Universiteit
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Masterproef scriptie

Recursive Monte Carlo

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Contents

Abstract

We will write this at the end. Also need a dutch abstract

1 Introduction

1.1 Introductory Example

In this subsection we introduce recursive Monte Carlo with our main example for initial value problems:

$$y' = y, y(0) = 1. \tag{1}$$

Integrating both sides of (1) obtains:

$$y(t) = 1 + \int_0^t y(s)ds. \tag{2}$$

Equation (2) is a recursive integral equation or to be more specific a linear Volterra integral equation of the second type. By estimating the recursive integral of equation (2) with Monte Carlo one derives following estimator:

$$Y(t) = 1 + ty(Ut). \tag{3}$$

With $U \sim \text{Uniform}(0, 1)$. If y is well behaved then $E[Y(t)] = y(t)$ but we can't calculate $Y(t)$ without accesses to $y(s), s < t$. Notice that we can replace y by a unbiased estimator of it without changing $E[Y(t)] = y(t)$ by the law of total expectance ($E[X] = E[E[X|Z]]$). By replacing y by Y itself we obtain a recursive expression for Y:

$$Y(t) = 1 + tY(Ut). \tag{4}$$

Equation (4) is a recursive random variable equation. If you would implement equation (4) with recursion it will run indefinitely. A biased way of around this is by approximating $Y(t) \approx 1$ near $t = 0$. Later we discuss Russian roulette (2.2.1) which can be used as an unbiased stopping mechanism.

Python Code 1.1.1 (implementation of (4))

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

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

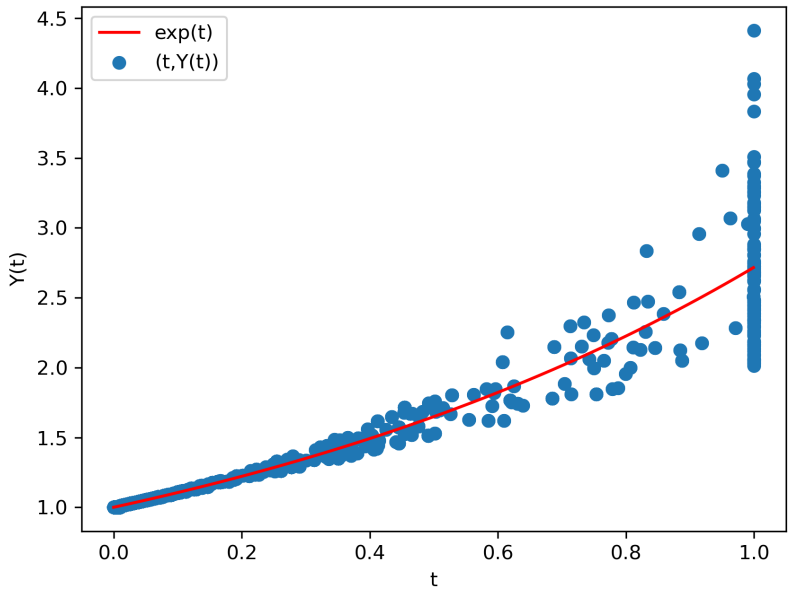

Figure 1: Recursive calls of (1.1.1)

An issue with (1.1.1) is that the variance increases rapidly when t increases. Later this is issue gets resolved in (3.3.1). Note that (1.1.1) keeps desirable properties from unbiased Monte Carlo methods such as being embarrassingly parallel and having simple error estimates.

1.2 Related Work

The main motivation for this thesis is the walk on sphere method for 2nd order elliptic PDEs with varying coefficients with Dirichlet boundary conditions discussed in [Saw+22]. This recursive Monte Carlo method is accurate even if the boundary conditions are geometric complex. We studied the mechanics behind these type of Monte Carlo techniques.

Related Work 1.2.1 (MC for IVPs ODEs)

Monte Carlo methods for initial value problems for systems of ordinary differential equations are little studied. The most significant works are:

- [JN09] describes a random Euler scheme for weak smoothness conditions.
- [Dau11] describes an randomized algorithm that achieves higher order of convergence order optimal even then deterministic algorithms under the same smoothness conditions by using polynomial extrapolation and control variates.
- [ET19], [ES21] study unbiased methods for linear problems and slightly biased for nonlinear based on the Volterra integral equations.

Previous Monte Carlo methods have limited applicability for initial value problems for systems of ordinary differential equations. From our personal perspective, the current literature on this subject lacks rewarding insights.

1.3 Contributions

A significant part of this thesis is dedicated to informally introducing recursive Monte Carlo with plenty of examples. The key contributions are:

- An unbiased Monte Carlo method (3.3.3) for linear initial value problems for systems of ordinary differential equations. This method achieves a higher order of convergence in the time step size that is comparable to explicit deterministic methods.
- Coupled recursion (2.5.2) and recursion in recursion (2.5.5) reformulations of the coupling in [VSJ21] and next flight in rendering see [Saw+22] the next flight version of walk on sphere.

2 Background

2.1 Notation

Notations used in this thesis include:

- $B(p) \sim \text{Bernoulli}(p) = \begin{cases} 1 & \text{if } U < p \\ 0 & \text{else} \end{cases}$.
- $H(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{else} \end{cases}$.
- $U \sim \text{Uniform}(0, 1)$.
- BVP = Boundary Value Problem
- 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 its self.
- RV = Random Variable.
- Random variables will be denoted with capital letters, e.g., X, Y or Z.

2.2 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.

Russian roulette is a MC technique commonly used in rendering. The main idea behind Russian roulette is to replace a random variable with a less computationally expensive approximation sometimes.

Definition 2.2.1 (Russian roulette)
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 the following way:

$$X \to \begin{cases} \frac{1}{p}(X - (1-p)Y_1) & \text{if } U < p \\ Y_2 & \text{else} \end{cases}. \tag{5}$$

Example 2.2.2 (Russian roulette)
Say that we are interested in estimating $E[Z]$ with Z defined in the following way:

$$Z = U + \frac{f(U)}{1000}. \tag{6}$$

where $f : \mathbb{R} \to [0, 1]$ expensive to compute. Estimating $E[Z]$ directly would require calling f each simulation. We can modify Z to

$$\tilde{Z} = U + B\left(\frac{1}{100}\right)\frac{f(U)}{10}. \tag{7}$$

Now $\tilde{Z}$ just requires calling f on average once every 100 simulations with the variance only increasing slightly compared to Z.

Related Work 2.2.3 (Russian roulette)
In example (2.2.2) 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 asymptotical optimal division of samples for each term.
In [Rat+22] they approximate optimal Russian roulette and splitting (RRS) factors with fixed-point iterations to maximize the efficiency in a render.

Example 2.2.4 (Russian roulette on (4))
Russian roulette can fix the indefinite recursion issue of equation (4) by approximating Y near $t = 0$ with 1 sometimes. Concretely we replace the t in front of the recursive term with $B(t)$ when $t < 1$.

$$Y(t) = \begin{cases} 1 + B(t)Y(Ut) & \text{if } t < 1 \\ 1 + tY(Ut) & \text{else} \end{cases}. \tag{8}$$

Python Code 2.2.5 (Russian roulette on (4))

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

Interestingly, $Y(t)$ is constrained to take on only integer values. This is visually evident on Figure 2.

