Multilevel Monte Carlo methods

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An outline personal history

- inspired by undergraduate numerical projects course while studying Maths at Cambridge, and working on summer projects at Rolls-Royce
- went to MIT for MSc and PhD in Aeronautical Engineering, then taught there for 7 years with research funding from Rolls-Royce
- RR helped me to move to Oxford in 1992 and I continued working on CFD until about 10 years ago – HYDRA CFD code is now the main analysis and design code at RR
- as a mid-career change, switched to computational finance and research on Monte Carlo methods for a wide range of applications with uncertainty
- (I also have a long-standing interest in High Performance Computing, including the use of GPUs)

Objectives

In presenting the multilevel Monte Carlo method, I hope to emphasise:

- the simplicity of the idea
- its flexibility – it's not prescriptive, more an approach
- there are lots of people working on a variety of applications

In doing this, I will focus on ideas rather than lots of numerical results, but I will begin with some motivation.

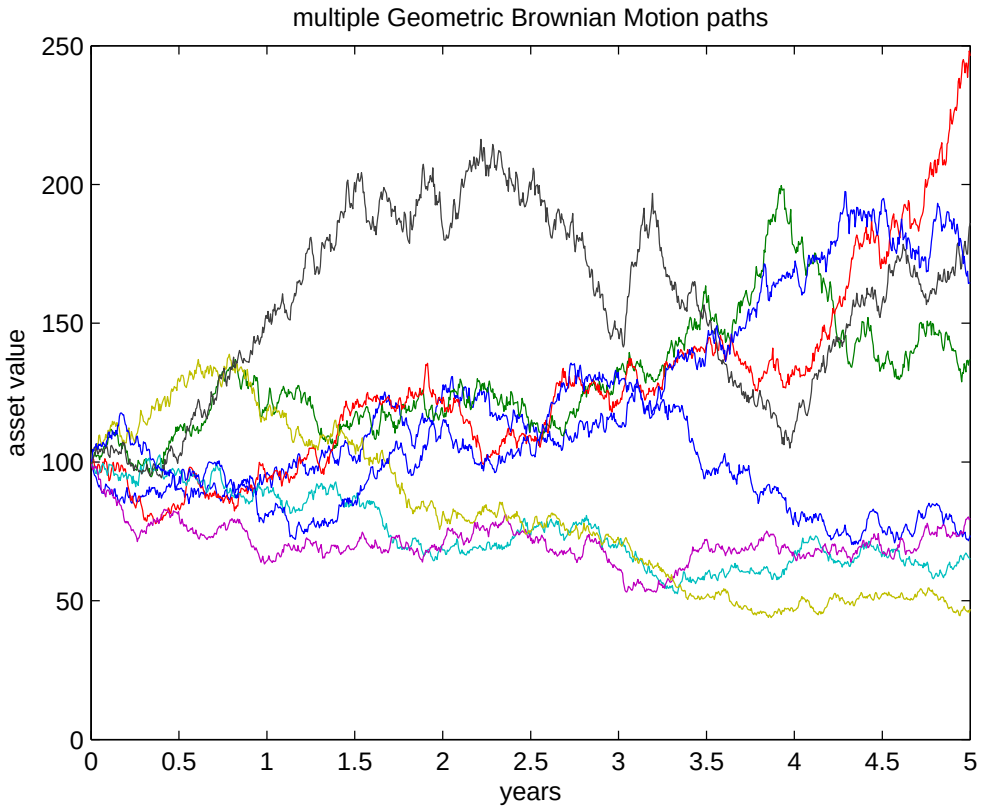
I'm a numerics / algorithms person – I collaborate a lot with others with interests in a wide variety of applications

Mathematical Finance: I

The movement of stock prices is modelled by stochastic differential equations such as

$$\mathrm{d}S_t = r\,S_t\,\mathrm{d}t + \sigma\,S_t\,\mathrm{d}W_t$$

where W_t is a Brownian path with $N(0, \mathrm{d}t)$ Normal increments



Mathematical Finance: II

Collaboration with Profs. Ben Hambly and Christoph Reisinger

Here, they looked at the evolution of a probability density function $p(x,t)$ for firms at a distance x from default at time t

