Multilevel and Multi-index Monte Carlo methods for the McKean-Vlasov equation

Abdul-Lateef Haji-Ali* Raúl Tempone†

*Mathematical Institute, University of Oxford, United Kingdom
†King Abdullah University of Science and Technology (KAUST), Saudi Arabia.

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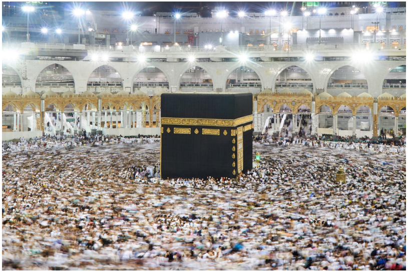
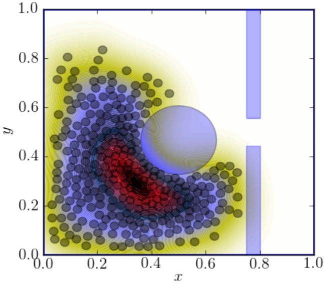
King Abdullah University of
Science and Technology

Particle Systems in the Mean-field

- Particle systems are a collection of coupled, usually identical and simple, models that can be used to model complicated phenomena.
  - Molecular dynamics, Crowd simulation, Oscillators, ...
- Certain stochastic particles systems have a mean-field limit when the number of particles increase. Such limits can be useful to understand their complicated phenomena.





Main reference

This presentation is based on the manuscript

• "Multilevel and Multi-index Monte Carlo methods for the McKean-Vlasov equation" by A. L. Haji Ali and R. Tempone. *arXiv:1610.09934*, 2016. To appear in Statistics and Computing.

A McKean-Vlasov process is a stochastic process described by a SDE whose coefficients depend on the distribution of the solution itself. They relate to the Vlasov model for plasma evolution and were first studied by Henry McKean in 1966. For $0 < t \leq T$ the process $X(t)$ solves

$$\begin{aligned} dX(t) =& a(X(t), \mu(t))dW(t) + b(X(t), \mu(t))dt, \\ \mu(t) =& \mathcal{L}(X(t)) \end{aligned}$$

and $\mu(0)$ given. **Goal:** approximate $E[g(X(T))]$ for some given g.

Convergence to the mean-field

For particles $X_{p|P}$, $p = 1, \ldots, P$, (evolving in a system of size P) define "shadow" particles $X_{p|\infty}$, (evolving in a system of ∞ size)

$$X_{p|P}(t) = x_p^0 + \int_0^t \left(a(X_{p|P}(t)) + \frac{1}{P}\sum_{q=1}^{P} A(X_{p|P}(t), X_{q|P}(t)) \right) \mathrm{d}t + \sigma W_p(t)$$

$$X_{p|\infty}(t) = x_p^0 + \int_0^t \left(a(X_{p|\infty}(t)) + \int A(X_{p|\infty}(t), y)\mu_\infty(t)(\mathrm{d}y) \right) \mathrm{d}t + \sigma W_p(t),$$

with $\mu_\infty(t)$ the marginal distribution for $X_{p|\infty}(t)$ for any p.

Consistency: The initial values x_p^0, $p = 1, \ldots, P$, are i.i.d. from $\mu_\infty(0)$.

For $t > 0$, and all x, the pdf of the *marginal distribution* $\mu_\infty(t)$ of the infinite size system satisfies a nonlinear Fokker Planck equation

$$\partial_t \rho_\infty(t,x) + div\left(\rho_\infty(t,x)(a(x) + \rho_\infty(t,\cdot) * A(x,\cdot))\right) = \sum_i \frac{\sigma_i^2}{2} \partial_i^2 \rho_\infty(t,x)$$

with a given initial condition $\rho_\infty(0,\cdot)$ and suitable b.c.

Question: What about the rate of weak convergence?

$$\mathrm{E}\left[g(X_{p|P}(T)) - g(X_{p|\infty}(T))\right] \lesssim \ldots$$

Kuramoto oscillator model †

For $p = 1, 2, \ldots, P$ consider equally coupled oscillators with intrinsic natural frequencies ϑ_p that follow a system of Itô SDEs

$$\mathrm{d}X_{p|P}(t) = \left(\vartheta_p + \frac{1}{P} \sum_{q=1}^{P} \sin(X_{p|P}(t) - X_{q|P}(t)) \right) \mathrm{d}t + \sigma \mathrm{d}W_{p|P}(t)$$
$$X_{p|P}(0) = x^0_{p|P}$$

where we are interested in

$$\text{Total order} = \left(\frac{1}{P} \sum_{p=1}^{P} \cos\left(X_{p|P}(T) \right) \right)^2 + \left(\frac{1}{P} \sum_{p=1}^{P} \sin\left(X_{p|P}(T) \right) \right)^2;$$

a real number between zero and one that measures the level of synchronization of the coupled oscillators.

† Y. Kuramoto, Chemical Oscillations, Waves, and Turbulence, Springer, Berlin, 1984.

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$$X_{p|P}(0) = x^0_{p|P}$$

where we are interested in: $$\phi_P = \frac{1}{P}\sum_{p=1}^{P} \cos\left(X_{p|P}(T)\right),$$

Mean-field limit: $\phi_P \to \phi_\infty = \mathrm{E}\left[\cos(X_{p|\infty(T)})\right]$ as $P \uparrow \infty$

$$\mathrm{d}X_{p|\infty} = \left(\vartheta_p + \int_{\mathbb{R}} \sin(X_{p|\infty}(t) - y)\mu_\infty(t, \mathrm{d}y)\right)\mathrm{d}t + \sigma \mathrm{d}W_{p|P}(t)$$

† Y. Kuramoto, Chemical Oscillations, Waves, and Turbulence, Springer, Berlin, 1984.

Kuramoto oscillator model [†], Euler-Maruyama

For $p = 1, 2, \ldots, P$ consider equally coupled oscillators with intrinsic natural frequencies ϑ_p that follow a system of Itô SDEs

$$X_{p|P}^{n|N} - X_{p|P}^{n-1|N} = \left(\vartheta_p + \frac{1}{P}\sum_{q=1}^{P} \sin(X_{p|P}^{n|N} - X_{q|P}^{n|N})\right)\frac{T}{N} + \sigma \Delta W_{p|P}^{n|N}$$

$$X_{p|P}^{0|N} = x_{p|P}^{0}$$

where we are interested in: $$\phi_P^N = \frac{1}{P}\sum_{p=1}^{P} \cos\left(X_{p|P}^{N|N}\right),$$

Mean-field limit: $\phi_P \to \phi_\infty = \mathrm{E}\left[\cos(X_{p|\infty(T)})\right]$ as $P \uparrow \infty$

$$\mathrm{d}X_{p|\infty} = \left(\vartheta_p + \int_{\mathbb{R}} \sin(X_{p|\infty}(t) - y)\mu_\infty(t, \mathrm{d}y)\right)\mathrm{d}t + \sigma \mathrm{d}W_{p|P}(t)$$

[†] Y. Kuramoto, Chemical Oscillations, Waves, and Turbulence, Springer, Berlin, 1984.

