Unlocking Efficiency in Complex Computations: Multilevel Bayesian Quadrature for Challenging Integrals

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This post introduces a novel Bayesian probabilistic numerical method proposed in the paper *Multilevel Bayesian Quadrature* published in the International Conference on Artificial Intelligence and Statistics (AISTATS), and selected for oral presentation. Besides, it was awarded the James Nelson Prize in 2024.Monte Carlo methods are common choices for scientists and engineers to solve complex integral problems. However, they can sometimes seem overwhelming when dealing with expensive scientific models, either from a computational or financial point of view. Our proposed method, Multilevel Bayesian Quadrature (MLBQ), has improved computational efficiency significantly, which means using the same computational resources for evaluation, our method achieves better accuracy.

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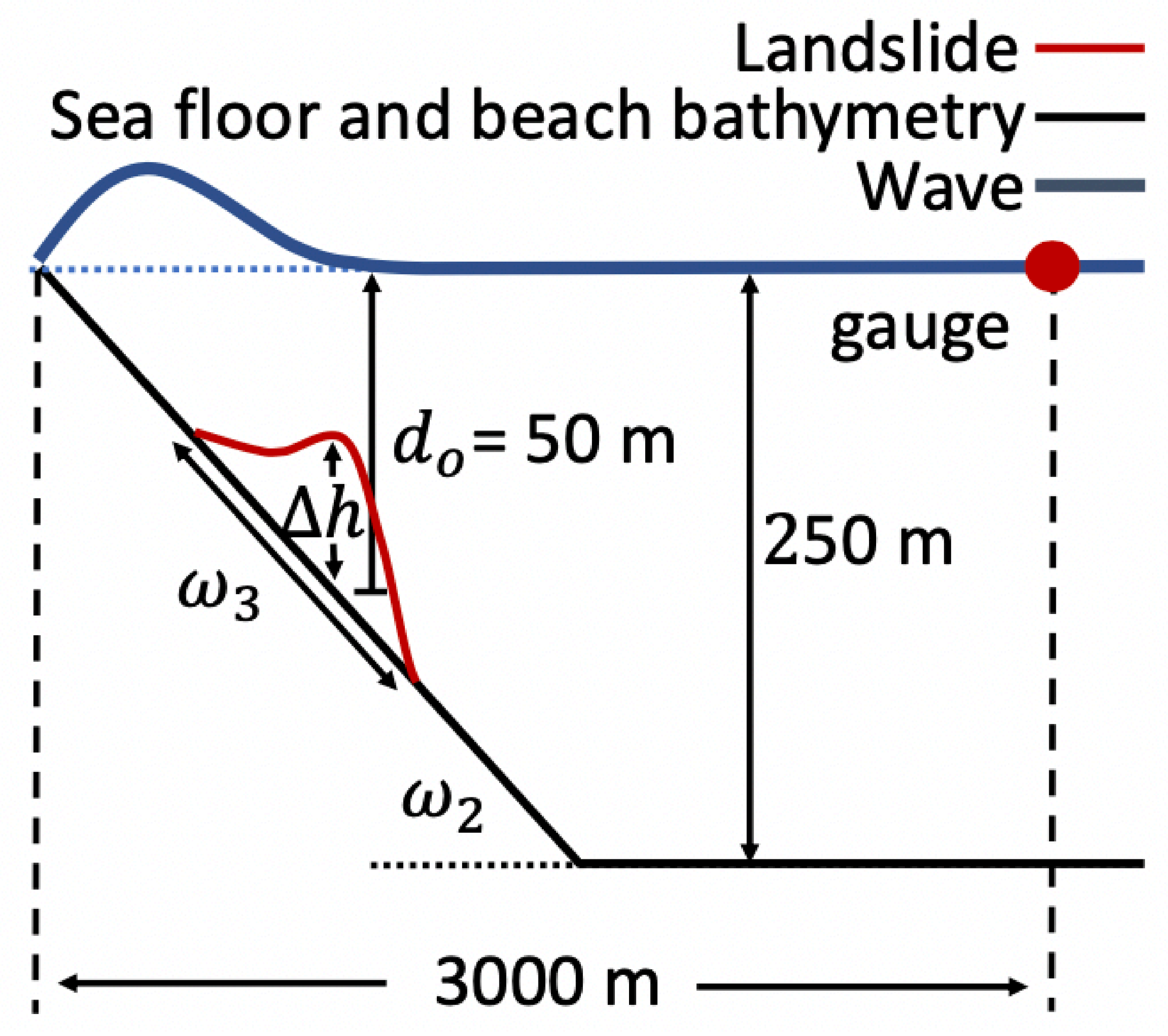
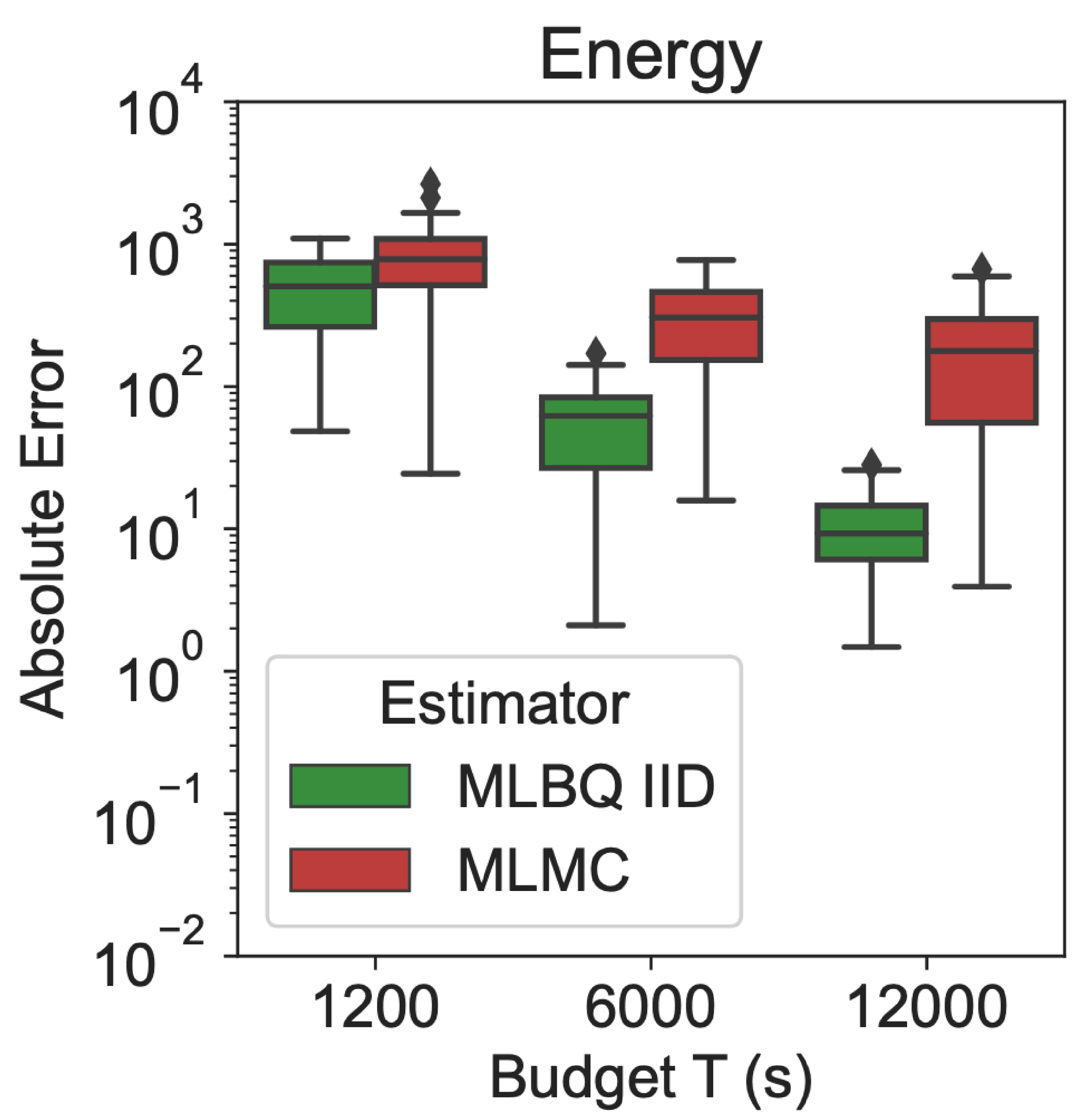