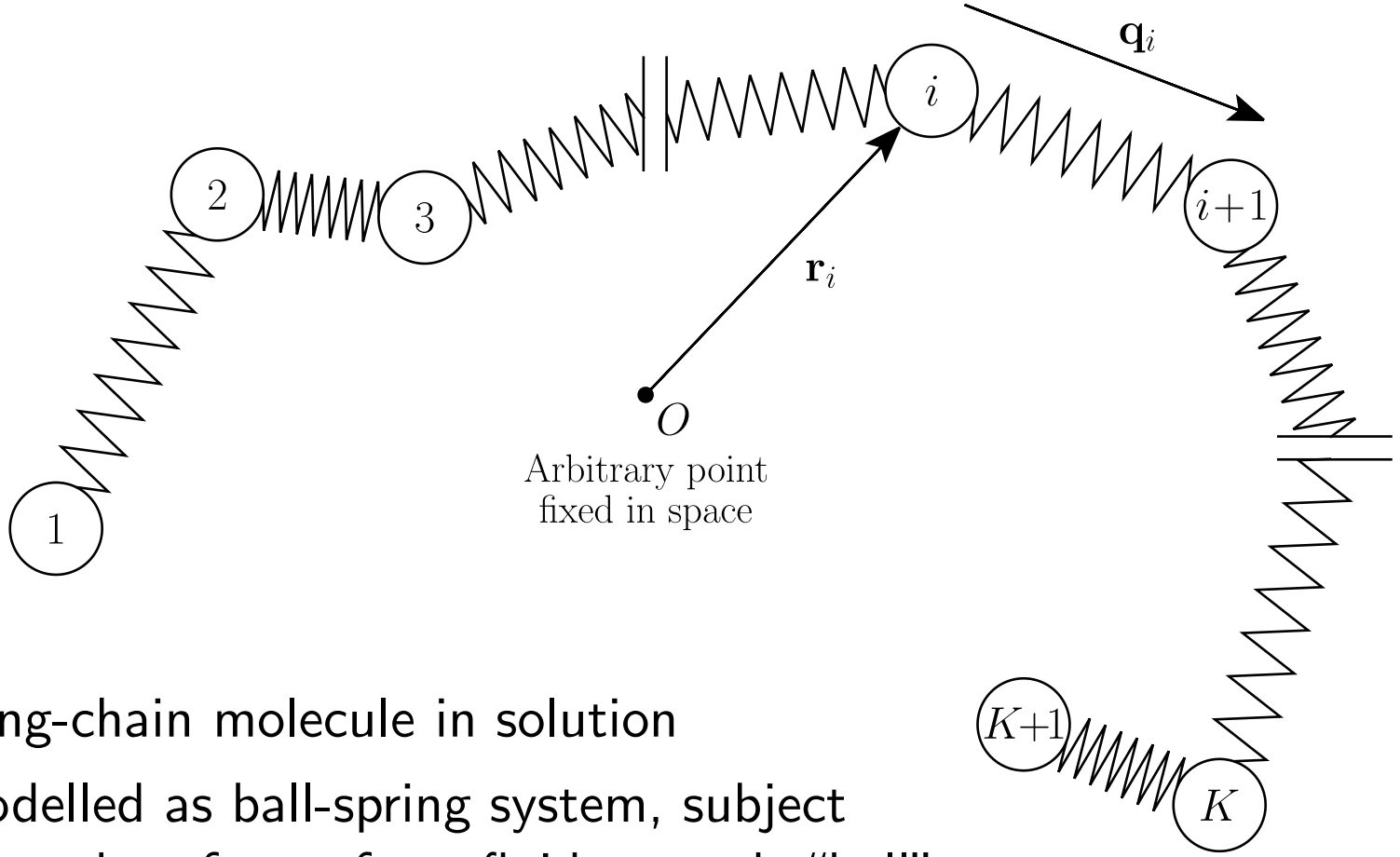
$$\mathrm{d}p = -\mu \frac{\partial p}{\partial x}\,\mathrm{d}t + \frac{1}{2}\frac{\partial^2 p}{\partial x^2}\,\mathrm{d}t + \sqrt{\rho}\,\frac{\partial p}{\partial x}\,\mathrm{d}W_t$$

with absorbing boundary $p(0,t) = 0$.

The diffusion behaviour is a large-limit effect of lots of different firms affected by individual (idiosyncratic) random effects, whereas the Brownian path W_t models the systemic effects which affect everyone.