Objective

Our objective is to build an estimator $\mathcal{A} \approx \phi_\infty$ with minimal work where

$$P(|\mathcal{A} - \phi_\infty| \leq \mathrm{TOL}) \;\geq 1 - \epsilon$$

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

Objective

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for a given accuracy TOL and a given confidence level determined by $0 < \epsilon \ll 1$. We instead impose the following, more restrictive, two constraints:

Bias constraint: $|\mathrm{E}[\mathcal{A}] - \phi_\infty| \leq \mathrm{TOL}/3,$

Statistical constraint: $P\left(|\mathcal{A} - \mathrm{E}[\mathcal{A}]| \geq 2\mathrm{TOL}/3\right)$

Objective

Our objective is to build an estimator $\mathcal{A} \approx \phi_\infty$ with minimal work where

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for a given accuracy TOL and a given confidence level determined by $0 < \epsilon \ll 1.$ We instead impose the following, more restrictive, two constraints:

$$\textbf{Bias constraint:} \qquad |\mathrm{E}[\mathcal{A}] - \phi_\infty| \leq \mathrm{TOL}/3,$$

$$\textbf{Variance constraint:} \qquad \mathrm{Var}[\mathcal{A}] \leq (2\mathrm{TOL}/3C_\epsilon)^2 \,.$$

assuming (at least asymptotic [a]) normality of the estimator, $\mathcal{A}$. Here, $0 < C_\epsilon$ is such that $\Phi(C_\epsilon) = 1 - \frac{\epsilon}{2}$, where Φ is the c.d.f. of a standard normal random variable.

[a] N. Collier, A.-L. Haji-Ali, E. von Schwerin, F. Nobile, and R. Tempone. "A continuation multilevel Monte Carlo algorithm". BIT Numerical Mathematics, 55(2):399-432, (2015).

Monte Carlo

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

$$\mathcal{A}_{\mathrm{MC}} = \frac{1}{M} \sum_{m=1}^{M} \phi_P^N(\boldsymbol{\omega}_P^m).$$

For a given P, N and M that we can choose to satisfy the error constraints and minimize the work. Here $\boldsymbol{\omega}_P^m = \left(\omega_p^m\right)_{p=1}^{P}$ and for each particle, ω_p^m denotes the independent, identically distributed (i.i.d.) samples of the set of underlying random variables that are used in calculating $X_{p|P}^{N|N}$, $1 \le p \le P$.

Monte Carlo work complexity

In our 1D example, we can check (at least numerically) that

Minimize total work: $\mathsf{Work}(\mathcal{A}_{\mathsf{MC}})$,

such that: $\mathsf{Bias}(\mathcal{A}_{\mathsf{MC}}) = \left|\phi_\infty - \mathrm{E}\left[\phi_P^N\right]\right| \leq \frac{\mathrm{TOL}}{3}$

and: $\mathrm{Var}[\mathcal{A}_{\mathsf{MC}}] = \frac{\mathrm{Var}\left[\phi_P^N\right]}{M} \leq \left(\frac{2\mathrm{TOL}}{3C_\epsilon}\right)^2$

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In our 1D example, we can check (at least numerically) that

Minimize total work: $\mathrm{Work}(\mathcal{A}_{\mathsf{MC}}) = \mathcal{O}\left(MNP^2\right)$

such that: $\mathrm{Bias}(\mathcal{A}_{\mathsf{MC}}) = \mathcal{O}\left(N^{-1}\right) + \mathcal{O}\left(P^{-1}\right) \leq \frac{\mathrm{TOL}}{3}$

and: $\mathrm{Var}[\mathcal{A}_{\mathsf{MC}}] = \frac{\mathcal{O}\left(P^{-1}\right)}{M} \leq \left(\frac{2\mathrm{TOL}}{3C_\epsilon}\right)^2$

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$$\textbf{Minimize total work:} \quad \mathrm{Work}(\mathcal{A}_{\mathrm{MC}}) = \mathcal{O}\left(MNP^2\right)$$

$$\textbf{such that:} \quad \mathrm{Bias}(\mathcal{A}_{\mathrm{MC}}) = \mathcal{O}\left(N^{-1}\right) + \mathcal{O}\left(P^{-1}\right) \leq \frac{\mathrm{TOL}}{3}$$

$$\textbf{and:} \quad \mathrm{Var}[\mathcal{A}_{\mathrm{MC}}] = \frac{\mathcal{O}\left(P^{-1}\right)}{M} \leq \left(\frac{2\mathrm{TOL}}{3C_\epsilon}\right)^2$$

In this case, we choose

$$P = \mathcal{O}\left(\mathrm{TOL}^{-1}\right), \quad N = \mathcal{O}\left(\mathrm{TOL}^{-1}\right), \quad M = \mathcal{O}\left(\mathrm{TOL}^{-1}\right)$$

and the total cost of a naive Monte Carlo is $\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$.

Observe: The cost of a "single cloud" naive method with $M = 1$ is $\mathcal{O}\left(\mathrm{TOL}^{-5}\right)$

Following (Heinrich, 2001) and (Giles, 2008), For a given $L \in \mathbb{N}$, define two hierarchies $\{N_\ell\}_{\ell=1}^L$ and $\{P_\ell\}_{\ell=1}^L$ satisfying $P_{\ell-1} \leq P_\ell$ and $N_{\ell-1} \leq N_\ell$ for all ℓ.
Recall the telescopic decomposition

$$\phi_\infty \approx \mathrm{E}\left[\phi_{P_L}^{N_L}\right] = \mathrm{E}\left[\phi_{P_0}^{N_0}\right] + \sum_{\ell=1}^{L} \mathrm{E}\left[\phi_{P_\ell}^{N_\ell} - \varphi_{P_{\ell-1}}^{N_{\ell-1}}\right]$$

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$$\text{where} \quad \Delta_\ell \phi = \begin{cases} \phi_{P_0}^{N_0} & \text{if } \ell = 0, \\ \phi_{P_\ell}^{N_\ell} - \varphi_{P_{\ell-1}}^{N_{\ell-1}} & \text{if } \ell > 0. \end{cases}$$

Here, we assume that the auxiliary estimator φ satisfies

$$\mathrm{E}\left[\varphi_{P_{\ell-1}}^{N_{\ell-1}}\right] = \mathrm{E}\left[\phi_{P_{\ell-1}}^{N_{\ell-1}}\right]$$

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

$$\mathcal{A}_{\mathrm{MLMC}} = \sum_{\ell=0}^{L} \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \Delta_\ell \phi(\omega_{P_\ell}^{\ell,m}).$$

where M_ℓ is optimally chosen. **High correlation is crucial** (between the pairs $(N_\ell, N_{\ell-1})$? $(P_\ell, P_{\ell-1})$?) to ensure that

$$\mathrm{Var}[\Delta_\ell \phi]$$

goes to zero sufficiently fast.

