Perfect Sampling for Gibbs Processes with a focus on Hard-sphere Models

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Abstract

We consider the problem of generating perfect samples from a Gibbs point process, a spatial process that is absolutely continuous with respect to a Poisson point process. Examples include area-interaction processes, Strauss processes, hard-sphere model and the Ising model. Traditionally, this problem is addressed using coupling from the past (CFTP) based methodologies. In this paper, we focus on acceptance-rejection based methods. Our key contribution is a novel importance sampling based acceptance-rejection methodology for generating perfect samples from Gibbs point processes, with a specific focus on a simpler setting of hard-sphere model (defined on a unit cube) that we analyze in an asymptotic regime where the number of spheres generated increases to infinity while the sphere radius decreases to zero at varying rates. We compare analytically and numerically, the computational effort required by the proposed method with naive acceptance-rejection based methods as well as with popular dominated CFTP based algorithms. Our analysis of the hard-sphere models relies upon identifying the large deviations decay rates of no overlap probability of spheres when their centers are distributed as a homogeneous Poisson point process; these results may also be of independent interest.

1 Introduction

Perfect sampling, that is, generating unbiased samples from a target distribution, is an important and exciting area of research in stochastic simulation. Perfect sampling is also referred to as perfect simulation or exact sampling. In this paper, we consider amongst the most important families of point processes known as Gibbs point processes, that is, the family of distributions that are absolutely continuous with respect to the distribution of a Poisson point process; hereafter, the distributions of Gibbs point processes are referred as Gibbs distributions. Examples include area-interaction processes, Strauss processes, spatial loss systems including hard-sphere models, Ising models, among others. We introduce and investigate a novel methodology for generating perfect samples from Gibbs distributions. This methodology combines importance sampling (IS) and acceptance-rejection (AR) techniques to achieve substantial performance improvement. In particular, we focus on simpler hard-sphere models. These models can be described as a set of spheres such that their centers constitute a Poisson point process on a bounded Euclidean space conditioned that no two spheres overlap with each other. In statistical physics, there is a large body of work related to the hard-sphere fluid model. See, for e.g., [30, 28, 1, 2, 27, 31, 22, 6]. The hard-sphere model is also important in modelling adsorption of latexes or proteins on solid surfaces [34, 33] and references therein]. Our results can be used to assess the stationary behaviour of Code Division Multiple Access (CDMA) wireless networks. Analysis of performance of CDMA involves viewing it as a spatial loss system where arrivals are typically assumed to be Poisson and a new call is accepted only if it guarantees that Signal-to-Interference-Noise-Ratio at each receiver
is at least above a threshold value; see, e.g., [4], [5] and references therein.

**Literature Review:** The existing literature offers several perfect sampling methods for Gibbs distributions, such as the dominated coupling from the past (dominated CFTP) [26, 25, 20], Fill’s algorithm [14] and the backward-forward algorithm (BFA) by Ferrari et al. [13]; also see [21, 17]. As mentioned in [17], all these methods are, in some sense, complementary to each other. They take advantage of an important property that any given Gibbs distribution can be realized as an invariant measure of a spatial birth-and-death process, call it the target process. For example, the main ingredient of the dominated CFTP method is to construct a birth-and-death process backward in time starting from its steady-state at time zero such that it dominates the target process, and then use thinning on the dominating process to construct coupled upper and lower bound processes forward in time such that the coalescence of these two bounding processes assures a perfect sample from the invariant measure of the target process. A crucial drawback of the dominated CFTP method is that it exhibits so called impatient-user bias (a bias induced by the dependence of the running time of the algorithm on the output sample). Fill’s algorithm is free of impatient-user bias, but applicable only under certain monotonicity properties (see [15] and [35]). The BFA is based on the construction of the clan of ancestors that uses thinning of a dominating process and extends the applicability to infinite-volume measures. This also exhibits the impatient-user bias.

**Our Contributions:** AR algorithms are applicable under more general stability conditions than those considered for other methods. They are free of impatient-user bias and involve neither thinning nor coupling (which are crucial for other methods). Despite being an obvious alternative to the existing methods, to the best of our knowledge, in the context of Gibbs point processes, the use of AR methods is still largely unexplored (except brief discussions, for e.g., in [16] and [21]). AR methods for Gibbs point processes are amenable to further algorithmic enhancements that may substantially decrease the expected running time of the algorithm. The proposed methodology provides one such enhancement. To highlight the significance of the proposed methodology, we compare its running time complexity for the hard-sphere model with that of both the naive AR and the dominated CFTP methods. This effectiveness analysis is based on our large deviations analysis of the no overlap probability of spheres when their centers are distributed as a homogeneous Poisson point process.

- Our key contribution is that we propose a novel IS based AR algorithm for generating perfect samples from Gibbs distributions by partitioning the underlying configuration space such that different IS techniques can be developed on different subsets of the partition. We consider a hard-sphere model that is absolutely continuous with respect to the homogeneous marked Poisson point process on $[0, 1]^d$ with intensity $\lambda$, where the mark associated with a point is the radius of the sphere centered at that point. We assume that the radii of the spheres are independent and identical in distribution to $R/\eta$ for some $\eta > 0$ and a bounded positive random variable $R$. The hard-sphere model is further divided into two, depending on the definition of spheres: In the Euclidean-hard-sphere model, each sphere is defined to be an Euclidean sphere, and in the torus-hard-sphere model, the space $[0, 1]^d$ is treated as a torus so that each boundary sphere can loop over to the opposite boundaries. Applicability of the proposed algorithm is illustrated using the above hard-sphere models in two scenarios. In the first scenario, all the spheres are assumed to be the same size with a fixed radius ($R$ is a fixed positive constant). We develop an IS technique under which spheres are generated sequentially such that each sphere is generated uniformly over the non-blocking region created by the existing spheres; here blocking means that the center of the sphere falling in this
set would create an overlap. In the second scenario, we consider the general case where spheres have i.i.d. radii. In this scenario, in addition to the above IS technique, we use exponential twisting on the radius distribution. In both the scenarios, the new method provably substantially improves the performance of the algorithm compared to the naive AR method.

- The implementation of the proposed IS technique for the hard-sphere model can be difficult because it involves identification of the non-blocking regions for generating the centers of the spheres, and knowing the non-blocking regions exactly may not be possible. To remedy this, we adapt the proposed method using a hyper-cubic grid on \([0, 1]^d\), where the non-blocking regions are approximated using the grid. We optimize the cell edge length of the grid for each \(\lambda\) to minimize the running time complexity of the algorithm.

- To compare the performance of the proposed method (as well the naive AR method) with the dominated CFTP method proposed by Kendall and Møller [26], we consider a spatial birth-and-death process known as a loss system, where births are marked points on an Euclidean space and each birth is accepted only if the resulting state of the system satisfies a given acceptance criteria. An accepted birth stays in the system for a mean one exponentially distributed random time. We derive a lower bound on the expected running time complexity of the dominated CFTP algorithm for generating perfect samples from the steady-state of the loss system. Furthermore, some of the alternative dominated CFTP methods proposed in the literature are discussed. These alternative methods are applicable if the target Gibbs point process is a pairwise interaction processes. One such method is by Huber [20] (also see [21]). Numerical comparisons are provided for all the methods discussed above.

- We conduct large deviations analysis of the non-overlapping probability of spheres as \(\lambda \to \infty\) when their centers constitute a homogeneous Poisson point process on the unit cube \([0, 1]^d\) with the total intensity \(\lambda\) and the radius of each sphere is independent and identical in distribution to \(R/\lambda^\eta\), \(\eta d > 0\), where again \(R\) is a positive bounded random variable. This large deviations analysis is useful in the study of the asymptotic behaviour of the expected running time complexities of the AR and the dominated CFTP methods for hard-sphere models; these large deviations results may also be of independent interest.

**Organization:** Section 2 provides definitions of spatial point processes and spatial birth-and-death processes. Section 3 and Section 4 present, respectively, a naive AR method and the proposed IS based AR method for generating perfect samples from Gibbs point processes. The expected running time complexity analysis of AR methods for the hard-sphere models are provided in Section 5. The grid based IS technique is presented in Section 6. In Section 7, a review of the dominated CFTP method proposed by Kendall and Møller [26] in the context of loss system is presented and a lower bound on its expected running time complexity is derived. This section also discusses an alternative dominated CFTP method proposed by Huber [20] for pairwise interaction processes. Section 8 illustrates the efficiency of the proposed methodology using simple numerical experiments. Paper is concluded in Section 9.

### 2 Spatial Point Processes

**Notation:** \(X \sim F\) denotes that the distribution of a random variable \(X\) is \(F\). \(\text{Poi}(\lambda)\) and \(\text{Bern}(p)\) denote, respectively, Poisson distribution with mean \(\lambda > 0\) and Bernoulli distribution with success probability \(p\). The uniform distribution on \([0, 1]\) is denoted by \(\text{Unif}([0, 1])\). The function \(I(A)\) takes value 1 if event \(A\) occurs, otherwise it takes value 0. A measure \(\mu_1\) is absolutely continuous...
with respect to measure $\mu_2$ on a measurable set $A$ if $\mu_1(B \cap A) = 0$ for any measurable $B$ such that $\mu_2(B \cap A) = 0$. For any probability measure $\mu$, $\mathbb{P}_\mu(A)$ denotes the probability of an event $A$ under the law $\mu$, and $\mathbb{E}_\mu[\cdot]$ denotes the associated expectation. Whenever possible, we drop the subscript and write $\mathbb{P}(\cdot)$ (and $\mathbb{E}[\cdot]$ for expectation); in this case, we make sure that all the random elements involved in the expression are well defined beforehand. For any non-negative real valued functions $f$ and $g$, write $f(x) = O(g(x))$ if $\limsup_{x \to \infty} \frac{f(x)}{g(x)} \leq c$ for some constant $c$, $f(x) = \Omega(g(x))$ if $g(x) = O(f(x))$, and $f(x) = o(g(x))$ if $\limsup_{x \to \infty} \frac{f(x)}{g(x)} = 0$. Write $f(x) = \Theta(g(x))$ if the both $f(x) = O(g(x))$ and $f(x) = \Omega(g(x))$ are true. For any real value $x$, the largest integer $n$ such that $n \leq x$ is denoted by $\lfloor x \rfloor$ and the smallest integer $n$ such that $n \geq x$ is denoted by $\lceil x \rceil$.

**Poisson Point Processes:** Consider a measurable space $\mathbf{G} \subseteq \mathbb{R}^d$ and a Radon measure $\nu$ on $\mathbf{G}$. Let $\mathcal{G}$ be the set of all locally finite multisets defined as follows:

$$\mathcal{G} = \{(x_1, x_2, \ldots, x_n) : n = 0, 1, 2, \ldots, \infty \text{ and } x_i \in \mathbf{G}, \forall i \leq n\},$$

where the case $n = 0$ corresponds to the empty set denoted by $\emptyset$. A point process is a random element $\mathbf{X}$ on $\mathcal{G}$. For any $\mathbf{X} \in \mathcal{G}$, $|A \cap \mathbf{X}|$ denotes the number of points of $\mathbf{X}$ in $A \subseteq \mathbb{R}^d$.

A random element $\mathbf{X} \in \mathcal{G}$ is called Poisson point process (PPP) with intensity measure $\nu$ if for any separable measurable subset $S \subseteq \mathbf{G}$ with $\nu(S) < \infty$, the finite multiset $\mathbf{X} \cap S = \{X_1, X_2, \ldots, X_N\}$ is an i.i.d. sequence such that $X_i \sim \nu(dx)/\nu(G)$ and $N \sim \text{Poi}(\nu(S))$. A PPP on $\mathbb{R}^d$ is called $\kappa$-homogeneous if the intensity $\nu(dx) = \kappa dx$ for some constant $\kappa > 0$. A binomial point process (BPP) with $n$ points and distribution $\nu(dx)/\nu(S)$ on a separable measurable subset $S \subseteq \mathbf{G}$ with $\nu(S) < \infty$ is a PPP conditioned that the total number of points in $S$ is $n$. If $\nu(dx)$ is uniform over $S$, then the BPP is called homogeneous. A marked point process (MPP) on $\mathbf{G} \times \mathcal{M}$ is a PPP on $\mathbf{G}$ such that each point of the PPP has an independent mark belonging to a mark space $\mathcal{M}$. An important MPP is the germ-grain model on $\mathbb{R}^d \times \mathcal{M}$, where a collection of points (called germs) in $\mathbb{R}^d$ constitute a PPP and, for some $m$, each point has an independent $\mathbb{R}^m$-valued mark to describe the compact Borel subset (called grain) of $\mathbb{R}^d$ at that point.

**Gibbs Point Processes:** Suppose that $\mu^0$ is the law of an MPP on $\mathbf{B} \times \mathcal{M}$ with intensity $\nu(d(x,y)) = \kappa(dx) \times \vartheta(dy)$, for some intensity measure $\kappa$ on $\mathbb{R}^d$ and mark distribution $\vartheta$ on the mark space $\mathcal{M}$, where the Borel set $\mathbf{B} \subseteq \mathbb{R}^d$ such that $\lambda := \kappa(B) < \infty$. Gibbs distribution $\mu$ restricted to $\mathbf{B}$ has a Radon-Nikodym derivative with respect to $\mu^0$ given by

$$\frac{d\mu}{d\mu^0}(\mathbf{X}) = \frac{\exp(-\beta V(\mathbf{X}))}{Z}, \quad (1)$$

for any locally finite multiset $\mathbf{X} \subseteq \mathbf{B} \times \mathcal{M}$, where $\beta \in \mathbb{R}$ is a constant known as inverse temperature, $V$ is known as potential function and is non-negative, and the normalizing constant $Z := Z(\kappa, \beta, V, \mathbf{B}) = \mathbb{E}_{\mu^0}[\exp(-\beta V(\mathbf{X}))]$. We assume that the potential function $V$ is non-degenerate (that is, $V(\{x\}) < \infty$) and hereditary (that is, $V(\mathbf{X}) \leq V(\mathbf{X}')$ for all $\mathbf{X} \subseteq \mathbf{X}'$). Until unless stated specifically, the above definitions of $\mu^0$, $\mu$, $\lambda$ and $Z$ are valid throughout the paper.

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1 Definition of a multiset (see [7]): A multiset is a collection of objects (called elements) in which elements may occur more than once. The number of times an element occurs in a multiset is called its multiplicity. The cardinality $|A|$ of a multiset $A$ is the sum of the multiplicities of its elements.
**Pairwise interaction point processes:** An important class of Gibbs point processes are pairwise interaction point processes (see, for e.g., [9]), which have a potential functions of the form

\[ V^I(\mathcal{X}) := c n + \sum_{1 \leq i < j \leq n} f(\|x_i - x_j\|), \text{ for } \mathcal{X} = \{x_1, x_2, \ldots, x_n\}, \]

for some constant \( c \in \mathbb{R} \) and function \( f : \mathbb{R}_+ \rightarrow \mathbb{R} \cup \{\infty\} \), where \( \|\cdot\| \) denotes the Euclidean norm. One important example is hard-sphere model with fixed radius, where \( \beta = 1, c = 0 \) and there exists a parameter \( r > 0 \) such that \( f(s) = \infty \) if \( s \leq 2r \), otherwise, \( f(s) = 0 \) (that is, if we assume that each point in \( \mathcal{X} \) is the center of a sphere with radius \( r \) then \( V^I(\mathcal{X}) = 1 \) if no two spheres overlap, otherwise, \( V^I(\mathcal{X}) = 0 \)). Another well studied model is Strauss process, where \( \beta > 0, c < 0 \) and \( f(s) = I(s \leq r) \) for some parameter \( r > 0 \). Refer to [24] for generalizations of pairwise interaction point processes, and refer to, for e.g., [9, 17] and [32] for more details on point processes.

### 2.1 Spatial Birth-and-death Processes

As highlighted earlier, every Gibbs distribution (recall Equation[1]) considered in this paper can be viewed as an invariant measure of a spatial birth-and-death point process. A process \( D = \{D(t) : t \in (-\infty, \infty)\} \) is called free birth-and-death process (or simply free process) if individuals arrive on space \( B \) with intensity \( \kappa(\cdot) \) and stay alive for random time exponentially distributed with mean one. Throughout the paper, we use the words birth and arrival interchangeably. Also, without loss of generality, we assume that all birth-and-death processes are càdlàg (right continuous with left limits). The generator of free process is given by

\[ \mathcal{A}^0 g(\mathcal{X}) = \int_{\mathbf{G}} \nu(x) \left[ g\left( \mathcal{X} \cup \{x\} \right) - g(\mathcal{X}) \right] dx + \sum_{x \in \mathcal{X}} \left[ g\left( \mathcal{X} \setminus \{x\} \right) - g(\mathcal{X}) \right], \]

and its invariant measure is \( \mu^0 \). Let \( \psi(\mathcal{X}) := \exp(-\beta V(\mathcal{X})) \), \( \mathcal{X} \subseteq \mathcal{G} \), and

\[ \ell(\mathcal{X}, x) := \frac{\psi(\mathcal{X} \cup \{x\})}{\psi(\mathcal{X})}, \quad \mathcal{X} \in \mathcal{G}, \ x \in \mathbf{G}, \]

where we take \( \ell(\mathcal{X}, x) = 0 \) when \( \psi(\mathcal{X}) = 0 \). The ratio \( \ell(\mathcal{X}, x) \) is well known as Papangelou conditional intensity. Assume that the following stability condition holds.

**Stability condition 1:** There exists a constant \( \sigma > 0 \) such that \( \ell(\mathcal{X}, x) \leq \sigma \) for all \( \mathcal{X} \in \mathcal{G}, x \in \mathbf{G} \).

The Stability condition 1 guarantees the hereditary of \( \psi \): \( \psi(\mathcal{X}) > 0 \) whenever \( \psi(\mathcal{Y}) > 0 \) for \( \mathcal{X} \subseteq \mathcal{Y} \). Let

\[ \mathcal{A} g(\mathcal{X}) = \int_{\mathbf{G}} \nu(x) \ell(\mathcal{X}, x) \left[ g(\mathcal{X} \cup \{x\}) - g(\mathcal{X}) \right] dx + \sum_{x \in \mathcal{X}} \left[ g(\mathcal{X} \setminus \{x\}) - g(\mathcal{X}) \right] \]

\[ = \int_{\mathbf{G}} \sigma \nu(x) \frac{\ell(\mathcal{X}, x)}{\sigma} \left[ g(\mathcal{X} \cup \{x\}) - g(\mathcal{X}) \right] dx + \sum_{x \in \mathcal{X}} \left[ g(\mathcal{X} \setminus \{x\}) - g(\mathcal{X}) \right]. \]

Suppose that \( \mathcal{A} \) is the generator of the birth-and-death process \( X = \{X(t) : t \in (-\infty, \infty)\} \). Then \( \mu \) is the unique invariant (up to a scaling factor) measure of \( X \); see, for e.g., [23]. The dynamics of the process \( X \) can be interpreted as follows: When \( X \) is in the state \( \mathcal{X} \in \mathcal{G} \), an individual arrives with intensity \( \sigma \nu(\cdot) \) and is accepted with probability \( \frac{\ell(\mathcal{X}, \cdot)}{\sigma} \). Every accepted birth stays for a random
time exponentially distributed with mean one. The process $X$ is referred as interacting process, since it is characterized by the interactions between the individuals alive.

**Loss System:** Loss system is a spatial birth-and-death process on a subset $B \subseteq \mathbb{R}^d$ such that there is an independent $\mathbb{R}^m$-valued mark associated with each birth that describes the compact grain at that point, and the steady-state distribution $\mu$ of the loss system is defined by

$$
\frac{d\mu}{d\mu_0}(X) = \frac{I(X \in \mathcal{A})}{\mathbb{P}_\mu(X \in \mathcal{A})}, \quad X \in \mathcal{G},
$$

where $\mathcal{A} \subset \mathcal{G}$ is called the set of all acceptable configurations. In other words, each birth is accepted only if the resulting state of the system belongs to $\mathcal{A}$ and every accepted birth stays in the system for a random time exponentially distributed with mean one. Here, we assume that the set $\mathcal{A}$ is such that the hereditary property is satisfied, that is, $I(X' \in \mathcal{A}) = 1$ implies that $I(X \in \mathcal{A}) = 1$ for all $X' \subseteq X$. One important example is the loss system driven by hard-spheres, where each birth is a point that denotes the center of a sphere and the associated mark denotes its radius. A birth is accepted only if it is not overlapping with any other sphere present in the system on its birth, that is, $\mathcal{A}$ is the set of all configurations with spheres that are not overlapping with each other (see Section 5).

### 3 Naive AR Algorithm

In this section, we present a simple naive acceptance-rejection based perfect sampling algorithm which applies to the Gibbs distributions under a more general stability condition. Recall (1) and that $\psi(X) = \exp(-\beta V(X))$. Assume $N \sim \text{Poi}(\lambda)$.

**Stability condition 2:** There exists a function $\sigma : \mathbb{N} \rightarrow \mathbb{R}_+$ such that $\mathbb{E}[\sigma(N)] < \infty$ and $\psi(X) \leq \sigma(n)$ for all $|X| = n, n \geq 0$.

