# Two Applications of Urn Processes: The Fringe Analysis of Search Trees and the Simulation of Quasi-Stationary Distributions of Markov Chains 

David Aldous ${ }^{1}$<br>Department of Statistics<br>University of California<br>Berkeley, CA 94720<br>Barry Flannery<br>Department of Mathematics and Computer Science<br>Valdosta State College<br>Valdosta, GA 31698<br>José Luis Palacios ${ }^{2}$<br>Universidad Simón Bolǐvar Departamento de Matemáticas y C. C.<br>Apartado 89.000<br>Caracas, Venezuela

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Department of Statistics
University of California
Berkeley, California

# Two Applications of Urn Processes: The Fringe Analysis of Search Trees and the Simulation of Quasi-Stationary Distributions of Markov Chains 

David Aldous ${ }^{1}$<br>Department of Statistics<br>University of California<br>Berkeley, CA 94720<br>Barry Flannery<br>Department of Mathematics and Computer Science<br>Valdosta State College<br>Valdosta, GA 31698<br>José Luis Palacios ${ }^{2}$<br>Universidad Simón Bolivar Departamento de Matemáticas y C. C.<br>Apartado 89.000<br>Caracas, Venezuela

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#### Abstract

From an urn containing colored balls draw one ball and replace a random number of differently-colored balls, with the distribution of the added balls depending only on the color of the ball drawn. Under mild regularity conditions, the proportions of different colors will converge to deterministic limits. Two applications of this standard result are described. The average efficiency of binary trees, 2-3 trees and other structures for information storage has been studied with diverse techniques. One such technique for estimation is called fringe analysis, and this turns out to involve urn processes. The other topic is the simulation of quasi-stationary distributions of Markov chains. These arise when the chain is conditioned to avoid a taboo set. Here urn processes are used to prove an analog of the classical result on convergence of empirical distributions to the stationary distribution.


Key Words: urn process, branching process, binary search tree, 2-3 trees, empirical convergence, quasi-stationary distribution.

AMS (MOS) Subject Classification: 60J20, 68P05

## 1. Urn Processes

In this section we define a class of urn processes and state a limit theorem. Except for minor differences in hypotheses, these processes and the limit theorem are those described in Athreya and Ney (1972) section V.9.

Let $\left(c_{1}, c_{2}, \ldots, c_{m}\right)$ be a vector of constants. Consider an urn and a supply of balls of $m$ colors. The composition of the urn after $n$ draws is described by a random vector $X(n)=\left(X_{1}(n), \ldots, X_{m}(n)\right)$, where $X_{i}(n)$ is the number of balls of color $i$. A draw is performed as follows: pick one ball from the urn, with each ball of color i having chance $\frac{c_{i}}{\sum_{i} c_{i} X_{i}(n)}$ of being drawn. We see that the vector $c$ gives the relative probability of an individual i-colored ball being drawn. Now, given that a ball of color $i$ has been drawn, remove it and replace it by $Z_{j}^{(i)}$ balls of color $j(1 \leq j \leq m)$. The random choices on each draw are independent. Finally, let the initial distribution $\mathrm{X}(0)$ be arbitrary.

This describes an urn process parametrized by $m$ constants ( $c_{1}, \ldots, c_{m}$ ) and $m$ distributions $\left(\mathrm{Z}_{\mathrm{j}}^{(\mathrm{i})}, 1 \leq \mathrm{j} \leq \mathrm{m}\right), 1 \leq \mathrm{j} \leq \mathrm{m}$. We make the following hypotheses concerning these parameters:
(1.1) $c_{i}>0$ for all $i$
(1.2) $Z_{j}^{(i)}$ is non-negative integer-valued, $\sum_{j} Z_{j}^{(i)} \geq 1$ for each $i$ and $P\left(\sum_{j} Z_{j}^{(i)}>1\right)>0$ for some i.
(1.3) $E\left(Z_{j}^{(i)} \log Z_{j}^{(i)}\right)<\infty$.

