Bayesian analysis for reversible Markov chains

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Abstract

We introduce a natural conjugate prior for the transition matrix of a reversible Markov chain. This allows estimation and testing. The prior arises from random walk with reinforcement in the same way the Dirichlet prior arises from Polya's urn. We give closed form normalizing constants, a simple method of simulation from the posterior and a characterization along the lines of W.E. Johnson's characterization of the Dirichlet prior.

Contents

1 Introduction

Modelling with Markov chains is an important part of time series analysis, genomics and many other applications. *Reversible* Markov chains are a mainstay of computational statistics through the Gibbs sampler, Metropolis algorithm and their many variants. Reversible chains are widely used natural models in physics and chemistry where reversibility (often called detailed balance) is a stochastic analog of the time reversibility of Newtonian mechanics.

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This paper develops tools for a Bayesian analysis of the transition probabilities, stationary distribution and future prediction of a reversible Markov chain. We observe $X_0 = v_0$, $X_1 = v_1$, $\ldots$, $X_n = v_n$ from a reversible Markov chain with a finite state space V. Neither the stationary distribution $\pi(v)$ nor the transition kernel $k(v, v')$ are assumed known. Reversibility entails $\pi(v)k(v, v') = \pi(v')k(v', v)$ for all $v, v' \in V$. We also assume we know which transitions are possible (for which $v, v' \in V$ is $k(v, v') > 0$).

In Section 2, we introduce a family of natural conjugate priors. These are defined via closed form densities and by a generalization of Polya's urn to random walk with reinforcement on a graph. The density gives normalizing constants needed for testing independence versus reversibility or reversibility versus a full Markovian specification. The random walk gives a simple method of simulating from the posterior (Section 4.5).

Properties of the prior are developed in Section 4. The family is closed under sampling (Proposition 4.1). Mixtures of our conjugates are shown to be dense (Proposition 4.5). A characterization of the priors via predictive properties of the posterior is given (Section 4.2).

Two practical examples are given in Section 5. Several simple hypotheses are tested for a data set arising from the DNA of the human HLA-B gene. Section 5 also contains remarks about statistical analysis for reversible chains.

2 A class of prior distributions

We observe $X_0 = v_0$, $X_1 = v_1$, $\ldots$,$X_n = v_n$ from a reversible Markov chain with a finite state space V and unknown transition kernel $k(\cdot, \cdot)$.

Let $G = (V, E)$ be the finite graph with vertex set V and edge set E defined as follows: $e = \{v, v'\} \in E$ (i.e. there is an edge between v and v') if and only if $k(v, v') > 0$. We assume that $k(v, v') > 0$ iff $k(v', v) > 0$. In particular, all edges of G are undirected and an edge is denoted by the set of its endpoints. For some vertices v, we may have $k(v, v) > 0$. Define the simplex

$$\Delta := \left\{ x = (x_e)_{e \in E} \in (0, 1]^E : \sum_{e \in E} x_e = 1 \right\}. \tag{2.1}$$

Recall that the distribution of a reversible Markov chain can be described by putting on the edge between v and v' the weight $x_{\{v,v'\}} := \pi(v)k(v, v') = \pi(v')k(v', v)$. If the weights are normalized so that $\sum_{e \in E} x_e = 1$, this is a unique way to describe the distribution of the Markov chain. A transition from v to v' is made with probability proportional to the weight $x_{\{v,v'\}}$. Denote by $Q_{v_0,x}$ the distribution of the Markov chain induced by the weights $x = (x_e)_{e \in E} \in \Delta$ which starts with probability 1 in v_0. Using this notation, our assumption says that the observed data comes from a distribution in the class

$$\mathcal{Q} := \{Q_{v_0,x} : v_0 \in V, x \in \Delta\}. \tag{2.2}$$

2.1 A minimal sufficient statistics

If the endpoints of an edge e agree, we call e a *loop*. Let

$$E_{\text{loop}} := \{e \in E : e \text{ is a loop}\}. \tag{2.3}$$

Let $\pi := (\pi_0, \pi_1, \ldots, \pi_n)$ be an admissible path in G. For $v \in V$ and $e \in E$, define

$$k_v(\pi) := |\{i \in \{1, 2, \ldots, n\} : (v, \pi_i) = (\pi_{i-1}, \pi_i)\}|, \text{ for } v \in V, \tag{2.4}$$

$$k_e(\pi) := \begin{cases} |\{i \in \{1, 2, \ldots, n\} : \{\pi_{i-1}, \pi_i\} = e\}| & \text{if } e \in E \setminus E_{\text{loop}}, \\ 2 \cdot |\{i \in \{1, 2, \ldots, n\} : \{\pi_{i-1}, \pi_i\} = e\}| & \text{if } e \in E_{\text{loop}}. \end{cases} \tag{2.5}$$

I.e. $k_v(\pi)$ equals the number of times the path π leaves vertex v; for an edge e which is not a loop, $k_e(\pi)$ is the number of traversals of e by π, and for a loop e, $k_e(\pi)$ is twice the number of traversals of e. Recall that the edges are undirected; hence $k_e(\pi)$ counts the traversals of e in *both* directions. Set

$$Z_n := (X_0, X_1, \ldots, X_n). \tag{2.6}$$

Proposition 2.1 *The vector of transition counts $(k_e(Z_n))_{e \in E}$ is a minimal sufficient statistic for the model $\mathcal{Q}_{v_0} := \{Q_{v_0,x} : x \in \Delta\}$.*

Proof. Let π be an admissible path in G. In order to prove that $(k_e(Z_n))_{e \in E}$ is a sufficient statistics, we need to show that

$$Q_{v_0,x}(Z_n = \pi | (k_e(Z_n))_{e \in E}) \tag{2.7}$$

does not depend on x. If π does not start in v_0, (2.7) equals zero. Otherwise, we have

$$Q_{v_0,x}(Z_n = \pi) = \frac{\prod_{e \in E} x_e^{k_e(\pi)}}{\prod_{v \in V} x_v^{k_v(\pi)}}. \tag{2.8}$$

It is not hard to see that $k_v(\pi)$ can be expressed in terms of the $k_e(\pi)$ and the first observation v_0. Hence, the $Q_{v_0,x}$-probability of π depends only on $k_e(\pi)$, $e \in E$, and v_0. Thus, (2.7) equals one divided by the number of admissible paths π' with starting point v_0 and $k_e(\pi') = k_e(Z_n)$ for all $e \in E$, which is independent of x.

Suppose $K := (k_e)_{e \in E}$ is not minimal. Then there exists a sufficient statistics K' which needs less information than K. Consequently, there exist two admissible paths π and π' starting in v_0 such that $K(\pi) \neq K(\pi')$ and $K'(\pi) = K'(\pi')$. Then

$$\frac{Q_{v_0,x}(Z_n = \pi | K'(Z_n) = K'(\pi))}{Q_{v_0,x}(Z_n = \pi' | K'(Z_n) = K'(\pi'))} = \frac{Q_{v_0,x}(Z_n = \pi)}{Q_{v_0,x}(Z_n = \pi')} = \prod_{e \in E} x_e^{k_e(\pi) - k_e(\pi')} \prod_{v \in V} x_v^{k_v(\pi') - k_v(\pi)}. \tag{2.9}$$

Since by assumption $(k_e(\pi))_{e \in E} \neq (k_e(\pi'))_{e \in E}$, the last quantity depends on x. This contradicts the fact that K' is a sufficient statistics. ■

2.2 Definition of the densities $\phi_{v_0,a}$

Our aim is to define a class of prior distributions in terms of measures on Δ. We prepare the definition with some notation.

For an edge e, denote the set of its endpoints by $\bar{e}$. Denote the cardinality of a set S by $|S|$. Recall the definition (2.3) of the set E_{loop}. Set

$$l := |V| + |E_{\text{loop}}| \quad \text{and} \quad m := |E|. \tag{2.10}$$

For $x = (x_e)_{e\in E} \in (0,\infty)^E$ and a vertex v, define x_v to be the sum of all components x_e with e incident to v:

$$x_v := \sum_{\{e : v \in \bar{e}\}} x_e. \tag{2.11}$$

In sums such as this the sum is over edges including loops. Similarly, define a_v for $a := (a_e)_{e\in E} \in (0,\infty)^E$.

There is a simple way to delineate a *generating set of cycles* of G. We call a maximal subgraph of G which contains all loops but no cycle a *spanning tree* of G. Choose a spanning tree T. Each edge $e \in E \setminus E_{\text{loop}}$ which is not in T forms a cycle c_e when added to T. (By definition, a loop is never a cycle and never contained in a cycle.) There are $m - l + 1$ such cycles and we enumerate them arbitrarily: $c_1, \ldots, c_{m-l+1}$. This set of cycles forms an additive basis for the homology H_1 and also serves for our purposes. In general, the first Betti number β_1 is the dimension of H_1. For the complete graph, $\beta_1(K_n) = \binom{n-1}{2}$. Further details can be found in Giblin ([Gib81], Section 1.16). In Section 3.4, we show how such a basis of cycles can be obtained for the complete graph.

Orient the cycles $c_1, \ldots, c_{m-l+1}$ and all edges $e \in E$ in an arbitrary way. For every $x \in \Delta$, define a matrix $A(x) = (A_{i,j}(x))_{1\le i,j\le m-l+1}$ by

$$A_{i,i}(x) = \sum_{e\in c_i} \frac{1}{x_e}, \quad A_{i,j}(x) = \sum_{e\in c_i\cap c_j} \pm\frac{1}{x_e} \text{ for } i \ne j, \tag{2.12}$$

where the signs in the last sum are chosen to be $+1$ or -1 depending on whether the edge e has in c_i and c_j the same orientation or not.

