergence speed of example (3.3.1) to be $O\left(\frac{h^{1.5}}{\sqrt{n_{\text{sim}}}}\right)$. While a 1.5 order of convergence is commendable for an unbiased method, it raises the question of how to attain even higher convergence orders. It is possible to emulate classical methods to achieve a higher order of convergence. This can be accomplished by eliminating lower order terms by using control variates, as demonstrated in the MC trapezoidal rule (see 2.4.2).

Example 3.3.3 (CV RRMC $y' = y$)

Let us control variate example (3.3.1).

$$y(t) = y(t_n) + \int_{t_n}^t y(s)ds, \quad t > t_n. \quad (62)$$

We build a control variate with a lower-order approximation of the integrand:

$$y(s) = y(t_n) + (s - t_n)y'(t_n) + O((s - t_n)^2) \quad (63)$$

$$\approx y(t_n) + (s - t_n)f(y(t_n), t_n) \quad (64)$$

$$\approx y(t_n) + (s - t_n) \left(\frac{y(t_n) - y(t_{n-1})}{t_n - t_{n-1}} \right) \quad (65)$$

$$\approx y(t_n)(1 + s - t_n). \quad (66)$$



Figure 7: Recursive calls of equation (61) when calling $Y_{out}(3, h)$ 30 times for different h .

Using the last one as a control variate for the integral:

$$y(t) = y(t_n) + \int_{t_n}^t y(s) ds \quad (67)$$

$$= y(t_n) + \int_{t_n}^t y(s) - y(t_n)(1 + s - t_n) + y(t_n)(1 + s - t_n) ds \quad (68)$$

$$= y(t_n) \left(1 + (1 - t_n)(t - t_n) + \frac{t^2 - t_n^2}{2} \right) + \int_{t_n}^t y(s) - y(t_n)(1 + s - t_n) ds. \quad (69)$$

We will not discuss turning this into an RRVE nor the implementation. The implementation is very similar to (3.3.6) and Figure 8 is a convergence plot for this example.

Related Work 3.3.4 (CV RRM)

[Dau11] similarly uses control variates to achieve a higher order of convergence.

RRMC is biased for our approach to non-linear problems. The inner recursions are correlated because they use the same information from the outer recursions, this does not mean that reducing root-mean-square error by splitting does not work, you just have to be careful with the bias. We conjecture that the bias in RRMC converges faster than the variance when decreasing h .

Example 3.3.5 (nonlinear RRM IVP)

Consider the following IVP:

$$y' = y^2 - t^4 + 2t, \quad y(0) = 0. \quad (70)$$

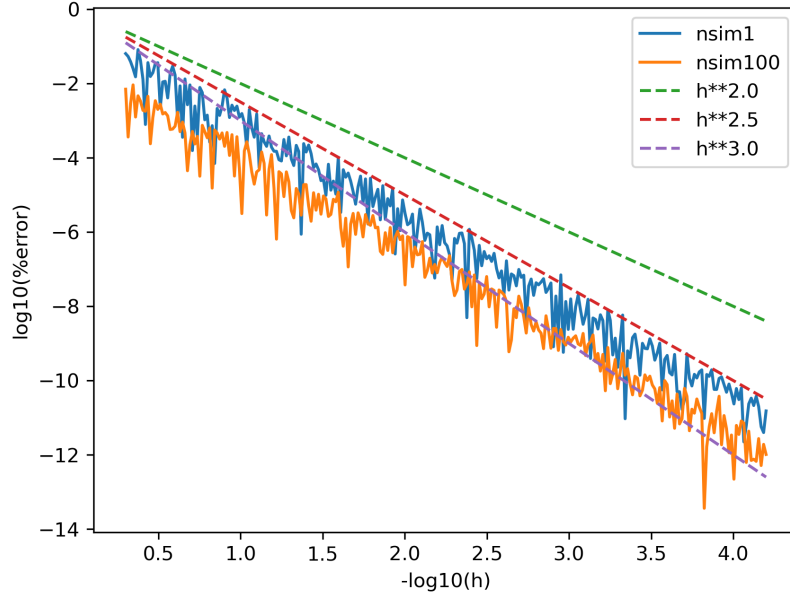


Figure 8: Log-log plot of the error for example (3.3.3) at $Y(10)$.

