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On the approximation of one Markov chain by another

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Abstract. Motivated by applications in Markov chain Monte Carlo, we discuss what it means for one Markov chain to be an approximation to another. Specifically included in that discussion are situations in which a Markov chain with continuous state space is approximated by one with finite state space. A simple sufficient condition for close approximation is derived, which indicates the existence of three distinct approximation regimes. Counterexamples are presented to show that these regimes are real and not artifacts of the proof technique. An application to the “ball walk” of Lovász and Simonovits is provided as an illustrative example.

1. Discussion

Monte Carlo algorithms compute approximate solutions to hard problems by extracting information from random samples. Markov chain Monte Carlo (MCMC) algorithms add an additional ingredient, namely Markov chain simulation, to this recipe. The idea is to devise a Markov chain \((X_t : t \in \mathbb{N})\) whose stationary distribution is the one from which we would like to sample. The required samples are drawn from a realisation of this Markov chain obtained by computer simulation. To avoid excessive bias, the samples must come from a time step of the realisation that is beyond the mixing time of the Markov chain, i.e., the time \(\tau\) at which \(X_\tau\) is close enough to stationarity.

The analysis of MCMC algorithms clearly requires us to bound the mixing time from above, and several approaches have been proposed for achieving this goal. However, the computer simulation of the Markov chain will in general be imperfect. The transition probabilities may not be exactly what they should be. Even worse, the state space may be uncountably infinite, so we cannot even represent the states exactly in the computer. Does this matter? Obviously, the answer depends on the accuracy with which the Markov chain is simulated. The aim of this note is to quantify the required accuracy.

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As a paradigmatic example, consider the (lazy) ball walk in a convex body, due to Lovász and Simonovits [7]. The state space in this instance is a convex body in $\mathbb{R}^n$, i.e., a compact convex set $K \subset \mathbb{R}^n$ of full dimension. The transition kernel of the ball walk (with step-size $r > 0$) is defined by the following trial: Suppose $X_t = x$. Choose a point $y$ uniformly at random (u.a.r.) from the ball of radius $r$ centred at $x$. If $y \in K$ then $X_{t+1}$ is $y$, otherwise $X_{t+1}$ is $x$. The state space is continuous, and the transition kernel also. In any implementation it would be necessary to approximate the states in the realisation of the ball walk by vectors of finite-precision real numbers; likewise, the transition kernel would need to be approximated by some discrete distribution.

This example motivates our general setting. There is an “ideal” ergodic Markov chain $(\Omega, P)$, with state space $\Omega$ and transition kernel $P$, whose stationary distribution and mixing time are known. Then there is a perturbed Markov chain $(\hat{\Omega}, \hat{P})$, which is the one actually implemented. We assume $\hat{\Omega} \subseteq \Omega$. Usually, $\hat{\Omega}$ will be finite, though we don’t assume this. Sometimes, as we have seen, $\Omega$ will be uncountably infinite. We no not assume that $(\hat{\Omega}, \hat{P})$ is necessarily ergodic. For example, in an implementation of the ball walk, the low order bits in the finite real number approximations might depend deterministically on those of the start state. In order to compare the $t$-step distributions of the two Markov chains, we regard $\hat{P}^t(x, \cdot)$ as a probability distribution on $\Omega$, using the convention $\hat{P}^t(x, A) := \hat{P}^t(x, A \cap \hat{\Omega})$.

Observe that in general $\hat{P}^t(x, \cdot)$ does not converge to $P^t(x, \cdot)$ in usual total variation distance (half $\ell_1$-norm). Indeed, any finite approximation to the ball walk will necessarily remain at total variation distance 1 throughout, since $\hat{\Omega}$ has measure zero in $\Omega$. It is clear, then, that any discussion of finite approximations to the ball walk must necessarily involve some underlying metric $d$ on $\Omega$. In the case of the ball walk it would be natural to take $d$ to be the Euclidean metric.

So regard $(\Omega, d)$ as a metric space, and look at convergence in Prohorov metric: for Borel probability measures $\pi$ and $\pi'$ on $\Omega$, define

$$\rho(\pi, \pi') := \inf \left\{ \varepsilon : \pi(A) \leq \pi'(A^\varepsilon) + \varepsilon \text{ for all closed } A \right\},$$

where $A^\varepsilon := \{ y : d(y, A) \leq \varepsilon \}$ and $d(y, A) := \inf \{ d(y, x) : x \in A \}$. (It can be shown that taking an infimum just over closed sets is equivalent to taking an infimum over all Borel sets.) The appearance of the Prohorov metric in this context is not novel, as it has been used by a few people, for example Diamond et al. [4], in studying approximations to dynamical systems. For reasons that will be mentioned in passing at the relevant moment, we need the technical condition that $(\Omega, d)$ is a separable metric space. This will always be the case in practice (e.g., for Euclidean space $(\mathbb{R}^n, \ell_2)$).

Upon reflection, there seem to be three prerequisites for $(\hat{\Omega}, \hat{P})$ to behave as a close approximation to $(\Omega, P)$:

1. $\hat{P}(x, \cdot)$ should be close to $P(x, \cdot)$ for all $x \in \hat{\Omega}$. This is the most obviously necessary condition. The ball-walk example suggests that “close” should be measured in the Prohorov metric, and not total variation.