Long-chain molecules in a fluid

Collaboration with Prof. Endre Süli



- Long-chain molecule in solution
- modelled as ball-spring system, subject to random forces from fluid on each "ball"
- interest is in mean stress exerted by molecules on fluid

Bio-chemical reactions

Collaboration with Prof. Ruth Baker

At high concentrations, chemistry is deterministic, resulting in ODEs

$$A + B \to C$$

$$\frac{\mathrm{d}c_A}{\mathrm{d}t} = -r\, c_A\, c_B, \quad \frac{\mathrm{d}c_B}{\mathrm{d}t} = -r\, c_A\, c_B, \quad \frac{\mathrm{d}c_C}{\mathrm{d}t} = +r\, c_A\, c_B.$$

where c_A, c_B, c_C are the concentrations in a well-stirred vessel.

However, at very low concentrations, it becomes stochastic:

$$\mathbb{P}(\text{reaction occurs in time } \mathrm{d}t) = R\, n_A\, n_B\, \mathrm{d}t$$

where n_A, n_B, n_C are the numbers of molecules. This results in a continuous-time Markov process.

Monte Carlo method

In stochastic models, we often have

$$\underset{\text{random input}}{\omega} \longrightarrow \underset{\text{intermediate variables}}{S} \longrightarrow \underset{\text{scalar output}}{P}$$

The Monte Carlo estimate for $\mathbb{E}[P]$ is an average of N independent samples $\omega^{(n)}$:

$$Y = N^{-1} \sum_{n=1}^{N} P(\omega^{(n)}).$$

This is unbiased, $\mathbb{E}[Y] = \mathbb{E}[P]$, and the Central Limit Theorem proves that as $N \to \infty$ the error becomes Normally distributed with variance $N^{-1}\mathbb{V}[P]$.

Monte Carlo method

In many cases, this is modified to

$$\underset{\text{random input}}{\omega} \longrightarrow \underset{\text{intermediate variables}}{\widehat{S}} \longrightarrow \underset{\text{scalar output}}{\widehat{P}}$$

where $\widehat{S}, \widehat{P}$ are approximations to S, P, in which case the MC estimate

$$\widehat{Y} = N^{-1} \sum_{n=1}^{N} \widehat{P}(\omega^{(n)})$$

is biased, and the Mean Square Error is

$$\mathbb{E}[\,(\widehat{Y} - \mathbb{E}[P])^2] \;=\; N^{-1}\,\mathbb{V}[\widehat{P}] + \Big(\mathbb{E}[\widehat{P}] - \mathbb{E}[P]\Big)^2$$

Greater accuracy requires larger N and smaller weak error $\mathbb{E}[\widehat{P}] - \mathbb{E}[P]$.

SDE Path Simulation

My interest was in SDEs (stochastic differential equations) for finance, which in a simple one-dimensional case has the form

$$\mathrm{d}S_t = a(S_t, t)\,\mathrm{d}t + b(S_t, t)\,\mathrm{d}W_t$$

Here $\mathrm{d}W_t$ is the increment of a Brownian motion – Normally distributed with variance $\mathrm{d}t$.

This is usually approximated by the simple Euler-Maruyama method

$$\widehat{S}_{t_{n+1}} = \widehat{S}_{t_n} + a(\widehat{S}_{t_n}, t_n)\,h + b(\widehat{S}_{t_n}, t_n)\,\Delta W_n$$

