Dedicated to Marius Iosifescu on the occasion of his 80th anniversary

A Gibbs sampler in a generalized sense

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ABSTRACT. We present, in the finite case, a generalization of the cyclic Gibbs sampler – the Gibbs sampler for short. The chain obtained we call the cyclic Gibbs sampler in a generalized sense – the Gibbs sampler in a generalized sense for short. The Gibbs sampler in a generalized sense belongs to our collection of hybrid Metropolis-Hastings chains from [U. Păun, A hybrid Metropolis-Hastings chain, *Rev. Roumaine Math. Pures Appl.* **56** (2011), 207–228] and we conjecture that it is the fastest chain in this collection in a sense which will be specified in article. We then present the wavy probability distributions, a generalized sense, a special one, for wavy probability distributions which is fast, attaining its stationarity in a finite number of steps, and, besides this, has other important properties – the computation of certain important probabilities iteratively and, for wavy probability distributions having normalization constant, the computation of this constant.

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1. Basic things

In this section, we present some basic things.

 Set

 $\operatorname{Par}(E) = \left\{ \Delta \mid \Delta \text{ is a partition of } E \right\},\$

where E is a nonempty set. We shall agree that the partitions do not contain the empty set.

Definition 1.1. Let $\Delta_1, \Delta_2 \in Par(E)$. We say that Δ_1 is finer than Δ_2 if $\forall V \in \Delta_1$, $\exists W \in \Delta_2$ such that $V \subseteq W$.

Write $\Delta_1 \preceq \Delta_2$ when Δ_1 is finer than Δ_2 .

In this article, a vector is a row vector and a stochastic matrix is a row stochastic matrix.

The entry (i, j) of a matrix Z will be denoted Z_{ij} or, if confusion can arise, $Z_{i \to j}$. Set

$$\begin{split} \langle m \rangle &= \{1, 2, ..., m\} \ (m \geq 1), \\ \langle \langle m \rangle \rangle &= \{0, 1, ..., m\} \ (m \geq 0), \\ N_{m,n} &= \{P \mid P \text{ is a nonnegative } m \times n \text{ matrix} \}, \end{split}$$

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 $S_{m,n} = \{P \mid P \text{ is a stochastic } m \times n \text{ matrix}\},\$

$$N_n = N_{n,n},$$
$$S_n = S_{n,n}.$$

Let $P = (P_{ij}) \in N_{m,n}$. Let $\emptyset \neq U \subseteq \langle m \rangle$ and $\emptyset \neq V \subseteq \langle n \rangle$. Set the matrices

$$P_U = (P_{ij})_{i \in U, j \in \langle n \rangle}, \ P^V = (P_{ij})_{i \in \langle m \rangle, j \in V}, \ \text{and} \ P^V_U = (P_{ij})_{i \in U, j \in V}.$$

Set

$$\begin{aligned} (\{i\})_{i \in \{s_1, s_2, \dots, s_t\}} &= (\{s_1\}, \{s_2\}, \dots, \{s_t\}); \\ (\{i\})_{i \in \{s_1, s_2, \dots, s_t\}} \in \operatorname{Par}\left(\{s_1, s_2, \dots, s_t\}\right). \end{aligned}$$

E.g.,

$$(\{i\})_{i \in \langle n \rangle} = (\{1\}, \{2\}, ..., \{n\}).$$

Definition 1.2. Let $P \in N_{m,n}$. We say that P is a generalized stochastic matrix if $\exists a \geq 0, \exists Q \in S_{m,n}$ such that P = aQ.

Definition 1.3. [8] Let $P \in N_{m,n}$. Let $\Delta \in \operatorname{Par}(\langle m \rangle)$ and $\Sigma \in \operatorname{Par}(\langle n \rangle)$. We say that P is a $[\Delta]$ -stable matrix on Σ if P_K^L is a generalized stochastic matrix, $\forall K \in \Delta, \forall L \in \Sigma$. In particular, a $[\Delta]$ -stable matrix on $(\{i\})_{i \in \langle n \rangle}$ is called $[\Delta]$ -stable for short.

Definition 1.4. [8] Let $P \in N_{m,n}$. Let $\Delta \in Par(\langle m \rangle)$ and $\Sigma \in Par(\langle n \rangle)$. We say that P is a Δ -stable matrix on Σ if Δ is the least fine partition for which P is a $[\Delta]$ -stable matrix on Σ . In particular, a Δ -stable matrix on $(\{i\})_{i \in \langle n \rangle}$ is called Δ -stable while a $(\langle m \rangle)$ -stable matrix on Σ is called stable on Σ for short. A stable matrix on $(\{i\})_{i \in \langle n \rangle}$ is called stable for short.

