Mathematical Finance, Vol. 11, No. 2 (April 2001), 245–265

FINDING GENERATORS FOR MARKOV CHAINS VIA EMPIRICAL TRANSITION MATRICES, WITH APPLICATIONS TO CREDIT RATINGS

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In this paper we identify conditions under which a true generator does or does not exist for an empirically observed Markov transition matrix. We show how to search for valid generators and choose the "correct" one that is the most compatible with bond rating behaviors. We also show how to obtain an approximate generator when a true generator does not exist. We give illustrations using credit rating transition matrices published by Moody's and by Standard and Poor's.

Key Words: generators, Markov chains, Markov processes, transition matrix, credit rating

1. INTRODUCTION

Since the seminal work of Jarrow, Lando, and Turnbull (1997), the use of credit rating transition matrices in credit risk modeling has received increasing attention. For example, Kijima and Komoribayashi (1998) provide an improvement on the estimation procedure in Jarrow et al. (1997); Belkin, Suchower, and Forest Jr. (1998) propose a one-factor Markov process to model credit rating transitions; Kijima (1998), from a technical perspective, explains how a Markov chain model can lead to the known empirical regularities such as memory in rating changes and long-term reversion of ratings; and Arvanitis, Gregory, and Laurent (1999) develop a framework within which credit rating migrations can exhibit the usual empirical regularities. In a useful note, Lando (2000) shows how a transition matrix can be used to value credit derivatives such as a default swap.

Rating transition matrices have also received increasing attention in the financial industry. Two major bond rating services in the United States, Moody's and Standard

The authors thank Melanie Cao, Ed Perkins, Jeremy Quastel, Peter Rosenthal, Tom Salisbury, two anonymous referees, and Stanley Pliska (the editor) for helpful comments and suggestions. They also thank David Lando for his communications with Jason Wei on the topic. Jeffrey Rosenthal acknowledges financial support by NSERC, and Jason Wei acknowledges financial support by SSHRC and the Connaught Fund of the University of Toronto.

Manuscript received January 2000; final revision received August 2000.

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and Poor's, now each publish an annual update of historical transition matrices, together with a wealth of other related information.

The shortest time interval within which a transition matrix is estimated is typically one year. The number of transition observations within a shorter period would be too small for a reliable transition matrix to be estimated. However, for valuation purposes (e.g., valuing a default swap), we frequently need a transition matrix for a period shorter than one year. If one can obtain a generator for a transition matrix P, meaning a matrix Q having row-sums 0 and nonnegative off-diagonal entries such that $\exp(Q) = P$, then one can set $P(t) = \exp(tQ)$ to obtain matrices for any time $t \geq 0$. Unfortunately, there is a lack of guidance in the finance literature as to when such a generator Q exists; or how to find such a matrix if indeed it exists.

Authors such as Lando (2000) and Arvanitis et al. (1999) simply assume the existence of such generators. The only authors in finance who have addressed the issue of estimating a generator are Jarrow et al. (1997) who obtain an approximate generator by assuming that the probability for one rating to make more than one transition in one year is small. To our knowledge, no one in the finance literature has addressed the issues of existence and identification of transition matrix generators.

The objective of this paper is to identify conditions under which a true generator does or does not exist. We will show how to search for valid generators and how to choose a "correct" generator that is the most compatible with bond rating behaviors. When a true generator does not exist, we will show how to obtain an approximate one.

Toward the later stage of our research, our attention was drawn to a study by Singer and Spilerman (1976) who examined similar issues in the context of social sciences. As they have succinctly summarized, to determine if an empirical transition matrix is compatible with a true generator or an underlying Markov process is an *embeddability* problem; to seek for the true generator once its existence is established is an *identification* problem. Some of our results turn out to be rediscoveries of those by Singer and Spilerman and earlier authors such as Elfving (1937), Kingman (1962), Chung (1967), and Johansen (1973, 1974); others are our own. We attempt to attribute the results to the earlier authors whenever called for.

The rest of the paper is presented in seven sections. Section 2 presents a simple method of finding a generator and identifies conditions under which this method works. Section 3 provides a "fix" to the method in Section 2 when negative off-diagonal entries are present in a candidate generator matrix. Section 4 discusses some examples from finance. Section 5 presents some further results on the existence and uniqueness of generators. In Section 6, an algorithm is outlined for searching a valid generator when the simple series method in Section 2 fails. Further discussions are given in Section 7. The paper is concluded in Section 8. Proofs of theorems are relegated to the Appendix.

2. FINDING A CANDIDATE GENERATOR

Let P be a time-homogeneous Markov transition matrix—that is, an $N \times N$ real matrix with nonnegative entries and with row-sums 1. We are interested in finding a generator Q, an $N \times N$ real matrix with nonnegative off-diagonal entries and with row-sums 0, such that $\exp(Q) = P$. (Here and throughout,

$$\exp(tQ) = I + tQ + (tQ)^2/2! + (tQ)^3/3! + \cdots ,$$

where I is the $N \times N$ identity matrix. Without loss of generality, we will assume that P is for one year, i.e. $t = 1$.)

Our computational starting point is given by the following theorem. To state it, let

$$S = \max\left\{(a-1)^2 + b^2;\ a+bi \text{ is an eigenvalue of } P, a, b \in \mathbf{R}\right\};$$

that is, S is computed by examining all of the (possibly complex) eigenvalues of P, of the form $a+bi$ where a and b are real, and computing the absolute-square of the eigenvalue minus 1 (i.e. $(a-1)^2+b^2$) and then taking the maximum of these absolute-squares over all of the eigenvalues of P.