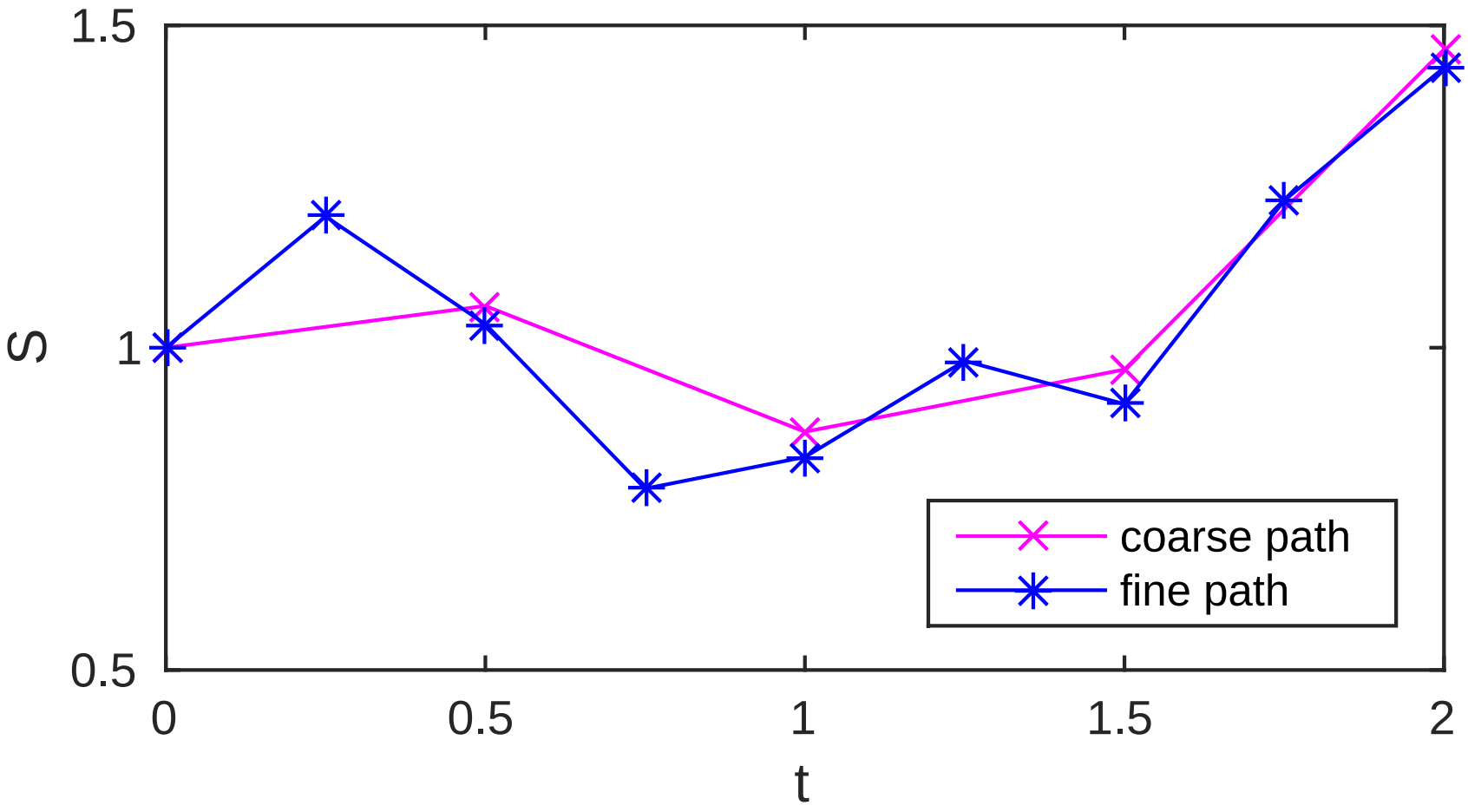
with uniform timestep h, and increments ΔW_n with variance h.

In simple applications, the output of interest is a function of the final value:

$$\widehat{P} \equiv f(\widehat{S}_T)$$

SDE Path Simulation

Geometric Brownian Motion: $\mathrm{d}S_t = r\,S_t\,\mathrm{d}t + \sigma\,S_t\,\mathrm{d}W_t$



SDE Path Simulation

Two kinds of discretisation error:

Weak error:

$$\mathbb{E}[\widehat{P}] - \mathbb{E}[P] = O(h)$$

Strong error:

$$\left(\mathbb{E}\left[\sup_{[0,T]}\left(\widehat{S}_t - S_t\right)^2\right]\right)^{1/2} = O(h^{1/2})$$

For reasons which will become clear, I prefer to use the Milstein discretisation for which the weak and strong errors are both $O(h)$.

SDE Path Simulation

The Mean Square Error is

$$N^{-1}\,\mathbb{V}[\widehat{P}] + \Big(\mathbb{E}[\widehat{P}] - \mathbb{E}[P]\Big)^2 \;\approx\; a\,N^{-1} + b\,h^2$$

If we want this to be ε^2, then we need

$$N = O(\varepsilon^{-2}), \qquad h = O(\varepsilon)$$

so the total computational cost is $O(\varepsilon^{-3})$.