Let
$$\Delta_1 \in \operatorname{Par}(\langle m \rangle)$$
 and $\Delta_2 \in \operatorname{Par}(\langle n \rangle)$. Set (see [8] for G_{Δ_1,Δ_2} and [9] for $\overline{G}_{\Delta_1,\Delta_2}$)
 $G_{\Delta_1,\Delta_2} = \{P \mid P \in S_{m,n} \text{ and } P \text{ is a } [\Delta_1] \text{-stable matrix on } \Delta_2 \}$

and

$$\overline{G}_{\Delta_1,\Delta_2} = \{P \mid P \in N_{m,n} \text{ and } P \text{ is a } [\Delta_1] \text{-stable matrix on } \Delta_2 \}.$$

When we study or even when we construct products of nonnegative matrices (in particular, products of stochastic matrices) using G_{Δ_1,Δ_2} or $\overline{G}_{\Delta_1,\Delta_2}$ we shall refer this as the *G* method. *G* comes from the verb to group and its derivatives.

Below we give an important result.

Theorem 1.1. [8] Let
$$P_1 \in G_{(\langle m_1 \rangle), \Delta_2} \subseteq S_{m_1, m_2}$$
, $P_2 \in G_{\Delta_2, \Delta_3} \subseteq S_{m_2, m_3}$, ..., $P_{n-1} \in G_{\Delta_{n-1}, \Delta_n} \subseteq S_{m_{n-1}, m_n}$, $P_n \in G_{\Delta_n, (\{i\})_{i \in \langle m_{n+1} \rangle}} \subseteq S_{m_n, m_{n+1}}$. Then

 $P_1 P_2 ... P_n$

is a stable matrix (i.e., a matrix with identical rows, see Definition 1.4).

Proof. See [8].

Definition 1.5. (See, e.g., [14, p. 80].) Let $P \in N_{m,n}$. We say that P is a rowallowable matrix if it has at least one positive entry in each row.

Let $P \in N_{m,n}$. Set

$$\overline{P} = (\overline{P}_{ij}) \in N_{m,n}, \ \overline{P}_{ij} = \begin{cases} 1 \text{ if } P_{ij} > 0, \\ 0 \text{ if } P_{ij} = 0, \end{cases}$$

 $\forall i \in \langle m \rangle, \forall j \in \langle n \rangle$. We call \overline{P} the incidence matrix of P (see, e.g., [5, p. 222]).

In this article, the transpose of a vector x is denoted x'. Set $e = e(n) = (1, 1, ..., 1) \in \mathbb{R}^n$, $\forall n \ge 1$.

In this article, some statements on the matrices hold eventually by permutation of rows and columns. For simplification, further, we omit to specify this fact.

Warning! In this article, if a Markov chain has the transition matrix $P = P_1 P_2 \dots P_s$, where $s \ge 1$ and P_1, P_2, \dots, P_s are stochastic matrices, then any 1-step transition of this chain is performed via P_1, P_2, \dots, P_s , i.e., doing s transitions: one using P_1 , one using P_2, \dots , one using P_s .

Let $S = \langle r \rangle$. (We work with this set for simplification; S can be any nonempty finite set.) Let $\pi = (\pi_i)_{i \in S} = (\pi_1, \pi_2, ..., \pi_r)$ be a positive probability distribution on S. One way to sample approximately or, at best, exactly from S when $r \geq 2$ is by means of our hybrid Metropolis-Hastings chain from [9]. Below we define this chain.

Let *E* be a nonempty set. Set $\Delta \succ \Delta'$ if $\Delta' \preceq \Delta$ and $\Delta' \neq \Delta$, where Δ , $\Delta' \in Par(E)$.

Let $\Delta_1, \Delta_2, ..., \Delta_{t+1} \in \operatorname{Par}(S)$ with $\Delta_1 = (S) \succ \Delta_2 \succ ... \succ \Delta_{t+1} = (\{i\})_{i \in S}$, where $t \ge 1$. $(\Delta_1 \succ \Delta_2 \text{ implies } r \ge 2$.) Let $Q_1, Q_2, ..., Q_t \in S_r$ such that

(C1) $\overline{Q}_1, \overline{Q}_2, ..., \overline{Q}_t$ are symmetric matrices;

(C2) $(Q_l)_K^L = 0, \forall l \in \langle t \rangle - \{1\}, \forall K, L \in \Delta_l, K \neq L$ (this assumption implies that Q_l is a block diagonal matrix and Δ_l -stable matrix on $\Delta_l, \forall l \in \langle t \rangle - \{1\}$);

(C3) $(Q_l)_K^U$ is a row-allowable matrix, $\forall l \in \langle t \rangle$, $\forall K \in \Delta_l$, $\forall U \in \Delta_{l+1}$, $U \subseteq K$.

