mimclib

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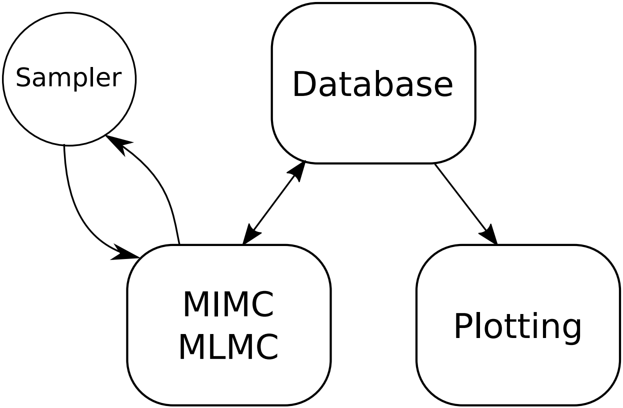
Outline

Vision (the ambitious version)

- Provide an **easy to use**, **customizable** and **extendable** open source library for UQ problems, both forward and inverse.
- Multilevel and Multi-index versions of Monte Carlo, Quasi Monte Carlo, Stochastic collocation, Least square projection among others.
- Support parallel computation whenever possible.
- Provide easy to use storage facility.
- Provide easy to customize plotting facility (for common plots).
- Provide easy to run test cases.
- Use `Python` for easier implementation of most parts of code and use object code (`C++` or `FORTRAN`) for computationally expensive parts.

What has been done, `mimclib 0.2.0.dev0`

- Multilevel and Multi-index versions of Monte Carlo.
- Provide easy to use storage facility in MySQL.
- Provide easy to customize plotting facility (for common plots).
- Provide easy to run test cases.
- Documentation is still in progress (these slides are part of it).
- Interface is written with the other features in mind.


Sampler
Database
MIMC
MLMC
Plotting

Why?

- Python
  - Open source. No need for licensing
  - An easy to use programming language. Familiar to MATLAB users (Especially with numpy and matplotlib)
  - Can call object code for computationally expensive parts, e.g., samplers.
- MySQL
  - Relatively easy data modifications and querying.
  - Allows asynchronous access which is ideal for parallel computation.
  - Allows remote access.
  - Optimal storage and data querying.

The central question

Given an $\mathbb{R}^n$-valued random variable, $\mathbf{X}$ with PDF $f(\mathbf{x}) : \mathbb{R}^n \to [0, \infty)$ and a function, $g : \mathbb{R}^n \to \mathbb{R}$, assume that we are interested in computing the quantity

$$\mathrm{E}[g(\mathbf{X})] = \int_{\mathbb{R}^n} g(\mathbf{x}) f(\mathbf{x}) \mathrm{d}\mathbf{x}.$$

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Possible difficulties:

- PDF, f, is inaccessible, only (approximate) samples of $\mathbf{X}$ can be generated.
    - E.g., $\mathbf{X}$ is the solution of an SDE.
- Dimension, n, is large or even infinite, hence the integral is expensive to approximate.
    - E.g., expansion of a random field.

Setup

Our objective is to build an estimator $\mathcal{A} \approx \mathrm{E}[g(\mathbf{X})]$ with minimal work where

$$P(|\mathcal{A} - \mathrm{E}[g(\mathbf{X})]| \leq \mathrm{TOL}) \geq \epsilon$$

for a given accuracy TOL and a given confidence level determined by $0 < \epsilon < 1$.

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Instead, we impose the following, more restrictive, two constraints:

$$\textbf{Bias constraint:} \qquad |\mathrm{E}[\mathcal{A} - g(\mathbf{X})]| \leq (1-\theta)\mathrm{TOL},$$

$$\textbf{Statistical constraint:} \qquad P\left(|\mathcal{A} - \mathrm{E}[\mathcal{A}]| \leq \theta \mathrm{TOL}\right) \geq \epsilon.$$

For some tolerance splitting, $\theta \in (0,1)$.

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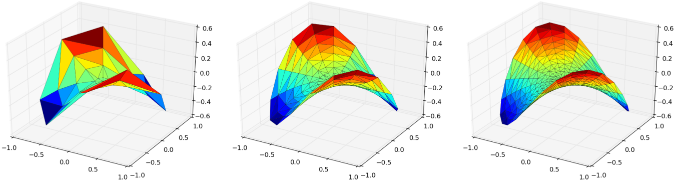
For some tolerance splitting, $\theta \in (0,1)$. Assuming (at least asymptotic) normality of the estimator, $\mathcal{A}$. Here, Φ^{-1} is the inverse of the standard normal CDF.

Numerical approximation

Notation: g_ℓ for $\ell \in \mathbb{N}$ is the approximation of g calculated based on discretization parameters $\mathbf{h}_\ell = (h_{\ell,i})_{i=1}^{d}$.



