Advances in Applied Mathematics 92 (2018) 122–143

Contents lists available at ScienceDirect

Advances in Applied Mathematics

www.elsevier.com/locate/yaama

Heat-bath random walks with Markov bases

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ARTICLE INFO

Article history:
Received 27 May 2016
Received in revised form 14 June 2017
Accepted 10 August 2017
Available online xxxx

MSC:
primary 05C81
secondary 37A25, 11P21

Keywords:
Heat-bath random walks
Sampling
Lattice points
Markov bases

ABSTRACT

Graphs on lattice points are studied whose edges come from a finite set of allowed moves of arbitrary length. We show that the diameter of these graphs on fibers of a fixed integer matrix can be bounded from above by a constant. We then study the mixing behaviour of heat-bath random walks, a generalization of the Glauber dynamics, on these graphs. We also state explicit conditions on the set of moves so that the heat-bath random walk mixes rapidly in fixed dimension.

1. Introduction

A *fiber graph* is a graph on the finitely many lattice points $\mathcal{F} \subset \mathbb{Z}^d$ of a polytope where two lattice points are connected by an edge if their difference lies in a finite set of allowed moves $\mathcal{M} \subset \mathbb{Z}^d$. The implicit structure of these graphs makes them a useful tool to explore the set of lattice points randomly: At the current lattice point $u \in \mathcal{F}$, an element $m \in \pm\mathcal{M}$ is sampled and the random walk moves along m if $u + m \in \mathcal{F}$ and

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http://dx.doi.org/10.1016/j.aam.2017.08.002
0196-8858/

stays at u otherwise. The corresponding Markov chain is irreducible if the underlying fiber graph is connected and the set $\mathcal{M}$ is called a *Markov basis* for $\mathcal{F}$ in this case. This paper investigates the *heat-bath* version of this random walk: At the current lattice point $u \in \mathcal{F}$, we sample $m \in \mathcal{M}$ and move to a random element in the integer ray $(u+\mathbb{Z}\cdot m)\cap\mathcal{F}$. The authors of [6] discovered that this random walk can be seen as a discrete version of the *hit-and-run* algorithm [15,26,16] that has been used frequently to sample from all the points of a polytope – not only from its lattice points. The popularity of the continuous version of the hit-and-run algorithm has not spread to its discrete analog, and not much is known about its mixing behaviour. One reason is that it is already challenging to guarantee that all points in the underlying set $\mathcal{F}$ can be reached by a random walk that uses moves from $\mathcal{M}$, whereas for the continuous version, a random sampling from the unit sphere suffices. However, in many situations where a Markov basis is known, the heat-bath random walk is evidently fast. For instance, it was shown in [3] that the heat-bath random walk on contingency tables mixes rapidly when the number of columns is fixed. To work around the connectedness issue, a *discrete hit-and-run* algorithm was introduced in [1] for arbitrary finite sets $\mathcal{F} \subset \mathbb{Z}^d$. In each step of this random walk, a subordinate and unrestricted random walk starts at the current lattice point $u \in \mathcal{F}$ and uses the unit vectors to collect a set of proposals $S \subset \mathbb{Z}^d$. The random walk then moves from u to a random point in $S \cap \mathcal{F}$. Generally speaking, the same methodology is applied by the heat-bath walk, but here, the set of proposals $S \cap \mathcal{F}$ is an integer ray through $\mathcal{F}$.

Random walks of the heat-bath type, such as the one presented above, have been studied recently in [8] in a more general context. In this paper, we explore the mixing behaviour of heat-bath random walks on the lattice points of polytopes with Markov bases. Throughout, we assume that a Markov basis has been found already and refer to the relevant literature for their computation [24,25,11,17,10,21]. We call the underlying graph of the heat-bath random walk a *compressed fiber graph* (Definition 2.5) and determine in Section 3 bounds on its graph-diameter. We prove that for any $A \in \mathbb{Z}^{m\times d}$ with $\ker_{\mathbb{Z}}(A) \cap \mathbb{N}^d = \{0\}$, the diameter of compressed fiber graphs on $\{u \in \mathbb{N}^d : Au = b\}$ that use a fixed Markov bases $\mathcal{M} \subset \ker_{\mathbb{Z}}(A)$ is bounded from above by a constant as b varies (Theorem 3.15). In contrast, we show that the diameter of conventional fiber graphs grow linearly under a dilation of the underlying polytope (Remark 3.9). This gives rise to slow mixing results for conventional fiber walks as observed in [27]. In Section 4, we study in more detail the combinatorial and analytical structure of the transition matrices of heat-bath random walks on lattice points and prove upper and lower bounds on their second largest eigenvalues. We also discuss how the distribution on the moves $\mathcal{M}$ affects the speed of convergence (Example 4.21). Theorem 5.8 establishes with the *canonical path approach* from [23] an upper bound on the second largest eigenvalue when the Markov basis is *augmenting* (Definition 5.1) and the stationary distribution is uniform. From that, we conclude fast mixing results for random walks on lattice points in fixed dimension.