A well known Ruelle stability condition has $\sigma(n) = r^n$ for $r > 0$. Suppose $X_n$ denotes the BPP on $B$ with $n$ points and distribution $\nu(N)$ such that $\frac{\nu(\cdot)}{\nu(N)}$. Let $M$ be an non-negative integer valued random variable with probability mass function (pmf) defined by

$$
\mathbb{P}(M = m) = \frac{e^{-\lambda} \sigma(m) \lambda^m}{m!}, \quad m \geq 0.
$$

(When Ruelle stability holds, $M \sim \text{Poi}(r \lambda)$.) By (1), the Gibbs measure

$$
\mu(A) = \frac{\mathbb{E}[\psi(X_n) I(X_n \in A)]}{\mathbb{E}[\psi(X_n)]} = \frac{1}{\mathbb{E}[\psi(X_n)]} \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} \mathbb{E}[\psi(X_n) I(X_n \in A)]
$$

$$
= \frac{\mathbb{E}[\sigma(N)]}{\mathbb{E}[\psi(X_n)]} \sum_{n=0}^{\infty} \frac{e^{-\lambda}}{n!} \frac{\lambda^n}{n!} \mathbb{E}[\psi(X_n) I(X_n \in A)]
$$

$$
= \frac{\mathbb{E}[\psi(X_M)] I(X_M \in A)}{\mathbb{E}[\psi(X_N)]} \frac{\mathbb{E}[\psi(X_N) I(X_N \in A)]}{\mathbb{E}[\psi(X_N)]} = \mathbb{P}(U \leq \frac{\psi(X_M) I(X_M \in A)}{\sigma(M) I(X_M \in A)}, X_M \in A),
$$

for every measurable $A \subseteq \mathcal{G}$, where $U \sim \text{Unif}([0,1]).$ Expression (4) leads to Algorithm (1) that generates perfect samples from $\mu$; the proof is straightforward and is omitted.


\textbf{Algorithm 1} Acceptance-Rejection Based Exact Sampling

1: Generate a sample $M$ (using (3))
2: Generate a realization $X_M$ of BPP with $M$ points and distribution $\nu(\cdot)/\nu(B)$
3: Generate $J \sim \text{Bern}(\psi(X_M)/\sigma(M))$
4: Return $X_M$ if $J = 1$. Otherwise, repeat from Step 1.

The probability that a configuration of $n$ points is accepted is proportional to $\sigma(n)\lambda^n P_n$, where $P_n := \frac{1}{\sigma(n)} E[\psi(X_n)]$.

\textbf{Remark 1} (Expected running time complexity). Let $T_{AR}$ be the average running time complexity of Algorithm 1 where the running time complexity denotes the expected number of elementary operations performed by the algorithm; every elementary operation takes at most a fixed amount of time. If we denote the acceptance probability and the running time complexity of an iteration, respectively, by $P_{acc}$ and $C_{itr}$, then the expected number of iterations to generate one sample is $1/P_{acc}$ and thus $T_{AR} = E[C_{itr}]/P_{acc}$.

\textbf{Remark 2} (Choice of $\sigma$). Note that

$$P_{acc} = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\sigma(n)\lambda^n}{n!} P_n = \frac{1}{E[\sigma(N)]} E_{\mu_\rho}[\psi(X)].$$

(5)

Therefore, if both $\sigma_1(\cdot)$ and $\sigma_2(\cdot)$ satisfying Stability condition 2 and $E[\sigma_1(N)] < E[\sigma_2(N)]$, then, by (5), it is always advisable to choose $\sigma_1(\cdot)$ over $\sigma_2(\cdot)$ (assuming that the complexity associated with generating samples using the pmf of $M$ for $\sigma_1(\cdot)$ is of the order of that for $\sigma_2(\cdot)$).

\textbf{Remark 3} (Insertion probability). Consider a birth-and-death process whose invariant measure is a Gibbs distribution. Insertion probability, or the probability that a birth in steady-state is accepted, is an important performance measure in statistical physics [36]. From the definition, births are Poisson and hence in the steady-state, the births see time averages (PASTA property holds), see, e.g., [37]. Thus the distribution of the number of customers seen by a birth in the steady-state is $\{\pi_n : n \geq 0\}$. Let $P_{ins}(n)$ be the conditional probability that the $n^{th}$ marked point is accepted given that the first $n-1$ marked points are accepted in a static experiment where $n$ marked points are generated in $G$ independently using the measure $\nu$. Then $P_{ins}(n+1) = P_{n+1}/P_n$ and that the insertion probability of a birth in the steady-state,

$$\frac{1}{\sum_{k=0}^{\infty} \sigma(k)\lambda^k P_k} \sum_{n=0}^{\infty} \sigma(n)\lambda^n P_n P_{ins}(n+1) = \frac{1}{\sum_{k=0}^{\infty} \sigma(k)\lambda^k P_k} \sum_{n=0}^{\infty} \sigma(n)\lambda^n P_{n+1},$$

can be easily estimated via simulation.

4 IS Based AR Algorithm

In this section, we further generalize the stability criteria and show how one can exploit IS techniques for enhancement of the performance of the AR method. The idea is to partition the configuration space $\mathcal{G}$ and identify separate IS measure on each subset of the partition such that the likelihood ratio associated with each IS measure is uniformly bounded. Such enhancements for the hard-sphere models are presented in Section 5. Let $\mathcal{G}_n := \{X \in \mathcal{G} : |X| = n\}$ and assume that
the following generalized stability condition holds.

**Stability condition 3:** For each $n \geq 0$, there exist $K_n \in \mathbb{N} \cup \{\infty\}$, a partition $\{D_{n,k}\}_{k=1}^{K_n}$ of $\mathcal{G}_n$, and a sequence of measures $\{\mu_{n,k}\}_{k=1}^{K_n}$ such that, for all $n \geq 0$, $\mu^0$ is absolutely continuous with respect to $\mu_{n,k}$ on $D_{n,k}$ with the likelihood ratio denoted by $L_{n,k}(\mathcal{X}) := \frac{d\mu_{n,k}}{d\mu} (\mathcal{X})$. Furthermore, suppose that $\{\sigma_{n,k}\}_{k=1}^{K_n}$ is a sequence of constants for each $n$ such that the following condition holds for each $n$ and each $k = 1, 2, \ldots, K_n$:

$$
\psi(\mathcal{X})L_{n,k}(\mathcal{X}) \leq \sigma_{n,k}, \text{ if } \mathcal{X} \in D_{n,k},
$$

and $\mathbb{E}\left[\sum_{k=1}^{K_n} \sigma_{n,k}\right] < \infty$, where $N \sim \text{Poi}(\lambda)$.

Under Stability condition 3, we write that

$$
\mu(A) \propto \mathbb{E}_{\mu^0}\left[\psi(\mathcal{X})I(\mathcal{X} \in A)\right] = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} \left(\sum_{k=1}^{K_n} \mathbb{E}_{\mu^0}\left[\psi(\mathcal{X})I(\mathcal{X} \in D_{n,k} \cap A)\right]\right)
$$

$$
= \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} \left(\sum_{k=1}^{K_n} \frac{\sigma_{n,k}}{\bar{\sigma}(n)} \mathbb{E}_{\mu_{n,k}}\left[\psi(\mathcal{X})L_{n,k}(\mathcal{X}) \frac{I(\mathcal{X} \in D_{n,k} \cap A)}{\sigma_{n,k}}\right]\right),
$$

where $\bar{\sigma}(n) := \sum_{k=1}^{K_n} \sigma_{n,k}$. Further by letting $C(\lambda) = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!}$ and $U \sim \text{Unif}([0, 1])$, we have

$$
\mu(A) \propto \frac{1}{C(\lambda)} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left(\sum_{k=1}^{K_n} \frac{\sigma_{n,k}}{\bar{\sigma}(n)} \mathbb{P}_{\mu_{n,k}}\left(U \leq \frac{\psi(\mathcal{X})L_{n,k}(\mathcal{X})}{\sigma_{n,k}}, \mathcal{X} \in D_{n,k} \cap A\right)\right).
$$

Let $M$ be a non-negative integer valued random variable with the pmf defined by,

$$
\mathbb{P}(M = m) = \frac{1}{C(\lambda)} \frac{\lambda^m \bar{\sigma}(m)}{m!}, \quad m \geq 0. \tag{6}
$$

This pmf is well defined under Stability condition 3, because $\mathbb{E}[\bar{\sigma}(N)] < \infty$. Algorithm 2 generates a perfect sample from the Gibbs distribution $\mu$.

**Algorithm 2** IS Based AR method

1. Generate a sample $M$ (using (6))
2. Generate $J$ with pmf $\mathbb{P}(J = k) = \sigma_{M,k}/\bar{\sigma}(M)$, $k = 1, 2, \ldots, K_M$
3. Generate a realization $\mathcal{X}$ of $M$ points under the measure $\mu_{M,J}$
4. Return $\mathcal{X}$ if $\text{Bern}\left(\frac{\psi(\mathcal{X})L_{M,J}(\mathcal{X})I(\mathcal{X} \in D_{M,J})}{\sigma_{M,J}}\right) = 1$. Otherwise, repeat from Step 1

**Remark 4** (Acceptance Probability). Suppose that $\tilde{P}_{\text{acc}} = \mathbb{P}(\tilde{J} = 1)$ denotes the probability of accepting the configuration generated in an iteration of Algorithm 2. Then

$$
\tilde{P}_{\text{acc}} = \frac{1}{C(\lambda)} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left(\sum_{k=1}^{K_n} \frac{\sigma_{n,k}}{\bar{\sigma}(n)} \mathbb{E}_{\mu_{n,k}}\left[\psi(\mathcal{X})L_{n,k}(\mathcal{X}) \frac{I(\mathcal{X} \in D_{n,k})}{\sigma_{n,k}}\right]\right) = \frac{1}{\mathbb{E}[\bar{\sigma}(N)]} \mathbb{E}_{\mu^0}\left[\psi(\mathcal{X})\right].
$$
where \( N \sim \text{Poi}(\lambda) \). Recall from (5) that \( P_{\text{acc}} = \frac{1}{\mathbb{E}_{\sigma(N)}[\psi(X)]} \) denotes the acceptance probability of the naive AR method, where \( \sigma(n)'s \) are selected so that Stability condition 1 is satisfied (see Section 3). Since \( \mathbb{E}_{\sigma(N)}[\psi(X)] \) is independent of \( \sigma(n)'s \) and \( \tilde{\sigma}(n)'s \), \( P_{\text{acc}} \mathbb{E}[\sigma(N)] = \tilde{P}_{\text{acc}} \mathbb{E}[\tilde{\sigma}(N)] \). Hence, it is reasonable to seek a partition \( \{D_{n,k}\}_{k=1}^{K_n} \) for each \( n \) (and the associated IS measures \( \{\mu_{n,k}\}_{k=1}^{K_n} \)) for which \( \mathbb{E}[\tilde{\sigma}(N)] \) is much smaller than \( \mathbb{E}[\sigma(N)] \) so that \( \tilde{P}_{\text{acc}} \) is much higher than \( P_{\text{acc}} \). In the following section, we present two applications of Algorithm 2 for hard-sphere models where \( \tilde{P}_{\text{acc}} \) is indeed much higher than \( P_{\text{acc}} \).

5 Hard-sphere Model - Running Time Complexity Analysis

In this section, we consider two hard-sphere models on the unit cube \([0, 1]^d\) with spheres of i.i.d. radii. In one model, called Euclidean-hard-sphere model, each sphere is an Euclidean sphere, and in the other model, called torus-hard-sphere model, the unit cube \([0, 1]^d\) is treated as a torus such that spheres on the boundaries are allowed to loop over to the opposite boundaries. These models are absolutely continuous with respect to a \( \lambda \)-homogeneous MPP and each sphere has a radius on average of order \( 1/\lambda^n \) for \( \eta > 0 \). Here, the goal is to compare the expected running time complexities of the naive AR and IS based AR methods for every \( \lambda \).

To define the models precisely, let \( R \) be a bounded strictly positive random variable and \( \mu^0 \) be the distribution of the \( \lambda \)-homogeneous MPP on \( G = [0, 1]^d \times M \), where the mark space \( M \) is the set of all values that \( R \) can possibly take. A typical element \((x, a) \in G\) of a realization of \( \mu^0 \) denotes the sphere centered at \( x \in [0, 1]^d \) with radius \( a/\lambda^0 \). Let \( \mathcal{A} \subset \mathcal{G} \) be the set of all configurations with non-overlapping spheres. Throughout the paper, we reserve \( r \) to denote an upper bound on \( R \), and if \( R \) is constant, we take \( R = r \).

- **Euclidean-hard-space model:** Every sphere is treated as a an Euclidean sphere, that is, the sphere \( S(x, a) \) centered at \( x \in [0, 1]^d \) with radius \( a > 0 \) is defined by

  \[
  S(x, a) := \left\{ y \in \mathbb{R}^d : \|x - y\| < a \right\},
  \]

  where \( \| \cdot \| \) is the \( d \)-dimensional Euclidean norm.

- **Torus-hard-sphere model:** The underlying space \([0, 1]^d\) is treated as a torus. On the torus, a sphere \( S(x, a) \) centered at \( x \in [0, 1]^d \) with radius \( a \) is defined by

  \[
  S(x, a) := \{(y_1 \mod 1, \ldots, y_d \mod 1) : y = (y_1, \ldots, y_d) \in S(x, a)\},
  \]

  where \( S(x, a) \) is the Euclidean sphere with center \( x \) and radius \( a \) and ‘mod’ denotes the modulo operation defined by Raymond [3]: for any real numbers \( a \) and \( b \neq 0 \), \( a \mod b \) is the unique \( c \in [0, b) \) such that \( a = nb + c \) for an integer \( n \).

Throughout the remaining paper, the phrase ’hard-sphere model’ refers to both the models, and assume that \( \lambda^0 > 2r \) to avoid the possibility of a sphere overlapping with itself. Note that the law \( \mu \) of the hard-sphere model has the following Radon-Nikodym derivative with respect to \( \mu^0 \):

\[
\frac{d\mu}{d\mu^0}(\mathcal{X}) = \frac{I(\mathcal{X} \in \mathcal{A})}{\mathcal{P}(\lambda)}, \quad (7)
\]

where the normalizing constant

\[
\mathcal{P}(\lambda) = \mathbb{P}_{\mu^0}(\mathcal{X} \in \mathcal{A}) \quad (8)
\]
is the non-overlapping probability. The following large deviations result, Theorem 1, on $P(\lambda)$ is useful for the running time complexity analysis of both the AR and the dominated CFTP methods for the hard-sphere model; a proof is given in Appendix A.1. Let $\hat{R}$ be a random variable identical in distribution to $R$, and define $m_1 := E \left[ \left( R + \hat{R} \right)^d \right]$. Hereafter, $\gamma = \pi^{d/2}/\Gamma(d/2 + 1)$, where $\Gamma(\cdot)$ is the gamma function. Define

$$\gamma' = \begin{cases} \gamma, & \text{for torus-hard-sphere model}, \\ \gamma/2^d, & \text{for Euclidean-hard-sphere model}. \end{cases}$$

(9)

**Theorem 1.** The non-overlapping probability $P(\lambda)$ satisfies

$$\lim_{\lambda \to \infty} P(\lambda) = \begin{cases} 1, & \text{if } \eta d > 2, \\ \exp \left( -\frac{\gamma m_1}{2} \right), & \text{if } \eta d = 2, \end{cases}$$

$$\lim_{\lambda \to \infty} \left[ \frac{1}{\lambda^{2-\eta d}} \log P(\lambda) \right] = -\frac{\gamma m_1}{2}, \quad \text{if } 1 < \eta d < 2,$$

and

$$\lim_{\lambda \to \infty} \left[ \frac{1}{\lambda} \log P(\lambda) \right] = -1, \quad \text{if } 0 < \eta d < 1.$$

When $\eta d = 1$, the limit $\delta := \lim_{\lambda \to \infty} \left[ \frac{1}{\lambda} \log P(\lambda) \right]$ exists and $-1 \leq \delta < 0$. Furthermore, $\delta \nearrow 0$ if $\gamma m_1 \searrow 0$, and $\delta \leq -\frac{1}{2} \left( 1 - \frac{1}{\gamma r^d} \right)^2$ if $R \equiv r$ and $\gamma' r^d > 1$. In addition, for torus-hard-sphere model,

$$\lim_{\lambda \to \infty} \left[ P(\lambda) \exp \left( \frac{\gamma m_1}{2} \lambda^{2-\eta d} \right) \right] = 1, \quad \text{if } 5/3 < \eta d < 2.$$

### 5.1 Naive AR Algorithm

We now establish bounds on the expected running time complexity $T_{AR}$ of the naive AR algorithm for the hard-sphere model, and provide its asymptotic behavior as $\lambda \nearrow \infty$ using Theorem 1.

To understand $T_{AR}$ for each $\lambda$, observe that the expected running time complexity to generate a sample of mean $\lambda$ Poisson random variable is of order $\log \lambda$ (see, for e.g., [12]). The data structures that are commonly known as self-balancing binary search trees offer to perform search, insertion and deletion operations in $O(\log n)$ time when the total number of nodes in the tree is $n$. Examples of such self-balancing binary trees include AVL tree and Red-black tree; see, for e.g., [10].

For hard-sphere models, Stability condition 2 holds with $\sigma(n) = 1$ for all $n \geq 0$, and this choice of $\sigma(n)$ is optimal (see Remark 2). So, the random variable $M$ in Step 1 of Algorithm 1 is a Poisson variable with mean $\lambda$. Therefore, Algorithm 1 for the hard-sphere model can be stated as follows: Generate $M$ spheres on $G$ and accept the configuration if no sphere overlaps with other spheres. Clearly, this can be implemented by generating $M$ spheres in a sequential order such that each sphere is inserted into a self-balancing binary tree constructed using centers of already generated spheres. We can check whether the inserted sphere is overlapping with existing spheres or not just by checking its center’s distance from that of its neighboring nodes. This operation takes at most a constant time because there can be at most three neighboring nodes in the binary tree. If the new sphere is overlapping with any of its neighbors then discard the whole configuration and go to the next iteration of the algorithm. Otherwise, generate the next sphere and repeat the same procedure until all the $M$ spheres are accepted. As stated earlier, the expected complexity of insertion for $n^{th}$
sphere is of order \( \log n \). The complexity associated with verification of the overlapping criteria for the new sphere is constant as the co-ordinates of the centers of the accepted spheres are sorted. We have the following result and a proof is given in Appendix A.2.

**Proposition 1.** The expected running time \( T_{AR} \) of Algorithm 1 (naive AR) for the hard-sphere model satisfies

\[
T_{AR} = \begin{cases} 
\Theta(\lambda \log \lambda) \frac{1}{P(\lambda)} & \text{if } \eta d \geq 2, \\
\eta d \Theta(\lambda^{\eta d/2} \log \lambda) \frac{1}{P(\lambda)} & \text{if } \eta d < 2.
\end{cases}
\]

(10)

Plugging in the asymptotic expression for \( P(\lambda) \) from Theorem 1,

\[
T_{AR} = \begin{cases} 
\Theta(\lambda \log \lambda), & \text{if } \eta d \geq 2, \\
\Theta(\lambda^{\eta d/2} \log \lambda) \exp \left( \left( \frac{2m_1}{\lambda} + o(1) \right) \lambda^{2-\eta d} \right), & \text{if } 1 < \eta d < 2, \\
\Theta(\lambda^{\eta d/2} \log \lambda) \exp (\delta \lambda), & \text{for some } 0 < \delta \leq 1, \text{ if } \eta d = 1, \\
\eta d \Theta(\lambda^{\eta d/2} \log \lambda) \exp \left( (1 + o(1)) \lambda \right), & \text{if } 0 < \eta d < 1.
\end{cases}
\]

**Remark 5** (Significance of \( P_{acc}(\lambda) \)). Observe that \( P_{acc}(\lambda) = P(\lambda) \), since \( M \) is distributed as \( Poi(\lambda) \). From (10), we see that for large values of \( \lambda \) and for \( \eta d < 2 \), \( T_{AR} \) is mainly governed by the acceptance probability \( P_{acc}(\lambda) = P(\lambda) \). This suggests that a significant improvement in the acceptance probability will result in a significant improvement in the running time complexity.

### 5.2 Importance Sampling

We now present an IS methodology for the hard-sphere model. Subsections 5.3 and 5.4 presents two applications of Algorithm 2 using this IS method to significantly improve the acceptance probability.

Recall that the distribution \( \mu \) of the hard-sphere model is given by (7). Let \( \tilde{\mu} \) be the IS measure under which \( n \) spheres are generated as follows (for any \( n \)):

1. Generate the center of the first sphere uniformly on \([0, 1]^d\).
2. For each \( i = 2, \ldots, n \), generate the center of the \( i \)th sphere uniformly over the non-blocking subset of \([0, 1]^d\) created by the spheres 1 to \( i - 1 \); here blocking means that the center of the \( i \)th sphere falling in this set would create an overlap.
3. If, for any sphere \( i < n \), the whole space is blocked, then assume that the remaining spheres \( i \) to \( n \) are centered at origin with unit radius, and terminate the procedure (such selection of fixed centers and radii for spheres \( i \) to \( n \) always leads to overlap of the spheres).

