# Explaining the Perfect Sampler

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**Abstract**

In 1996, Propp and Wilson introduced Coupling from the Past (`CFTP`), an algorithm for generating a sample from the exact stationary distribution of a Markov chain. In 1998, Fill proposed another so–called *perfect sampling* algorithm. These algorithms have enormous potential in Markov Chain Monte Carlo (`MCMC`) problems because they eliminate the need to monitor convergence and mixing of the chain. This article provides a brief introduction to the algorithms, with an emphasis on understanding rather than technical detail.

## 1 Setting

A Markov chain is a sequence of random variables $\{X_t\}$ that can be thought of as evolving over time, and where the distribution of $X_{t+1}$ depends on $X_t$, but not on $X_{t-1}, X_{t-2}, \ldots$ . When used in Markov chain Monte Carlo (`MCMC`) algorithms, Markov chains are usually constructed from a *Markov transition kernel* $K$, a conditional probability density on $\mathcal{X}$ such that $X_{t+1}|X_t \sim K(X_t, X_{t+1})$. Interest is usually in the *stationary distribution* of the chain, the distribution $\pi$ that satisfies

$$\int_{\mathcal{X}} K(x, B)\, d\pi(x) = \pi(B) \text{ for any } B \subset \mathcal{X}.$$

Thus, if $X_t \sim \pi$ then $X_{t+1} \sim \pi$. In a common application $\pi$ is the posterior distribution from a Bayesian analysis and $K$ is constructed to have stationary distribution $\pi$.

Here is an example that we follow throughout the article.

**Beta-Binomial** Following Casella and George (1992), and for some suitable parameters $n$, $\alpha$ and $\beta$, let $\theta \sim \text{Beta}(\alpha, \beta)$ and $X|\theta \sim \text{Bin}(n, \theta)$, leading to the joint density

$$\pi(x, \theta) \propto \binom{n}{x} \theta^{x+\alpha-1}(1-\theta)^{n-x+\beta-1}$$

and the conditional density $\theta|x \sim \text{Beta}(\alpha + x, \beta + n - x)$.

We can construct a Markov chain, in fact a Gibbs sampler, having $\pi$ as its stationary distribution by using the following transition rule for $(X_t, \theta_t) \mapsto (X_{t+1}, \theta_{t+1})$:

1. choose $\theta_{t+1} \sim \text{Beta}(\alpha + x_t, \beta + n - x_t)$, and
2. choose $X_{t+1} \sim \text{Bin}(n, \theta_{t+1})$.

This transition rule has transition kernel

$$\begin{aligned} K((x_t, \theta_t), (x_{t+1}, \theta_{t+1})) &= f((x_{t+1}, \theta_{t+1})|(x_t, \theta_t)) \\ &\propto \binom{n}{x_{t+1}} \theta^{x_{t+1}+\alpha+x_t-1}(1-\theta)^{\beta+2n-x_t-x_{t+1}-1}. \end{aligned}$$

For future reference we note that the subchain $\ldots, X_t, X_{t+1}, \ldots$ is a Markov chain with $X_{t+1}|x_t \sim \text{BetaBin}(n, \alpha + x_t, \beta + n - x_t)$ and transition kernel

$$\begin{aligned} &K(x_t, x_{t+1}) = f(x_{t+1}|x_t) \propto \\ &\binom{n}{x_{t+1}} \frac{\Gamma(\alpha+\beta+n)\Gamma(\alpha+x_t+x_{t+1})\Gamma(\beta+2n-x_t-x_{t+1})}{\Gamma(\alpha+x_t)\Gamma(\beta+n-x_t)\Gamma(\alpha+\beta+2n)}. \end{aligned}$$

■

Theorems about stationary distributions and ergodicity apply when the Markov chain satisfies the three properties of *irreducibility*, *reversibility* and *aperiodicity*, defined in Appendix 6.1. See Robert and Casella (1999, Chap. 4) for a brief description or Meyn and Tweedie (1993) and Resnick (1992) among others for book-length treatments. These properties are assumed true for the rest of this article.

The *stationary distribution* of the Markov chain is also a *limiting distribution*: $X_t$ converges in distribution to $X \sim \pi$. For `MCMC` purposes two useful consequences of our assumptions are that $\frac{1}{M}\sum_{j=1}^{M} h(X_j) \to \mathrm{E}_\pi[h(X)]$ (sometimes called the ergodic theorem) and that a central limit theorem holds.