THEOREM 2.1. *Let P be an $N \times N$ Markov transition matrix, and suppose that $S < 1$. Then the series*

$$\widetilde{Q} = (P-I) - (P-I)^2/2 + (P-I)^3/3 - (P-I)^4/4 + \cdots \tag{2.1}$$

converges geometrically quickly, and gives rise to an $N \times N$ matrix $\widetilde{Q}$ having row-sums 0, *such that* $\exp(\widetilde{Q}) = P$ *exactly.*

This theorem is proved in the Appendix (as are all the other theorems). The series (2.1) has been considered in this context by others. Indeed, a proof of Theorem 2.1 can be found in Zahl (1955, p. 96), using a result of Wedderburn (1934, pp. 122–123), and is also discussed by Singer and Spilerman (1976, p. 8). It provides a simple method (in terms of summing a series of matrices) for obtaining a matrix $\widetilde{Q}$ that automatically has most of the desired properties of a generator.

REMARK 2.1. We wish to emphasize that, even if the series (2.1) fails to converge, or converges to a matrix $\widetilde{Q}$ that is not a valid generator, this does not preclude the possibility that a valid generator for P still exists; see Section 5.

We note that in practice it is not too important to check the condition $S < 1$. Indeed, as long as the series (2.1) converges absolutely, the conclusions that $\widetilde{Q}$ has row-sums 0 and that $\exp(\widetilde{Q}) = P$ are automatically satisfied, so that the condition $S < 1$ is no longer necessary. Furthermore, for many transition matrices arising in the credit risk literature, the condition that $S < 1$ is satisfied automatically via the following result.

THEOREM 2.2. *Suppose the diagonal entries of a transition matrix P are all greater than $\frac{1}{2}$ (i.e., $p_{ii} > 0.5$ for all i). Then $S < 1$; that is, the convergence of the series* (2.1) *is guaranteed.*

REMARK 2.2. In matrix language, the condition of Theorem 2.2 is equivalent to the transition matrix P being *strictly diagonally dominant* (e.g., see Horn and Johnson 1985, p. 302). Furthermore, it is proved by Cuthbert (1972, 1973) that, under this condition, P can have at most one generator: if a generator exists then it is unique.

We emphasize that the condition is only a *sufficient* one, in that the series (2.1) may well converge, and we may well have $S < 1$, even if some of the diagonal entries of P are less than 0.5.

REMARK 2.3. Elfving (1937) was the first to pose the problem of identifying test criteria on the entries of a transition matrix P so that there is a valid generator Q with $\exp(Q) = P$. This problem became known as the embedding problem.

REMARK 2.4. In the case where P is diagonalizable with all eigenvalues real and positive, summing the series (2.1) (if it converges) is equivalent to first diagonalizing P, then replacing the diagonal entries by their logarithms, and then converting back to the original basis. This is analogous to the approach of finding the nth root of P by diagonalizing and then replacing diagonal entries by their nth roots (see e.g., Press et al., 1988, Chap. 11). However, we note that this method does not guarantee that the resulting nth root matrix will have nonnegative entries. Moreover, it is not clear as to which root to choose when more than one real root exists.

3. THE NONNEGATIVITY CONDITION

The main drawback of Theorem 2.1 is that the matrix $\widetilde{Q}$ is not guaranteed to have nonnegative off-diagonal entries. (Several examples from finance are given in Section 4 below; for an example from sociology see Singer and Spilerman 1976.) This is problematic since if $\widetilde{Q}$ has a negative off-diagonal entry, then so will $P_t = \exp(t\widetilde{Q})$ for sufficiently small $t > 0$. This means that P_t will not be a proper Markov transition matrix, which is unacceptable.

However, any negative off-diagonal entries of $\widetilde{Q}$ will usually be quite small. Therefore, it is possible to correct the problem simply by replacing these negative entries with 0, and adding the appropriate value back into the corresponding diagonal entry to preserve the property of having row-sums 0. That is, once we have obtained $\widetilde{Q}$, we can obtain a new matrix Q by setting

$$q_{ij} = \max(\tilde{q}_{ij}, 0), \quad j \neq i; \qquad q_{ii} = \tilde{q}_{ii} + \sum_{j \neq i} \min(\tilde{q}_{ij}, 0). \tag{3.1}$$

(This modification technique is also considered in Zahl 1955.) The new matrix Q will still have row-sums 0, and will have nonnegative off-diagonal entries. However, it will no longer satisfy $\exp(Q) = P$ exactly.

A different version of Q can be obtained by adding the negative values back into *all* the entries of the same row (not just the diagonal one) which have the correct sign, proportional to their absolute values. That is, we could instead let

$$G_i = |\tilde{q}_{ii}| + \sum_{j \neq i} \max(\tilde{q}_{ij}, 0); \qquad B_i = \sum_{j \neq i} \max(-\tilde{q}_{ij}, 0)$$

be the "good" and "bad" totals for each row i, and then set

$$q_{ij} = \begin{cases} 0, & i \neq j \text{ and } \tilde{q}_{ij} < 0 \\ \tilde{q}_{ij} - B_i|\tilde{q}_{ij}|/G_i & \text{otherwise if } G_i > 0 \\ \tilde{q}_{ij}, & \text{otherwise if } G_i = 0. \end{cases} \tag{3.1$'$}$$

(Note that since $\sum_j \tilde{q}_{ij} = 0$, we always have $G_i \geq B_i$; hence, (3.1′) guarantees that $q_{ij} \geq 0$ for $i \neq j$.) When $\widetilde{Q}$ has only slightly negative off-diagonal elements, and the values $-q_{ii}$ are reasonably large, (3.1) and (3.1′) will usually be fairly similar.

