Clustered Multilevel Monte Carlo (C-MLMC)

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1 Problem Setup and Notation

We aim to estimate $\mathbb{E}[P]$ for a path-dependent payoff P under an SDE model. Using the Multilevel Monte Carlo (MLMC) framework, we define level-wise differences:

$$\Delta P_{\ell} = \begin{cases} P_0, & \text{if } \ell = 0, \\ P_{\ell} - P_{\ell-1}, & \text{if } \ell \geq 1. \end{cases}$$

Let $V_{\ell} = \text{Var}[\Delta P_{\ell}]$, and C_{ℓ} be the average cost per sample on level ℓ . Classical MLMC chooses:

$$N_\ell \propto \sqrt{rac{V_\ell}{C_\ell}}$$

to meet the MSE constraint:

$$\sum_{\ell=0}^{L} \frac{V_{\ell}}{N_{\ell}} \le (1-\theta)\varepsilon^{2}.$$

2 Motivation for Clustering

When the variance is concentrated in rare modes of the input space, uniform sampling becomes inefficient. C-MLMC improves efficiency by:

- Extracting features from simulation details,
- \bullet Clustering samples via K-means into n_c variance modes,
- Estimating per-cluster statistics $(P_{\ell,c}, V_{\ell,c})$,
- Allocating samples proportional to $\sqrt{P_{\ell,c}V_{\ell,c}}$.

3 C-MLMC Algorithm

Algorithm 1 Clustered MLMC Estimator

Require: Simulator $f(\ell, N, \texttt{return_details})$, feature extractor φ , tolerance ε , pilot size N_0 , clusters n_c

- 1: Initialize level count $L \leftarrow L_{\min}$, precision control $\theta \in (0,1)$
- 2: for each level $\ell \leq L$ do
- 3: Run pilot: simulate $\{(Y_i, d_i)\}_{i=1}^{N_0} \leftarrow f(\ell, N_0, \text{true})$
- 4: Extract features: $\phi_i \leftarrow \varphi(d_i)$
- 5: Cluster $\{\phi_i\}$ into n_c clusters using K-means
- 6: Compute:

$$P_{\ell,c} = \frac{\#\{\text{samples in cluster } c\}}{N_0}, \quad V_{\ell,c} = \text{Var}\left(Y_i \mid \phi_i \in \text{cluster } c\right)$$

- 7: Store cluster-wise sums $S_{\ell,c} = \sum Y_i$, and counts $N_{\ell,c}$
- 8: end for
- 9: while not converged do
- 10: Aggregate level stats: $V_{\ell} = \sum_{c=1}^{n_c} P_{\ell,c} V_{\ell,c}, C_{\ell} = \frac{\text{total cost}}{N_{\ell}}$
- 11: Allocate level-wise samples: $N_{\ell} \propto \sqrt{V_{\ell}/C_{\ell}}$
- 12: Allocate cluster-wise samples:

$$N_{\ell,c} \propto \sqrt{P_{\ell,c} V_{\ell,c}}$$
 s.t. $\sum_{c} N_{\ell,c} = N_{\ell}$

- 13: **for** each level $\ell > 0$, cluster c **do**
- 14: Sample until $N_{\ell,c}$ accepted samples with cluster label c
- 15: Accumulate cluster sum $S_{\ell,c} \leftarrow S_{\ell,c} + \sum Y_i$
- 16: Update counts $N_{\ell,c} \leftarrow N_{\ell,c} + \#\text{new samples}$
- 17: end for
- 18: Bias check: extrapolate tail bias using $\widehat{\mathbb{E}}[\Delta P_{\ell}] \sim \mathcal{O}(2^{-\alpha \ell})$; if large, increment L
- 19: end while
- 20: Final estimator:

$$\hat{P} = \frac{1}{N_0} \sum_{i=1}^{N_0} Y_{0,i} + \sum_{\ell=1}^{L} \sum_{c=1}^{n_c} \frac{S_{\ell,c}}{N_{\ell,c}}$$

4 Optimal Allocation via $\sqrt{P_c V_c}$

To minimize the estimator variance:

$$\operatorname{Var}(\hat{Y}) = \sum_{c=1}^{n_c} \frac{P_c^2 V_c}{N_c}, \quad \text{subject to} \quad \sum_{c=1}^{n_c} N_c = N,$$

the optimal allocation is:

$$N_c \propto P_c \sqrt{V_c} \quad \Rightarrow \quad \text{weights} \propto \sqrt{P_c V_c}.$$

5 Estimator Properties

Each cluster-wise estimator

$$\hat{Y}_{\ell,c} = \frac{S_{\ell,c}}{N_{\ell,c}}$$

is unbiased for its conditional mean, and the full estimator

$$\hat{P} = \sum_{\ell=0}^{L} \hat{Y}_{\ell}, \quad \hat{Y}_{\ell} = \begin{cases} \frac{1}{N_0} \sum_{i=1}^{N_0} Y_{0,i}, & \ell = 0, \\ \sum_{c=1}^{n_c} \frac{S_{\ell,c}}{N_{\ell,c}}, & \ell \ge 1 \end{cases}$$

is an unbiased estimator of $\mathbb{E}[P_L]$. Bias $\mathbb{E}[P-P_L]$ is controlled via extrapolation on the last levels.

6 Conclusion

C-MLMC enhances standard MLMC by stratifying variance-heavy simulations via clustering and allocating samples proportionally to $\sqrt{P_cV_c}$. This stratified estimator preserves unbiasedness while improving computational efficiency in high-variance regimes.