It is typical in practice to have `MCMC` algorithms begin from an arbitrarily chosen state at time $t = 0$, say, and run for a long time $T$, say, in the hope that $X_T$ is a draw from $\pi$. One typically discards $X_0, \ldots, X_{T-1}$ and estimates $\mathrm{E}_\pi[h(X)]$ as $\frac{1}{M}\sum_{j=T}^{T+M-1} h(X_j)$. A serious practical problem is determining the "burn-in" time $T$. A second practical problem is determining the correlation between $X_t$ and $X_{t+1}$, which is used to calculate the variance of the estimate. Perfect sampling avoids both problems because it produces independent draws having distribution $\pi$ precisely.

Indeed, the major drawback with using MCMC methods is that their validity is only asymptotic: if we run the sampler kernel until the end of time, we are bound to explore the entire distribution of interest; but, since computing and storage resources are not infinite, we are bound to stop the MCMC sampler at some point. The influence of this stopping time on the distribution of the chain is not harmless and in some cases may induce serious biases (Roberts and Rosenthal, 1998). Perfect sampling alleviates this difficulty by producing exactly the same chain as one running an infinite number of steps, by simply replacing the starting time with $-\infty$ and $\infty$ with 0. And, at no additional cost, it also removes the dependence on the starting value! In other words, the burn-in time becomes infinite and the chain is indeed in the stationary distribution at time 0.

## 2 Coalescence

The first step in obtaining a perfect sample is to find a way to make $X_t$ independent of the starting value. The answer is to work with coupled parallel chains.

Suppose there are $k$ states in $\mathcal{X}$, and we start a Markov chain in each state at time $t = 0$. These are *parallel chains*. Parallel chains can be *coupled* through a *transition rule* $\phi$ and random numbers $U_t$. A transition rule determines $X_{t+1}$ as a function of $X_t$ and $U_{t+1}$. Note that the same $\phi$ and same $\ldots, U_t, U_{t+1}, \ldots$ are used for each chain. A common and convenient choice is to let $U_{t+1} \sim \mathrm{Uniform}(0, 1)$ and take $X_{t+1} = \phi(x_t, u_{t+1}) = F^{-1}_{X_{t+1}|x_t}(u_{t+1})$, the inverse-cdf function of $X_{t+1}|x_t$ determined by the kernel $K$. For illustration we return to the Beta-Binomial example.

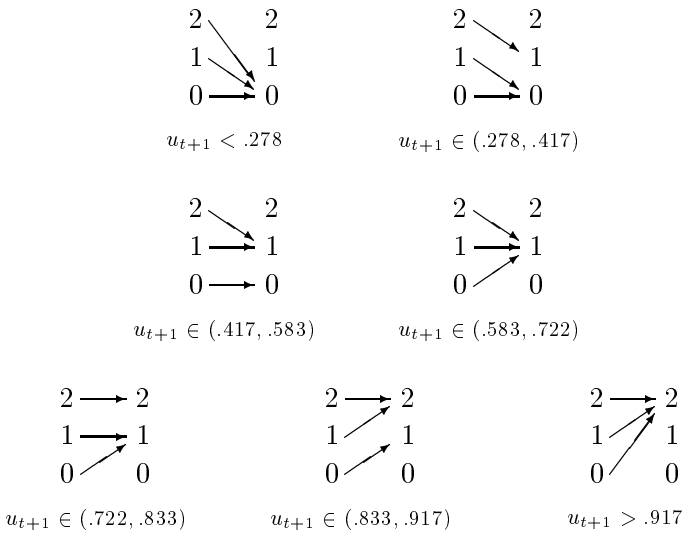



Figure 1: All possible transitions for the Beta-Binomial(2,2,4) example

**Beta-binomial, continued.** Consider the $\{X_t\}$ subchain from the previous example, and let $n = 2$, $\alpha = 2$ and $\beta = 4$. The state space is $\mathcal{X} = \{0, 1, 2\}$. The transition probabilities are

$$\begin{aligned} &\Pr(0 \mapsto 0) = .583, \quad \Pr(0 \mapsto 1) = .333, \quad \Pr(0 \mapsto 2) = .083, \\ &\Pr(1 \mapsto 0) = .417, \quad \Pr(1 \mapsto 1) = .417, \quad \Pr(1 \mapsto 2) = .167, \\ &\Pr(2 \mapsto 0) = .278, \quad \Pr(2 \mapsto 1) = .444, \quad \Pr(2 \mapsto 2) = .278 \end{aligned}$$

Thus we can draw $U_{t+1} \sim \text{Uniform}(0, 1)$ and make the transitions illustrated by Figure 1.

■

Figure 1 shows that coupled chains will all go to the same state, or *coalesce* if there is ever a time $t$ such that either $U_t < .278$ or $U_t > .917$. Once coupled chains coalesce at time $t$, they remain coalesced at all times greater than $t$. And because the $U_t$'s are mutually independent coalescence is guaranteed to happen eventually. The next theorem gives some general results about coalescence.