Definition 2.2 *For all $v_0 \in V$ and $a := (a_e)_{e\in E} \in (0,\infty)^E$, define*

$$\phi_{v_0,a}(x) := Z_{v_0,a}^{-1} \frac{\prod_{e\in E\setminus E_{\text{loop}}} x_e^{a_e - \frac{1}{2}} \prod_{e\in E_{\text{loop}}} x_e^{\frac{a_e}{2}-1}}{x_{v_0}^{\frac{a_{v_0}}{2}} \prod_{v\in V\setminus\{v_0\}} x_v^{\frac{a_v+1}{2}}} \sqrt{\det(A(x))} \tag{2.13}$$

($x := (x_e)_{e\in E} \in \Delta$) with

$$Z_{v_0,a} := \frac{\prod_{e\in E}\Gamma(a_e)}{\Gamma(\frac{a_{v_0}}{2}) \prod_{v\in V\setminus\{v_0\}} \Gamma(\frac{a_v+1}{2}) \prod_{e\in E_{\text{loop}}} \Gamma(\frac{a_e+1}{2})} \cdot \frac{(m-1)!\pi^{\frac{l-1}{2}}}{2^{1-l+\sum_{e\in E} a_e}}. \tag{2.14}$$

The definition of $\phi_{v_0,a}$ does *not* depend on the choice of the cycles c_i used in the definition of $A(x)$. Let us explain why: Let $\mathcal{T}$ denote the set of all spanning trees of G. Then

$$\det A(x) = \sum_{T\in\mathcal{T}} \prod_{e\notin E(T)} \frac{1}{x_e}. \tag{2.15}$$

Clearly, the right-hand side of (2.15) does not depend on the choice of the cycles c_i.

The identity (2.15) is proved for graphs without loops in [Mau76] (page 145, theorem 3'). By definition, $A(x)$ does not depend on x_e, $e \in E_{\text{loop}}$. Furthermore, since every spanning tree contains all loops, the right-hand side of (2.15) does not depend on x_e, $e \in E_{\text{loop}}$ either. In particular, both sides of (2.15) are the same for G and the graph obtained from G by removing all loops; hence they are equal.

2.3 Random walk with reinforcement

Let σ denote the Lebesgue measure on Δ, normalized such that $\sigma(\Delta) = 1$. The measures $\phi_{v_0,a}d\sigma$ on Δ arise in the study of edge-reinforced random walk, as was observed by Coppersmith and Diaconis (see [Dia88]). Let us explain this connection: The edges of G are given strictly positive weights; at time 0 edge e has weight $a_e > 0$. Edge-reinforced random walk on G with starting point v_0 is defined as follows: The process starts at v_0 at time 0. In each step, the random walker traverses an edge with probability proportional to its weight. Each time an edge $e \in E \setminus E_{\text{loop}}$ is traversed, its weight is increased by 1. Each time a loop $e \in E_{\text{loop}}$ is traversed, its weight is increased by 2.

Denote the set of non-negative integers by $\mathbb{N}_0$. Let Ω be the set of all $(v_i)_{i\in\mathbb{N}_0} \in V^{\mathbb{N}_0}$ such that $\{v_i, v_{i+1}\} \in E$ for all $i \in \mathbb{N}_0$. Let $X_n : V^{\mathbb{N}_0} \to V$ denote the projection onto the nth coordinate. Recall that $Z_n = (X_0, X_1, \ldots, X_n)$. Denote by $P_{v_0,a}$ the distribution on Ω of an edge-reinforced random walk with starting point v_0 and initial edge weights $a = (a_e)_{e\in E}$.

Let $\alpha_e(Z_n) := k_e(Z_n)/n$ be the proportion of traversals of edge e up to time n. It was observed by Coppersmith and Diaconis that $\alpha(Z_n) := (\alpha_e(Z_n))_{e\in E}$ converges almost surely to a random variable with distribution $\phi_{v_0,a}d\sigma$ (see [Dia88] and also [KR00]). In particular, $\phi_{v_0,a}d\sigma$ is a probability measure on Δ. This fact is not at all obvious from the definition of $\phi_{v_0,a}$.

It turns out that edge-reinforced random walk on G is a mixture of reversible Markov chains, where the mixing measure described as a measure on edge weights $(x_e)_{e\in E}$ is given by $\phi_{v_0,a}d\sigma$. This is made precise by the following theorem:

Theorem 2.3 *Let $(X_n)_{n\in\mathbb{N}_0}$ be edge-reinforced random walk with initial weights $a = (a_e)_{e\in E}$ starting at v_0, and let $Z_n = (X_0, X_1, \ldots, X_n)$. For any admissible path $\pi = (v_0, \ldots, v_n)$, the following holds:*

$$P_{v_0,a}(Z_n = \pi) = \int_\Delta \prod_{i=1}^n \frac{x_{\{v_{i-1},v_i\}}}{x_{v_{i-1}}} \phi_{v_0,a}(x)\, d\sigma(x); \tag{2.16}$$

here $x := (x_e)_{e\in E}$. Hence, if $\mathbb{P}_{v_0,a}$ is the mixture of Markov chains where the mixing measure, described as a measure on edge weights $(x_e)_{e\in E}$, is given by $\phi_{v_0,a}d\sigma$, then

$$\boxed{P_{v_0,a} = \mathbb{P}_{v_0,a}.} \tag{2.17}$$

Proof. If G has no loops, then the claim is true by Theorem 3.1 of [Rol03].

Let G be a graph with loops. Define a graph $G' := (V', E')$ as follows: Replace every loop of G by an edge of degree 1 incident to the same vertex (see Figure 1). More precisely, for all $e \in E_{\text{loop}}$, let $v(e)$ be the vertex e is incident to and let $v'(e)$ be an additional vertex, different from all the others. Then, set $g(e) := \{v(e), v'(e)\}$ and

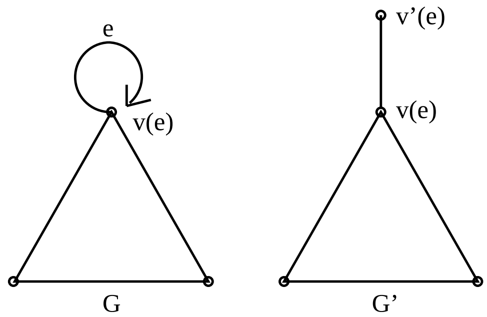
$$V' := V \cup \{v'(e) : e \in E_{\text{loop}}\}, \tag{2.18}$$
$$E' := [E \setminus E_{\text{loop}}] \cup \{g(e) : e \in E_{\text{loop}}\}. \tag{2.19}$$

The graph G' has no loops and the claim of the theorem is true for G'.

Let $P'_{v_0,b}$ be the distribution of a reinforced random walk on G' starting at v_0 with initial weights $b = (b_{e'})_{e'\in E'}$ defined by

$$b_{e'} := \begin{cases} a_{e'} & \text{if } e' \in E \setminus E_{\text{loop}} \\ a_e & \text{if } e' = g(e) \text{ for some } e \in E_{\text{loop}}. \end{cases} \tag{2.20}$$

Figure 1: Transformation of loops



Any finite admissible path $\pi = (\pi_0 = v_0, \pi_1, \ldots, \pi_n)$ in G can be mapped to an admissible path $\pi' = (\pi'_0 = v_0, \pi'_1, \ldots, \pi'_{n'})$ in G' by mapping every traversal of a loop $e \in E_{\text{loop}}$ in π to a traversal of $(v(e), v'(e), v(e))$ in π' (i.e. a traversal of the edge $g(e)$ back and forth in π'). The probability that the reinforced random walk on G traverses π agrees with the probability that the reinforced random walk on G' traverses π'. (Note that for G and G' the following is true: Between any two successive visits to $v(e)$, the sum of the weights of all edges incident to $v(e)$ increases by 2.) Since the claim of the theorem is true for G', it follows that

$$P_{v_0,a}(Z_n = \pi) = P'_{v_0,b}(Z_{n'} = \pi') = \int_\Delta \prod_{i=1}^{n'} \frac{x_{\{\pi'_{i-1},\pi'_i\}}}{x_{\pi'_{i-1}}} \phi'_{v_0,b}(x)\, d\sigma(x), \tag{2.21}$$

where $\phi'_{v_0,b}$ denotes the density corresponding to G', starting point v_0, and initial weights b. We claim that the right-hand side of (2.21) equals

$$\int_\Delta \prod_{i=1}^{n} \frac{x_{\{\pi_{i-1},\pi_i\}}}{x_{\pi_{i-1}}} \phi_{v_0,a}(x)\, d\sigma(x). \tag{2.22}$$