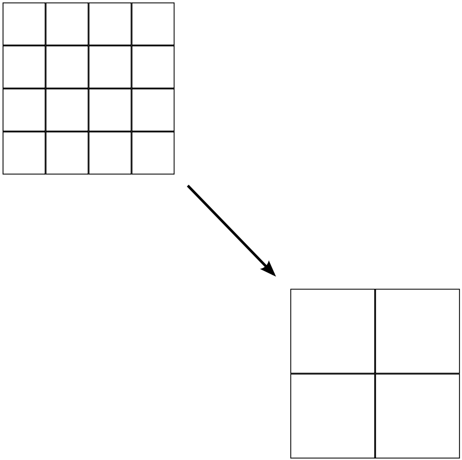
Monte Carlo

The simplest (and most popular) estimator is the Monte Carlo estimator

$$\mathcal{A}_{\mathrm{MC}}[g_L; M] = \frac{1}{M} \sum_{m=1}^{M} g_L(\mathbf{X}^{(m)}),$$

for a given level, L, and number of samples, M, that we can choose to satisfy the error constraints and minimize the work.

MLMC main idea: Variance reduction



Multilevel Monte Carlo (MLMC) (Heinrich, 1998) and (Giles, 2008)

Observe the telescopic identity

$$\mathrm{E}[g] \approx \mathrm{E}[g_L] = \mathrm{E}[g_0] + \sum_{\ell=1}^{L} \mathrm{E}[g_\ell - g_{\ell-1}]$$

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where

$$\Delta_\ell g = \begin{cases} g_0 & \text{if } \ell = 0, \\ g_\ell - g_{\ell-1} & \text{if } \ell > 0. \end{cases}$$

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Then, using Monte Carlo to approximate each difference independently, the MLMC estimator can be written as

$$\mathcal{A}_{\mathrm{MLMC}}[g; L] = \sum_{\ell=0}^{L} \mathcal{A}_{\mathrm{MC}}[\Delta g_\ell; M_\ell].$$

Main idea: variance reduction using cheaper approximations.

Optimal number of samples

Given the following estimates

$$V_\ell = \begin{cases} \mathrm{Var}[g_0] & \ell = 0, \\ \mathrm{Var}[g_\ell - g_{\ell-1}] & \ell \geq 1, \end{cases}$$

$$W_\ell = \begin{cases} \text{Work of a single sample of } g_0 & \ell = 0, \\ \text{Work of a single sample of } (g_\ell - g_{\ell-1}) & \ell \geq 1. \end{cases}$$

Then, using simple Lagrangian optimization of the total work subject to the variance constraint then, we can obtain the optimal number of samples

$$M_\ell \approx \left(\frac{\theta \mathrm{TOL}}{\Phi^{-1}\left(\frac{\epsilon+1}{2}\right)} \right)^{-2} \sqrt{\frac{V_\ell}{W_\ell}} \left(\sum_{i=0}^{L} \sqrt{V_i W_i} \right), \quad \text{for } 0 \leq \ell \leq L.$$

Assumptions

Assumption MC1 (Bias): $|\mathrm{E}[g - g_\ell]| \lesssim \exp(-w\ell)$,
Assumption MC2 (Work): $\mathrm{Work}[g_\ell] \lesssim \exp(d\gamma\ell)$,
Assumption MLMC3 (Variance): $\mathrm{Var}[g_\ell - g_{\ell-1}] \lesssim \exp(-s\ell)$

for all $\ell \in \mathbb{N}$ and positive constants γ, w, s.

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The optimal work of MLMC is

$$\begin{cases} \mathcal{O}\left(\mathrm{TOL}^{-2}\right) & s > d\gamma \\ \mathcal{O}\left(\mathrm{TOL}^{-2}\right)\left(\log\left(\mathrm{TOL}^{-1}\right)\right)^2 & s = d\gamma \\ \mathcal{O}\left(\mathrm{TOL}^{-2-\frac{d\gamma-s}{w}}\right) & s < d\gamma \end{cases}$$

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Recall: Optimal cost of Monte Carlo is $\mathcal{O}\left(\mathrm{TOL}^{-2-\frac{d\gamma}{w}}\right)$

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Notice: the cost exponentially increases with increasing d.

Continuation MLMC

- To compute M_ℓ we need to find L and find estimates of V_ℓ.

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- To compute M_ℓ we need to find L and find estimates of V_ℓ.
- Instead of running for the small required TOL, CMLMC runs a sequence of MLMC realizations, for decreasing tolerances, ending with the required TOL.
- In each step, estimates of V_ℓ are generated using a Bayesian setting which uses **Assumption MLMC3** coupled with the generated samples to produce good estimates even with a small number of samples.
- The value of L is also chosen in each step to minimize the work. This allows choosing a better splitting parameter, θ.
- CMLMC does not have to reuse samples between iterations, ensuring an unbiased estimator for level L approximation.

mimclib showcase

- Code required for basic MLMC run.
- Show single run of `mimclib`.
- Show plots in pdf.
- Show database in mysql.