**Theorem 1** *Suppose we have k coupled Markov chains,* $X^{(1)}, X^{(2)}, \ldots, X^{(k)}$, *where*

*(i). $X^{(j)}$ starts in state $j$ (so one chain starts in each state of $\mathcal{X}$)*

*(ii). updating is performed according to $X_{t+1}^{(j)} = \phi(x_t^{(j)}, u_{t+1})$, where the $U_i$ are mutually independent.*

*Then*

*(a). The time $T$ to coalescence is a random variable that depends only on $U_1, U_2, \ldots$.*

*(b). The random variable $X_T$, the common value at coalescence, is independent of any starting values.*

**Proof**: Part $(a)$ is immediate by construction, and part $(b)$ follows since $X_T$ is a function only of $U_1, \ldots, U_T$ and not of $X_0$.

■

Conclusion (b) of Theorem 1 says that $T$ is a time at which the initial state of the chain has "worn off". One might therefore hope that $X_T$ is a draw from the stationary distribution $\pi$. This hope is false. It is true that if $T^*$ is a *fixed* time, and $X_{T^*}$ is independent of $X_0$, then $X_{T^*} \sim \pi$. Unfortunately, $T$ is a random time and in general, $X_T \not\sim \pi$, as the following example illustrates.

> **Two-state** Consider the Markov chain with state space $\{1, 2\}$ and transition kernel $K(1,1) = K(1,2) = .5$; $K(2,1) = 1$; $K(2,2) = 0$. The stationary distribution is $\pi(1) = 2/3$; $\pi(2) = 1/3$. A little thought shows that parallel chains can coalesce only in $X_T = 1$ and therefore $X_T \not\sim \pi$.

■

# 3 Propp and Wilson

Propp and Wilson (1996) discovered how to take advantage of coalescence while sampling the chain at a fixed time, thereby producing a random variable having distribution $\pi$, exactly. Their algorithm is called *Coupling from the Past* (`CFTP`), and is based on the idea that if a chain were started at time $t = -\infty$ in any state $X_{-\infty}$, it would be in equilibrium by time $t = 0$, so $X_0$ would be a draw from $\pi$. This would happen since the chain would have run for an infinite length of time.

To implement this idea in an algorithm, we use the coalescence strategy. We first find a time $-T$ such that $X_0$ does not depend on $X_{-T}$ (coalescence occurs between time $-T$ and time 0), and then we determine $X_0$ by starting chains from all states at time $t = -T$ and following them to time $t = 0$.

`CFTP` is an algorithm for finding $-T$ and $X_0$, and goes as follows.

(1). Start chains $X^{(1)}, X^{(2)}, \ldots, X^{(k)}$ at time $t = -1$ from every state of $\mathcal{X}$. Generate $U_0$.

(2). Update each chain to time $t = 0$ by applying the transition rule $X_0^{(j)} = \phi(x_{-1}^{(j)}, u_0)$. If the chains have coalesced at time $t = 0$, then $-T = -1$ and the common value $X_0$ is a draw from $\pi$.

(3). Otherwise, move back to time $t = -2$, generate $U_{-1}$, and update each chain using $X_{-1}^{(j)} = \phi(x_{-2}^{(j)}, u_{-1})$ and $X_0^{(j)} = \phi(x_{-1}^{(j)}, u_0)$. If the chains have coalesced at time $t = 0$, then $-T = -2$ and the common value $X_0$ is a draw from $\pi$.

(4). Otherwise, move back to time $t = -3$ and continue.

It is crucial, when going back to $t = -2$, to use the same $U_0$ that was already drawn. Specifically, we start chains at time $t = -2$ from every state; draw $U_{-1}$; use $U_{-1}$ to update all the chains to time $t = -1$; use the $U_0$ from before to update all the chains to time $t = 0$; check for coalescence; and either accept $T = -2$ and $X_0$ if the chains have coalesced or go back to time $t = -3$ if they haven't. The algorithm continues backing through time until coalescence occurs.

**Theorem 2** *The `CFTP` algorithm returns a random variable distributed exactly according to the stationary distribution of the Markov chain.*

**Proof**: The proof is based on establishing the following three facts:

(1). The $k$ Markov chains will coalesce at some finite time into one chain, call it $X_t^*$.

(2). For each $j = 1, 2, \ldots, k$, $X_{-t}^{(j)} \to X \sim \pi$ as $t \to \infty$

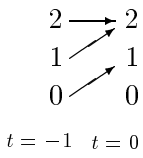
(3). For each $j = 1, 2, \ldots, k$, $X_{-t}^{(j)} \to X_0^*$ as $t \to \infty$

It then follows that $X_0^*$ and $X$ have the same distribution and, in particular, $X_0^* \sim \pi$. See Appendix 6.2 for details.

