

# Rapid Mixing in Markov Chains

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## 1. Examples

We consider “counting problems”, where there is an implicitly defined finite set  $X$  and one wishes to compute exactly or approximately  $|X|$ . In many situations, the approximate counting problem can be reduced to the problem of generating uniformly at random an element of  $X$  (the random generation problem). This is often the relatively easier part. Then, the generation problem is solved by devising a Markov Chain with set of states  $X$  with uniform steady state probabilities and then showing that this chain “mixes rapidly” - i.e., is close to the steady state distribution after a number of steps which is bounded above by a polynomial in the length of the input. [The proof of rapid mixing is often the challenging part.] We will illustrate the problem settings and scope of the area by means of three examples in this section. Then we will outline some tools for proving rapid mixing and describe very briefly how the tools are applied in some examples. This paper presents a cross-section of methods and results from the area. A more comprehensive survey can be found in [19].

Our first example is the permanent of a  $n \times n$  matrix  $A$ . Valiant [36] showed that the *exact* computation of the permanent is  $\# P$  - hard, i.e., every problem in a class of problems called  $\# P$  is reducible to the exact computation of the permanent of a matrix; thus it is conjectured that it is not solvable in polynomial time. The hardness result holds even for the case with each entry a 0 or a 1 whence the problem is to find  $|X|$  where  $X = \{\sigma \in S_n : A_{i,\sigma(i)} = 1 \forall i\}$ . Note that  $X$  here is implicitly defined by  $A$ . In the general case, we may think of  $A$  as specifying a weight  $\prod_i A_{i,\sigma(i)}$  on each  $\sigma$  in  $X$ .

As usual, we measure running time as a function of  $n$ , a natural parameter of the problem (like the  $n$  above) and  $1/\epsilon$ , where  $\epsilon > 0$  is the relative error allowed. Our primary aim is a **polynomial** (in  $n, 1/\epsilon$ ) **time** bounded algorithm; but, we will also discuss methods which help improve the polynomial. A recent breakthrough due to Jerrum, Sinclair, Vigoda [22] gives an approximation algorithm with such a time bound for the permanent (of a matrix with non-negative entries) settling this important open problem.

Our second example starts with the classical problem of computing the volume of a compact convex set in Euclidean  $n$ - space  $\mathbf{R}^n$ . Dyer, Frieze and the author [17]

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gave polynomial time algorithm for estimating the volume to any specified relative error  $\epsilon$ . They first reduce the problem to that of drawing a random point from the convex set (with uniform probability density). They then impose a grid on space and do a “coordinate random walk” - from current grid point  $x$  in  $K$ , pick one of the  $2n$  coordinate neighbours  $y$  of  $x$  at random and go to  $y$  if  $y \in K$ ; otherwise, stay at  $x$ . Under mild conditions, it is easy to show that the steady state distribution is uniform (over the grid points in the set); they show that in a polynomial (in  $n$ ) number of steps, we are “close” to the steady state. [The number of states of the chain can be exponentially large.]

Lovász and Simonovits [27] have devised a continuous state space random walk called the “ball walk” which performs better. In this, we choose at the outset a “step size”  $\delta > 0$ . From the current point  $x$ , we pick at random (with uniform density) a point  $y$  in a ball of radius  $\delta$  with  $x$  as center. We go to  $y$  if it is in  $K$ , otherwise, we stay at  $x$ .

More generally, we may consider the integration (a “continuous” analog of counting) of a function over a convex set  $K$ . Of particular interest are logarithmically-concave (a positive real valued function  $F$  is log-concave over a domain if  $\log F$  is concave over the domain) functions, since many families of familiar probability density functions like the multi-variate normal are log-concave. One may use the Metropolis version of the random walks for convex set (cf section 1.). Rapid mixing has been proved for this general case too [4].