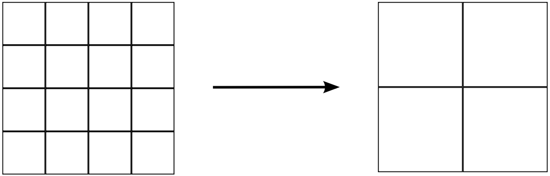
Variance reduction

Recall:

$$\mathrm{Var}[\mathcal{A}_{MC}] = \frac{1}{M_L}\mathrm{Var}[S_L].$$

$$\mathrm{Var}[\mathcal{A}_{\mathrm{MLMC}}] = \frac{1}{M_0}\mathrm{Var}[S_0] + \sum_{\ell=1}^{L}\frac{1}{M_\ell}\mathrm{Var}[\Delta_\ell S].$$

Main point: MLMC reduces the variance of the deepest level using samples on coarser (less expensive) levels!



Recall: MLMC optimal work complexity [‡] [§]

$$
\begin{aligned}
\textbf{Bias:} \quad & |\mathrm{E}[\Delta_\ell S]| = \mathcal{O}\left(\exp(-w\ell)\right), \\
\textbf{Variance:} \quad & \mathrm{Var}[\Delta_\ell S] = \mathcal{O}\left(\exp(-s\ell)\right), \\
\textbf{Work:} \quad & \mathrm{Work}[\Delta_\ell S] = \mathcal{O}\left(\exp(\gamma\ell)\right).
\end{aligned}
$$

[‡] Cliffe, K.A. and Giles, M.B. and Scheichl, R. and Teckentrup, A. Computing and Visualization in Science, "Multilevel Monte Carlo methods and applications to elliptic PDEs with random coefficients" (2011).

[§] Giles, Acta Numerica 2015.

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\textbf{Work:} \quad & \mathrm{Work}[\Delta_\ell S] = \mathcal{O}\left(\exp(\gamma\ell)\right).
\end{aligned}
$$

The optimal work of MLMC is

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

Recall the total cost of Monte Carlo is

$$
\mathcal{O}\left(\mathrm{TOL}^{-2-\frac{\gamma}{w}}\right)
$$

[‡] Cliffe, K.A. and Giles, M.B. and Scheichl, R. and Teckentrup, A. Computing and Visualization in Science, "Multilevel Monte Carlo methods and applications to elliptic PDEs with random coefficients" (2011).

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- In the following, we look at different settings in which either P_ℓ or N_ℓ depends on ℓ while the other parameter is constant for all ℓ.
- We begin by recalling the optimal convergence rates of MLMC when applied to a generic real valued random variable, Y, for the case when there are two discretization parameters:
  - ℓ, that is a function of the level,
  - $\mathcal{L}$, that is fixed for all levels.

Corollary (Optimal MLMC complexity)

Let $Y_{\mathcal{L},\ell}$ be an approximation of Y for every $(\mathcal{L},\ell) \in \mathbb{N}^2$. Consider the MLMC estimator

$$\mathcal{A}_{\mathsf{MLMC}}(L,\mathcal{L}) = \sum_{\ell=0}^{L} \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} (Y_{\mathcal{L},\ell} - Y_{\mathcal{L},\ell-1})$$

with $Y_{\mathcal{L},-1} = 0$ and assume the following

1. $\left|\mathrm{E}\left[Y - Y_{\mathcal{L},\ell}\right]\right| \lesssim \exp(-\widetilde{w}\mathcal{L}) + \exp(-w\ell)$
2. $\mathrm{Var}\left[Y_{\mathcal{L},\ell} - Y_{\mathcal{L},\ell-1}\right] \lesssim \exp(-\widetilde{c}\mathcal{L})\exp(-s\ell)$
3. $W Y_{\mathcal{L},\ell} - Y_{\mathcal{L},\ell-1} \lesssim \exp(\widetilde{\gamma}\mathcal{L})\exp(\gamma\ell)$.

The optimal work of MLMC in this setting is

$$W(\mathcal{A}_{\mathsf{MLMC}}) \lesssim \begin{cases} \mathrm{TOL}^{-(2-\widetilde{c})-\frac{\widetilde{\gamma}}{\widetilde{w}}} & \text{if } s > \gamma, \\ \mathrm{TOL}^{-(2-\widetilde{c})-\frac{\widetilde{\gamma}}{\widetilde{w}}} \log\left(\mathrm{TOL}^{-1}\right)^2 & \text{if } s = \gamma, \\ \mathrm{TOL}^{-(2-\widetilde{c})-\frac{\widetilde{\gamma}}{\widetilde{w}}-\frac{\gamma-s}{w}} & \text{if } s < \gamma. \end{cases}$$

MLMC in number of time-steps, N

- $P_\ell = P_L$ and $N_\ell = 2^\ell$.
- Build correlated samples by using the same Brownian paths discretized with different meshes 2^ℓ and $2^{\ell-1}$ (Recall that we are using Euler-Maruyama discretization).

$$\varphi_{P_L}^{N_{\ell-1}}(\boldsymbol{\omega}_{P_L}^{\ell,m}) = \phi_{P_L}^{N_{\ell-1}}(\boldsymbol{\omega}_{P_L}^{\ell,m})$$