It is not hard to see that \( \mu^0 \) is absolutely continuous with respect to \( \tilde{\mu} \) on \( \mathcal{A} \), and the associated likelihood ratio is given by

\[
L(\mathcal{X}) = \frac{d\mu^0}{d\tilde{\mu}}(\mathcal{X}) := \prod_{i=1}^{n} \left( 1 - B_i \right), \tag{11}
\]
Figure 1: Illustration of the proposed IS on $[0,1]^2$. All the spheres (dark circles) have the same radius $r/\lambda\eta$. In (a) (respectively, in (b)), the solid dark area together with the hatched area represents the blocking area seen by the second disk (respectively, the third disk).

for any configuration $X \in \mathcal{G}_n \cap \mathcal{A}$, where $B_i = B_i(X)$ is the volume of the blocking region seen by the $i^{th}$ sphere. Figure 1 illustrates this IS on two dimensional space.

Observe that the blocking volume contribution (or the blocking volume added) by $i^{th}$ sphere is at least $\gamma'(\frac{R_i}{R})^d$, where $\gamma'$ is defined by (9). This is because for the torus-hard-sphere model, the entire volume within an accepted sphere is added to blocking volume, and for the Euclidean-hard-sphere model, at least $1/2^d$ fraction of an accepted sphere is added to the blocking volume (this minimum blocking volume is achieved when the sphere is centered at a corner of the unit cube). Thus

$$B_i \geq \min \left(1, \frac{\gamma'}{\lambda^{\eta d}} \sum_{j=1}^{i-1} R_j^d \right),$$

for every configuration in $\mathcal{A}$. The significance of (12) is seen in the following subsections.

### 5.3 IS Based AR Algorithm – Fixed Radius

We consider an application of Algorithm 2 for the hard-sphere model under assumption that all the spheres are of the same size with a fixed radius $r/\lambda\eta$ for some constant $r > 0$. From (12), $B_i \geq \min \left(1, (i-1) \frac{\gamma'^d}{\lambda^{\eta d}} \right)$, for every configuration in $\mathcal{A}$. Assign $\sigma_{0,1} = 1$ and

$$\sigma_{n,1} = \prod_{i=1}^{n} \left(1 - (i-1) \frac{\gamma'^d}{\lambda^{\eta d}} \right)^+$$

(13)
for all \( n \geq 1 \), where \( x^+ = \max(0, x) \).

For each \( n \geq 0 \), let \( K_n = 1, D_{n,1} \equiv \mathcal{G}_n, \tilde{\sigma}(n) = \sigma_{n,1} \), and \( \mu_{n,1} = \bar{\mu} \). Thus, \( L_{n,1}(X) = L(X) \) for all \( n \geq 0 \). Note that for the hard-sphere model, \( \psi(X) = I(X \in \mathscr{A}) \). By the absolute continuity of \( \mu^0 \) with respect to \( \bar{\mu} \), for all \( n \geq 0 \), write \( \psi(X)L_{1}(X) = I(X \in \mathscr{A})L(X) \leq \tilde{\sigma}(n) \), if \( X \in D_{n,1} \equiv \mathcal{G}_n \). Therefore Stability condition 3 holds. Furthermore, the pmf of \( M \) is given by

\[
\mathbb{P}(M = m) = \frac{1}{C(\lambda)} \frac{\tilde{\sigma}(m)\lambda^m}{m!}, \quad m \geq 0,
\]

where \( C(\lambda) = \sum_{m=0}^{\infty} \frac{\tilde{\sigma}(m)\lambda^m}{m!} \). Then Algorithm 2 can be restated as Algorithm 3.

**Algorithm 3** IS Based AR Method for Fixed Radii Hard-sphere Model

1. Generate a sample \( M \) (using (6)). If \( M = 0 \), output the empty state \( \varnothing \) and terminate.
2. Generate a realization \( X \) with \( M \) spheres under \( \bar{\mu} \)
3. Generate \( J \sim \text{Bern} \left( \frac{\prod_{i=1}^{M} (1 - B_i)}{\tilde{\sigma}(M)} \right) \)
4. Return \( X \) if \( J = 1 \). Otherwise, repeat from Step 1

By Remark 4, the acceptance probability \( \tilde{P}_{\text{acc}}(\lambda) \) of Algorithm 3 is equal to \( \frac{1}{E[\tilde{\sigma}(N)]} \mathcal{P}(\lambda) \), and thus

\[
\frac{\tilde{P}_{\text{acc}}(\lambda)}{P_{\text{acc}}(\lambda)} = \frac{1}{E[\tilde{\sigma}(N)]}.
\]

(15)

Let \( T_{IS} \) be the expected running time complexity of Algorithm 3. We have Proposition 2 proved in Section A.3

**Proposition 2.** Suppose that all the spheres in the hard-sphere model have a constant radii \( r / \lambda^d \), for some \( r > 0 \). Then there exist a constant \( c > 0 \) such that

\[
T_{IS} \leq c \min(1, \eta d) \frac{\lambda^{\min(1, \eta d)}}{E[\tilde{\sigma}(N)]} \log \frac{\lambda}{\mathcal{P}(\lambda)},
\]

for all \( \eta d > 0 \), where \( N \sim \text{Poi}(\lambda) \). Furthermore,

\[
\limsup_{\lambda \to \infty} \left[ \frac{1}{\lambda^{2-\eta d}} \log E[\tilde{\sigma}(N)] \right] \leq -\frac{\gamma' r d}{2}, \quad \text{if } \eta d > 1, \quad \text{and}
\]

\[
\limsup_{\lambda \to \infty} \left[ \frac{1}{\lambda} \log E[\tilde{\sigma}(N)] \right] \leq -b, \quad \text{if } 0 < \eta d \leq 1, \quad \text{for some constant } b > 0.
\]

The following result is a trivial consequence of Proposition 1 and Proposition 2

**Corollary 1.** If \( \eta d \geq 2 \), the expected running time complexity \( T_{IS} \) of Algorithm 3 is of order \( T_{AR} \), and if \( 0 < \eta d < 2 \), then there exist a constant \( c > 0 \) such that \( T_{IS} \leq c E[\tilde{\sigma}(N)] \lambda^{\min(1, \eta d)} T_{AR} \).

**Remark 6** (Random radii bounded below by a positive constant). The above choice of \( \sigma(\cdot) \) and the corresponding improvement in the acceptance probability hold even when the spheres have random radii that are bounded below by a constant \( r > 0 \). Furthermore, a similar analysis can be established when the spheres are replaced with i.i.d. convex shapes such that each shape occupies a minimum positive volume.
Remark 7 (Better choice of $\tilde{\sigma}(n)$ for Euclidean-hard-sphere model). If spheres are Euclidean, further improvements in $\sigma_{n,1}$ can be obtained by accounting for boundary effects. For instance, for $d = 2$, there can be at most 4 spheres at corners, while the remaining spheres must block twice as much area as these do.

5.4 IS Based AR Algorithm – Random Radius

We now consider another application of Algorithm 2 for the hard-sphere model when each sphere has an i.i.d. random radius. Recall that in the previous section where each radius was fixed, the proposed IS ensured that small uniform bound on the likelihood ratio could be obtained for all large $n$ along acceptable configurations. This however, may no longer be true in the random radius setting on sample paths where the generated radii are unusually small (because the associated blocking area is small). We address this issue by partitioning the state space into two sets for all sufficiently large $n$: One where the sum of volumes is well behaved for a well chosen fraction, call it $\delta$, of the spheres. This ensures that the remaining spheres along this set see sufficient amount of blocked volume so that importance sampling that places these spheres in the non-blocking area results in a small likelihood ratio on this set. On the other set, the sum of volumes is unusually small for the fraction $\delta$ of spheres. The IS scheme for the second set involves exponentially twisting (see, e.g., [3]) the generated radius raised to the power $d$ so that sum of the volume of fraction $\delta$ of generated samples taking small values now occurs with high probability. This results in a small uniform bound on the likelihood ratio on the second set of acceptable configurations. We adjust the structuring parameters for improved performance.

Recall that $R$ denotes a random variable such that $R/\lambda^n$ is distributed as the radius of each generated sphere. Let $F$ be the distribution of $R^d$ and $\alpha = E[R^d]$. The logarithmic moment generating function associated with $F$ is defined by $\Lambda(\theta) := \log \left( E\left[ e^{\theta R^d}\right] \right)$ for every $\theta \in \mathbb{R}$. Let $D = \{ \Lambda'(\theta) : \theta \in \mathbb{R} \}$, where $\Lambda'$ denotes the derivative of $\Lambda$. We assume that $(0, \alpha) \in D$. Let $\tilde{\theta}$ be such that $\Lambda'(\tilde{\theta}) = \rho$ for some $\rho \in (0, \alpha)$. Observe that $\tilde{\theta} < 0$; see, for e.g., [11]. Consider the distribution $\tilde{F}$ obtained by exponentially twisting $F$ by amount $\tilde{\theta}$, i.e.,

$$
\tilde{dF}(dx) = \exp \left( \tilde{\theta}x - \Lambda(\tilde{\theta}) \right) dF(x).
$$

Fix any $\delta \in (0, 1)$ (we later show that $\delta = 1/2$ optimizes the performance of the algorithm). Define, for each $n$,

$$
H_n := \left\{ (r_1, r_2, \ldots, r_{\lceil n\delta \rceil}) : \frac{1}{\lceil n\delta \rceil} \sum_{i=1}^{\lceil n\delta \rceil} r_i \geq \rho \right\}.
$$

Let $\Lambda^*(\cdot)$ denote the Legendre-Fenchel transform of $\Lambda$. This also corresponds to the large deviations rate function associated with the empirical average of i.i.d. samples from $F$ (see, e.g., [11]). Also, $\Lambda^*(\rho) := \tilde{\theta}\rho - \Lambda(\tilde{\theta}) > 0$. Denote the complement of $H_n$ by $H_n^c$. Since $\tilde{\theta} < 0$,

$$
\exp \left( \tilde{\theta} \sum_{i=1}^{\lceil n\delta \rceil} r_i - \lceil n\delta \rceil \Lambda(\tilde{\theta}) \right) = \exp \left( \tilde{\theta} \sum_{i=1}^{\lceil n\delta \rceil} (r_i - \rho) + \lceil n\delta \rceil \Lambda^*(\rho) \right) \geq \exp \left( \lceil n\delta \rceil \Lambda^*(\rho) \right),
$$

for all $(r_1, r_2, \ldots, r_{\lceil n\delta \rceil}) \in H_n^c$, and thus

$$
\prod_{i=1}^{\lceil n\delta \rceil} \frac{dF(r_i)}{\tilde{dF}} \leq \exp \left( -\lceil n\delta \rceil \Lambda^*(\rho) \right). \quad (16)
$$
Recall the definition of the distribution $\mu$ of the hard-sphere model given by (7). To apply Algorithm 2, select $K_n$ and the associated IS measures $\{\mu_{n,1}, \ldots, \mu_{n,K_n}\}$, for each $n \geq 0$, as follows.

**Case 1: $n \leq 1/\delta$:** Let $K_n = 1$, $D_{n,1} = \mathcal{G}$ and $\mu_{n,1} = \mu^0$ and $\sigma_{n,1} = 1$. That is, there is no partition and no change of measure involved when $n \leq 1/\delta$. All the $n$ spheres are generated independently and identically.

**Case 2: $n > 1/\delta$:** Let $K_n = 2$ and define

$$D_{n,1} := \left\{ \mathcal{X} = \{(x_1, t_1), \ldots, (x_n, t_n)\} : (t_1^d, \ldots, t_{n\delta}^d) \in H_n \right\},$$

and

$$D_{n,2} := D_{n,1}^c = \left\{ \mathcal{X} = \{(x_1, t_1), \ldots, (x_n, t_n)\} : (t_1^d, \ldots, t_{n\delta}^d) \in H_n^c \right\},$$

where $\mathcal{X} = \{(x_1, t_1), \ldots, (x_n, t_n)\}$ is a typical configuration that denotes the set of $n$ spheres where the $i^{th}$ sphere is centered at $x_i$ with radius $t_i/\lambda^d$. The IS measures $\mu_{n,1}$ and $\mu_{n,2}$ are defined as follows.

- Take $\mu_{n,1} = \tilde{\mu}$, where $\tilde{\mu}$ is the IS measure introduced in the previous subsection. In other words, to generate $n$ spheres, we first generate their radii $R_1/\lambda^d, \ldots, R_n/\lambda^d$, where $R_1, \ldots, R_n$ are i.i.d. such that $R_i^d \sim F$. Then generate center of each sphere uniformly over the non-blocking region created by already generated spheres.

The associated likelihood ratio $L_1(\mathcal{X})$ is given by (11), that is, $L_1(\mathcal{X}) = \prod_{i=1}^n \left(1 - B_i\right)$, $\mathcal{X} \in \mathcal{G}_n$, where $B_i$ is the volume of the blocking region seen by the $i^{th}$ sphere. By (12), $B_i \geq \min \left(1, \frac{\gamma_i |n\delta|}{\lambda^{nd}}\right)$ on $D_{n,1} \cap \mathcal{A}$ for all $i \geq \lfloor n\delta \rfloor + 1$ because $\frac{1}{|n\delta|} \sum_{j=1}^{\lfloor n\delta \rfloor} R_j^d \geq \varrho$ over the set $H_n$. Consequently, we have by (11) that

$$L_1(\mathcal{X}) \leq \left[\left(1 - \frac{\gamma_i |n\delta|}{\lambda^{nd}}\right)^+\right]^{n(1-\delta)} := \sigma_{n,1},$$

for all $\mathcal{X} \in D_{n,1} \cap \mathcal{A}$.

- The measure $\mu_{n,2}$ is induced by the following procedure: Generate i.i.d. samples $R_1^d, \ldots, R_{\lfloor n\delta \rfloor}^d$ from $\tilde{F}$, and generate i.i.d. samples $R_{\lfloor n\delta \rfloor + 1}^d, \ldots, R_n^d$ from $F$. For $i = 1, \ldots, n$, the $i^{th}$ sphere has radius $R_i/\lambda^d$ with the center generated uniformly over non-blocking region in $[0, 1]^d$. The contribution to the likelihood ratio due to placing the generated spheres in the non-blocking regions is bounded from above by 1. Since $R_1^d, \ldots, R_{\lfloor n\delta \rfloor}^d$ are sampled from $\tilde{F}$, by (16), their contribution to the likelihood ratio,

$$L_2(\mathcal{X}) = \prod_{i=1}^{\lfloor n\delta \rfloor} \frac{dF}{d\tilde{F}}(x_i) \leq \exp \left(-|n\delta| \Lambda^*(\varrho)\right) := \sigma_{n,2}.$$

In summary, with the above choice of $K_n$’s and the IS measures, Stability condition 3 holds and Algorithm 3 generates perfect samples from $\mu$. 

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Notice that $\bar{\sigma}(n) = \sigma_{n,1} + \sigma_{n,2}$ for each $n \geq 0$. By Remark 4, $\bar{P}_{\text{acc}}(\lambda) = \frac{1}{\mathbb{E}[\bar{\sigma}(N)']} P_{\text{acc}}(\lambda)$, where $N \sim \text{Poi}(\lambda)$. Observe that $\sigma_{n,1} \leq \exp \left(\frac{-\gamma' n^2 \delta (1-\delta)}{\lambda^d} \varrho \right)$. The proof of Proposition 2 can be extended to current scenario to show that $T_{IS} \leq c \min(1, \eta d) \mathbb{E}[\bar{\sigma}(N)] \frac{\lambda^{\min(1, \eta d)} \log \lambda}{\mathcal{P}(\lambda)}$, for some constant $c > 0$, and

$$\limsup_{\lambda, \delta \to \infty} \left[ \frac{1}{\lambda^{2-\eta d}} \log \mathbb{E}[\sigma_{N,1}] \right] \leq -\gamma' \delta (1-\delta) \varrho, \text{ if } \eta d > 1, \text{ and}$$

$$\limsup_{\lambda, \delta \to \infty} \left[ \frac{1}{\lambda} \log \mathbb{E}[\sigma_{N,1}] \right] \leq -b, \text{ if } 0 < \eta d \leq 1, \text{ for some constant } b > 0.$$

It is now clear that a good choice for $\delta$ is $1/2$ because that value maximises $\delta (1-\delta)$. Furthermore,

$$\mathbb{E}[\sigma_{N,2}] \leq \exp \left( -\lambda \left(1 - e^{-\Lambda^* / 2} \right) \right),$$

using the moment generating function of Poisson random variable. Therefore:

**Proposition 3.** For the hard-sphere model considered above, $T_{IS} \leq c \min(1, \eta d) \mathbb{E}[\bar{\sigma}(N)] \frac{\lambda^{\min(1, \eta d)} \log \lambda}{\mathcal{P}(\lambda)}$ for some constant $c > 0$, where $N \sim \text{Poi}(\lambda)$. Furthermore, for all large values of $\lambda$,

$$\limsup_{\lambda, \delta \to \infty} \left[ \frac{1}{\lambda^{2-\eta d}} \log \mathbb{E}[\bar{\sigma}(N)] \right] \leq -\gamma' \varrho / 4, \text{ if } \eta d > 1, \text{ and}$$

$$\limsup_{\lambda, \delta \to \infty} \left[ \frac{1}{\lambda} \log \mathbb{E}[\bar{\sigma}(N)] \right] \leq -b, \text{ if } 0 < \eta d \leq 1, \text{ for some constant } b > 0.$$

**Remark 8** (Optimal $\varrho$). By Proposition 3, the smaller $\mathbb{E}[\bar{\sigma}(N)]$, the better the upper bound on $T_{IS}$. Clearly, $\mathbb{E}[\bar{\sigma}(N)]$ is minimum if $\varrho$ is selected for each $n \geq 2$ to equal $\arg\min_{\varrho \in (0, \alpha)} \left(\sigma_{n,1} + \sigma_{n,2}\right)$. Observe that $\sigma_{n,1}$ decreases and $\sigma_{n,2}$ increases as functions of $\varrho$.

The above decompositions were chosen to illustrate ideas simply. More complex decompositions are easily created for further performance improvement. For instance, we could have defined $H_n$ above as

$$H_n := \left\{ (r_1, r_2, \ldots, r_n) : \frac{1}{m} \sum_{i=1}^{m} r_i \geq \varrho_m, \forall m \leq n \right\},$$

and then arrived at appropriate $\{\varrho_m\}_{m \leq n}$ and appropriate changes of measures for configurations in $H_n$ and $H_n^c$. While this should lead to substantial performance improvement, it also significantly complicates the analysis.

### 6 Grid based IS for Hard-sphere Model

When the dimension $d = 1$, spheres become line segments and thus it is easy to implement the IS $\bar{\mu}$. However, such an implementation may not be possible when $d \geq 2$ as it can be difficult to identify the non-blocking regions. In addition, implementation of Step 3 of Algorithm 3 relies on the fact that the volumes of blocking regions $B_i$’s are known exactly. To overcome this, in Subsection 6.1, we propose a simple grid based methodology for approximating the blocking regions.
This method involves partitioning the underlying space $[0, 1]^d$ into a cubic grid, and generating centers of the spheres uniformly over the non-blocking cells. Naturally, grid with smaller cells gives a better approximation of blocking regions. However, decrease in the cell size increases the number of operations and hence the running time of the algorithm. In Subsection 6.2, we optimize the cell size as a function of $\lambda$ (the total intensity) and $n$ (the number of spheres generated) for the hard-sphere model with spheres of a fixed radius. These ideas can be extended to the hard-sphere model with random radii.

6.1 Algorithm

Suppose that we need to generate $n$ spheres with radii $R_1/\lambda^n, \ldots, R_n/\lambda^n$. The first step in the implementation of the grid method is to partition the space $[0, 1]^d$ into a regular cubic grid of cell edge length $\varepsilon$ such that $1/\varepsilon$ is an integer.

Initially, all the cells are marked as non-blocking. We generate $i^{th}$ sphere uniformly over the non-blocking cells, for all $i \leq n$. Here a cell is marked as a blocking cell for the $i^{th}$ sphere if the cell is strictly within the distance of $R_{j} + R_i/\lambda^n$ from the center of one of the $j^{th}$ sphere, for any $j = 1, 2, \ldots, i - 1$; see Figure 2. This is done as follows:

1. If $n = 0$ then the algorithm terminates by outputting the empty configuration $\emptyset$, or if $n = 1$ then the algorithm terminates by outputting a sphere with the center uniformly generated on $[0, 1]^d$. In both the cases, the associated likelihood ratio takes the value 1.

2. For $n \geq 2$, suppose that $i - 1$ spheres are already generated for some $i \leq n$. Denote the centers of these spheres by $X_1, X_2, \ldots, X_{i-1}$.

3. If all the cells are blocked, then assume that the spheres $i$ to $n$ are centered at origin with unit radius and terminate the procedure (in this case, the likelihood ratio takes value 0).