2. $P(x, \cdot)$ should vary smoothly with $x$. This condition is necessary to exclude “chaotic” systems whose stationary distribution is very sensitive to small changes in $P$. 


3. \((\Omega, P)\) should be rapidly mixing. Otherwise \((\Omega, P)\) and \((\hat{\Omega}, \hat{P})\) might diverge slowly over time, even if conditions (1) and (2) are met. Consider, e.g., a random walk on \([0, 1, \ldots, 2^n - 1]\) with a drift of order \(2^{-n}\).

Conditions (1) and (3) were noted by Azar et al. [3], whose motivation was similar to ours, but who considered the more restricted situation \(\hat{\Omega} = \Omega\). They had no need of (2) since they were dealing only with Markov chains with discrete state spaces.

Aside from Azar et al., there is also related work on the simulation of dynamical systems, for example, by Shardlow and Stuart [9]. Here, the dynamical system may be in continuous time, and any computer simulation will involve discretisation of time as well as of the state space. (Indeed, it is fair to say that the discretisation of time is a greater concern in this setting.) Where this work diverges from that in the dynamical systems literature is in the emphasis on non-asymptotic bounds that explore the dependence of errors on some measure of the size or complexity of the Markov chain. For example, in the simple random walk example from condition (3) above, we are interested in quantifying, in terms of the size of the state space of the random walk, how close the transition kernel \(\hat{P}(x, \cdot)\) must be to \(P(x, \cdot)\) to achieve an adequate approximation. In the case of the ball walk, we may want to quantify the closeness of approximation in terms of the dimension \(n\), step-size \(r\), and the diameter of the convex body \(K\). This concern seems less of an issue in the dynamical systems literature.

Although Theorem 2 is billed as the main result, it must be admitted that its conclusion is unsurprising and its proof banal. Nevertheless, it may have some utility in justifying the use of theoretical mixing-time upper bounds in imperfect computer simulations, where real numbers are carried to bounded accuracy and random variables are sampled from not quite the right distributions. An example application is given in §5. The main theoretical contribution of this note is in §4 where it is shown, through a sequence of counterexamples, that the three possible behaviours described in Theorem 2 are real, and not artifacts of the proof. These examples will hopefully shed light on the main mechanisms at work in this setting.

2. Definitions and preliminaries

Observe that the two occurrences of \(\varepsilon\) in definition (1) have different functions: one limits variation in position, and the other variation in probability. In questions of asymptotic convergence it is fine to lump these together. In quantitative work, we want to separate them, since we need to establish greater control over the former than the latter. In light of this, define a parametric version of the Prohorov metric

\[
\varrho_{\lambda}(\pi, \pi') := \inf \left\{ \varepsilon : \pi(A) \leq \pi'(A^{2\varepsilon}) + \varepsilon \text{ for all closed } A \right\}.
\]

A metric such as this is not entirely unknown in the literature, see Rachev [8, eq. (3.2.22)].

There is an alternative definition, due to Strassen [10, Cor. to Thm 11], of the Prohorov metric in terms of an optimal coupling. The (parameterised) Ky Fan
distance $K_{\lambda}(X, Y)$ between random variables (r.v’s) $X, Y$ on $\Omega$ is defined as

$$K_{\lambda}(X, Y) := \inf \{ \epsilon : \Pr[d(X, Y) > \lambda \epsilon] \leq \epsilon \}.$$  

Denote by $\mathcal{L}(X)$ the law (distribution) of r.v. $X$.

**Theorem 1.** Suppose $\pi$ and $\pi'$ are probability distributions on $\Omega$. Then $\varrho_{\lambda}(\pi, \pi')$ is the infimum of $K_{\lambda}(X, Y)$ over all pairs $(X, Y)$ of coupled $\Omega$-valued r.v’s such that $\mathcal{L}(X) = \pi$ and $\mathcal{L}(Y) = \pi'$.

(The theorem in this form is from García-Palomares and Giné [5].)

**Remark 1.** Strassen states Theorem 1 for the case $\lambda = 1$, but the proof clearly holds for arbitrary $\lambda \geq 0$. (To avoid delving into the proof, one could simply scale the metric $d$.) The case $\lambda = 0$ is the well-known Optimal Coupling Theorem. It is in the proof of Theorem 1 that the technical assumption of separability is used.

One last definition, and we’ll be ready to formalise conditions (1)–(3). The total variation distance between two measures $\pi$ and $\pi'$ on $\Omega$ is

$$\|\pi - \pi'\|_{TV} := \varrho_0(\pi, \pi') = \sup \{|\pi(A) - \pi'(A)| : A \text{ closed, } A \subseteq \Omega\}.$$  

The the variation threshold time [2, §4.3] of the Markov chain $(\Omega, P)$ is defined to be

$$\tau_1 := \min \{ t : \|P^t(x, \cdot) - P^t(x', \cdot)\|_{TV} \leq e^{-1}, \text{ for all } x, x' \in \Omega \}.$$  

The choice of threshold $e^{-1}$ is somewhat arbitrary. There are other, slightly different notions of $\ell_1$ mixing, but they are equivalent for our purposes. In algorithmic applications, one often estimates the probability $\pi(A)$ of some event $A$ in the stationary distribution by taking a suitably sized sample from the $t$-step distribution $P^t(x, \cdot)$. There are two sources of error in this process: the sampling error, and the error occasioned by using $P^t(x, \cdot)$ in place of $\pi(\cdot)$. The variation threshold time is important precisely because it is a worst-case bound on the latter.