MLMC in number of time-steps, N

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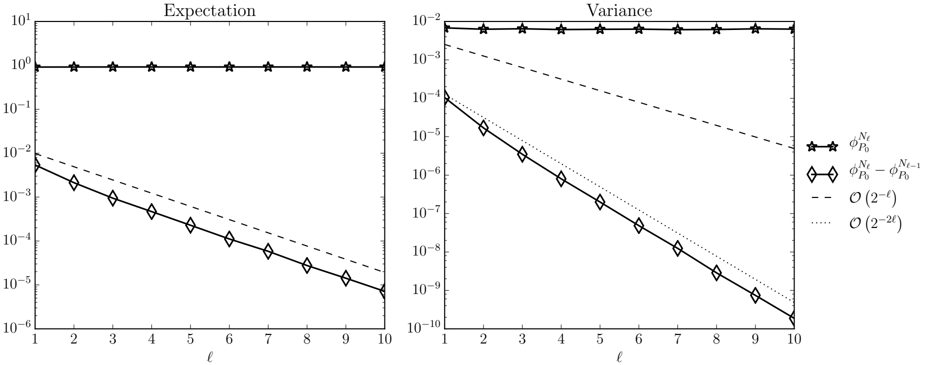
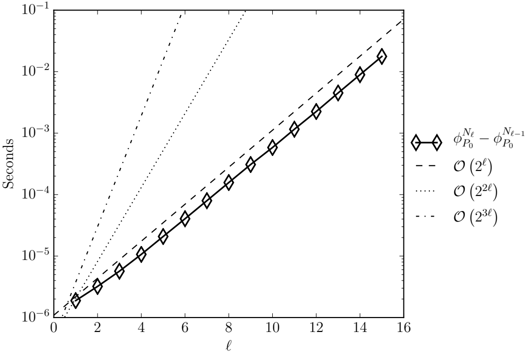


Bias, $w = 1, s = 2$

MLMC in number of time-steps, N

- $P_\ell = P_L$ and $N_\ell = 2^\ell$.



Work, $\gamma = 1$

MLMC in number of time-steps, N

- $P_\ell = P_L$ and $N_\ell = 2^\ell$.

- **Summary:** $w = 1, s = 2, \gamma = 1$
- Fixing P_L, the optimal work of biased MLMC is $\mathcal{O}\left(\mathrm{TOL}^{-2}\right)$.

MLMC in number of time-steps, N

- $P_\ell = P_L$ and $N_\ell = 2^\ell$.

- **Summary:** $w = 1, s = 2, \gamma = 1$
- Fixing P_L, the optimal work of biased MLMC is $\mathcal{O}\left(\mathrm{TOL}^{-2}\right)$.
- To control bias $\mathcal{O}\left(P_L^{-1}\right)$, choose $P_L = \mathcal{O}\left(\mathrm{TOL}^{-1}\right)$
  - Cost per sample: $\mathcal{O}\left(P_L^2 N_\ell\right)$
  - Variance: $\mathcal{O}\left(P_L^{-1} N_\ell^{-1}\right)$
  - **Summary:** $\tilde{w} = 1, \tilde{c} = 1, \tilde{\gamma} = 2$

  then the total cost becomes

$$\mathcal{O}\left(\mathrm{TOL}^{-3}\right) = \mathcal{O}\left(\mathrm{TOL}^{-(2-\tilde{c})-\frac{\tilde{\gamma}}{\tilde{w}}}\right).$$

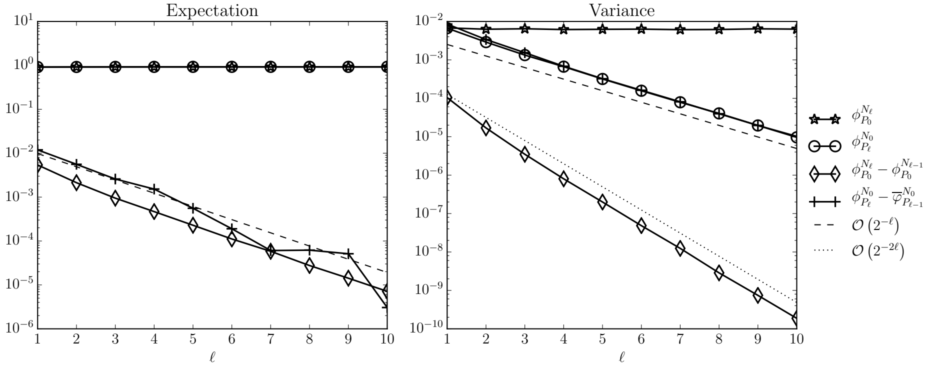
MLMC in number of particles, P

- $P_\ell = 2^\ell$ and $N_\ell = N_L$.
- Build correlated samples by sampling 2^ℓ and sub-sampling $2^{\ell-1}$ particles out of them (e.g. the first $2^{\ell-1}$). Use the same initial conditions, Brownian paths or any other random variables associated to a particle.

$$\varphi^{N_L}_{P_{\ell-1}}(\boldsymbol{\omega}^{\ell,m}_{P_\ell}) = \phi^{N_L}_{P_{\ell-1}}\left(\left(\omega^{\ell,m}_p\right)_{p=1}^{P_{\ell-1}}\right)$$

MLMC in number of particles, P

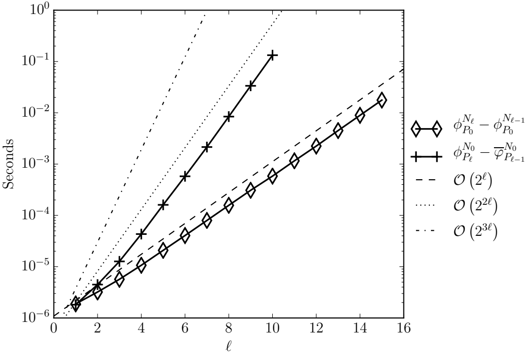
- $P_\ell = 2^\ell$ and $N_\ell = N_L$.



$$s = w = 1$$

MLMC in number of particles, P

- $P_\ell = 2^\ell$ and $N_\ell = N_L$.



Work, $\gamma = 2$

MLMC in number of particles, P

- $P_\ell = 2^\ell$ and $N_\ell = N_L$.
- **Summary:** $w = 1, s = 1, \gamma = 2$
- Fixing N_L, the optimal work of biased MLMC is $\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$.

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MLMC in number of particles, P

- $P_\ell = 2^\ell$ and $N_\ell = N_L$.

- **Summary:** $w = 1, s = 1, \gamma = 2$
- Fixing N_L, the optimal work of biased MLMC is $\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$.
- To control bias $\mathcal{O}\left(N_L^{-1}\right)$, choose $N_L = \mathcal{O}\left(\mathrm{TOL}^{-1}\right)$
  - Cost per sample: $\mathcal{O}\left(N_L P_\ell\right)$
  - Variance: $\mathcal{O}\left(P_\ell^{-1}\right)$
  - **Summary:** $\tilde{w} = 1, \tilde{c} = 0, \tilde{\gamma} = 1$

  then the total cost becomes

$$\mathcal{O}\left(\mathrm{TOL}^{-4}\right) = \mathcal{O}\left(\mathrm{TOL}^{-(2+\frac{\gamma-s}{w})-\frac{\tilde{\gamma}}{\tilde{w}}}\right).$$

- No advantage of MLMC over MC? Need a more correlated estimator!