Our third set of examples concerns the Ising model and other Statistical Mechanics problems. (see [21] and references there). The computational problem arising from the Ising model is the following : we are given a real symmetric  $n \times n$  matrix  $V$  (the entries of  $V$  arise as pairwise interaction energies), a real number  $B$  (the external field) and a positive real number  $\beta$  (the temperature). The Ising partition function is defined as

$$Z = Z(V_{ij}, B, \beta) = \sum_{\sigma \in \{-1, +1\}^n} e^{-\beta H(\sigma)}, \quad \text{where } H(\sigma) = -\sum_{i,j} V_{ij} \sigma_i \sigma_j - B \sum_k \sigma_k.$$

Jerrum and Sinclair [21] presented a polynomial time approximation algorithm to compute  $Z$  in the case when all  $V_{ij}$  are non-negative (called the ferromagnetic case).

Their algorithm for the ferromagnetic case first reduces the problem to the corresponding sampling problem and then more interestingly reduces this sampling problem to another one where we are given a graph (explicitly)  $G(V, E)$  with positive edge weights  $w(e)$ . The problem is to pick a subset of edges of  $G$  at random such that the probability of picking a particular subset  $T$  is proportional to

$$w(T) = \mu^{|\text{odd}(T)|} \prod_{e \in T} w(e),$$

where  $\mu$  is a given positive number and  $\text{odd}(T)$  denotes the set of odd degree vertices in  $T$ . [Note that in this case  $X$  is the set of all subsets of edges and we have probabilities  $\mathcal{P}$  on  $X$  as given above, where  $X, \mathcal{P}$  are implicitly defined by giving  $G, w$ .]

## 2. Preliminaries, Eigenvalue Connection

Most of what we say extends naturally to continuous state space chains (where the set of states is (possibly uncountably) infinite) under mild conditions of measurability, but for ease of notation, here we state it for chains with a finite number of states. If  $P$  is the transition probability matrix with  $P_{xy}$  denoting the probability of transition from state  $x$  to state  $y$ , for any natural number  $t$ , the matrix power  $P^t$  denotes the  $t$ -step transition probabilities. All our chains will be connected and aperiodic and thus have steady state probabilities -  $\pi(y) = \lim_{t \rightarrow \infty} P_{x,y}^t$ . ( $\pi(y)$  exists and is independent of the start state  $x$ ). [The notation  $\pi(\cdot)$  will be used throughout for steady state probabilities.] We let the vector  $p^{(t)} = p^{(0)}P^t$  denote the probabilities at time  $t$  where we start with the initial distribution  $p^{(0)}$ . All our chains will be “time-reversible”, i.e.,  $\pi(x)P_{xy} = \pi(y)P_{yx}$  will be valid for all pairs  $x, y$ .

From Linear algebra, we get that the eigenvalues of  $P$  are  $1 = \lambda_1 > \lambda_2 \geq \lambda_3 \dots \lambda_N \geq -1$  (where  $N$  is the number of states). Standard techniques yield :

**Theorem 1.** *For a finite time-reversible Markov Chain, with  $\pi_0 = \min_x \pi(x)$ , for any  $t$ ,*

$$\sum_x \left| p^{(t)}(x) - \pi(x) \right| \leq \frac{1}{\pi_0} [\max(|\lambda_2|, |\lambda_N|)]^t.$$

Modifying a Markov Chain by making it stay at the current state with probability  $1/2$  and move according to its transition function with probability  $1/2$  ensures that  $\lambda_N > 0$  while only increasing the (expected) running time by a factor of 2; so in the maximum above, we need only consider  $\lambda_2$ . We call a chain “lazy” if  $P_{xx} \geq \frac{1}{2} \forall x$ . We will use the phrase **mixing time** to denote the least positive real  $\tau$  such that for any  $p^{(0)}$ ,  $\sum_x |p^{(\tau)}(x) - \pi(x)| \leq 1/4$ . It is known [1] that then for  $t \geq \tau \log(1/\epsilon)$ , we have  $\sum_x |p^{(t)}(x) - \pi(x)| \leq \epsilon$ .

If we have a time-reversible Markov Chain on a finite set of states with transition probability matrix  $P$  with steady state probabilities  $\pi(x)$  and  $F$  is a positive real valued function on the states, there is a simple modification of the chain with steady state probabilities -  $\pi(x)F(x) / \sum_y F(y)$ , called the the **Metropolis** modification. It has transition probabilities -  $P'_{xy} = P_{xy} \text{Min}(1, \frac{F(y)}{F(x)})$  for  $x \neq y$ . This construction is used in many instances including as mentioned in the introduction for sampling according to log-concave functions.

