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Random sampling: Billiard Walk algorithm ☆

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ABSTRACT

Hit-and-Run is known to be one of the best random sampling algorithms, its mixing time is polynomial in dimension. However in practice, the number of steps required to obtain uniformly distributed samples is rather high. We propose a new random walk algorithm based on billiard trajectories. Numerical experiments demonstrate much faster convergence to the uniform distribution.

1. Introduction

Generating points uniformly distributed in an arbitrary bounded region $Q \subset \mathbb{R}^n$ finds applications in many computational problems (Tempo, Calafiore, & Dabbene, 2004; Rubinstein & Kroese, 2008).

Straightforward sampling techniques are usually based on one of the three approaches: rejection, transformation, and composition. In the rejection approach, the region of interest Q is embedded into a region with available uniform sampler B (usually a box or a ball). At the next step, samples that do not belong to Q are rejected. Assume Q is the unit ball, and the bounding region B is the box $[-1,1]^n$. Then for $n = 2k$, the ratio of the volumes of the box and the ball is equal to $q = \frac{\mathrm{Vol}(Q)}{\mathrm{Vol}(B)} = \frac{\pi^k}{k!2^k}$, thus $q \approx 10^{-8}$ for $n = 20$, so that one has to generate $\sim 10^8$ samples to obtain just a few of them in Q. For polytopes this ratio can be much smaller. Another way to exploit pseudo-random number generator for a simple region B is to map B onto Q via a smooth deterministic function with constant Jacobian. For instance, to obtain uniform samples in $Q = \{x : x^T A x < 1\}$, A being a positive definite matrix, it suffices to generate samples y uniformly in the unit ball $||y||_2 < 1$ and transform them as $x = A^{-1/2} y$. Unfortunately, such a transformation exists just for a limited class of regions. In the composition approach, the set Q is partitioned into a finite number of sets that can be efficiently sampled. For instance, a polytope can be partitioned into simplices, but the large number of them makes the procedure computationally hard.

Other sampling procedures use modern versions of the Monte Carlo technique based on the Markov Chain Monte Carlo (MCMC) approach (Gilks, Richardson, & Spiegelhalter, 1996; Diaconis, 2009). For instance, efficient algorithms for computing volumes using random walks can be found in Dyer, Frieze, and Kannan (1991), Lovasz and Somonovits (1993), Lovasz and Deak (2012). One of the most famous and efficient algorithms of the MCMC type is Hit-and-Run (HR), which was originally proposed by Turchin (1971) and independently by Smith (1984). The brief description of the HR algorithm is as follows. At every step HR generates a random direction uniformly over the unit sphere and picks the next point uniformly on the segment of the straight line in the given direction in Q. HR is applicable to various control and optimization problems (Polyak & Gryazina, 2008; Polyak & Gryazina, 2011; Dabbene, Shcherbakov, & Polyak, 2010) as well as to simulation-based multiple criteria decision analysis (Tervonen, van Valkenhoef, Basturk, & Postmus, 2013). Unfortunately, even for simple "bad" sets, such as level sets of ill-posed functions, HR techniques fail or become computationally inefficient.

A variety of applications and drawbacks of the existing techniques provides much room for improving and developing new sampling algorithms. For instance, there were attempts to exploit the approach proposed for interior-point methods of convex optimization (Nesterov & Nemirovsky, 1994) and to combine it with MCMC algorithms. As a result, the Barrier Monte Carlo method (Polyak & Gryazina, 2010) generates random points with better uniformity properties as compared to the standard Hit-and-Run.

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On the other hand, the complexity of every iteration is in general high enough (the calculation of $\left(\nabla^2 F(x)\right)^{-1/2}$ is required, where $F(x)$ is a barrier function of the set). Moreover, the Barrier Monte Carlo method does not accelerate convergence for simplex-like sets.

In this paper we propose a new random walk algorithm motivated by physical phenomena of gas diffusing in a vessel. A particle of gas moves with a constant speed until it meets the boundary of the vessel, then it reflects (the angle of incidence equals the angle of reflection) and so on. When a particle hits another one, its direction and speed change. In our simplified model we assume that the direction changes randomly, while the speed remains the same. Thus our model combines the ideas of the Hit-and-Run technique and use of the billiard trajectories. There exists a vast literature on mathematical billiards, and many useful facts can be extracted from there (Tabachnikov, 1995; Galperin & Zemlyakov, 1990; Sinai, 1970; Sinai, 1978; Kozlov & Treshchev, 1991). The traditional theory addresses the behavior of one particular billiard trajectory in different billiard tables, their ergodic properties, and the conditions for the existence of periodic orbits. In stochastic analogs of the classical billiard (Evans, 2001), a direction after reflection is chosen randomly uniformly. Shake-and-Bake algorithms are based on stochastic billiards and generate points on the boundary of a convex set (Boender et al., 1991). The recently proposed version of the Shake-and-Bake algorithm (Dieker & Vempala, xxxx) exhibits polynomial-time convergence to the uniform distribution. Our algorithm is aimed at sampling the interior of a set (actually, later in the text we consider open regions). Besides that, we extend billiard trajectories of random length keeping the standard reflection law. Such an incorporation of randomness also improves the ergodic properties.