Although Q_l , $l \in \langle t \rangle$, are not irreducible matrices if $l \geq 2$, we define the matrices P_l , $l \in \langle t \rangle$, as in the Metropolis-Hastings case (see, e.g., [6, pp. 63–66] for this case), namely,

$$P_l = \left(\left(P_l \right)_{ij} \right) \in S_{r_i}$$

$$(P_l)_{ij} = \begin{cases} 0 & \text{if } j \neq i \text{ and } (Q_l)_{ij} = 0, \\ (Q_l)_{ij} \min\left(1, \frac{\pi_j(Q_l)_{ji}}{\pi_i(Q_l)_{ij}}\right) & \text{if } j \neq i \text{ and } (Q_l)_{ij} > 0, \\ 1 - \sum_{k \neq i} (P_l)_{ik} & \text{if } j = i, \end{cases}$$

 $\forall l \in \langle t \rangle$. Set $P = P_1 P_2 \dots P_t$.

Theorem 1.2. [9] Concerning P above we have $\pi P = \pi$ and P > 0.

Proof. See [9].

By Theorem 1.2, $P^n \to e'\pi$ as $n \to \infty$. We call the Markov chain with transition matrix P the hybrid Metropolis-Hastings chain. In particular, we call this chain the hybrid Metropolis chain when $Q_1, Q_2, ..., Q_t$ are symmetric matrices.

2. Our Gibbs sampler in a generalized sense

In this section, we consider a generalization of the cyclic Gibbs sampler – the Gibbs sampler for short – which we call the cyclic Gibbs sampler in a generalized sense – the Gibbs sampler in a generalized sense for short. The Gibbs sampler in a generalized sense belongs to our collection of hybrid Metropolis-Hastings chains presented in Section 1 and, moreover, we conjecture that it is the fastest chain in this collection in a sense which will be specified in this section.

Theorem 2.1. Consider a hybrid Metropolis-Hastings chain with state space $S = \langle r \rangle$ and transition matrix $P = P_1 P_2 \dots P_t$, P_1 , P_2 , \dots , P_t corresponding to Q_1, Q_2, \dots, Q_t , respectively. Suppose that $\forall l \in \langle t \rangle, \forall i, j \in S$,

$$(Q_l)_{ij} = \frac{\pi_j}{\sum\limits_{k \in S, (Q_l)_{ik} > 0}} if \ (Q_l)_{ij} > 0$$

(see Section 1 again for Q_l , $l \in \langle t \rangle$, $\pi = (\pi_i)_{i \in S}$, ...). Then

$$P_l = Q_l, \ \forall l \in \langle t \rangle$$

Proof. Obvious.

We call the hybrid Metropolis-Hastings chain from Theorem 2.1 the cyclic Gibbs sampler in a generalized sense – the Gibbs sampler in a generalized sense for short. Recall that we work with $S = \langle r \rangle$ for simplification; S, here, can be any finite set with $|S| \geq 2$ ($|\cdot|$ is the cardinal).

We use the convention that an empty term vanishes.

Let π be a positive probability distribution on $S = \langle \langle h \rangle \rangle^n$, $h, n \ge 1$ (more generally, on $S = \langle \langle h_1 \rangle \rangle \times \langle \langle h_2 \rangle \rangle \times \ldots \times \langle \langle h_n \rangle \rangle$, $h_1, h_2, \ldots, h_n, n \ge 1$). Let $x = (x_1, x_2, \ldots, x_n) \in S$. Set

$$x[k|l] = (x_1, x_2, \dots, x_{l-1}, k, x_{l+1}, \dots, x_n), \forall k \in \langle \langle h \rangle \rangle, \forall l \in \langle n \rangle.$$

Obviously, $x[k|l] \in S$, $\forall k \in \langle \langle h \rangle \rangle$, $\forall l \in \langle n \rangle$. The (usual) cyclic Gibbs sampler - the Gibbs sampler for short - on $S = \langle \langle h \rangle \rangle^n$, $h, n \ge 1$ (more generally, on $S = \langle \langle h_1 \rangle \rangle \times \langle \langle h_2 \rangle \rangle \times \ldots \times \langle \langle h_n \rangle \rangle$, $h_1, h_2, \ldots, h_n, n \ge 1$) is a Markov chain with state space S and transition matrix $P = P_1 P_2 \ldots P_n$, where

$$(P_l)_{xy} = \begin{cases} 0 & \text{if } y \neq x \left[k \mid l \right], \forall k \in \langle \langle h \rangle \rangle, \\ \frac{\pi_{x\left[k \mid l \right]}}{\sum\limits_{j \in \langle \langle h \rangle \rangle} \pi_{x\left[j \mid l \right]}} & \text{if } y = x \left[k \mid l \right] \text{ for some } k \in \langle \langle h \rangle \rangle, \end{cases}$$

 $\forall l \in \langle n \rangle$, $\forall x, y \in S$. (For the Gibbs sampler, see, e.g., [2], [4, Chapter 5], and [6, pp. 69-81].)