3. Main result

Now all the definitions are in place we can state the main result.

**Theorem 2.** Suppose for some $\lambda, C, \delta \geq 0$:

1. $\varrho_{\lambda}(\hat{P}(x, \cdot), P(x, \cdot)) \leq \delta$, for all $x \in \hat{\Omega}$;
2. $\varrho_{\lambda}(P(x, \cdot), P(x', \cdot)) \leq C d(x, x')$, for all $x, x' \in \Omega$;
3. The Markov chain defined by $P$ is ergodic, with stationary distribution $\pi$, and variation threshold time $\tau_1$.

Then $\varrho_{\lambda}(\hat{P}^t(x, \cdot), \pi) \leq \delta$ provided $t \geq t_\varepsilon := \lceil \ln(2\varepsilon/\delta) / \tau_1 \rceil$ and, additionally:

- in the case $\lambda C < 1$,  
  $$\delta \leq \left( \frac{1 - \lambda C}{2t_\varepsilon} \right) \varepsilon;$$  

- in the case $\lambda C \geq 1$,
• in the case $\lambda C = 1$,
  \[ \delta \leq \frac{\varepsilon}{t_\varepsilon(t_\varepsilon + 1)}; \]
• and in the case $\lambda C > 1$,
  \[ \delta \leq \frac{(\lambda C - 1)^2 \varepsilon}{2(\lambda C)t_\varepsilon + 1}. \]

Remark 2. • The key point is that if $\lambda C < 1$ then $\hat{P}$ does not need to approximate $P$ to excessive accuracy, but only to within $O(\tau_1^{-1})$. In contrast, when $\lambda C > 1$, the required accuracy scales exponentially with $\tau_1$. So, for example, real arithmetic would have to be carried out to a number of significant digits scaling linearly with $\tau_1$. In the boundary situation, $\lambda C = 1$, the required accuracy scales as $O(\tau_1^{-2})$.

• All three behaviours described in Theorem 2 actually occur, and are not artifacts of the proof. Examples will be provided in §4.

• In §5 we shall see that the ball-walk, at least of the lazy kind, fits the most favourable case, $\lambda C < 1$.

• We can recover something akin to one of Azar et al.’s results [3] by setting $\lambda = 0$, $C = 1$ and $d$ to be the discrete metric. Observe that condition 2 of the theorem becomes vacuous, and $\varrho_0$ is just total variation distance. Note that Azar et al. express their condition 3 in terms of $\ell^2$ mixing time (spectral gap).

Proof of Theorem 2. Set $t = t_\varepsilon = \lceil \ln(2\varepsilon) / \tau_1 \rceil$. Let $(X_i)$ and $(\hat{X}_i)$ be Markov chains with transition kernels $P$ and $\hat{P}$, respectively, starting at a fixed state $X_0 = \hat{X}_0 = a \in \hat{\Omega}$. Note that $t$ has been chosen so that $\varrho_\lambda(L(X_t), \pi) \leq \|L(X_t) - \pi\|_{TV} \leq \varepsilon/2$. (See, e.g., Aldous and Fill [2, §4, Lemma 5].)

We’ll couple $(\hat{X}_i)$ and $(X_i)$ so that
\[ \varrho_\lambda(L(\hat{X}_i), L(X_i)) \leq \varepsilon/2. \] (3)

This will be possible provided $\delta$ satisfies the appropriate condition laid down in the statement of Theorem 2. To see this, let $D_i := d(\hat{X}_i, X_i)$ denote the divergence of the two Markov chains at time $i$. Consider the situation at time $i - 1$. Suppose we have constructed a realisation of the coupled process
\[ (a, a) = (\hat{X}_0, X_0), (\hat{X}_1, X_1), \ldots, (\hat{X}_{i-1}, X_{i-1}) = (\hat{b}, b). \]

Conditioned on $(\hat{X}_{i-1}, X_{i-1}) = (\hat{b}, b)$ we have
\[
\varrho_\lambda(L(\hat{X}_i), L(X_i)) \leq \varrho_\lambda(L(\hat{X}_i), \hat{P}(\hat{b}, \cdot)) + \varrho_\lambda(\hat{P}(\hat{b}, \cdot), L(X_i)) \\
= \varrho_\lambda(\hat{P}(\hat{b}, \cdot), P(\hat{b}, \cdot)) + \varrho_\lambda(P(\hat{b}, \cdot), P(b, \cdot)) \\
\leq \delta + CD_{i-1},
\]
where the final inequality uses conditions (1) and (2) of the theorem. According to Theorem 1, we may couple $\hat{X}_i$ and $X_i$ so that
\[ \Pr[D_i > \lambda(CD_{i-1} + \delta)] \leq CD_{i-1} + \delta. \]
Iterating this construction, it follows, by induction on \( i \), that

\[
\Pr \left[ D_t > \lambda \delta \sum_{i=0}^{t-1} (\lambda C)^i \right] \leq \delta \sum_{i=0}^{t-1} (t-i)(\lambda C)^i. \tag{4}
\]