## 3. Techniques for proving Rapid Mixing

### 3.1. Conductance

Alon and Milman [3] and Sinclair and Jerrum [34] related  $\lambda_2$  to a combinatorial quantity called “conductance” (in what may be looked on as a discrete analog of Cheeger’s inequality for manifolds). This has turned out to be of great use in practice; often, first proofs of polynomial time convergence use conductance.

For any two subsets  $S, T$  of states, the *ergodic flow* from  $S$  to  $T$  (denoted  $Q(S, T)$ ) is defined as  $Q(S, T) = \sum_{x \in S, y \in T} \pi(x) P_{xy}$ . The conductance  $\Phi$  is defined by :

$$\Phi(S) = \frac{Q(S, \bar{S})}{\pi(S)} \quad \Phi = \min_{S: 0 < \pi(S) < 3/4} \Phi(S).$$

$\Phi(S)$  is the probability of escaping from  $S$  to  $\bar{S}$  conditioned on starting in  $S$  in the steady state; since  $p^{(0)}$  may be this distribution, it is intuitively clear that if the conductance of any set is low, then the mixing time is high. More interestingly, [3] and [34] show also a converse.

**Theorem 2.** *For a time-reversible, lazy, ergodic Markov chain with conductance  $\Phi$ , we have*

$$1 - 2\Phi \leq \lambda_2 \leq 1 - \frac{1}{2}\Phi^2.$$

While conductance has helped bound the mixing time for some complicated chains (including the three examples mentioned in the introduction), it is not a fine enough tool to give the correct bounds for some simple chains. For example, consider the lazy version of the random walk on the  $2^n$  vertices on the  $n$ -**cube**, where in each step, one picks at random one of the  $n$  neighbours of the current vertex to go to. The mixing time is known to be  $O(n \log n)$ . Conductance is  $\Theta(1/n)$  for this example, yielding only a mixing time of  $O(n^3)$  by Theorems (2) and (1).

A striking contrast is the random walk on the vertices of the **cube truncated** by a half-space (i.e., the set of 0-1 vectors satisfying a given linear inequality.) Morris and Sinclair [29] showed that the conductance of this walk is at least  $1/p(n)$  for a polynomial  $p(\cdot)$ .

We now discuss a recent improvement of conductance for chains with a finite number of states from [26], [23]; similar results hold for chains with infinite number of states. In addition to measuring the ergodic flow from  $S$  to  $\bar{S}$ , we now also see if the flow is “well-spread out” in the sense that we “block” a set  $B \subseteq \bar{S}$ , and then see if  $Q(S, \bar{S} \setminus B)$  is still high. We now define for  $S$  with  $0 < \pi(S) \leq 3/4$ ,

$$\Psi(S) = \sup_{\alpha \in (0, \pi(S))} \min_{B \subseteq \bar{S}; \pi(B) \leq \alpha} \frac{\alpha Q(S, \bar{S} \setminus B)}{\pi(S)^2}.$$

It is easy to show that a set  $B$  with  $\pi(B) \leq \frac{1}{2}Q(S, \bar{S})$ , blocks at most  $1/2$  of the flow from  $S$  to  $\bar{S}$ , so we have  $\Psi(S) \geq \frac{1}{4}\Phi(S)^2$ . Thus, an assertion that mixing time is  $O(\log(1/\pi_0) \min_S \Psi(S))$  would be at least as strong a result as we get from Theorems (2) and (1). We prove a theorem which implies this assertion; indeed, instead of taking  $\min_S \Psi(S)$ , the theorem takes an “average” of this quantity over different set sizes. We say that  $\psi : [0, 3/4] \rightarrow [0, 1]$  is a “blocking conductance function” (b.c.f.) if (the second condition is technical)

$$\forall S, 0 < \pi(S) \leq 3/4, \quad \Psi(S) \geq \psi(\pi(S)) \quad \text{and} \quad \psi(t) \leq 2\psi(t') \quad \forall 0 \leq t \leq t' \leq \frac{4}{3}t.$$

