

Efficient sampling in condensing particle systems

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Driven diffusive systems are models from non-equilibrium statistical mechanics where discrete and identical particles move on a fixed lattice. These systems conserve the number of particles and are used to model traffic dynamics, granular systems and various biological processes. Often these systems exhibit a condensation transition, [1]. This means there exists some critical density such that below this critical density sites occupations are distributed according to some stationary measure and the system is known to be in a fluid phase. As the density is increased above the critical density, a finite fraction of particles will accumulate on a single site while the surrounding sites will remain in the fluid phase. We wish to further understand the link between the condensation phenomena and attractivity in particle systems.

Certain classes of driven diffusive systems, known as Misanthrope processes, exhibit factorisable stationary distributions called product measures, [2] [3]. That is, the joint distribution of site occupations is factorisable and implies that single sites are distributed independently (and identically in the homogeneous case). In the grand-canonical ensemble, the stationary measures are parametrised by a number called the fugacity which controls the average number of particles in the system. In the canonical ensemble, the stationary measure is unique and can be expressed as the conditional version of the grand-canonical measure. For such models the mixing and relaxation times often scale like N^2 , where N is the number of particles in the system. For the zero-range process with constant rates see [4]. Methods of calculating mixing times are discussed in [5].

The main goal of this PhD project will be to sample from the generalized canonical distributions which are not necessarily of product form, with an improved computation time when comparing to the usual Markov chain Monte Carlo techniques. We will investigate various techniques to achieve this goal. One such method is to construct a basic coupling between two processes, which can be interpreted as a method of simulating two processes in parallel, one with N particles and the other with $N + 1$. Finding the probability of the extra particle given a particular configuration will allow us to define a growth rule which will give us configurations distributed according to the canonical stationary measure. This coupling technique is limited to attractive particle systems and therefore, this process will not allow us to sample from the stationary measure in general.

For simpler models with product measures the single-site marginal in the grand-canonical ensemble are known explicitly. Thus, we propose a method of sampling from the canonical measure, analogous to the binary search algorithm, as follows; Fix the number of lattice sites, say L , and distribute L independent uniform random variables between $[0, 1]$. Initialise a fugacity parameter and calculate the number of particles in the system using the grand-canonical measure. If the total number of particles is not as desired, change the fugacity parameter as appropriate.

For homogeneous Misanthrope processes, it can be shown that condensation cannot occur if the process is attractive. However, attractivity does not necessarily imply that the condensation phenomena cannot occur in other processes. For example, the so called chipping model, [6], where either all the particles at a site jump together or one particle is chipped of a site and added to a neighbour, [7]. Similar to Misanthrope processes, the transition from a fluid phase to condensed phase occurs at some critical density ρ_c . However, unlike the Misanthrope process, the chipping model does not exhibit stationary product measures. In fact it has been shown that the validity of a mean-field approximation depends on whether the dynamics is symmetric or asymmetric.

Within the next 6 months we plan to fully understand the most efficient sampling mechanisms for

models with stationary product measures, and study the chipping model and related processes as particular examples. A first step will be to simulate the various methods of sampling and compare them to numerical values of the product measure, when numerical values are accessible. Simulations should take the transition rates, system size and particle number as an input and outputs a sample of configurations distributed according to the canonical measure. Sampling methods can be compared directly by looking at simulation time for the algorithm.

References

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