Considering first the case \( \lambda C < 1 \), we may sum the series in (4) to obtain

\[
\Pr \left[ D_t > \frac{\lambda \delta (1 - (\lambda C)^t)}{1 - \lambda C} \right] \leq \frac{\delta t}{1 - \lambda C} = \frac{\lambda \delta C (1 - (\lambda C)^t)}{(1 - \lambda C)^2}, \tag{5}
\]

which entails

\[
\Pr \left[ D_t > \frac{\lambda \delta}{1 - \lambda C} \right] \leq \frac{\delta t}{1 - \lambda C}. \tag{6}
\]

Our goal is to attain

\[
\Pr [D_t > \lambda \varepsilon / 2] \leq \varepsilon / 2, \tag{7}
\]

since this implies inequality (3) through Theorem 1. The analysis of the case \( \lambda C < 1 \) is completed by noting that to achieve the goal it is sufficient that \( \delta \leq (1 - \lambda C)\varepsilon / 2t \).

Now turn to the case \( \lambda C = 1 \). Summing the series in (4) in this case yields

\[
\Pr [D_t > \lambda \delta t] \leq \frac{\delta t(t+1)}{2}. \]

We achieve (7) provided \( \delta \leq \varepsilon / t(t+1) \).

The final case, \( \lambda C > 1 \) is handled in a very similar manner to the first. In this case we find

\[
\Pr \left[ D_t > \frac{\lambda \delta ((\lambda C)^t - 1)}{\lambda C - 1} \right] \leq \frac{\lambda \delta C ((\lambda C)^t - 1)}{(\lambda C - 1)^2}, \tag{8}
\]

and that (3) is achieved provided

\[
\delta \leq \frac{(\lambda C - 1)^2 \varepsilon}{2(\lambda C)^{t+1}}.
\]

In conclusion, we have shown that

\[
\varrho_L(\mathcal{L}(\hat{X}_t), \pi) \leq \varrho_L(\mathcal{L}(\hat{X}_t), \mathcal{L}(X_t)) + \varrho_L(\mathcal{L}(X_t), \pi) \leq \varepsilon / 2 + \varepsilon / 2 = \varepsilon,
\]

as required. If \( t > t_\varepsilon \), we simply delay starting the coupling until \( t_\varepsilon \) steps from the end. \( \square \)

4. Counterexamples

We demonstrate in this section that the dependence on \( \tau_1 \) indicated by Theorem 2 is correct: i.e., linear in the case \( \lambda C < 1 \), exponential in the case \( \lambda C > 1 \), and quadratic at the boundary.

In applications we are thinking mainly of uncountable state spaces. However, for convenience, the counterexamples will all be finite Markov chains.
4.1. “Convergent” case

The heading is intended to indicate the case $\lambda C < 1$. We’ll set $\lambda = 0$ (i.e., our measure of convergence is total variation distance) and $C = 1$, though the construction would work equally well for a range of $\lambda, C$ satisfying $\lambda C < 1$.

The state space in this counterexample is $\Omega := \{\omega_j : 0 \leq j < n\}$. Identify the state $\omega_j$ with the point $(n \cos(2j\pi/n), n \sin(2j\pi/n))$ in $\mathbb{R}^2$, so that the states are equally spaced points around a circle of radius $n$. The metric $d$ is just Euclidean distance.

Define transition probabilities for the Markov chain (from state $\omega_j$) according to the following trial:

- With probability $1/n$, set $j' := 0$.
- Otherwise (with probability $1 - 1/n$), set $j' := (j + 1) \mod n$.

The new state is $\omega_{j'}$. Informally, we move relentlessly anticlockwise around the circle, except that with probability $1/n$ we perform a “reset” and return to distinguished vertex $\omega_0$. Since $C = 1$ and the Euclidean distance between any pair of states is at least 1, condition (2) of Theorem 2 is vacuously true.

It is easy to verify, by coupling, that the variation threshold time $\tau_1$ is $O(n)$. Simply take two copies of the Markov chain and couple the resets. A synchronised reset occurs within $n$ steps with probability at least $1 - e^{-1}$, so $\tau_1 \leq n$. (See, e.g., Aldous [1, Lemma 3.6].)

Define $\hat{P}$ as $P$ but with reset probability $4/n$ in place of $1/n$. We claim that with $\hat{P}$ there is significantly lower probability of observing $j \geq n/2$. Thus the stationary distributions are quite far apart in total variation distance (which is Prohorov metric with parameter $\lambda = 0$).

The justification of this claim runs as follows. Assume for convenience that $n$ is even, and fix a time step $t \geq n$. The probability that we observe $j \geq n/2$ in the $\hat{P}$ version is at least

$$\Pr(\text{no reset in past \(n/2\) steps} \land \text{at least one reset in past \(n\) steps})$$

This for large $n$ is close to $e^{-1/2}(1 - e^{-1/2}) \approx 0.238$. In contrast, for the $\hat{P}$ version, the probability that we observe $j \geq n/2$ is at most

$$\Pr(\text{no reset in past \(n/2\) steps}),$$

which for large $n$ is close to $e^{-2} \approx 0.136$. Comparing with previous bound, it will be seen that the two stationary distributions differ by at least $0.1$ in total variation distance.