Installation

- Prerequisites: `gcc` (supporting `c++11`), `python2.7`, `pip`, `mysql-server`, `mysql-client`.
- First step:

```
> git clone \
      https://github.com/StochasticNumerics/mimclib.git
> cd mimclib
> make pip
```

- Note: to update to latest version

```
> git pull
```

- Done! Sort of.

Setting up the database

- Make sure `mysql-server`, `mysql-client`, and `libmysqlclient-dev` are installed on your data server.
- Create `mimclib` database on data server

```
> python -c 'from mimclib.db import MIMCDatabase ; \
         print MIMCDatabase().DBCreationScript();' \
         | mysql -u root -p
```

- Create database user for `mimclib` (hint: you can use local username)

```
      > mysql -u root -p
mysql> CREATE USER 'USER'@'%' \
                IDENTIFIED BY 'password';
mysql> GRANT ALL PRIVILEGES ON mimc.* TO \
               'USER'@'%' WITH GRANT OPTION;
```

Other useful MySQL commands

- Change password

```
      > mysql -u USER -p
mysql> SET PASSWORD FOR 'USER'@'%' \
       = PASSWORD('newpassword');
```

MIMC Database

tbl_runs

run_id	int	[PK]
creation_date	DATETIME	
TOL	REAL	
done_flag	int	
dim	int	
tag	VARCHAR(128)	
params	mediumblob	
comment	TEXT	

tbl_data

data_id	int	[PK]
run_id	int	[U, FK]
TOL	REAL	
bias	REAL	
stat_error	REAL	
creation_date	DATETIME	
totalTime	REAL	
Qparams	mediumblob	
userdata	mediumblob	
iteration_idx	int	[U]

tbl_lvls

data_id	int	[U, FK]
lvl	text	
lvl_hash	varchar(35)	[U]
El	REAL	
Vl	REAL	
Wl	REAL	
Tl	REAL	
Ml	int	
psums_delta	mediumblob	
psums_fine	mediumblob	

Legend

[FK]	Foreign Key
[PK]	Primary key
[U]	Unique constraint

Created by SQL::Translator 0.11021

Installation for Debian/Ubuntu

- ```
  > git clone \
        https://github.com/StochasticNumerics/mimclib.git
  > cd mimclib
  > ./mimc_install.sh
  ```
- Updates all packages on the system
- Installs all prerequisites
- Clones and installs the library
- Creates a database with the current user and no password.
- Standard GBM Example is ready to run.
  ```

Problem setup: Geometric Brownian Motion

Given $S(0), \mu$ and σ, define

$$\mathrm{d}S(t) = \mu S(t)\mathrm{d}t + \sigma S(t)\mathrm{d}W(t)$$

Euler-Maruyama discretization

$$\begin{aligned} S_{n+1} &= S_n + \mu S_n \Delta t + \sigma S_n \Delta W_n \\ &= S_n \left(1 + \mu \Delta t + \sigma \Delta W_n\right) \end{aligned}$$

We can find (using Itô integral and a log transformation)

$$\begin{aligned} \mathrm{E}[S(t)] &= S(0) e^{\mu t} \\ \mathrm{Var}[S(t)] &= (S(0))^2 e^{2\mu t} \left(e^{\sigma^2 t} - 1\right) \end{aligned}$$

Numerical ex.: PDE with random coeffs., [H-ANTT, 2015]

We solve a 3D elliptic PDE with random coefficient and forcing term

$$
\begin{aligned}
-\nabla \cdot \left(e^{\kappa(\mathbf{x},\mathbf{y})}\, \nabla u(\mathbf{x},\mathbf{y})\right) &= 1 \quad \text{in} \quad \mathcal{D} = [0,1]^3 \\
u(\mathbf{x},\mathbf{y}) &= 0 \quad \text{on} \quad \partial\mathcal{D},
\end{aligned}
$$

where

$$\kappa(\mathbf{x},\mathbf{y}) = \sum_{k=0}^{n} y_k \sqrt{3}\exp(-k)\Psi_k(\mathbf{x}).$$

Here $\{y_k\}_{k=1}^n$ are i.i.d. $\mathcal{U}[-1,1]$. Moreover, Ψ_k is a tensorizable cosine/sine basis. Quantity of interest is:

$$g = \left(2\pi\sigma^2\right)^{-\frac{3}{2}} \int_{\mathcal{D}} \exp\left(-\frac{\|\mathbf{x}-\mathbf{x}_0\|_2^2}{2\sigma^2}\right) u(\mathbf{x}) d\mathbf{x},$$

for $\mathbf{x}_0 \in \mathcal{D}$ and $\sigma > 0$.

Using 2nd order Finite Difference Method with GMRES linear solver, for this problem we have $\gamma \approx 1$, $w = 2$ (isotropic case).

The end

- Slides can be found on GitHub under "docs" `https://github.com/StochasticNumerics/mimclib`.
- You can post questions in the "Issues" page.
- Next time
  - Next, next time: Multi-index Monte Carlo applied on PDEs in 3D.