Summary

Method	Work complexity
Monte Carlo	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
MLMC in N	$\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$
MLMC in P	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$

Reducing the variance w.r.t P; partitioning sampler

- The crucial element is how fast $\mathrm{Var}[\Delta\phi_\ell]$ goes to zero compared to how much it costs to compute $\Delta\phi_\ell$.
- Better choice of $\varphi(\cdot)$ to reduce $\mathrm{Var}[\Delta_\ell\phi]$.

Reducing the variance w.r.t P; partitioning sampler

- The crucial element is how fast $\mathrm{Var}[\Delta\phi_\ell]$ goes to zero compared to how much it costs to compute $\Delta\phi_\ell$.
- Better choice of $\varphi(\cdot)$ to reduce $\mathrm{Var}[\Delta_\ell\phi]$.
- If $P_{\ell-1} = P_\ell/2$, then given a group of P_ℓ particles, we can subsample *two identically-distributed, independent groups* that have $P_{\ell-1}$ particles and average the QoI

$$\varphi^{N_L}_{P_{\ell-1}}(\boldsymbol{\omega}^{\ell,m}_{P_\ell}) = \frac{1}{2}\left(\phi^{N_L}_{P_{\ell-1}}\left(\left(\omega^{\ell,m}_p\right)^{P_{\ell-1}}_{p=1}\right) + \phi^{N_L}_{P_{\ell-1}}\left(\left(\omega^{\ell,m}_p\right)^{P_\ell}_{p=1+P_{\ell-1}}\right)\right)$$

MLMC in number of particles P, with partitioning samplers

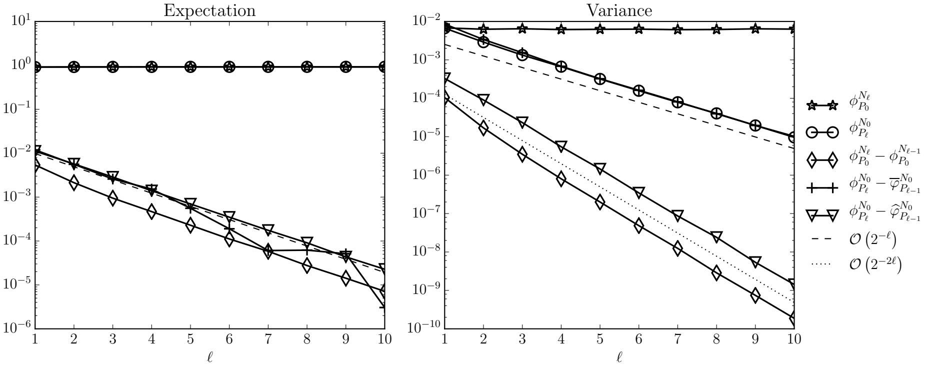
- $P_\ell = 2^\ell$ and $N_\ell = N_L$.

- Build correlated samples by sampling 2^ℓ and sub-sampling two identically-distributed, independent groups of $2^{\ell-1}$ particles out of them. Use the same initial conditions, Brownian paths or any other random variables associated to a particle.

$$\varphi^{N_L}_{P_{\ell-1}}(\boldsymbol{\omega}^{\ell,m}_{P_\ell}) = \frac{1}{2}\left(\phi^{N_L}_{P_{\ell-1}}\left(\left(\omega^{\ell,m}_p\right)^{P_{\ell-1}}_{p=1}\right) + \phi^{N_L}_{P_{\ell-1}}\left(\left(\omega^{\ell,m}_p\right)^{P_\ell}_{p=1+P_{\ell-1}}\right)\right)$$

MLMC in number of particles P, with partitioning samplers

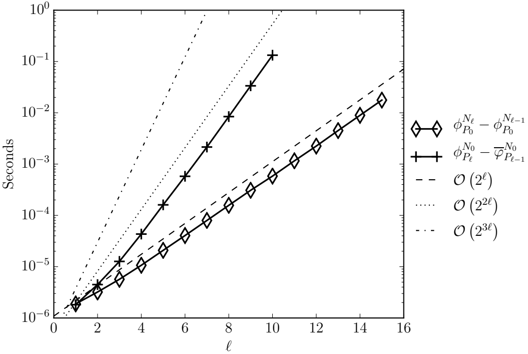
- $P_\ell = 2^\ell$ and $N_\ell = N_L$.



Bias, $w = 1, s = 2$

MLMC in number of particles P, with partitioning samplers

- $P_\ell = 2^\ell$ and $N_\ell = N_L$.



Work, $\gamma = 2$

MLMC in number of particles P, with partitioning samplers

- $P_\ell = 2^\ell$ and $N_\ell = N_L$.

- **Summary:** $w = 1, s = 2, \gamma = 2$
- Fixing N_L, the optimal work of biased MLMC is $\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$.

MLMC in number of particles P, with partitioning samplers

- $P_\ell = 2^\ell$ and $N_\ell = N_L$.

- **Summary:** $w = 1, s = 2, \gamma = 2$
- Fixing N_L, the optimal work of biased MLMC is $\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$.
- To control bias $\mathcal{O}\left(N_L^{-1}\right)$, choose $N_L = \mathcal{O}\left(\mathrm{TOL}^{-1}\right)$
    - Cost per sample: $\mathcal{O}\left(N_L P_\ell\right)$
    - Variance: $\mathcal{O}\left(P_\ell^{-1}\right)$
    - **Summary:** $\tilde{w} = 1, \tilde{c} = 0, \tilde{\gamma} = 1$

  then the total cost becomes

$$\mathcal{O}\left(\mathrm{TOL}^{-3}\left(\log \mathrm{TOL}\right)^2\right) = \mathcal{O}\left(\mathrm{TOL}^{-2-\frac{\tilde{\gamma}}{\tilde{w}}} \log\left(\mathrm{TOL}^{-1}\right)^2\right).$$

- Can we do better?