![Figure 2](image)

Figure 2: A typical realization with 10 circles using the grid based IS for an hard-sphere model with fixed radii Euclidean circles (dark gray), where the grid size is $100 \times 100$ and the radius is 0.1. The bigger circle around each circle is the actual region blocked by the circle. The set of gray cells denotes the blocking region for the $11^{th}$ circle.
4. Generate the center $X_i$ of the $i^{\text{th}}$ sphere uniformly over a cell that is selected uniformly from the non-blocking cells created by the existing spheres for the $i^{\text{th}}$ sphere. If the $i^{\text{th}}$ sphere is overlapping with the existing spheres, then again assume that the spheres $i + 1$ to $n$ are centered at origin with unit radius and terminate the procedure (in this case, $I(\mathcal{X}_n \in \mathcal{A}) = 0$). Otherwise, continue the procedure for generating the other spheres.

5. If all the $n$ spheres are generated successfully without overlap, then output the configuration $\{X_1, X_2, \ldots, X_n\}$ and the likelihood ratio $\prod_{i=1}^n \left(1 - \hat{B}_i\right)$, where $\hat{B}_i$ is the volume of the blocked cells at the time of the $i^{\text{th}}$ sphere generation.

Suppose that $\hat{\mu}$ is the probability measure induced by the above procedure. Then the measure $\mu^0$ is absolutely continuous with respect to $\hat{\mu}$ on $\mathcal{A}$. Let $N_i$ be the number of blocked cells at the time of $i^{\text{th}}$ sphere generation (clearly $N_1 = 0$). Suppose that the output configuration of the above procedure is given by $\mathcal{X}_n = \{X_1, X_2, \ldots, X_n\}$. Since the volume of each cell is $\varepsilon^d$, we have $\hat{B}_i = N_j \varepsilon^d$ and the likelihood ratio $\hat{L}(\mathcal{X}_n) := \frac{d\mu^0}{d\hat{\mu}}(\mathcal{X}_n) = \prod_{i=1}^n \left(1 - N_i \varepsilon^d\right)$.

### 6.2 Optimal Cell Edge Length

Consider the hard-sphere model on $[0, 1]^d$ with fixed radii $r/\lambda^n$, where $r, \eta > 0$. For a fixed total intensity $\lambda$, let $\varepsilon_{\lambda,n}$ be the cell edge length for generating $n \geq 2$ spheres under the grid based IS such that $1/\varepsilon_{\lambda,n}$ is an integer (note that construction of a grid is not needed for $n = 0, 1$).

Since the largest diagonal size of a cell is $\sqrt{d} \varepsilon_{\lambda,n}$, within every generated sphere, there exists a small sphere with the same center and radius $r_{\lambda,n} := \left(\frac{r}{\lambda^n} - \sqrt{d} \varepsilon_{\lambda,n}\right)^+$ such that the small sphere is always blocked for all the spheres generated afterwards. This implies, $\sum_{j=1}^i N_j \varepsilon_{\lambda,n}^d \geq \min \left(1, (i - 1) \gamma r_{\lambda,n}^d\right)$ (compare this expression with (12)). Thus,

$$\hat{L}(\mathcal{X}_n) \leq \prod_{i=1}^n \left(1 - (i - 1) \gamma r_{\lambda,n}^d\right)^+ =: \tilde{\sigma}(n)$$

for all configurations $\mathcal{X}_n$ with $n$ spheres. Suppose that $M$ is a random variable with the pmf defined by

$$\mathbb{P}(M = m) = \frac{1}{C(\lambda)} \frac{\tilde{\sigma}(m) \lambda^m}{m!}, \ m \geq 0,$$

where $C(\lambda) = \sum_{m=0}^\infty \frac{\tilde{\sigma}(m) \lambda^m}{m!}$. In Algorithm 3, by replacing the measure $\hat{\mu}$ with the new measure $\tilde{\mu}$, we can generate perfect samples for the hard-sphere model of constant radii. That is, in each iteration of the Algorithm 3, generate a sample of $M$ using the distribution (17). Generate a configuration of $M$ spheres $\mathcal{X} = \{X_1, X_2, \ldots, X_M\}$ under the measure $\tilde{\mu}$ and accept the $\mathcal{X}$ with probability $\frac{\hat{L}(\mathcal{X})}{\tilde{\sigma}(M)}$.

Suppose that $\hat{P}_{\text{acc}}(\lambda)$ and $\hat{T}_{\text{AR}}$ are, respectively, the acceptance probability and the expected running time complexity of the grid based IS algorithm. If $\hat{C}_{\text{itr}}$ denotes the running time complexity of an iteration of the algorithm, then

$$\hat{T}_{\text{AR}} = \frac{\mathbb{E}[\hat{C}_{\text{itr}}]}{\hat{P}_{\text{acc}}(\lambda)}.$$  

(18)
Proposition 4 shows that the optimal cell edge length for each \( \lambda \) and \( n \) is of order \( \lambda^{\eta(d-1)}/n^2 \), proved in Section A.4.

**Proposition 4.** Let \( \{\varepsilon_{\lambda,n}^* : n \geq 1\} \) be the sequence of optimal cell edge lengths that minimize \( \bar{F}_{AR} \) such that \( \varepsilon_{\lambda,n}^* < \frac{r}{2\sqrt{d}n^\eta} \). Then \( M \leq \frac{\lambda^{\eta d}}{2^d n^\eta} + 1 \) and there exist constants \( c_1, c_2 > 0 \) (independent of \( r, \lambda \) and \( n \)) such that, for all \( \lambda > (2r)^{1/\eta} \) and \( n \leq \frac{\lambda^{\eta d}}{2^d n^\eta} + 1 \),

\[
 c_1 \min \left( \frac{r \cdot \lambda^{\eta(d-1)}}{\lambda^0 \cdot n^2 r^{d-1}} \right) \leq \varepsilon_{\lambda,n}^* \leq c_2 \min \left( \frac{r \cdot \lambda^{\eta(d-1)}}{\lambda^0 \cdot n^2 r^{d-1}} \right).
\]

**Remark 9.** In Proposition 4, the assumption that \( 2\sqrt{d}\varepsilon_{\lambda,n} < \frac{r}{\lambda^\theta} \) is important to make sure that each generated sphere encircles at least one cell; otherwise, it makes no sense to use the grid to approximate the blocking volume. This assumption also implies that \( r_{\lambda,n} > 0 \). As mentioned in Section 5, \( \lambda > (2r)^{1/\eta} \) is required to avoid the possibility of a sphere overlapping with itself in the torus-hard-sphere model. The proof of Proposition 4 suggests that one possible option is to choose \( c_1 = \min \left( \frac{1}{2\sqrt{d}}, \frac{2(1 - 1/2^d)}{\sqrt{d} \gamma'} \right) \) and \( c_2 = \max \left( \frac{1}{2\sqrt{d}}, \frac{2^{d+1}}{\sqrt{d} \gamma'} \right) \). In our numerical experiments, \( d = 2 \) and \( \varepsilon_{\lambda,n}^* \approx 1/ \max \left( 4\lambda^0/r, 4n^2r/\lambda^0 \right) \).

## 7 Comparison of AR and Dominated CFTP Methods

This section provides an analytical comparison between the expected running time complexities of AR and dominated CFTP methods. We do it in the context of the loss system defined in Section 2.1. A review of the dominated CFTP by Kendall and Møller for generating perfect sample from the steady-state distribution of the loss system presented in Section 7.1 refers to [26] to see the dominated CFTP for general Gibbs point processes (this method is first proposed for area-interaction processes by Kendall [25]). A lower bound on the expected running time complexity of the dominated CFTP is established in Section 7, and it is compared with the complexity of the naive and the proposed AR methods. These results are specialized to the hard-sphere models in Section 7.3. Two alternative dominated CFTP methods for pairwise interaction processes with substantial performance improvement are discussed in Section 7.4.

### 7.1 Algorithm (Kendall and Møller [26])

Kendall and Møller [26] proposed a dominated CFTP technique that uses spatial birth-and-death processes to perform perfect sampling. This method is applicable to finite-volume Gibbs measures. It consists of two steps: i) construct the dominating process, free process \( D \), backward in time, and ii) use thinning on the dominating process to obtain two appropriate processes that upper bound and lower bound a version of the interacting process \( X \). The coalescence of the upper and lower bound processes results in the output of a perfect sample from the invariant measure of \( X \).

Recall that \( \mu^0 \) is the law of MPP on \( G = B \times \mathcal{M} \) for \( B \subseteq \mathbb{R}^d \) with intensity \( \nu (d(x,y)) = \kappa(dx) \times \vartheta(dy) \) such that the total volume \( \lambda := \kappa(B) \) is finite. Also recall that \( \psi(\mathcal{X}) = \exp \left( -\beta V(\mathcal{X}) \right) \), \( \mathcal{X} \subseteq \mathcal{G} \). Further assume that Stability condition 1 holds.

Let \( D = \{D(t) : t \in \mathbb{R}\} \) and \( X = \{X(t) : t \in \mathbb{R}\} \) be the associated free process (with intensity \( \sigma\nu \)) and the interacting process, respectively, as defined in Section 2.1. From the definitions, \( \mu^0 \)
and $\mu$ are the invariant measures of free process and interacting process, respectively.

Let $\cdots < t_{-2} < t_{-1} < t_0 = 0 < t_1 < t_2 < \cdots$ be the event instants of the process $D$, where event can be either a birth or a death. Consider the simple setting of the loss system defined in Section 2.1. From the definition, $\psi(X) = I(X \in \mathcal{A})$ and thus the Papangelou conditional intensity is given by

$$\ell(X, x) := \frac{I(X \cup \{x\} \in \mathcal{A})}{I(X \in \mathcal{A})} = I(X \cup \{x\} \in \mathcal{A}), \quad (19)$$

where recall that $\mathcal{A}$ is the set of all the acceptable configurations. Observe that Stability condition 1 is satisfied with $\sigma \equiv 1$.

We now use partial ordering of the state space $\mathcal{A}$ and a coupling argument to construct the interacting process $X(t)$ (also referred as target process) such that it is dominated by $D(t)$, where dominating means that $X(t) \subseteq D(t)$ for all $t$. Suppose that $\mathcal{Y}$ and $\mathcal{X} \subseteq \mathcal{Y}$ are the states of dominating and target processes, respectively, just before an event instant $t_i$. If a point $y$ is born in the dominating process $D$ at time $t_i$, that is, $D(t_i) = \mathcal{Y} \cup \{y\}$ then take $X(t) = \mathcal{X} \cup \{y\}$, $t_i \leq t < t_{i+1}$ if $\ell(X, y) = 1$, otherwise, $X(t)$ is unchanged over $[t_i, t_{i+1})$. Every death of $D$ is reflected in the target process $X$; here, by reflected we mean that $X(t) = \mathcal{X} \setminus \{y\}$ for all $t_i \leq t < t_{i+1}$.

For each $n \leq 1$, construct two processes $L_n$ and $U_n$ starting at $t_{-n}$ and satisfying $L_n(t) \subseteq X(t) \subseteq U_n(t) \subseteq D(t)$ over the time interval $t_{-n} \leq t \leq 0$. These processes are known as lower and upper bound processes, respectively. Observe that the process $D$ is time-reversible, and hence one can generate $\{D(-t) : 0 \leq t \leq T\}$ for any finite $T > 0$ just by generating a copy $\{\tilde{D}(t) : 0 \leq t \leq T\}$ of the dominating process $\{D(t) : 0 \leq t \leq T\}$ and taking $D(-t) = \tilde{D}(t)$ for $0 \leq t \leq T$. Define,

$$\alpha^l(\mathcal{X}^l, \mathcal{X}^u, x) := \ell(\mathcal{X}^u, x) = I(\mathcal{X}^u \cup \{x\} \in \mathcal{A}), \quad \text{and} \quad \alpha^u(\mathcal{X}^l, \mathcal{X}^u, x) := \ell(\mathcal{X}^l, x) = I(\mathcal{X}^l \cup \{x\} \in \mathcal{A}).$$

Observe from the hereditary of $\mathcal{A}$ that $\alpha^l \leq \alpha^u$. Construct $\{L_n(t) : t \geq t_{-n}\}$ and $\{U_n(t) : t \geq t_{-n}\}$ as follows: Let $L_n(t_{-n}) = \emptyset$ and $U_n(t_{-n}) = D(t_{-n})$. Suppose that $\mathcal{X}^l = L_n(t_i)$ and $\mathcal{X}^u = U_n(t_i)$ for $-n \leq i < 0$ then assign $L_n(t) = \mathcal{X}^l$ and $U_n(t) = \mathcal{X}^u$ for $t_i \leq t < t_{i+1}$. In case it is a birth at $x$ in the dominating process $D$ at time $t_{i+1}$, set $L_n(t_{i+1}) = \mathcal{X}^l \cup \{x\}$ if $\alpha^l(\mathcal{X}^l, \mathcal{X}^u, x) = 1$; otherwise, it will remain unchanged, that is, $L_n(t_{i+1}) = \mathcal{X}^l$. Similarly, set $U_n(t_{i+1}) = \mathcal{X}^u \cup \{x\}$ if $\alpha^u(\mathcal{X}^l, \mathcal{X}^u, x) = 1$; otherwise, set $U_n(t_{i+1}) = \mathcal{X}^u$. Every death in the dominating process reflects in both the lower and upper bound processes. Note that a birth is accepted by the lower bound process if the resulting state of the upper bound process is in $\mathcal{A}$, and vice versa. Algorithm 4 generates perfect samples from $\mu$; refer to [26] for a proof.

Consider the \textit{backward coalescence} time $N^* = \min \{n \geq 0 : L_n(0) = U_n(0)\}$. The average running time complexity of Algorithm 4 depends on the number of operations involved within $N^*$.

7.2 Expected Running Time Complexity

Let $T_{DC}$ be the expected running time complexity of the dominated CFTP for generating a perfect sample from the steady-state distribution $\mu$ of the loss system. To derive lower bound on $T_{DC}$, view the entire dominating process $D$ as a Poisson Boolean model on a higher dimensional space and use an extension of FKG inequality [29] (alternatively, see Theorem 2.2 in [29]). To this
Hence, on average the running time complexity doubles at each iteration. From the definition of the lower bound (20) is a loose bound, because the bound is established by considering the running time complexity only up to the time at which the lower bound process receives its first arrival. This can be much smaller than the running time complexity until the coalescence of the upper and lower bound processes. As a result, (21) is also a loose bound. Our numerical results highlight this point; refer to Section 8.

end, we make some remarks on the dominated CFTP, specifically, in the context of the loss system.

At each iteration, the length of the dominating process \( D(t) \) is doubled backwards in time. Hence, on average the running time complexity doubles at each iteration. From the definition of \( N^* \), the length of the last iteration is \( 2^{\lceil \log_2 N^* \rceil} \geq N^* \). Let

\[
N^f = \min \{ n \geq 0 : L_0(t_n) = U_0(t_n) \}
\]

be the forward coalescence time. Due to the reversibility of the dominating process, it can be shown that \( N^* \) and \( N^f \) are identical in distribution \([3]\), and hence the expected computational effort for constructing the dominating, upper bound and lower bound processes up to the forward coalescence time \( N^f \), starting from time 0, is a lower bound on the expected running time of the algorithm.

Let \( s_0 = 0 \) and \( s_i \) be the instant of the \( i \)th arrival in the dominating process after time zero. Let \( C(\mathcal{X}, \mathcal{X}^u, \mathcal{X}^l) \) be the running time complexity of updating the dominating, upper bound and lower bound processes at the instant of an arrival when their respective states are \( \mathcal{X}, \mathcal{X}^u \) and \( \mathcal{X}^l \). Without loss of generality, assume that \( C(\mathcal{X}, \mathcal{X}^u, \mathcal{X}^l) \) is an increasing function in each argument under the partial order on \( \mathcal{G} \), because the updating cost increases with the number of points involved. For example, in the first argument, \( C(\mathcal{X}, \mathcal{X}^u, \mathcal{X}^l) \leq C(\mathcal{X} \cup \{x\}, \mathcal{X}^u, \mathcal{X}^l) \) for any \( x \in \mathcal{G} \). We have the following result.

**Theorem 2.** Suppose that \( \mathbb{E}_{\mu^0}[C^2(\mathcal{X}, \mathcal{X}, \emptyset)] < \infty \). The running time complexity \( T_{DC} \) of the dominated CFTP algorithm satisfies

\[
T_{DC} \geq \frac{\mathbb{E}_{\mu^0}[C(\mathcal{X}, \mathcal{X}, \emptyset)]}{\mathbb{P}_{\mu^0}(\mathcal{X} \in \mathcal{G})}. \tag{20}
\]

Furthermore, if \( T_{AR} \) is the expected running time of the naive AR method for the loss system, then

\[
T_{AR} \leq \frac{\mathbb{E}[C_{itr}]}{\mathbb{E}_{\mu^0}[C(\mathcal{X}, \mathcal{X}, \emptyset)T_{DC}]}. \tag{21}
\]

where \( C_{itr} \) is the running time complexity of an iteration of the naive AR algorithm.

**Remark 10.** The lower bound (20) is a loose bound, because the bound is established by considering the running time complexity only up to the time at which the lower bound process receives its first arrival. This can be much smaller than the running time complexity until the coalescence of the upper and lower bound processes. As a result, (21) is also a loose bound. Our numerical results highlight this point; refer to Section 8.

**Algorithm 4 Dominated CFTP**

1: Generate \( D(0) \sim \mu^0 \) and \( M_{-1/2} \sim \text{Unif}([0, 1]) \), and assign \( D(t_{-1/2}) = D(0) \) and \( n = 1 \)
2: Return \( \emptyset \) if \( D(0) = \emptyset \)
3: Extend \( D \) backwards in time from \( \{D(t) : t \in [t_{-n/2}, 0]\} \) to \( \{D(t) : t \in [t_{-n}, 0]\} \)
4: Generate \( M_{i} \sim \text{Unif}([0, 1]) \) for \( i = n/2, n/2 + 1, \ldots, n \)
5: Construct \( \{L_n(t) : t_{-n} \leq t \leq 0\} \) and \( \{U_n(t) : t_{-n} \leq t \leq 0\} \)
6: Return \( U_n(0) \) if \( L_n(0) = U_n(0) \)
7: Take \( n \leftarrow 2 \times n \) and go to Step 3
7.3 Hard-sphere Model

Observe that the loss system driven by hard-spheres is a special case of the general loss system considered in Section 7.2. As a consequence of Theorem 2, for the hard-sphere model we now establish a lower bound on the expected running time \( T_{DC} \) of the dominated CFTP proposed in 7.1. The asymptotic behavior of \( T_{DC} \) as \( \lambda \to \infty \) is established using Theorem 1.

**Proposition 5.** The expected running time complexity \( T_{DC} \) of Algorithm 4 (dominated CFTP) for the hard-sphere model satisfies

\[
T_{DC} \geq c \log \frac{\lambda}{P(\lambda)},
\]

for some constant \( c > 0 \). Furthermore,

\[
T_{DC} = \begin{cases} 
\Omega \left( \lambda \log^2 \lambda \right), & \text{if } \eta d \geq 2, \\
\Omega \left( (\log \lambda) \exp \left( \left( \frac{\eta d}{2} + o(1) \right) \lambda^{2-\eta d} \right) \right), & \text{if } 1 < \eta d < 2, \\
\Omega \left( (\log \lambda) \exp \left( (1 + o(1)) \lambda \right) \right), & \text{if } 0 < \eta d \leq 1.
\end{cases}
\]

Corollary 2 is a consequence of Propositions 1, 3 and 5, and the fact that \( \lim_{\lambda \to \infty} P(\lambda) > 0 \) for all \( \eta d \geq 2 \). Refer to Proposition 3 to see asymptotic bounds on \( E[\tilde{\sigma}(N)] \).

**Corollary 2.** There exist constants \( c_1, c_2, c_3, c_4 > 0 \) such that, with \( N \sim \text{Poi}(\lambda) \),

\[
T_{IS} \leq \begin{cases} 
c_3 \frac{1}{\log \lambda} T_{DC}, & \text{if } \eta d \geq 2, \\
c_4 E[\tilde{\sigma}(N)] \eta d \lambda^{\min(1,\eta d)} T_{DC}, & \text{if } 0 < \eta d < 2,
\end{cases}
\]

and

\[
T_{AR} \leq \begin{cases} 
c_1 \frac{1}{\log \lambda} T_{DC}, & \text{if } \eta d \geq 2, \\
c_2 \eta d \lambda^{\eta d/2} T_{DC}, & \text{if } 0 < \eta d < 2.
\end{cases}
\]

7.4 Other Dominated CFTP Methods for Pairwise Interaction Processes

If the target point process is a repulsive pairwise interaction Gibbs point process \((\beta < 0)\), there are alternative constructions of upper and lower bound processes that are shown to be more effective compared to the earlier construction. Here we discuss two such constructions. First, recall from the definition that a pairwise interaction point process has a potential function of the form given by

\[
V^f(\mathcal{X}) := cn + \sum_{1 \leq i < j \leq n} f(\|x_i - x_j\|), \text{ for } \mathcal{X} = \{x_1, x_2, \ldots, x_n\},
\]

for some constant \( c \in \mathbb{R} \) and function \( f : \mathbb{R}_+ \to \mathbb{R} \cup \{\infty\} \). Define

\[
\tilde{\ell}(\mathcal{X}, x) := \exp \left( \beta c - \beta \sum_{y \in \mathcal{X}} f(\|y - x\|) \right).
\]

We assume that \( \tilde{\ell}(\mathcal{X}, x) \) satisfies Stability condition 1.