REMARK 3.1. It may be possible to improve still further the choice of where to add the extra back in for the modification Q, by optimizing this choice as a multivariate function. However, it appears that this further improvement would rarely make a substantial difference to the distance of $\exp(Q)$ to P, so we do not pursue it here.

Is it possible that a valid generator still exists even if the $\widetilde{Q}$ computed by Theorem 2.1 is not a valid one? The answer is yes. Furthermore, it may be possible that there exists more than one valid generator for a given matrix P. Such issues and related examples are discussed in Section 5.

Is it possible to conclude the nonexistence of a generator for a given transition matrix P under certain conditions? The answer is again yes. For example, we have the following theorem. (Part (a) of the theorem is also stated in Kingman 1962; part (b) is proved as Theorem 6.1 in Goodman 1970; and part (c) follows from the standard Lévy Dichotomy, see, e.g., Chung 1967 and Grimmett and Stirzaker 1992.) To state it, recall that a state j is *accessible* from a state i if there is a sequence of states $k_0 = i, k_1, k_2, \ldots, k_m = j$ such that $p_{k_\ell\, k_{\ell+1}} > 0$ for each ℓ.

THEOREM 3.1. *Let P be a transition matrix, and suppose that*

(a) $\det(P) \le 0$, *or*
(b) $\det(P) > \prod_i p_{ii}$, *or*
(c) *there are states i and j such that j is accessible from i, but* $p_{ij} = 0$.

Then there does not exist an exact generator for P.

REMARK 3.2. We note that if $p_{ii} > 0.5$ for all i as in Theorem 2.2 then we necessarily have $\det(P) > 0$, so that Theorem 3.1(a) never applies. To see this, we can write $P = mI + (1-m)R$ for a stochastic matrix R, where $m = \min_i p_{ii} > 0.5$. Hence, setting $A_s = sP + (1-s)I$, we have $A_s = (1-s+sm)I + s(1-m)R$, so that A_s is invertible for all $0 \le s \le 1$ (since $1-s+sm > s(1-m)$). But then $\det(A_s)$ is a real continuous nonzero function of $s \in [0, 1]$, which is positive at $s = 0$, hence it is also positive at $s = 1$.

Some further results about the existence and uniqueness of generators are presented in Section 5. We first pause to consider some numerical examples.

4. SOME EXAMPLES FROM FINANCE

In finance, the finite state space $\Omega = \{1, 2, \ldots, N\}$ covers possible bond ratings, with state 1 being the highest rating and state N being Default. Typically, $\Omega = \{$AAA, AA, A, BBB, BB, B, CCC, Default$\}$. Insofar as a lower rating presents a higher credit risk, a rating transition matrix should satisfy one of the two conditions outlined by Jarrow et al. (1997) and given here in the following lemma.

LEMMA 4.1. *Let Q be a valid generator for P. Then the following two conditions are equivalent*:

(a) $\sum_{j\ge k} p_{ij}$ *is a nondecreasing function of i for every fixed k.*
(b) $\sum_{j\ge k} q_{ij} \ge \sum_{j\ge k} q_{i+1,\,j}$ *for all i and k such that* $k \ne i+1$.

Proof. See Jarrow et al. (1997, p. 495). □

REMARK 4.1. In the language of Markov chains, the above conditions are equivalent to requiring that the underlying Markov chain be "stochastically monotonic."

Let us first examine the annual transition matrix considered by Jarrow et al. (1997), which is based on empirical observations from *Standard and Poor's Credit Review* (1993), for the years 1981 through 1991. After distributing the "Not Rated" weights to the other entries via their equation (31), they obtain the following average transition matrix (their Table 3):

$$P = \begin{pmatrix} 0.8910 & 0.0963 & 0.0078 & 0.0019 & 0.0030 & 0.0000 & 0.0000 & 0.0000 \\ 0.0086 & 0.9010 & 0.0747 & 0.0099 & 0.0029 & 0.0029 & 0.0000 & 0.0000 \\ 0.0009 & 0.0291 & 0.8894 & 0.0649 & 0.0101 & 0.0045 & 0.0000 & 0.0009 \\ 0.0006 & 0.0043 & 0.0656 & 0.8427 & 0.0644 & 0.0160 & 0.0018 & 0.0045 \\ 0.0004 & 0.0022 & 0.0079 & 0.0719 & 0.7764 & 0.1043 & 0.0127 & 0.0241 \\ 0.0000 & 0.0019 & 0.0031 & 0.0066 & 0.0517 & 0.8246 & 0.0435 & 0.0685 \\ 0.0000 & 0.0000 & 0.0116 & 0.0116 & 0.0203 & 0.0754 & 0.6493 & 0.2319 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 1.0000 \end{pmatrix}.$$

Here the eight columns and rows represent, in order, the credit ratings AAA, AA, A, BBB, BB, B, CCC, and Default.