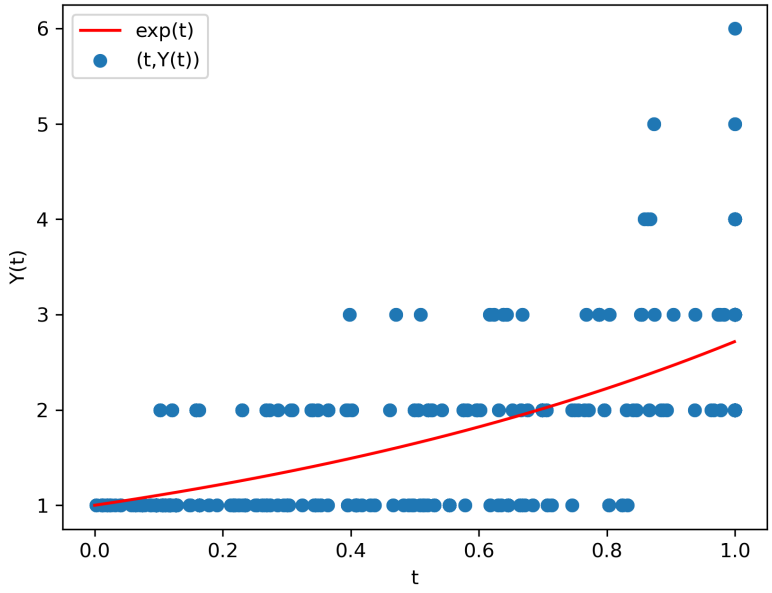

Figure 2: Recursive calls $(t, Y(t))$ of (2.2.5)

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 samples) which reduces the variance.

Definition 2.2.6 (splitting)
Splitting X means using multiple $X_j \sim X$ not independent per se to lower variance by averaging them:

$$\bar{X} = \frac{1}{N} \sum_{j=1}^{N} X_j. \tag{9}$$

Splitting the recursive term in a RRVE can lead to (additive) branching recursion, which requires extra care to ensure that the branches get terminated quickly to avoid an exponential increase in computational complexity. This can be achieved by employing termination strategies that have already been discussed. Later on, we will discuss the use of coupled recursion as a technique for alleviating additive branching recursion in RRVEs (see (3.2.3)).

Example 2.2.7 (splitting on (4))
We can "split" the recursive term of (4) in 2:

$$Y(t) = 1 + \frac{t}{2}(Y_1(Ut) + Y_2(Ut)). \tag{10}$$

with $Y_1(t), Y_2(t)$ i.i.d. $Y(t)$.

Python Code 2.2.8 (splitting on (4))

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

Definition 2.2.9 (2-level MC)
2-level MC on X with parameters $\tilde{X}, Y : E[\tilde{X}] = E[Y]$:

$$X \to X - \tilde{X} + Y. \tag{11}$$

Definition 2.2.10 (control variates)
Control variate on $f(X)$ is

$$f(X) \to f(X) - \tilde{f}(X) + E[\tilde{f}(X)]. \tag{12}$$

Control variates are a special case of 2-level MC. Usually $\tilde{f}$ is an approximation of f to reduce variance.

Example 2.2.11 (control variate on (4))
To make a control variate for (4) that reduces variance we use following approximation of $y(t) \approx 1 + t$:

$$Y(t) = 1 + t + \frac{t^2}{2} + t(Y(Ut) - 1 - Ut). \tag{13}$$

Notice that we can cancel the constant term of the control variate but that would affect the Russian roulette negatively.

Python Code 2.2.12 (control variate on (4))

```
from random import random as U
def Y(t):
    u = U()
    if t > 1: return 1+t**2/2 + t*(Y(u*t)-u*t)
    return 1 + t + t**2/2 + (Y(u*t)-1-u*t if U() < t else 0)
def y(t, nsim): return sum(Y(t) for _ in range(nsim))/nsim
print(f"y(1) approx {y(1,10**3)}")
# y(1) approx 2.734827303480301
```

Related Work 2.2.13 (MC modification)
Our favorite work that discusses these techniques is [Vea]. More interesting MC techniques can be found in rendering. 2-level gets discussed in [Gil13].

2.3 Monte Carlo Trapezoidal Rule

We present in this subsection a MC trapezoidal rule with similar convergence behavior to methods discussed later. The MC trapezoidal rule will just be regular MC control variated with the normal trapezoidal rule.

Definition 2.3.1 (MC trapezoidal rule)
Define the MC trapezoidal rule for f on $[x, x+dx]$ the following way:

$$\int_x^{x+dx} f(s)ds \approx \frac{f(x)+f(x+dx)}{2} + f(S_x) - f(x) - \frac{S_x - x}{dx}\left(f(x+dx) - f(x)\right) \quad (14)$$

with $S_x = \text{Uniform}(x, x+dx)$.

Defining the composite MC trapezoidal rule as the sum of MC trapezoidal rules on equally divided intervals is possible but expensive. Every interval would add a function call compared to the normal composite MC trapezoidal rule. Instead you can aggressively Russian roulette into the normal trapezoidal rule such that the increase in functions calls is arbitrarily small.

Definition 2.3.2 (composite MC trapezoidal rule)
Define the composite MC trapezoidal rule for f on $[a, b]$ with n intervals and a Russian roulette rate l the following way:

$$\int_a^b f(s)ds \approx \quad (15)$$

$$\sum_x \frac{f(x)+f(x+dx)}{2} + lB\left(\frac{1}{l}\right)\left(f(S_x) - f(x) - \frac{S_x - x}{dx}(f(x+dx) - f(x))\right) \quad (16)$$

with $S_x = \text{Uniform}(x, x+dx)$.

Python Code 2.3.3 (implementation of (2.3.2))
We implement (2.3.2) for $\int_0^1 e^s ds$.

```
from random import random as U
from math import exp
import numpy as np
def f(x): return exp(x)
def trapezium(n): return sum((f(x)+f(x+1/n))/2
    for x in np.arange(0, 1, 1/n))/n
def MCtrapezium(n, l=100):
    sol = 0
    for j in range(n):
        if U()*l < 1:
            x, xx = j/n, (j+1)/n
            S = x + U()*(xx-x)  # \sim Uniform(x,xx)
            sol += l*(f(S)-f(x)-(S-x)*(f(xx)-f(x))*n)/n
    return sol+trapezium(n)
def exact(a, b): return exp(b)-exp(a)
def error(s): return (s-exact(0, 1))/exact(0, 1)
print(f"  error:{error(trapezium(10000))}")
print(f"MCerror:{error(MCtrapezium(10000,100))}")
# error:8.333344745642098e-10
# MCerror:8.794793540941216e-11
```

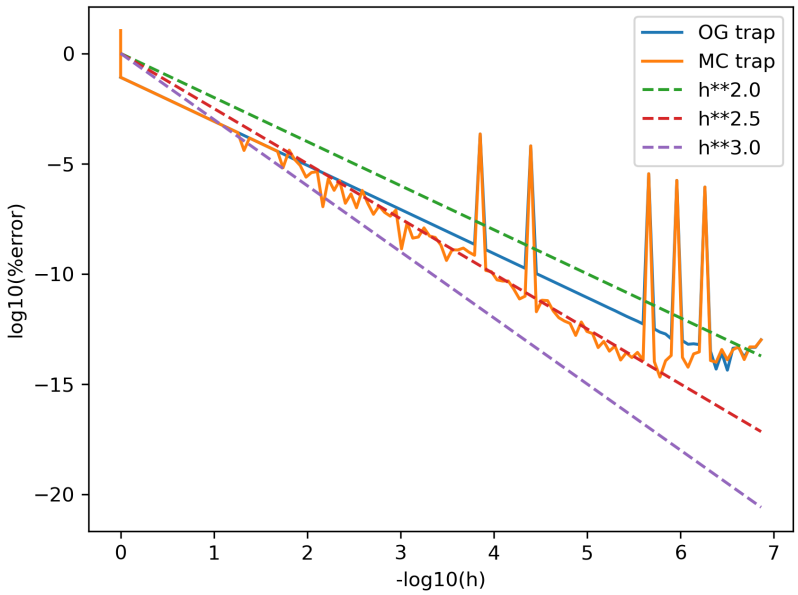

Figure 3: Log-log plot of (2.3.2) for $\int_0^1 e^s ds$ with $l = 100$.

