Exotic forests and new higher order methods for the invariant measure of ergodic SDEs on Riemannian manifolds

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In many applications, such as stochastic optimization, molecular dynamics or statistical learning, one is interested in the long time behavior of stochastic dynamics evolving under geometrical constraints. Usual approaches often rely on penalization methods or extrinsic discretizations, which can lead to heavy computations, embeddings in high-dimensional spaces and strong restrictions on the time step. We consider a general class of ergodic stochastic differential equations evolving on Riemannian manifolds, which includes the Riemannian Langevin dynamics, and we develop numerical methods aimed at sampling their invariant measure specifically. As the analysis of the convergence order involves technical Taylor expansion, we introduce an algebraic formalism of exotic Butcher forests to systematically describe the algebraic operations underlying the intrinsic analysis for the invariant measure.
We present numerical experiments on different manifolds to illustrate the improved accuracy of the new methods.

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