So we certainly need to insist on $\delta < 4/n - 1/n = 3/n$ if we want to guarantee that the stationary distributions of the two Markov chains are closer than $\varepsilon = 0.1$ in variation distance. In particular, we could not replace the $\tau_1$ factor in the first case of Theorem 2 by anything growing more slowly.
4.2. “Neutral” case

This is the boundary case $\lambda C = 1$. The state space for this example is $\Omega := \{\omega_{i,j} : 0 \leq i, j < n\}$. Identify state $\omega_{i,j}$ with the point $(n \cos(2j\pi/n), n \sin(2j\pi/n), 5i/n^2)$ in $\mathbb{R}^3$. (There are $n$ circles, in $n$ layers closely packed the $z$-dimension, each containing $n$ evenly spaced states.) The metric $d$ is again Euclidean distance. Define

$$r(i) := \begin{cases} 
1/n & \text{if } i < n/5; \\
5i/n^2 & \text{if } n/5 \leq i < 4n/5; \\
4/n & \text{if } i \geq 4n/5. 
\end{cases}$$

Define transition probabilities (from state $\omega_{i,j}$) according to the following trial:

1. With probability $r(i)$, set $j' := 0$;
2. Otherwise (with probability $1 - r(i)$), set $j' := j + 1 \mod n$.

The new state is $\omega_{i',j'}$. Informally: owing to the drift in the $z$-dimension, we quickly gravitate to $i = 0$ layer and stay close to it. Within the layer, we move clockwise around the cycle, except that with probability $r(i)$ we perform a “reset” and return to one of the distinguished states $\omega_{i,0}$.

We set $\lambda = 1$, in other words we measure convergence in the standard Prohorov metric. It is routine to verify that $\varrho(P(x, \cdot), P(x', \cdot)) \leq d(x, x')$, so that $C = 1$, and we are in the $\lambda C = 1$ (boundary) regime. (We need only check pairs of states of the form $(x, x') = (\omega_{i,j}, \omega_{i,j'})$, i.e., pairs which agree in their second index, since other pairs of states have separation $d(x, x') > 1$. Indeed, by the triangle inequality, we need only check pairs of the form $(x, x') = (\omega_{i,j}, \omega_{i+1,j})$. There is a natural coupling of transitions from these adjacent states $x$ and $x'$ such that the new states are within distance $5/n^2$ of each other with probability at least $1 - 5/n^2$.)

As before, we can show that $\tau_1 = O(n)$ using a coupling argument. Consider two copies of the Markov chain started in different states. In the first phase, couple on $i$ using the identity coupling. Coupling (of the $i$-index) occurs at or before the first occasion at which both copies have visited $i = 0$ layer. After this point the coupled versions always agree as to the level. This happens with high probability within $4n$ steps. In the second phase, we couple on $j$. We do the natural thing and synchronise the resets (just as in the case $\lambda C < 1$). Again, we can arrange for a synchronised reset within $2n$ steps with high probability.

Define $\tilde{P}$ as $P$ but with drift on $i$ reversed. The intuition is that we quickly gravitate to layer $i = n - 1$ and remain close to it. We then circle as before, but with much higher reset probability. We claim, as before, that with $\tilde{P}$ there is a lower probability of observing $j \geq n/2$. Thus the stationary distributions are quite far apart in Prohorov metric.

The justification of this claim runs as follows. Denote by $E$ the event (in the $P$ Markov chain)

“in the previous $n$ steps, $i$ has remained in range $[0, n/5]$”

Fix a time step $t \geq 6n$. The probability that we observe $j \geq n/2$ (in the $P$ version) is at least
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$$\Pr(\mathcal{E} \land \text{no reset in past } n/2 \text{ steps} \land \text{at least one reset in past } n \text{ steps})$$

$$= \Pr(\mathcal{E}) \Pr(\text{no reset in past } n/2 \text{ steps} \land \text{at least one reset in past } n \text{ steps} | \mathcal{E}).$$

This for large $n$ is close to $e^{-1/2} (1 - e^{-1/2}) \geq 0.238$. In contrast, for the $\hat{P}$ version, denote by $\mathcal{E}'$ the event

“in the previous $n$ steps, $i$ has remained in range $[4n/5, n]$”,

the probability that we observe $j \geq n/2$ is at most

$$\Pr(\neg \mathcal{E}' \lor \text{no reset in past } n/2 \text{ steps})$$

$$\leq \Pr(\neg \mathcal{E}') + \Pr(\text{no reset in past } n/2 \text{ steps} | \mathcal{E}').$$

The latter probability for large $n$ is close to $e^{-2} \leq 0.136$. Comparing with the previous estimate, we see the two stationary distributions differ by at least $0 \cdot \frac{1}{n}$ in the Prohorov metric.

So we certainly need to insist on $\delta < 10n^{-2}$ to bring the stationary distributions of the two Markov chains within $\varepsilon = 0.1$ in the Prohorov metric.