We postulate that this MC composite rule enhances the convergence rate by 0.5 orders compared to the standard composite rule for each dimension, provided that the appropriate conditions of smoothness are met. To substantiate this conjecture, we shall outline our rationale concerning the accumulation of unbiased polynomial errors.

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

$$\int_0^h s^2 ds = O(h^3). \tag{17}$$

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 like:

$$\int_0^h s^2 ds - h(hU)^2 = \int_0^h s^2 ds - h^3 U^2 = O(h^3). \tag{18}$$

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:

$$\sqrt{\text{Var}\left(\sum_{j=1}^{n}\int_0^h s^2 ds - h^3 U_j^2\right)} = \sqrt{\text{Var}\left(\sum_{j=1}^{n} h^3 U_j^2\right)} \tag{19}$$

$$= h^3\sqrt{\text{Var}\left(\sum_{j=1}^{n} U_j^2\right)} \tag{20}$$

$$= h^3\sqrt{\sum_{j=1}^{n}\text{Var}(U_j^2)} \tag{21}$$

$$= h^3\sqrt{n\text{Var}(U^2)} \tag{22}$$

$$= h^3\sqrt{n}\sqrt{\text{Var}(U^2)} \tag{23}$$

$$= O(h^{2.5}). \tag{24}$$

Related Work 2.3.4
Optimal theoretical bounds on randomized algorithms can be found in: (see literature randomized trapezoidal rule) [Wu20]. The half order convergence that randomized gains over determinstic isn't the same gain we consider.

2.4 Unbiased Non-Linearity

In this subsection we introduce techniques to deal with non-linearity. At first it may looks only possible to deal with linear problems in an unbiased way but by using independent samples it possible to deal with polynomial non-linearity's (which theoretically extend to any continuos functions by the Weierstrass approximation theorem). It is not always easy to transform non-linearity into polynomials but it is not difficult to come up with biased alternative approaches based on linearization or approximate polynomial non-linearity.

Example 2.4.1 ($y' = y^2$)
Let's do following example:

$$y' = y^2, y(1) = -1. \tag{25}$$

This has solution $-\frac{1}{t}$. Integrate both sides of equation (25) to arrive at following integral equation:

$$y(t) = -1 + \int_1^t y(s)y(s)ds. \tag{26}$$

To estimate the recursive integral in equation (2) we use 2 independent $Y_1, Y_2 \sim Y$:

$$Y(t) = -1 + (t-1)Y_1(S)Y_2(S). \tag{27}$$

With $S \sim \text{Uniform}(1, t)$. This is a branching RRVE this is typical when dealing with non-linearity.

Python Code 2.4.2 ($y' = y^2$)

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

Example 2.4.3 ($e^{E[X]}$)

$e^{\int x(s)ds}$ is 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:

$$e^{E[X]} = \sum_{n=0}^{\infty} \frac{E^n[X]}{n!} \tag{28}$$

$$= 1 + \frac{1}{1}E[X]\left(1 + \frac{1}{2}E[X]\left(1 + \frac{1}{3}E[X]\left(1 + ...\right)\right)\right). \tag{29}$$

Change the fractions of equation (29) to Bernoulli processes and replace all X with independent X_j with $E[X] = E[X_i]$.

$$e^{E[X]} = E\left[1 + B\left(\frac{1}{1}\right)E[X_1]\left(1 + B\left(\frac{1}{2}\right)E[X_2]\left(1 + B\left(\frac{1}{3}\right)E[X_3]\left(1 + ...\right)\right)\right)\right] \tag{30}$$

$$= E\left[1 + B\left(\frac{1}{1}\right)X_1\left(1 + B\left(\frac{1}{2}\right)X_2\left(1 + B\left(\frac{1}{3}\right)X_3\left(1 + ...\right)\right)\right)\right] \tag{31}$$

$$\tag{32}$$

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

Python Code 2.4.4 ($e^{E[X]}$)

The following python code estimates $e^{\int_0^t s^2 ds}$:

```python
from random import random as U
from math import exp
def X(t): return -t**3*U()**2
def num_B(i):  # = depth of Bernoulli's = 1
    return num_B(i+1) if U()*i < 1 else i-1
def res(n, t): return 1 + X(t)*res(n-1, t) if n != 0 else 1
def expE(t): return res(num_B(0), t)

t, nsim = 1, 10**3
sol = sum(expE(t) for _ in range(nsim))/nsim
exact = exp(-t**3/3)
print(f"sol = {sol} %error={(sol- exact)/exact}")
#sol = 0.7075010309320893 %error=-0.01260277046
```

Related Work 2.4.5
A similar approach to non-linearity can be found in [ET19]. We have more papers on how to deal with non-linearity stashed, no idea if they are worth mentioning.

2.5 Recursion

In this subsection we discuss recursion related techniques.

Technique 2.5.1 (coupled recursion)
The idea behind coupled recursion is sharing recursion calls of multiple RRVEs for simulation. This does make them dependent. It is like assuming 2 induction hypotheses at the same time and proving both inductions steps at the same time vs doing separate induction proofs. Which should be easier because you have accesses to more assumptions at the same time.

Example 2.5.2 (coupled recursion)
Lets say you are interested in calculating the sensitivity of the solution of an ODE to a parameter a:

$$y' = ay, y(0) = 1 \Rightarrow \tag{33}$$
$$\partial_a y' = y + a\partial_a y \tag{34}$$

Turn (33) and (34) into RRVEs. To emphasize that they are coupled, that they should recurse together we write them in a matrix equation:

$$\begin{bmatrix} Y(t) \\ \partial_a Y(t) \end{bmatrix} = X(t) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} + t \begin{bmatrix} a & 0 \\ 1 & a \end{bmatrix} X(Ut). \tag{35}$$

Notice how this gets rid of the additive branching recursion of equation (34).

Python Code 2.5.3 (implementation of (35))

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

Related Work 2.5.4 (coupled recursion)
Example (2.5.2) is inspired by [VSJ21]. Coupling feels close to percolation [Dum19].

Technique 2.5.5 (recursion in recursion)
Recursion in recursion is what is sounds like. It is like proving an induction step of an induction proof with induction.

Related Work 2.5.6 (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 support recursion but this comes with restrictions like maximum recursion depth and performance issues. When possible tail recursion is a way to implement recursion that solves those issues.

Technique 2.5.7 (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 straightforwardly 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. To retain some of these intermediate values while still partly optimizing for performance, it is possible to combine tail recursion with normal recursion.

Python Code 2.5.8 (tail recursion on (35))
We implement (35) but this time with tail recursion. We collect addition operations in a vector *sol* and multiplication in a matrix W.

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

Related Work 2.5.9 (branching tail recursion)
This blog discusses branching tail recursion: https://jeroenvanwijgerden.me/post/recursion-1/.

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. Before defining green functions we do some examples.

Example 3.1.1 ($y' = y$ average condition)
Let's solve

$$y' = y. \tag{36}$$

but this time with the following condition:

$$\int_0^1 y(s)ds = e - 1. \tag{37}$$

This still has solution $y(t) = e^t$. We define the corresponding source green function $G(t, x)$ for y' and this type of condition as follows:

$$G' = \delta(x - t), \int_0^1 G(s, x)ds = 0. \tag{38}$$

Solving this obtains:

$$G(t, x) = H(t - x) + x - 1. \tag{39}$$

Note that we could have used a different green function corresponding to a different linear differential operator.

