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Implementation and tuning of Hamiltonian Monte Carlo for large linear inverse problems

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The Hamiltonian Monte Carlo method is a powerful tool for geophysical inverse problems. The sampler can draw much more informed models from a posterior probability using gradient information of the misfit functional than typical sampler such as the Metropolis-Hastings algorithm. Of course, the usefulness of the method is determined by the complexity of calculating the gradient of the misfit.

In this study a code is developed for linear inverse problems with Gaussian uncertainties in both prior and data. The code uses a freely available parallel linear algebra package to run large inversions (number of parameters > 10,000) on computing clusters.

At first, optimal tuning settings from the sampler are derived from the theory, leaving only one parameter for the user to tune. Mass matrix can be optimally chosen using the prior and data covariance matrices and forward model. Oscillation trajectory length and related tuning parameters can easily be inferred from this. For alternate (positive definite) mass matrices, the code also supplies automated methods to determine trajectory tuning parameters. Also ergodicity, correlated prior distributions and choice of kinetic energy are discussed.

As illustration, the posterior of a linear traveltime tomography model of 10201 blocks is appraised. When using an optimal tuned mass matrix based completely on prior information, proposal of only a 1,000 samples gives means subject to little change as the number of samples increases. It is shown that for alternate choices of mass matrices this convergence is much slower or even unpractical, due to unequal oscillations through phase space.