

Geometry-independent Hit-and-Run via ensemble sampler

Abstract

We study Markov chain Monte Carlo algorithms for sampling from a uniform distribution on high-dimensional convex bodies. Motivated by affine-invariant ensemble samplers, we introduce an ensemble version of hit-and-run for convex-body sampling. Our algorithm evolves a collection of walkers whose proposals are constructed by combining random chords with affine-invariant ensemble moves, yielding dynamics that are robust to severe anisotropy while preserving the simplicity and fast mixing behavior of hit-and-run. Our results potentially imply an $O(n^4)$ mixing time on any convex body without an isotropic assumption. Numerical experiments on highly elongated hyperrectangles further support this geometry-independence, showing essentially dimension-only mixing behavior across a wide range of condition numbers.

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 stretch-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 $h \in \mathbb{S}^{n-1}$ denote n -dimensional directions, 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.

We define a symmetric body centered at x as $T(x, c) = \{x + hr | h \in \mathbb{S}^{n-1}, r \in [-c\ell(h), c\ell(h)]\}$. Note that T is exactly a scaling of the difference body $K - K$ with a factor c , thus T is convex. We define $\alpha_x(h)$ as the distance start from x with direction h to the boundary of K , thus $\alpha_x(h) + \alpha_x(-h)$ is the length of chord through x with direction h . We define $\kappa(x, c) = \int_{\{h | \alpha_x(h) \geq \ell(h), h \in \mathbb{S}^{n-1}\}} f_H(h) du$ and $\kappa_\rho(x, c) = \int_{\{h | \alpha_x(h) \geq \rho(h), h \in \mathbb{S}^{n-1}\}} f_H(h) du$ and let $K_r := \{x | x \in K, \kappa(x, r) \geq \frac{15}{16}\}$.

Algorithm 1 Ensembled Hit-and-Run

Require: Convex body $K \subset \mathbb{R}^n$; number of particles d ; number of iterations T ; initial distribution ν (an ε -warm start for target π), i.e.
 $\forall S \subseteq \mathbb{R}^n$ measurable, $|\nu(S) - \pi(S)| \leq \varepsilon$.

Ensure: Particle ensemble $\{X_T^i\}_{i=1}^d \subset K$.

- 1: **Initialize:** draw $X_0^1, \dots, X_0^d \sim \nu$ (e.g. i.i.d.) with $X_0^i \in K$.
- 2: **for** $t = 0, 1, \dots, T - 1$ **do**
- 3: **for** $i = 1, 2, \dots, d$ **do**
- 4: Sample (j, k) uniformly at random from $\{1, \dots, d\} \setminus \{i\}$ with $j \neq k$.
- 5: Set direction
$$h \leftarrow \frac{X_t^j - X_t^k}{\|X_t^j - X_t^k\|}.$$
- 6: Define the chord of K through X_t^i in direction h as the line-section
$$\ell(X_t^i, h) = \{X_t^i + \alpha h | \alpha \in \mathbb{R}\} \cap K.$$
- 7: Sample $X_{t+1}^i \sim \text{Unif}(\ell(X_t^i, h))$.
- 8: **end for**
- 9: **end for**
- 10: **return** $\{X_T^i\}_{i=1}^d$.

3 A Road Map

The mixing time analysis of the ensemble sampler is typically hard. For simplicity, we adopt the warm-start assumption. In addition, in this note, we analyze an alternative dynamics: we assume that when each particle is updated, it forms the direction of its random walk by uniformly sampling two independent points from the convex body K , rather than sampling two points from other particles. This differs from the true dynamics and introduces a bias, but it typically does not affect the order of the mixing time.

4 Ensembled Hit-and-Run

The major difference in ensembled Hit-and-Run is that the choice of direction is dependent on the geometry of the convex body K instead of a uniformly random direction. To start with, we analyze the distribution of a

Algorithm 2 Analyzed version of ensembled Hit-and-Run

Require: Convex body $K \subset \mathbb{R}^n$; number of particles d ; number of iterations T ; initial distribution ν (an ε -warm start for target π), i.e. $\forall S \subseteq \mathbb{R}^n$ measurable, $|\nu(S) - \pi(S)| \leq \varepsilon$.

Ensure: Particle ensemble $\{X_T^i\}_{i=1}^d \subset K$.

