# Multilevel Monte Carlo for Data Assimilation via coupling algorithms

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# Outline

# Orientation

Aim: Approximately sample from sequence of probability distributions $\eta_{\infty,m}$, which need to be approximated by some $\eta_{L,m}$, for $m = 1, 2, \ldots,$ each given by a Bayesian inversion.

Solution: The multilevel Monte Carlo (MLMC) framework is extended to the multilevel particle and ensemble Kalman filters (MLPF and MLEnKF).

- MLMC methods *reduce cost to* error$= \mathcal{O}(\varepsilon)$, can be used in the case that $\eta_{L,m}$ can be sampled from directly [G08].
- Here it is assumed that $\eta_{\infty,m}$ and $\eta_{L,m}$ cannot be sampled from directly.
- Particle filters are sequential Monte Carlo (SMC) algorithms which provide consistent approximations of such distributions [D04].
- EnK filters are SMC algorithms which provide approximations of such distributions [E06].

# Outline

# Example: expectation for SDE [G08]

Estimation of expectation of solution of intractable stochastic differential equation (SDE).

$$dX = f(X)dt + \sigma(X)dW, \quad X_0 = x_0 \ .$$

Aim: estimate $\mathbb{E}(g(X_T))$.
We need to

(1) Approximate, e.g. by Euler-Maruyama method with resolution $h$:

$$X_{n+1} = X_n + hf(X_n) + \sqrt{h}\sigma(X_n)\xi_n, \quad \xi_n \sim N(0,1).$$

(2) Sample $\{X_{N_T}^{(i)}\}_{i=1}^N$, $N_T = T/h$.

# Single level Monte Carlo

Aim: Approximate $\eta_\infty(g) := \mathbb{E}_{\eta_\infty}(g)$ for $g : E \to \mathbb{R}$.

Monte Carlo approach

- Discretize the space $\Rightarrow$ *approximate* distribution $\eta_L$.
- Sample $U_L^{(i)} \sim \eta_L$ i.i.d., and approximate

$$\eta_L(g) := \mathbb{E}_{\eta_L}(g) \approx \widehat{Y}_L^{N_L} := \frac{1}{N_L} \sum_{i=1}^{N_L} g(U_L^{(i)}).$$

- Mean square error (MSE) $\mathbb{E}\{\widehat{Y}_L^{N_L} - \mathbb{E}_{\eta_\infty}[g(U)]\}^2$ splits into

$$\underbrace{\mathbb{E}\{\widehat{Y}_L^{N_L} - \mathbb{E}_{\eta_L}[g(U)]\}^2}_{\text{variance}=\mathcal{O}(N_L^{-1})} + \underbrace{\{\mathbb{E}_{\eta_L}[g(U)] - \mathbb{E}_{\eta_\infty}[g(U)]\}^2}_{\text{bias}}$$

- Cost to achieve MSE$= \mathcal{O}(\varepsilon^2)$ is Cost$(U_L^{(i)}) \times \varepsilon^{-2}$.

# Multilevel Monte Carlo I

Introduce a hierarchy of discretization levels $\{\eta_l\}_{l=1}^{L}$ and define $Y_l = \{\mathbb{E}_{\eta_l}[g(U)] - \mathbb{E}_{\eta_{l-1}}[g(U)]\}$, with $\eta_{-1} := 0$.
Observe the telescopic sum

$$\mathbb{E}_{\eta_L}[g(U)] = \sum_{l=0}^{L} Y_l.$$

Each term can be unbiasedly approximated by

$$Y_l^{N_l} = \frac{1}{N_l} \sum_{i=1}^{N_l} \{g(U_l^{(i)}) - g(U_{l-1}^{(i)})\}$$

where $g(U_{-1}^{(i)}) := 0$.