**Theorem 3.** *If  $\psi$  is a blocking conductance function of a lazy, ergodic, time-reversible, finite Markov chain, with  $\pi_0 = \min_x \pi(x)$ , then, the mixing time is at most*

$$500 \int_{t=\pi_0}^{3/4} \frac{1}{t\psi(t)} dt.$$

This has been used to improve the analysis of the ball walk for convex sets in [26] and also some other examples in [30]. Also, [5] uses Theorem (3) to argue that the mixing time of the grid lattice, (in a fixed number of dimensions) where some edges have failed according to a standard percolation model is still within a constant of the mixing time of the whole.

### 3.2. Coupling

Another important technique for proving rapid mixing is “Coupling” [1]. A *coupling* is a stochastic process  $(X_t, Y_t), t = 0, 1, 2, \dots$ , where each of  $\{X_t, t = 0, 1, \dots\}$  and  $\{Y_t, t = 0, 1, 2, \dots\}$  is marginally a copy of the chain. [They may be mutually dependent.] So, we run “two copies” of the chain  $(X_t, Y_t)$  in tandem. If  $Y_0$  is distributed according to  $\pi$ , the steady state distribution, then, the distribution  $p^{(t)}$  of  $X_t$ , satisfies

$$\sum_x |p^{(t)}(x) - \pi(x)| \leq \Pr(X_t \neq Y_t).$$

To apply this, one must construct a coupling  $(X_t, Y_t)$  for which  $X_t$  and  $Y_t$  “meet” as fast as possible. This can prove difficult. Path coupling introduced by Bubley and Dyer [8] which we describe now simplifies the task quite a bit. In path coupling, we have an underlying connected directed graph  $G$  on the set of states. ( $G$  could just be the graph of the Markov Chain.)  $G$  defines distances between pairs of states - namely the length of the shortest path in  $G$ . We only need to define a coupling of adjacent pairs of vertices, with the property that for every pair of adjacent (in  $G$ ) vertices  $(u, v)$ , the expected distance between the next states of  $u, v$  is at most  $\beta < 1$ . They then show that

**Theorem 4.** *If  $D$  is the diameter (of  $G$ ), then for any  $t > 0$ ,  $\Pr(X_t \neq Y_t) \leq D\beta^t$ .*

Propp and Wilson [31] have designed a method they call **Coupling from the Past**. This applies to chains with a partial order on the set of states with a least state  $\underline{0}$  and a greatest state  $\underline{1}$ . They show that running two copies of the Chain backwards - one from  $\underline{0}$  and one from  $\underline{1}$  - with a coupling satisfying a certain monotonicity condition until they “meet” gives us a good upper bound on the number of steps needed to mix. We refer the reader to [31] for details.

### 3.3. Other Methods

One way to prove a lower bound on conductance for a chain with a finite set of states  $X$  is to construct a family of  $|X|^2$  paths - one from each state to each other using as edges the transitions of the Markov Chain, so that no transition is “overloaded” by

too many paths. We do not supply here any more details of this technique referred to as the method of “canonical paths” and used by Jerrum and Sinclair [20].

We may look upon the construction of these paths as routing a multi-commodity flow through the network and apply techniques from Network Flows. [33] pursues this. [13] uses different measures of congestion to achieve improved results in some cases and their methods are applied in [15].

Another important method is the use of logarithmic Sobolev inequalities, where, we use (relative) entropy -  $\text{Ent}(p^{(t)}) = \sum_x p^{(t)}(x) \log \frac{p^{(t)}(x)}{\pi(x)}$  as the measure of distance. It is known that for ergodic Markov Chains, this distance declines exponentially [12]; i.e., there is a constant  $\alpha \in (0, 1)$  such that

$$\text{Ent}(p^{(t)}) \leq \alpha^t \text{Ent}(p^{(0)}).$$

Note that  $\text{Ent}(p^{(0)}) \leq \log(1/\pi_0)$ . So, it suffices to choose  $t = (\log \log \frac{1}{\pi_0} + \log(1/\epsilon)) / (1 - \alpha)$  to reduce the entropy to  $\epsilon$ ; the dependence on  $1/\pi_0$  is thus better. But we need to determine  $\alpha$  which is only known for simple chains. It is known that  $\alpha > \lambda_2$ , so the most that this method could save over using something like Theorem (1) is the  $\log(1/\pi_0)$  factor. [16] and [30] contain several comparisons between the log-Sobolev inequalities, eigenvalue bounds and conductance. [18] uses the log-Sobolev inequality to prove better bounds on the Metropolis version of the coordinate random walk for log-concave functions.