- 1: **Initialize:** draw $X_0^1, \dots, X_0^d \sim \nu$ (e.g. i.i.d.) with $X_0^i \in K$.
- 2: **for** $t = 0, 1, \dots, T-1$ **do**
- 3: **for** $i = 1, 2, \dots, d$ **do**
- 4: Sample Y_1, Y_2 uniformly at random from K .
- 5: Set direction

$$h \leftarrow \frac{Y_1 - Y_2}{\|Y_1 - Y_2\|}.$$
- 6: Define the chord of K through X_t^i in direction h as the line-section

$$\ell(X_t^i, h) = \{X_t^i + \alpha h | \alpha \in \mathbb{R}\} \cap K.$$
- 7: Sample $X_{t+1}^i \sim \text{Unif}(\ell(X_t^i, h))$.
- 8: **end for**
- 9: **end for**
- 10: **return** $\{X_T^i\}_{i=1}^d$.

random direction in a convex body K .

Lemma 1. Suppose that π is a uniform distribution on a convex body $K \subset \mathbb{R}^n$ with maximum diameter $2D$, and i.i.d random variables $X, Y \sim \pi$. Denote $Z = X - Y$. Suppose that H is the direction of Z , i.e $H = \frac{Z}{\|Z\|}$. Assume that $\frac{|K|}{\pi_{n-1} D^{n-1} \ell(h)} \gg \frac{1}{n}$. Then the density of H satisfies

$$\frac{c_1}{|K|n^2} \left(\frac{\ell(h)}{c_2} \right)^n \leq f_H(h) \leq \frac{\ell(h)^n}{n(n+1)|K|}$$

where $\ell(h)$ is the maximum of the length of the chord of direction h , and c_1, c_2 is small constant independent of n .

Lemma 2. Define $f_u(x)$ as the probability distribution of a step from u . Then

$$f_u(A) = \int_A \frac{f_H(u_x)}{\ell(x, u)|x-u|^{n-1}} dx$$

where $u_x = \frac{x-u}{\|x-u\|}$.

Recall that the direction h has density $f_H(h)$, and by Lemma 1 we have

$$c_1 \ell(h) \leq (n^2 |K| f_H(h))^{\frac{1}{n}} \leq \ell(h).$$

The analysis relies on a vital fact that K_r should be convex:

Conjecture 1. K_r , defined by $K_r := \{x|x \in K, \kappa(x, r) \geq \frac{15}{16}\}$, is convex if K is convex.

We aim to follow the analysis in [7] by using an isoperimetric inequalities. The following lemmas serve as preliminaries.

Lemma 3. *For any convex body K , we have*

$$\frac{|K_r|}{|K|} \geq 1 - cnr \quad \text{possibly } \sqrt{n} \text{ here} \quad (1)$$

for some constant $c > 0$.

Lemma 4. *For any $h \in K$, suppose that x is generated by first sampling a direction $h \sim f_H(h)$ then uniformly choosing a point on the chord through u with direction h . We have*

$$\mathbb{P}\left(\frac{|x - u|}{\rho\left(\frac{x-u}{\|x-u\|}\right)} \leq c\right) \leq \frac{c}{c'} + \bar{\kappa}(u, c')$$

Lemma 5. *For any $u \in K_r$, we have*

$$F(u) \geq \frac{1}{16}r.$$

Lemma 6. *Suppose that $u, v \in K$ satisfies $\frac{|v-u|}{\rho\left(\frac{v-u}{\|v-u\|}\right)} \leq \frac{c_1}{n} F(u)$, then $d(P_v, P_u) \leq 1 - c$ for some $c > 0$.*

The following corollary discloses the edge of a geometry-aware direction sampling compared to a uniform direction sampling, which is the independence of the maximum radius R .

Corollary 1. *Let $K = S_1 \cup S_2$ be a partition of K . Let*

$$\begin{aligned} S'_1 &:= \{x \in S_1 \cap K_r : P_x(S_2) \leq \frac{5c}{16}\}. \\ S'_2 &:= \{x \in S_2 \cap K_r : P_x(S_1) \leq \frac{5c}{16}\}. \end{aligned}$$

Then

$$d_K(S'_1, S'_2) \geq \frac{r}{n}.$$

Finally we are ready to present the main theorem.

Theorem 1. *The conductance Φ of the proposed MCMC algorithm satisfies*

$$\Phi \geq \frac{cr}{n} = O\left(\frac{1}{n^2}\right)$$

Thus the mixing time start from a ϵ -warm start is roughly $O(n^4)$.

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Advances in Neural Information Processing Systems, 35:31684–31696, 2022.