REMARK 4.2. In this paper, we are implicitly assuming (as have Jarrow et al. 1997 and other authors) that the credit ratings process is time-homogeneous and Markovian. In reality, both assumptions are open to debate, and likely neither one is precisely true for real credit ratings. In fact, the empirical question of whether the time-homogeneous Markov model is suitable for bond rating transitions has yet to be addressed in the literature. We do not consider such issues here, but rather implicitly assume a time-homogeneous Markov model throughout.

It can be shown that condition (a) in Lemma 4.1 is violated for this transition matrix. For example, when $k = 4$ and $i = 6$, we compute that $\sum_{j\geq 4} p_{6j} = 0.9949$ and $\sum_{j\geq 4} p_{7j} = 0.9885$. It turns out that condition (a) is also violated in the other matrices we will examine in this section. Since whether a transition matrix is stochastically monotonic has very little bearing on the existence of a generator, and since any "fixing" would be necessarily guided by arbitrary, ad hoc rules, we will leave the matrices as they are. In cases where the monotone condition is crucial (as in estimation of risk premiums), researchers may make some adjustments of the transition matrix based on their best judgments.

By Theorem 3.1(c), the transition matrix P does not have an exact generator. For example, $p_{12} > 0$ and $p_{26} > 0$, but $p_{16} = 0$. Thus, it will be useful to find an approximate generator Q, such that $\exp(Q)$ is approximately equal to P, and that a transition matrix for any time t can be approximated by $\exp(Qt)$.

REMARK 4.3. It may be considered disappointing that this transition matrix P does not have an exact generator. It is possible that an empirical matrix P estimated from many more years of data would have no zero entries and would in fact be embeddable, though we lack sufficient data to test this. In the absence of such data, it may be tempting to use the "trick" of simply raising the given matrix P to a high power, as a stand-in for an empirical transition matrix for many more years. However, this trick does not help with the embeddability problem. Indeed, clearly if P is not embeddable then neither is any power of P (moreover, if P is embeddable then any power of P has the same set of valid generators as P does).

Jarrow et al. (1997) obtain an approximate generator Q_{JLT} for this P by assuming that there is never more than one transition per year. Their method leads to the general formula

$$q_{ii} = \log(p_{ii}); \qquad q_{ij} = p_{ij} \log(p_{ii})/(p_{ii} - 1) \quad (i \neq j). \tag{4.1}$$

To continue the above example, their approximate generator is

$$Q_{JLT} = \begin{pmatrix} -0.1154 & 0.1019 & 0.0083 & 0.0020 & 0.0031 & 0.0000 & 0.0000 & 0.0000 \\ 0.0091 & -0.1043 & 0.0787 & 0.0105 & 0.0030 & 0.0030 & 0.0000 & 0.0000 \\ 0.0010 & 0.0309 & -0.1172 & 0.0688 & 0.0107 & 0.0048 & 0.0000 & 0.0010 \\ 0.0007 & 0.0047 & 0.0713 & -0.1711 & 0.0701 & 0.0174 & 0.0020 & 0.0049 \\ 0.0005 & 0.0025 & 0.0089 & 0.0813 & -0.2530 & 0.1181 & 0.0144 & 0.0273 \\ 0.0000 & 0.0021 & 0.0034 & 0.0073 & 0.0568 & -0.1929 & 0.0479 & 0.0753 \\ 0.0000 & 0.0000 & 0.0142 & 0.0142 & 0.0250 & 0.0928 & -0.4318 & 0.2856 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \end{pmatrix}.$$

This approximate generator Q_{JLT} does indeed have row-sums 0 and nonnegative off-diagonal entries.

Furthermore we calculate that

$$\exp(Q_{JLT})$$
$$= \begin{pmatrix} 0.891431 & 0.091476 & 0.011075 & 0.002650 & 0.002847 & 0.000339 & 0.000025 & 0.000062 \\ 0.008198 & 0.902501 & 0.070932 & 0.011685 & 0.003332 & 0.003028 & 0.000093 & 0.000231 \\ 0.001042 & 0.027907 & 0.892718 & 0.060232 & 0.011116 & 0.005288 & 0.000231 & 0.001465 \\ 0.000676 & 0.005202 & 0.062348 & 0.847319 & 0.057651 & 0.018185 & 0.002246 & 0.006373 \\ 0.000457 & 0.002533 & 0.010214 & 0.066701 & 0.781647 & 0.095894 & 0.012458 & 0.030092 \\ 0.000025 & 0.001947 & 0.003751 & 0.008390 & 0.046273 & 0.829090 & 0.035518 & 0.074915 \\ 0.000016 & 0.000317 & 0.011507 & 0.012042 & 0.020256 & 0.069455 & 0.651072 & 0.235331 \\ 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 1.000000 \end{pmatrix}.$$

We thus see that $\exp(Q_{JLT})$ is close to, but not exactly equal to, the original P.