Summary

Method	Work complexity
Monte Carlo	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
MLMC in N	$\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$
MLMC in P	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
MLMC in P, partitioning	$\mathcal{O}\left(\mathrm{TOL}^{-3}\log(\mathrm{TOL}^{-1})^2\right)$

MLMC in P and N, with partitioning samplers

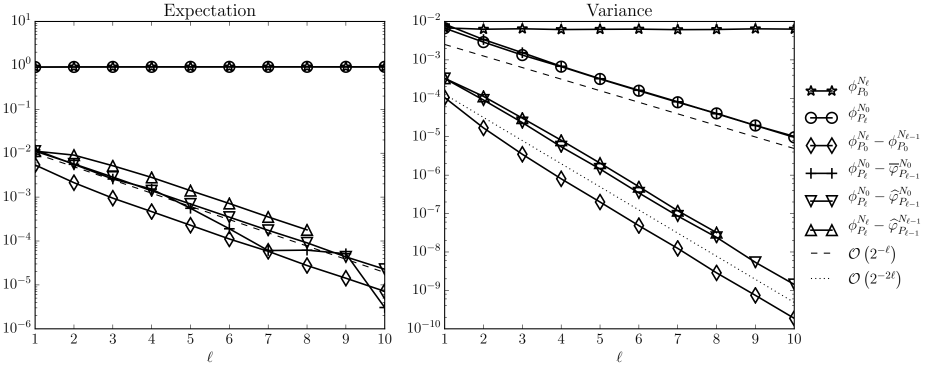
- $P_\ell = 2^\ell$ and $N_\ell = 2^\ell$.

- Build correlated samples by
  - Sampling 2^ℓ and sub-sampling two identically-distributed, independent groups of $2^{\ell-1}$ particles out of them. Use the same initial conditions, Brownian paths or any other random variables associated to a particle
  - At the same time, by using the same Brownian paths discretized with different meshes 2^ℓ and $2^{\ell-1}$.

$$\varphi_{P_{\ell-1}}^{N_{\ell-1}}(\boldsymbol{\omega}_{P_\ell}^{\ell,m}) = \frac{1}{2}\left(\phi_{P_{\ell-1}}^{N_{\ell-1}}\left(\left(\omega_p^{\ell,m}\right)_{p=1}^{P_{\ell-1}}\right) + \phi_{P_{\ell-1}}^{N_{\ell-1}}\left(\left(\omega_p^{\ell,m}\right)_{p=1+P_{\ell-1}}^{P_\ell}\right)\right)$$

MLMC in P and N, with partitioning samplers

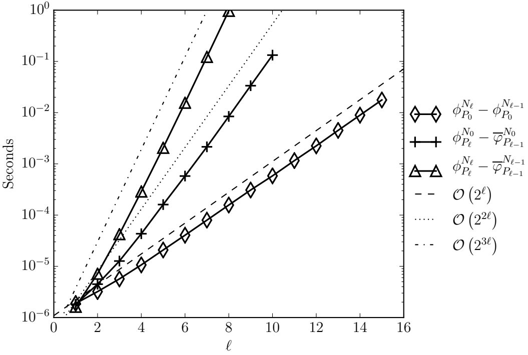
- $P_\ell = 2^\ell$ and $N_\ell = 2^\ell$.



$$w = 1, s = 2$$

MLMC in P and N, with partitioning samplers

- $P_\ell = 2^\ell$ and $N_\ell = 2^\ell$.



Work, $\gamma = 3$

MLMC in P and N, with partitioning samplers

- $P_\ell = 2^\ell$ and $N_\ell = 2^\ell$.

- **Summary:** $w = 1, s = 2, \gamma = 3$
- The optimal work of asymptotically unbiased MLMC is

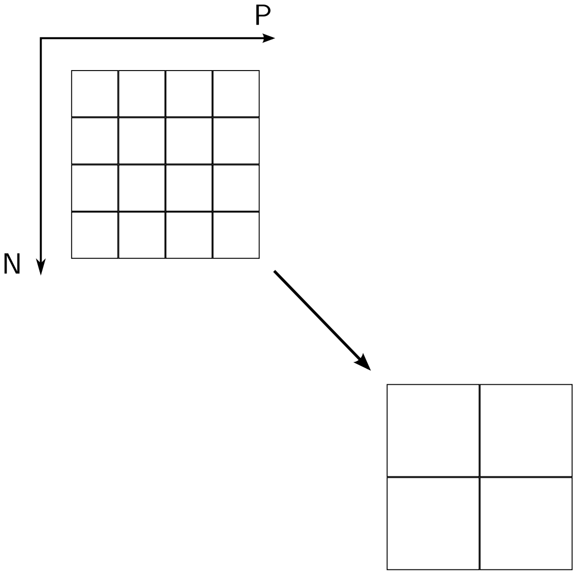
$$\mathcal{O}\left(\mathrm{TOL}^{-3}\right) = \mathcal{O}\left(\mathrm{TOL}^{-(2+\frac{\gamma-s}{w})}\right).$$

- The number of particles is not helping. Can we do better?

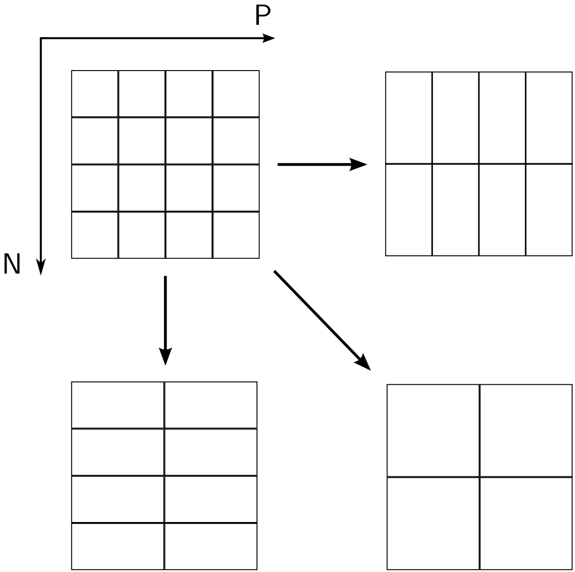
Summary

Method	Work complexity
Monte Carlo	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
MLMC in N	$\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$
MLMC in P	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
MLMC in P, partitioning	$\mathcal{O}\left(\mathrm{TOL}^{-3} \log(\mathrm{TOL}^{-1})^2\right)$
MLMC in P and N	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
MLMC in P and N, partitioning	$\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$

Variance reduction: MLMC



Variance reduction: Further potential



MIMC Estimator[¶]

For $\boldsymbol{\alpha} = (\alpha_1, \alpha_2) \in \mathbb{N}^2$, let $P_{\alpha_1} = 2^{\alpha_1}$ and $N_{\alpha_2} = 2^{\alpha_2}$. Define the first order mixed difference

$$\begin{aligned} \boldsymbol{\Delta}_{\boldsymbol{\alpha}} \phi &= \Delta_{1,\boldsymbol{\alpha}}(\Delta_{2,\boldsymbol{\alpha}} \phi) \\ &= (\phi_{P_{\alpha_1}}^{N_{\alpha_2}} - \phi_{P_{\alpha_1}}^{N_{\alpha_2 - 1}}) - (\varphi_{P_{\alpha_1 - 1}}^{N_{\alpha_2}} - \varphi_{P_{\alpha_1 - 1}}^{N_{\alpha_2 - 1}}). \end{aligned}$$

[¶] A.-L. Haji-Ali, F. Nobile, and R. Tempone. "Multi-Index Monte Carlo: When Sparsity Meets Sampling". Numerische Mathematik, 1-40, (2015)

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Then the MIMC estimator can be written as

$$\mathcal{A}_{\text{MIMC}} = \sum_{\boldsymbol{\alpha} \in \mathcal{I}} \frac{1}{M_{\boldsymbol{\alpha}}} \sum_{m=1}^{M_\alpha} \boldsymbol{\Delta}_{\boldsymbol{\alpha}} \phi(\omega_{\boldsymbol{\alpha},m})$$

for some *properly chosen* index set $\mathcal{I} \subset \mathbb{N}^2$ and optimal number of samples $M_{\boldsymbol{\alpha}}$ for every $\boldsymbol{\alpha} \in \mathcal{I}$.