Let $Q=\left(q_{i, j}\right)$ be the matrix with entries $q_{i, j}=E Z_{j}^{(i)}$. We make the last assumption
(1.4) $Q$ is irreducible, that is to say for each pair $i, j$ there exists an $n$ such that $\mathrm{q}_{\mathrm{i}, \mathrm{j}}^{\mathrm{n}}>0$.
Next, let $\hat{X}(n)$ be the vector of proportions after $n$ draws:

$$
\hat{X}_{i}(n)=\frac{X_{i}(n)}{\sum_{j} X_{j}(n)}
$$

Let $\mathbb{R}$ be the matrix with entries $\mathrm{r}_{\mathrm{ij}}=\mathrm{c}_{\mathrm{i}}\left(\mathrm{q}_{\mathrm{i}, \mathrm{j}}-\delta_{\mathrm{i}, \mathrm{j}}\right)$, where $\delta_{\mathrm{i}, \mathrm{j}}=1_{(\mathrm{i}=\mathrm{j})}$.
Theorem 1.5. Consider an urn process satisfying (1.1) - (1.4). Then
(a) the equations $\sum_{\mathrm{i}} \mathrm{x}_{\mathrm{i}} \mathrm{r}_{\mathrm{i}, \mathrm{j}}=\lambda \mathrm{x}_{\mathrm{j}}, 1 \leq \mathrm{j} \leq \mathrm{m}$ have a unique solution $(\mathrm{x}, \lambda)$ for which $\mathrm{x}_{\mathrm{i}}>0, \Sigma \mathrm{x}_{\mathrm{i}}=1$ and $\lambda>0$.
(b) $\hat{\mathrm{X}}(\mathrm{n}) \rightarrow \mathrm{x}$ a.s. as $\mathrm{n} \rightarrow \infty$, where x is the eigenvector in (a).

This theorem is essentially the result of Athreya and Ney (1972), except for some minor changes in hypotheses; they use the hypotheses
(1.1)' $c_{i}=1$ for each $i$
(1.2)' the drawn ball is replaced, so that $Z_{i}^{(i)} \geq 1$ for all $i$ and
(1.3)' the matrix $\mathbf{Q}$ is regular, that is to say there exists $n$ such that $q_{i, j}^{n}>0$ for all pairs $\mathbf{i , j}$.

The proof uses the natural embedding of the urn process into a continuous-time multitype branching process, where individuals of type $i$ have exponential (mean 1) lifetimes and on death are replaced by $\mathrm{Z}_{\mathrm{j}}^{(\mathrm{i})}(1 \leq \mathrm{j} \leq \mathrm{m})$ offspring of type j . Minor modifications of the proof allow our relaxations to be made. To modify (1.1)' make type i individuals have exponential (with rate $\mathrm{c}_{\mathrm{i}}$ ) lifetimes. Condition (1.2)' is used to ensure that the branching process is supercritical with extinction probability 0 , and our hypothesis (1.2) has the same effect. Finally, we see (1.3)' is to guarantee that the process is "positive regular", and our weaker hypothesis (1.4) does the job.

For later use, we remark that in the context of Theorem 1.5,

$$
\begin{equation*}
\text { if } \sum_{j} q_{i, j} c_{j}=c_{i}+1 \text { for all } i \text {, then } \lambda=1 \tag{1.6}
\end{equation*}
$$

To show this, we observe

$$
\begin{aligned}
\lambda \sum_{j} c_{j} x_{j} & =\sum_{j} \sum_{i} c_{j} x_{i} r_{i, j} \quad \text { using (a) } \\
& =\sum_{i} \sum_{j} c_{j} x_{i} c_{i}\left(q_{i, j}-\delta_{i, j}\right) \text { by definition of } r_{i, j} \\
& =\sum_{i} c_{i} x_{i} \text { by (1.6). }
\end{aligned}
$$

The purpose of this paper is to exhibit two completely different applications of this theorem. The "novel content" of the paper is simply the (trivial) observation that the urn result does apply to the problems discussed (without this observation, the problems look more difficult). We have chosen to describe the problems in Section 2 in some detail, rather than refer to other papers. They would perhaps make interesting nontraditional examples in a course on branching processes or urn models.

## 2. Fringe Analysis of Search Trees

Binary search trees are a well-known structure for storage, retrieval and addition of information labelled by numerical keys. Perhaps the simplest example is that described in Knuth (1973). Keys are stored at the internal nodes. To search for a key $x$, one compares $x$ with the key $y$ (say) occupying the top node. If $x \neq y$, then move
to the left or right according to whether $x<y$ or $x>y$, respectively. At the next mode, a comparison is made with the key located there. Ultimately, either x is located or the search terminates at an external node. In the latter case, $x$ may be appended at that node thus creating two new external nodes. The figure below shows the effect of adding keys 13 and 1 to the tree. A standard convention is to depict internal nodes with ovals and external nodes with squares.