4.3. "Divergent" case

The state space here is $\Omega := \{2^{-ni} : 0 \leq i < 2^n\}$, and the metric $d : \Omega^2 \to \mathbb{R}^+$ is given by $d(x, y) := |x - y|$. Define the function $G : \Omega \to \Omega$ by

$$G(x) := \begin{cases} 2x, & \text{if } x < 1/2; \\ 2(1 - 2^{-n} - x), & \text{if } x \geq 1/2. \end{cases}$$

(This is the Lorenz “tent map” of dynamical systems [11, eq. (2.5.2)], adapted to the discrete situation.) Then the transition kernel

$$P(x, y) := \begin{cases} 1/2, & \text{if } y \in \{G(x), G(x) + 2^{-n}\}; \\ 0, & \text{otherwise}, \end{cases}$$

defines an ergodic Markov chain with stationary distribution $\pi$ uniform on $\Omega$. Why is this? View $x = 0.x_1x_2 \ldots x_n \in \Omega$ as an $n$-bit binary fraction. Then

$$G(x) = \begin{cases} 0.x_2x_3 \ldots x_n0, & \text{if } x < 1/2; \\ 0.\tilde{x}_2\tilde{x}_3 \ldots \tilde{x}_n0, & \text{if } x \geq 1/2, \end{cases}$$

where $\tilde{x}_i := 1 - x_i$. That is to say, $G$ can be viewed as a left shift, followed (possibly) by complementation. (C.f. two’s complement arithmetic.) So one step of the Markov chain can be viewed as a left shift, followed (possibly) by complementation, and concluded by appending a random bit. Thus $P'(x)$ for any $x \in \Omega$ and $t \geq n$ is a binary fraction formed of independent, symmetric Bernoulli r.v’s. We see from this argument that $\tau_1 = n$. (Notice that distance from stationarity drops from 1/2 to 0 between time $t = n - 1$ and time $t = n$!) Set $\lambda = 1$, and observe that $\phi(P(x, \cdot), P(x', \cdot)) \leq 2d(x, x')$, so that we are $\lambda C > 1$ regime. (In light of the triangle inequality, we just need to check pairs $(x, x')$ with $x' = x + 2^{-n}$.)
Now define an approximating Markov chain: 

$$\hat{P}(x,y) := \begin{cases} 
3/4, & \text{if } y = G(x) \text{ and } 2^{n-1}G(x) \text{ is even;} \\
1/4, & \text{if } y = G(x) \text{ and } 2^{n-1}G(x) \text{ is odd;} \\
3/4, & \text{if } y = G(x) + 2^{-n} \text{ and } 2^{n-1}G(x) \text{ is odd;} \\
1/4, & \text{if } y = G(x) + 2^{-n} \text{ and } 2^{n-1}G(x) \text{ is even;} \\
0, & \text{otherwise.} 
\end{cases}$$

Note that $$\varrho(\hat{P}(x,\cdot), P(x,\cdot)) \leq 2^{-n}.$$ The interpretation of the Markov chain defined by $$\hat{P}$$ in terms of binary fractions is similar to before, only now the random bit appended is with probability $$3/4$$ equal to the bit immediately to its left. So, for any $$t \geq n$$, $$\hat{P}^t(x,A) = 3/4,$$ where $$A = \Omega \cap ([0, 1/4) \cup [3/4, 1)).$$ In contrast, $$P^t(x,A') = 2/3,$$ where $$A' = \Omega \cap ([0, 1/3) \cup [2/3, 1)).$$ Now $$A' \supseteq A$$ with $$\varepsilon = 1/12.$$ Thus 

$$\varrho(\hat{P}^t(x,\cdot), \pi) = \varrho(\hat{P}^t(x,\cdot), P^t(x,\cdot)) \geq 1/12,$$

where $$\pi$$ is the stationary (uniform) distribution. The bottom line is that the transition kernels $$\hat{P}$$ and $$P$$ are very close and variation threshold time is short, but that the stationary distributions of the two Markov chains are nevertheless far apart. The exponential dependence of $$\delta$$ on $$\tau_1$$ in the third case of Theorem 2 is unavoidable.

5. Application: ball walk of Lovász and Simonovits

Recall the ball walk of Lovász and Simonovits [7] in its “lazy” version. The situation is as follows. $$K \subseteq \mathbb{R}^n$$ is a convex body in $$n$$-dimensional Euclidean space. For $$x \in \mathbb{R}^n$$ and $$r \in \mathbb{R}_+^+, B_n(x,r)$$ denotes the $$n$$-dimensional (closed) ball centred at $$x$$. Procedurally, the lazy walk $$(X_t : t \in \mathbb{N})$$ is described by the following trial (where the current state is $$X_t = x \in \mathbb{R}^+$$):

1. Choose $$y \in B_n(x,r)$$ u.a.r.
2. If $$y \in K$$ then $$X_{t+1} := y$$ else $$X_{t+1} := x$$.

Alternatively, the transition kernel is

$$P(x,A) := \begin{cases} 
\mu_n(B_n(x,r) \cap (\Omega \cup A))/v_n(r), & \text{if } x \in A; \\
\mu_n(B_n(x,r) \cap K \cap A)/v_n(r), & \text{otherwise,} 
\end{cases}$$

where $$\mu_n$$ is Lebesgue measure, $$\Omega$$ denotes the complement of $$K$$, and $$v_n(r) := \mu_n(B_n(0,r))$$ the volume of the $$n$$-dimensional ball of radius $$r$$.