**Dominated CFTP without swaps:** Recall that the Papangelou conditional intensity \( \ell(\mathcal{X}, x) \) defined by (22) is used in the construction of the upper and lower bound processes. Suppose that in this construction \( \ell(\mathcal{X}, x) \) is replaced with \( \tilde{\ell}(\mathcal{X}, x) \). Now we argue that this replacement is indeed
a better option to increase the speed of the algorithm for pairwise interaction processes. For example consider the hard-sphere model with fixed radii $r$. Then $\ell(\mathcal{X}, x) = 1$ if no two points in $\mathcal{X} \cup \{x\}$ are within $2r$ distance from each other, otherwise, $\ell(\mathcal{X}, x) = 0$; see (19). On the other hand, $\hat{\ell}(\mathcal{X}, x) = 1$ if the point $x$ is $2r$ distance far from every point in $\mathcal{X}$, otherwise $\hat{\ell}(\mathcal{X}, x) = 0$. As a consequence, under the new construction, the lower bound process accepts births more often and hence the upper bound process accepts births less often when compared with the earlier construction given in Section 7.1. This implies that the coalescence time is shorter if we use $\hat{\ell}(\mathcal{X}, x)$ instead of $\ell(\mathcal{X}, x)$.

**Dominated CFTP with swaps:** A different approach for dominated CFTP for repulsive pairwise interaction processes has been proposed by Huber [20]. Here, we discuss main ingredients of the method for hard-sphere model. Refer to [20] and [21] for detailed discussion on how to apply this method to Strauss process and to general repulsive pairwise interaction processes.

In this method, the dominating process is again the free process $D(t)$. However, the interaction process is different and is known as spatial birth-death swap process, whose invariant distribution is the target hard-sphere model. In addition to births and deaths of spheres, this process also allows swap moves; here swap move is an event where an existing sphere is replaced by an arrival if it is the only sphere that is overlapping with the arrival. The lower and upper bounding processes are constructed as follows: At the $i$th iteration of Algorithm 4, $n = 2^i$ and the upper and lower bound processes, respectively, $U_n(t)$ and $L_n(t)$ are constructed for $t_{n-1} \leq t \leq 0$ as follows: As usual let $U_n(t_{n-1}) = D(t_{n-1})$ and $L_n(t_{n-1}) = \emptyset$. For any $0 < k < n$, if $t_{n-k}$ is an instant of a death in the dominating process $D(t)$ then the death is reflected in both upper and lower bound processes. Now suppose that $x \in D(t_{n-k})$ is born at $t_{n-k}$.

**Case 1:** There is at most one sphere $y \in U_n(t_{n-k})$ overlapping with the arrival sphere $x$. Then $y$ is removed from $U_n(t_{n-k})$ (from $L_n(t_{n-k})$ if it is present) and $x$ is added to both $U_n(t_{n-k})$ and $L_n(t_{n-k})$.

**Case 2:** There are at least two spheres in $L_n(t_{n-k})$ overlapping with $x$. Then $x$ is rejected by both $U_n(t_{n-k})$ and $L_n(t_{n-k})$.

**Case 3:** There is at most one sphere $y$ in $L_n(t_{n-k})$, and at least two spheres in $U_n(t_{n-k})$ overlapping with $x$. Then $x$ is added to $U_n(t_{n-k})$ (but not to $L_n(t_{n-k})$) and $y$ is removed from $L_n(t_{n-k})$.

**Remark 11.** Note that the results presented in Section 7.3 are not necessarily true for the dominated CFTP methods discussed in this section. See Section 8 for numerical comparison of the AR and the dominated CFTP methods.

## 8 Simulations

We compare the effectiveness of the proposed IS based AR method by comparing with the naive AR and the dominated CFTP (DCFTP) methods using numerical experiments. For this, we consider the hard-sphere model of Euclidean spheres with fixed radii on 2-dimensional square $[0, 1]^2$ and compute the expected number of spheres (or, circles as we call them here) generated per sample using these methods for different values of the total intensity $\lambda$ and different values of $\eta$. We compare the estimated average number of circles per one sample generation instead of comparing the expected running time complexities to keep the discussion independent of the underlying
data structures used in the implementation of the algorithms.

The experimental set-up is as follows. For each value of $\lambda$, the radius of each sphere is $r/\lambda^n$. The DCFTP (Kendall and Møller) is implemented as it is. In the naive AR method (Algorithm 1) implementation, in each iteration, spheres are generated in a sequential order such that the iteration is terminated when there is an overlap of spheres and go to the next iteration; this helps in reducing the complexity of the algorithm. Finally, in the implementation of the IS based AR, grid has the cell edge length $\varepsilon_{\lambda,n} = 1/\max\left(4\lambda^n r, 4n^2 r/\lambda^n\right)$ for each $\lambda$ and $n$ (see Section 5). Recall the two DCFTP methods discussed in Section 7.4. As mention earlier, these two methods are useful to generate perfect samples from pairwise interaction processes. Since the hard-sphere model is a pairwise interaction process, simulation results for these two methods also included in every experiment presented below. From all the three experiments, it can be seen that the order of the complexities of these two algorithms is the same up to a multiplicative constant.

Suppose that $T$ denotes the total number of perfect samples of the hard-sphere model generated for constructing the required estimators. Let $\#S_{NAR}(i)$ be the number of circles generated during the $i^{th}$ perfect sample generation using the naive AR. Then the average number of circles generated per generation of a perfect sample using the naive AR method is estimated by the empirical average $\hat{S}_{NAR} := \frac{1}{T} \sum_{i=1}^{T} \#S_{NAR}(i)$. Similarly we can define the average number of circles generated per a perfect sample for other methods as well. Let $\hat{S}_{ISAR}, \hat{S}_{DLS}, \hat{S}_{DWOS}$ and $\hat{S}_{DWS}$ be the estimated average number of circles generated per generation of a perfect sample using, respectively, IS based AR (Algorithm 3), the dominated CFTP for the loss system (Algorithm 4 with (19) as Papangelou condition intensity), the dominated CFTP for pairwise interaction processes without swaps (Algorithm 4 with (22) as Papangelou condition intensity) and the dominated CFTP for pairwise interaction processes with swaps (Algorithm 4 with spatial birth-death swap process). These quantities are compared in Figures 3 - 6 for different values of $\eta$ and $\lambda$. In each experiment, $T = 200$.

**Experiment 1:** Here $r = 1$ and $\eta = 0.40$ (that is, $\eta d = 0.80$). Simulation results as a function of $\lambda$ are shown in Figure 3. This experiment suggests that the proposed IS AR method can perform significantly better than every other method. In the figure, we see a jump in $\log \hat{S}_{ISAR}$ between $\lambda = 9$ and $\lambda = 10$. This is because the support of the pmf of the random variable $M$ increases; see Proposition 4.

**Experiment 2:** Here $\eta = 0.50$ (that is, $\eta d = 1$). This is an important and historically well studied regime. It is equivalent to the regime where the underlying space is $[0, \sqrt{\lambda}]^2$ and each sphere has $r$ radius. One would like to compare methods as $\lambda$ increases. See Figure 3 (where $r = 1$) and Figure 5 (where $r = 0.05$) for simulation results. In this regime also we see that the proposed IS based AR method can perform significantly better than every other method (even when $r$ is small).

**Experiment 3:** Here $r = 1$ and $\eta = 0.75$ (that is, $\eta d = 1.5$). In this regime, the two DCFTP methods for pairwise interaction processes may eventually perform better than the proposed method. See Figure 6.
In this paper we considered the problem of perfect sampling from Gibbs point processes. These are processes that are absolutely continuous with respect to spatial Poisson point processes and include area-interaction processes, loss processes, Strauss processes and the Ising model. We discussed the performance of the naive acceptance-rejection method and introduced importance sampling based enhancements to it. We also compared these methods to some of the popular coupling from the past based techniques prevalent in the existing literature. The performance analysis and comparison (of expected running time complexity) was conducted in a simpler setting of hard-sphere models where we developed an asymptotic regime where the Poisson process intensity $\lambda$ of spheres in a hyper cube $[0, 1]^d$ increased to infinity, while the sphere volume of order $\lambda^{-\eta d}$ decreased to zero. We conducted this analysis for different ranges of $\eta$. Our one conclusion was

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Figure 3}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Figure 4}
\end{figure}

9 Conclusion

In this paper we considered the problem of perfect sampling from Gibbs point processes. These are processes that are absolutely continuous with respect to spatial Poisson point processes and include area-interaction processes, loss processes, Strauss processes and the Ising model. We discussed the performance of the naive acceptance-rejection method and introduced importance sampling based enhancements to it. We also compared these methods to some of the popular coupling from the past based techniques prevalent in the existing literature. The performance analysis and comparison (of expected running time complexity) was conducted in a simpler setting of hard-sphere models where we developed an asymptotic regime where the Poisson process intensity $\lambda$ of spheres in a hyper cube $[0, 1]^d$ increased to infinity, while the sphere volume of order $\lambda^{-\eta d}$ decreased to zero. We conducted this analysis for different ranges of $\eta$. Our one conclusion was
that while the recently proposed dominated coupling from the past methods perform better for $1 < \eta d < 2$ for large $\lambda$, our importance sampling based methods provide an improved performance for $\eta d \leq 1$ and $\eta d \geq 2$.

Enroute, we established large deviations results for the probability that spheres with centers generated as a Poisson process in a hyper cube $[0, 1]^d$ do not overlap with each other. We did this even when the radius of the spheres was randomly distributed. Finally, to operationalize the proposed importance sampling based acceptance-rejection methods, we introduced and analyzed grid based importance sampling. We also conducted extensive numerical experiments to validate our asymptotic results.

The proposed importance sampling based acceptance-rejection methods rely on clever parti-
tioning of the underlying configuration space and arriving at an appropriate change of measure to generate the spatial process on each partition. While we showed how this may be effectively conducted in a few settings, further research is needed to develop effective implementations for perfect sampling from a broad class of Gibbs processes.

Appendix A Proofs

The following lemmas are useful for proving our results. Lemma 1 is a standard Chernoff bound for Poisson random variables and Lemma 2 is Hoeffding’s inequality for U-statistics [19].

Lemma 1 (Chernoff bound for Poisson). Let \( N \sim \text{Poi}(\lambda) \). Then, for any \( 0 < \epsilon < 1 \),

\[
P(N \leq (1 - \epsilon)\lambda) \leq \exp \left(-\frac{\lambda \epsilon^2}{2}\right) \quad \text{and} \quad P(N \geq (1 + \epsilon)\lambda) \leq \exp \left(-\frac{\lambda \epsilon^2}{3}\right).
\]

Lemma 2 (Hoeffding, 1963). Suppose that \( \xi_1, \xi_2, \ldots, \xi_n \) are i.i.d. random variables and \( g : \mathbb{R}^k \to [0, 1] \) is a bounded function. Set \( Y_n = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq n} g(\xi_{i_1}, \xi_{i_2}, \ldots, \xi_{i_k}) \) for an integer \( k \leq n \) (this is known as U-statistics of order \( k \)). Then, for any \( \epsilon > 0 \),

\[
P(Y_n \geq \binom{n}{k} \left( \mathbb{E}[g(\xi_1, \xi_2, \ldots, \xi_k)] + \epsilon \right)) \leq 2 \exp \left(-2|n/k|\epsilon^2\right).
\]

The same estimate holds for \( P(Y_n \leq \binom{n}{k} \left( \mathbb{E}[g(\xi_1, \xi_2, \ldots, \xi_k)] - \epsilon \right) \).

A.1 Proof of Theorem 1

Remember that in Section 5, the hard-sphere model is considered in two scenarios according to the definition of the spheres. In the first scenario, each sphere is an Euclidean sphere. In the second scenario the space \([0, 1]^d\) is a torus and hence each sphere close to the boundary loops over to the opposite boundaries. All the results stated and proved below are true for both the scenarios.

Recall that \( \lambda > 0 \), \( \eta > 0 \), and \( \{R_1, \ldots, R_n\} \) are the radii of \( n \) spheres whose centers are independently and uniformly generated on the \( d \)-dimensional unit cube \([0, 1]^d\), where \( R_1, R_2, \ldots, R_n \) are i.i.d. strictly positive random variables bounded above by a constant \( r \). Define, for all \( i \geq 1 \),

\[
m_i := \mathbb{E}[(R_1 + R_2)^{id}] . \quad (23)
\]

Suppose that the centers of the spheres constitute a homogeneous BPP \( \{X_1, X_2, \ldots, X_n\} \) on the \( d \)-dimensional unit cube \([0, 1]^d\), where \( X_i \) denotes the center of the \( i \)th sphere. Let \( P_n(\lambda) \) be the probability that these \( n \) spheres do not overlap with each other. A typical configuration with \( n \) points is denoted by \( \mathcal{X} = \{(X_1, R_1), (X_2, R_2), \ldots, (X_n, R_n)\} \).

The volume of a sphere with radius \( x \) is given by \( \gamma x^d \), where \( \gamma = \pi^{d/2}/\Gamma(d/2 + 1) \) and \( \Gamma(\cdot) \) is the gamma function. We conclude the proof of Theorem 1 as a consequence of the lemmas that are stated and proved below. Our large deviations analysis exploits the IS technique introduced in Section 4. Recall that \( \tilde{\mu} \) denotes the IS measure, and \( \mu^0 \) is absolutely continuous with respect to \( \tilde{\mu} \) over \( \mathcal{A} \) with the associated likelihood ratio \( L(\mathcal{X}) \) is given by (11). It is useful to note and easy to
observe that \( L(\mathcal{X}) = 0 \) if and only if \( \mathcal{X} \) is an overlapping configuration. Then, by the definition of \( \mathcal{P}_n(\lambda) \),

\[
\mathcal{P}_n(\lambda) = \mathbb{P}_{\mu^0}(\mathcal{X} \in \mathcal{A}) = \mathbb{E}_{\tilde{\mu}} \left[ I(\mathcal{X} \in \mathcal{A}) \prod_{i=1}^{n} \left(1 - B_i\right) \right] = \mathbb{E}_{\tilde{\mu}} \left[ \prod_{i=1}^{n} \left(1 - B_i\right) \right].
\]

(24)

The following bound holds trivially,

\[
B_i \leq \frac{\gamma}{\lambda^{nd}} \sum_{j=1}^{i-1} (R_j + R_i)^d.
\]

(25)

Let \( \theta_{n,\lambda} = \frac{\gamma(2r)^d n}{\lambda^{nd}} \). We have the following upper and lower bounds on \( \mathcal{P}_n(\lambda) \).

**Lemma 3.** Under the above set-up,

\[
\mathcal{P}_n(\lambda) \geq \exp \left( -n \sum_{j=1}^{\infty} \left( \frac{\gamma n}{\lambda^{nd}} \right)^j \frac{m_j}{j(j+1)} \right),
\]

(26)

and, for any \( \epsilon > 0 \),

\[
\mathcal{P}_n(\lambda) \leq N_{n,\lambda} \left[ \exp \left( -\frac{\gamma n(n-1)(m_1-\epsilon)}{2\lambda^{nd}} \right) + 2 \exp \left( -\frac{(n-1)\epsilon^2}{(2r)^2d} \right) \right],
\]

(27)

for any \( n \) and \( \lambda \) such that \( \theta_{n,\lambda} < 1 \), where \( N_{n,\lambda} \) is a function of \( n, \lambda \) and \( r \) such that

\[
\lim_{\lambda \to \infty} \frac{1}{\lambda^{2-\eta d}} \log N_{\lambda,\lambda} = 0, \text{ if } \eta d > 1.
\]

(28)

In particular, for torus-hard-sphere model,

\[
\lim_{\lambda \to \infty} N_{\lambda,\lambda} = 1, \text{ if } \eta d > 3/2.
\]

(29)

**Proof of Lemma 3**  **Lower Bound:** To prove (26) notice that, by (24),

\[
\mathcal{P}_n(\lambda) = \mathbb{E}_{\tilde{\mu}} \left[ \exp \left( \sum_{i=1}^{n} \log \left(1 - B_i\right) \right) \right] = \mathbb{E}_{\tilde{\mu}} \left[ \exp \left( \sum_{i=1}^{n} \sum_{j=1}^{\infty} \frac{1}{j} B_i^j \right) \right],
\]

here we used the Taylor’s expansion \( \log(1 - x) = -\sum_{j=1}^{\infty} x^j/j \), for \( 0 \leq x \leq 1 \). By Jensen’s inequality and (25), we write that

\[
\mathcal{P}_n(\lambda) \geq \exp \left( -\sum_{i=1}^{n} \sum_{j=1}^{\infty} \frac{1}{j} \mathbb{E}_{\tilde{\mu}} \left[ B_i^j \right] \right) \geq \exp \left( -\sum_{i=1}^{n} \sum_{j=1}^{\infty} \frac{\gamma j}{j\lambda^{nd}} \mathbb{E}_{\tilde{\mu}} \left[ \left( \sum_{l=1}^{i-1} (R_l + R_i)^d \right)^j \right] \right)
\]

\[
= \exp \left( -\sum_{i=1}^{n-1} \sum_{j=1}^{\infty} \frac{\gamma j}{i\lambda^{nd}} \mathbb{E}_{\tilde{\mu}} \left[ \left( \frac{1}{i-1} \sum_{l=1}^{i-1} (R_l + R_i)^d \right)^j \right] \right).
\]
Again by Jensen’s inequality,  
\[ \left( \frac{1}{i-1} \sum_{i=1}^{i-1} (R_l + R_i)^d \right)^{\gamma} \leq \frac{1}{i-1} \left( \sum_{i=1}^{i-1} (R_l + R_i)^d \right)^{\gamma} \], 
and thus \( \mathcal{P}_n(\lambda) \geq \exp \left( - \sum_{j=1}^{\infty} \frac{\gamma j m_j}{j^{\gamma d}} \sum_{i=1}^{n} (i - 1)^j \right) \). We establish (26) using \( \sum_{i=1}^{n} (i - 1)^j \leq \int_{x=0}^{n} x^j \, dx = \frac{n^{j+1}}{j + 1} \).