# Multilevel Monte Carlo II

Multilevel Monte Carlo approach:

- Sample i.i.d. $(U_l, U_{l-1})^{(i)} \sim \bar{\eta}^l$, such that $\int \bar{\eta}^l du_{l-1,l} = \eta_{l,l-1}$, and approximate
$$\eta_L(g) \approx \widehat{Y}_{L,\text{Multi}} := \sum_{l=0}^{L} Y_l^{N_l} .$$
- Mean square error (MSE) given by
$$\mathbb{E}\{\widehat{Y}_{L,\text{Multi}} - \mathbb{E}_{\eta_\infty}[g(U)]\}^2 = \underbrace{\mathbb{E}\{\widehat{Y}_{L,\text{Multi}} - \mathbb{E}_{\eta_L}[g(U)]\}^2}_{\text{variance}=\sum_{l=0}^{L} V_l/N_l} + \underbrace{\{\mathbb{E}_{\eta_L}[g(U)] - \mathbb{E}_{\eta_\infty}[g(U)]\}^2}_{\text{bias}} .$$
- Fix bias by choosing $L$. Minimize cost $C = \sum_{l=0}^{L} C_l N_l$ as a function of $\{N_l\}_{l=0}^{L}$ for fixed variance $\Rightarrow N_l \propto \sqrt{V_l/C_l}$.

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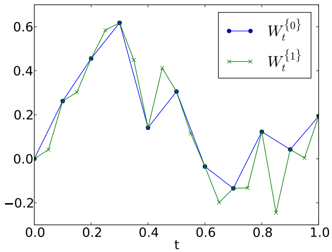
# Illustration of pairwise coupling

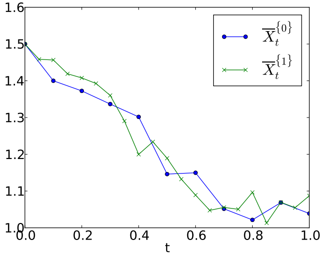
Pairwise coupling of trajectories of an SDE:

$$X^1_{n+1} = X^1_n + hf(X^1_n) + \sqrt{h}\sigma(X^1_n)\xi_n, \quad \xi_n \sim N(0,1), \quad n = 0, \ldots, N_1$$

$$X^0_{n+1} = X^0_n + (2h)f(X^0_n) + \sqrt{2h}\sigma(X^0_n)(\xi_{2n} + \xi_{2n+1}), \ \ n = 0, \ldots, (N_1 - 1)/2.$$




(a) Weiner process $W^1_n = \sqrt{h}\sum_{i=0}^n \xi_n$, $W^0_n = W^1_{2n}$.




(b) Stochastic process driven by Weiner process.

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# Multilevel vs. Single level

Assume $h_l = 2^{-l}$ and there are $\alpha$, and $\beta > \zeta$ such that

(i) weak error $|\mathbb{E}[g(U_l) - g(U)]| = \mathcal{O}(h_l^\alpha)$.

(ii) strong error $\mathbb{E}|g(U_l) - g(U)|^2 = \mathcal{O}(h_l^\beta) \Rightarrow V_l = \mathcal{O}(h_l^\beta)$,

(iii) computational cost for a realization of $g(U_l) - g(U_{l-1})$, $C_l \propto h_l^{-\zeta}$.

Both cases require $h_L^\alpha = \mathcal{O}(\varepsilon) \Rightarrow L \propto |\log \varepsilon|$.

- Single level cost $C = \mathcal{O}(\varepsilon^{-\zeta/\alpha-2})$ : cost per sample is $C_L \propto \varepsilon^{-\zeta/\alpha}$, and fixed $V \propto \varepsilon^2 \Rightarrow N_L \propto \varepsilon^{-2}$.
- Multilevel cost $C_{\mathrm{ML}} = \mathcal{O}(\varepsilon^{-2})$ : $N_l \propto \varepsilon^{-2} K_L h_l^{(\beta+\zeta)/2}$, so $V \propto \varepsilon^2$ and $C \propto \varepsilon^{-2} K_L^2$ for $K_L = \sum_{l=0}^{L} h_l^{(\beta-\zeta)/2} = \mathcal{O}(1)$ [G08] – cost of simulating a scalar random variable.
- Example: Milstein solution of SDE

$$C = \mathcal{O}(\varepsilon^{-3}) \quad \text{vs.} \quad C_{\mathrm{ML}} = \mathcal{O}(\varepsilon^{-2}).$$