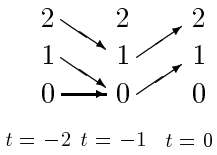
■

We use the Beta-Binomial example for illustration.

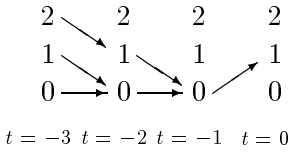
**Beta-Binomial, continued.** Begin at time $t = -1$ and draw $U_0$. Suppose $U_0 \in (.833, .917)$. The next picture shows the result of updating all chains.




The chains have not coalesced, so we go to time $t = -2$ and draw $U_{-1}$. Suppose $U_{-1} \in (.278, 417)$. The next picture shows the result of updating all chains.




The chains have still not coalesced so we go to time $t = -3$. Suppose $U_{-2} \in (.278, .417)$. The next picture shows the result of updating all chains.




All chains have coalesced into $X_0 = 1$. We accept $X_0$ as a draw from $\pi$ . Note: even though the chains have coalesced at $t = -1$, we do not accept $X_{-1} = 0$ as a draw from $\pi$.

■

In `CFTP`, $T$ and $X_0$ are dependent random variables. Therefore, a user who gets impatient or whose computer crashes and who therefore restarts

runs when $T$ gets too large will generate biased samples. Another algorithm, due to Fill (1998), generates samples from $\pi$ in a way that is independent of the number of steps.

# 4 Fill's algorithm

A simple version of Fill's algorithm (`Fill`) is:

1. Arbitrarily choose a time $T$ and state $x_T = z$.
2. Generate $X_{T-1}|x_T$, $X_{T-2}|x_{T-1}$, ... , $X_0|x_1$.
3. Generate $[U_1|x_0, x_1]$, $[U_2|x_1, x_2]$, ... , $[U_T|x_{T-1}, x_T]$
4. Begin chains in all states at time $T = 0$ and use the common $U_1$, ... , $U_T$ to update all chains
5. If the chains have coalesced by time $T$ (and are in state $z$ at time $T$), then accept $x_0$ as a draw from $\pi$
6. Otherwise begin again, possibly with a new $T$ and $z$.

We note that the $U_1, \ldots, U_T$ used for the coalescing chains are generated in such a way to insure that $x \to z$. (We write $x \to z$ to denote that the chain goes from state $x$ to state $z$ in $T$ steps.) So, for example, generate $U_1$ to be uniform on the set $\{u : x_1 = \phi(x_0, u)\}$, $U_2$ to be uniform on the set $\{u : x_2 = \phi(x_1, u)\}$ etc. See the example for a further illustration.

There are two ways to prove that `Fill` is correct. We present one here and one in the appendix. Let $C_T(z)$ be the event that all chains have coalesced and are in state $z$ at time $T$.

*First proof:* `Fill` delivers a value only if $C_T(z)$ occurs, so we need to prove $\Pr[X_0 = x|C_T(z)] = \pi(x)$. This probability is

$$\Pr[X_0 = x|C_T(z)] = \frac{\Pr[z \to x]\Pr[C_T(z)|x \to z]}{\sum_{x'} \Pr[z \to x']\Pr[C_T(z)|x' \to z]}.$$

Now because the coalescence event entails each $x' \to z$, we have for every $x'$

$$\Pr[C_T(z)|x' \to z] = \frac{\Pr[C_T(z) \text{ and } x' \to z]}{\Pr[x' \to z]} = \frac{\Pr[C_T(z)]}{\Pr[x' \to z]}, \qquad (1)$$

and writing $\Pr[x' \to z] = K^T(x', z)$ the probability becomes

$$\begin{aligned}\Pr[X_0 = x | C_T(z)] &= \frac{K^T(z,x)\Pr[C_T(z)]/K^T(x,z)}{\sum_{x'} K^T(z,x')\Pr[C_T(z)]/K^T(x',z)} \\ &= \frac{K^T(z,x)/K^T(x,z)}{\sum_{x'} K^T(z,x')/K^T(x',z)},\end{aligned}$$

Using the detailed balance condition we have $K^T(z,x)/K^T(x,z) = \pi(x)/\pi(z)$, and thus,

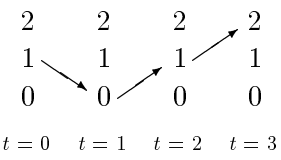
$$\Pr[X_0 = x | C_T(z)] = \frac{\pi(x)/\pi(z)}{\sum_{x'} \pi(x')/\pi(z)} = \pi(x).$$

■

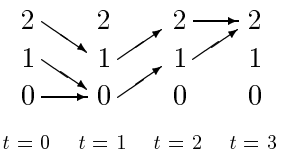
We follow the Beta-binomial (2,2,4) example through the steps in `Fill`.