To improve this cost we need to

- reduce N – variance reduction or Quasi-Monte Carlo methods
- reduce the cost of each path (on average) – MLMC

Two-level Monte Carlo

If we want to estimate $\mathbb{E}[\widehat{P}_1]$ but it is much cheaper to simulate $\widehat{P}_0 \approx \widehat{P}_1$, then since

$$\mathbb{E}[\widehat{P}_1] = \mathbb{E}[\widehat{P}_0] + \mathbb{E}[\widehat{P}_1 - \widehat{P}_0]$$

we can use the estimator

$$N_0^{-1} \sum_{n=1}^{N_0} \widehat{P}_0^{(0,n)} \;+\; N_1^{-1} \sum_{n=1}^{N_1} \left(\widehat{P}_1^{(1,n)} - \widehat{P}_0^{(1,n)} \right)$$

Benefit: if $\widehat{P}_1 - \widehat{P}_0$ is small, its variance will be small, so won't need many samples to accurately estimate $\mathbb{E}[\widehat{P}_1 - \widehat{P}_0]$, so cost will be reduced greatly.

Multilevel Monte Carlo

Natural generalisation: given a sequence $\widehat{P}_0, \widehat{P}_1, \ldots, \widehat{P}_L$

$$\mathbb{E}[\widehat{P}_L] = \mathbb{E}[\widehat{P}_0] + \sum_{\ell=1}^{L} \mathbb{E}[\widehat{P}_\ell - \widehat{P}_{\ell-1}]$$

we can use the estimator

$$N_0^{-1} \sum_{n=1}^{N_0} \widehat{P}_0^{(0,n)} \; + \; \sum_{\ell=1}^{L} \left\{ N_\ell^{-1} \sum_{n=1}^{N_\ell} \left(\widehat{P}_\ell^{(\ell,n)} - \widehat{P}_{\ell-1}^{(\ell,n)} \right) \right\}$$

with independent estimation for each level of correction

Multilevel Monte Carlo

If we define

- C_0, V_0 to be cost and variance of $\widehat{P}_0$
- C_ℓ, V_ℓ to be cost and variance of $\widehat{P}_\ell - \widehat{P}_{\ell-1}$

then the total cost is $\displaystyle\sum_{\ell=0}^{L} N_\ell\, C_\ell$ and the variance is $\displaystyle\sum_{\ell=0}^{L} N_\ell^{-1} V_\ell$.

Using a Lagrange multiplier μ^2 to minimise the cost for a fixed variance

$$\frac{\partial}{\partial N_\ell} \sum_{k=0}^{L} \left(N_k\, C_k + \mu^2 N_k^{-1} V_k \right) = 0$$

gives

$$N_\ell = \mu \sqrt{V_\ell / C_\ell} \quad \Longrightarrow \quad N_\ell\, C_\ell = \mu \sqrt{V_\ell\, C_\ell}$$

Multilevel Monte Carlo

Setting the total variance equal to ε^2 gives

$$\mu = \varepsilon^{-2} \left(\sum_{\ell=0}^{L} \sqrt{V_\ell \, C_\ell} \right)$$

and hence, the total cost is

$$\sum_{\ell=0}^{L} N_\ell \; C_\ell \;=\; \varepsilon^{-2} \left(\sum_{\ell=0}^{L} \sqrt{V_\ell C_\ell} \right)^2$$

in contrast to the standard cost which is approximately $\varepsilon^{-2} \, V_0 \, C_L$.

The MLMC cost savings are therefore approximately:

- V_L/V_0, if $\sqrt{V_\ell C_\ell}$ increases with level
- C_0/C_L, if $\sqrt{V_\ell C_\ell}$ decreases with level

Multilevel Path Simulation

With SDEs, level ℓ corresponds to approximation using M^ℓ timesteps, giving approximate payoff $\widehat{P}_\ell$ at cost $C_\ell = O(h_\ell^{-1})$.

Simplest estimator for $\mathbb{E}[\widehat{P}_\ell - \widehat{P}_{\ell-1}]$ for $\ell > 0$ is

$$\widehat{Y}_\ell = N_\ell^{-1} \sum_{n=1}^{N_\ell} \left(\widehat{P}_\ell^{(n)} - \widehat{P}_{\ell-1}^{(n)} \right)$$

using same driving Brownian path for both levels.