**Upper Bound:** Let \( R_{(1)}, R_{(2)}, \ldots, R_{(n)} \) be the order statistics of \( R_1, R_2, \ldots, R_n \). Since the non-overlapping probability \( \mathcal{P}_n(\lambda) \) is independent of the order in which the spheres are generated, without loss of generality assume that the \( i^{th} \) sphere has radius \( R_{(i)} \). Let, for each \( 1 \leq j \leq i - 1 \), \( \tilde{B}_i(j) \) be the volume of the blocked region seen by the \( j^{th} \) sphere when the \( j + 1, j + 2, \ldots, i - 1 \) spheres are ignored, where \( \tilde{B}_i(0) = 0 \). One can think of \( \tilde{B}_i(j) - \tilde{B}_i(j - 1) \) as the blocking volume contributed by the \( j^{th} \) sphere for the \( i^{th} \) sphere. Under the new measure \( \bar{\mu} \), the blocking volume seen by the \( i^{th} \) sphere, \( B_i = \sum_{j=1}^{i-1} \left( \tilde{B}_i(j) - \tilde{B}_i(j - 1) \right) \). Consider the sets

\[ \mathcal{N}^{(i)} := \left\{ j \in \{1, 2, \ldots, i - 1\} : \tilde{B}_i(j) - \tilde{B}_i(j - 1) = \frac{\gamma}{\lambda^{nd}} (R_{(j)} + R_{(i)})^d \right\}, \]

for \( i \leq n \) and take \( \tilde{\mathcal{N}}^{(i)} := \{1, 2, \ldots, i - 1\} \setminus \mathcal{N}^{(i)} \). Using the inequality \( 1 - x \leq e^{-x} \) and (24),

\[ \mathcal{P}_n(\lambda) \leq \mathbb{E}_{\bar{\mu}} \left[ \exp \left( - \sum_{i=1}^{n} B_i \right) \right] \]
\[ = \mathbb{E}_{\bar{\mu}} \left[ \exp \left( - \sum_{i=1}^{n} \sum_{j=1}^{i-1} \left( \tilde{B}_i(j) - \tilde{B}_i(j - 1) \right) \right) \right] \]
\[ \leq \mathbb{E}_{\bar{\mu}} \left[ \exp \left( - \frac{\gamma}{\lambda^{nd}} \sum_{i=1}^{n} \sum_{j \in \mathcal{N}^{(i)}} (R_{(j)} + R_{(i)})^d \right) \right] \]
\[ = \mathbb{E}_{\bar{\mu}} \left[ \exp \left( - \frac{\gamma}{\lambda^{nd}} \sum_{i=1}^{n} \sum_{j \in \mathcal{N}^{(i)}} (R_{(j)} + R_{(i)})^d \right) \right] \]
\[ \leq \mathbb{E}_{\bar{\mu}} \left[ \exp \left( - \frac{\gamma}{\lambda^{nd}} \sum_{i=1}^{n} \sum_{j \in \mathcal{N}^{(i)}} (R_{(j)} + R_{(i)})^d \right) \right], \]

where \( Y_n = \sum_{i=1}^{n} \sum_{j=1}^{i-1} \left( \frac{R_{(j)} + R_{(i)}}{2r} \right)^d \), and the last inequality holds because of the assumption that each radius \( R_i \) is upper bounded by \( r \). Since \( R_{(i)} \) is non-decreasing with \( i \), from the definition of \( \mathcal{N}^{(i)} \), it is easy to see that \( |\mathcal{N}^{(i)}| \) is a non-decreasing with \( i \). Therefore,

\[ \mathcal{P}_n(\lambda) \leq \mathbb{E}_{\bar{\mu}} \left[ \exp \left( - \frac{\gamma}{\lambda^{nd}} Y_n + \theta_{n,\lambda,|\mathcal{N}^{(n)}|} \right) \right] \]
\[ = \mathbb{E} \left[ \exp \left( - \frac{\gamma}{\lambda^{nd}} Y_n \right) \mathbb{E}_{\bar{\mu}} \left[ \exp \left( \theta_{n,\lambda,|\mathcal{N}^{(n)}|} \right) \right] \mathbb{E}_{\bar{\mu}} \left[ \exp \left( \theta_{n,\lambda,|\mathcal{N}^{(n)}|} \right) R_1, \ldots, R_n \right] \right]. \]

We now show that \( |\mathcal{N}^{(n)}| \) is stochastically bounded by a binomial random variable, and as a consequence, the conditional expectation \( \mathbb{E}_{\bar{\mu}} \left[ \exp \left( \theta_{n,\lambda,|\mathcal{N}^{(n)}|} \right) \right] \mathbb{E}_{\bar{\mu}} \left[ \exp \left( \theta_{n,\lambda,|\mathcal{N}^{(n)}|} \right) \right] \) is uniformly bounded by a constant, which is function of \( n, \lambda \) and \( r \). Let

\[ q_j = \mathbb{P}_{\bar{\mu}} \left( \tilde{B}_n(j) - \tilde{B}_n(j - 1) < \frac{\gamma}{\lambda^{nd}} (R_{(j)} + R_{(n)})^d \right). \]
Clearly, \( q_j \) is increasing with \( j \), and therefore \( q_j \leq q_{n-1} \) for all \( j \leq n - 1 \). This implies that \(|\mathcal{Y}^{(n)}|\) is stochastically bounded by a binomial random variable with parameters \( n \) and \( q_{n-1} \), and thus
\[
\mathbb{E}_\tilde{\mu} \left[ \exp \left( \theta_{n,\lambda} |\mathcal{Y}^{(n)}| \right) \right] R_1, \ldots, R_n \leq \left( q_{n-1} \exp \left( \theta_{n,\lambda} \right) - (1 - q_{n-1}) \right)^n.
\]
Due to the boundary effect, \( q_{n-1} \) for the Euclidean-hard-sphere model is different from that of the torus-hard-sphere model. Observe that, for the Euclidean-hard-sphere model, \( \tilde{B}_n(n - 1) - \tilde{B}_n(n - 2) < \frac{\gamma(R(j) + R(n))d}{\lambda^d} \) if either

1. the center of the \((n - 1)^{th}\) sphere is within \((R(j) + R(n) + 2R(n))/\lambda^n \) distance from the center of \( j^{th} \) sphere for some \( j \leq n - 2 \), or
2. the center of \((n - 1)^{th}\) sphere is within \((R(n) + R(n))/\lambda^n \) distance form the boundary of the unit cube.

Note that the boundary event (2) is irrelevant for the torus-hard-sphere model. The probability of the event (1) is maximized by \( \frac{\gamma}{\lambda^d} \sum_{j=1}^{n-2} \left( \frac{R(j) + R(n) + 2R(n)}{1 - B_n} \right)^d \), while that for the event (2) is maximized by \( \frac{1 - (1 - 2(R(n) + R(n))/\lambda^n)^d}{1 - B_n} \). Since \( R_i \)'s are bounded by \( \tilde{r} \) and \( B_n \leq \theta_{n,\lambda} \) (from (25)), we have
\[
q_{n-1} \leq \bar{q}_{n,\lambda} := \left\{\begin{array}{ll}
2d\theta_{n,\lambda} & \text{for Euclidean-hard-sphere model} \\
\frac{1 - \theta_{n,\lambda}}{2} & \text{for torus-hard-sphere model}
\end{array}\right.
\]
for any \( n \) and \( \lambda \) such that \( \theta_{n,\lambda} < 1 \), and for some constant \( c \).

Let \( N_{n,\lambda} = \left(1 + \bar{q}_{n,\lambda} \left( \exp \left( \theta_{n,\lambda} \right) - 1 \right) \right)^n \), then \( \mathcal{P}_n(\lambda) \leq N_{n,\lambda} \mathbb{E} \left[ \exp \left( - \frac{\gamma}{\lambda^d} Y_n \right) \right] \). Since \( Y_n = \sum_{i=1}^n \sum_{j=1}^{i-1} \left( \frac{R_i + R_j}{2\tilde{r}} \right)^d \), for any \( \epsilon > 0 \),
\[
\mathbb{E} \left[ \exp \left( - \frac{\gamma}{\lambda^d} (2r)^d Y_n \right) \right] \leq \exp \left( - \frac{\gamma n(n - 1)}{2\lambda^d} \left( m_1 - \epsilon \right) \right) \mathbb{P} \left( Y_n < \frac{n(n - 1)}{2} \left( \frac{m_1 - \epsilon}{(2r)^d} \right) \right) .
\]
By Lemma 2 (with \( k = 2 \)), \( \mathbb{P} \left( Y_n < \frac{n(n - 1)}{2} \left( \frac{m_1 - \epsilon}{(2r)^d} \right) \right) \leq 2 \exp \left( - \frac{(n - 1)^2}{2(2r)^d} \right) \), and thus (27) is established.

It is now remain to prove (28) and (29). Assume that \( \eta d > 1 \). Then \( \lim_{\lambda \to \infty} \theta_{n,\lambda} = 0 \) and hence \( \lim_{\lambda \to \infty} \bar{q}_{n,\lambda} = 0 \). Since \( N_{n,\lambda} \leq \exp \left( \lambda \bar{q}_{n,\lambda} \left[ \exp \left( \theta_{n,\lambda} \right) - 1 \right] \right) \), using Taylor’s expansion of exponential function,
\[
0 \leq \lim_{\lambda \to \infty} \frac{1}{\lambda^2 \eta d} \log N_{n,\lambda} \leq \lim_{\lambda \to \infty} \left[ \bar{q}_{n,\lambda} \sum_{j=0}^{\infty} \frac{\gamma^{(j+1)}(2r)^j}{(j+1)!} \lambda^{j(\eta d - 1)} \right] = 0.
\]
Thus (28) holds. In particular, for torus-hard-sphere model with \( \eta d > 3/2 \),
\[
\lambda \bar{q}_{n,\lambda} \left[ \exp \left( \theta_{n,\lambda} \right) - 1 \right] = \lambda \frac{2d\theta_{n,\lambda}}{1 - \theta_{n,\lambda}} \left[ \exp \left( \theta_{n,\lambda} \right) - 1 \right] = \frac{2d}{1 - \theta_{n,\lambda}} \sum_{j=2}^{\infty} \frac{\gamma j^d}{j!} \lambda^{1 - j(\eta d - 1)}
\]
go to 0 as \( \lambda \to \infty \), and hence (29) holds. \( \square \)
Recall that the non-overlapping probability $\mathcal{P}(\lambda)$ defined by (8).

**Lemma 4.** Suppose that $1 < \eta d \leq 2$ and $R \leq r$ almost surely for some constant $r > 0$. Then, for any $0 < a < 0.5$,

$$\mathcal{P}(\lambda) \geq \exp \left( -\sum_{j=1}^{\infty} \frac{\lambda^{j(1-\eta d)+1} (1 + \frac{1}{\lambda^a})^{j+1} \gamma^j m_j}{j(j+1)} \right) [1 - o(1)]. \quad (30)$$

Furthermore, let $\bar{\lambda} = [\lambda(1 - \frac{1}{2^a})]$ for some constant $a$ such that $0 < a < \frac{\eta d - 1}{2}$. Then, for any $\epsilon > 0$,

$$\mathcal{P}(\lambda) \leq N_{\lambda,\lambda} \exp \left( -\gamma \lambda^2 (m_1 - \epsilon) \right) [1 + o(1)], \quad (31)$$

where $N_{\lambda,\lambda}$ satisfies (28) and (29). In particular, (30) holds with $\epsilon = 0$ if $\eta d > 5/3$ and $2 - \eta d < a < \frac{\eta d - 1}{2}$.

**Proof.** The number of spheres in a $\lambda$-homogeneous PPP on the unit cube $[0, 1]^d$ is a Poisson random variable, denote it by $N$, with mean $\lambda$. Thus the non-overlapping probability

$$\mathcal{P}(\lambda) = \mathbb{E}[\mathcal{P}_N(\lambda)], \quad (32)$$

where $\mathcal{P}_n(\lambda)$ is the non-overlapping probability of $n$ spheres as defined in the last section.

**Lower Bound:** Fix $a$ such that $0 < a < 0.5$. Notice that $\mathcal{P}_n(\lambda)$ is a decreasing function of $n$ for any given $\lambda$. Therefore, by Lemma 3, we can say that for all $n < \lambda (1 + \frac{1}{\lambda^a})$,

$$\mathcal{P}_n(\lambda) \geq \exp \left( -\sum_{j=1}^{\infty} \frac{\lambda^{j(1-\eta d)+1} (1 + \frac{1}{\lambda^a})^{j+1} \gamma^j m_j}{j(j+1)} \right),$$

and from (32) and the Chernoff bound for the Poisson variable $N$ (see Lemma 1),

$$\mathcal{P}(\lambda) \geq \mathbb{E} \left( \mathcal{P}_N(\lambda); N < \lambda \left(1 + \frac{1}{\lambda^a}\right) \right) \geq \Pr \left( N < \lambda \left(1 + \frac{1}{\lambda^a}\right) \right) \exp \left( -\sum_{j=1}^{\infty} \frac{\lambda^{j(1-\eta d)+1} (1 + \frac{1}{\lambda^a})^{j+1} \gamma^j m_j}{j(j+1)} \right) \geq \left( 1 - \exp \left( -\frac{1}{3} \lambda^{1-2a} \right) \right) \exp \left( -\sum_{j=1}^{\infty} \frac{\lambda^{j(1-\eta d)+1} (1 + \frac{1}{\lambda^a})^{j+1} \gamma^j m_j}{j(j+1)} \right).$$

We have (30) because $\exp \left( -\frac{1}{3} \lambda^{1-2a} \right) = o(1)$ as a function of $\lambda$.

**Upper Bound:** From (32),

$$\mathcal{P}(\lambda) = \mathbb{E}[\mathcal{P}_N(\lambda)] \leq \mathbb{E}[\mathcal{P}_N(\lambda); N \geq \bar{\lambda}] + \Pr(N < \bar{\lambda}) \leq \mathcal{P}_\bar{\lambda}(\lambda) + \Pr(N < \bar{\lambda}), \quad (33)$$

where the last inequality holds due the fact that $\mathcal{P}_n(\lambda)$ is a decreasing function of $n$ for any given $\lambda$. We analyze $\mathcal{P}_\bar{\lambda}(\lambda)$ and $\Pr(N < \bar{\lambda})$ separately.
By Lemma 3 for any $\epsilon > 0$,

\[
\mathcal{P}_\lambda (\lambda) \leq N_{\lambda, \lambda} \left[ \exp \left( -\frac{\gamma \lambda (\lambda - 1) (m_1 - \epsilon)}{2 \lambda^{\eta d}} \right) + 2 \exp \left( -\frac{\lambda \epsilon^2}{(2r)^{2d}} \right) \right] \\
\leq N_{\lambda, \lambda} \left[ \exp \left( -\frac{\gamma \lambda^2 (m_1 - \epsilon)}{2 \lambda^{\eta d}} \right) \exp \left( \frac{\gamma m_1}{2 \lambda^{\eta d - 1}} \right) + 2 \exp \left( -\frac{\lambda \epsilon^2}{(2r)^{2d}} \right) \right],
\]

where we used the fact that $\bar{\lambda} \leq \lambda$. We rewrite the above expression as follows:

\[
\mathcal{P}_\lambda (\lambda) \leq N_{\lambda, \lambda} \exp \left( -\frac{\gamma \lambda^2 (m_1 - \epsilon)}{2 \lambda^{\eta d}} \right) \left( \exp \left( \frac{\gamma m_1}{2 \lambda^{\eta d - 1}} \right) + 2 \exp \left( -\frac{\lambda \epsilon^2}{(2r)^{2d}} \right) \right).
\]

Notice that $\frac{\gamma \lambda^2 m_1}{2 \lambda^{\eta d}} = O (\lambda^2 - \eta d)$ and $\frac{\lambda \epsilon^2}{(2r)^{2d}} = \Omega (\lambda)$. Since $\eta d > 1$,

\[
2 \exp \left( \frac{\gamma \lambda^2 m_1}{2 \lambda^{\eta d}} - \frac{\lambda \epsilon^2}{(2r)^{2d}} \right) \leq 2 \exp \left( -\bar{\lambda} \left( \frac{\epsilon^2}{(2r)^{2d}} - \frac{\gamma m_1}{2 \lambda^{\eta d - 1}} \right) \right) \rightarrow 0, \text{ as } \lambda \to \infty,
\]

and since $\lim_{\lambda \to \infty} \exp \left( \frac{\gamma m_1}{2 \lambda^{\eta d - 1}} \right) = 1$, we can say that the first term $\mathcal{P}_\lambda (\lambda)$ in (33) satisfies the following inequality,

\[
\mathcal{P}_\lambda (\lambda) \leq N_{\lambda, \lambda} \exp \left( -\frac{\gamma \lambda^2 (m_1 - \epsilon)}{2 \lambda^{\eta d}} \right) [1 + o(1)].
\]

By Lemma 1,

\[
\mathbb{P} \left( N \leq \lambda \right) \leq \mathbb{P} \left( N \leq \lambda \left( 1 - \frac{1}{\lambda^a} \right) \right) \leq \exp \left( -\frac{\lambda^{1-2a}}{2} \right).
\]

It is important to note that $2a < 1$ because $\eta d \leq 2$. By the definition of $a$, we have $1 - 2a > 2 - \eta d$, and hence using (35) and the fact that $N_{\lambda, \lambda} \geq 1$,

\[
\exp \left( \frac{\gamma \lambda^2 (m_1 - \epsilon)}{2 \lambda^{\eta d}} \right) \mathbb{P} \left( N \leq \lambda \right) \leq \exp \left( \frac{\gamma \lambda^2 (m_1 - \epsilon)}{2 \lambda^{\eta d}} - \frac{\lambda^{1-2a}}{2} \right) \rightarrow 0, \text{ as } \lambda \to \infty,
\]

and hence (31) follows from (33) and (36).

In particular if $\eta d > 5/3$, we can choose $a$ such that $2 - \eta d < a < \frac{\eta d - 1}{2}$. Let $\epsilon = 1/\lambda^a$. Then (34) and (36) holds. We complete the proof using the fact that $\lim_{\lambda \to \infty} \exp \left( \frac{\gamma \lambda^2 \epsilon}{2 \lambda^{\eta d}} \right) = 1$.

**Proof of Theorem 1.** The following upper and lower bounds together complete the proof.

**Lower Bounds:** Consider the inequality (30).

**Case: $\eta d > 2$.** It is given that the spheres have bounded radii, that is, $R \leq r$ almost surely for some constant $r > 0$. Hence, $m_j \leq (2r)^j d$ and for all values of $\eta d > 2$, and thus all the terms in the exponent of the right-hand side of (30) go to zero asymptotically. In other words, for any $0 < a < 0.5$,

\[
\lim_{\lambda \to \infty} \sum_{j=1}^{\infty} \frac{\lambda^j (1-\eta d + 1) (1 + \frac{1}{\lambda^a})^j + 1}{j (j + 1)} \gamma^j m_j = 0.
\]

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That means, \( \lim_{\lambda \to \infty} \mathcal{P}(\lambda) = 1 \), for \( \eta d > 2 \).

**Case: 3/2 < \eta d \leq 2.** From \([30]\),

\[
\mathcal{P}(\lambda) \exp \left( \frac{2m_1}{2} \lambda_2 - \eta d \right) \geq \exp \left( O \left( \lambda^2 - \eta d - a \right) - \sum_{j=2}^{\infty} \frac{\lambda^j (1-\eta d) + 1}{j(j+1)} \right) [1 - o(1)].
\]

By fixing \( a > 2 - \eta d \), we see that the right-hand side of the above expression goes to one as \( \lambda \to \infty \). Thus, \( \liminf_{\lambda \to \infty} \left[ \mathcal{P}(\lambda) \exp \left( \frac{2m_1}{2} \lambda^2 - \eta d \right) \right] \geq 1 \).

**Case: 1 < \eta d \leq 3/2.** By applying \( \log \) on both the sides of \([30]\), we have for any \( 0 < a < 0.5 \) that

\[
\log \mathcal{P}(\lambda) \geq \log (1 - o(1)) - \sum_{j=1}^{\infty} \frac{\lambda^j (1-\eta d) + 1}{2} \frac{\gamma^1 m_1}{j(j+1)},
\]

and see that

\[
\frac{1}{\lambda^2 - \eta d} \sum_{j=1}^{\infty} \frac{\lambda^j (1-\eta d) + 1}{2} \frac{\gamma^1 m_1}{j(j+1)} = \frac{\gamma^1 m_1}{2} + \sum_{j=2}^{\infty} \frac{(1 + \frac{1}{\lambda})^j \gamma^j m_j}{\lambda (j-1)(\eta d - 1) j(j+1)}.
\]

Now write \( \liminf_{\lambda \to \infty} \frac{1}{\lambda^{2-\eta d}} \log \mathcal{P}(\lambda) \geq -\frac{2m_1}{2} \) as a consequence of \( \eta d > 1 \).

**Case: 0 < \eta d \leq 1.** Configurations with one sphere or no sphere is always accepted, that is, \( \mathcal{P}_1(\lambda) = \mathcal{P}_0(\lambda) = 1 \). The probability of generating no sphere is \( e^{-\lambda} \). Consequently, \( \mathcal{P}(\lambda) > e^{-\lambda} \) and for any \( \eta d > 0 \),

\[
\liminf_{\lambda \to \infty} \left[ \frac{1}{\lambda} \log \mathcal{P}(\lambda) \right] \geq -1.
\]

(37)

In particular, assume that \( \eta d = 1 \). For this case, first we show that the limit \( \delta := \lim_{\lambda \to \infty} \left[ \frac{1}{\lambda} \log \mathcal{P}(\lambda) \right] \) exists. To prove this, partition the cube \([0,1]^d\) into a cubic grid of cell edge length \( x^{1/d} \in (0,1) \).

Ignore the cells at the boundary with edge length strictly smaller than \( x^{1/d} \). So, the total intensity of the underlying PPP over a cell is \( \lambda x \).

When \( \eta d = 1 \), radius of each sphere is identical in distribution to \( R/\lambda \). It is important to observe that the non-overlapping probability of the spheres restricting to a cell is \( \mathcal{P}(\lambda x) \) (see the definition of the non-overlapping probability). Since the total number of cells is at least \( 1/x \), the non-overlapping probability \( \mathcal{P}(\lambda) \) is bounded above by \( (\mathcal{P}(\lambda x))^{1/x} \), and thus \( \frac{1}{\lambda} \log \mathcal{P}(\lambda) \leq \frac{1}{x} \log \mathcal{P}(\lambda x) \).