# Outline

# Filtering Problem

Framework:

$$X_{n+1} \sim Q(X_n, \cdot)\,,$$

$$Y_n | X_n \text{ has density } G(y_n, x_n).$$

Objective: Approximate $\mathbb{E}(\varphi(X_n)|y_1, \ldots, y_n)$, where $y_k \in \mathbb{R}^m$ is a realization of $Y_k$ and $\varphi : \mathbb{R}^d \to \mathbb{R}$.

The joint probability density of state and observations given initial data $X_0 \sim \eta_0$ is

$$\prod_{i=1}^{n} G(y_i, x_i) Q(x_{(i-1)}, x_i) \eta_0(x_0).$$

Further assume we can only approximate $X^\ell_{n+1} \sim Q^\ell(X^\ell_n, \cdot)$, at resolutions indexed by $\ell = 0, 1, 2, \ldots$, where $Q^\infty := Q$.

# Outline

# Particle filter

$Q^L(x,\cdot)$ : kernel associated to level $L$ with initial condition $x$. This will be Euler-Maruyama discretization of an SDE.

Generate $\widehat{\eta}^{N_L}_{L,m} = \frac{1}{N_L}\sum_{i=1}^{N_L} \delta_{\widehat{U}^{L,i}_m} \approx \widehat{\eta}_{L,m}$ using

**Particle filter algorithm**:

**For** $i = 1, \ldots, N_L$, draw $\widehat{U}^{L,i}_0 \sim \mu_0$.

**Initialize** $m = 1$. **Do**

(i) **For** $i = 1, \ldots, N_L$, draw $U^{L,i}_m \sim Q^L(\widehat{U}^{L,i}_{m-1}, \,\cdot\,)$;

(ii) **For** $k = 1, \ldots, N_L$, draw $I^{L,k}_m$ according to multinomial distribution $\{w^i_m\}_{i=1}^{N_L}$, where $w^i_m := G_m(U^{L,i}) / \sum_{j=1}^{N_L} G_m(U^{L,j})$.

(iii) $\widehat{U}^{L,k}_m \leftarrow U^{L,I^{L,k}_m}_m$.

$m \leftarrow m+1$

# Outline

# Multilevel particle filter

$M^\ell([x,y],\cdot)$ : coupled kernel with marginals $Q^\ell(x,\cdot)$ and $Q^{\ell-1}(y,\cdot)$.

Generate $\widehat{\eta}^{ML}_{L,m} = \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} (\delta_{\widehat{U}^{\ell,i}_{m,1}} - \delta_{\widehat{U}^{\ell,i}_{m,2}}) \approx \widehat{\eta}_{L,m}$, with $\delta_{\widehat{U}^{0,i}_{m,2}} := 0$, using

**Multilevel particle filter algorithm**:

**For** $\ell = 0,1,\ldots,L$ and $i = 1,\ldots,N_\ell$, draw $\widehat{U}^{\ell,i}_{0,1} \sim \mu_0$, and let $\widehat{U}^{\ell,i}_{0,2} = \widehat{U}^{\ell,i}_{0,1}$.

**Initialize** $m = 1$. **Do**

(i) **For** $\ell = 0,1,\ldots,L$ and $i = 1,\ldots,N_\ell$, draw $(U^{\ell,i}_{m,1}, U^{\ell,i}_{m,2}) \sim M^\ell((\widehat{U}^{\ell,i}_{m-1,1}, \widehat{U}^{\ell,i}_{m-1,2}), \ \cdot\ )$;

(ii) **For** $\ell = 0,1,\ldots,L$ and $k = 1,\ldots,N_\ell$, draw $(I^{\ell,k}_{m,1}, I^{\ell,k}_{m,2})$ according to the coupled resampling procedure;

(iii) $(\widehat{U}^{\ell,k}_{m,1}, \widehat{U}^{\ell,k}_{m,2}) \leftarrow (U^{\ell,I^{\ell,k}_1}_{m,1}, U^{\ell,I^{\ell,k}_2}_{m,2})$ for $k = 1,\ldots,N_\ell$.

