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Utilizing Cramers-van Mises distance for the Global Sensitivity Analysis of Monte Carlo Models

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An important aspect in the interpretation of a molecular simulation model is to quantify which parameter uncertainties have the most influence on the simulation results. We present an approach to such Global Sensitivity Analysis (GSA) on basis of the Cramers-von Mises distance. Unlike revalent approaches to GSA it combines the following properties: i) it is equally suited for deterministic as well as stochastic model outputs, ii) it is free of gradients, and iii) it can be estimated from (almost) any numerical quadrature. Using Low-Discrepency Sequences for quadrature and a prototypical first-principles kinetic Monte Carlo models, we examine the performance of the approach. We find that the approach converges in a modest number of quadrature points. Furthermore, it seems to be robust against even extreme relative noise. These properties make the method particularly suited for expensive (kinetic) Monte Carlo models, because only a relatively small number of rather inaccurate Monte Carlo estimates is needed.

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