The exact solution to this problem is given by $y(t) = t^2$. We can express the solution as an integral equation:

$$y(t) = y(t_n) + \int_{t_n}^t y^2(s)ds - \frac{t^5 - t_n^5}{5} + (t^2 - t_n^2). \quad (71)$$

By control variating $y^2(s)$ up to the second order using Taylor expansion, we have:

$$y^2(t) \approx y^2(t_n) + 2(t - t_n)y(t_n)y'(t_n) + ((t - t_n)y'(t_n))^2 + O((t - t_n)^2) \quad (72)$$

$$\approx y^2(t_n) + 2(t - t_n)y(t_n)y'(t_n) + O((t - t_n)^2) \quad (73)$$

Integrating the control variate yields:

$$\int_{t_n}^t y^2(t_n) + 2(s - t_n)y(t_n)y'(t_n)ds \quad (74)$$

$$= (t - t_n)y^2(t_n) + 2\left(\frac{t^2 - t_n^2}{2} - t_n(t - t_n)\right)y(t_n)y'(t_n). \quad (75)$$

We implement this example in (3.3.6).

Python Code 3.3.6 (implementation of (3.3.5))

```

1 from random import random as U
2 def Y_in(t, tn, yn, dyn, h, l):
3     sol = yn # initial conditon
4     sol += t**2-tn**2 - (t**5-tn**5)/5 # source
5     sol += (t-tn)*yn**2 # 0 order

```



```

6     sol += 2*((t**2-tn**2)/2 - tn*(t-tn))*yn*dyn # 1 order
7     if U()*l < (t-tn)/h:
8         S = tn + U()*(t-tn) # \sim Uniform(T,t)
9         sol += l*h*(Y_in(S, tn, yn, dyn, h, 1)*
10             Y_in(S, tn, yn, dyn, h, 1) - yn**2-2*(S-tn)*yn*dyn)
11     return sol
12 def Y_out(t, h, l):
13     yn, tn = 0, 0
14     while tn < t:
15         tt = tn+h if tn+h < t else t
16         dyn = yn**2 - tn**4+2*tn
17         yn = Y_in(tt, tn, yn, dyn, tt-tn, l)
18         tn = tt
19     return yn

```

4 Limitations and Future Work

We have not dedicated significant attention, if any at all, to the convergence analysis of RMC methods for Fredholm equations. Figure 6 illustrates that arbitrary RMC do not converge.

Similarly to classic methods, RRMC struggles with big negative coefficients in front of the recursive parts which may appear in stiff problems. In addition to the challenges with stiff problems, we have not conducted a comparison between RRMC and traditional methods, and we do not anticipate that RRMC in this form outperforms other classic methods. The reason for this is that RRMC involves many function calls in the inner recursion without updating the current control variate. Proper testing requires precise tuning of the MC techniques utilized. We do believe that RRMC could potentially offer advantages in atypical scenarios. In the following example, we examine an ODE with a random parameter.

Example 4.0.1 (random ODEs)

Consider the problem given by the initial value problem

$$Y' = AY, \quad Y(0) = 1, \quad A \sim \text{Uniform}(0, 1). \quad (76)$$

The solution to this problem is given by $Y(t) = e^{tA}$, which is a RV. In order to compute expectations of functions of $Y(t)$, we use unbiased estimates X of the simulations of the solution.

Given an analytic function f , we can obtain $E[f(Y(t))]$ by conditioning on the value of A and using the law of total expectation:

$$E_A[f(Y(t))] = E_A[f(Y(t)) \mid A] \quad (77)$$

$$= E_A[f(E_X[X(t, A)]) \mid A]. \quad (78)$$

To estimate $f(E_X[X(t, A)])$, we use the approach outlined in (2.5.3). For the specific