$m \leftarrow m+1$

# Coupled resampling I

Given $\{\{U_{m,1}^{\ell,i}, U_{m,2}^{\ell,i}\}_{i=1}^{N_\ell}\}_{\ell=0}^{L}$,

For $\ell = 0, 1, \ldots, L$ define

$$w_{m,1}^{\ell,i} = \frac{G_m(U_{m,1}^{\ell,i})}{\sum_{j=1}^{N_\ell} G_m(U_{m,1}^{\ell,j})} \quad \text{and} \quad w_{m,2}^{\ell,i} = \frac{G_m(U_{m,2}^{\ell,i})}{\sum_{j=1}^{N_\ell} G_m(U_{m,2}^{\ell,j})}.$$

# Coupled resampling II

**Coupled resampling procedure**:

**a.** with probability $\alpha_m^\ell = \sum_{i=1}^{N_\ell} w_{m,1}^{\ell,i} \wedge w_{m,2}^{\ell,i}$, draw $I_{m,1}^{\ell,k}$ according to

$$\mathbb{P}(I_{m,1}^{\ell} = i) = \frac{w_{m,1}^{\ell,i} \wedge w_{m,2}^{\ell,i}}{\sum_{j=1}^{N_\ell} w_{m,1}^{\ell,j} \wedge w_{m,2}^{\ell,j}}, \qquad i = 1, \ldots, N_\ell.$$

and let $I_{m,2}^{\ell,k} = I_{m,1}^{\ell,k}$.

**b.** with probability $1 - \alpha_m^\ell$, draw $(I_{m,1}^{\ell,k}, I_{m,2}^{\ell,k})$ *independently* according to the probabilities

$$\mathbb{P}(I_{m,1}^{\ell} = i) = [w_{m,1}^{\ell,i} - w_{m,1}^{\ell,i} \wedge w_{m,2}^{\ell,i}]/(\sum_{j=1}^{N_\ell} w_{m,1}^{\ell,j} - w_{m,1}^{\ell,j} \wedge w_{m,2}^{\ell,j});$$

$$\mathbb{P}(I_{m,2}^{\ell} = i) = [w_{m,2}^{\ell,i} - w_{m,1}^{\ell,i} \wedge w_{m,2}^{\ell,i}]/(\sum_{j=1}^{N_\ell} w_{m,2}^{\ell,j} - w_{m,1}^{\ell,j} \wedge w_{m,2}^{\ell,j}),$$

for $i = 1, \ldots, N_\ell$.

Assuming 1-step strong error convergence order $\beta$, weak error order $\alpha$, and cost $\zeta$ (for Euler-Maruyama $\alpha = \beta = \zeta = 1$), the following theorem holds:

### Theorem (JKLZ15)

*Under suitable regularity assumptions on $M^\ell$ and G, for any $\varphi \in \mathcal{B}_b(\mathbb{R}^d) \cap Lip(\mathbb{R}^d)$*

$$\mathbb{E}[\{\widehat{\eta}_m^{ML}(\varphi) - \widehat{\eta}_m^{L}(\varphi)\}^2] \lesssim \sum_{\ell=1}^{L} \frac{h_\ell^{\beta/2}}{N_\ell}$$

*In particular, for $\beta/2 > \zeta$, L and $\{N_\ell\}_{\ell=0}^{L}$ can be chosen such that MSE$= \mathcal{O}(\varepsilon^2)$ for computational cost$= \mathcal{O}(\varepsilon^{-2})$.*