Analysis gives MSE $= \displaystyle\sum_{\ell=0}^{L} N_\ell^{-1} V_\ell + \Big(\mathbb{E}[\widehat{P}_L] - \mathbb{E}[P] \Big)^2$

To make RMS error less than ε

- choose $N_\ell \propto \sqrt{V_\ell / C_\ell}$ so total variance is less than $\frac{1}{2}\,\varepsilon^2$
- choose L so that $\Big(\mathbb{E}[\widehat{P}_L] - \mathbb{E}[P] \Big)^2 < \frac{1}{2}\,\varepsilon^2$

Multilevel Path Simulation

For Lipschitz payoff functions $P \equiv f(S_T)$, we have

$$\begin{aligned} V_\ell \;\equiv\; \mathbb{V}\left[\widehat{P}_\ell - \widehat{P}_{\ell-1}\right] \;&\leq\; \mathbb{E}\left[(\widehat{P}_\ell - \widehat{P}_{\ell-1})^2\right] \\ &\leq\; K^2\,\mathbb{E}\left[(\widehat{S}_{T,\ell} - \widehat{S}_{T,\ell-1})^2\right] \\ &=\; \begin{cases} O(h_\ell), & \text{Euler-Maruyama} \\ O(h_\ell^2), & \text{Milstein} \end{cases} \end{aligned}$$

and hence

$$V_\ell\, C_\ell = \begin{cases} O(1), & \text{Euler-Maruyama} \\ O(h_\ell), & \text{Milstein} \end{cases}$$

MLMC Theorem

(Slight generalisation of version in 2008 *Operations Research* paper)

If there exist independent estimators $\widehat{Y}_\ell$ based on N_ℓ Monte Carlo samples, each costing C_ℓ, and positive constants $\alpha, \beta, \gamma, c_1, c_2, c_3$ such that $\alpha \geq \frac{1}{2}\min(\beta, \gamma)$ and

i) $\left|\mathbb{E}[\widehat{P}_\ell - P]\right| \leq c_1\, 2^{-\alpha\,\ell}$

ii) $\mathbb{E}[\widehat{Y}_\ell] = \begin{cases} \mathbb{E}[\widehat{P}_0], & \ell = 0 \\ \mathbb{E}[\widehat{P}_\ell - \widehat{P}_{\ell-1}], & \ell > 0 \end{cases}$

iii) $\mathbb{V}[\widehat{Y}_\ell] \leq c_2\, N_\ell^{-1} 2^{-\beta\,\ell}$

iv) $\mathbb{E}[C_\ell] \leq c_3\, 2^{\gamma\,\ell}$

MLMC Theorem

then there exists a positive constant c_4 such that for any $\varepsilon < 1$ there exist L and N_ℓ for which the multilevel estimator

$$\widehat{Y} = \sum_{\ell=0}^{L} \widehat{Y}_\ell,$$

has a mean-square-error with bound $\mathbb{E}\left[\left(\widehat{Y} - \mathbb{E}[P]\right)^2\right] < \varepsilon^2$

with an expected computational cost C with bound

$$C \le \begin{cases} c_4\, \varepsilon^{-2}, & \beta > \gamma, \\ c_4\, \varepsilon^{-2} (\log \varepsilon)^2, & \beta = \gamma, \\ c_4\, \varepsilon^{-2-(\gamma-\beta)/\alpha}, & 0 < \beta < \gamma. \end{cases}$$

MLMC Theorem

Two observations of optimality:

- MC simulation needs $O(\varepsilon^{-2})$ samples to achieve RMS accuracy ε. When $\beta > \gamma$, the cost is optimal — $O(1)$ cost per sample on average.

  (Would need multilevel QMC to further reduce costs)

- When $\beta < \gamma$, another interesting case is when $\beta = 2\alpha$, which corresponds to $\mathbb{E}[\widehat{Y}_\ell]$ and $\sqrt{\mathbb{E}[\widehat{Y}_\ell^2]}$ being of the same order as $\ell \to \infty$.

  In this case, the total cost is $O(\varepsilon^{-\gamma/\alpha})$, which is the cost of a single sample on the finest level — again optimal.

MLMC work on SDEs

- Milstein discretisation for path-dependent options – G (2008)
- numerical analysis – G, Higham, Mao (2009), Avikainen (2009), G, Debrabant, Rößler (2012)
- financial sensitivities ("Greeks") – Burgos (2011)
- jump-diffusion models – Xia (2011)
- Lévy processes – Dereich (2010), Marxen (2010), Dereich & Heidenreich (2011), Xia (2013), Kyprianou (2014)
- American options – Belomestny & Schoenmakers (2011)
- Milstein in higher dimensions without Lévy areas – G, Szpruch (2014)
- adaptive timesteps – Hoel, von Schwerin, Szepessy, Tempone (2012), G, Lester, Whittle (2014)

SPDEs

- quite natural application, with better cost savings than SDEs due to higher dimensionality