example of (76), we can compute the first two moments of $Y(t)$ as

$$E_A[Y(t)] = \frac{e^t}{t} - \frac{1}{t}, \quad (79)$$

$$E_A[Y^2(t)] = \frac{e^{2t}}{2t} - \frac{1}{2t}. \quad (80)$$

Python Code 4.0.2 (implementation of (4.0.1))

```

1 from random import random as U
2 from math import exp
3 def X(t, a):
4     if t < 1: return 1+a*X(U()*t, a) if U() < t else 1
5     return 1+t*a*X(U()*t, a)
6 def eY(t): return X(t, U())
7 def eY2(t):
8     A = U()
9     return X(t, A)*X(t, A)
10 t, nsim = 3, 10**4
11 sol = sum(eY(t) for _ in range(nsim))/nsim
12 sol2 = sum(eY2(t) for _ in range(nsim))/nsim
13 s = exp(t)/t - 1/t # analytic solution
14 s2 = exp(2*t)/(2*t) - 1/(2*t) # analytic solution
15 print(f"E(Y({t})) is approx {sol},%error = {(sol - s)/s}")
16 print(f"E(Y^2({t})) is approx {sol2},%error = {(sol2 - s2)/s2}")
17 # E(Y(3)) is approx 6.5683, %error = 0.0324
18 # E(Y^2(3)) is approx 64.5843, %error = -0.0370

```

4.1 Heat Equation

In this subsection, we introduce the relation between the heat equation and Brownian motion.

Definition 4.1.1 (1D heat equation Dirichlet)

We define the 1D heat equation for u on connected domain Ω with Dirichlet boundary conditions the following way:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}. \quad (81)$$

Given $u(x, t) = \psi(x, t), \forall (x, t) \in \partial\Omega : t < \sup\{t | (x, t) \in \Omega\}$.

Lemma 4.1.2 (Brownian motion and the heat equation)

For problem (4.1.1) if $|\psi|$ is bounded then there holds:

$$u(x, t) = E[\psi(Y_\tau, \tau) | Y_t = x]. \quad (82)$$

With $dY_s = dW_{-s}, \tau = \sup\{s | (Y_s, s) \notin \Omega\}$.

Proof. Discretize the heat equation with a regular rectangular mesh that includes (x, t) with equally spaced intervals over space and time $(\Delta x, \Delta t)$ with the corresponding difference equation:

$$\frac{u(x, t) - u(x, t - \Delta t)}{\Delta t} = \frac{u(x + \Delta x, t) - 2u(x, t) + u(x - \Delta x, t)}{\Delta x^2}. \quad (83)$$

Isolate $u(x, t)$:

$$u(x, t) = \frac{\Delta t}{2\Delta t + \Delta x^2} (u(x + \Delta x, t) + u(x - \Delta x, t)) + \frac{\Delta x^2}{2\Delta t + \Delta x^2} (u(x, t - \Delta t)). \quad (84)$$

Because $u(x + \Delta x, t) \approx u(x - \Delta x, t) \approx u(x, t - \Delta t) \approx$ right-hand side of equation (84) we may Russian roulette to remove branching recursion and generate a recursion path instead of a tree.

$$Z(x, t) = \begin{cases} \psi(\operatorname{argmin}_{b \in \partial\Omega} \|(x, t) - b\|) & \text{when } (x, t) \notin \Omega \\ \begin{cases} Z(x + \Delta x, t) & \text{with chance } \frac{\Delta t}{2\Delta t + \Delta x^2} \\ Z(x - \Delta x, t) & \text{with chance } \frac{\Delta t}{2\Delta t + \Delta x^2} \\ Z(x, t - \Delta t) & \text{with chance } \frac{\Delta x^2}{2\Delta t + \Delta x^2} \end{cases} & \text{else .} \end{cases} \quad (85)$$

This is a RRVE, Z has finite variance because $|\psi|$ is bounded and $E[Z(x, t)]$ is the solution to the discretized heat equation. Taking the limit makes the discrete solution converge to the real solution. For (85) the limit makes the recursion path go to Brownian motion Y_t .

$$Z(x, t) \rightarrow \psi(Y_\tau, \tau). \quad (86)$$

Finishing the proof. □

Related Work 4.1.3

(4.1.2) is a subcase of the Feynman-Kac formula. For a proof and an in-depth discussion of the Feynman-Kac formula see [Øks03].

Abstract

Deze scriptie onderzoekt recursieve Monte Carlo voor het oplossen van lineaire gewone differentiaalvergelijkingen met het oog op partiële differentiaalvergelijkingen. De voorgestelde algoritmes maken gebruik van de geschikte combinatie van Monte Carlo technieken. Deze Monte Carlo technieken worden geïntroduceerd met voorbeelden en code.

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