Let us now instead use the series method presented in Theorem 2.1. By Theorem 2.2, we automatically have $S < 1$ in this case, so that Theorem 2.1 does apply. Indeed, we find that the series (2.1) for $\widetilde{Q}$ converges very quickly. In fact, summing just the first sixteen terms of the series, we compute that the effect of subsequent terms is less than 10^{-8}, thus giving extremely high accuracy. Retaining six digits, we obtain that

$$\widetilde{Q} = \begin{pmatrix} -0.115931 & 0.107466 & 0.004208 & 0.001334 & 0.003372 & -0.000409 & -0.000014 & -0.000025 \\ 0.009566 & -0.106131 & 0.083233 & 0.008115 & 0.002567 & 0.002942 & -0.000114 & -0.000168 \\ 0.000831 & 0.032362 & -0.121382 & 0.074626 & 0.009028 & 0.004013 & -0.000274 & 0.000589 \\ 0.000623 & 0.003572 & 0.075556 & -0.177517 & 0.079050 & 0.013991 & 0.001350 & 0.003277 \\ 0.000440 & 0.002181 & 0.005768 & 0.088535 & -0.261178 & 0.129535 & 0.013816 & 0.020800 \\ -0.000027 & 0.002086 & 0.002711 & 0.004655 & 0.063962 & -0.199781 & 0.059016 & 0.067268 \\ -0.000015 & -0.000420 & 0.014447 & 0.013639 & 0.024547 & 0.101298 & -0.435344 & 0.281980 \\ 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{pmatrix}.$$

We then compute that

$$\exp(\widetilde{Q}) = P$$

exactly, to at least six decimal places (i.e., to within 10^{-6}). Furthermore, our $\widetilde{Q}$ has row-sums 0, as it must.

Unfortunately, our $\widetilde{Q}$ has some (small) negative off-diagonal entries. We thus replace $\widetilde{Q}$ by Q as in equation (3.1), to obtain

$$Q = \begin{pmatrix} -0.116380 & 0.107466 & 0.004208 & 0.001334 & 0.003372 & 0.000000 & 0.000000 & 0.000000 \\ 0.009566 & -0.106414 & 0.083233 & 0.008115 & 0.002567 & 0.002942 & 0.000000 & 0.000000 \\ 0.000831 & 0.032362 & -0.121656 & 0.074626 & 0.009028 & 0.004013 & 0.000000 & 0.000589 \\ 0.000623 & 0.003572 & 0.075556 & -0.177517 & 0.079050 & 0.013991 & 0.001350 & 0.003277 \\ 0.000440 & 0.002181 & 0.005768 & 0.088535 & -0.261178 & 0.129535 & 0.013816 & 0.020800 \\ 0.000000 & 0.002086 & 0.002711 & 0.004655 & 0.063962 & -0.199808 & 0.059016 & 0.067268 \\ 0.000000 & 0.000000 & 0.014447 & 0.013639 & 0.024547 & 0.101298 & -0.435779 & 0.281980 \\ 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{pmatrix}.$$

This Q now has nonnegative off-diagonal entries and still has row-sums 0. However, it no longer exactly satisfies that $\exp(Q) = P$. In fact,

$$\exp(Q) = \begin{pmatrix} 0.890600 & 0.096265 & 0.007798 & 0.001901 & 0.003010 & 0.000351 & 0.000026 & 0.000048 \\ 0.008597 & 0.900745 & 0.074680 & 0.009899 & 0.002901 & 0.002906 & 0.000097 & 0.000175 \\ 0.000900 & 0.029092 & 0.889158 & 0.064893 & 0.010102 & 0.004511 & 0.000211 & 0.000935 \\ 0.000600 & 0.004300 & 0.065591 & 0.842700 & 0.064400 & 0.016000 & 0.001808 & 0.004501 \\ 0.000401 & 0.002202 & 0.007899 & 0.071900 & 0.776400 & 0.104299 & 0.012698 & 0.024100 \\ 0.000024 & 0.001911 & 0.003100 & 0.006600 & 0.051699 & 0.824577 & 0.043491 & 0.068498 \\ 0.000014 & 0.000323 & 0.011610 & 0.011599 & 0.020296 & 0.075384 & 0.649019 & 0.231854 \\ 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 1.000000 \end{pmatrix},$$

which is very close to, but not exactly equal to, the original transition matrix P.

It is useful to know which approximation is more accurate. One method of comparison is to compute the L^1-norm (i.e., the sum of the absolute values of the 64 matrix entries) of $P - \exp(Q_{JLT})$ and of $P - \exp(Q)$, to see which is smaller. We compute that

$$\mathrm{norm}[P - \exp(Q_{JLT})] = 0.116900; \qquad \mathrm{norm}[P - \exp(Q)] = 0.002736.$$

We thus see that, in terms of closeness of $\exp(Q)$ to P, the choice of Q is better than Q_{JLT} by a factor of $0.116900/0.002736 \approx 42.7$.

In fact, if we instead use the alternative approximation (3.1′), we then compute that

$$\text{norm}[P - \exp(Q)] = 0.002686,$$

which is a slight additional improvement.

We thus tentatively conclude that, although our method requires the awkward transformation of $\widetilde{Q}$ to Q, it can be substantially better than the method of Jarrow et al. (1997) whereby we must assume away multiple transitions in a single year.

REMARK 4.4. As an aside, we note that the row entries of this example matrix P do not add exactly to 1, presumably due to round-off errors. As a check, we slightly modified the diagonal entries of P so that the row entries sum to exactly 1; but this had negligible effect on any of the resulting matrices or distances.