Note that a traversal of $e \in E_{\text{loop}}$ contributes $x_e/x_{v(e)}$ to the integrand in (2.22), whereas a traversal of $(v(e), v'(e), v(e))$ contributes $x_{g(e)}/x_{v(e)}$ to the integrand in (2.21). Furthermore, $e \in E_{\text{loop}}$ contributes

$$\frac{\Gamma\left(\frac{a_e+1}{2}\right)}{\Gamma(a_e)} \cdot 2^{a_e} \cdot (x_e)^{\frac{a_e}{2}-1} \tag{2.23}$$

to $\phi_{v_0,a}$, whereas the contribution of the edge $g(e)$ and the vertex $v'(e)$ to the density $\phi'_{v_0,b}$ equals

$$\begin{aligned} \frac{\Gamma\left(\frac{a_{v'(e)}+1}{2}\right)}{\Gamma(a_e)} \cdot 2^{a_e} \cdot \frac{(x_{g(e)})^{a_e-\frac{1}{2}}}{(x_{v'(e)})^{\frac{a_{v'(e)}+1}{2}}} &= \frac{\Gamma\left(\frac{a_e+1}{2}\right)}{\Gamma(a_e)} \cdot 2^{a_e} \cdot \frac{(x_{g(e)})^{a_e-\frac{1}{2}}}{(x_{g(e)})^{\frac{a_e+1}{2}}} \\ &= \frac{\Gamma\left(\frac{a_e+1}{2}\right)}{\Gamma(a_e)} \cdot 2^{a_e} \cdot (x_{g(e)})^{\frac{a_e}{2}-1}. \end{aligned} \tag{2.24}$$

Finally, $|V| + |E_{\text{loop}}| = |V'|$ and $|E| = |E'|$. Consequently, the expression in (2.22) agrees with the right-hand side of (2.21) and the claim follows. ■

Definition 2.4 *Let* $\mathcal{D} := \left\{\mathbb{P}_{v_0,a} : v_0 \in V, a = (a_e)_{e\in E} \in (0,\infty)^E\right\}$ *with* $\mathbb{P}_{v_0,a}$ *as in Theorem 2.3.*

We will prove in Section 4.2 that $\mathcal{D}$ is a natural family of prior distributions for reversible Markov chains.

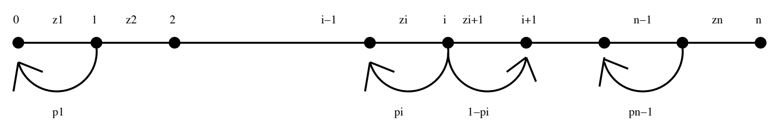
3 The density $\phi_{v_0,a}$ for special graphs

In this section, we write down the densities $\phi_{v_0,a}$ for some special graphs.

3.1 The line graph (Birth and death chains)

Consider the line graph with vertex set $V = \{i : 0 \le i \le n\}$ and edge set $E = \{\{i, i+1\} : 0 \le i \le n-1\}$. Given $a = (a_{\{i-1,i\}})_{1\le i\le n}$, let $b_i := a_{\{i-1,i\}}$. The variables in the simplex Δ are denoted $z_i := x_{\{i-1,i\}}$.

Figure 2: The line graph



Recall that the density of the beta distribution with parameters $b_1, b_2 > 0$ is given by

$$\beta[b_1, b_2](p) := \frac{\Gamma(b_1+b_2)}{\Gamma(b_1)\Gamma(b_2)} p^{b_1-1}(1-p)^{b_2-1} \quad (0 < p < 1). \tag{3.1}$$

Set

$$p_i = \frac{z_i}{z_i + z_{i+1}}, \qquad 1 \le i \le n-1, \tag{3.2}$$

and $p := (p_i)_{1\le i\le n-1}$. Clearly p_i is the probability that the Markov chain with edge weights z_i makes a transition to $i-1$ given it is at i. If we make the change of variables (3.2) in the density $\phi_{v_0,a}$, then we obtain the transformed density $\widetilde{\phi}_{v_0,a}$ given by

$$\widetilde{\phi}_{0,a}(p) = \begin{cases} \displaystyle\prod_{i=1}^{n-1} \beta\left[\frac{b_i+1}{2}, \frac{b_{i+1}}{2}\right](p_i) \quad \text{if } v_0 = 0, \\ \displaystyle\left[\prod_{i=1}^{v_0-1} \beta\left[\frac{b_i}{2}, \frac{b_{i+1}+1}{2}\right](p_i)\right] \beta\left[\frac{b_{v_0}}{2}, \frac{b_{v_0}}{2}\right](p_{v_0}) \left[\prod_{i=v_0+1}^{n-1} \beta\left[\frac{b_i+1}{2}, \frac{b_{i+1}}{2}\right](p_i)\right] \\ \text{if } v_0 \in \{1, 2, \ldots, n-1\}, \\ \displaystyle\prod_{i=1}^{n-1} \beta\left[\frac{b_i}{2}, \frac{b_{i+1}+1}{2}\right](p_i) \quad \text{if } v_0 = n; \end{cases} \tag{3.3}$$

here the empty product is defined to be 1.

With the change of variables (3.2), the conjugate prior can be described as a product of independent beta variables with carefully linked parameters. If loops are allowed, the edge weights are independent Dirichlet by a similar argument (see Section 3.2). The next example contains a generalization.

3.2 Trees with loops

Recall that the density of the Dirichlet distribution with parameters $b_i > 0$, $1 \le i \le d$ is given by

$$D[b_i; 1 \le i \le d](p_i; 1 \le i \le d) := \frac{\Gamma\left(\sum_{i=1}^{d} b_i\right)}{\prod_{i=1}^{d} \Gamma(b_i)} \prod_{i=1}^{d} p_i^{b_i - 1}, \quad \left(p_i \ge 0, \sum_{i=1}^{d} p_i = 1\right). \tag{3.4}$$

Let $T = (V, E)$ be a tree. Suppose that there is a loop attached to every vertex, i.e. $\{v\} \in E$ for all $v \in V$. Let $v_0 \in V$. For every $v \in V \setminus \{v_0\}$ there exists a unique shortest path from v_0 to v. Let $e(v)$ be the unique edge incident to v which is traversed by the shortest path from v_0 to v. Let $E_v := \{e \in E : v \in \bar{e}\}$ be the set of all edges incident to v. Set

$$p_e := \frac{x_e}{x_v} \quad \text{for } v \in V,\ e \in E_v, \tag{3.5}$$

$p := (p_e)_{e \in E}$, and $\vec{p}_v := (p_e)_{e \in E_v}$. If we make the change of variables (3.5) in the density $\phi_{v_0,a}$, the transformed density $\widetilde{\phi}_{v_0,a}$ is given by

$$\widetilde{\phi}_{v_0,a}(p) = D\left[\frac{a_e}{2}, e \in E_{v_0}\right](\vec{p}_{v_0}) \prod_{v \in V \setminus \{v_0\}} D\left[\frac{a_{e(v)} + 1}{2}, \frac{a_e}{2}, e \in E_v \setminus \{e(v)\}\right](\vec{p}_v). \tag{3.6}$$

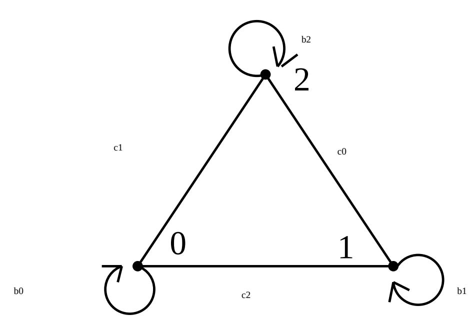
Thus again, in the reparametrization (3.5), the conjugate prior is seen as a product of independent choices of edge weights. This is not true in the following example.

The fact that the density $\phi_{v_0,a}$ for a tree has this particular form, was first observed by Pemantle [Pem88].

3.3 The triangle

Consider the triangle with loops attached to all vertices. Let the vertex set be $V = \{0, 1, 2\}$ and the edge set $E = \{\{0\}, \{1\}, \{2\}, \{0,1\}, \{0,2\}, \{1,2\}\}$ (see Figure 3). Let b_i be the initial weight of the loop at vertex i and let c_i be the initial weight of the edge opposite of vertex i. Similarly, let $y_i := x_{\{i\}}$ and let $z_0 := x_{\{1,2\}}$, $z_1 := x_{\{0,2\}}$, $z_2 := x_{\{0,1\}}$.

Figure 3: The triangle with loops



The density $\phi_{0,a}$ for $a = (b_0, b_1, b_2, c_0, c_1, c_2)$ is given by

$$\phi_{0,a}(y_0, y_1, y_2, z_0, z_1, z_2) = Z_{0,a}^{-1} \cdot \frac{y_0^{\frac{b_0}{2}-1} y_1^{\frac{b_1}{2}-1} y_2^{\frac{b_2}{2}-1} z_0^{c_0-1} z_1^{c_1-1} z_2^{c_2-1} \sqrt{z_0 z_1 + z_0 z_2 + z_1 z_2}}{(z_1+z_2)^{\frac{b_0+c_1+c_2}{2}} (z_0+z_2)^{\frac{b_1+c_0+c_2+1}{2}} (z_0+z_1)^{\frac{b_2+c_0+c_1+1}{2}}} \quad (3.7)$$

with

$$Z_{0,a} = \frac{\Gamma(c_0)\Gamma(c_1)\Gamma(c_2)\Gamma\left(\frac{b_0}{2}\right)\Gamma\left(\frac{b_1}{2}\right)\Gamma\left(\frac{b_2}{2}\right)}{\Gamma\left(\frac{b_0+c_1+c_2}{2}\right)\Gamma\left(\frac{b_1+c_0+c_2+1}{2}\right)\Gamma\left(\frac{b_2+c_0+c_1+1}{2}\right)} \cdot \frac{480\pi}{2^{c_0+c_1+c_2}}. \quad (3.8)$$

To calculate $Z_{0,a}$ from (2.14), use the identity

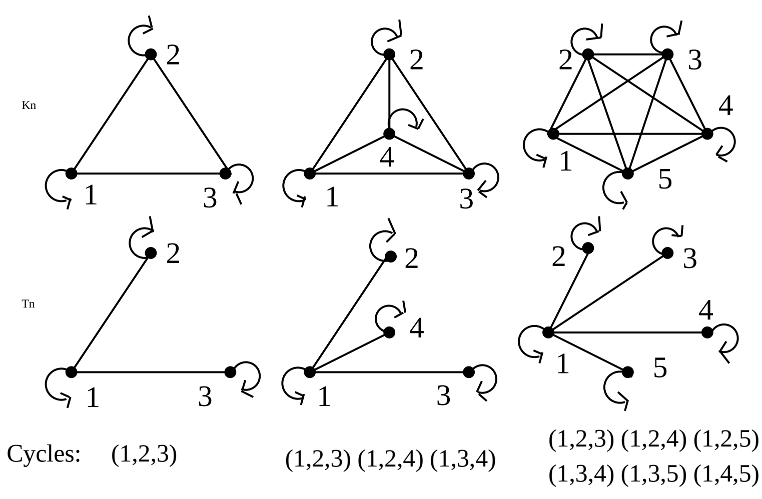
$$\frac{\Gamma(b_i)}{2^{b_i}\Gamma\left(\frac{b_i+1}{2}\right)} = \frac{\Gamma\left(\frac{b_i}{2}\right)}{2\sqrt{\pi}} \qquad (i = 0, 1, 2). \quad (3.9)$$

For the triangle without loops, a derivation of the formula for the density $\phi_{0,a}$ can be found e.g. in [Kea90].

