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Ensemble Sampler For Infinite-Dimensional Inverse Problems

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Abstract : We introduce a Markov chain Monte Carlo (MCMC) sam-pler for infinite-dimensional inverse problems. Our sam-pler is based on the affine invariant ensemble sampler, which uses interacting walkers to adapt to the covariance structure of the target distribution. We extend this ensem-ble sampler for the first time to infinite-dimensional func-tion spaces, yielding a highly efficient gradient-free MCMC algorithm. Because our ensemble sampler does not require gradients or posterior covariance estimates, it is simple to implement and broadly applicable. In many Bayes-ian inverse problems, Markov chain Monte Carlo (MCMC) meth-ods are needed to approximate distributions on infinite-dimensional function spaces, for example, in groundwater flow, medical imaging, and traffic flow. Yet designing efficient MCMC methods for function spaces has proved challenging. Recent gradi-ent-based MCMC methods preconditioned MCMC methods, and SMC methods have improved the computational efficiency of functional random walk. However, these samplers require gradi-ents or posterior covariance estimates that may be challenging to obtain. Calculating gradients is difficult or impossible in many high-dimensional inverse problems involving a numerical integra-tor with a black-box code base. Additionally, accurately estimating posterior covariances can require a lengthy pilot run or adaptation period. These concerns raise the question: is there a functional sampler that outperforms functional random walk without requir-ing gradients or posterior covariance estimates? To address this question, we consider a gradient-free sampler that avoids explicit covariance estimation yet adapts naturally to the covariance struc-ture of the sampled distribution. This sampler works by consider-ing an ensemble of walkers and interpolating and extrapolating between walkers to make a proposal. This is called the affine in-variant ensemble sampler (AIES), which is easy to tune, easy to parallelize, and efficient at sampling spaces of moderate dimen-sionality (less than 20). The main contribution of this work is to propose a functional ensemble sampler (FES) that combines func-tional random walk and AIES. To apply this sampler, we first cal-culate the Karhunen–Loeve (KL) expansion for the Bayesian prior distribution, assumed to be Gaussian and trace-class. Then, we use AIES to sample the posterior distribution on the low-wavenumber KL components and use the functional random walk to sample the posterior distribution on the high-wavenumber KL components. Alternating between AIES and functional random walk updates, we obtain our functional ensemble sampler that is efficient and easy to use without requiring detailed knowledge of the target dis-tribution. In past work, several authors have proposed splitting the Bayesian posterior into low-wavenumber and high-wavenumber components and then applying enhanced sampling to the low-wavenumber components. Yet compared to these other samplers, FES is unique in its simplicity and broad applicability. FES does not require any derivatives, and the need for derivative-free sam-plers has previously been emphasized. FES also eliminates the requirement for posterior covariance estimates. Lastly, FES is more efficient than other gradient-free samplers in our tests. In two nu-merical examples, we apply FES to challenging inverse problems that involve estimating a functional parameter and one or more scalar parameters. We compare the performance of functional random walk, FES, and an alternative derivative-free sampler that explicitly estimates the posterior covariance matrix. We conclude that FES is the fastest available gradient-free sampler for these challenging and multimodal test problems.

Keywords : Bayesian inverse problems, Markov chain Monte Carlo, infinite-dimensional inverse problems, dimensionality reduction
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