Assessment of two MCMC algorithms convergence for Bayesian estimation of the particle size distribution from multiangle dynamic light scattering measurements

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Dynamic light scattering (DLS) is a standard technique widely used to assess the particle size distribution (PSD) of a sample composed of particles dispersed in a liquid [1]. The size of particles ranges from a few nanometers to several micrometers. The increasing success of the DLS technique comes from the fact that it is easy to handle, non-destructive, fast, and requires no calibration process. Several instruments are commercially available, among them the Nano DS from CILAS. This technique is based on the analysis of the temporal fluctuations of light intensity scattered at a given angle by the dispersed particles illuminated by a Laser beam. Retrieving the PSD information from DLS measurements (time autocorrelation function (ACF)) that are generally corrupted by noise is known as a high ill-posed inverse problem [2].

Methods based on Bayesian inference have been recently investigated to solve this inverse problem [3-5]. In [6], we have proposed a new Bayesian inference method applied directly to the multiangle DLS measurements to improve multimodal PSDs estimation. The posterior probability density of interest is sampled using MCMC Metropolis-Hasting algorithm one variable at time. Figure 1 shows improvement of multimodal PSD estimation using the proposed method.

Since MCMC methods are associated in practice with unknown rates of convergence, the aim of the present work is to assess the convergence of the method proposed in [6] and of some other MCMC algorithms that can be used to sample the posterior probability density of interest [7]. To this end, we propose to use the simulation method recently proposed by the authors of [8] and which method help assess the MCMC algorithms efficiency. This simulation method is based on the evaluation of the Kullback divergence criterion requiring an estimate of the entropy of the algorithm successive densities.

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