**Beta-Binomial, continued.**

1. We arbitrarily choose $T = 3$ and $X_T = 2$.
2. Our chain is reversible, so $[X_2 | X_3 = 2] = [X_3 | X_2 = 2] = \text{BetaBin}(2,4,4)$. The probabilities are given on page 4. We generate $X_2$. Suppose it turns out to equal 1. Similarly, $X_1 | X_2 = 1 \sim \text{BetaBin}(2,3,5)$; suppose we get $X_1 = 2$; $X_0 | X_1 = 2 \sim \text{BetaBin}(2,4,4)$; suppose we get $X_0 = 1$. The next picture shows the transitions we've generated.




3. $X_0 = 1$, $X_1 = 0$, $X_2 = 1$ and $X_3 = 2$ imply $U_1 \sim \text{U}(0, .417)$; $U_2 \sim \text{U}(.583, .917)$; and $U_3 \sim \text{U}(.833, 1)$. (See Figure 1.) Suppose we generate $U_1 \in (.278, .417)$, $U_2 \in (.833, .917)$ and $U_3 > .917$.
4. Begin chains in states 0, 1 and 2.
5. The next picture follows the chains through time $t = 3$.



6. The chains coalesce in $X_3 = 2$; so we accept $X_0 = 1$ as a draw from $\pi$.

■

`Fill` depends on an arbitrary choice of $T$ and $X_T$. To get some feeling for how big $T$ needs to be and whether the choice of $X_T$ is important, we ran `Fill` on a Beta-binomial$(16, 2, 4)$ example. For each of $X_T = 0, 2, \ldots, 16$, we ran `Fill` in a loop with $T = 1, 3, \ldots$ successively until the algorithm returned a value. The whole simulation was repeated 50 times. Figure 2 is a boxplot, sorted by $X_T$, of the $T$ for which coalescence was achieved. The horizontal axis is the value of $X_T$ which we fixed in advance. The vertical axis is the value of $T$ for which coalescence occurred. The figure shows that coalescence occurred much more quickly when we chose either $X_T = 0$ or $X_T = 16$ than any other value of $X_T$.

# 5 Discussion

- A potentially troublesome point is detecting whether coalescence has occurred. In general, starting and keeping track of chains from every state is computationally infeasible. In (partially) ordered state spaces with a *monotone* transition rule it is only necessary to keep track of chains started from the maximal and minimal members. A monotone transition rule is one in which $X_t \geq Y_t \Rightarrow X_{t+1} = \phi(X_t, u_{t+1}) \geq Y_{t+1} = \phi(Y_t, u_{t+1})$. If our transition function is an inverse-cdf function that is stochastically ordered, then the transition rule will be monotone.

  This is the case in our example, where a chain started from state 1 is sandwiched between chains started from states 0 and 2. Therefore it is only necessary to keep track of chains started from 0 and 2 to determine whether coalescence has occurred. In fact, if there exist maximal and minimal elements, coalescence is detectable even with a continuous state space. Non-monotone transition rules or state spaces without minimal and maximal elements require more sophisticated methods. See Fill et al. (1999) or Green and Murdoch (1999) for details and extensions.

- In describing `CFTP` we set $T$ successively equal to -1, -2, .... In fact, any decreasing sequence would do as well. Propp and Wilson (1996) argue that $T = -1, -2, -4, -8, \ldots$ is near optimal. In `Fill`, if $X_0$ is