The Gibbs sampler on $\langle \langle h \rangle \rangle^n$ belongs to our collection of hybrid Metropolis-Hastings chains, see [10] – this follows considering the partitions

$$\Delta_{1} = (S) ,$$

$$\Delta_{l+1} = \left(K_{(x_{1}, x_{2}, \dots, x_{l})} \right)_{x_{1}, x_{2}, \dots, x_{l} \in \langle \langle h \rangle \rangle} , \forall l \in \langle n \rangle .$$

where

$$K_{(x_1, x_2, \dots, x_l)} = \{(y_1, y_2, \dots, y_n) \mid (y_1, y_2, \dots, y_n) \in S \text{ and } y_i = x_i, \forall i \in \langle l \rangle \},\$$

 $\forall l \in \langle n \rangle$, $\forall x_1, x_2, ..., x_l \in \langle \langle h \rangle \rangle$ (so, $\Delta_1 = (S) \succ \Delta_2 \succ ... \succ \Delta_{n+1} = (\{x\})_{x \in S}$), and matrices $Q_l, l \in \langle n \rangle$,

$$Q_l = P_l, \ \forall l \in \langle n \rangle.$$

Obviously – now, it is obvious –, the Gibbs sampler on $\langle\langle h \rangle\rangle^n$ is a special case of our Gibbs sampler in a generalized sense on $\langle\langle h \rangle\rangle^n$.

Remark 2.2. The matrices Q_l , $l \in \langle n \rangle$, of Gibbs sampler on $\langle \langle h \rangle \rangle^n$ have the property:

$$\begin{array}{ll} (Q_l)_K^U \text{ has in each row just one positive entry,} \\ \forall l & \in & \langle n \rangle , \ \forall K \in \Delta_l, \ \forall U \in \Delta_{l+1} \text{ with } U \subseteq K. \end{array}$$

Therefore, a subcollection - an interesting subcollection - of our collection of Gibbs samplers in a generalized sense is that of the Gibbs samplers in a generalized sense having the above property, i.e., satisfying the condition (c4) from [9].

Let $P = (P_{ij}) \in N_{m,n}$. P is called 0-1 matrix if $P_{ij} \in \langle \langle 1 \rangle \rangle, \forall i \in \langle m \rangle, \forall j \in \langle n \rangle$.

We conjecture that the Gibbs sampler in a generalized sense is the fastest chain in our collection of hybrid Metropolis-Hastings chains in a sense which is specified below.

Conjecture 2.3. Fix $S = \langle r \rangle$. Fix $\Delta_1, \Delta_2, ..., \Delta_{t+1} \in Par(S)$ with $\Delta_1 = (S) \succ \Delta_2 \succ ... \succ \Delta_{t+1} = (\{i\})_{i \in S}$, where $t \geq 1$. Fix the 0-1 matrices $V_1, V_2, ..., V_t \in N_r$ having the properties (C1)-(C3) from Section 1 – we extend these properties for matrices from N_r . Fix the target probability distribution $\pi = (\pi_i)_{i \in S}$ (on S). Fix w, a probability distribution on S. Consider the subcollection of hybrid Metropolis-Hastings chains corresponding to π (each chain from this subcollection is constructed using π) with $Q_1, Q_2, ..., Q_t \in S_r$ having the properties (C1)-(C3) and, moreover,

$$\overline{Q}_l = V_l, \ \forall l \in \langle t \rangle$$

(these equations simply say that all the chains from this subcollection have the same neighbor system; $V_1, V_2, ..., V_t$ are fixed, not $Q_1, Q_2, ..., Q_t$ – the latter are only fixed for each chain from subcollection). Then the Gibbs sampler in a generalized sense from this subcollection (there exists a unique Gibbs sampler in a generalized sense in this subcollection) is the fastest chain in this subcollection, i.e., for any hybrid Metropolis-Hastings chain from this subcollection,

$$||p_n - \pi||_1 \le ||s_n - \pi||_1, \ \forall n \ge 1,$$

where p_n = the probability distribution of Gibbs sampler in a generalized sense (from this subcollection) at time n, s_n = the probability distribution of hybrid Metropolis-Hastings chain at time n, $\forall n \geq 0$, $p_0 = s_0 = w$ (all the chains from this subcollection have the same initial probability distribution, w).

Obviously, the word "fastest" from the above conjecture refers to Markov chains strictly, not to computers. The running time of our hybrid chains on a computer is another matter (the computational cost per step is the main problem; on a computer, a step of a Markov chain can be performed or not).