It shouldn't be clear from this point but with this green function we form following integral equation for (36):

$$y(t) = e - 1 + \int_0^1 G(t, s)y(s)ds. \tag{40}$$

Turning equation (40) into a RRVE with recursive MC gives:

$$Y(t) = e - 1 + 2B\left(\frac{1}{2}\right)Y(S)(H(t - S) + S - 1). \tag{41}$$

With $S \sim U$. We will be skipping over the python implementation of equation (41) because it adds nothing new. Instead we plot realizations of equation (41) in Figure 4.

Example 3.1.2 ($y'' = y$ mixed boundary conditions)
Lets solve the following boundary problem:

$$y'' = y, y(0) = 1, y'(1) = e. \tag{42}$$

This has solution $y(t) = e^t$. We define the source green function $G(t, x)$ for y'' and Dirichlet/Neumann boundary conditions in the following way:

$$G'' = \delta(t - x), G(0) = 0, G'(1) = 0. \tag{43}$$

Solving this obtains:

$$G(t, x) = \begin{cases} -t & \text{if } t < x \\ -x & \text{if } t \geq x \end{cases}. \tag{44}$$

The boundary green function $P(t, x)$ (for $x \in \{0, 1\}$) for y'' and Dirichlet/Neumann boundary conditions is defined the following way:

$$P'' = 0, (P(0, x), P'(1, x)) = \begin{cases} (1, 0) & \text{if } x = 0 \\ (0, 1) & \text{if } x = 1 \end{cases}. \tag{45}$$

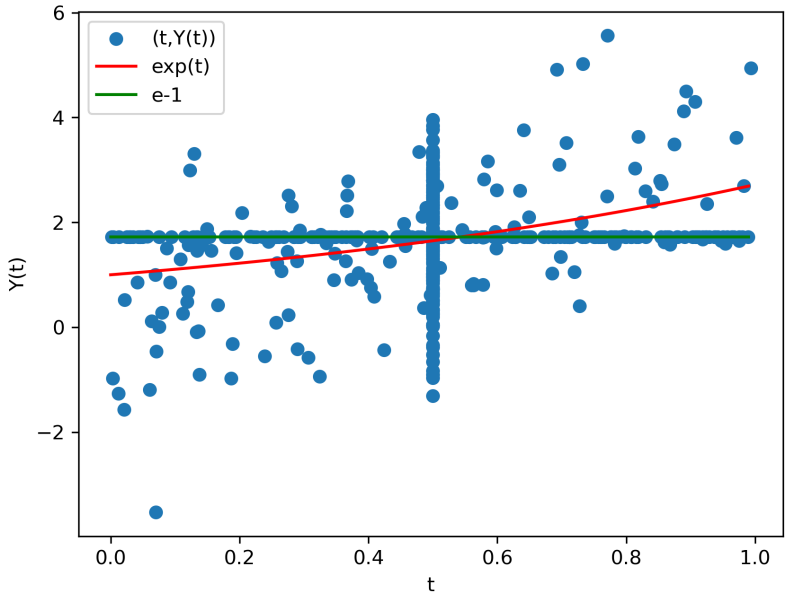

Figure 4: Recursive calls of (41) when calling $Y(0.5)$ 300 times. Points accumulate on the green line due to the Russian roulette, and at $t = 0.5$ because it is the starting value of the simulation.

Which is just a basis for the homogenous solutions for now. Solving this gives:

$$P(t,x) = \begin{cases} 1 & \text{if } x = 0 \\ t & \text{if } x = 1 \end{cases}. \tag{46}$$

Again it shouldn't be clear from this point but with these set of green functions we form following integral equation for (42):

$$y(t) = P(t,0)y(0) + P(t,1)y(1) + \int_0^1 G(t,s)y(s)ds. \tag{47}$$

Equation (47) looks like:

$$Y(t) = 1 + te + lB\left(\frac{1}{l}\right) G(t,S)Y(S). \tag{48}$$

With $S \sim U$ and $l > 1 \in \mathbb{R}$. We visualize equation (48) on Figure 5.

Related Work 3.1.3 ($y'' = y$ mixed boundary conditions)
[Saw+23] discusses an algorithm for mixed boundary conditions.

Definition 3.1.4 (green function)
Vaguely speaking we define the green function as a type of kernel function that we use to solve linear problems with linear conditions. The Green's function is the kernel that we need to put in front of the linear conditions or the source term that we integrate over and to obtain the solution and the green function has the property that it satisfies either null linear conditions and a Dirac delta source term, or vice versa.

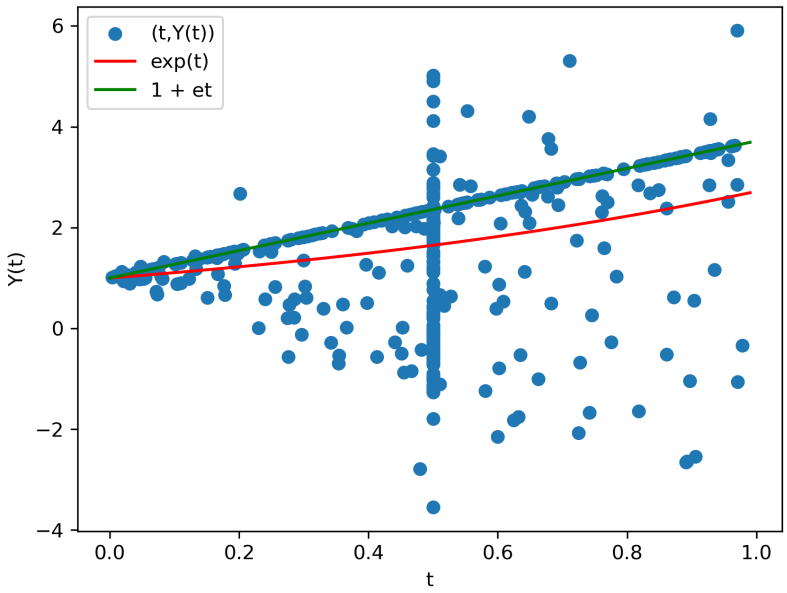

Figure 5: Recursive calls of (48), $l = 2$ when calling $Y(0.5)$ 300 times.

Related Work 3.1.5 (green function)
Our notion of green function is similar to that in [HGM01].

3.2 Fredholm Integral Equations

The integral equations acquired in the last subsection are Fredholm integral equations of the second kind. In this subsection we introduce coupled splitting a technique for RMC for this kind of equations.

Definition 3.2.1 (Fredholm equation of the second kind)
A Fredholm equation of the second kind for φ is of the following form:

$$\varphi(t) = f(t) + \lambda \int_a^b K(t,s)\varphi(s)ds. \tag{49}$$

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

If both K and f are nice, then for sufficiently small λ, it is straightforward to establish the existence and uniqueness of solutions for Fredholm equations of the second kind using a fix point argument.