3.4 The complete graph

Perhaps the most important example is where all transitions are possible. This involves the complete graph K_n on n vertices with loops attached to all vertices. Let $V = \{1, 2, 3, \ldots, n\}$. Let T_n be the spanning tree with edges $\{1, i\}$ and loops $\{i\}$, $1 \leq i \leq n$. This spanning tree induces the basis of cycles given by all triangles $(1, i, j)$, $2 \leq i < j \leq n$. Figure 4 shows K_3, K_4, and K_5 together with T_3, T_4, and T_5.

Figure 4: The complete graphs K_3, K_4, K_5 with loops together with a spanning tree



We remark that a different basis of cycles is given by $(i, i+1, j)$ for $1 \leq i < j+1 \leq n$. This may be proved by induction using the Mayer-Vietoris decomposition theorem based on K_{n-1} and a point.

Let $a = \left(a_{\{i,j\}}\right)_{1\le i,j\le n}$ be given. For K_n, set $b_i := a_{\{i\}}$, $a_i = \sum_{j=1}^n a_{\{i,j\}}$, and $b := \sum_{1\le i,j\le n} a_{\{i,j\}}$. The variables of the simplex are $x = (x_{\{i,j\}})_{1\le i,j\le n}$. Abbreviating $y_i := x_{\{i\}}$ and $x_i = \sum_{j=1}^n x_{\{i,j\}}$, the density $\phi_{1,a}$ is given by

$$\phi_{1,a}(x) = Z_{1,a}^{-1} \cdot \frac{\prod\limits_{1\le i<j\le n} x_{\{i,j\}}^{a_{\{i,j\}}-\frac{1}{2}} \prod\limits_{i=1}^n y_i^{\frac{b_i}{2}-1}}{x_1^{\frac{a_1}{2}} \prod\limits_{i=2}^n x_i^{\frac{a_i+1}{2}}} \sqrt{\det(A_n(x))} \tag{3.10}$$

with $A_n(x)$ defined in (2.12) and

$$Z_{1,a} = \frac{\prod\limits_{1\le i,j\le n} \Gamma\left(a_{\{i,j\}}\right)}{\Gamma\left(\frac{a_1}{2}\right) \prod\limits_{i=2}^n \Gamma\left(\frac{a_i+1}{2}\right) \prod\limits_{i=1}^n \Gamma\left(\frac{b_i+1}{2}\right)} \cdot \frac{\left(\frac{n(n+1)}{2}-1\right)! \pi^{n-\frac{1}{2}}}{2^{1-2n+b}}. \tag{3.11}$$

4 Properties of the family of priors

4.1 Closure under sampling

Recall the definition (2.5) of $k_e(\pi)$ and recall that $Z_n = (X_0, \dots, X_n)$.

Proposition 4.1 *Under the prior distribution $\mathbb{P}_{v_0,a}$ with observations $X_0 = v_0$, $X_1 = v_1$, ..., $X_n = v_n$, the posterior is given by $\mathbb{P}_{v_n,(a_e+k_e(Z_n))_{e\in E}}$. In particular, the family $\mathcal{D}$ is closed under sampling.*

Proof. Suppose we are given $n+1$ observations $\pi = (\pi_0, \pi_1, \dots, \pi_n)$ sampled from $\mathbb{P}_{v_0,a}$. Then $\pi_0 = v_0$. We claim that the posterior is given by $\mathbb{P}_{\pi_n,(a_e+k_e(\pi))_{e\in E}}$. Recall that the posterior distribution is the $\mathbb{P}_{v_0,a}$-distribution of $\{X_{n+k}\}_{k\ge 0}$ given $Z_n = \pi$. By Theorem 2.3, $\mathbb{P}_{v_0,a} = P_{v_0,a}$. The $P_{v_0,a}$-distribution of $\{X_{n+k}\}_{k\ge 0}$ given $Z_n = \pi$ is the distribution of an edge-reinforced random walk starting at the vertex π_n with initial values $a_e + k_e(\pi)$. Using the identity (2.17) from Theorem 2.3 again, it follows that the posterior equals $\mathbb{P}_{\pi_n,(a_e+k_e(\pi))_{e\in E}}$, which is an element of $\mathcal{D}$. ■

4.2 Uniqueness

In this section, we give a characterization of our priors along the lines of W.E. Johnsons characterization of the Dirichlet prior. See Zabell [Zab82] for history and Zabell [Zab95] for a version for non-reversible chains. The closely related topic of de Finetti's theorem for Markov chains is developed by Diaconis and Freedman ([Fre62], [DF80]). See also Regazzini et al. [FLPR02].

Definition 4.2 *Two finite admissible paths π and π' are called* equivalent *if they have the same starting point and satisfy $k_e(\pi) = k_e(\pi')$ for all $e \in E$. We define P to be* partially exchangeable *if $P(Z_n = \pi) = P(Z_n = \pi')$ for any equivalent paths π and π' of length n.*

For $n \in \mathbb{N}_0$ and $v \in V$, define

$$k_n(v) \quad := \quad |\{i \in \{0, 1, \dots, n\} : X_i = v\}|. \tag{4.1}$$

It seems natural to take a class $\mathcal{P}$ of distributions for Z_n with the following properties:

P 1 *For all* $P \in \mathcal{P}$ *there exists* $v_0 \in V$ *such that* $P(X_0 = v_0) = 1$.

P 2 *For all* $P \in \mathcal{P}$, v_0 *as in P 1, and any admissible path* π *of length* $n \geq 1$ *starting at* v_0, *we have* $P(Z_n = \pi) > 0$.

P 3 *Every* $P \in \mathcal{P}$ *is partially exchangeable.*

P 4 *For all* $P \in \mathcal{P}$, $v \in V$, *and* $e \in E$ *there exists a function* $f_{P,v,e}$ *taking values in* $[0,1]$ *such that for all* $n \geq 0$

$$P(X_{n+1} = v|Z_n) = f_{P,X_n,\{X_n,v\}}(k_n(X_n), k_{\{X_n,v\}}(Z_n)).$$

The condition P 4 says that given $X_0, X_1, \ldots, X_n$, the probability that $X_{n+1} = v$ depends only on the following quantities: the observation X_n, the number of times X_n has been observed so far, the edge $\{X_n, v\}$, and the number of times transitions between X_n and v (and between v and X_n) have been observed so far.

We make the following assumptions on the graph G:

G 1 *For all* $v \in V$ *degree*$(v) \neq 2$.

G 2 *The graph* G *is* 2*-edge-connected, i.e. removing an edge does not make* G *disconnected.*

For example, a triangle with loops or the complete graph K_n, $n \geq 4$, with or without loops satisfies G 1 and G 2 while a path fails both G 1 and G 2.

Recall that $Q_{v_0,x}$ is the distribution of the reversible Markov chain starting in v_0, making a transition from v to v' with probability proportional to $x_{\{v,v'\}}$ whenever $\{v, v'\} \in E$.

Theorem 4.3 *Suppose the graph* G *satisfies G 1 and G 2.*

1. *The set* $\mathcal{D}$ *defined in Definition 2.4 satisfies P 1 – P 4.*
2. *On the other hand, if P 1 – P 4 are satisfied for a set* $\mathcal{P}$ *of probability distributions, then for all* $P \in \mathcal{P}$ *there exist* $v_0 \in V$ *and* $a \in (0,\infty)^E$ *such that either*

$$\begin{aligned} &P(X_{n+1} = v|Z_n, k_n(X_n) \geq 3) = \mathbb{P}_{v_0,a}(X_{n+1} = v|Z_n, k_n(X_n) \geq 3) \quad \text{for all } n \geq 0 \quad \text{or} \\ &P(X_{n+1} = v|Z_n, k_n(X_n) \geq 3) = Q_{v_0,a}(X_{n+1} = v|Z_n, k_n(X_n) \geq 3) \quad \text{for all } n \geq 0. \end{aligned} \tag{4.2}$$

The second part of the theorem states that either P and $\mathbb{P}_{v_0,a}$ or P and $Q_{v_0,a}$ essentially agree; only the conditional probabilities to leave from a state which has been visited at most twice could be different.