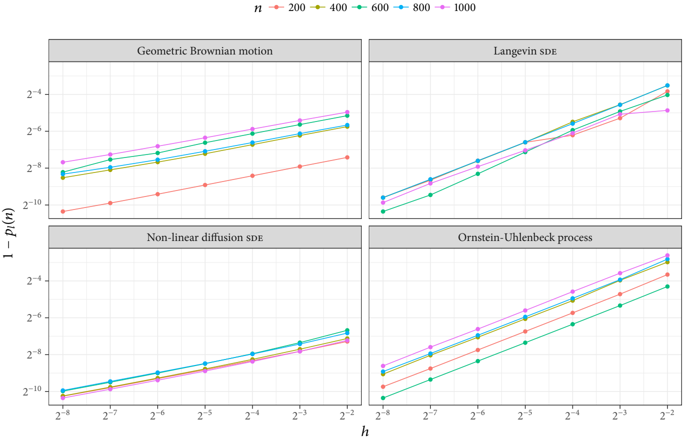
Note that the coupled resampling effectively reduces rate $\beta \to \beta/2$.

# Numerical examples

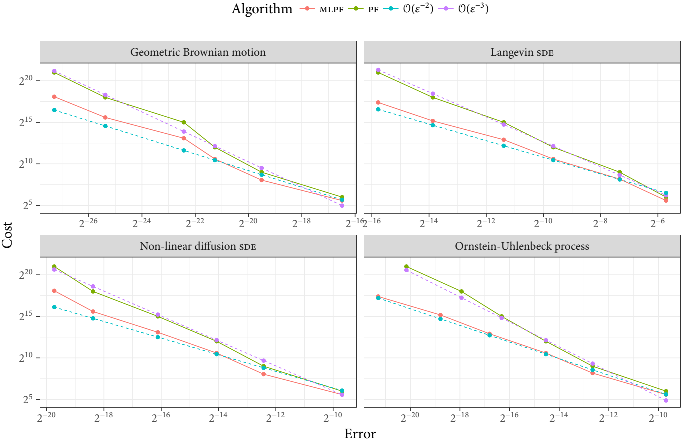
- $dX_t = a(X_t)dt + b(X_t)dW_t, \qquad X_0 = x_0,$
  with $X_t \in \mathbb{R}^d$, $t \geq 0$ and $\{W_t\}_{t\in[0,T]}$ a Brownian motion of appropriate dimension.
- Partial observations $\{y_1, \ldots, y_n\}$ available and $Y_k|X_k$ has a density function $G(y_k, x_k)$.
- Euler Maruyama discretization with $h_\ell = 2^{-\ell}$. For constant diffusion $\beta = 2$, for non-constant diffusion $\beta = 1$.

| Example | $a(x)$ | $b(x)$ | $G(y;x)$ | $\varphi(x)$ |
|---|---|---|---|---|
| OU | $\theta(\mu - x)$ | $\sigma$ | $\mathcal{N}(x, \tau^2)$ | $x$ |
| GBM | $\mu x$ | $\sigma x$ | $\mathcal{N}(\log x, \tau^2)$ | $x$ |
| Langevin | $\frac{1}{2}\nabla \log \pi(x)$ | $\sigma$ | $\mathcal{N}(0, \tau^2 e^x)$ | $\tau^2 e^x$ |
| NLM | $\theta(\mu - x)$ | $\frac{\sigma}{\sqrt{1+x^2}}$ | $\mathcal{L}(x, s)$ | $x$ |