To apply Theorem 2, we want to find a constant $$C$$ such that

$$\varrho(\hat{P}(x,\cdot), P(x',\cdot)) \leq C \|x - x'\|_2,$$

since $$d$$ is here Euclidean distance. For this part of the calculation the value of $$\lambda$$ is immaterial (even $$\lambda = 0$$ will do), so we’ll defer the choice of $$\lambda$$ until later.

We could work directly from (9), but it seems easier to go via Theorem 1. Let $$d = \|x - x'\|_2.$$ For convenience, let $$x = du_0/2$$ and $$x' = -du_0/2,$$ where $$u_0$$ is the unit vector parallel to the first coordinate axis. Define a coupling $$(Y,Y')$$ with $$\mathcal{L}(Y) = P(x,\cdot)$$ and $$\mathcal{L}(Y') = P(x',\cdot)$$ according to the trial...
1. Choose \( y \in B_n(x, r) \) u.a.r.
2. If \( y \in B_n(x', r) \) then \( y' := y \) else \( y' := \bar{y} \), where \( \bar{y} \) is the reflection of \( y \) in the plane \( \xi \cdot u_0 = 0 \).
3. \( \bullet \) If \( y \in K \) then \( Y := y \) else \( Y := x' \).
   \( \bullet \) If \( y' \in K \) then \( Y' := y' \) else \( Y' := x' \).

Note that \( Y = Y' \) unless \( y \in B_n(x, r) \setminus B_n(x', r) \). Now \( \mu_\lambda(B_n(x, r) \setminus B_n(x', r)) \) is bounded above by the volume of an \( n \)-dimensional cylinder with height \( d \) and cross-sectional \((n-1)\)-dimensional volume \( v_{n-1}(r) \). Thus \( \Pr(Y \neq Y') \leq d \frac{v_{n-1}(r)}{v_n(r)} \), and hence

\[
\varrho_\lambda(P(x, \cdot), P(x', \cdot)) \leq \frac{v_{n-1}(r)}{v_n(r)} d \leq C d
\]

where \( C = \Theta(\sqrt{n}/r) \). (Note that the inequality holds for any \( \lambda \), even \( \lambda = 0 \).) By setting \( \lambda = 1/2C = \Theta(r/\sqrt{n}) \) we place ourselves in the first (most favourable) case of Theorem 2.

Now, under the simplifying assumption that the convex body \( K \) does not have sharp corners, the variation threshold time is

\[
\tau_1 = O \left( \frac{D^2n^2 \ln(D/r)}{r^2} \right),
\]

where \( D \) is the diameter of \( K \).

Remark 3. See [6, Thm 6.7 and Cor. 6.8] for more detail, including a precise explanation of the requirement of having no “sharp corners”. Note that the radius of the ball defining the ball walk is usually denoted \( \delta \); we have used \( r \) instead to avoid a notational clash. For general convex bodies \( K \), the mixing time is essentially as given in (10), but one has to take care over the distribution of the start state of the walk, since the ball walk in its lazy variant may get trapped for long periods near points on the boundary of \( K \) of tight curvature.

From the above considerations, it can be seen that the transition kernel \( \tilde{P} \) of the ball walk as implemented is not required to approximate the ideal transition kernel very closely; specifically we require, according to Theorem 2, \( \varrho_\lambda(\tilde{P}(x, \cdot), P(x, \cdot)) \leq \delta \), where

\[
\delta = O \left( \frac{\varepsilon r^2}{D^2n^2 \ln(D/r)} \right).
\]

This is consistent with Lovász and Simonovits’s observation that for their algorithm real numbers need only be carried to \( O(\log n) \) digits.

Some concise notes on how to achieve (11). Assume, as a starting point, procedures that sample points from distributions that are close to \( N(0, 1) \) (Gaussian with mean 0 and variance 1) and to \( U(0, 1) \) (uniform on \([0, 1]\)). A standard approach to sampling a point u.a.r. from \( B_n(0, r) \) is the following (with step 2 omitted):

\footnote{In applications of the ball walk, the radius \( r \) is typically of order \( 1/\sqrt{n} \), so that \( \lambda = \Theta(1/n) \).}
1. Let $\Phi_1, \Phi_2, \ldots, \Phi_n$ be i.i.d. samples from $N(0, 1)$.
2. If $R = \sqrt{\Phi_1^2 + \Phi_2^2 + \cdots + \Phi_n^2} < \frac{1}{2} \sqrt{n}$ declare the trial void and start again at step 1.
3. Set $S = r(\Phi_1, \Phi_2, \ldots, \Phi_n)/R$.
4. Let $U$ be a sample from the uniform distribution on $[0, 1]$, and return $W = U^{1/n} S$.