Proof of Theorem 4.3. It is straightforward to check that $\mathcal{D}$ has the properties P 1 – P 4. For the converse, let $P \in \mathcal{P}$. By P 3, P is partially exchangeable. Hence, if G has no loops, then Theorem 1.2 of [Rol03] implies that there exist $v_0 \in V$ and $a \in (0,\infty)^E$ such that either (4.2) holds or $P(X_{n+1} = v|Z_n, k_n(X_n) \geq 3) = P_{v_0,a}(X_{n+1} = v|Z_n, k_n(X_n) \geq 3)$ for all n. In this case, the claim follows from (2.17).

If G has loops, consider the graph G' defined in the proof of Theorem 2.3 and the induced process $X' := (X'_n)_{n\in\mathbb{N}_0}$ on G' with reflection at the vertices $v'(e)$, $e \in E_{\text{loop}}$. The process X' satisfies P 1 – P 4. Hence, the claim holds for X' and consequently for $(X_n)_{n\in\mathbb{N}_0}$. ■

Remark 4.4 *The preceding theorem holds under the assumption that the graph G is 2-edge-connected (G 2). If G is not 2-edge-connected, a similar statement can be proved for a different class of priors: One replaces the class $\mathcal{D}$ defined in Definition 2.4 by the mixing measures of so called* modified edge-reinforced random walk*; for the definition of this process see Definition 2.1 of [Rol03]. A uniqueness statement similar to Theorem 4.3 follows from Theorem 2.1 of [Rol03].*

4.3 The priors are dense

As shown by Dalal and Hall [DH83] and Diaconis and Ylvisaker [DY85] for classical exponential families, mixtures of conjugate priors are dense in the space of all priors. This holds for reversible Markov chains.

Proposition 4.5 *The set of convex combinations of priors in $\mathcal{D}$ is weak-star dense in the set of all prior distributions on reversible Markov chains on G.*

Proof. For an infinite admissible path $\pi = (\pi_0, \pi_1, \pi_2, \dots)$ in G, define $\alpha(\pi) := (\alpha_e(\pi))_{e\in E}$ by $\alpha_e(\pi) := \lim_{n\to\infty} k_e(\pi_0, \pi_1, \dots, \pi_n)/n$ to be the limiting fraction of crossings of the edge e by the path π. Let $Z_\infty := (Z_0, Z_1, Z_2, \dots)$. Note that $\alpha(Z_\infty)$ is defined $\mathbb{P}_{v_0,a}$-a.s. Define τ_n to be the n^{th} return time to v_0. Since G is finite, $\tau_n < \infty$ $\mathbb{P}_{v_0,a}$-a.s. for all $n \in \mathbb{N}$ and all $a \in (0,\infty)^E$.

Let $f : \Delta \to \mathbb{R}$ be bounded and continuous. Denote the expectation with respect to $\mathbb{P}_{v_0,a}$ by $\mathbb{E}_{v_0,a}$. Since $X_{\tau_n} = v_0$, Proposition 4.1 implies that $\mathbb{P}_{v_0,(a_e+k_e(Z_{\tau_n}))_{e\in E}}(\cdot) = \mathbb{P}_{v_0,a}(\cdot|Z_{\tau_n})$. Hence,

$$\mathbb{E}_{v_0,(a_e+k_e(Z_{\tau_n}))_{e\in E}}[f(\alpha(Z_\infty))] = \mathbb{E}_{v_0,a}[f(\alpha(Z_\infty))|Z_{\tau_n}] := M_n. \tag{4.3}$$

Clearly, $(M_n)_{n\geq 0}$ is a bounded martingale. Hence, by the martingale convergence theorem,

$$\begin{aligned}\lim_{n\to\infty} \mathbb{E}_{v_0,(a_e+k_e(Z_{\tau_n}))_{e\in E}}[f(\alpha(Z_\infty))] &= \mathbb{E}_{v_0,a}[f(\alpha(Z_\infty))|Z_\infty] \\ &= f(\alpha(Z_\infty)) = \int f(\alpha(Z_\infty))\, d\delta_{\alpha(Z_\infty)} \end{aligned}\tag{4.4}$$

$\mathbb{P}_{v_0,a}$-a.s.; here δ_a denotes the point mass in a. Since Δ is compact, there is a countable dense subset of the set of bounded continuous functions on Δ. Hence, the above shows that for $\mathbb{P}_{v_0,a}$-almost all Z_∞,

$$\mathbb{P}_{v_0,(a_e+k_e(Z_{\tau_n}))_{e\in E}}(\alpha(Z_\infty) \in \cdot) \Rightarrow \delta_{\alpha(Z_\infty)}(\cdot) \quad \text{weakly as } n \to \infty. \tag{4.5}$$

The $\mathbb{P}_{v_0,a}$-distribution of $\alpha(Z_\infty)$ is absolutely continuous with respect to Lebesgue measure on Δ with the density $\phi_{v_0,a}$ which is strictly positive in the interior of Δ. Hence, for Lebesgue-almost all $a \in \Delta$ there is a sequence $a_n \in \Delta$ such that $\mathbb{P}_{v_0,a_n}(\alpha(Z_\infty) \in \cdot) \Rightarrow \delta_a(\cdot)$ weakly. By the Krein-Milman theorem, convex combinations of point masses are weak-star dense in the set of all measures on Δ. Using a standard argument it follows that the set of convex combinations of distributions of the form $\mathbb{P}_{v_0,a}(\alpha(Z_\infty) \in \cdot)$ is dense in the set of all probability measures on Δ. Consequently, the set of convex combinations of distributions of the form $\mathbb{P}_{v_0,a}$ is dense in the set of all prior distributions. ■

4.4 Computing some moments

For any edge $e_0 \in E$, we can calculate the probability that the mixture of Markov chains with mixing measure $\phi_{v_0,a} d\sigma$ traverses e_0 back and forth starting at an endpoint of e_0. This gives a closed form for certain moments of the prior $\mathbb{P}_{v_0,a}$.

Proposition 4.6 *For $e_0 \in E \setminus E_{\text{loop}}$ with endpoints v and v' we have*

$$\int_\Delta \frac{(x_{e_0})^2}{x_v x_{v'}} \phi_{v_0,a}(x) d\sigma(x) = \begin{cases} \dfrac{a_{e_0}(a_{e_0}+1)}{(a_v+1)(a_{v'}+1)} & \text{if } v_0 \notin \{v, v'\}, \\ \dfrac{a_{e_0}(a_{e_0}+1)}{a_v(a_{v'}+1)} & \text{if } v = v_0. \end{cases} \tag{4.6}$$

For a loop $e_0 \in E_{\text{loop}}$ incident to v we have

$$\int_\Delta \frac{x_{e_0}}{x_v} \phi_{v_0,a}(x) d\sigma(x) = \begin{cases} \dfrac{a_{e_0}}{a_v+1} & \text{if } v \neq v_0, \\ \dfrac{a_{e_0}}{a_v} & \text{if } v = v_0. \end{cases} \tag{4.7}$$

Proof. *Case $e_0 \in E \setminus E_{\text{loop}}$:* Suppose v_0 is an endpoint of e_0, say $v = v_0$. Then,

$$\int_\Delta \frac{(x_{e_0})^2}{x_v x_{v'}} \phi_{v_0,a}(x) d\sigma(x) = \mathbb{P}_{v_0,a}(X_0 = v_0, X_1 = v', X_2 = v_0); \tag{4.8}$$

this is the probability that the mixture of Markov chains traverses the edge e_0 back and forth starting at v_0. By (2.17), $\mathbb{P}_{v_0,a} = P_{v_0,a}$. Hence (4.8) equals the probability that an edge-reinforced random walk traverses e_0 back and forth, namely

$$P_{v_0,a}(X_0 = v_0, X_1 = v', X_2 = v_0) = \frac{a_{e_0}(a_{e_0}+1)}{a_v(a_{v'}+1)}. \tag{4.9}$$

Here we used that the sum of the weights of all edges incident to v' equals $a_{v'}+1$ after e_0 has been traversed once. This proves the claim in the case $v_0 \in \bar{e}_0$.

Suppose $v_0 \notin \bar{e}_0$. Define $b := (b_e)_{e \in E}$ by $b_{e_0} := a_{e_0} + 2$ and $b_e := a_e$ for $e \in E \setminus \{e_0\}$. Then, using the definition of $\phi_{v_0,a}$, we obtain

$$\frac{(x_{e_0})^2}{x_v x_{v'}} \phi_{v_0,a}(x) = \frac{Z_{v_0,b}}{Z_{v_0,a}} \phi_{v_0,b}(x) \qquad \text{for all } x \in \Delta. \tag{4.10}$$

Using the definition of the normalizing constants $Z_{v_0,a}$ and $Z_{v_0,b}$ and the identity $\Gamma(z+1) = z\Gamma(z)$, it follows that

$$\frac{Z_{v_0,b}}{Z_{v_0,a}} = \frac{\Gamma(\frac{a_v+1}{2})\Gamma(\frac{a_{v'}+1}{2})\Gamma(a_{e_0}+2)}{4\Gamma(\frac{a_v+3}{2})\Gamma(\frac{a_{v'}+3}{2})\Gamma(a_{e_0})} = \frac{a_{e_0}(a_{e_0}+1)}{(a_v+1)(a_{v'}+1)}. \tag{4.11}$$