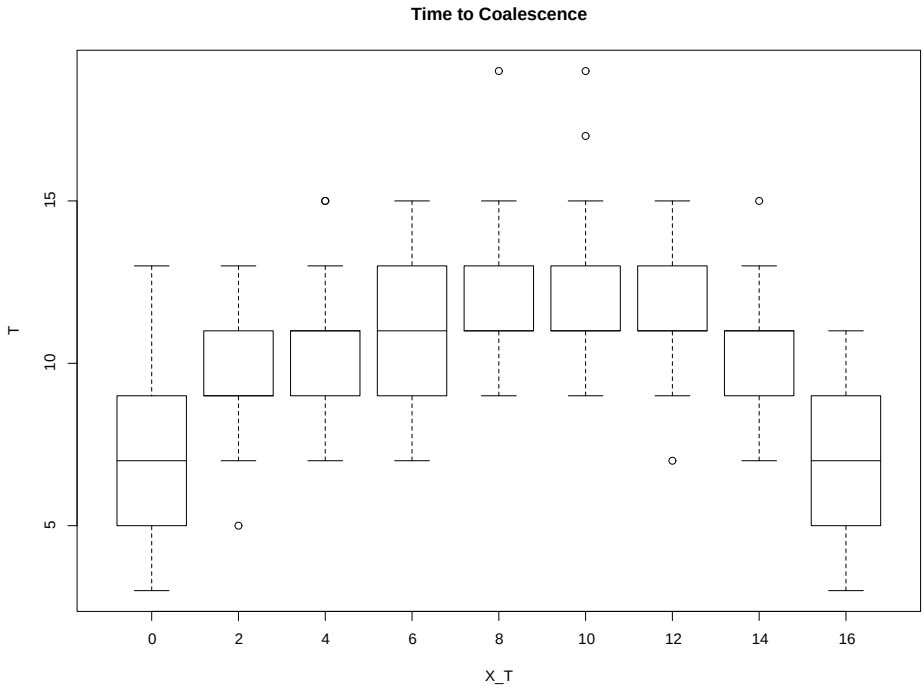



Figure 2: Time to coalescence for 50 runs of Fill's algorithm, for each value of $X_T$.

rejected, or if one is generating many realizations, one may wish to choose new values of $T$ and $z$ for the next proposal. Figure 2 shows that some combinations of $(T, z)$ are more likely to lead to coalescence than others. There is no general theory at present to guide the choice of $(T, z)$. In practice the results of early iterations may guide the choice of $(T, z)$ in later iterations.

- In his original algorithm described here, when running the $k$ chains for coalescence, Fill used constrained uniform variables $U_1, \ldots, U_T$ conditional on $X_0, \ldots, X_T$, generating $[U_1|x_0, x_1]$, $[U_2|x_1, x_2]$, $\ldots$ , $[U_T|x_{T-1}, x_T]$. This insures that the chain starting in $x$ will end up in $z$. This is practical as long as the conditional distribution of the $U_i$'s given the $X_i$'s is not too difficult.

  An alternative to the algorithm described in `Fill` is to generate the $U_i$'s unconditionally. (Typically $U_i \sim U(0, 1)$.) Using these $U_i$'s, check whether $x_0 \to z$. If yes, then also check for $C_T(z)$ and either accept or reject $X_0$ accordingly. Otherwise, discard the $U_i$'s and generate another set until finding one such that $x_0 \to z$. Ultimately we will accept $x_0$ with probability $\Pr[C_T(z)|x_0 \to z]$, as required.

- Some practical applications of Markov chains iterate between a discrete $X$ and a parameter $\theta$ which might be either discrete or continuous. In such cases we can obtain perfect samples from the joint distribution of both $X$ and $\theta$. For example, consider modeling the data $Y$ as a mixture of Normal distributions. The model is usually extended to include indicator variables $X$, which are not observed but which indicate which $Y$'s come from the same mixture components. Conditional on $X$, the model is a straightforward collection of Normals. Let $\theta$ denote all unknown parameters other than $X$. The posterior is typically analyzed through a Gibbs sampler that iterates between $[X|\theta]$ and $[\theta|X]$. The iterates of $X$ form a subchain on a finite state space and are amenable to perfect sampling. Given a perfect sample of $X$, one can simulate from $[\theta|X]$ to obtain a perfect sample of $\theta$.

  This remark extends to other latent variable models, but one must keep in mind that the size of the finite parameter space of $X$ in the mixture example is $k^n$, which rapidly gets unmanageable unless monotonicity features can be exhibited, as in Hobert et al. (1999).

- To remove the difficulty with continuous state space chains, another promising direction relies on *slice sampling*. This technique is a special

case of Gibbs sampling (See Robert and Casella 1999, Sect. 7.1.2) and takes advantage of the fact that the marginal (in $x$) of the uniform distribution on $\{(x,u);\ u \le \pi(x)\}$ is $\pi(x)$. The idea, detailed in Mira et al. (1999), is that, if $x_0'$ is a variable generated from the uniform distribution on $\{x;\ \pi(x) \ge \epsilon\pi(x_0)\}$, it can also be taken as a variable generated from the uniform distribution on $\{x;\ \pi(x) \ge \epsilon\pi(x_1)\}$ for all $x_1$'s such that $\epsilon\pi(x_0) \le \epsilon\pi(x_1) \le \pi(x_0')$ by a simple accept–reject argument. Therefore, assuming a bounded state space $\mathcal{X}$, if one starts with $x_0'$ generated uniformly on $\mathcal{X}$, a finite sequence $x_0', \ldots, x_T'$ can be used instead of the continuum of possible starting values, with $x_i'$ being generated from a uniform distribution on $\{x;\ \pi(x) \ge \pi(x_{i-1}')\}$, and $T$ being such that $\pi(x_T') \ge \epsilon \sup \pi(x)$. Moreover, slice sampling exhibits natural monotonicity structures which can be exploited to further reduce the number of chains. The practical difficulty of this approach is that uniform distributions on $\{x;\ \pi(x) \ge \epsilon\pi(x_0)\}$ may be hard to simulate, as shown in Casella et al. (1999) in the setup of mixtures.