# Numerical examples: rate



# Numerical examples: cost



# Outline

# EnKF

Observation $\quad G(u_i, y_i) \propto \exp(-\frac{1}{2}|\Gamma^{-\frac{1}{2}}(Hu_i - y_i)|^2) \quad ,$

$$\text{Prediction} \quad \begin{cases} u_{j+1}^{L,n} & \sim Q^L(\widehat{u}_j^{L,n}, \cdot\,),\; n = 1, \dots, N, \\ m_{j+1}^L & = \frac{1}{N}\sum_{n=1}^N u_{j+1}^{L,n}\,, \\ C_{j+1}^L & = \frac{1}{N-1}\sum_{n=1}^N (u_{j+1}^{L,n} - m_{j+1}^L)(u_{j+1}^{L,n} - m_{j+1}^L)^T\,. \end{cases}$$

$$\text{Analysis} \quad \begin{cases} K_{j+1}^L & = C_{j+1}^L H^T (H C_{j+1}^L H^T + \Gamma)^{-1}, \\ \widehat{u}_{j+1}^{L,n} & = (I - K_{j+1}^L H) u_{j+1}^{L,n} + K_{j+1} y_{j+1}^{L,n},\; n = 1, \dots, N, \\ y_{j+1}^n & = y_{j+1} + \xi_{j+1}^n,\; n = 1, \dots, N. \end{cases}$$

with $\xi_{j+1}^n \sim N(0, \Gamma)$ i.i.d.

# EnKF converges under weak assumptions

$$\text{Prediction} \begin{cases} \overline{u}^L_{j+1} & \sim Q^L(\widehat{\overline{u}}^L_j, \cdot\,), \\ \overline{m}^L_{j+1} & = \mathbb{E}[\overline{u}^L_{j+1}], \\ \overline{C}^L_{j+1} & = \mathbb{E}[(\overline{u}^L_{j+1} - \overline{m}^L_{j+1})(\overline{u}^L_{j+1} - \overline{m}^L_{j+1})^T]. \end{cases}$$

$$\text{Analysis} \begin{cases} \overline{K}^L_{j+1} & = \overline{C}^L_{j+1} H^T (H\overline{C}^L_{j+1} H^T + \Gamma)^{-1}, \\ \widehat{\overline{u}}^L_{j+1} & = (I - \overline{K}^L_{j+1} H)\overline{u}^L_{j+1} + \overline{K}^L_{j+1} \overline{y}_{j+1}, \\ \overline{y}_{j+1} & = y_{j+1} + \xi_{j+1}. \end{cases}$$

Then for suitable $\varphi$

$$\left\| \frac{1}{N} \sum_{n=1}^{N} \varphi(u_j^{L,n}) - \mathbb{E}[\varphi(\overline{u}^L_j)] \right\|_p \leq C N^{-1/2}$$

# Outline

# MLEnKF [HLT16]

**For** $\ell = 1, \ldots, L$, and $n = 1, \ldots, N_\ell$, draw $(u_{1,1}^{\ell,n}, u_{1,2}^{\ell,n}) \overset{\text{i.i.d.}}{\sim} M^\ell((u_0, u_0), \cdot)$. And draw $u_1^{0,n} \sim Q^0(u_0, \cdot)$.
**Initialize** $j = 1$. **Do**

(i) Compute the MLMC Kalman gain estimator $K_j^{\mathrm{ML}}$.

(ii) **For** $\ell = 1, \ldots, L$, and $n = 1, \ldots, N_\ell$, independently draw $y_j^{\ell,n} \sim N(y_j, \Gamma)$, and for $i = 1, 2$ compute

$$\widehat{u}_{j,i}^{\ell,n} = (I - K_j^{\mathrm{ML}} H) u_{j,i}^{\ell,n} + K_j^{\mathrm{ML}} y_j^{\ell,n} .$$

Set $j = j + 1$.

(iii) **For** $\ell = 1, \ldots, L$, and $n = 1, \ldots, N_\ell$, independently draw $(u_{j,1}^{\ell,n}, u_{j,2}^{\ell,n}) \overset{\text{i.i.d.}}{\sim} M^\ell((\widehat{u}_{j-1,1}^{\ell,n}, \widehat{u}_{j-1,2}^{\ell,n}), \cdot)$. And draw $U_j^{0,i} \sim Q^0(\widehat{u}_{j-1}^{0,n}, \cdot)$.