For the random walk on the cube a simple coupling argument, which, moves both  $X_t$  and  $Y_t$  in the same coordinate, trying to make them equal - shows that mixing time is  $O(n \log n)$ . Some sophisticated Fourier Transform methods have been used to get much more exact results here and the results are applicable in other contexts too.

A traditional approach to sampling from a probability distribution involves the so-called “Stopping Rules” [1], where one specifies a rule for when to stop the Markov Chain and shows that if we follow the rule, we sample (exactly) from the desired distribution. [2] contain results about the expected time needed for certain stopping rules, which then serves as an upper bound on the number of steps needed to converge.

We also mention two general techniques for deriving convergence rates of a Markov Chain from the knowledge of convergence rates for a simpler-to-analyze chain. The first one is called Comparison and is developed in [11]. The second technique is called Decomposition [32]; here one decomposes the chain into chains on subsets of states and derives a bound on the convergence rate of the whole chain based on the rates for the “sub-chains” and the interconnections between them.

## 4. Solution of Sampling and Counting problems

### PERMANENT

We consider the permanent of a  $n \times n$  0-1 matrix  $A$ . We may define a bipartite graph corresponding to the matrix. Each  $\sigma \in S_n$  with  $A_{i, \sigma(i)} = 1$  for all  $i$  corresponds to a perfect matching in the graph. Let  $\mathcal{M}$  be the set of perfect matchings in the graph.

Unfortunately, no rapidly mixing Markov Chain with only  $\mathcal{M}$  as the set of states is known. Broder [7] first defined the following Markov Chain. We also include the set of “near- perfect” matchings -  $\mathcal{M}'$  (a near-perfect matching has  $\frac{n}{2} - 1$  edges, no two incident to the same vertex). Transitions of the Markov Chain are as follows : In any current state,  $M$ , we pick an edge  $e = (u, v)$  of the graph uniformly at random (all edges are equally likely) and

- if  $M \in \mathcal{M}_n$  and  $e \in M$ , move to  $M' = M - e$ .
- If  $M \in \mathcal{M}_{n-1}$  and  $u$  and  $v$  are both unmatched in  $M$ , then move to  $M' = M + e$ .
- $M \in \mathcal{M}_{n-1}$ ,  $u$  is matched to  $w$  in  $M$  and  $v$  unmatched, then move to  $M' = (M + e) - (u, w)$ ; make a symmetric move if  $v$  is matched and  $u$  unmatched.
- In all other cases, stay at  $M$ .

[20] showed that if  $A$  is dense (each row has at least  $n/2$  1's), then the chain above mixes rapidly and in addition that  $|\mathcal{M}'| \leq p(n)|\mathcal{M}|$  for a polynomial  $P(\cdot)$ . Thus, rejection sampling - accept result of a run of the chain if the result is in  $\mathcal{M}$  yields a polynomial time sampling procedure.

Jerrum, Sinclair and Vigoda [22] develop an algorithm for the general 0-1 permanent (including the non-dense case). Here is very brief sketch of their algorithm : An edge-weighting  $w$  assigns a (positive) real weight  $w(e)$  to each edge. For a matching  $M$   $w(M) = \prod_{e \in M} w(e)$  is its weight. For a set  $S$  of matchings,  $w(S) = \sum_{M \in S} w(M)$ . Finally, for each pair of vertices  $(u, v)$ , define  $w'(u, v)$  to be the ratio of the weight of all perfect matchings to the weight of all near-perfect matchings which leave  $u, v$  unmatched. Then define the “modified weight”  $w'(M)$  of a matching  $M$  to be  $w(M)$  if  $M$  is perfect and  $w(M)w'(u, v)$  if  $M$  leaves  $u, v$  unmatched. They first show that a Metropolis version of the above random walk to sample according to  $w'(M)$  mixes rapidly. But the  $w'$  are not known; they argue that if we start with the complete graph and go through a sequence of graphs, where in each step, we lower the edge weight of a non-edge of  $G$  by a factor, then we can successively estimate  $w'$  for each edge-weighting (of the complete graph) in the sequence. The final element of the sequence has low enough weights for the non-edges that it gives a good approximation to the permanent.