Conjecture 2.3 is supported by [11]-[13]; each of these articles is based on a Gibbs sampler in a generalized sense which is fast – we refer, here, both the Markov chains and computers – and, moreover, has other interesting properties. (For more information, see Section 3.)

3. Wavy probability distributions

In this section, we construct a class of probability distributions which contains the wavy probability distribution(s) of first type from [10] as a special case. The probability distributions from this class we call the wavy probability distributions.

Let $S = \langle r \rangle$. Let $\pi = (\pi_i)_{i \in S}$ be a positive probability distribution (on S). Let Δ_1 , Δ_2 , ..., $\Delta_{t+1} \in \operatorname{Par}(S)$ with $\Delta_1 = (S) \succ \Delta_2 \succ ... \succ \Delta_{t+1} = (\{i\})_{i \in S}$, where $t \ge 1$. $(\Delta_1 \succ \Delta_2 \text{ implies } r \ge 2$.) Consider that $\Delta_l = \left(K_1^{(l)}, K_2^{(l)}, ..., K_{u_l}^{(l)}\right)$, $K_1^{(l)}$ having the first $\left|K_1^{(l)}\right|$ elements of S, $K_2^{(l)}$ having the next $\left|K_2^{(l)}\right|$ elements of S (this condition and the next ones vanish when l = 1), ..., $K_{u_l}^{(l)}$ having the last $\left|K_{u_l}^{(l)}\right|$ elements of S, $\forall l \in \langle t+1 \rangle$. Consider that

(c1)
$$\left|K_{1}^{(l)}\right| = \left|K_{2}^{(l)}\right| = \dots = \left|K_{u_{l}}^{(l)}\right|, \forall l \in \langle t+1 \rangle \text{ with } u_{l} \ge 2;$$

(c2) $r = r_1 r_2 \dots r_t$ with $r_1 r_2 \dots r_l = |\Delta_{l+1}|, \forall l \in \langle t-1 \rangle$, and $r_t = |K_1^{(t)}|$ (this condition is compatible with $\Delta_1 \succ \Delta_2 \succ \dots \succ \Delta_{t+1}$).

The above conditions are noted (c1) and (c2) as in [9]. The condition (c2) is superfluous because it follows from (c1) and $\Delta_1 \succ \Delta_2 \succ ... \succ \Delta_{t+1}$.

We have

$$K_{v}^{(l)} = \bigcup_{s \in D_{v,b_{l}} \cup \{vb_{l}\}} K_{s}^{(l+1)}, \; \forall l \in \langle t \rangle, \; \forall v \in \langle u_{l} \rangle,$$

where

$$b_l = \frac{|\Delta_{l+1}|}{|\Delta_l|}, \ \forall l \in \langle t \rangle$$

and

$$D_{v,b_l} = \{ (v-1) \, b_l + 1, \ (v-1) \, b_l + 2, \ \dots, \ v b_l - 1 \}, \ \forall l \in \langle t \rangle, \ \forall v \in \langle u_l \rangle.$$

Suppose that $\forall l \in \langle t \rangle$, $\forall v \in \langle u_l \rangle$, $\forall s \in D_{v,b_l}$, $\exists \alpha_s^{(l,v)} > 0$ such that

$$\pi_{i+d_s^{(l,v)}} = \alpha_s^{(l,v)} \pi_i \text{ (direct proportionality), } \forall i \in K_{(v-1)b_l+1}^{(l+1)}$$

where

$$d_{s}^{(l,v)} = \left| K_{(v-1)b_{l}+1}^{(l+1)} \right| + \left| K_{(v-1)b_{l}+2}^{(l+1)} \right| + \dots + \left| K_{s}^{(l+1)} \right|$$

 $\forall l \in \langle t \rangle, \forall v \in \langle u_l \rangle, \forall s \in D_{v,b_l}.$

Definition 3.1. The probability distribution $\pi = (\pi_i)_{i \in S}$ having the above property we call the *wavy probability distribution*.

To define the wavy probability distribution, we considered $S = \langle r \rangle$ $(r \geq 2)$ for simplification; moreover, $S = \langle r \rangle$ was equipped with the usual order relation $\langle (1 < 2 < ... < r)$ for simplification too. S can be any finite set for which the conditions (c1) and (c2) hold, setting r = |S|. In this case, supposing that $\pi = (\pi_i)_{i \in S}$ is given, to see if π is a wavy probability distribution on S, we must consider, excepting $S = \langle r \rangle$ equipped with the usual order relation \langle , order relations on S or bijective functions (i.e., coding functions; for coding functions, see, e.g., [3, p. 643]) from S to $\langle |S| \rangle$, equipping the latter set with the usual order relation \langle .

