Geometry-independent Hit-and-Run via ensemble sampler

Abstract

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1 Introduction

Sampling from high-dimensional convex bodies and, more generally, from log-concave distributions constrained to convex sets, is a central topic in modern algorithms, statistics, and optimization. Applications range from randomized algorithms for volume estimation and convex programming to Bayesian inference under hard constraints and high-dimensional combinatorial optimization. The widely-used algorithms for these tasks are almost all Markov chain Monte Carlo (MCMC) methods, whose efficiency is measured by mixing time bounds that scale polynomially in the dimension. The first randomized polynomial-time algorithm for approximating the volume of a convex body via a random walk was raised by [1]. Through a grid walk, they obtained approximately uniform samples. In [2], the ball walk was used in the sampling algorithm, and they use isoperimetric inequalities and the "localization" method to give an $O(n^6 \log n)$ bound. A later refinement achieves an $O^*(n^5)$ oracle calls in [3].

Subsequent work [4] developed a systematic geometric theory of log-concave functions, demonstrating that for well-rounded (near-isotropic) convex bodies both the ball walk and variants of hit-and-run mix in $O^*(n^3)$ steps from a warm start, and that this suffices to obtain $O^*(n^3)$ algorithms for sampling and integration of log-concave densities. [5] later combined these ideas with an "accelerated Gaussian cooling" schedule to achieve $O^*(n^3)$ algorithms for both volume and Gaussian volume, further improving constants and clarifying the role of rounding and warm starts.

Hit-and-run and its variants Hit-and-run is one of the most effective volume algorithms, conducted simply by choosing a random chord and doing a random walk on the 1-dim chord each time. The method was formalized and generalized to arbitrary absolutely continuous target distributions in the early 1990s [6]. In a landmark result, [7] showed that hit-and-run mixes rapidly on any convex body: starting from a warm start in a reasonably rounded body, the mixing time is $O^*(n^2\frac{R}{r})$ where R and r are the radius of the circumscribed and inscribed balls, which implies a $O^*(n^3)$ complexity after preprocessing $R = O(\sqrt{n})$. [8] then achieves $O^*(n^3)$ in sampling from a log-concave distribution on convex body. The bound of sampling on an isotropic convex body was recently sharpened by [9] to $\tilde{O}(n^2/\psi_n^2)$ via localization schemes [10], where ψ_n is the best isoperimetric (KLS) constant for isotropic log-concave distributions.

Ensemble MCMC and affine-invariant ensemble samplers The idea of evolving a collection of walkers simultaneously appears in several guises (e.g., differential evolution MCMC, ensemble Kalman methods [11, 12]), but perhaps the most influential example is the affine-invariant ensemble sampler [13]. The ensemble sampler has been shown, theoretically and empirically, to be effective in preconditioning the system and reducing the condition number of the problem, which is credited to the affine invariant nature of the ensemble sampler. The idea of affine invariance has been incorporated in the strech-move, Hamilton Monte Carlo, regression, and neural network [14, 15, 16, 17].

Other geometric MCMC for convex bodies Beyond ball walk and hit-and-run, several more recent geometric MCMC schemes have been proposed for sampling from convex bodies. Vaidya and John walks construct proposals using, respectively, volumetric-logarithmic and John-ellipsoid barriers, leading to affine-invariant random walks on polytopes with improved mixing-time bounds compared to the Dikin walk [18]. Building on similar ideas, John's Walk [19] uses successive approximations of John's ellipsoids to define an affine-invariant proposal that adapts to the local geometry of an arbitrary convex body. The In-and-Out algorithm [20] takes a different, diffusion-based perspective, alternating forward and backward heat flows to obtain sharp convergence guarantees in several information-theoretic distances. In parallel, constrained Riemannian Hamiltonian Monte Carlo methods [21] define Hamiltonian dynamics on a Riemannian manifold tailored to the convex constraints, providing a non-reversible alternative with favorable scaling for high-dimensional constrained targets.

Contribution In this paper, we take a step towards bridging the two lines of research by designing and analyzing an ensemble version of hit-and-run for sampling from high-dimensional convex bodies. Our algorithm adapts the Goodman–Weare affine-invariant ensemble ideas to the setting of convex-body random walks, which improves the geometry-dependence of the current random walk algorithm on convex bodies, while preserving the fast-mixing of the hit-and-run algorithm. Our result potentially implies an $O(n^2)$ mixing time on any convex body without an isotropic assumption. The numerical experiments further support this result by showing a consistent mixing time over elongated hyper-rectangular.

2 Preliminary

Let $K \subset \mathbb{R}^n$ be a convex body, and π be the uniform distribution on K, i.e., $\pi(\cdot) \propto \mathbf{1}_K(\cdot)$. Denote the volume of K by $|K|$. Let $h \in \mathbb{S}^{n-1}$ be a direction, and let $\ell(x, h)$ denotes the length of the chord in K passing through x with direction h and define $\ell(h) := \max_{x \in K} \ell(x, h)$. We use $\| \cdot \|$ denote the ℓ_2 norm of a vector.

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