We assume throughout that arithmetic is exact, in order to focus on sampling errors. Assume that $\Phi_1, \Phi_2, \ldots, \Phi_n$ and $U$ are sampled perfectly from distributions $N(0, 1)$ and $U(0, 1)$, respectively. Then $\Phi_1, \Phi_2, \ldots, \Phi_n$ is distributed according to an $n$-dimensional symmetric Gaussian distribution, and is in particular rotationally symmetric. Thus, with or without step 2, $S$ is distributed uniformly over the surface of $B_n(0, r)$. The final step spreads the distribution uniformly into the interior of $B_n(0, r)$. The unusual step 2 is included to avoid a small error being blown up in the unlikely event that $R$ is close to 0.

Without loss of generality, assume that ball walk is at the origin at time step 0. Its location $Y$ at time step 1 is obtained by applying the rejection rule to the r.v. $W$; explicitly, $Y = W$ if $W \in K$, and $Y = 0$ otherwise. Now suppose that we have only approximations $\hat{\Phi}_1$ and $\hat{U}$ to the perfect samples. Specifically, suppose

$$\varrho(L(\hat{\Phi}_1), N(0, 1)) = O(\delta/n) \quad \text{and} \quad \varrho(L(\hat{U}), U(0, 1)) = O(\delta^2).$$

where $\delta$, given by (11), is the deviation we are prepared to tolerate in $L(\hat{Y})$, the approximate version of $Y$. (Specifically, we are aiming at $\varrho_{L}(L(\hat{Y}), L(Y)) \leq \delta$.)

Suppose that we run through the above trial, replacing the perfectly distributed r.v.’s by their hatted, imperfect approximations $\hat{S}$, $\hat{W}$ and finally $\hat{Y}$, which arises from the rejection rule: $\hat{Y} = \hat{W}$ if $\hat{W} \in K$, and $\hat{Y} = 0$ otherwise.

Now couple the hatted and unhatted r.v.’s as suggested by Theorem 1. The build-up of errors is summarised in the following table. The penultimate row relates to the approximate proposal move $\hat{W}$ for the ball walk, sampled according to the four-step trial described earlier, and the final row to the result of applying the rejection rule. The interpretation of (say) the third line of the table is that we may couple $S$ and $\hat{S}$ so that $\|S - \hat{S}\|_2 = O(r\delta/n)$ with probability $1 - O(\delta)$.

| Random variable $\hat{X}$ | $\|X - \hat{X}\|_2$ bounded by... except with probability... |
|--------------------------|--------------------------------------------------|
| $\hat{\Phi}_1$          | $O(\delta/n)$                                   | $O(\delta/n)$       |
| $(\hat{\Phi}_1, \hat{\Phi}_2, \ldots, \hat{\Phi}_n)$ | $O(\delta/\sqrt{n})$                           | $O(\delta)$         |
| $\hat{S}$                | $O(r\delta/n)$                                  | $O(\delta) + O(\delta/n) = O(\delta)$ |
| $\hat{W}$                | $O(r\delta/n)$                                  | $O(\delta) + O(\delta) = O(\delta)$ |
| $\hat{Y}$                | $O(r\delta/n)$                                  | $O(\delta) + O(\delta) = O(\delta)$ |

The rows of the table may be checked as follows. Row 2 is straightforward. In row 3 we need to be concerned about the trial being declared void in the hatted trial
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and not in the unhatted, or vice versa. For this to occur, $R$ must be within $O(\delta/\sqrt{n})$ of $\frac{1}{2}\sqrt{n}$, an event whose probability may be (crudely) bounded by $O(\delta/\sqrt{n}) \times O(1/\sqrt{n}) = O(\delta/n)$. (The density of the r.v. $R$ is unimodal, and achieves its maximum at the point $\sqrt{n} - 1$; so the density of $R$ at $\frac{1}{2}\sqrt{n}$ can be at most $O(1/\sqrt{n})$.)

In row 4, we need to be concerned about errors being magnified when $U$ is close to 0. We deal with this simply by giving everything away if $\hat{U} = O(\delta)$. In the final row, our concern is with the event $\hat{Y} \in K$ and $Y \notin K$ (or vice versa). For this event, we must have $Y \in (K^\eta \setminus K) \cap B(0, r)$, where, as usual, $K^\eta$ denotes the Minkowski sum of $K$ and a ball of radius $\eta$, and $\eta = O(r\delta/n)$. Now

$$\mu_n((K^\eta \setminus K) \cap B(0, r)) \leq \mu_n(B(0, r)^\eta \setminus B(0, r)),$$

and so

$$\frac{\mu_n((K^\eta \setminus K) \cap B(0, r))}{\mu_n(B(0, r))} \leq \frac{\mu_n(B(0, r)^\eta \setminus B(0, r))}{\mu_n(B(0, r))} = O(\delta).$$

Recall that we have set $\lambda = \Theta(r/\sqrt{n})$, from which it follows that $r\delta/n = O(\lambda \delta)$. In summary, then, to obtain a close approximation to the ball-walk it is enough that the various samples from the Gaussian and uniform distributions satisfy (12), where $\delta$ is given by (11).

Remark 4. It is unlikely that one would want, in the analysis of a new algorithm, to repeat a calculation such as the one given above in a similar level of detail. Nevertheless, it would be comforting to verify, in practical situations, that one was working in one of the two favourable cases in Theorem 2: it would then follow by more informal reasoning that logarithmic (number of bits or significant digits) accuracy would suffice.

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