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Recall that $\mathbb{R}^+=\{x\mid x\in\mathbb{R} \text{ and } x>0\}$. Recall that in [10] the probability distribution

$$\pi = (c_0, c_0 a, \dots, c_0 a^w, c_1, c_1 a, \dots, c_1 a^w, \dots, c_h, c_h a, \dots, c_h a^w, c_0, c_0 a, \dots, c_0 a^w, c_1, c_1 a, \dots, c_1 a^w, \dots, c_h, c_h a, \dots, c_h a^w, \dots, c_0, c_0 a, \dots, c_0 a^w, c_1, c_1 a, \dots, c_1 a^w, \dots, c_h, c_h a, \dots, c_h a^w)$$

(the sequence $c_0, c_0 a, ..., c_0 a^w, c_1, c_1 a, ..., c_1 a^w, ..., c_h, c_h a, ..., c_h a^w$ appears $(h+1)^{n-t-1}$ times if $0 \le t < n$ and $c_0, c_0 a, ..., c_0 a^w$ only appears if t = n) on $\langle \langle h \rangle \rangle^n$ equipped with the lexicographic order, where $w = (h+1)^t - 1$, $0 \le t \le n$, $c_0, c_1, ..., c_h, a \in \mathbb{R}^+$, was called the *wavy probability distribution of first type*. This probability distribution is, according to Definition 3.1, a wavy probability distribution. Below we illustrate this in a simple case.

Example 3.1. Consider $S = \langle \langle 1 \rangle \rangle^3$ (h = 1, n = 3) equipped with the lexicographic order and

$$\pi = \left(c_0, c_0 a, c_0 a^2, c_0 a^3, c_1, c_1 a, c_1 a^2, c_1 a^3\right).$$

 π is a wavy probability distribution (according to Definition 3.1). To show this, we consider (see Section 2, where we showed that the (usual) Gibbs sampler belongs to our collection of hybrid Metropolis-Hastings chains) the sets

$$\begin{split} K_{(0)} &= \left\{ (0,0,0) \,, \ (0,0,1) \,, \ (0,1,0) \,, \ (0,1,1) \right\} \,, \\ K_{(1)} &= \left\{ (1,0,0) \,, \ (1,0,1) \,, \ (1,1,0) \,, \ (1,1,1) \right\} \,, \\ K_{(0,0)} &= \left\{ (0,0,0) \,, \ (0,0,1) \right\} \,, \ K_{(0,1)} &= \left\{ (0,1,0) \,, \ (0,1,1) \right\} \,, \\ K_{(1,0)} &= \left\{ (1,0,0) \,, \ (1,0,1) \right\} \,, \ K_{(1,1)} &= \left\{ (1,1,0) \,, \ (1,1,1) \right\} \,, \\ K_{(0,0,0)} &= \left\{ (0,0,0) \right\} \,, \ K_{(0,0,1)} &= \left\{ (0,0,1) \right\} \,, \ \ldots , \ K_{(1,1,1)} &= \left\{ (1,1,1) \right\} \end{split}$$

and partitions

$$\Delta_{1} = (S) = \left(\left\langle \left\langle 1 \right\rangle \right\rangle^{3} \right),$$

$$\Delta_{2} = \left(K_{(0)}, \ K_{(1)} \right),$$

$$\Delta_{3} = \left(K_{(0,0)}, \ K_{(0,1)}, \ K_{(1,0)}, \ K_{(1,1)} \right),$$

$$\Delta_{4} = \left(K_{(0,0,0)}, \ K_{(0,0,1)}, \ \dots, \ K_{(1,1,1)} \right)$$

Obviously,

$$\begin{split} \Delta_1 \succ \Delta_2 \succ \Delta_3 \succ \Delta_4, \\ \left| K_{(0)} \right| &= \left| K_{(1)} \right| = 4, \\ K_{(0,0)} \right| &= \left| K_{(0,1)} \right| = \left| K_{(1,0)} \right| = \left| K_{(1,1)} \right| = 2, \\ \left| K_{(0,0,0)} \right| &= \left| K_{(0,0,1)} \right| = \dots = \left| K_{(1,1,1)} \right| = 1, \\ \pi_{(1,0,0)} &= \frac{c_1}{c_0} \pi_{(0,0,0)}, \ \pi_{(1,0,1)} &= \frac{c_1}{c_0} \pi_{(0,0,1)}, \\ \pi_{(1,1,0)} &= \frac{c_1}{c_0} \pi_{(0,1,0)}, \ \pi_{(1,1,1)} &= \frac{c_1}{c_0} \pi_{(0,1,1)} \end{split}$$

(the proportionality factor is $\frac{c_1}{c_0}$),

$$\pi_{(0,1,0)} = a^2 \pi_{(0,0,0)}, \ \pi_{(0,1,1)} = a^2 \pi_{(0,0,1)}$$

(the proportionality factor is a^2),

$$\pi_{(1,1,0)} = a^2 \pi_{(1,0,0)}, \ \pi_{(1,1,1)} = a^2 \pi_{(1,0,1)}$$

(the proportionality factor is also a^2),

$$\pi_{(0,0,1)} = a\pi_{(0,0,0)}, \ \pi_{(0,1,1)} = a\pi_{(0,1,0)},$$

$$\pi_{(1,0,1)} = a\pi_{(1,0,0)}, \ \pi_{(1,1,1)} = a\pi_{(1,1,0)}$$

(the proportionality factor is a in all these last cases). Therefore, π is a wavy probability distribution (according to Definition 3.1).