- range of applications
  - Graubner & Ritter (Darmstadt) – parabolic
  - G, Reisinger (Oxford) – parabolic
  - Cliffe, G, Scheichl, Teckentrup (Bath/Nottingham) – elliptic
  - Barth, Jenny, Lang, Meyer, Mishra, Müller, Schwab, Sukys, Zollinger (ETH Zürich) – elliptic, parabolic, hyperbolic
  - Harbrecht, Peters (Basel) – elliptic
  - Efendiev (Texas A&M) – numerical homogenization
  - Vidal-Codina, G, Peraire (MIT) – reduced basis approximation

Engineering Uncertainty Quantification

Simplest possible example:

- 3D elliptic PDE, with uncertain boundary data
- grid spacing proportional to $2^{-\ell}$ on level ℓ
- cost is $O(2^{+3\ell})$, if using an efficient multigrid solver
- 2nd order accuracy means that

$$\widehat{P}_\ell(\omega) - P(\omega) \approx c(\omega)\, 2^{-2\ell}$$

$$\Longrightarrow \quad \widehat{P}_{\ell-1}(\omega) - \widehat{P}_\ell(\omega) \approx 3\, c(\omega)\, 2^{-2\ell}$$

- hence, $\alpha=2,\ \beta=4,\ \gamma=3$
- cost is $O(\varepsilon^{-2})$ to obtain ε RMS accuracy
- this compares to $O(\varepsilon^{-3/2})$ cost for one sample on finest level, so $O(\varepsilon^{-7/2})$ for standard Monte Carlo

Non-geometric multilevel

Almost all applications of multilevel in the literature so far use a geometric sequence of levels, refining the timestep (or the spatial discretisation for PDEs) by a constant factor when going from level ℓ to level $\ell + 1$.

Coming from a multigrid background, this is very natural, but it is **NOT** a requirement of the multilevel Monte Carlo approach.

All MLMC needs is a sequence of levels with

- increasing accuracy
- increasing cost
- increasingly small difference between outputs on successive levels

Reduced Basis PDE approximation

Vidal-Codina, Nguyen, G, Peraire (2014) take a fine FE discretisation:

$$A(\omega)\, u = f(\omega)$$

and use a reduced basis approximation

$$u \approx \sum_{k=1}^{K} v_k\, u_k$$

to obtain a low-dimensional reduced system

$$A_r(\omega)\, v = f_r(\omega)$$

- larger $K \Longrightarrow$ greater accuracy at greater cost
- in multilevel treatment, K_ℓ varies with level
- brute force optimisation determines the optimal number of levels, and reduced basis size on each level

Other MLMC applications

- parametric integration, integral equations (Heinrich)
- multilevel QMC (Dick, G, Kuo, Scheichl, Schwab, Sloan)
- stochastic chemical reactions (Anderson & Higham, Tempone)
- mixed precision computation on FPGAs (Korn, Ritter, Wehn)
- MLMC for MCMC (Scheichl, Schwab, Stuart, Teckentrup)
- Coulomb collisions in plasma (Caflisch)
- nested simulation (Haji-Ali & Tempone, Hambly & Reisinger)
- invariant distribution of contractive Markov process (Glynn & Rhee)
- invariant distribution of contractive SDEs (G, Lester & Whittle)

Three MLMC extensions

- unbiased estimation – Rhee & Glynn (2015)
  - randomly selects the level for each sample
  - no bias, and finite expected cost and variance if $\beta > \gamma$
- Richardson-Romberg extrapolation – Lemaire & Pagès (2013)
  - reduces the weak error, and hence the number of levels required
  - particularly helpful when $\beta < \gamma$
- Multi-Index Monte Carlo – Haji-Ali, Nobile, Tempone (2015)
  - important extension to MLMC approach, combining MLMC with sparse grid methods

Multi-Index Monte Carlo

Standard "1D" MLMC truncates the telescoping sum

$$\mathbb{E}[P] = \sum_{\ell=0}^{\infty} \mathbb{E}[\Delta \widehat{P}_\ell]$$

where $\Delta \widehat{P}_\ell \equiv \widehat{P}_\ell - \widehat{P}_{\ell-1}$, with $\widehat{P}_{-1} \equiv 0$.