[¶] A.-L. Haji-Ali, F. Nobile, and R. Tempone. "Multi-Index Monte Carlo: When Sparsity Meets Sampling". Numerische Mathematik, 1-40, (2015)

MIMC optimal work complexity

$$\begin{aligned} \textbf{Bias:} \quad & |\mathrm{E}[\Delta_{\boldsymbol{\alpha}} \phi]| = \mathcal{O}\left(\exp(-w_1 \alpha_1 - w_2 \alpha_2)\right), \\ \textbf{Variance:} \quad & \mathrm{Var}[\Delta_{\boldsymbol{\alpha}} \phi] = \mathcal{O}\left(\exp(-s_1 \alpha_1 - s_2 \alpha_2)\right), \\ \textbf{Work:} \quad & \mathrm{Work}[\Delta_{\boldsymbol{\alpha}} \phi] = \mathcal{O}\left(\exp(\gamma_1 \alpha_1 + \gamma_2 \alpha_2)\right). \end{aligned}$$

MIMC optimal work complexity

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The optimal set $\mathcal{I}$

$$\mathcal{I}(L) = \Big\{(\alpha_1, \alpha_2) \in \mathbb{N}^2 \ : \ (2w_1 + \gamma_1 - s_1)\,\alpha_1 + (2w_2 + \gamma_2 - s_2)\alpha_2 \leq L\Big\}$$

MIMC optimal work complexity

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The optimal set $\mathcal{I}$

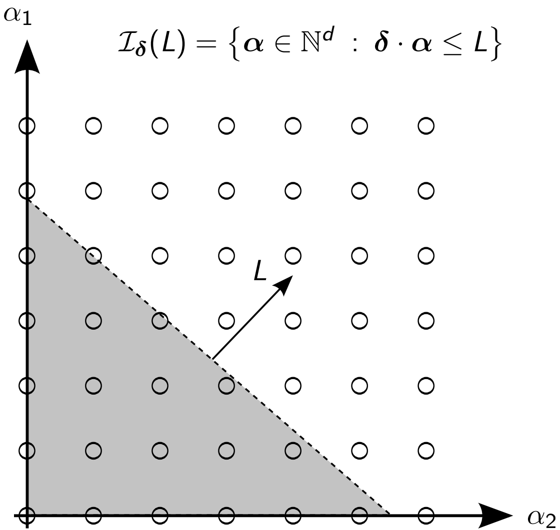
$$\mathcal{I}(L) = \Big\{(\alpha_1, \alpha_2) \in \mathbb{N}^2 \;: \\ (2w_1 + \gamma_1 - s_1)\,\alpha_1 + (2w_2 + \gamma_2 - s_2)\alpha_2 \le L\Big\}$$

Letting $\zeta = \max\left(\frac{\gamma_1 - s_1}{2w_1}, \frac{\gamma_2 - s_2}{2w_2}\right)$, then the optimal work of MIMC is

$$\mathcal{O}\left(\mathrm{TOL}^{-2(1+\max(0,\zeta))} \log\left(\mathrm{TOL}^{-1}\right)^{\mathfrak{p}}\right)$$

for $\mathfrak{p} \ge 0$.

Optimal choice of $\mathcal{I}$: Total degree set

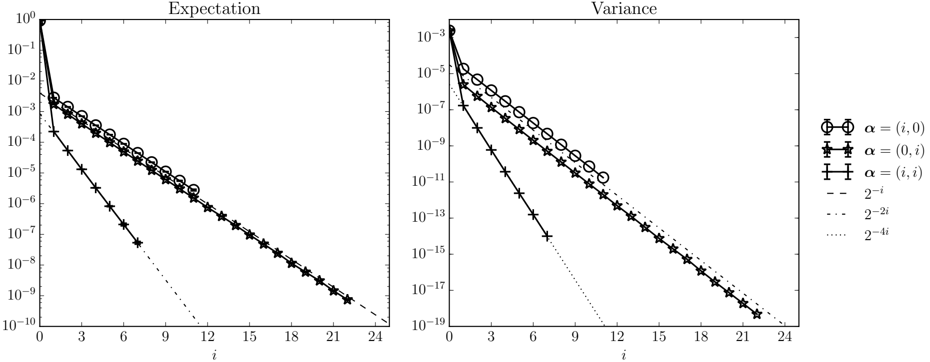


MIMC, with partitioning samplers

- Let $P_{\alpha_1} = 2^{\alpha_1}$ and $N_{\alpha_2} = 2^{\alpha_2}$.
- Build correlated samples by
  - Sampling 2^{α_1} and sub-sampling two identically-distributed, independent groups of $2^{\alpha_1 - 1}$ particles out of them.
  - At the same time, by using the same Brownian paths discretized with different meshes 2^{α_2} and $2^{\alpha_2 - 1}$.
  - Use MIMC levels: Mixed differences!

MIMC, with partitioning samplers

- Let $P_{\alpha_1} = 2^{\alpha_1}$ and $N_{\alpha_2} = 2^{\alpha_2}$.

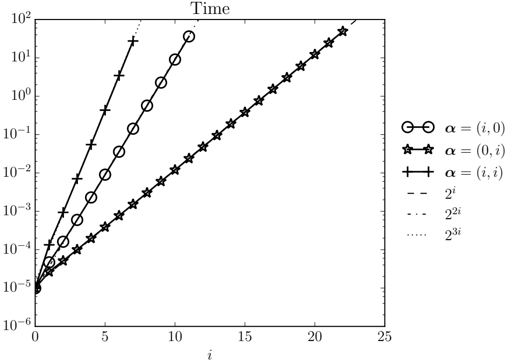


$w_1, w_2 = 1, s_1 = s_2 = 2$

Notice higher rates for mixed difference.