The Mallows model through Cayley metric and that through Kendall metric and Potts model on the tree are three interesting examples of wavy probability distributions. It is easy to show these statements using [11]-[13]. (For the first two models (models for ranked data), see also [7]; for the last model (a model used in statistical physics and other fields), see also [6, Chapter 6].)

Below we give the main result of this section.

Theorem 3.1. Let $S = \langle r \rangle$. Let $\pi = (\pi_i)_{i \in S}$ be a wavy probability distribution (on S). Consider a Gibbs sampler in a generalized sense with state space S and transition matrix $P = P_1 P_2 \dots P_t$ ($t \ge 1$), where (we use the notation from the definition of wavy probability distribution)

$$(P_l)_{i+d_s^{(l,v)} \to \xi} = \begin{cases} \frac{\pi_{i+d_u^{(l,v)}}}{\sum\limits_{w \in \{0\} \cup D_{v,b_l}} \pi_{i+d_w^{(l,v)}}} & \text{if } \xi = i + d_u^{(l,v)} \text{ for some } u \in \{0\} \cup D_{v,b_l}, \\ 0 & \text{if } \xi \neq i + d_u^{(l,v)}, \ \forall u \in \{0\} \cup D_{v,b_l}, \end{cases}$$

 $\begin{array}{l} \forall l \in \langle t \rangle, \ \forall v \in \langle u_l \rangle, \ \forall i \in K_{(v-1)b_l+1}^{(l+1)}, \ \forall s \in \{0\} \cup D_{v,b_l}, \ \forall \xi \in S, \ setting \ d_0^{(l,v)} = 0, \\ \forall l \in \langle t \rangle, \ \forall v \in \langle u_l \rangle. \ Then \end{array}$

$$P = e'\pi$$

(therefore, the chain attains its stationarity at time 1, its stationary probability distribution being, obviously, π).

Proof. We have

$$(P_l)_{i+d_s^{(l,v)} \to \xi} = \begin{cases} \frac{1}{1+\sum\limits_{w \in D_{v,b_l}} \alpha_w^{(l,v)}} & \text{if } \xi = i, \\ \frac{\alpha_u^{(l,v)}}{1+\sum\limits_{w \in D_{v,b_l}} \alpha_w^{(l,v)}} & \text{if } \xi = i + d_u^{(l,v)} \text{ for some } u \in D_{v,b_l}, \\ 0 & \text{if } \xi \neq i + d_u^{(l,v)}, \ \forall u \in \{0\} \cup D_{v,b_l}, \end{cases}$$

 $\forall l \in \langle t \rangle, \forall v \in \langle u_l \rangle, \forall i \in K^{(l+1)}_{(v-1)b_l+1}, \forall s \in \{0\} \cup D_{v,b_l}, \forall \xi \in S. \text{ It follows that}$ $P_l \in G_{\Delta_l, \Delta_{l+1}}, \forall l \in \langle t \rangle$

(for Δ_l , $l \in \langle t+1 \rangle$, see the definition of wavy probability distribution). Since $P = P_1 P_2 \dots P_t$, by Theorem 1.1, P is a stable matrix. Consequently, $\exists \psi, \psi$ is a probability distribution on S, such that

$$P = e'\psi$$

On the other hand, by Theorem 1.2 we have

$$\pi P = \pi$$

Finally, we have

so,

$$\pi = \pi P = \pi e' \psi = \psi,$$
$$P = e' \pi.$$

Theorem 3.1 supports Conjecture 2.3. Each of articles [11]-[13] contains a special case of Theorem 3.1 (in Theorem 3.1, $S = \langle r \rangle$ for simplification ...). So, [11]-[13] support Conjecture 2.3 too.

Below, in Theorem 3.2 and Remarks 3.3 and 3.4, we give three important applications of Theorem 3.1.