We can increase \( \lambda \) and decrease the cell edge length \( x^{1/d} \) such that \( y := \lambda x \) is fixed. Then the following inequality holds

\[
\limsup_{\lambda \to \infty} \left[ \frac{1}{\lambda} \log \mathcal{P}(\lambda) \right] \leq \frac{1}{y} \log \mathcal{P}(y) < 0.
\]

Now the existence of the required limit is established by applying limit on \( y \):

\[
\limsup_{\lambda \to \infty} \left[ \frac{1}{\lambda} \log \mathcal{P}(\lambda) \right] \leq \liminf_{y \to \infty} \left[ \frac{1}{y} \log \mathcal{P}(y) \right].
\]

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To show that $\delta \nearrow 0$ as $\gamma m_1 \searrow 0$, assume that $\gamma m_1 < \epsilon$ for a constant $\epsilon \in (0, 1)$. By (24) and (25),

$$\mathcal{P}_n(\lambda) \geq \mathbb{E} \left[ \prod_{i=1}^{n-1} \left( 1 - \frac{\gamma}{\lambda} \sum_{k=1}^{i} (R_k + R_i)^d \right)^+ \right].$$

Consider the following partial order on $\mathbb{R}_n$: for any $y, y' \in \mathbb{R}_n$, we say that $y \preceq y'$ if $y_i \leq y'_i$ for all $i = 1, \ldots, n$. A function $f : \mathbb{R}_n^+ \to \mathbb{R}$ is called increasing (or decreasing) if $f(y) \leq f(y')$ (or $f(y) \geq f(y')$) for all $y, y' \in \mathbb{R}_n$ such that $y \preceq y'$. If $f$ and $g$ are either increasing or decreasing functions then Theorem 2.4 of [18] (FKG inequality) can trivially extended to show that $\mathbb{E}[f(Y)g(Y)] \geq \mathbb{E}[f(Y)]\mathbb{E}[g(Y)]$. Clearly the following function $f_i$ is a decreasing function on $\mathbb{R}_n^+$.

$$f_i(y) = \left( 1 - \frac{\gamma}{\lambda} \sum_{k=1}^{i} (y_k + y_i)^d \right)^+.$$ 

Therefore,

$$\mathbb{E} \left[ \prod_{i=1}^{n-1} \left( 1 - \frac{\gamma}{\lambda} \sum_{k=1}^{i} (R_k + R_i)^d \right)^+ \right] \geq \prod_{i=1}^{n-1} \mathbb{E} \left[ \left( 1 - \frac{\gamma}{\lambda} \sum_{k=1}^{i} (R_k + R_i)^d \right)^+ \right].$$

Using the convexity of the function $x^+$ and Jensen’s inequality, for each $i$,

$$\mathbb{E} \left[ \left( 1 - \frac{\gamma}{\lambda} \sum_{k=1}^{i} (R_k + R_i)^d \right)^+ \right] \geq \left( 1 - i \frac{\gamma m_1}{\lambda} \right)^+,$$

and thus $\mathcal{P}_n(\lambda) \geq \prod_{i=1}^{n-1} \left( 1 - i \frac{\gamma m_1}{\lambda} \right)^+$. With $\Lambda = [\lambda + \lambda^0.75]$ and $N \sim \text{Poi}(\lambda)$,

$$\mathcal{P}(\lambda) = \sum_{n=0}^{\infty} e^{-\lambda} \frac{\lambda^n}{n!} \mathcal{P}_n(\lambda) \geq \sum_{n=0}^{\Lambda} e^{-\lambda} \frac{\lambda^n}{n!} \mathcal{P}_n(\lambda) \geq \mathcal{P}_\Lambda(\lambda) \mathbb{P}(N \leq \Lambda).$$

By applying log on both the sides of the above inequality and scaling with $1/\lambda$,

$$\frac{1}{\lambda} \log \mathcal{P}(\lambda) \geq \frac{1}{\lambda} \log \mathcal{P}_\Lambda(\lambda) + \frac{1}{\lambda} \log \mathbb{P}(N \leq \Lambda).$$

From the definition of $\Lambda$ and Lemma 1, the second term, $\frac{1}{\lambda} \log \mathbb{P}(N \leq \Lambda)$, goes to zero as $\lambda \nearrow \infty$. We now focus on the first term, $\frac{1}{\lambda} \log \mathcal{P}_\Lambda(\lambda)$. Since $\gamma m_1 < \epsilon < 1$, for all $i \leq \Lambda$,

$$\frac{i \gamma m_1}{\lambda} \epsilon < \frac{\lambda \gamma m_1}{\lambda} \epsilon \leq \left( 1 + \frac{1}{\lambda^{0.25}} \right) \frac{\gamma m_1}{\epsilon} \leq 1,$$

for large values of $\lambda$. Thus, we can write using Bernoulli’s inequality that

$$\mathcal{P}_\Lambda(\lambda) \geq \prod_{i=1}^{\Lambda} \left( 1 - i \frac{\gamma m_1}{\lambda} \right) = \prod_{i=1}^{\Lambda} \left( 1 - \epsilon \frac{i \gamma m_1}{\lambda} \right) \geq \prod_{i=1}^{\Lambda} \left( 1 - \epsilon \frac{i \gamma m_1}{\lambda} \right),$$

for large values of $\lambda$. Therefore, by combining the trivial bound (37) and the above conclusions,

$$\delta \geq \max \left( -1, \frac{\gamma m_1}{2} \left[ \log(1 - \epsilon) \right] \right) \to 0 \text{ as } \gamma m_1 \searrow 0.$$
Upper Bounds: We have a complete proof of the large deviation of \( \mathcal{P}(\lambda) \) for the case \( \eta d > 2 \). So, it is now remain to prove the theorem for \( 0 < \eta d \leq 2 \). We first prove the required upper bounds for the case \( 1 < \eta d \leq 2 \). If \( 0 < a < 0.5 \) and \( \bar{\lambda} = [\lambda(1 - \frac{1}{\lambda^d})] \), then from Lemma 4 for any \( \epsilon > 0 \),

\[
\mathcal{P}(\lambda) \leq N_{\lambda, \lambda} \exp \left( -\frac{\gamma \lambda^2 (m_1 - \epsilon)}{2 \lambda^d} \right) [1 + o(1)].
\]

(38)

Case: \( \eta d > 1 \). By applying \( \log \) on both the sides of (38) and then dividing by \( \lambda^2 - \eta d \), we see that

\[
\frac{1}{\lambda^2 - \eta d} \log \mathcal{P}(\lambda) \leq -\frac{\gamma (m_1 - \epsilon)}{2} \left( 1 + \frac{1}{\lambda^d} \right)^2 + \frac{1}{\lambda^2 - \eta d} \log N_{\lambda, \lambda} + \frac{1}{\lambda^2 - \eta d} \log [1 + o(1)].
\]

As a consequence of Lemma 3, \( \limsup_{\lambda \to \infty} \frac{1}{\lambda^2 - \eta d} \log \mathcal{P}(\lambda) \leq -\frac{\gamma (m_1 - \epsilon)}{2} \). Now take \( \epsilon \searrow 0 \).

In particular, consider torus-hard-sphere model with \( 5/3 < \eta d \leq 2 \). We can fix \( a \) such that \( 2 - \eta d < a < \frac{\eta d - 1}{2} \). From Lemma 4, (38) holds with \( \epsilon = 0 \). Therefore,

\[
\mathcal{P}(\lambda) \exp \left( \frac{\gamma m_1}{2} \lambda^2 - \eta d \right) \leq N_{\lambda, \lambda} \exp \left( O \left( \lambda^2 - \eta d \right) \right) [1 + o(1)],
\]

and hence \( \limsup_{\lambda \to \infty} [\mathcal{P}(\lambda) \exp \left( \frac{\gamma m_1}{2} \lambda^2 - \eta d \right)] \leq 1 \) from Lemma 3.

Case: \( 0 < \eta d < 1 \). Let \( \lambda = [\lambda^{\frac{\eta d}{d}}] \) and \( N \sim Poi(\lambda) \). From the definition

\[
\mathcal{P}(\lambda) = \mathbb{E} [\mathcal{P}_N(\lambda)] \leq \mathbb{P} (N \leq \lambda) + \mathbb{E} [\mathcal{P}_N(\lambda); N \geq \lambda + 1].
\]

(39)

For any \( \epsilon > 0 \), let \( H_n(\epsilon) := \left\{ \frac{1}{n} \sum_{i=1}^{n} R_i^d > \epsilon \right\} \). From (12),

\[
\mathcal{P}_{n+1}(\lambda) \leq \mathbb{E} \left[ \prod_{i=1}^{n} \left( 1 - \frac{\gamma}{\lambda^d} \sum_{j=1}^{i} R_j^d \right)^{+} \right] \leq \mathbb{P} \left( H^c_n \left( \frac{\lambda^{\eta d}}{\gamma n} \right) \right) \leq \mathbb{P} \left( H^c_n \left( \frac{\lambda^{\eta d}}{\lambda n} \right) \right),
\]

where the second inequality holds because \( \left( 1 - \frac{\gamma}{\lambda^d} \sum_{j=1}^{n} R_j^d \right)^+ = 0 \) on \( H_n \left( \frac{\lambda^{\eta d}}{\gamma n} \right) \). Since \( \eta d < (\eta d + 1)/2 < 1 \), see that \( \frac{\lambda^{\eta d}}{\gamma^2} \searrow 0 \) as \( \lambda \nearrow \infty \), and thus for every \( \epsilon > 0 \) there exists \( \lambda_\epsilon \) such that

\[
\mathcal{P}_{n+1}(\lambda) \leq \mathbb{P} \left( H^c_n (\epsilon) \right),
\]

for all \( \lambda > \lambda_\epsilon \) and \( n > \lambda \).

Suppose there is a constant \( c > 0 \) such that \( R \geq c \). Then for all sufficiently small values of \( \epsilon \), \( \mathbb{P} \left( H^c_n (\epsilon) \right) = 0 \) for all \( n > \lambda \). Thus for large values of \( \lambda \), \( \mathcal{P}(\lambda) \leq \mathbb{P} (N \leq \lambda) \leq e^{-\lambda \lambda_\epsilon} \), and from the definition of \( \lambda_\epsilon \)

\[
\limsup_{\lambda \to \infty} \frac{1}{\lambda} \log \mathcal{P}(\lambda) \leq -1 + \limsup_{\lambda \to \infty} \left[ \frac{\lambda \log \lambda}{\lambda} \right] = -1.
\]

So we can assume that \( \mathbb{P}(R < \epsilon) > 0 \) for every \( \epsilon > 0 \). Recall that \( \mathbb{P}(R > 0) = 1 \), \( F \) is the distribution of \( R^d \), and \( \Lambda(\theta) \) is the logarithmic moment generating function of \( F \). As a consequence of positivity of \( R \), we see that \( \Lambda(\theta) \searrow -\infty \) as \( \theta \searrow -\infty \). Let \( \Lambda^*(x) = \sup_{\theta \in \mathbb{R}} \{ \theta x - \Lambda(\theta) \} \). As a
consequence of the assumption that $P(R < \epsilon) > 0$ for every $\epsilon > 0$, we can show $\Lambda^*(x) \nrightarrow \infty$ as $x \searrow 0$. From Theorem 2.2.3 of [11],

$$P(H^n_\epsilon(\epsilon)) \leq 2 \exp \left( -n \inf_{x \leq \epsilon} \Lambda^*(x) \right) = 2 \exp (-n \Lambda^*(\epsilon))$$

for all $n > \lambda$ and $\epsilon < \mathbb{E}[R^d_1]$, where the last inequality holds because $\Lambda^*(x)$ is non-decreasing over $0 < x \leq \mathbb{E}[R^d_1]$. By (39),

$$P(\lambda) \leq P(N \leq \lambda) + P(H^c_N(\epsilon); N \geq \lambda + 1) \leq P(N \leq \lambda) + P(H^c_N(\epsilon))$$

$$\leq P(N \leq \lambda) + 2 \exp \left( -\lambda \left( 1 - e^{-\Lambda^*(\epsilon)} \right) \right),$$

for all $\lambda \geq \lambda_*$. To conclude that $\limsup_{\lambda \to \infty} \frac{1}{\lambda} \log P(\lambda) \leq -1$, see from the definition of Poisson distribution and $\lambda$ that

$$P(N \leq \lambda) = \sum_{n=0}^{\lambda} e^{-\lambda} \frac{\lambda^n}{n!} \leq \lambda e^{-\lambda} \left( \frac{\lambda}{\lambda} \right)^{\lambda} \leq e^{-\lambda} \frac{\lambda}{\lambda},$$

where we used the fact that $\lambda^{n-1}/(n-1)! < \lambda^n/n!$ for all $n < \lambda$. Hence,

$$P(\lambda) \leq 2 \exp \left( -\lambda \left( 1 - e^{-\Lambda^*(\epsilon)} \right) \right) \left( 1 + \lambda \exp ( -\lambda \Lambda^*(\epsilon)) \right)$$

$$= 2 \exp \left( -\lambda \left( 1 - e^{-\Lambda^*(\epsilon)} \right) \right) \left( 1 + \exp \left( -\lambda \left( \Lambda^*(\epsilon) - \frac{1}{\lambda} \log \lambda \right) \right) \right).$$

From the definition of $\lambda_*$ see that $\frac{1}{\lambda} \log \lambda \searrow 0$ as $\lambda \nrightarrow \infty$, and hence $\exp \left( -\lambda \left( \Lambda^*(\epsilon) - \frac{1}{\lambda} \log \lambda \right) \right)$ goes to zero as $\lambda \nrightarrow \infty$. Therefore,

$$\limsup_{\lambda \to \infty} \frac{1}{\lambda} \log P(\lambda) \leq - \left( 1 - e^{-\Lambda^*(\epsilon)} \right).$$

We have the required result by taking $\epsilon \searrow 0$.

**Case: $\eta d = 1$.** It is now remain to show that $\delta \leq -\frac{1}{2} \left( 1 - \frac{1}{r^{\gamma / d}} \right)^2$ if $R \equiv r$ and $\gamma / r^d > 1$. Since, from [12], $\mathcal{P}_{n+1}(\lambda) \leq \prod_{i=1}^n \left( 1 - \frac{\gamma}{r^d} \right) = 0$, for all $n > \lambda \frac{\lambda}{r^d}$, we have $\mathcal{P}(\lambda) \leq \mathbb{P} \left( N \leq \lambda \frac{\lambda}{r^d} \right)$. The proof is completed using Lemma 1.

### A.2 Proof of Proposition 1

From Remark 1 and (8), the expected running time complexity $T_{AR}$ of the naive AR method for hard-spheres model is given by

$$T_{AR} = \frac{E[C_{itr}]}{\mathcal{P}(\lambda)},$$

where $C_{itr}$ is the running time complexity in an iteration.
Let \( M' \) be the number of spheres generated sequentially, independently and identically before seeing an overlap. Then \( \mathbb{E}[C_{itr}] = c \mathbb{E} \left[ \sum_{n=1}^{\min(M, M')} \log(n) \right] \) for some constant \( c \), where \( M \sim \text{Poi}(\lambda) \) as mentioned in Section 5.1. To simplify the discussion take \( c = 1 \). Furthermore, observe that

\[
\mathbb{E}[C_{itr}] = \mathbb{E} \left[ \sum_{n=1}^{\min(M, M')} \log(n) \right] = \mathbb{E} \left[ \sum_{n=1}^{M} \log(n) I(M' \geq n) \right] = \mathbb{E} \left[ \sum_{n=1}^{M} \log(n + 1) \mathcal{P}_n(\lambda) \right],
\]

where the last equality follows from the fact that \( \mathbb{P}(M' > n) = \mathcal{P}_n(\lambda) \).

**Upper bounds:** Our proof depends on the following bounds on \( \mathcal{P}_n(\lambda) \). Recall from (24) that \( \mathcal{P}_n(\lambda) = \mathbb{E}_{\bar{M}} \left[ \prod_{i=1}^{n} \left( 1 - B_i \right) \right] \). As a consequence of (12),

\[
\mathcal{P}_n(\lambda) \leq \mathbb{E} \left[ \exp \left( -\frac{\gamma^d}{\lambda} \sum_{1 \leq j < n} R_j^d \right) \right] = \mathbb{E} \left[ \exp \left( -\frac{\gamma^d}{\lambda} \sum_{1 \leq j < n} \frac{R_j^d}{d^d} \right) \right],
\]

where \( r \) is an upper bound on \( R_j^d \)'s. Let \( \alpha = \mathbb{E}[R_1^d] \) and apply Hoeffding's inequality (Lemma 2) on the sequence \( \{R_1^d/r^d, R_2^d/r^d, \ldots, R_n^d/r^d\} \) with \( \epsilon = \alpha/2r^d \), \( k = 2 \) and \( g(x, y) = x \). Then

\[
\mathcal{P}_n(\lambda) \leq \exp \left( -\frac{\gamma^d}{2\lambda} \frac{\alpha}{2} \right) + \exp \left( -\frac{n\alpha^2}{4r^2d^2} \right).
\]

Let \( a = \sqrt{\frac{2\alpha^2}{\gamma^d}} \). Then from the above expression,

\[
\sum_{n=1}^{\infty} \log(n + 1) \mathcal{P}_n(\lambda) \leq \sum_{n=1}^{\infty} \log(n + 1) \exp \left( -\frac{n^2}{2a^2} \right) + \sum_{n=1}^{\infty} \log(n + 1) \exp \left( -\frac{n\alpha^2}{4r^2d^2} \right).
\]

If we define \( p = 1 - \exp \left( -\frac{\alpha^2}{4r^2d^2} \right) \), then the second term on the right side of the above inequality is \( 1/p \) times the expectation of \( \log(1 + \text{geom}) \) plus a geometric random variable with success probability \( p \) and support \( \{1, 2, 3, \ldots \} \). Since \( \log \) is a concave function, with application of Jensen’s inequality, \( \sum_{n=1}^{\infty} \log(n + 1) \exp \left( -\frac{n\alpha^2}{4r^2d^2} \right) \) is upper bounded by \( (1/p) \log(1/p + 1) \), which is a constant. On the other hand,

\[
\sum_{n=1}^{\infty} \log(n + 1) \exp \left( -\frac{n^2}{2a^2} \right) \leq \int_{0}^{\infty} \log(x + 1) \exp \left( -\frac{x^2}{2a^2} \right) dx = \sqrt{\frac{\pi}{2a}} \mathbb{E} \left[ \log \left( \mathcal{N}(0, a^2) \right) + 1 \right],
\]

where \( \mathcal{N}(0, a^2) \) is a Gaussian random variable with mean 0 and variance \( a^2 \). Again using the concavity of the \( \log \) function, Jensen’s inequality and the fact that the mean of the folded Gaussian variable \( |\mathcal{N}(0, a^2)| \) is \( \sqrt{\pi/a} \),

\[
\sum_{n=1}^{\infty} \log(n + 1) \exp \left( -\frac{n^2}{2a^2} \right) \leq \sqrt{\frac{\pi}{2a}} \log \left( \sqrt{\frac{\pi}{2a}} + 1 \right).
\]

Using the definition of \( a \) and the above conclusions, there exists a constant \( c \) such that

\[
\sum_{n=1}^{\infty} \log(n + 1) \mathcal{P}_n(\lambda) \leq c \eta d \lambda^{nd/2} \log(\lambda).
\]
We now establish the required upper bounds case-by-case basis. For \( \eta d < 2 \), the proof is straightforward from (42) and (40) since \( \mathbb{E}[C_{itr}] = \mathbb{E}\left[\sum_{n=1}^{M} \log(n+1)P_n(\lambda)\right] \leq \sum_{n=1}^{\infty} \log(n+1)P_n(\lambda) \).

Suppose that \( \eta d \geq 2 \) and see that

\[
\mathbb{E}\left[\sum_{n=1}^{M} \log(n+1)P_n(\lambda)\right] \leq \mathbb{E}[M \log(M)] = \lambda \log \lambda + \lambda \mathbb{E}\left[\frac{M}{\lambda} \log \left(\frac{M}{\lambda}\right)\right].
\]

Using the fact that \( n \log n \leq n^2 \), write \( \mathbb{E}\left[\left(\frac{M}{\lambda} \log \left(\frac{M}{\lambda}\right)\right)\right] \leq \mathbb{E}\left[\left(\frac{M}{\lambda}\right)^2\right] = \frac{1}{\lambda^2} \mathbb{E}[M^2] \), which is uniformly bounded by 2 for all \( \lambda \geq 1 \) since \( M \) is a mean \( \lambda \) Poisson random variable and \( \mathbb{E}[M^2] = \lambda(1 + \lambda) \). Thus, there exists a constant \( c > 0 \) such that \( \frac{\mathbb{E}[M \log(M)]}{\lambda \log \lambda} \leq c \), for all \( \lambda \geq 1 \), and the required upper bounds are established.

**Lower bounds:** Let \( \epsilon' = \min(1, \eta d/2) \). Then from (41),

\[
\mathbb{E}[C_{itr}] \geq P\left(M \geq \frac{\lambda \epsilon'}{2}\right) \sum_{n=1}^{\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor} \log(n)P_n(\lambda) \geq P_{\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor}(\lambda) \log \left(\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor!\right).
\]

From (26),

\[
P_{\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor}(\lambda) = \exp \left( -\frac{\lambda \epsilon'}{2} \sum_{j=1}^{\infty} \frac{\gamma \lambda \epsilon'}{2 \lambda \eta d} \right) \geq \exp \left( -\frac{\lambda \epsilon'}{2} \sum_{j=1}^{\infty} \frac{\gamma \lambda \epsilon'}{2 \lambda \eta d} \frac{m_j}{j} \right),
\]

where \( m_j = \mathbb{E}\left[(R_1 + R_2)^j\right] \). Note that \( m_j \leq (2r)^j \) since \( R_i \)'s are bounded by \( r \). Therefore,

\[
P_{\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor}(\lambda) \geq \exp \left( -\frac{\lambda \epsilon'}{2} \sum_{j=1}^{\infty} \frac{1}{j} \left( \frac{\gamma (2r)^d}{2 \lambda \eta d} \right)^j \right).
\]

Using Taylor’s expansion of \( \log(1-x) \) for \( 0 < x < 1 \), and the fact that \( \frac{\gamma (2r)^d}{2 \lambda \eta d} < 1 \), for sufficiently large values of \( \lambda \),

\[
P_{\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor}(\lambda) \geq \exp \left( \frac{\lambda \epsilon'}{2} \log \left(1 - \frac{\gamma (2r)^d}{2 \lambda \eta d} \right)\right) = \left(1 - \frac{\gamma (2r)^d}{2 \lambda \eta d} \right)^{\frac{\lambda \epsilon'}{2}}.
\]

From the definition of \( \epsilon' \),

\[
\lim_{\lambda \to \infty} \left[ \left(1 - \frac{\gamma (2r)^d}{2 \lambda \eta d} \right)^{\frac{\lambda \epsilon'}{2}} \right] = \begin{cases} 1, & \text{if } \eta d > 2, \\ \exp \left(-\gamma (2r)^d/4\right), & \text{if } 0 < \eta d \leq 2. \end{cases}
\]

In addition, from the definition of \( \epsilon' \) and Lemma 1, \( \lim_{\lambda \to \infty} P\left(M \geq \frac{\lambda \epsilon'}{2}\right) = 1 \). Therefore, there exists a constant \( c \) such that \( \mathbb{E}[C_{itr}] \geq c \log \left(\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor!\right) \).