Figures 1 and 2 here.

Another scheme for information storage, called " $2-3$ tree" (see Yao (1978)) allows the internal nodes to contain either 1 or 2 keys and has all the external nodes at the same bottom level. To put a new key into a node that contains only one key, we simply insert it as a second key. If the node already contains 2 keys, the node is split into two nodes containing respectively the minimum and the maximum of the three keys and the middle key is inserted into the parent node by repeating the process. When thee is no node above, a new root is created to hold the middle key. For example, to this 2-3 tree

Figure 3 here.
we add the keys 20 and 65 to obtain:

Figure 4 here.

Write $t_{n}$ to denote a tree with $n$ keys. With such a tree one may associate various statistics, $f\left(t_{n}\right)$, which measure aspects of the "efficiency" of using the search tree. For instance, one may be interested in the average number of comparisons needed in a search or the height of the tree. Consider any tree with $\mathrm{j}-1$ keys in it. These $\mathrm{j}-1$ keys divide all possible key values into $j$ intervals (notice that there are as many such intervals as external nodes). The insertion of a new key into the tree is said to be a random insertion if the new key has equal probabilities of being in any of the j intervals defined before. A random insertion is accomplished if we take as the successive keys $K_{1}, K_{2}, \ldots$ a sequence of i.i.d. continuous random variables. Any given algorithm for tree construction will then generate a random sequence of trees $T_{n}$, and we will speak of 'random binary trees", 'random 2-3 trees", etc.

One may compare different algorithms by choosing a measure, f , of efficiency and comparing the random variables $f\left(T_{n}\right)$. It turns out that the algorithm for 2-3 trees is efficient whereas that of the binary tree is inefficient. The latter algorithm can be
improved by means of a simple heuristic proposed and analyzed by Poblete and Munro (1985). Trees of the form shown in the following diagram are produced. To this tree

Figure 5 here.
we add the record 8 . The elementary addition algorithm would yield

Figure 6 here.

But this new algorithm would yield the more balanced tree

Figure 7 here.
this algorithm may be described as follows: as comparisons are being made, if the basic algorithm would dictate a new level to be created emanating from the last node while the prior level (from this same node) is not full, then rotate the three keys in order that the median of the three keys is at the top, and the least key is at the left and the largest is at the right.

Let us define the fringe of a tree as the set of subtrees at the bottom of the tree which contain the external nodes. Then the algorithm just described produces trees of two types at the fringe:

Figure 8 here.

Let $\left(\mathrm{x}_{1}(\mathrm{n}), \mathrm{x}_{2}(\mathrm{n})\right)$ be the number of type 1 and type 2 subtrees in the fringe of the tree $t_{n}$ produced by this algorithm. Of course, this pair will not uniquely determine the tree, but it turns out that most statistics $f\left(t_{n}\right)$ can be either computed or bounded by functions $g\left(x_{1}(n), x_{2}(n)\right)$. The same thing can be said of the 2-3 trees, whose fringe exhibits subtrees of either of these two types:

Figure 9 here.

This technique of estimating efficiency by analyzing the vector $x(n)$ was introduced by Yao (1978) and is now called fringe analysis. It was further studied in Eisenbarth et al (1982), who proposed the following general framework. Given an algorithm, suppose we can define $m$ types of subtrees such that
(2.1) the fringe of the sequences of trees, $t_{n}$, produced by the algorithm consists only of subtrees of these $m$ types (in our examples $m$ is 2 );
(2.2) when an element is inserted into a subtree $\hat{\mathrm{t}}$, say, of the fringe, the other subtrees of the fringe are unaffected, and $\hat{\mathfrak{t}}$ is changed into one or more subtrees in a way depending only on the type of $\hat{\mathbf{t}}$.
Consider now the random trees $T_{n}$ grown from i.i.d. keys $K_{1}, K_{2}, \ldots$ and let $X(n)=\left(X_{1}(n), \ldots, X_{m}(n)\right)$ count the number of subtrees of types 1 to $m$ in the fringe of $T_{n}$. Then $X(n)$ is an urn process as described in Section 1 for which:
$\mathrm{Z}_{\mathrm{j}}{ }^{(\mathrm{i})}$ is the (usually deterministic) number of type j subtrees created by the insertion into a type i subtree;
$c_{i}$ is the number of external nodes in a type $i$ subtree (= the number of subintervals that the keys of a type $i$ subtree determine).
A draw of a ball is the arrival of a new key, and to select a ball of color i means now to have the new coming key landing in any one of the subtrees of type in the fringe ( $c_{i}$ "good"' places to land out of a total of $\Sigma c_{i} X_{i}(n)$ places, yielding the appropriate value of the probability).