# MLMC Kalman gain

$$K_j^{\mathrm{ML}} = C_j^{\mathrm{ML}} H^T (H C_{+,j}^{\mathrm{ML}} H^T + \Gamma)^{-1} ,$$

with $C_{+,j}^{\mathrm{ML}}$ the positive semi-definite modification of the multilevel covariance estimate $C_j^{\mathrm{ML}}$, given by

$$C_j^{\mathrm{ML}} = \frac{1}{N_0} \sum_{i=1}^{N_0} u_j^{0,i} (u_j^{0,i})^T - \left( \frac{1}{N_0} \sum_{i=1}^{N_0} u_j^{0,i} \right) \left( \frac{1}{N_0} \sum_{i=1}^{N_0} u_j^{0,i} \right)^T$$
$$+ \sum_{\ell=1}^{L} \left[ \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \left( u_{j,1}^{\ell,i} (u_{j,1}^{\ell,i})^T - u_{j,2}^{\ell,i} (u_{j,2}^{\ell,i})^T \right) - \right.$$
$$\left. \left( \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} u_{j,1}^{\ell,i} \right) \left( \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} u_{j,1}^{\ell,i} \right)^T + \left( \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} u_{j,2}^{\ell,i} \right) \left( \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} u_{j,2}^{\ell,i} \right)^T \right] .$$

# MLEnKF

Denote $\mu_{L,m}^{ML} := \sum_{\ell=0}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} (\delta_{u_{m,1}^{\ell,i}} - \delta_{u_{m,2}^{\ell,i}}) \approx \mu_{L,m}$, with $\delta_{u_{m,2}^{0,i}} := 0$, where $\mu_{L,m}$ is the level $L$ limiting measure.

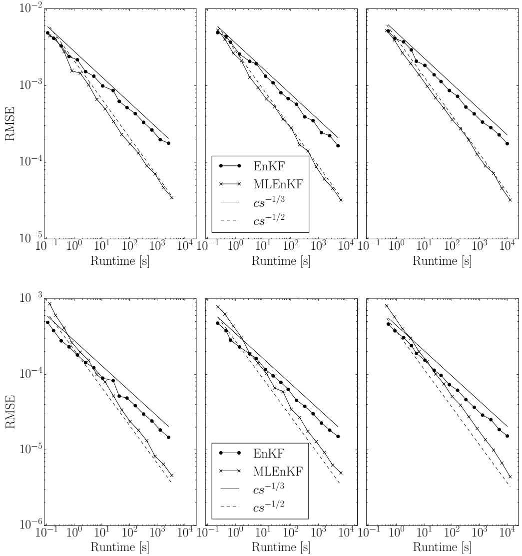
**Theorem (HLT16)**

*Assume the coefficients of the SDE are globally Lipschitz, the initial condition is in $L^p$ for all $p \geq 2$, and $\beta > \zeta$. Then, for appropriate $\varphi$, and for $\varepsilon > 0$, one can choose $L$ and $\{N_\ell\}_{\ell=0}^{L}$ so that*

$$\left\| \mu_{L,m}^{ML}(\varphi) - \mu_{L,m}(\varphi) \right\|_p \leq C\varepsilon$$

*for some $C > 0$, for a cost of $\mathcal{O}((\log \varepsilon)^{2n} \varepsilon^{-2})$.*

# Error of MLEnKF for OU SDE



# Outline

# Summary

- Multilevel particle filter (MLPF) can perform asymptotically as well as MLMC.
- Cost-to-$\varepsilon$ can be asymptotically the same as for a scalar random variable!
- MLPF strong error is effectively reduced by coupled resampling $\beta \to \beta/2$.
- Using approximate coupling on the smoothing distribution, and importance sampling, strong error can be preserved: illustrated with particle MCMC in [JKLZ17].
- MLEnKF has a spurious n-dependent logarithmic penalty $(\log \varepsilon)^{2n}$ on cost (not present in simulations).
- MLEnKF for spatial models (PDE) recently introduced [CHLNT17].

# https://sites.google.com/site/kodyjhlaw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# Thank you!