Example 3.2.2 (Dirichlet $y'' = y$)
The following problem will be the main testing example for boundary value problems:

$$y'' = y, y(b_0), y(b_1). \tag{50}$$

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

$$P(t,x) = \begin{cases} \frac{b_1 - t}{b_1 - b_0} & \text{if } x = b_0 \\ \frac{t - b_0}{b_1 - b_0} & \text{if } x = b_1 \end{cases} \tag{51}$$

$$G(t,s) = \begin{cases} -\frac{(b_1 - t)(s - b_0)}{b_1 - b_0} & \text{if } s < t \\ -\frac{(b_1 - s)(t - b_0)}{b_1 - b_0} & \text{if } t < s \end{cases}. \tag{52}$$

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

$$y(t) = P(t,b_0)y(b_0) + P(t,b_1)y(b_1) + \int_{b_0}^{b_1} G(t,s)y(s)ds \tag{53}$$

$$Y(t) = P(t,b_0)y(b_0) + P(t,b_1)y(b_1) + lB\left(\frac{1}{l}\right)(b_1 - b_0)G(t,S)y(S). \tag{54}$$

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

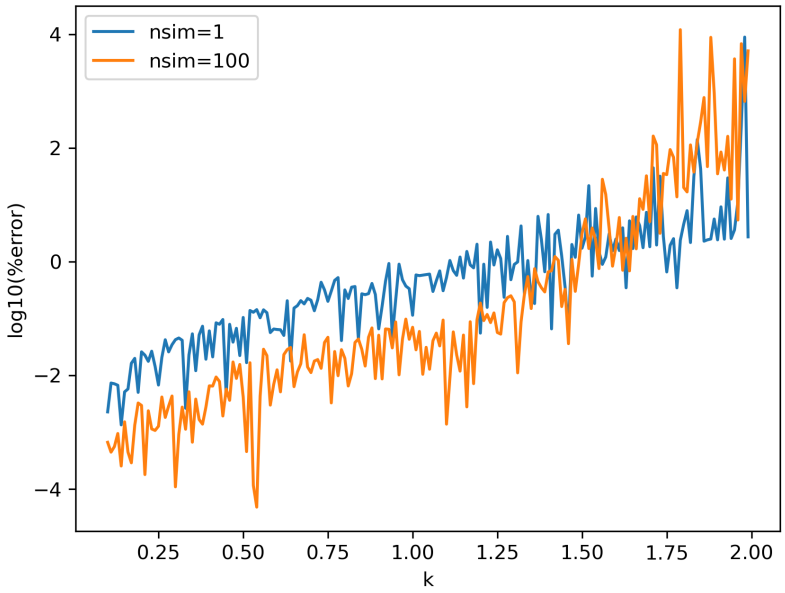

Figure 6: The logarithmic percentage error of $Y(0)$ for (54), with $l = 1.2$ and initial conditions $y(-k) = e^{-k}$ and $y(k) = e^{k}$, displays an exponential increase until approximately $k = 1.5$, beyond which additional simulations fail to reduce the error, indicating that the variance doesn't exist.

Example 3.2.3 (coupled splitting on (3.2.2))

Next to normal splitting (2.2.6) we can also split the domain in equation (53):

$$y(t) = P(t,b_0)y(b_0) + P(t,b_1)y(b_1) + \frac{1}{2}\int_{b_0}^{b_1} G(t,s)y(s)ds + \frac{1}{2}\int_{b_0}^{b_1} G(t,s)y(s)ds \tag{55}$$

$$y(t) = P(t,b_0)y(b_0) + P(t,b_1)y(b_1) + \int_{b_0}^{\frac{b_1+b_0}{2}} G(t,s)y(s)ds + \int_{\frac{b_1+b_0}{2}}^{b_1} G(t,s)y(s)ds \tag{56}$$

Coupling can get rid of the additive branching recursion in the RRVEs corresponding to (55) and (56). Resulting in following RRVE:

$$X(t_1,t_2) = \begin{bmatrix} P(t_1,b_0) & P(t_1,b_1) \\ P(t_2,b_0) & P(t_2,b_1) \end{bmatrix} \begin{bmatrix} y(b_0) \\ y(b_1) \end{bmatrix} + W \begin{bmatrix} G(t_1,S_1) & G(t_1,S_2) \\ G(t_2,S_1) & G(t_2,S_2) \end{bmatrix} X(S_1,S_2). \tag{57}$$

With W the right weighting matrix (see code (3.2.4) for an example) and S_1, S_2 can be chosen in various ways.

Python Code 3.2.4 (implementation of (57))
We implemented equation (57) in example (3.2.3) with recursion but in this case it is actually possible to implement it forwardly because the time proces is nice.

```
from random import random as U
from math import exp
import numpy as np
def Pb0(t, b0, b1): return (b1-t)/(b1-b0)
def Pb1(t, b0, b1): return (t-b0)/(b1-b0)
def G(t, s, b0, b1): return - (b1-s)*(t-b0)/(b1-b0) if t < s
    else - (b1-t)*(s-b0)/(b1-b0)
def X(T, y0, y1, b0, b1):
    yy = np.array([y0, y1])
    bb = np.diag([(b1-b0)/len(T)]*len(T))
    PP = np.array([[Pb0(t, b0, b1), Pb1(t, b0, b1)] for t in T])
    sol = PP @ yy
    l = 1.2  # russian roulette rate
    if U()*l < 1:
        u = U()
        SS = [b0+(u+j)*(b1-b0)/len(T) for j in range(len(T))]
        GG = np.array([[G(t,S,b0,b1) for S in SS] for t in T])
        sol += l*GG @ bb @ X(SS, y0, y1, b0, b1)
    return sol
```

Figure 7 resembles a fixed point iterations, leading us to hypothesize that coupled splitting can achieve convergence in most cases where a fixed point argument holds true and that 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 usually done when approaching the bottleneck. Alternatively when reaching the bottleneck it is possible to rely on MC convergence.

Coupled splitting was tested on the example shown in Figure 6, but it did not contribute to the convergence of the method. This suggests that a fix point argument

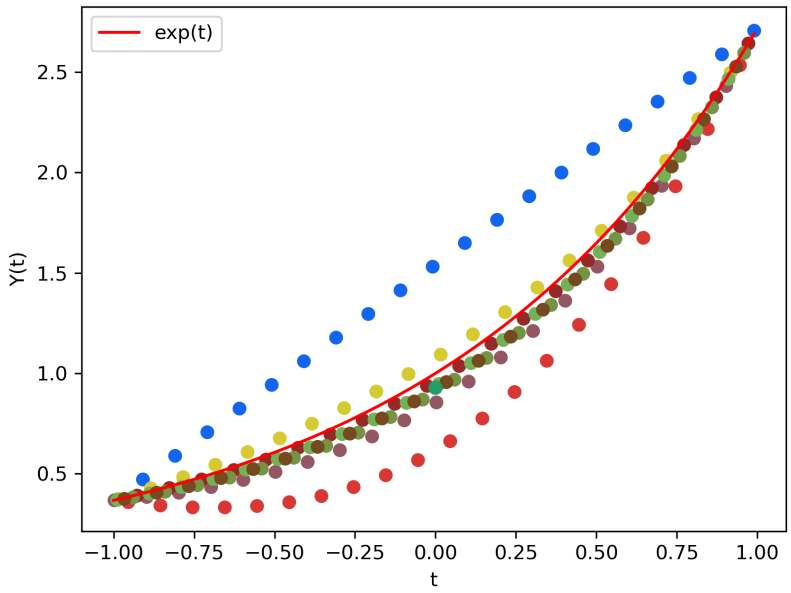

Figure 7: Recursive calls of equation (57) when calling $X(0)$ once, with a split size of 20, S_j coupled such they're equally spaced (they don't have to be independent) and coupling is colored. The initial conditions for this call are $y(-1) = e^{-1}$ and $y(1) = e^1$, with Russian roulette rate $l = 1.2$.

would not be effective for this particular example with this Russian roulette setup.