We will assume

$$
\begin{equation*}
\text { the matrix } Q \text { with } q_{i j}=E Z_{j}^{(i)} \text { is irreducible. } \tag{2.3}
\end{equation*}
$$

This hypothesis is met by every reasonable algorithm that creates random trees, the reason being the cyclic nature of the creating process: usually insertion into a type i subtree ( $\mathrm{i}<\mathrm{m}$ ) originates a type $\mathrm{i}+1$ subtree and insertion into a type m subtree originates trees of several types including type 1. Of course, more complicated situations preserving irreducibility can arise. As the hypotheses (1.1) - (1.3) are automatically satisfied we may apply Theorem (1.5). The conclusion may be simplified by using some special structure. Because the binary tree grows one node at a time, the urn processes arising here have a special property:

$$
\begin{equation*}
\sum_{\mathrm{j}} \mathrm{c}_{\mathrm{j}} \mathrm{Z}_{\mathrm{j}}^{(\mathrm{i})}=\mathrm{c}_{\mathrm{i}}+1 ; \quad 1 \leq \mathrm{i} \leq \mathrm{m} \tag{2.4}
\end{equation*}
$$

and hence

$$
\begin{equation*}
\sum_{j} c_{j} q_{i, j}=c_{i}+1 \tag{2.5}
\end{equation*}
$$

This allows us to apply (1.6) and conclude that in Theorem 1.5 we have $\lambda=1$. Also, since the number of external nodes in a search tree equals the number of intervals determined by the first $n$ keys ( $n+1$ such intervals) we can conclude that

$$
\begin{equation*}
\sum_{i} c_{i} X_{i}(n)=n+1 \tag{2.6}
\end{equation*}
$$

Theorem 1.5 says

$$
\frac{\sum_{i} c_{i} X_{i}(n)}{\sum_{i} X_{i}(n)} \rightarrow b=\sum_{i} c_{i} x_{i}
$$

and then (2.6) gives

$$
\frac{1}{n} \sum_{i} X_{i}(n) \rightarrow 1 / b
$$

Thus in Theorem 1.5 we can substitute normalization by $n$ for normalization by $\sum_{i} X_{i}(n)$, to obtain the following result. Recall $r_{i, j}=c_{i}\left(q_{i, j}-\delta_{i, j}\right)$.
Theorem 2.7. In a fringe analysis satisfying (2.3), $\mathrm{X}_{\mathrm{i}}(\mathrm{n}) / \mathrm{n} \rightarrow \mathrm{x}_{\mathrm{i}} / \mathrm{b}$ a.s. as $\mathrm{n} \rightarrow \infty$, where $x$ is the unique solution of $\sum_{i} x_{i} r_{i, j}=x_{j}, 1 \leq j \leq m ; x_{i}>0 ; \Sigma x_{i}=1$, and where $b=\sum_{i} c_{i} x_{i}$.
Remarks. Previous fringe analysis - Yao (1978), Eisenbarth et al (1982), Poblete and Munro (1985), Cunto and Gascón (1987) and references therein - used recurrence relations for $E X_{i}(n)$ in order to conclude convergence of $E X_{i}(n) / n$ to the same limit. The urn process representation gives the stronger conclusion of a.s. convergence. Bagchi and Pal (1985) noted that the fringe of 2-3 trees had an urn process representation, and gave a proof of a central limit theorem: however, they gave an ad hoc proof, rather than exploiting known theory of urn processes.