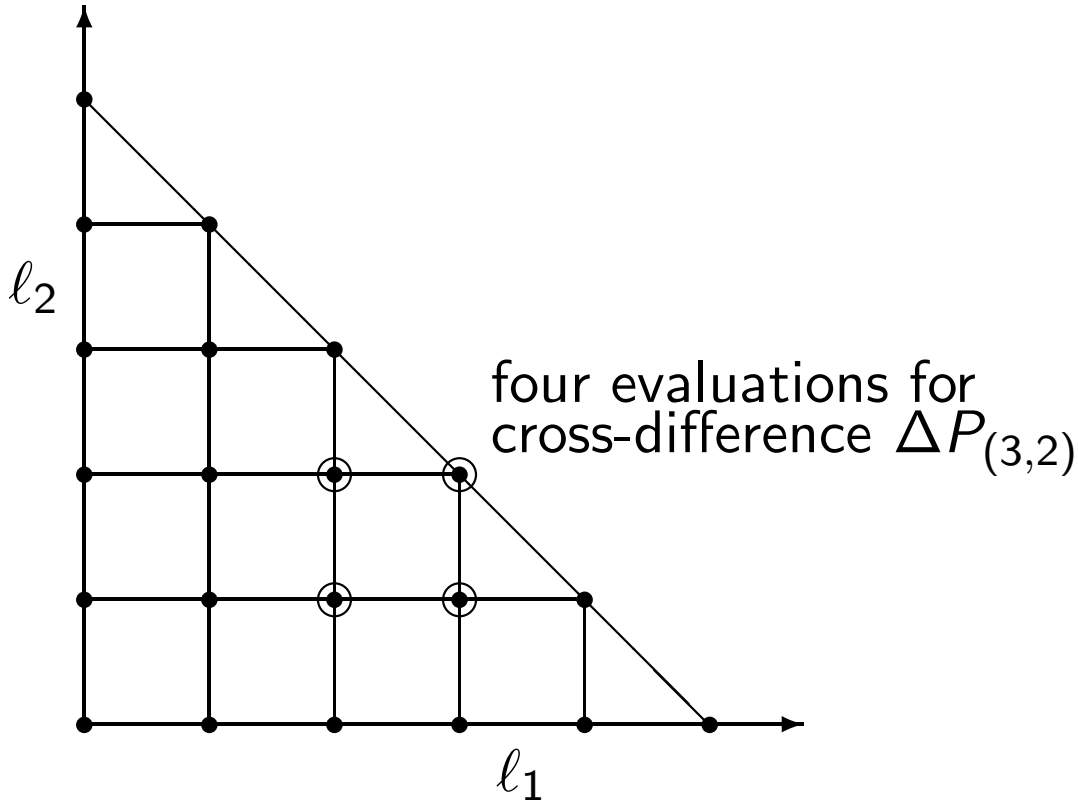
In "2D", MIMC truncates the telescoping sum

$$\mathbb{E}[P] = \sum_{\ell_1=0}^{\infty} \sum_{\ell_2=0}^{\infty} \mathbb{E}[\Delta \widehat{P}_{\ell_1,\ell_2}]$$

where $\Delta \widehat{P}_{\ell_1,\ell_2} \equiv (\widehat{P}_{\ell_1,\ell_2} - \widehat{P}_{\ell_1-1,\ell_2}) - (\widehat{P}_{\ell_1,\ell_2-1} - \widehat{P}_{\ell_1-1,\ell_2-1})$

Different aspects of the discretisation vary in each "dimension" – for a 2D PDE, could use grid spacing $2^{-\ell_1}$ in direction 1, $2^{-\ell_2}$ in direction 2

Multi-Index Monte Carlo



MIMC truncates the summation in a way which minimises the cost to achieve a target MSE – quite similar to sparse grids.

Can achieve $O(\varepsilon^{-2})$ complexity for a wider range of SPDE and other applications than plain MLMC.

Conclusions

- multilevel idea is very simple; key question is how to apply it in new situations, and perform the numerical analysis
- discontinuous output functions can cause problems, but there is a lot of experience now in coping with this
- there are also "tricks" which can be used in situations with poor strong convergence
- being used for an increasingly wide range of applications; biggest computational savings when coarsest (reasonable) approximation is much cheaper than finest
- currently, getting at least 100$\times$ savings for SPDEs and stochastic chemical reaction simulations

References

Webpages for my research papers and talks:

`people.maths.ox.ac.uk/gilesm/mlmc.html`
`people.maths.ox.ac.uk/gilesm/slides.html`

Webpage for new 70-page *Acta Numerica* review and MATLAB test codes:

`people.maths.ox.ac.uk/gilesm/acta/`

– contains references to almost all MLMC research

Webpage with details of those working in this area:

`people.maths.ox.ac.uk/gilesm/mlmc_community.html`