We now consider some additional examples. First we consider the average one-year transition matrix from Moody's (1999), which covers the period of 1980–1998. After reassigning the "Not Rated" weights to the other entries, we obtain the following transition matrix:

$$P = \begin{pmatrix} 0.886583 & 0.102937 & 0.010169 & 0.000000 & 0.000311 & 0.000000 & 0.000000 & 0.000000 \\ 0.010787 & 0.887045 & 0.095530 & 0.003423 & 0.001452 & 0.001452 & 0.000000 & 0.000311 \\ 0.000625 & 0.028759 & 0.902053 & 0.059185 & 0.007398 & 0.001771 & 0.000104 & 0.000104 \\ 0.000529 & 0.003386 & 0.070680 & 0.852291 & 0.060523 & 0.010052 & 0.000846 & 0.001587 \\ 0.000328 & 0.000765 & 0.005571 & 0.056806 & 0.835809 & 0.080839 & 0.005353 & 0.014638 \\ 0.000109 & 0.000435 & 0.001738 & 0.006519 & 0.065950 & 0.827032 & 0.027597 & 0.070621 \\ 0.000000 & 0.000000 & 0.006600 & 0.010500 & 0.030500 & 0.061100 & 0.629700 & 0.261600 \\ 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 1.000000 \end{pmatrix}.$$

We again see from Theorem 3.1(c) that there does not exist an exact generator for this transition matrix. Hence, we search for an approximate generator.

Using the method of Jarrow et al. in equation (4.1) to compute the approximate generator Q_{JLT}, we can then calculate the L^1-norm as

$$\text{norm}[P - \exp(Q_{JLT})] = 0.100047.$$

Using the series method (2.1) together with the modification (3.1) yields a different approximate generator Q, which gives an L^1 distance of $\exp(Q)$ to P of

$$\text{norm}[P - \exp(Q)] = 0.001401.$$

Once again, using the modification (3.1′) instead gives a slightly better approximation, with

$$\text{norm}[P - \exp(Q)] = 0.001371.$$

Compared with Q_{JLT}, the generators obtained above represent an improvement on the order of 71.4 and 73.0 respectively.

As another example, we consider the transition matrix from Standard and Poor's (1999) which covers a longer period than the one considered by Jarrow et al. After reassigning the "Not Rated" weights, we obtain the following annual transition matrix:

$$P = \begin{pmatrix} 0.919347 & 0.074592 & 0.004829 & 0.000822 & 0.000411 & 0.000000 & 0.000000 & 0.000000 \\ 0.006396 & 0.918085 & 0.067575 & 0.005984 & 0.000619 & 0.001135 & 0.000310 & 0.000000 \\ 0.000730 & 0.022725 & 0.916814 & 0.051183 & 0.005629 & 0.002502 & 0.000104 & 0.000417 \\ 0.000425 & 0.002658 & 0.055609 & 0.878894 & 0.048272 & 0.010207 & 0.001701 & 0.002339 \\ 0.000441 & 0.000991 & 0.006058 & 0.077542 & 0.814847 & 0.078973 & 0.011125 & 0.010133 \\ 0.000000 & 0.001019 & 0.002830 & 0.004641 & 0.069496 & 0.827957 & 0.039615 & 0.054556 \\ 0.001860 & 0.000000 & 0.003720 & 0.007439 & 0.024294 & 0.121237 & 0.604557 & 0.237010 \\ 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 1.000000 \end{pmatrix}.$$

Once again, we see by Theorem 3.1(c) that an exact generator for this P does not exist.

Following the same procedures as above, we compute the L^1-norm for the Jarrow et al. method and the series method (based on (3.1) and (3.1′)) as

$$\text{norm}[P - \exp(Q_{JLT})] = 0.103516; \quad \text{norm}[P - \exp(Q)] = 0.001096 \text{ (based on (3.1))};$$
$$\text{norm}[P - \exp(Q)] = 0.001088 \text{ (based on (3.1′))}.$$

It can be seen that the improvement factor is over 90 for both adjustment methods.

REMARK 4.5. It is possible that our method has applications in other fields as well. For an example of Alzheimer's Disease therapy evaluation, see Stewart, Philips, and Dempsey (1998).

5. FURTHER RESULTS ON THE EXISTENCE AND UNIQUENESS OF GENERATORS

According to Kingman (1962), the embeddability problem is completely solved for the case of 2×2 matrices by D. G. Kendall, who proves that a 2×2 transition matrix is compatible with a continuous Markov process if and only if the sum of the two diagonal entries is larger than 1. For matrices with higher dimensions, it is no longer clear-cut, as we have seen in Sections 2 and 3. In this section, we consider some additional results applicable to higher-dimensional transition matrices. Again, many of our results have appeared previously in other papers (especially Singer and Spilerman 1976), as we shall indicate.

One might hope that, if the series (2.1) converges to a matrix $\widetilde{Q}$ which does *not* have all its off-diagonal entries nonnegative, then perhaps this proves that no generator for P can possibly exist. Unfortunately, this is not true in general, as the following proposition shows. Intuitively, the series (2.1) only represents the principal branch of $\log(P)$; other branches of $\log(P)$ may still provide valid generators.

PROPOSITION 5.1. *For a given stochastic matrix P, the fact that a real matrix Q_1 with row-sums 0 and some negative off-diagonal entries satisfies* $\exp(Q_1) = P$ *does not preclude the possibility that there is a valid generator Q_2 for P. This is true even if Q_1 is equal to the matrix $\widetilde{Q}$ obtained from the series* (2.1).

Proof. We prove the proposition by citing an example. Let

$$P = \begin{pmatrix} .284779445 & .284035268 & .283826586 & .147358701 \\ .284191780 & .284779445 & .284035268 & .146993507 \\ .283487477 & .284191780 & .284779445 & .147541298 \\ .284543931 & .283487477 & .284191780 & .147776812 \end{pmatrix}.$$

Then the eigenvalues of P are 1, 0.0010572 (with multiplicity two), and 7.46905×10^{-7}. It follows that $S = (1 - 7.46905 \times 10^{-7})^2$, so that $S < 1$.