Example (3.2.3) isn't the best example to demonstrate coupled splitting. We don't exploit locality and smoothness of the problem. We conjecture that this algorithm is useful for linear Fredholm equations of the second kind in cases where MC integration win over classic integration: high dimensional, non-smooth kernels or nasty domains.

Related Work 3.2.5 (coupled splitting)
Coupled splitting is partly inspired by how [SM09] reduces variance by using a bigger submatrices . Use cases for MC for differential equations under weak smoothness conditions get discussed in [JN09].

See [GH21] for a discussion on convergence of recursive stochastic algorithms. We highly recommend watching the following video [Abh20] before reading previous paper.

3.3 Initial Value Problems

Right now we don't have a RMC algorithm for IVPs that can guarantee a reasonable variance or even existence when increasing the time domain. Classing IVP solvers rely on shrinking the time steps for convergence. Recursion in Recursion MC (RRMC) for IVPs tries to emulate this behavior.

Example 3.3.1 (RRMC $y' = y$)

Let's us explain RRMC for IVPs with our main example. Imagine we have a time stepping sheme (t_n) $(t_n > t_{n-1})$ then following integral equations hold:

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

Turn these in following class of RRVEs:

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

A problem with these RRVEs is that we don't know $y(t_n)$. Instead we can replace it with an unbiased estimate y_n which we keep frozen:

$$Y_n(t) = y_n + (t - t_n)Y_n((t - t_n)U + t_n), t > t_n \tag{60}$$

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

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))

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

We measured the convergence speed to be $O\left(\frac{h^{1.5}}{\sqrt{\text{nsim}}}\right)$.

1.5 order of convergence is cool but this begs the question on how to achieve higher order of convergence in h. Again it is easy to imitate classical methods to achieve higher order convergence. We do this by removing lower order terms (which requires smoothness) with control variates like the MC trapezoidal rule (2.3.2).

Example 3.3.3 (CV RRMC $y' = y$)
Let us control variate example (3.3.1). Start with:

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

We need a lower order approximation of the integrand:

$$y(s) = y(t_n) + (s - t_n)y'(t_n) + O((s - t_n)^2) \tag{63}$$

$$\approx y(t_n) + (s - t_n)f(y(t_n), t_n) \tag{64}$$

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

$$\approx y(t_n)(1 + s - t_n). \tag{66}$$

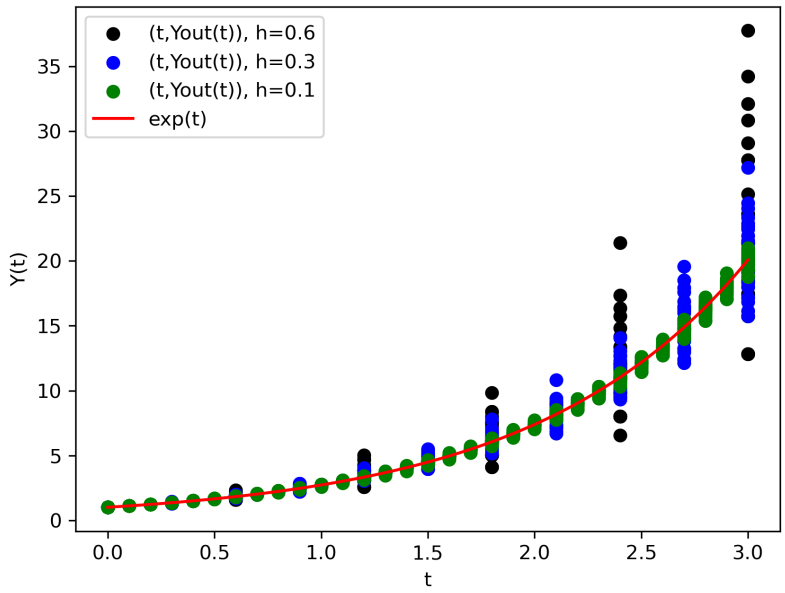

Figure 8: Recursive calls of equation (61) when calling $Y_{\text{out}}(3, h)$ 30 times for different h.

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

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

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

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

We won't discuss turning this into an RRVE nor the implementation. The implementation is very similar to (3.3.6) and Figure 9 is a convergence plot for this example.

Related Work 3.3.4 (CV RRMC)

[Dau11] also 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 info from the outer recursions, this doesn't mean that reducing root mean square error by splitting doesn't work, you just have to be careful with the bias. We conjecture that the bias in RRMC converges faster then the variance.

Example 3.3.5 (nonlinear RRMC IVP)

Consider:

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

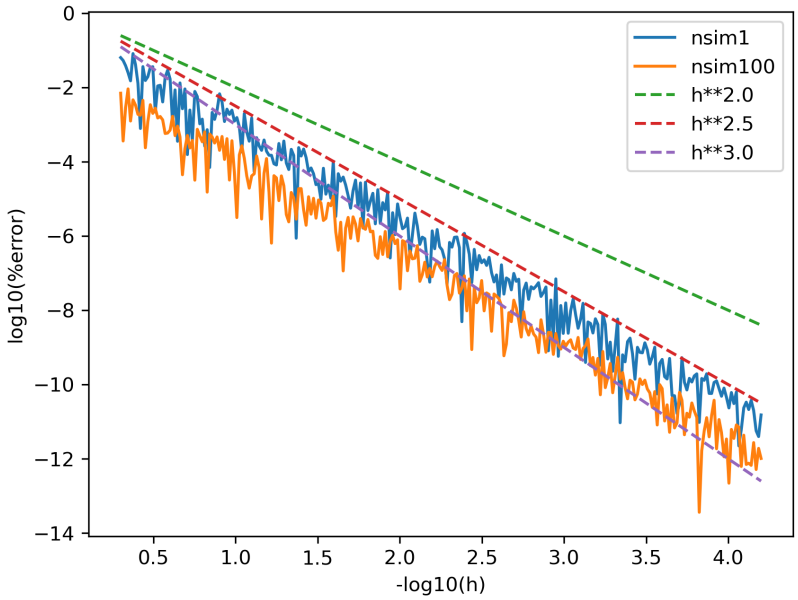

Figure 9: Log-log plot of example (3.3.3).

with solution: $y(t) = t^2$. With integral equation:

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

control variating $y^2(s)$ up to second order (via Taylor):

$$\begin{aligned} y^2(t) &\approx y^2(t_n) + 2(t-t_n)y(t_n)y'(t_n) + ((t-t_n)y'(t_n))^2 + O((t-t_n)^2) && (72)\\ &\approx y^2(t_n) + 2(t-t_n)y(t_n)y'(t_n) + O((t-t_n)^2) && (73) \end{aligned}$$

Then we have to integrate the control variate:

$$\begin{aligned} &\int_{t_n}^{t} y^2(t_n) + 2(s-t_n)y(t_n)y'(t_n)ds && (74)\\ &\quad = (t-t_n)y^2(t_n) + 2\left(\frac{t^2 - t_n^2}{2} - t_n(t-t_n)\right)y(t_n)y'(t_n). && (75) \end{aligned}$$

Python Code 3.3.6 (implementation of (3.3.5))

```
from random import random as U
def Y_in(t, tn, yn, dyn, h, l):
    sol = yn  # initial conditon
    sol += t**2-tn**2 - (t**5-tn**5)/5  # source
    sol += (t-tn)*yn**2  # 0 order
    sol += 2*((t**2-tn**2)/2 - tn*(t-tn))*yn*dyn  # 1 order
    if U()*l < (t-tn)/h:
        S = tn + U()*(t-tn)  # \sim Uniform(T,t)
        sol += l*h*(Y_in(S, tn, yn, dyn, h, l)*
```

```
            Y_in(S, tn, yn, dyn, h, l) - yn**2-2*(S-tn)*yn*dyn)
    return sol
def Y_out(t, h, l):
    yn, tn = 0, 0
    while tn < t:
        tt = tn+h if tn+h < t else t
        dyn = yn**2 - tn**4+2*tn
        yn = Y_in(tt, tn, yn, dyn, tt-tn, l)
        tn = tt
    return yn
```

Similarly to classic methods, RRMC struggles with big negative coefficients in front of the recursive parts. DRRMC is a potential solution to this problem but we don't think it is effective.