For completeness, let us give some examples, even though the numerical calculations are the same as those in the original papers. We can apply simultaneously Theorem 2.7 to the trees created by the Poblete-Munro algorithm (P.M. trees from now on) and to the 2-3 trees. In both cases we have $c_{1}=2, c_{2}=3$ and $Q$ is the irreducible matrix $\left[\begin{array}{ll}0 & 1 \\ 2 & 0\end{array}\right]$. The equations have solution

$$
\left(\mathrm{x}_{1}, \mathrm{x}_{2}\right)=(2 / 3,1 / 3) ; \mathrm{b}=7 / 3
$$

so that almost surely we have the convergence:

$$
\begin{gather*}
{\left[\frac{X_{1}(n)}{X_{1}(n)+X_{2}(n)}, \frac{X_{2}(n)}{X_{1}(n)+X_{2}(n)}\right] \rightarrow\left(\frac{2}{3}, \frac{1}{3}\right]}  \tag{2.8}\\
{\left[\frac{X_{1}(n)}{n}, \frac{X_{2}(n)}{n}\right] \rightarrow\left[\frac{2}{7}, \frac{1}{7}\right] .} \tag{2.9}
\end{gather*}
$$

Now in order to be able to compute statistics of the efficiency of the trees using the above results, we need equations relating the fringe to the totality of the tree. Let $v(n)$ and $\mu(n)$ denote respectively the number of nodes above the fringe and the
number of internal nodes of a search tree. For P.M. trees we have the equality:

$$
\begin{equation*}
X_{1}(n)+X_{2}(n)=v(n)-1 \tag{2.10}
\end{equation*}
$$

which is a simple consequence of the fact that for binary trees the number of external nodes equals the number of internal nodes minus one. For the 2-3 trees we have a set of inequalities (Yao (1978) Lemma 2.2):

$$
\begin{equation*}
\frac{3}{2}\left(X_{1}(n)+X_{2}(n)\right)-\frac{1}{2} \leq \mu(n) \leq 2\left(X_{1}(n)+X_{2}(n)\right)-1 \tag{2.11}
\end{equation*}
$$

Using (2.9) in (2.10) we can conclude that for P.M. trees

$$
\frac{v(n)}{n} \rightarrow \frac{3}{7} \approx 0.43
$$

which is a measure of the balance of these trees, because for a perfectly balanced complete binary tree $\frac{v(n)}{n}=\frac{2^{K}}{2^{K+1}-1} \approx 0.5$ whereas for a totally imbalanced tree (a linear array) $\frac{v(n)}{n}=0$. For the 2-3 trees, using (2.9) in (2.11) we get:

$$
0.64 \approx \frac{9}{14} \leq \lim _{n} \frac{\mu(n)}{n} \leq \frac{6}{7} \approx 0.86
$$

which is basically the corollary to Theorem 2.7 in Yao, except that there, $\mu(n)$ is replaced by the expected value $\mathrm{E} \mu(\mathrm{n})$. Yao defines the storage utilization for a 2-3 tree of $n$ keys as $\frac{n}{2 E \mu(n)}$ (if all internal nodes had two keys, there would be $\frac{n}{2}$ of them, so the storage utilization is the ratio $\frac{\text { smallest possible \# of internal nodes }}{\text { expected \# of internal nodes }}$; Eisenbarth et.al. (1982) discuss the inverse of this measure) and gives the asymptotic value $\log 2 \approx 0.69$ for the storage utilization of a $B$ tree (a generalization of 2-3 trees). Here, using (2.9) and (2.11) we can obtain for the point storage utilization the inequalities:

$$
\begin{equation*}
0.58 \approx \frac{7}{12} \leq \lim _{n} \frac{n}{2 \mu(n)} \leq \frac{14}{18} \approx 0.78 \tag{2.12}
\end{equation*}
$$

Our result (2.7) also applies in more complicated settings such as the generalized k - t binary search trees of Cunto and Gascón (1987), a generalization of P.M.-trees where there are up to $t$ keys per node and rotations are made each time there is a linear array of $2 \mathrm{k}-1$ nodes in the fringe. As a final example, Yao's second order analysis of 2-3 trees (i.e., the consideration of the two bottom tiers of nodes) from our viewpoint is simply the fringe problem for which $\left(c_{1}, c_{2}, c_{3}, c_{4}, c_{5}, c_{6}, c_{7}\right)=$ $(4,5,6,6,7,8,9)$ and $Q$ is the (irreducible) matrix

$$
\left(\begin{array}{ccccccc}
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 / 5 & 3 / 5 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
6 / 7 & 0 & 0 & 0 & 0 & 4 / 7 & 0 \\
3 / 4 & 3 / 4 & 0 & 0 & 0 & 0 & 1 / 4 \\
2 / 3 & 2 / 3 & 2 / 3 & 0 & 0 & 0 & 0
\end{array}\right] .
$$