The paper is organized as follows. In Section 2 we present a novel sampling algorithm and prove that it produces asymptotically uniformly distributed samples in Q. In Section 3 we pay much attention to some properties of the Billiard Walk (BW), implementation issues are discussed as well. Simulation of BW for particular test domains is presented in Section 4. Much attention is devoted to the capability of BW to get out of the corner, in comparison with HR. Here we consider just the most demonstrative types of geometry. In Section 4.6 we briefly discuss possible applications of the algorithm.

2. Algorithm

Assume there is a bounded, open connected set $Q \subset \mathbb{R}^n, n \geqslant 2$, and a point $x^0 \in Q$. Our aim is to generate asymptotically uniform samples $x^i \in Q, i = 1, \ldots, N$.

The new BW algorithm generates a random direction uniformly over the unit sphere. Then the next sample is chosen as the end-point of the billiard trajectory of length ℓ. This length is chosen randomly; i.e., we assume that the probability of collision with another particle is proportional to δt for small time instances δt, this validates the formula for ℓ in the algorithm below. The scheme of the method is given in Fig. 1, while the precise routine is as follows.

2.1. Algorithm of Billiard Walk (BW)

1. Take $x^0 \in Q; \ i = 0, x = x^0$.
2. Generate the length of the trajectory $\ell = -\tau \log \xi, \xi$ being uniform random on $[0,1]$, τ is a specified constant parameter of the algorithm.
3. Pick a random direction $d \in \mathbb{R}^n$ uniformly distributed over the unit sphere (i.e., $d = \xi / \|\xi\|$, where $\xi \in \mathbb{R}^n$ has the standard Gaussian distribution). Construct a billiard trajectory starting at x^i and having initial direction d. When the trajectory meets the boundary with internal normal $s, ||s|| = 1$, the direction is changed as
$$d \to d - 2(d,s)s,$$
where (d,s) is the scalar product.
4. If a point with nonsmooth boundary is met or the number of reflections exceeds R, go to step 2. Otherwise proceed until the length of the trajectory equals ℓ.
5. $i = i + 1$, take the end-point as x^{i+1} and go to step 2.

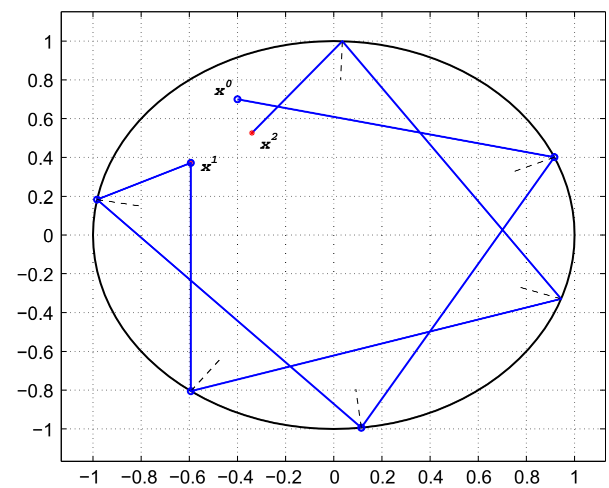

Fig. 1. Billiard walk.

The algorithm involves two parameters τ and R and we discuss their choice below.

We prove asymptotical uniformity of the samples produced by BW for convex and nonconvex cases separately. The requirements on Q are different for these two cases, while the sampling algorithm remains the same. Consider the Markov Chain induced by the BW algorithm $x^0, x^1, \ldots$. For an arbitrary measurable set $A \subseteq Q$, denote by $\mathbf{P}(A|x)$ the probability of obtaining $x^{i+1} \in A$ for $x^i = x$ by the BW algorithm. Then $\mathbf{P}_N(A|x)$ is the probability to get $x^{i+N} \in A$ for $x^i = x$. We also denote by $p(y|x)$ the probability density function for $\mathbf{P}(A|x)$, i.e. $\mathbf{P}(A|x) = \int_A p(y|x)dy$.

Theorem 1. *Assume Q is an open bounded convex set in $\mathbb{R}^n$, the boundary of Q is piecewise smooth. Then the distribution of points x^i generated by the BW algorithm tends to the uniform one over Q, i.e.*
$$\lim_{N\to\infty} \mathbf{P}_N(A|x) = \lambda(A)$$
for any measurable $A \subseteq Q$, $\lambda(A) = \mathrm{Vol}(A)/\mathrm{Vol}(Q)$ and any starting point x.

Proof. First, the algorithm is well-defined: at step 4 with zero probability the algorithm sticks at a point with nonsmooth boundary. On the other hand ℓ and d are chosen in such a way that, with positive probability, x^{i+1} is obtained by less than R reflections (see detailed discussion of "bad" situations in SubSections 3.1 and 3.2).

In view of Theorem 2 in Smith (1984) based on the asymptotic properties of Markov Chains, the two assumptions on $p(y|x)$ imply that the uniform distribution over Q is a unique stationary distribution, and it is achieved for any starting point $x \in Q$. The first assumption requires the existence of $p(y|x)$ and its symmetry; the second assumption claims its positivity $p(y|x) > 0$ for all $x, y \in Q$.