Theorem 3.2. Let $S = \langle r \rangle$. Let $\pi = (\pi_i)_{i \in S}$ be a wavy probability distribution (on S). Suppose that

$$\pi_i = \frac{\nu_i}{Z}, \ \forall i \in S,$$

where

$$Z = \sum_{i \in S} \nu_i,$$

Z is the normalization constant ($\nu_i \in \mathbb{R}^+$, $\forall i \in S$, so, $Z \in \mathbb{R}^+$). Then (we use the notation from the definition of wavy probability distribution and Theorem 3.1)

$$Z = \nu_1 \prod_{l \in \langle t \rangle} \left(1 + \sum_{w \in D_{1,b_l}} \alpha_w^{(l,1)} \right)$$

Proof. We know that

$$\pi_1 = \frac{\nu_1}{Z}.$$

On the other hand, by Theorem 3.1, using the equation $P = e'\pi$, we can compute π_1 because $S = K_1^{(1)} \supset K_1^{(2)} \supset ... \supset K_1^{(t+1)} = \{1\}$, P_l is a block diagonal matrix, $\forall l \in \langle t \rangle - \{1\}$, and $P_l \in G_{\Delta_l, \Delta_{l+1}}, \forall l \in \langle t \rangle$ (moreover, P_l is a Δ_l -stable matrix on $\Delta_{l+1}, \forall l \in \langle t \rangle$); we obtain

$$\pi_1 = \frac{1}{\prod\limits_{l \in \langle t \rangle} \left(1 + \sum\limits_{w \in D_{1,b_l}} \alpha_w^{(l,1)} \right)}.$$

So,

$$Z = \nu_1 \prod_{l \in \langle t \rangle} \left(1 + \sum_{w \in D_{1,b_l}} \alpha_w^{(l,1)} \right).$$

Each of articles [11]-[13] contains a special case of Theorem 3.2 (in Theorem 3.2, $S = \langle r \rangle$ for simplification ...). Moreover, in [13], by Z (this computation way using Z is known, see, e.g., [1, p. 6]) it is computed the expectation for the Potts model on the tree.

Remark 3.3. When the transition probabilities from Theorem 3.1 can be computed, this theorem gives an exact Markovian method to sample from S according to the wavy probability distribution π . Since $P = P_1 P_2 \dots P_t$, this method has t steps and it is fast when the transition probabilities from Theorem 3.1 can be computed fast. See [11]-[13] for examples.

Remark 3.4. The important probabilities $P(K_v^{(l)})$, $l \in \langle t+1 \rangle$, $v \in \langle u_l \rangle$, can be computed for wavy probability distributions iteratively. Indeed, this can be done using Theorem 3.1 and Uniqueness Theorem from [10]. See [11]-[13] for examples.

The Gibbs sampler in a generalized sense is good, very good, at least for wavy probability distributions when its transition probabilities from Theorem 3.1 can be computed fast (no problem for the models from [11]-[13]). This is our final conclusion.

References

- J. Beck, Inevitable Randomness in Discrete Mathematics, American Mathematical Society, Providence, Rhode Island, 2009.
- [2] G. Casella, E.I. George, Explaining the Gibbs sampler, Amer. Statist. (1992) 46, 167–174.
- [3] L. Devroye, Non-Uniform Random Variate Generation, Springer-Verlag, New York, 1986; also available at http://cg.scs.carleton.ca/~luc/rnbookindex.html.
- [4] D. Gamerman, H.F. Lopes, Markov Chain Monte Carlo: Stochastic Simulation for Bayesian Interference, 2nd Edition, Chapman & Hall, Boca Raton, 2006.
- [5] M. Iosifescu, Finite Markov Processes and Their Applications, Wiley, Chichester & Ed. Tehnică, Bucharest, 1980; corrected republication by Dover, Mineola, N.Y., 2007.
- [6] N. Madras, *Lectures on Monte Carlo Methods*, American Mathematical Society, Providence, Rhode Island, 2002.
- [7] J.I. Marden, Analyzing and Modeling Rank Data, Chapman & Hall, London, 1995.
- [8] U. Păun, G_{Δ_1,Δ_2} in action, Rev. Roumaine Math. Pures Appl. (2010) 55, 387–406.
- [9] U. Păun, A hybrid Metropolis-Hastings chain, Rev. Roumaine Math. Pures Appl. (2011) 56, 207–228.
- [10] U. Păun, G method in action: from exact sampling to approximate one, Submitted.
- [11] U. Păun, G method in action: fast exact sampling from set of permutations of order n according to Mallows model through Cayley metric, Braz. J. Probab. Stat. (to appear).
- [12] U. Păun, G method in action: fast exact sampling from set of permutations of order n according to Mallows model through Kendall metric, *Submitted*.
- [13] U. Păun, G method in action: normalization constant, important probabilities, and fast exact sampling for Potts model on trees, Submitted.
- [14] E. Seneta, Non-negative Matrices and Markov Chains, 2nd Edition, Springer-Verlag, Berlin, 1981; revised printing, 2006.

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