Since $\int_\Delta \phi_{v_0,b}(x) d\sigma(x) = 1$, the claim follows by integrating both sides of (4.10) over Δ.
Case $e_0 \in E_{\text{loop}}$: The proof follows the same line as in the case $e_0 \notin E_{\text{loop}}$. Let $e_0 = \{v\}$ be incident to v. We prove only the case $v \neq v_0$. Defining b as above, (4.10) is valid with

$$\frac{Z_{v_0,b}}{Z_{v_0,a}} = \frac{\Gamma(\frac{a_v+1}{2})\Gamma(\frac{a_{e_0}+1}{2})\Gamma(a_{e_0}+2)}{4\Gamma(\frac{a_v+3}{2})\Gamma(\frac{a_{e_0}+3}{2})\Gamma(a_{e_0})} = \frac{a_{e_0}(a_{e_0}+1)}{(a_v+1)(a_{e_0}+1)} = \frac{a_{e_0}}{(a_v+1)}; \tag{4.12}$$

here we used again the identity $\Gamma(z+1) = z\Gamma(z)$. The claim follows. ■

Recall the definitions (2.4) and (2.5) of $k_v(\pi)$ and $k_e(\pi)$ for a finite admissible path π in G. Abbreviate $k_v := k_v(\pi)$, $k_e := k_e(\pi)$. For $x = (x_e)_{e\in E} \in \Delta$, denote by $Q_x(\pi)$ the probability that the reversible Markov chain with transition probabilities induced by the weights $(x_e)_{e\in E}$ on the edges traverses the path π. Note that if π is a *closed* path, i.e. if the starting and endpoint of π agree, then $Q_x(\pi)$ is independent of the starting point of π. The argument as in the proof of Proposition 4.6 gives

Proposition 4.7 *For any finite admissible path π starting at v_0, we have*

$$\int_\Delta Q_x(\pi)\phi_{v_0,a}(x)d\sigma(x) = \frac{\left[\prod_{e\in E\setminus E_{\mathrm{loop}}} \prod_{i=0}^{k_e-1}(a_e+i)\right]\left[\prod_{e\in E_{\mathrm{loop}}} \prod_{i=0}^{k_e/2-1}(a_e+2i)\right]}{\prod_{i=0}^{k_{v_0}-1}(a_{v_0}+2i) \prod_{v\in V\setminus\{v_0\}} \prod_{i=0}^{k_v-1}(a_v+1+2i)}. \tag{4.13}$$

For any finite admissible path π with the same starting and endpoint which avoids v_0, we have

$$\int_\Delta Q_x(\pi)\phi_{v_0,a}(x)d\sigma(x) = \frac{\left[\prod_{e\in E\setminus E_{\mathrm{loop}}} \prod_{i=0}^{k_e-1}(a_e+i)\right]\left[\prod_{e\in E_{\mathrm{loop}}} \prod_{i=0}^{k_e/2-1}(a_e+2i)\right]}{\prod_{v\in V} \prod_{i=0}^{k_v-1}(a_v+1+2i)}. \tag{4.14}$$

Here the empty product is defined to be 1.

If π is a closed path, we call $Q_x(\pi)$ a *cycle probability.* The transition probabilities of a Markov chain with finite state space V that visits every state with probability 1 are completely determined by all its cycle probabilities (see e.g. [Fre62], Corollary on page 116).

4.5 Simulating from the posterior

In this subsection, we show how the posterior distribution of the unknown stationary distribution for the underlying Markov chain can be simulated using reinforced random walks.

Suppose our posterior distribution is $\mathbb{P}_{v_0,a} = \phi_{v_0,a}d\sigma$. Let $X^{(i)} := (X_n^{(i)})_{n\geq 0}$, $i \geq 1$, be independent reinforced random walks with the same initial edge weights $a = (a_e)_{e\in E}$. Let $Z_n^{(i)} := (X_0^{(i)}, X_1^{(i)}, \dots, X_n^{(i)})$ and recall that $k_e(Z_n^{(i)})$ equals the number of traversals of edge e by the process $X^{(i)}$ up to time n.

Proposition 4.8 *For any interval $I \subseteq \mathbb{R}$ and all $e \in E$, we have*

$$\lim_{n\to\infty}\lim_{m\to\infty}\frac{1}{m}\left|\left\{i\leq m : \frac{k_e(Z_n^{(i)})}{n}\in I\right\}\right| = \mathbb{P}_{v_0,a}(x_e\in I). \tag{4.15}$$

Proof. For every n, the random variables $k_e(Z_n^{(i)})/n$, $i \geq 1$, are i.i.d. Hence, by the Glivenko-Cantelli theorem, for all $x \in \mathbb{R}$,

$$\lim_{m\to\infty}\frac{1}{m}\left|\left\{i\leq m : \frac{k_e(Z_n^{(i)})}{n}\leq x\right\}\right| = P_{v_0,a}\left(\frac{k_e(Z_n)}{n}\leq x\right) = \mathbb{P}_{v_0,a}\left(\frac{k_e(Z_n)}{n}\leq x\right). \tag{4.16}$$

For the last equality, we used (2.17). Since $\mathbb{P}_{v_0,a}$ is a mixture of Markov chains, $k_e(Z_n)/n$ converges to the normalized weight of the edge e $\mathbb{P}_{v_0,a}$-a.s. and hence weakly. Since the $\mathbb{P}_{v_0,a}$-distribution of x_e is continuous,

$$\lim_{n\to\infty} \mathbb{P}_{v_0,a}\left(\frac{k_e(Z_n)}{n} \leq x\right) = \mathbb{P}_{v_0,a}(x_e \leq x), \tag{4.17}$$

and the claim follows. ■

Proposition 4.9 *For all $e \in E$,*

$$\lim_{n\to\infty} \int \frac{k_e(Z_n)}{n} dP_{v_0,a} = \int x_e \, d\mathbb{P}_{v_0,a}. \tag{4.18}$$

Proof. By (2.17), $P_{v_0,a} = \mathbb{P}_{v_0,a}$. Since the proportion $k_n(e)/n$ converges $\mathbb{P}_{v_0,a}$-a.s. to the normalized weight of the edge e, the claim follows from the dominated convergence theorem. ■

Remark 4.10 *The Markov chain with distribution induced by the edge weights $(x_e)_{e\in E} \in \Delta$ has the stationary distribution $\pi(v) = \frac{x_v}{2} = \frac{1}{2}\sum_{e\in E_v} x_e$. Thus, Propositions 4.8 and 4.9 allow simulation of the $\mathbb{P}_{v_0,a}$-distribution and the mean of $\pi(v)$.*

5 Applications

Reversibility can serve as a natural intermediate beween independence and fully non-parametric Markovian dependence. On $|V|$ states, with no restrictions the number of free parameters is $|V| - 1$ with independence, $|V|(|V| - 1)$ for full Markov and $\frac{|V|(|V|-1)}{2} - 1$ for reversibility. As Table 1 below indicates, these numbers vary widely for $|V|$ large.

Table 1: Degrees of freedom for independent, reversible, and full Markov specification

$\lvert V\rvert$	3	4	5	10	20	50	100	1000
independent $\lvert V\rvert - 1$	2	3	4	9	19	49	99	999
reversible $\lvert V\rvert(\lvert V\rvert - 1)/2 - 1$	2	5	9	44	189	1224	4949	499499
full Markov $\lvert V\rvert(\lvert V\rvert - 1)$	6	12	20	90	380	2450	9900	999000

In this section, we illustrate the use of our priors for testing a variety of simple hypotheses. As a first numerical illustration, we use a small data set (Table 2) generated by asking a student to generate a random sequence of length 100 with the symbols "red (R), white (W), blue (B)". The data is listed in order left to right and from top to bottom. It is well known that human generated sequences of this type fail simple tests of randomness (Bar-Hillel and Wagenaar [BHW91]). This example is simply illustrative.

Table 4 shows a genetic data set from the DNA sequence of the humane HLA-B gene. This gene plays a central role in the immune system. The data displayed in Table 4 is downloaded from the webpage of the National Center for Biotechnology Information (http://www.ncbi.nlm.nih.gov/genome/guide/human/).

In Example a, we test i.i.d. $\frac{1}{3}$ versus i.i.d. for the data from Table 2 and we test i.i.d. $\frac{1}{4}$ versus i.i.d. for the DNA-data. In Example b, we test i.i.d. versus reversible. In Example c, we test reversible versus full Markov. In Example d, we compare i.i.d. with full Markov.

Table 2: Sequence of length 100 consisting of "R", "W", "B"

RRWBRWWBRR	WBRWWBBRWB	BRBRWWBRWW	WRRBRWBRRW
BBRWBRWRWB	WWBRWBBRWB	RWWRWBBRWB	WRWRRWBRWB
BBRBRWBRWR	BRWBBWRWBR		

Let n_R, n_w, and n_B denote the number of occurrences of R, W, and B, respectively. Then

$$n_R = 34, \quad n_W = 34, \quad n_B = 32.$$

Table 3: Occurrences N_{ij} of the string ij for $i, j \in \{R, W, B\}$

	R	W	B
R	5	24	4
W	7	7	20
B	21	3	8

Table 4: The humane HLA-B gene. Part of the DNA sequence of length 3370.