(a)



(b)

Figure 1: (a)：Sketch of submerged landslide-generated tsunami. (b)：Absolute error of multilevel Monte Carlo estimates and multilevel Bayesian quadrature estimates for the integral estimation of tsunami example

Figure 1 illustrates an example of tsunamis. Scientists modelling such landslide-generated tsunamis must solve a complex system of differential equations describing wave evolution. In this context, designers of tsunami-resistant buildings and prevention structures might be interested in estimating quantities that are functions of the solutions of the differential equations, such as energy flux. However, there will usually be some uncertainty associated with certain physical parameters, such as those characterising the slope or size of the landslide. This uncertainty is represented through probability distributions, necessitating the computation of the expected value of the quantities of interest.

The main challenge here is that, in order to obtain highly accurate estimates, standard Monte Carlo methods would require very fine time and space meshes to solve the differential equations and evaluate the integrand at a fixed high accuracy level, leading to significant costs. Furthermore, in some cases, a high-resolution simulation of tsunamis in the realistic world can take a few minutes per run, making thousands or hundreds of thousands of runs infeasible, as Monte Carlo methods require large samples.

In contrast, multilevel Bayesian quadrature utilises several approximations with different meshes (each corresponding to a level) and employs fewer evaluations of the expensive levels. At each accuracy level, multilevel Bayesian quadrature employs a Bayesian nonparametric method, Bayesian quadrature, to estimate the integral of increments between each two consecutive levels. With a fixed computational budget, this allows multilevel Bayesian quadrature to obtain much more accurate estimates than standard Monte Carlo methods. Multilevel Bayesian quadrature combines the advantages of multilevel Monte Carlo and Bayesian quadrature, enabling it to incorporate prior knowledge as well as utilise multifidelity models. The fast convergence property of multilevel Bayesian quadrature makes it potentially valuable in fields where complex models may be involved, such as geophysics, engineering, etc.

References

1. Li, K., Giles, D., Karvonen, T., Guillas, S. and Briol, F. X. (2023). Multilevel Bayesian Quadrature. In International Conference on Artificial Intelligence and Statistics (AISTATS), pp. 1845-1868. PMLR 1.

Kaiyu Li
Kaiyu is interested in uncertainty quantification, computational statistics and machine learning. Her work involves developing and applying new methods to investigate and quantify uncertainties in computer models.
https://ceciliakaiyu.github.io/