### THE ISING MODEL

Recall the subgraph sampling problem in section 1. Here is the random walk they use. The states of the Markov Chain are the subsets of  $E$ . Their chain is the Metropolis version of the following simple Markov Chain whose steady state probabilities are uniform over all subsets of the edges, namely : at any current subset  $T$  of  $E$ , pick uniformly at random an edge  $e \in E$ ; if  $e \in T$ , then go to  $T' = T - e$ , otherwise go to  $T' = T + e$ . They also make the chain lazy. The proof of a lower bound on conductance relies on a canonical paths argument.

The algorithm that is preferred by physicists is the one due to Swendsen and Wang [35]. This algorithm switches the signs on large blocks of vertices of the graph at once. But while this seems to work well in practice, no proof of rapid mixing is known.

### CONVEX SETS, LOG-CONCAVE FUNCTIONS

Consider the ball walk in a convex set  $K$  in  $\mathbf{R}^n$  with balls of radius  $\delta$ . We

use the notation  $P_{xy}$  for the transition probability density from  $x$  to  $y$  here. The conductance of a (measurable) subset  $S$  of  $K$  is now defined as

$$\frac{\int_{x \in S} \int_{y \in K \setminus S} \pi(x) P_{xy}}{\min(\pi(S), 1 - \pi(S))}.$$

Let  $\partial S$  be the boundary of  $S$  interior to  $K$ . Since points  $x \in S$  on or near  $\partial S$ , intuitively have a high  $\int_y P_{xy}$ , a lower bound on  $\text{Vol}_{n-1}(\partial S)$  would seem to imply a lower bound on conductance. This is indeed the case. Lower bounds on  $\text{Vol}_{n-1}(\partial S)$  have been the subject of much effort. The most general result known is the following.

**Theorem 5. Isoperimetry** *Suppose  $K$  is a compact convex set in  $\mathbf{R}^n$  of diameter  $d$  and  $F$  is a positive real-valued log-concave function on  $K$ . Then for any measurable  $S \subseteq K$  with  $\int_S F \leq (1/2) \int_K F$ , and measurable boundary  $\partial S$  interior to  $K$ , we have*

$$\int_{\partial S} F \geq \frac{2}{d} \int_S F.$$

The theorem was first proved for the case  $F \equiv 1$  by Lovász and Simonovits [27] and independently also by Khachiyan and Karzanov [25]. The result was generalized to the case of general log-concave measures  $F$  by Applegate and Kannan [4] using the same techniques. We may add an extra factor of  $\ln(\int_K F / \int_S F)$  to the right hand side; this was proved independently in [26] and also by Bobkov [6]. The most recent algorithm for computing the volume of convex sets is in [24], where references to earlier papers may be found.

#### OTHER EXAMPLES

There are many other counting problems on which progress has been made using this method. Again, we are not able to present a comprehensive review here.

A notable result is the one for the truncated cube already mentioned in section 3.. Another example of interest is Contingency Tables - where we are given  $m, n$  (positive integers) and the row and column sums of an  $m \times n$  matrix  $A$ . The problem is to sample uniformly at random from the set of  $m \times n$  matrices with non-negative integer entries with these row and column sums. The problem remains open, but there are several partial results [14],[10].

There are many **tiling problems**, where the problem is to pick a random tiling of say a large square in the plane by dominoes of a given shape. These problems arise in Statistical Mechanics. For regular shapes, it is often possible to devise a polynomial time algorithm to count the number exactly. But it is important to devise algorithms with low polynomial time bounds. There has been much progress here - see [28] and references there. Random generation of colorings and independent sets of a graph has received much attention lately due to connections to Statistical Mechanics [9].

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