Definition 3.3.7 (DRRMC)
Consider a general linear ODE IVP problem:

$$x' = Ax + g, x(0) = x_0. \tag{76}$$

Sometimes repeatedly multiplying by A is unstable. Diagonal RRMC adds a positive diagonal matrix D to A and hopes that it stabilizes.

$$x' + Dx = (A + D)x + g. \tag{77}$$

Following integral equation can be derived by using integrating factor:

$$x(t) = e^{D(t_n - t)}x(t_n) + \int_{t_n}^{t} e^{D(s-t)}(A + D)x(s)ds + \int_{t_n}^{t} e^{D(s-t)}g(s)ds. \tag{78}$$

Remember that the exponential of a diagonal matrix is the exponential of its elements. The recursive integral has the following trivial control variate:

$$\int_{t_n}^{t} e^{D(s-t)}(A + D)x(t_n)ds = D^{-1}(I - e^{D(t_n - t)})(A + D)x(t_n). \tag{79}$$

Note that D may be chosen differently every recursion.

Related Work 3.3.8 (DRRMC)
DRRMC is inspired by $\bar{\sigma}$ parameter in [Saw+22] but instead of importance sampling and weight window we use control variates to deal with nonlinearity introduced by the exponential because it needs to work over an entire vector at the same time. Similar manipulations can also be found in exponential integrator methods.

4 Brownian Motion

Current RMC algorithms for PDEs are linked to Brownian motion. In this section build up to recursive first passage sampling which is similar to walk on sphere.

Definition 4.0.1 (Brownian Motion)
Define Brownian motion W_t as the limit/logical generalization when $n \to \infty$ of

following discrete proces defined as:

$$\begin{cases} X_t^n = X_{t-\frac{1}{n}}^n + Z_n \\ X_0^n = 0 \end{cases} . \tag{80}$$

With $Z_n \sim N(0, \frac{1}{n})$ i.i.d . From this definition it is easily seen that $W_t \sim N(0, t)$.

Lemma 4.0.2 (self-affinity Brownian motion)
Brownian motion is self affine as a random proces that means you can cut a small part of it move so it starts in 0 and scale time to the original size and space such that the variance stays the same to get back the whole Brownian motion.

$$\forall c \in \mathbb{R}_0^+ : \frac{W_{ct}}{\sqrt{c}} \sim W_t. \tag{81}$$

Theorem 4.0.3 (Feyman-Kac formula (wikipedia))
Consider the partial differential equation

$$\frac{\partial u}{\partial t}(x,t) + \mu(x,t)\frac{\partial u}{\partial x}(x,t) + \frac{1}{2}\sigma^2(x,t)\frac{\partial^2 u}{\partial x^2}(x,t) - V(x,t)u(x,t) + f(x,t) = 0, . \tag{82}$$

defined for all $x \in \mathbb{R}$ and $t \in [0,T]$, subject to the terminal condition

$$u(x,T) = \psi(x), . \tag{83}$$

where μ, σ, ψ, V, f are known functions, T is a parameter, and $u : \mathbb{R} \times [0,T] \to \mathbb{R}$ is the unknown. Then the Feynman-Kac formula tells us that the solution can be written as a conditional expectation

$$u(x,t) = E^Q \left[\int_t^T e^{-\int_t^r V(X_\tau,\tau)d\tau} f\left(X_r, r\right) dr + e^{-\int_t^T V(X_\tau,\tau)d\tau} \psi\left(X_T\right) \mid X_t = x \right]. \tag{84}$$

under the probability measure Q such that X is an Itô process driven by the equation

$$dX_t = \mu(X,t)dt + \sigma(X,t)dW_t^Q. \tag{85}$$

with $W^Q(t)$ is a Wiener process (also called Brownian motion) under Q, and the initial condition for $X(t)$ is $X(t) = x$.

4.1 First Passage Sampling

Definition 4.1.1 (first passage sampling)
In the first passage sampling we try to sample states when a proces reaches a boundary or specified state of the system for the first time (the first passage). We are specifically interested in first passage problem with Brownian motion for a closed time space barrier.

The first passage distribution of Brownian motion is in fact the boundary green function for the heat equation this can be easily seen by using the Feynman-Kac formula (4.0.3).

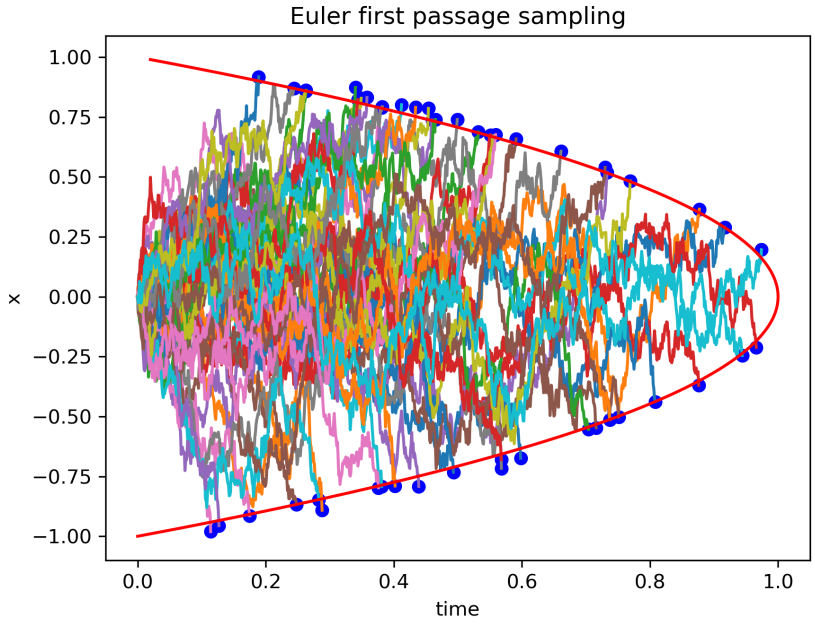

Figure 10: 50 realizations of Euler first passage sampling with step size 0.001.

Example 4.1.2 (Euler first passage sampling)
In this example we naively sample first passage exit point of Brownian motion for a parabolic barrier by simulating Brownian motion with the Euler scheme.

Technique 4.1.3 (recursive first passage sampling)
The idea behind recursive first passage sampling is to break down a first passage sampling on a bigger domain to contained smaller domains by using the fact you can't leave the big domain without leaving the smaller first (intermediate value theorem). When you sample the exit from the smaller domain it is the start point of a new first passage sampling problem and then you recurse until you are close to the stopping condition.

Related Work 4.1.4 (recursive first passage sampling)
Recursive first passage sampling get discussed in [HT16] and extension for processes with jumps in [HM21].

Example 4.1.5 (recursive first passage sampling)
In this example we recursively first passage sample the exit point of Brownian motion for a triangular barrier by resampling and scaling (using (4.0.2)) from a precomputed Euler scheme to sample a exit point from a parabolic barrier.

Instead of resampling from a Euler scheme it is also possible to tabloid the inverse cumulative probability function for the triangular case. Something similar gets done in [HGM01].