MIMC, with partitioning samplers

- Let $P_{\alpha_1} = 2^{\alpha_1}$ and $N_{\alpha_2} = 2^{\alpha_2}$.



$$\gamma_1 = 2, \gamma_2 = 1$$

MIMC, with partitioning samplers

- Let $P_{\alpha_1} = 2^{\alpha_1}$ and $N_{\alpha_2} = 2^{\alpha_2}$.
- **Summary:**

$$\left.\begin{array}{c} w_1 = w_2 = 1 \\ s_1 = s_2 = 2 \\ \gamma_1 = 2\gamma_2 = 2 \end{array}\right\} \Longrightarrow \zeta = \max\left(\frac{\gamma_1 - s_1}{2w_1}, \frac{\gamma_2 - s_2}{2w_2}\right) = 0$$

- The optimal set

$$\mathcal{I}(L) = \left\{(\alpha_1, \alpha_2) \in \mathbb{N}^2 \ : \ 2\alpha_1 + 3\alpha_2 \leq L\right\}$$

- The optimal work of the asymptotically unbiased MIMC is

$$\mathcal{O}\left(\mathrm{TOL}^{-2} \log\left(\mathrm{TOL}^{-1}\right)^2\right)$$

Summary

Method	Work complexity
Monte Carlo	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
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MLMC in P and N	$\mathcal{O}\left(\mathrm{TOL}^{-4}\right)$
MLMC in P and N, partitioning	$\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$
MIMC	$\mathcal{O}\left(\mathrm{TOL}^{-2}\log\left(\mathrm{TOL}^{-1}\right)^2\right)$

Numerical Example: MIMC vs. MLMC

$$X_{p|P}^{n|N} - X_{p|P}^{n-1|N} = \left(\vartheta_p + \frac{0.4}{P} \sum_{q=1}^{P} \sin(X_{p|P}^{n|N} - X_{q|P}^{n|N}) \right) \frac{T}{N} + 0.4 \Delta W_{p|P}^{n|N}$$

$$X_{p|P}^{0|N} \sim \mathcal{N}(0, 0.2)$$

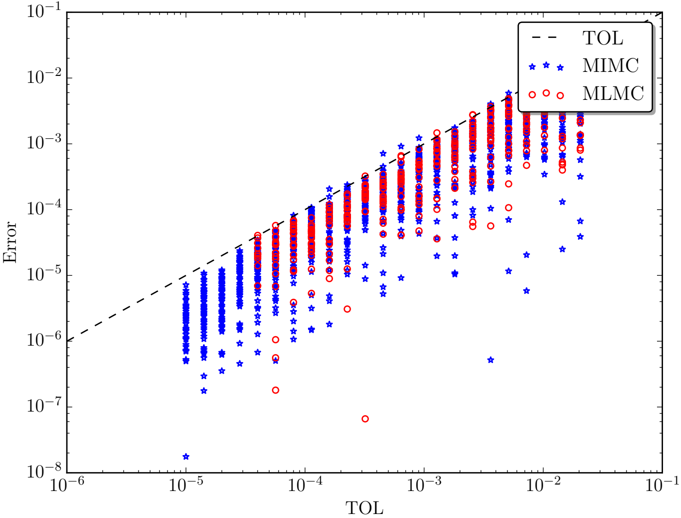
where $\vartheta_p \sim \mathcal{U}(-0.2, 0.2)$. The quantity of interest is

$$\phi_P^N = \frac{1}{P} \sum_{p=1}^{P} \cos\left(X_{p|P}^{N|N} \right).$$

for $T = 1$.

Numerical Example: MIMC vs. MLMC

for $T = 1$.



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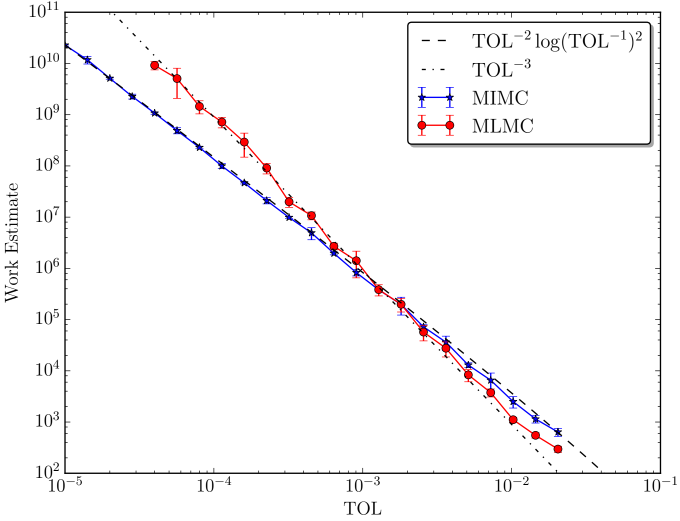
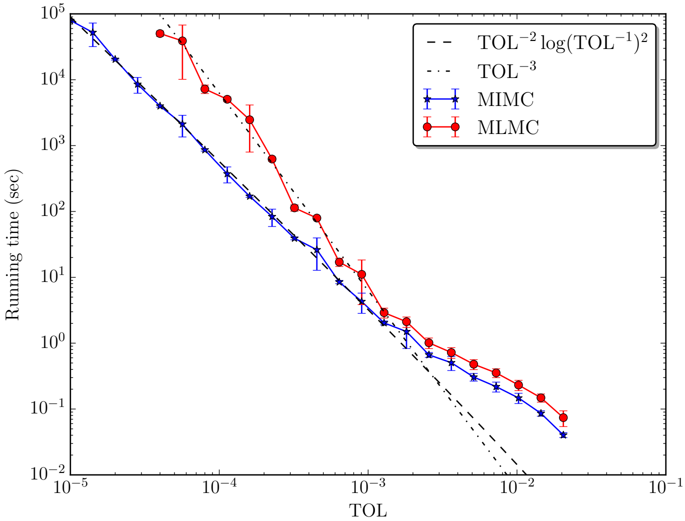
for $T = 1$.



Numerical Example: MIMC vs. MLMC

for $T = 1$.



Conclusions

- MLMC applied to particle systems in the mean-field limit is not trivial since the variance of the quantity of interest depends on the number of particles, P.
- The partitioning estimator achieves much better L^2 convergence rate w.r.t. P.
- Considerable computational saving by using MIMC, from TOL^{-4} to $\mathrm{TOL}^{-2} \log^2(\mathrm{TOL})$.
- Other applications: higher dimension particle systems (e.g. crowd flow).
- MLMC and MIMC Theory: working on estimates on mixed differences.