An application of (2.7) yields

$$
\begin{aligned}
& x_{1}=\frac{138}{485} \approx 0.28, x_{2}=\frac{132}{485} \approx 0.27, x_{3}=\frac{304}{3395} \approx 0.09 \\
& x_{4}=\frac{396}{3395} \approx 0.12 \quad x_{5}=\frac{15}{97} \approx 0.15 \quad x_{6}=\frac{20}{291} \approx 0.07 \quad x_{7}=\frac{4}{291} \approx 0.01 \\
& b=\frac{7991}{1455} \approx 5.49 .
\end{aligned}
$$

Another combinatorial equation (Yao's lemma 2.8) relates $\mu(\mathrm{n})$ to the two bottom tiers of nodes:

$$
\frac{7}{2} \sum_{i=1}^{3} X_{i}(n)+\frac{9}{2} \sum_{i=4}^{7} X_{i}(n)-\frac{1}{2} \leq \mu(n) \leq 4 \sum_{i=1}^{3} X_{i}(n)+5 \sum_{i=4}^{7} X_{i}(n)-1 .
$$

Taking limits after dividing by $n$ and using the values for $b$ and the $x_{i}$ 's just found we get

$$
0.70=\frac{78501}{111874} \leq \lim _{n} \frac{\mu(n)}{n} \leq \frac{44343}{55937} \cong 0.79
$$

the a.s. result analogous to Theorem 2.12 of Yao. We see also that our inequalities in (2.12) for the storage utilization are improved now to

$$
0.63 \approx \frac{55937}{88686} \leq \lim _{n} \frac{n}{2 \mu(n)} \leq \frac{55937}{78561} \cong 0.71
$$

## 3. Empirical Convergence to Quasi-Stationary Distributions

Let $Y_{n}$ be a Markov chain in a finite state space I with irreducible and aperiodic transition matrix P. Classical limit theory gives existence and uniqueness of a stationary distribution $\pi$ satisfying

$$
\begin{gather*}
\sum_{i} \pi_{i} P_{i, j}=\pi_{j} \text { for all } j ; \pi_{j}>0 ; \Sigma \pi_{j}=1  \tag{3.1}\\
P\left(Y_{n}=j\right) \rightarrow \pi_{j} \text { as } n \rightarrow \infty  \tag{3.2}\\
N^{-1} \sum_{n=1}^{N} 1_{\left(Y_{n}=j\right)} \rightarrow \pi_{j} \text { a.s. as } N \rightarrow \infty . \tag{3.3}
\end{gather*}
$$

So (3.2) asserts convergence of the distribution of $Y_{n}$, while (3.3) gives convergence of the empirical distribution. Next we fix $A \subset I$, and let $\hat{P}$ be the matrix $P$ with the rows and columns corresponding to states in $A^{c}$ deleted. We suppose $\hat{P}$ is aperiodic and irreducible as well. Furthermore, let $T$ be the first hitting time of $Y_{n}$ on $A^{c}$. Formally, $\mathrm{T}=\min \left\{\mathrm{n}: \mathrm{Y}_{\mathrm{n}} \in \mathrm{A}^{\mathrm{c}}\right\}$. Then there exists a unique quasi-stationary distribution $\alpha$ on A satisfying

$$
\begin{equation*}
\sum_{i \in A} \alpha_{i} \hat{P}_{i, j}=\lambda \alpha_{j} ; \alpha_{j}>0 ; \Sigma \alpha_{j}=1 \tag{3.4}
\end{equation*}
$$

where $\lambda$ is the largest eigenvalue of $\hat{\mathrm{P}}, 0<\lambda<1$, and $\lambda$ is real. See e.g. Darroch and Seneta (1965). This $\alpha$ has the interpretation of being the limiting distribution of the process $\mathrm{Y}_{\mathrm{n}}$ conditioned on $\{\mathrm{T}>\mathrm{n}\}$ :

$$
\begin{equation*}
P\left(Y_{n}=j \mid T>n\right) \rightarrow \alpha_{j} \text { as } n \rightarrow \infty . \tag{3.5}
\end{equation*}
$$

Now (3.4) and (3.5) are plainly analogous to (3.1) and (3.2). There is no immediate analog of (3.3), but we shall motivate an indirect analog.