We then compute the series (2.1), which converges very slowly since S is very close to 1, and obtain

$$Q_1 \equiv \widetilde{Q} = \begin{pmatrix} -6.194496074 & 2.807322994 & 1.374197570 & 2.012975514 \\ 3.882167062 & -6.194496074 & 2.807322994 & -.494993979 \\ -.954631245 & 3.882167062 & -6.194496074 & 3.266960260 \\ 6.300566216 & -.954631245 & 3.882167062 & -9.228102034 \end{pmatrix},$$

a matrix with some negative off-diagonal entries. (Of course, we still have $\exp(Q_1) = P$, as we must.)

However, the matrix

$$Q_2 = \begin{pmatrix} -5.642931358 & 5.642931358 & 0.000000000 & 0.000000000 \\ 0.000000000 & -5.642931358 & 5.642931358 & 0.000000000 \\ 0.000000000 & 0.000000000 & -5.642931358 & 5.642931358 \\ 61.410871840 & 0.000000000 & 0.000000000 & -61.410871840 \end{pmatrix}$$

is indeed a valid generator for P, since $\exp(Q_2) = P$ and Q_2 has row-sums 0 and positive off-diagonal entries. $\square$

This proposition shows that even if the $\widetilde{Q}$ from Theorem 2.1 does not satisfy the nonnegativity condition, a valid generator for P may still exist. (Similarly, an example where the series (2.1) fails to converge, but where a valid generator still exists, is given by Singer and Spilerman 1976, Ex. 4.)

On the other hand, even if the existence of a generator for P is established, the generator may not be *unique*, as the following example shows. (A similar example is given in Singer and Spilerman 1976, Ex. 12.)

PROPOSITION 5.2. *There exist transition matrices P which have more than one valid generator.*

Proof. Let $b = e^{-4\pi}$, and let

$$P = \begin{pmatrix} (2+3b)/5 & (2-2b)/5 & (1-b)/5 \\ (2-2b)/5 & (2+3b)/5 & (1-b)/5 \\ (2-2b)/5 & (2-2b)/5 & (1+4b)/5 \end{pmatrix}$$

$$Q_1 = \begin{pmatrix} -2\pi & 2\pi & 0 \\ 0 & -2\pi & 2\pi \\ 4\pi & 0 & -4\pi \end{pmatrix}$$

$$Q_2 = \begin{pmatrix} -12\pi/5 & 8\pi/5 & 4\pi/5 \\ 8\pi/5 & -12\pi/5 & 4\pi/5 \\ 8\pi/5 & 8\pi/5 & -16\pi/5 \end{pmatrix}.$$

It can be verified that Q_1 and Q_2 both qualify as generators, and $\exp(Q_1) = \exp(Q_2) = P$. Thus, Q_1 and Q_2 are both valid generators for P. □

REMARK 5.1. This last result raises this question: When a transition matrix P has multiple valid generators Q, which generator is the "best"? This question could be important, because different generators lead to different values of $P_t = \exp(tQ)$ for most t (e.g., for all sufficiently small t). Mathematically, the notion of "desirability" of a generator is not well defined, since any valid generator is as good as any other. However, in practice, it is indeed meaningful to ask which valid generator will represent the empirical transition matrices the best. To shed some light on this issue, realize that with most empirical transition matrices (such as the ones presented in Section 4), it is generally unlikely for a rating to migrate to a remote rating in a short time period. Thus, one method of choosing among valid generators is to take the one with the smallest value of

$$J = \sum_{i,j} |j-i||q_{ij}|,$$

which ensures that the chance of jumping too far too quickly is minimized. In the example from the above proposition, we have

$$J_1 = 2\pi + 2\pi + 2(4\pi) = 12\pi \doteq 37.70$$

and

$$J_2 = 8\pi/5 + 2(4\pi/5) + 8\pi/5 + 4\pi/5 + 2(8\pi/5) + 8\pi/5 = 52\pi/5 \doteq 32.67.$$

We therefore might conclude that Q_2 is a better choice than Q_1. For discussions of somewhat related issues in rather different contexts, see Cuthbert (1972) and Singer and Spilerman (1976, Sec. 4).

Despite the difficulties raised in Proposition 5.2, it is sometimes possible to prove the uniqueness of generators for P, as the following result shows. (Part (c) below also appears in Cuthbert 1972, 1973.) To state it, we will use $\log(P)$ to denote the principal branch of the logarithm of P. This will be equal to the sum of the series (2.1) whenever the series converges. It always satisfies $\exp(\log(P)) = P$, and if P has row-sums 1 then $\log(P)$ has row-sums 0.

THEOREM 5.1. *Let P be a transition matrix.*

(a) *If* $\det(P) > 1/2$, *then P has at most one generator.*
(b) *If* $\det(P) > 1/2$ *and* $\|P - I\| < 1/2$ *(using any operator norm), then the only possible generator for P is* $\log(P)$.
(c) *If P has distinct eigenvalues and* $\det(P) > e^{-\pi}$, *then the only possible generator for P is* $\log(P)$.

In addition, we have the following result, which is also observed by Singer and Spilerman (1976, pp. 29–30).