You can transform first passage sampling problems for others processes back to Brownian Motion by doing the right time and space bending. For example geometric Brownian motion can be made into Brownian motion by taking the log.

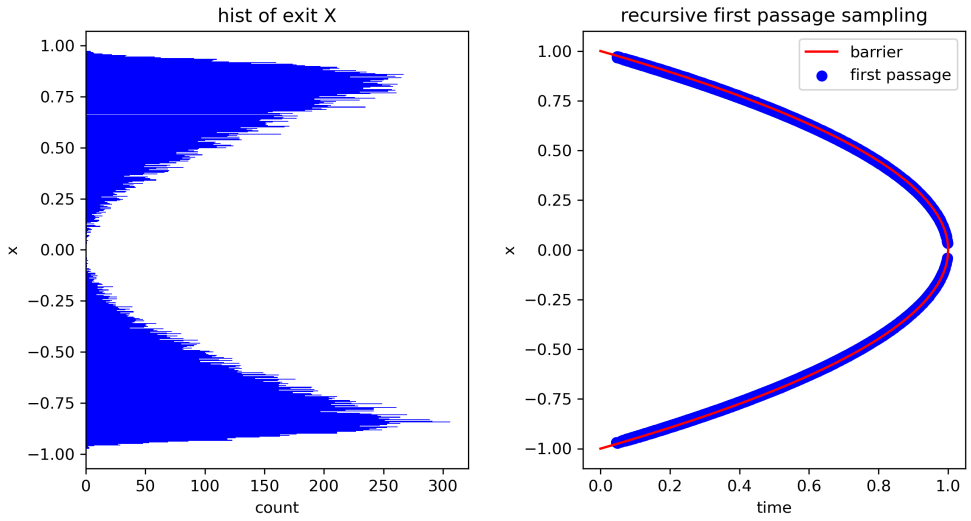

Figure 11: 50000 of realizations of recursive first passage sampling. The precomputed sample of 1000 first passages of a triangular barrier uses the Euler scheme with step size 0.001.

4.2 Extending First Passage Sampling

Sometimes we're interested in a specific property of a first passage sampled path like the max or the average. The naif way would be sampling full paths and calculating the desired property instead you can sample only the required information to calculate the desired property. In the case of the max and the average for example you only need the sample the max/average of the subpaths and combined that to the max/average of the whole path.

Example 4.2.1 (recursive first passage average sampling)
This is the same as example (4.1.5) but now we have to keep track of the average.

Doing the same thing for geometric Brownian motion is difficult because the average behaves bad under transformation unlike the max. You can think of the average as an extra dimension to keep track of. What you would need for geometric Brownian motion is the first passage distribution of the average and exit point for every different position of the begin point for subpaths.
And nothing holds you back of changing methods midway if you didn't the precompute a situation.

Technique 4.2.2 (path stitching)
Instead of thinking in sampling first passage points you can also sample whole paths to the first passage. The same way as before you need to be able to generate paths for a simple first passage problem and "stich" these paths together into one for a complicated one.

Example 4.2.3 (path stitching parabola)

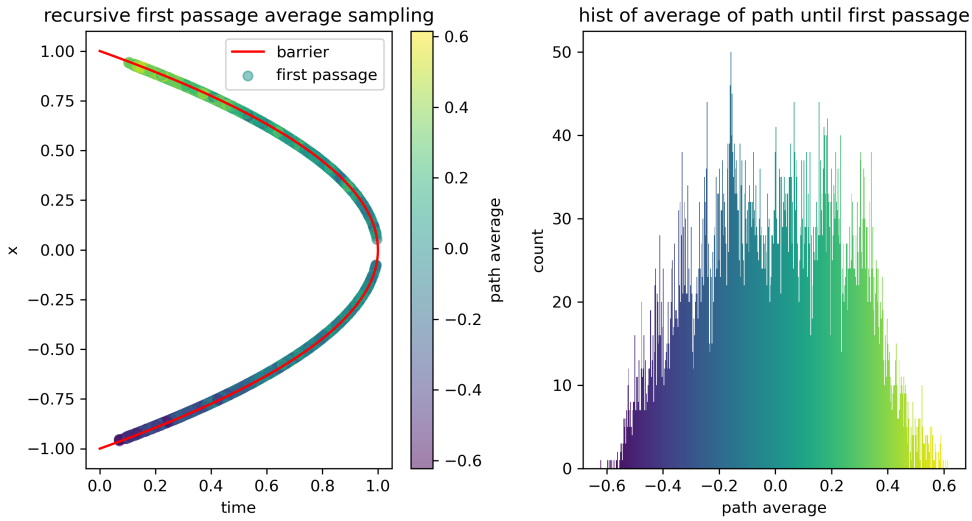

Figure 12: 10000 of realizations of recursive first passage sampling (for the average). The precomputed sample of 1000 first passages and averages of a triangular barrier uses the Euler scheme with step size 0.001.

This is the same as example (4.1.5) but now we have to keep track of the whole resampled Euler scheme generated paths.

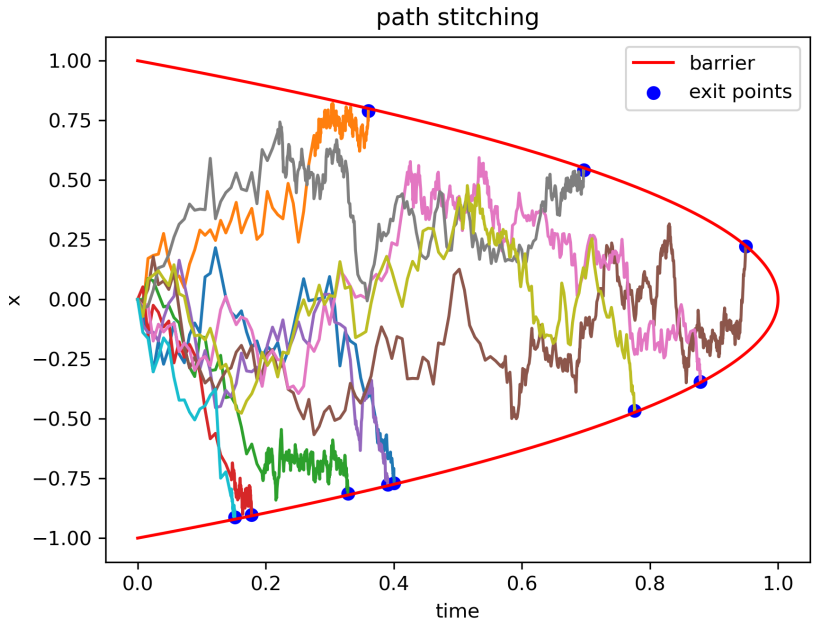

Figure 13: 10 paths build with path stitching build out of precomputed Euler scheme generated paths with step size 0.01.

For plotting the path we needed to accesses to all of its points. An advantage over normally generating paths is that a path can be represented by its subpaths and their scalings requiring way less memory then a full path. This can be useful in case

where the whole path isn't needed. Even if accesses to the whole path is needed this can be done in a slightly more efficient manor then a normal Euler scheme because it can almost be done in parallel vs step for step generation. The only downsides are that the time steps are inhomogeneous and it requires a precomputation.

A way around scaling base samples is limiting scaling to a discrete set and pick the biggest scaling that fits, instead of generating base samples for 1 scale and scaling it dynamically precompute all the discrete scalings.

Similar precomputing tricks can be used for geometric Brownian motion requiring and extra dimension of precomputing based on transformations.

Related Work 4.2.4 (path stitching)
Path stitching appears frequently in rendering and also in [Das+15] and [JL12].

5 Limitations and Future Work

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