Consider the setting (3.1) - (3.2). In applications we are usually interested not in the distribution $\pi$ itself, but in distributions or expectations of functions defined on the state space. Since the distribution of a function $g$ can be obtained from expectations of functions $f(i)=1_{(g(i) \leq x)}$, we need only consider expectations. We know the longrun averages converge:

$$
\begin{equation*}
N^{-1} \sum_{n=1}^{N} f\left(Y_{n}\right) \rightarrow \Sigma f(i) \pi_{i}, \text { a constant. } \tag{3.6}
\end{equation*}
$$

To calculate this constant we have two options:
a) Solve (3.1) for $\pi$; or
b) run a computer simulation of the chain for N steps, and use the observed value of (3.6) to estimate the limit.

Method (a) is preferable, but when the number of states is large it becomes impractical, and 9 b ) becomes more attractive.

The same issue arises in consideration of the quasi-stationary distribution, $\alpha$. Here (3.5) implies $E\left(f\left(Y_{n}\right) \mid T>n\right) \rightarrow \Sigma f(i) \alpha_{i}$, and in the case of a large state space we would like a method of estimating $\Sigma \mathrm{f}(\mathrm{i}) \alpha_{\mathrm{i}}$ without having to solve equations (3.4).
In this setting, simulations to estimate $\alpha$ by running the chain and discarding runs that hit $\mathrm{A}^{\mathrm{c}}$ are unsatisfactory because $\mathrm{P}(\mathrm{T}>\mathrm{n})$ may be small. Instead, we define a process whose empirical distribution converges to $\alpha$. First, pretend we know $\alpha$, and consider a process $V_{n}$ on $A$ defined as follows: $V_{n}$ evolves as $Y_{n}$ until the first hit on $A^{c}$, at which point the hit on $A^{c}$ is not counted as a transition and instead the chain is put back into $A$ according to the distribution $\alpha$. The process $V_{n}$ defined in this manner is
a Markov chain with stationary distribution $\alpha$. And (3.3) shows that the empirical distribution $\theta_{N}$ converges to $\alpha$, where $\theta_{N}(j)=N^{-1} \sum_{n=1}^{N} 1_{\left(V_{n}=j\right)}$. Of course, since we do not know $\alpha$, we cannot simulate this process. However, we can simulate the natural "adaptive" process for which a transition at step $\mathrm{N}+1$ which would go into $\mathrm{A}^{\mathrm{c}}$ is instead sent into $A$ according to the empirical distribution $\theta_{\mathrm{N}}$. Theorem 3.8 below says for this adaptive process, the empirical distribution does, in fact, converge to $\alpha$. We define this Markov process formally.
Definition 3.7. Let $M$ be the set of counting measures on $A$, and let $\delta_{j}(i)=1_{(i=j)}$. Let $\left(V_{n}, \mu_{n}\right)$ be the $A \times M$-valued Markov chain with $V_{1}=i_{1}, \mu_{1}=\delta_{i_{1}}$, and with transitions

$$
P\left(V_{n+1}=j, \mu_{n+1}=\mu+\delta_{j} \mid V_{n}=i, \mu_{n}=\mu\right)=P_{i, j}+\mu(j) \sum_{k \in A^{c}} P_{i, k}
$$