Using \( n! \geq \sqrt{2\pi} n^{n+1/2} e^{-n} \), write \( \log \left(\left\lfloor \frac{\lambda \epsilon'}{2} \right\rfloor!\right) \geq c \lambda \epsilon' \log \left(\lambda \epsilon'\right) = \epsilon' \lambda' \log \left(\lambda \epsilon'\right) \) for some constant \( \epsilon' \) and for all \( \lambda \geq 1 \). the proof of lower bounds follow from the definition of \( \epsilon' \) and (40). Now the proof of the Proposition 1 can be completed using Theorem 1.
A.3 Proof of Proposition 2

Suppose that $\hat{C}_{itr}$ is the running time complexity of an iteration of Algorithm 3. Just like in the case of naive AR algorithm, we can show using i.i.d. property of the iterations that

$$T_{IS} = \frac{E[\hat{C}_{itr}]}{P_{acc}(\lambda)}.$$  

Suppose $\eta d > 1$, then observe from (14) that the number of spheres generated in a typical iteration of Algorithm 3 is stochastically dominated by a Poisson random variable with mean $\lambda$. Therefore, $E[\hat{C}_{itr}] \leq c \lambda \log \lambda$ for some constant $c$ and for $\eta d > 1$; see the proof of Proposition 1.

On the other hand, if $0 < \eta d \leq 1$, the expected number of spheres generated per iteration is of order $\lambda^{\eta d}$ as the expected volume of each sphere is of order $1/\lambda^{\eta d}$. It is clear that there exists a constant $c > 0$ such that $E[\hat{C}_{itr}] \leq c \eta d \lambda^{\eta d} \log \lambda$. Thus, by (15) and Proposition 1,

$$T_{IS} \leq c \min(1, \eta d) \frac{\lambda^{\min(1, \eta d)} \log \lambda}{P_{acc}} = c E[\tilde{\sigma}(N)] \min(1, \eta d) \frac{\lambda^{\min(1, \eta d)} \log \lambda}{P_{acc}},$$

for some constant $c > 0$. Furthermore, from the definition of $\tilde{\sigma}(\cdot)$ and $N$,

$$E[\tilde{\sigma}(N)] \leq E\left[ \exp\left( -\sum_{i=0}^{N} (i - 1) \gamma r^d \right) \right] = E\left[ \exp\left( -\gamma^d \frac{r^d \lambda^{d} (N - 1) N}{2} \right) \right].$$

By Chernoff bound (Lemma 1), for any $0 < \epsilon < 1$,

$$E\left[ \exp\left( -\gamma^d \frac{r^d \lambda^{d} (N - 1) N}{2} \right) \right] \leq E\left[ \exp\left( -\gamma^d \frac{r^d \lambda^{d} (N - 1) N}{2} \right) : N > \lambda (1 - \epsilon) \right] + \mathbb{P}\left( N \leq \lambda (1 - \epsilon) \right) \leq \exp\left( -\gamma^d \frac{r^d}{2} (1 - \epsilon) \lambda^{2d} \right) + \exp\left( -\frac{\lambda^2}{2} \right).$$

If $\eta d > 1$, then the second term on the right-hand side of the above expression decreases at faster rate than the first term, and thus the claim holds true. For $\eta d = 1$, take $\epsilon = 1/2$, then we have the required result with $b = \min\left(1/8, \gamma r^d/4\right)$. Furthermore, if $0 < \eta d < 1$ then the first term decreases faster than the second one, and hence the proof is completed by taking $b = 1/2$.

A.4 Proof of Proposition 4

From (18) and Remark 4, $\hat{T}_{AR} = \frac{E[\hat{C}_{itr}] E[\tilde{\sigma}(N)]}{P_{acc}(\lambda)}$, where $N \sim \text{Poi}(\lambda)$. In an iteration of the grid method, suppose the number of spheres generated is $n$. The expected cost for each sphere generation is $a/\epsilon^d_{\lambda,n}$ for some constant $a > 0$, since the expected number of cells that are verified for marking is proportional to $1/\epsilon^d_{\lambda,n}$. From (17),

$$E[\hat{C}_{itr}] = \frac{1}{C(\lambda)} \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \tilde{\sigma}(n) a \frac{\epsilon}{\epsilon^d_{\lambda,n}}.$$

From the definition of $C(\lambda) = e^\lambda E[\tilde{\sigma}(N)]$. Thus

$$\hat{T}_{AR} = \frac{a}{P_{acc}(\lambda)} \sum_{n=0}^{\infty} \frac{e^{-\lambda} \lambda^n}{(n - 1)!} \frac{\tilde{\sigma}(n)}{\epsilon^d_{\lambda,n}},$$

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It implies that $\mathcal{T}_{AR}$ is minimum if the sequence $\{\varepsilon^*_\lambda,n : n \geq 1\}$ of cell edge lengths is such that

$$\varepsilon^*_\lambda,n = \arg\min_{\varepsilon_\lambda,n \in (0, \frac{r}{2\sqrt{d}\lambda^n})} \frac{\hat{\sigma}(n)}{\varepsilon_\lambda,n}.$$  

Recall from the definition that $\hat{\sigma}(n) = \prod_{i=1}^{n} \left(1 - (i - 1)\gamma' \left(\frac{r}{\lambda^n} - \sqrt{d} \varepsilon_\lambda,n\right)\right)^{+}$. To prove that $M \leq \frac{\lambda^{nd}}{\gamma^{nd}} + 1$ for the optimal cell edge lengths $\varepsilon^*_\lambda,n$, we need to show that for $n > \frac{\lambda^{nd}}{\gamma^{nd}} + 1$, there exists $\varepsilon_\lambda,n \in \left(0, \frac{r}{2\sqrt{d}\lambda^n}\right)$ such that $\hat{\sigma}(n) = 0$. In other words, for every $n > \frac{\lambda^{nd}}{\gamma^{nd}} + 1$, we need to show that there exists a constant $c \in (0,1)$ such that the selection of $\varepsilon^*_\lambda,n = \frac{r}{\sqrt{2d}\lambda^n}$ implies $(n - 1)\gamma' \left(\frac{r}{\lambda^n} - \frac{r}{2\lambda^n}\right)^d = 1$. This is easy to see because $(n - 1)\gamma' \frac{r}{\lambda^n} > 1$ and thus one can select $c \in (0,1)$ such that

$$(n - 1)\gamma' \left(\frac{r}{\lambda^n} - c \frac{r}{2\lambda^n}\right)^d = (n - 1)\gamma' \frac{r}{\lambda^n} (1 - c/2)^d \geq 1.$$  

So, from (43), we never generate a configuration with $n$ spheres when $n > \frac{\lambda^{nd}}{\gamma^{nd}} + 1$.

Now fix $n \leq \frac{\lambda^{nd}}{\gamma^{nd}} + 1$ and let $\zeta(x) := \gamma' \left(\frac{r}{\lambda^n} - \sqrt{d} x\right)^d$. Note that $(i - 1)\zeta(x) \in (0,1)$ for all $0 < x < r/(2\sqrt{d}\lambda^n)$ and $i \leq n$, and thus $\hat{\sigma}(n) = \prod_{i=1}^{n} \left(1 - (i - 1)\zeta(\varepsilon_\lambda,n)\right)$. From (43), $\varepsilon^*_\lambda,n$ is the solution of the optimization problem

$$\min_{x} \left[ \prod_{i=1}^{n-1} \left(1 - i\zeta(x)\right) \right] \text{ subjected to } x \leq \frac{r}{2\sqrt{d}\lambda^n}.$$  

By defining $f(x) := \sum_{i=1}^{n-1} \log \left(1 - i\zeta(x)\right) - d \log x$ and using the monotonicity of log function, one can see that $\varepsilon^*_\lambda,n$ is a solution of

$$\min_{x} f(x) \text{ subjected to } x \leq \frac{r}{2\sqrt{d}\lambda^n}.$$  

Further we see that

$$f'(x) = -\frac{d}{x} - \zeta'(x) \sum_{i=1}^{n-1} \frac{i}{1 - i\zeta(x)} \quad \text{and} \quad \zeta'(x^*) = -d\sqrt{d}\gamma' \left(\frac{r}{\lambda^n} - \sqrt{d} x^*\right)^{d-1}.$$  

So, $f'(x^*) = 0$ when $x^*$ is the solution of $x = -\frac{d}{\zeta'(x^*)} \sum_{i=1}^{n-1} \frac{1}{(1 - i\zeta(x^*))}$. Notice from the definition of the function $\zeta$ that $f'(x) \leq 0$ for all $x \leq \min \left(x^*, r/(2\sqrt{d}\lambda^n)\right)$. Also notice that if $x^* \leq r/(2\sqrt{d}\lambda^n)$, then $f'(x) \geq 0$ for all $\min \left(x^*, r/(2\sqrt{d}\lambda^n)\right) \leq x \leq r/(2\sqrt{d}\lambda^n)$.

As a consequence, the optimal solution $\varepsilon^*_\lambda,n = \min \left(x^*, r/(2\sqrt{d}\lambda^n)\right)$. Now it is sufficient to show that whenever $x^* \leq r/(2\sqrt{d}\lambda^n)$ there exist positive constants $c_1$ and $c_2$ (independent of $n$ and $\lambda$) such that

$$c_1 \frac{\lambda^{(d-1)}}{n^2} \leq x^* \leq c_2 \frac{\lambda^{(d-1)}}{n^2},$$  

(44)
for all \( \lambda > (2r)^{1/\eta} \). Since \( n \leq \frac{\lambda \nu}{r^{1/\eta}} + 1 \), for such \( x^* \), \( 1 - i \zeta(x^*) \geq 1 - (n - 1)\zeta(0) \geq 1 - \frac{1}{2^i} \), for all \( i \leq n - 1 \). Thus

\[
\sum_{i=1}^{n-1} \frac{i}{(1 - i \zeta(x^*))} \leq \frac{n(n - 1)}{2} \frac{1}{1 - \frac{1}{2^i}} \leq an^2,
\]

where \( a = \frac{1}{2^{(1-1)/2^i}} \). On the other hand, using the fact that \( 0 < 1 - i \zeta(x^*) \leq 1, i \leq n - 1 \),

\[
\sum_{i=1}^{n-1} \frac{i}{(1 - i \zeta(x^*))} \geq \sum_{i=1}^{n-1} i \geq bn^2,
\]

where \( b = 1/4 \). Using the constraints on the values of \( x^* \),

\[
\frac{r^{d-1}}{2^{d-1} \chi \eta(d-1)} \leq \left( \frac{r}{\chi \eta} - \sqrt{d} x^* \right)^{d-1} \leq \frac{r^{d-1}}{\chi \eta(d-1)}.
\]

From (45) - (47) and the definition of \( x^* \), we have (44) with \( c_1 = \min \left( \frac{1}{2\sqrt{d}}, \frac{2(1 - 1/2^d)}{\sqrt{d} \gamma} \right) \) and \( c_2 = \max \left( \frac{1}{2\sqrt{d}}, \frac{2^{d+1}}{\sqrt{d} \gamma} \right) \).

### A.5 Proof of Theorem 2

Since \( U_0(0) = D(0) \) and \( L_0(0) = \emptyset \), on \( \bigcap_{j=0}^t \{ D(s_j) \notin \mathcal{A} \} \), for all \( t \leq s_i \),

\[
L_0(t) = \emptyset \quad \text{and} \quad U_0(t) = D(t).
\]  

Thus, \( L_0(t) \neq U_0(t) \) for all \( t \leq s_i \) on \( \bigcap_{j=0}^i \{ D(s_j) \notin \mathcal{A} \} \). Take \( \tau = \inf \{ i \geq 0 : D(s_i) \notin \mathcal{A} \} \). From the above conclusion, it is clear that \( N^f \geq \tau \). Then,

\[
\mathcal{T}_{DC} \geq \mathbb{E} \left[ \sum_{i=0}^{N^f} C \left( D(s_i), U_0(s_i), L_0(s_i) \right) \right] \geq \mathbb{E} \left[ \sum_{i=0}^{\tau} C \left( D(s_i), U_0(s_i), L_0(s_i) \right) \right] \]

\[
= \sum_{i=0}^{\infty} \mathbb{E} \left[ C \left( D(s_i), U_0(s_i), L_0(s_i) \right) ; \tau \geq i \right] = \sum_{i=0}^{\infty} \mathbb{E} \left[ C \left( D(s_i), U_0(s_i), L_0(s_i) \right) ; \bigcap_{j=0}^{i-1} \{ D(s_j) \notin \mathcal{A} \} \right] \]

\[
= \sum_{i=0}^{\infty} \mathbb{E} \left[ C \left( D(s_i), D(s_i), \emptyset \right) ; \bigcap_{j=0}^{i-1} \{ D(s_j) \notin \mathcal{A} \} \right],
\]

where \( I \left( \bigcap_{j=0}^{i-1} \{ D(s_j) \notin \mathcal{A} \} \right) = 1 \) and the last equality follows from (48).

One can think of dominating process \( \{ D(t) : t \in \mathbb{R} \} \) as a Poisson Boolean model on \( (B \times \mathbb{R}) \times (\mathbb{R}^m \times \mathbb{R}_+) \), where Poisson points take values in \( B \times \mathbb{R} \) and the last coordinate is interpreted as time. Associated to each point there is a mark in \( \mathbb{R}^m \times \mathbb{R}_+ \), where the last coordinate denotes the life duration of the point.

Suppose that \( \mathcal{D} \) is the state space of the entire process \( \{ D(t) : t \in \mathbb{R} \} \). Then we can define a simple partial order on \( \mathcal{D} \) as follows: For any \( \omega, \omega' \in \mathcal{D} \), we say \( \omega \preceq \omega' \) if and only if every grain
present in $\omega$ is also present in $\omega'$, that is, either $\omega = \omega'$ or $\omega'$ is obtained by adding grains to $\omega$. Define the following notion of increasing functions: A real valued function on $\mathcal{D}$ is increasing if $f(\omega) \leq f(\omega')$ for all $\omega, \omega' \in \mathcal{D}$ such that $\omega \leq \omega'$.

Clearly, $C\left(D(s_i), D(s_i), \emptyset\right)$ is an increasing function in each argument under the above partial order. Furthermore, under the hereditary property, $I(D(s_i), \emptyset)$ is also an increasing function. It is important to observe that the dominating process is started in steady-state, and hence $D(s_i)$ has steady-state distribution, which is same as $\mu^0$, thanks to the PASTA property. That is, \(\{D(s_i)\}_{i \geq 0}\) is a sequence of identically distributed configurations with the distribution $\mu^0$. Hence, \(\{C\left(D(s_i), D(s_i), \emptyset\right)\}_{i \geq 0}\) is a sequence of identically distributed random variables such that

$$E \left[ C^2 \left(D(s_i), D(s_i), \emptyset\right) \right] = E_{\mu^0} \left[ C^2(\mathcal{X}, \mathcal{X}, \emptyset) \right] < \infty$$

(from the given hypothesis). By FKG inequality, Theorem 2.2 in [29], we have that

$$E \left[ C \left(D(s_j), D(s_i), \emptyset\right) : \bigcap_{j=0}^{i-1} \{D(s_j) \notin \mathcal{A}\} \right] \geq E \left[ C \left(D(s_i), D(s_i), \emptyset\right) \right] \prod_{j=0}^{i-1} P(D(s_j) \notin \mathcal{A}),$$

and thus,

$$\tau_{DC} \geq \frac{E \left[ C \left(D(s_0), D(s_0), \emptyset\right) \right]}{1 - P(D(s_0) \notin \mathcal{A})} = \frac{E_{\mu^0} \left[ C(\mathcal{X}, \mathcal{X}, \emptyset) \right]}{P_{\mu^0}(\mathcal{X} \in \mathcal{A})}.$$

Furthermore, from Remark 1, the expected running time $\tau_{AR}$ of the naive AR method for the loss system satisfies $\tau_{AR} = \frac{E[C_{\text{itr}}]}{P_{\text{acc}}}$, where $P_{\text{acc}}$ is the acceptance probability of the naive AR algorithm. Observe that Stability condition 1 required for the naive AR method is satisfied with $\sigma(n) = 1$ for all $n \geq 0$ (see Section 3) and this choice of $\sigma(n)$ is optimal by Remark 2. So, the configuration generated in each iteration of Algorithm 1 has distribution $\mu^0$. Thus, $P_{\text{acc}} = P_{\mu^0}(\mathcal{X} \in \mathcal{A})$. So, $\tau_{AR} = \frac{E[C_{\text{itr}}]}{P_{\mu^0}(\mathcal{X} \in \mathcal{A})}$. This completes the proof.

### A.6 Proof of Proposition 5

Recall that $C(\mathcal{X}, \mathcal{X}^u, \mathcal{X}^d)$ is the running time complexity of updating the dominating, upper bound and lower bound processes at the instant of an arrival when their respective states are $\mathcal{X}, \mathcal{X}^u$ and $\mathcal{X}^d$. As explained in Section 5.1 (using self-balancing binary tree), the updating cost

$$C(\mathcal{X}, \mathcal{X}^u, \mathcal{X}^d) = \Omega(\log |\mathcal{X}|),$$

(49)

because of insertion of the new arrival into the data structure associated with the dominating process. Since $|\mathcal{X}|$ is a mean $\lambda$ Poisson random variable, $E_{\mu^0} \left[ C(\mathcal{X}, \mathcal{X}, \emptyset) \right] = \Omega(\log \lambda)$ if $\mathcal{X} \sim \mu^0$. From the definition, $L_0(t) \subseteq U_0(t) \subseteq D(t)$, $t \geq 0$. Hence, at an arrival if the state of the dominating process is $\mathcal{X}$ then the number of operations involved is at most of order $|\mathcal{X}|^2$. So, $C(\mathcal{X}, \mathcal{X}, \emptyset) = O(|\mathcal{X}|^2)$ and thus $E_{\mu^0} \left[ C^2(\mathcal{X}, \mathcal{X}, \emptyset) \right] < \infty$. From Theorem 2 and (8), $\tau_{DC} \geq \frac{c \log \lambda}{P(\lambda)}$, for some constant $c > 0$. Furthermore, the required conclusions for $0 < \eta < 2$ follows from Theorem 1.
We now prove the result for the case \( \eta d \geq 2 \). Let \( S \) be the minimum time such that after \( S \) none of the initial spheres is present in the system. From the definition, \( L_0(0) = \emptyset \) and \( U_0(0) = D(0) \). Consequently, \( L_0(t) \neq U_0(t) \) for all \( t < S \). If we let \( \tau \) be the number of births within \( S \), then again we have \( N_f \geq \tau \), where \( N_f \) is the forward coalescence time; see Section 7.2 for the definition of \( N_f \).

Similar to the reasoning given in the proof of Theorem 2, we can show using (49) that

\[
T_{DC} \geq \mathbb{E} \left[ \sum_{i=0}^{N_f} C(D(s_i), U_0(s_i), L_0(s_i)) \right] \geq \mathbb{E} \left[ \sum_{i=0}^{\tau} \log |D(s_i)| \right] = c \mathbb{E}[\tau] \log \lambda,
\]

for some constant \( c > 0 \).

Since each accepted sphere stays for a random time independently and exponentially distributed with mean \( 1 \), \( \mathbb{E}(S \mid |D(0)| = m) = H(m) \), where \( H(m) = \sum_{i=1}^{m} \frac{1}{i} \) is the \( m \)th harmonic number. Furthermore, \( \left( \tau \mid |D(0)| = m \right) \sim \text{Poi}(\lambda H(m)) \) and hence \( \mathbb{E}[\tau] = \lambda \mathbb{E}[H(|D(0)|)] \). Using the bound \( H(m) > \log m \) and the fact that \( |D(0)| \) is a mean \( \lambda \) Poisson variable, we write \( \mathbb{E}[\tau] \geq \lambda \log \lambda \), and thus \( T_{DC} \geq \frac{c \lambda (\log \lambda)^2}{\mathbb{E}[\tau]} \), for some constant \( c > 0 \).

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