1	tggtgtagga	gaagagggat	caggacgaag	tcccaggtcc	cggacggggc	tctcagggtc
61	tcaggctccg	agggccgcgt	ctgcaatggg	gaggcgcagc	gttggggatt	ccccactccc
121	ctgagtttca	cttcttctcc	caacttgtgt	cgggtccttc	ttccaggata	ctcgtgacgc
181	gtccccactt	cccactccca	ttgggtattg	gatatctaga	gaagccaatc	agcgtcgccg
241	cggtcccagt	tctaaagtcc	ccacgcaccc	acccggactc	agagtctcct	cagacgccga
301	gatgctggtc	atggcgcccc	gaaccgtcct	cctgctgctc	tcggcggccc	tggccctgac
361	cgagacctgg	gccggtgagt	gcgggtcggg	agggaaatgg	cctctgccgg	gaggagcgag
421	gggaccgcag	gcgggggcgc	aggacctgag	gagccgcgcc	gggaggaggg	tcgggcgggt
481	ctcagcccct	cctcaccccc	aggctcccac	tccatgaggt	atttctacac	ctccgtgtcc
541	cggcccggcc	gcggggagcc	ccgcttcatc	tcagtgggct	acgtggacga	cacccagttc
601	gtgaggttcg	acagcgacgc	cgcgagtccg	agagaggagc	cgcgggcgcc	gtggatagag
661	caggaggggc	cggagtattg	ggaccggaac	acacagatct	acaaggccca	ggcacagact
721	gaccgagaga	gcctgcggaa	cctgcgcggc	tactacaacc	agagcgaggc	cggtgagtga
781	ccccggcccg	gggcgcaggt	cacgactccc	catcccccac	gtacggcccg	ggtcgccccg
841	agtctccggg	tccgagatcc	gcctccctga	ggccgcggga	cccgcccaga	ccctcgaccg
901	gcgagagccc	caggcgcgtt	tacccggttt	cattttcagt	tgaggccaaa	atccccgcgg
961	gttggtcggg	gcggggcggg	gctcgggggа	ctgggctgac	cgcggggccg	gggccagggt
1021	ctcacaccct	ccagagcatg	tacggctgcg	acgtggggcc	ggacgggcgc	ctcctccgcg
1081	ggcatgacca	gtacgcctac	gacggcaagg	attacatcgc	cctgaacgag	gacctgcgct
1141	cctggaccgc	cgcggacacg	gcggctcaga	tcacccagcg	caagtgggag	gcggcccgtg
1201	aggcggagca	gcggagagcc	tacctggagg	gcgagtgcgt	ggagtggctc	cgcagatacc
1261	tggagaacgg	gaaggacaag	ctggagcgcg	ctggtaccag	gggcagtggg	gagccttccc
1321	catctcctat	aggtcgccgg	ggatggcctc	ccacgagaag	aggaggaaaa	tgggatcagc
1381	gctagaatgt	cgccctccgt	tgaatggaga	atggcatgag	ttttcctgag	tttcctctga
1441	gggcccсctc	ttctctctag	acaattaagg	aatgacgtct	ctgaggaaat	ggaggggaag
1501	acagtcccta	gaatactgat	caggggtccc	ctttgacccc	tgcagcagcc	ttgggaaccg
1561	tgacttttcc	tctcaggcct	tgttctctgc	ctcacactca	gtgtgtttgg	ggctctgatt
1621	ccagcacttc	tgagtcactt	tacctccact	cagatcagga	gcagaagtcc	ctgttccccg
1681	ctcagagact	cgaactttcc	aatgaatagg	agattatccc	aggtgcctgc	gtccaggctg
1741	gtgtctgggt	tctgtgcccc	ttccccaccc	caggtgtcct	gtccattctc	aggctggtca
1801	catgggtggt	cctagggtgt	cccatgaaag	atgcaaagcg	cctgaatttt	ctgactcttc
1861	ccatcagacc	ccccaaagac	acacgtgacc	caccacccca	tctctgacca	tgaggccacc
1921	ctgaggtgct	gggccctggg	tttctaccct	gcggagatca	cactgacctg	gcagcgggat
1981	ggcgaggacc	aaactcagga	cactgagctt	gtggagacca	gaccagcagg	agatagaacc
2041	ttccagaagt	gggcagctgt	ggtggtgcct	tctggagaag	agcagagata	cacatgccat
2101	gtacagcatg	aggggctgcc	gaagcccctc	accctgagat	ggggtaagga	gggggatgag
2161	gggtcatatc	tcttctcagg	gaaagcagga	gcccttcagc	agggtcaggg	cccctcatct
2221	tcccctcctt	tcccagagcc	gtcttcccag	tccaccgtcc	ccatcgtggg	cattgttgct
2281	ggcctggctg	tcctagcagt	tgtggtcatc	ggagctgtgg	tcgctgctgt	gatgtgtagg
2341	aggaagagtt	caggtaggga	aggggtgagg	ggtggggtct	gggttttctt	gtcccactgg
2401	gggtttcaag	ccccaggtag	aagtgttccc	tgcctcatta	ctgggaagca	gcatgcacac
2461	aggggctaac	gcagcctggg	accctgtgtg	ccagcactta	ctcttttgtg	cagcacatgt
2521	gacaatgaag	gatggatgta	tcaccttgat	ggttgtggtg	ttggggtcct	gattccagca
2581	ttcatgagtc	aggggaaggt	ccctgctaag	gacagacctt	aggagggcag	ttggtccagg
2641	acccacactt	gctttcctcg	tgtttcctga	tcctgccctg	ggtctgtagt	catacttctg
2701	gaaattcctt	ttgggtccaa	gactaggagg	ttcctctaag	atctcatggc	cctgcttcct
2761	cccagtgccc	tcacaggaca	ttttcttccc	acaggtggaa	aaggagggag	ctactctcag
2821	gctgcgtgta	agtggtgggg	gtgggagtgt	ggaggagctc	acccacccca	taattcctcc
2881	tgtcccacgt	ctcctgcggg	ctctgaccag	gtcctgtttt	tgttctactc	caggcagcga
2941	cagtgcccag	ggctctgatg	tgtctctcac	agcttgaaaa	ggtgagattc	ttggggtcta
3001	gagtgggtgg	ggtggcgggt	ctgggggtgg	gtggggcaga	ggggaaaggc	ctgggtaatg
3061	gggattcttt	gattgggatg	tttcgcgtgt	gtggtgggct	gtttagagtg	tcatcgctta
3121	ccatgactaa	ccagaatttg	ttcatgactg	ttgttttctg	tagcctgaga	cagctgtctt
3181	gtgagggact	gagatgcagg	atttcttcac	gcctcccctt	tgtgacttca	agagcctctg
3241	gcatctcttt	ctgcaaaggc	acctgaatgt	gtctgcgtcc	ctgttagcat	aatgtgagga
3301	ggtggagaga	cagcccaccc	ttgtgtccac	tgtgacccct	gttcgcatgc	tgacctgtgt
3361	ttcctcccca					

Let n_a, n_c, n_g, and n_t denote the number of occurrences of a, c, g, and t, respectively. Then

$$n_a = 621, \quad n_c = 974, \quad n_g = 1064, \quad n_t = 711.$$

Table 5: Occurrences N_{ij} of the string ij for $i, j \in \{a, c, g, t\}$

	a	c	g	t
a	91	160	261	108
c	213	351	161	249
g	251	224	388	201
t	66	239	254	152

Example 1a. A Bayes test of H_0: i.i.d.($\frac{1}{3}$) versus H_1: i.i.d.(unknown) for the data from Table 2.

A 'standard' test can be based on the Bayes factor

$$\frac{P(data|H_0)}{P(data|H_1)}.$$

See Good [Goo68] for an extensive discussion. For H_1, we use a Dirichlet(1,1,1) prior. This gives

$$\begin{aligned} P(data|H_0) &= \left(\frac{1}{3}\right)^{100} \approx 1.94033 \cdot 10^{-48}, \\ P(data|H_1) &= \frac{\Gamma(3)\Gamma(n_R+1)\Gamma(n_W+1)\Gamma(n_B+1)}{\Gamma(n_R+n_W+n_B+3)} = \frac{\Gamma(3)\Gamma(35)\Gamma(35)\Gamma(33)}{\Gamma(103)} \\ &\approx 4.77096 \cdot 10^{-50}, \end{aligned}$$

and the bayes factor equals

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 41.$$

This is not surprising since the observed number of R, W, B are 34, 34, 32, respectively.

Example 2a. A Bayes test of H_0: i.i.d.($\frac{1}{4}$) versus H_1: i.i.d.(unknown) for the DNA-data.

In this case, we use a Dirichlet(1,1,1,1) prior for H_1. This yields

$$\begin{aligned} P(data|H_0) &= \left(\frac{1}{4}\right)^{3370} \approx 1.142429015368253 \cdot 10^{-2029}, \\ P(data|H_1) &= \frac{\Gamma(4)\Gamma(n_a+1)\Gamma(n_c+1)\Gamma(n_g+1)\Gamma(n_t+1)}{\Gamma(n_a+n_c+n_g+n_t+4)} \\ &= \frac{\Gamma(4)\Gamma(622)\Gamma(975)\Gamma(1065)\Gamma(712)}{\Gamma(3374)} \approx 1.140417804695619 \cdot 10^{-1999}, \end{aligned}$$

and hence the Bayes factor equals

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 1.00176 \cdot 10^{-30}.$$

Thus, H_0 is strongly rejected. Again, this is not surprising since the observed number of a, c, g, t are $n_a = 621$, $n_c = 974$, $n_g = 1064$, $n_t = 711$, respectively.

Example 1b. A Bayes test of H_0: i.i.d.(unknown) versus H_1: reversible for the data from Table 2.