(Here we are using the following notational convention: $\mu$ is an arbitrary vector, $\mu_{n}$ is the empirical counting measure at time n , and $\mu(\mathrm{j})$ is the jth entry of the arbitrary vector.)
Theorem 3.8. For the process defined in (3.7), $\mathrm{n}^{-1} \mu_{\mathrm{n}} \rightarrow \alpha$ a.s. as $\mathrm{n} \rightarrow \infty$, where $\alpha$ is the quasi-stationary distribution (3.4).
This result was proved in Flannery (1986) in a direct, but complicated manner. It can be deduced easily from Theorem 1.5. To do so, include in the definition (3.7) the count $C_{n}$ of the number of aborted visits to $A^{c}$ prior to step $n$. Precisely, let $C_{1}=0$ and rewrite (3.7) as

$$
\begin{gathered}
P\left(X_{n+1}=j, \mu_{n+1}=\mu+\delta_{j}, C_{n+1}=c \mid X_{n}=i, \mu_{n}=\mu, C_{n}=c\right)=P_{i, j} \\
P\left(X_{n+1}=j, \mu_{n+1}=\mu+\delta_{j}, C_{n+1}=c+1 \mid X_{n}=i, \mu_{n}=\mu, C_{n}=c\right)=\mu(j) \underset{k \in A^{c}}{ } P_{i, k} .
\end{gathered}
$$

Next, let $S_{n}=\min \left\{m: C_{m}=n\right\}$ be the time of the $n^{\text {th }}$ aborted visit to $A^{c}$, and let $\nu_{n}=\mu_{S_{n}}$ be the empirical counting measure at that time. It is easy to see that $v_{n}$ is the urn process where, for each $i, c_{i}=1$ and the distribution of $\left(Z_{j}^{(i)} ; j \in A\right)$ is the distri-

$$
\mathrm{T}-1
$$

bution of $\left(\sum_{n=0}^{T-1} 1_{\left(V_{n}=j\right)} ; j \in A\right)$ given $V_{0}=i$. We want to apply Theorem 1.5. Hypotheses (1.1) - (1.3) are clearly satisfied. For $\mathrm{Q}=\left(\mathrm{q}_{\mathrm{i}, \mathrm{j}}\right)$ defined above (1.4),

$$
\begin{aligned}
q_{i, j} & =E Z_{j}^{(i)} \\
& =E\left(\sum_{n=0}^{T-1} 1_{\left(V_{n}=j\right)} \mid V_{0}=i\right) \\
& =E\left(\sum_{n=0}^{\infty} 1_{\left(V_{n}=j, T>n\right)} \mid V_{0}=i\right)
\end{aligned}
$$

$$
=\sum_{n=0}^{\infty} \hat{P}_{i, n}^{(n)}, \text { for } \hat{P} \text { as in (3.4). }
$$

In other words,

$$
\begin{equation*}
\mathrm{Q}=\sum_{\mathrm{n}=0}^{\infty} \hat{\mathrm{P}}^{\mathrm{n}} . \tag{3.9}
\end{equation*}
$$

In particular, the hypothesis of irreducibility of $\hat{\mathbf{P}}$ implies irreducibility of $\mathbf{Q}$, condition (1.4). Setting $r_{i, j}=q_{i, j}-\delta_{i, j}$ and taking ( $\lambda, \alpha$ ) as in (3.4), we see that (3.4) implies

$$
\sum_{i \in A} \alpha_{i} r_{i, j}=\frac{\lambda}{1-\lambda} \alpha_{j}
$$

Applying Theorem 1.5 we see that $\alpha$ is the required eigenvector and $\frac{v_{n}}{\sum_{\mathrm{j}} v_{\mathrm{n}}(\mathrm{j})} \rightarrow \alpha$ a.s. That is

$$
\begin{equation*}
\frac{\mu_{\mathrm{S}_{\mathrm{n}}}}{\mathrm{~S}_{\mathrm{n}}} \rightarrow \alpha \text { a.s. } \tag{3.10}
\end{equation*}
$$

Since the state space is finite, $\mathrm{E}\left(\mathrm{S}_{\mathrm{n}+1}-\mathrm{S}_{\mathrm{n}}\right)^{\mathbf{2}}$ is bounded, and this easily implies

$$
\begin{equation*}
\frac{S_{n+1}}{S_{n}} \rightarrow 1 \text { a.s. } \tag{3.11}
\end{equation*}
$$

Noting that $\mu_{n}$ is monotone in $n$, the desired conclusion $\frac{\mu_{n}}{n} \rightarrow \alpha$ a.s. follows from (3.10) and (3.11) by simple analysis.

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Figure 1


Figure 2


Figure 3


Figure 4


Figure 5


Figure 6


Figure 7

type 2

Figure 8


Figure 9

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