- Perfect sampling is currently an active area of research. David Wilson maintains a web site of papers on perfect sampling at `http://dimacs.rutgers.edu:80/~dbwilson/exact.html`. The interested reader can find links to articles ranging from introductory to the latest research.

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# 6 Appendix

## 6.1 A Markov Chain Glossary

We will work with discrete state space Markov chains. The following definitions can be extended to continuous state spaces as long as the usual measurability complications are carefully dealt with.

A Markov chain $X_1, X_2, \ldots$, is *irreducible* if the chain can move freely throughout the state space; that is, for any two states $x$ and $x'$ with $\pi(x') > 0$, there exists an $n$ such that $\Pr[X_n = x' | X_0 = x] > 0$. Moreover, as the chains we are considering are all *positive*, that is, the stationary distribution

is a probability distribution, irreducibility also implies that the chain is *recurrent*. A recurrent chain is one in which the average number of visits to an arbitrary state is infinite.

A state $x$ has *period* $d$ if $P(X_{n+t} = x|X_t = x) = 0$ if $n$ is not divisible by $d$, $d$ being the largest integer with this property. For example, if a chain starts ($t = 0$) in a state with period 3, the chain can only return to that state at times $t = 3, 6, 9, \ldots$. If a state has period $d = 1$, it is *aperiodic*. In an irreducible Markov chain, all states have the same period. If that period is $d = 1$, the Markov chain is aperiodic.

We then have the following theorems.

**Theorem 3 Convergence to the stationary distribution** *If the countable state space Markov chain $X_1, X_2, \ldots$, is positive, recurrent and aperiodic with stationary distribution $\pi$, then from every initial state*

$$X_n \to X \sim \pi.$$

A positive, recurrent and aperiodic Markov chain is often called *ergodic*, a name also given to the following theorem, a cousin of the Law of Large Numbers.

**Theorem 4 Convergence of Sums** *If the countable state space Markov chain $X_1, X_2, \ldots$, is ergodic with stationary distribution $\pi$, then from every initial state*

$$\frac{1}{n}\sum_{i=1}^{n} h(X_i) \to E_\pi h(X)$$

*provided* $E_\pi|h(X)| < \infty$

Adding the property of *reversibility* will get us a Central Limit Theorem. A Markov chain is *reversible* if the distribution of $X_{t+1}$ conditional on $X_{t+2} = x$ is the same as the distribution of $X_{t+1}$ conditional on $X_t = x$. For any set $B$ we have

$$\sum_{y\in\mathcal{X}}\sum_{x\in B} K(y, x) = \sum_{y\in\mathcal{X}}\sum_{x\in B} K(x, y)$$

so the transition probabilities are the same whether we go forward or backward along the chain.

**Theorem 5 Central Limit Theorem** *If the countable state space Markov chain $X_1, X_2, \ldots$, is ergodic and reversible with stationary distribution $\pi$, then from every initial state*

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} [h(X_i) - E_\pi h(X)] \to \mathcal{N}(0, \sigma^2),$$

*provided* $0 < \sigma^2 = \text{Var } h(X_0) + \sum_{i=1}^{\infty} \text{Cov}_\pi(h(X_0), h(X_i)) < \infty$

## 6.2 Proof of Theorem 2

We will establish the three facts stated in the outline of the proof of Theorem 2, and fill in the gaps in the arguments. First, we show that the $k$ Markov chains will coalesce at some finite time with probability 1. We adapt the proof presented in Thönnes (1999).

Recall that we have $k$ coupled Markov chains, $X^{(1)}, X^{(2)}, \ldots, X^{(k)}$, where $X^{(j)}$ starts in state $j$ (so one chain starts in each state of $\mathcal{X}$). As each chain is irreducible, we can find $N_j$ such that

$$P(X_{N_j}^{(j)} = x | X_0^{(j)} = j) > 0, \text{ for all } x \in \mathcal{X}.$$

Set $N = \max\{N_1, N_2, \ldots, N_k\}$. It then follows that each chain has positive probability of being in any state at time $N$, and that for some $\varepsilon > 0$

$$P(X_N^{(1)} = X_N^{(2)} = \cdots = X_N^{(k)}) > \varepsilon.$$

Now run the `CFTP` algorithm in blocks of size $N$ as follows.