Here we use a Dirichlet(1,1,1) prior for the null hypothesis and the prior based on the complete graph K_3 with loops (see Figure 3) and all edge weights equal to 1. Then, $P(data|H_0)$ is as in Example 1a. In order to calculate $P(data|H_1)$, we first determine the transition counts k_e for our data (see Table 3):

$$k_{\{R,W\}} = 31,\ k_{\{R,B\}} = 25,\ k_{\{B,W\}} = 23,\ k_{\{R\}} = 10,\ k_{\{W\}} = 14,\ k_{\{B\}} = 16,$$

and also $k_v = n_v - \delta_R(v)$: $k_R = 33$, $k_W = 34$, $k_B = 32$. Using the first part of Proposition 4.7, we obtain

$$\begin{aligned} P(data|H_1) &= \frac{\prod_{e\in\{\{R,W\},\{R,B\},\{B,W\}\}} \prod_{i=0}^{k_e-1}(1+i) \prod_{j\in\{R,W,B\}} \prod_{i=0}^{k_{\{j\}}/2-1}(1+2i)}{\prod_{i=0}^{k_R-1}(3+2i) \prod_{j\in\{W,B\}} \prod_{i=0}^{k_j-1}(4+2i)} \\ &= \frac{(31)!(25)!(23)! \prod_{i=0}^{4}(1+2i) \prod_{i=0}^{6}(1+2i) \prod_{i=0}^{7}(1+2i)}{\prod_{i=0}^{32}(3+2i) \prod_{i=0}^{33}(4+2i) \prod_{i=0}^{31}(4+2i)} \\ &\approx 2.63663 \cdot 10^{-49} \end{aligned}$$

So the Bayes factor is

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 0.180949$$

and the null hypothesis is rejected.

Example 2b. A Bayes test of H_0: i.i.d.(unknown) versus H_1: reversible for the DNA-data.

Here we use a Dirichlet(1,1,1,1) prior for the null hypothesis and the prior based on the complete graph K_4 with loops (see Figure 4) and all edge weights equal to 1. The probability $P(data|H_0)$ is calculated in Example 2a. In order to calculate $P(data|H_1)$, we first determine the transition counts k_e for our data (see Table 6) and also $k_v = n_v - \delta_a(v)$:

$$k_a = 620, \quad k_c = 974, \quad k_g = 1064, \quad k_t = 711. \tag{5.1}$$

Table 6: The undirected transition counts $k_{\{i,j\}}$, $i, j \in \{a, c, g, t\}$

	a	c	g	t
a	182	373	512	174
c	373	702	385	488
g	512	385	776	455
t	174	488	455	304

We abbreviate $E' = \{\{a,c\},\{a,g\},\{a,t\},\{c,g\},\{c,t\},\{g,t\}\}$. By the first part of Proposition 4.7,

$$
\begin{aligned}
P(data|H_1) =& \frac{\prod_{e\in E'}\prod_{i=0}^{k_e-1}(1+i)\prod_{j\in\{a,c,g,t\}}\prod_{i=0}^{k_{\{j\}}/2-1}(1+2i)}{\prod_{i=0}^{k_t-1}(4+2i)\prod_{j\in\{a,c,g\}}\prod_{i=0}^{k_j-1}(5+2i)} \\
=& \frac{(373)!(512)!(174)!(385)!(488)!(455)!\prod_{i=0}^{90}(1+2i)\prod_{i=0}^{350}(1+2i)\prod_{i=0}^{387}(1+2i)\prod_{i=0}^{151}(1+2i)}{\prod_{i=0}^{710}(4+2i)\prod_{i=0}^{619}(5+2i)\prod_{i=0}^{973}(5+2i)\prod_{i=0}^{1063}(5+2i)} \\
\approx& 2.166939224648291\cdot 10^{-1961}.
\end{aligned}
$$

So the Bayes factor is

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 5.2628\cdot 10^{-39}$$

and the null hypothesis is strongly rejected.

Example 1c. A Bayes test of H_0: reversible versus H_1: full Markov for the data from Table 2.

Here we use our conjugate prior on reversible chains with all constants chosen as one. We use product Dirichlet measure for the rows in the full Markov case. Now,

$$
\begin{aligned}
P(data|H_1) &= \frac{\Gamma(3)\Gamma(6)\Gamma(25)\Gamma(5)}{\Gamma(36)}\cdot\frac{\Gamma(3)\Gamma(8)\Gamma(8)\Gamma(21)}{\Gamma(37)}\cdot\frac{\Gamma(3)\Gamma(22)\Gamma(4)\Gamma(9)}{\Gamma(35)} \\
&\approx 9.62182\cdot 10^{-42}.
\end{aligned}
$$

$P(data|H_0)$ was calculated in Example 1b. Hence,

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 2.74026\cdot 10^{-8}.$$

We see that a straight-forward Bayes test strongly rejects reversibility. This is not surprising since the transition counts are far from symmetric.

Example 2c. A Bayes test of H_0: reversible versus H_1: full Markov for the DNA-data.

Again, we use our conjugate prior on reversible chains with all constants chosen as one. We use product Dirichlet measure for the rows in the full Markov case. This yields

$$
\begin{aligned}
P(data|H_1) &= \prod_{i\in\{a,c,g,t\}}\Gamma(4)\frac{\prod_{j\in\{a,c,g,t\}}\Gamma(N_{ij}+1)}{\Gamma(k_i+4)} \\
&= \Gamma(4)^4\frac{\Gamma(92)\Gamma(161)\Gamma(262)\Gamma(109)}{\Gamma(624)}\cdot\frac{\Gamma(214)\Gamma(352)\Gamma(162)\Gamma(250)}{\Gamma(978)} \\
&\quad\cdot\frac{\Gamma(252)\Gamma(225)\Gamma(389)\Gamma(202)}{\Gamma(1068)}\cdot\frac{\Gamma(67)\Gamma(240)\Gamma(255)\Gamma(153)}{\Gamma(715)} \\
&\approx 4.16382063735625\cdot 10^{-1956}.
\end{aligned}
$$

The probability $P(data|H_0)$ was calculated in Example 2b. Hence,

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 5.20421 \cdot 10^{-6}.$$

We see that a straight-forward Bayes test rejects reversibility.

Example 1d. A Bayes test of H_0: i.i.d.(unknown) versus H_1: full Markov for the data from Table 2.

Using the Bayes factors computed above, we see strong rejection of i.i.d. versus Markov:

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 4.95848 \cdot 10^{-9}.$$

Of course, an i.i.d. process is a reversible Markov chain.

Example 2d. A Bayes test of H_0: i.i.d.(unknown) versus H_1: full Markov for the DNA-data.

Again, with the Bayes factors as above, the null hypothesis is strongly rejected:

$$\frac{P(data|H_0)}{P(data|H_1)} \approx 2.73887 \cdot 10^{-44}.$$

In using the Dirichlet prior for testing uniformity with multinomial data and for testing independence in contingency tables I.J. Good found the symmetric Dirichlet prior with density proportional to $\prod_{i=1}^{d} x_i^{c-1}$ an important tool. Good's many insights into these testing problems may be accessed through his book [Goo68] and the survey article [GC87].

We have used the analog of the symmetric Dirichlet for the reversible Markov chain context with all edge weights a_e equal to a constant c say. As c tends to infinity, this prior tends to a point mass supported on the simple random walk on the graph. As c tends to zero this prior tends to an improper prior which gives the maximum likelihood as its posterior.

Good also worked with c-mixtures of symmetric Dirichlet priors. We suspect that parallel, useful things can be done in our case as well.

We have not found *any* literature about statistical analysis of reversible Markov chains with unknown transitions and append two data analytic remarks here. First, under reversibility, the count $N(v, v')$ of v to v' transitions has the same expectation as the count $N(v', v)$ of v' to v transitions, namely $\pi(v)k(v, v')$. This suggests looking at ratios $N(v, v')/N(v', v)$ or differences $N(v, v') - N(v', v)$. For example, from Table 3, $\frac{N_{RW}}{N_{WR}} = \frac{24}{7}$, $\frac{N_{RB}}{N_{BR}} = \frac{4}{21}$, $\frac{N_{WB}}{N_{BW}} = \frac{20}{3}$; these are way off.

In large samples, these counts have limiting normal distributions by results of Höglund [Hög74]. A second data analytic tool would be to estimate the stationary distribution (perhaps by the method of moments estimator $\hat{\pi}(v) = \frac{1}{n}|\{i \le n : X_i = v\}|$) and also estimate the transition matrix, and then compare $\hat{\pi}(v)\hat{k}(v, v')$ with $\hat{\pi}(v')\hat{k}(v', v)$.

An interesting problem not tackled here is finding natural priors on the set of reversible Markov chains *with a fixed stationary distribution*. For definiteness, consider the uniform stationary distribution. Then the problem is to put a prior on $\mathcal{S}(n)$, the symmetric doubly stochastic $n \times n$ matrices. We make two remarks. First, determining the Euclidean volume of $\mathcal{S}(n)$ is a long-standing open problem, see Clara Chan and al. [CRY00] for recent results. Second, $\mathcal{S}(n)$ is a compact, convex subset of $\mathbb{R}^{n^2}$. Its extreme points are well known to be the *symmetrized* permutation matrices (see Stanley [Sta78]). Thus, if π is a permutation matrix on n letters with $e(\pi)$ the usual $n \times n$ permutation matrix, let $\tilde{e}(\pi) = \frac{1}{2}[e(\pi) + e(\pi^{-1})]$. The extreme points of $\mathcal{S}(n)$ are $(\tilde{e}(\pi))$ as π ranges over permutations in S_n. We may put a prior on $\mathcal{S}(n)$ by taking a random convex combination of the $\tilde{e}(\pi)$. Alas, $\mathcal{S}(n)$ is *not* a simplex, so symmetric weights on the extreme points may not lead to symmetric measures on $\mathcal{S}(n)$.

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