(i). Starting at time $-N$, run the $k$ coupled chains to time 0. If they have not coalesced

(ii). Starting at time $-2N$, run the $k$ coupled chains to time 0. If they have not coalesced

(iii). $\vdots$

Define the event

$$C_i = \{ \text{ The } k \text{ chains coalesce in } (-iN, -(i-1)N) \}.$$

From the above argument we have that $P(C_i) > \varepsilon$. Moreover, the $C_i$ are independent because coalescence in $(-iN, -(i-1)N)$ only depends on $U_{-iN}, U_{-iN-1}, \ldots, U_{-(i-1)N}$ (which are independent of all of the other $U$s)

and does not depend on the initial states. This is because we restart each iteration from all states, allowing us to recreate the chains using only the $U$s. (This last point is crucial, and shows why we must run the chains from the past to the present. If we went forward, we could not restart in every state, so coalescence might depend on the initial conditions. Only by running the chains from the past to the present, starting one chain in each state, can we guarantee independence from the initial conditions, and hence the independence of the $C_i$s.)

Finally, we observe that

$$\begin{aligned} P(\text{ No coalescence after } I \text{ iterations}) &= 1 - \prod_{i=1}^{I} [1 - P(C_i)] \\ &< (1-\varepsilon)^I \\ &\to 0 \text{ as } I \to \infty, \end{aligned}$$

showing that the probability of coalescence is 1. We can, in fact, make the stronger conclusion that the coalescence time is almost surely finite by noting that

$$\sum_{i=1}^{\infty} P(C_i) = \infty \Rightarrow P(C_i \text{ infinitely often }) = 1,$$

from the Borel-Cantelli Lemma.

We next show that for $j = 1, 2, \ldots, k$,

$$X_{-t}^{(j)} \to X \sim \pi \text{ as } t \to \infty \tag{2}$$

and

$$X_{-t}^{(j)} \to X_0^* \text{ as } t \to \infty. \tag{3}$$

Since $X_t^{(j)}$ is a Markov chain with a limiting distribution, $X_t^{(j)} \to X \sim \pi$ as $t \to \infty$. Now (2) follows by reversibility, that is, the forward chain and the backward chain have the same transitions.

Result (3) is a consequence of the fact that the `CFTP` algorithm starts with a Markov chain in every state. This means that the realization of *any* Markov chain starting at $-\infty$ will, at some time $-t$, couple with one of the `CFTP` chains and thereafter be equal to $X_t^*$. Therefore $X_0^*$ and $X$ have the same distribution and, in particular, $X_0^* \sim \pi$.

■

### 6.3 Alternate Proof of `Fill`

We can view `Fill` as a rejection algorithm: generate and propose $X_0 = x$; then accept $x$ as a draw from $\pi$ if $C_T(z)$ has occurred. The proposal distribution is the $T$-step transition density $K^T(z, \cdot)$. `Fill` is a valid rejection algorithm if we accept $X_0 = x$ with probability

$$\frac{1}{M}\frac{\pi(x)}{K^T(z,x)} \text{ where } M \geq \sup_x \frac{\pi(x)}{K^T(z,x)}.$$

From detailed balance we can write $\pi(x)/K^T(z,x) = \pi(z)/K^T(x,z)$ and, since $\Pr[C_T(z)] \leq K^T(x',z)$ for any $x'$, and hence $\Pr[C_T(z)] \leq \min_{x'} K^T(x',z)$, we have the bound

$$\frac{\pi(x)}{K^T(z,x)} = \frac{\pi(z)}{K^T(x,z)} \leq \frac{\pi(z)}{\min_{x'} K^T(x',z)} \leq \frac{\pi(z)}{\Pr[C_T(z)]} = M.$$

So we accept $X_0 = x$ with probability $\frac{1}{M}\frac{\pi(x)}{K^T(z,x)}$, which is quite difficult to compute. However,

$$\frac{1}{M}\frac{\pi(x)}{K^T(z,x)} = \frac{\Pr[C_T(z)]}{\pi(z)}\frac{\pi(x)}{K^T(z,x)} = \frac{\Pr[C_T(z)]}{\pi(z)}\frac{\pi(z)}{K^T(x,z)} = \frac{\Pr[C_T(z)]}{K^T(x,z)},$$

where we have again used detailed balance. But now, from (1), we have that $\frac{\Pr[C_T(z)]}{K^T(x,z)} = \Pr[C_T(z)|x \to z]$, exactly the event that `Fill` simulates.

■

Finally, note that the algorithm is more efficient if $M$ is as small as possible, so choosing $z$ to be the state that minimizes $\pi(z)/\Pr[C_T(z)]$ is a good choice. This, also, will be a difficult calculation, but in running the algorithm, these probabilities can be estimated.