THEOREM 5.2. *Let P be a transition matrix that has real distinct eigenvalues.*

(a) *If all eigenvalues of P are positive, then* $\log(P)$ *is the only real matrix Q such that* $\exp(Q) = P$.
(b) *If P has any negative eigenvalues, then there is no real matrix Q such that* $\exp(Q) = P$.

The two preceding theorems provide some further validity to our matrix $\widetilde{Q}$ from Theorem 2.1. In particular, they immediately show the following.

COROLLARY 5.1. *Let P be a transition matrix such that at least one of the following three conditions hold*:

(i) $\det(P) > \frac{1}{2}$ *and* $\|P - I\| < \frac{1}{2}$, *or*
(ii) *P has distinct eigenvalues and* $\det(P) > e^{-\pi}$, *or*
(iii) *P has distinct real eigenvalues.*

Suppose further that the series (2.1) *converges to a matrix $\widetilde{Q}$ with negative off-diagonal entries. Then there does not exist a valid generator for P.*

There are other known conditions on the eigenvalues of P which either preclude or establish the possibility of a valid generator Q. For example, Elfving (1937) proves that if P has a (complex) eigenvalue other than 1 of absolute value 1, or if P has a negative (real) eigenvalue of odd multiplicity, then no valid generator exists for P. A more refined result is obtained by Runnenberg (1962), who proves that if an $N \times N$ matrix P has a valid generator then each (complex) eigenvalue of P must lie within the region of the complex plane having boundary curve

$$\Big\{\big(\exp\left(-s + s\cos(2\pi/N)\right)\cos\left(s\sin(2\pi/N)\right),$$
$$\exp\left(-s + s\cos(2\pi/N)\right)\sin\left(s\sin(2\pi/N)\right)\big);\ 0 \le s \le \frac{\pi}{\sin(2\pi/N)}\Big\}$$

together with its reflection about the real axis. Each of these conditions is a further necessary condition for P to have a valid generator, in the spirit of Theorem 3.1 or Theorem 5.2(b).

Finally, we note that it is possible to provide a more quantitative version of Theorem 3.1(c) (the Lévy Dichotomy), as follows.

THEOREM 5.3. *If P does have a valid generator, then its entries must satisfy that*

$$p_{ik} \geq m^m r^r (m+r)^{-m-r} \sum_j (p_{ij} - b_m)(p_{jk} - b_r) \mathbf{1}_{p_{ij} > b_m,\, p_{jk} > b_r},$$

for any positive integers m and r. Here $b_m = \sum_{\ell=m+1}^{\infty} e^{-\lambda}\lambda^\ell/\ell! = 1 - \sum_{\ell=0}^{m} e^{-\lambda}\lambda^\ell/\ell!$, which equals the probability that $N' > m$, where N' is a Poisson random variable with mean $\lambda \equiv \max_i(-Q_{ii})$. Furthermore $\mathbf{1}_B$ is the indicator function of the Boolean event B.

For example, for the first matrix in Section 4, we have from equation (A.1) that

$$\lambda \equiv \max_i(-Q_{ii}) \leq -\mathrm{trace}(Q) = -\log\det(P) \doteq 1.417263, \tag{5.1}$$

and also that, for example, $p_{7,3} = 0.0116$ and $p_{3,2} = 0.0291$. Choosing $r = 5$ and $m = 4$, we compute that $b_5 \leq 0.00339622$ and $b_4 \leq 0.0149457$. The theorem then tells us that for a valid generator to exist we would require $p_{7,2} \geq 4^4 5^5 9^{-9}(p_{7,3} - b_4)(p_{3,2} - b_5) \geq 2.39779 \times 10^{-7}$. (This bound could perhaps be tightened somewhat by choosing different values of r and m, and summing over all possible intermediate states j, rather than just $j = 3$.) We thus see that this quantitative bound is not sufficiently large to rule out, say, the possibility that $P_{7,2} = 10^{-5}$ but only appears to be 0 because of rounding off.

REMARK 5.2. An improved bound could be obtained if we had a way of bounding $\max_i(-Q_{ii})$ better than the one presented in (5.1).

REMARK 5.3. We note that, even if a generator for P does not exist, it is still possible that, for example, there is a valid transition matrix $P_{1/2}$ such that $\left(P_{1/2}\right)^2 = P$. On the other hand, it is shown by Kingman (1962, Prop. 7) that if P is nonsingular, and if for *all* positive integers n there is a matrix $P_{1/n}$ such that $\left(P_{1/n}\right)^n = P$, then there *does* exist a generator for P.

6. AN ALGORITHM TO SEARCH FOR A VALID GENERATOR

If the series (2.1) fails to converge, or converges to a matrix that has some negative off-diagonal terms, then the results of the previous section indicate that it is still possible that a generator exists. In theory, it is possible to find this generator by checking all branches of the logarithm function and computing $\log(P)$ for each one, each time checking to see if the nonnegativity condition is satisfied.

If P has distinct eigenvalues, then this search is finite, as the following result shows.

THEOREM 6.1. *If P has distinct eigenvalues and if Q is a generator for P, then each eigenvalue λ of Q satisfies that $|\mathrm{Im}\lambda| \leq |\ln(\det(P))|$. In particular, there are only a finite number of possible branch values of $\log(P)$ which could possibly be generators of P. (Note that, by Theorem 3.1(a), if $\det(P) \leq 0$ then no generator exists.)*

In light of this theorem, whenever P has distinct eigenvalues, it is possible to construct a finite algorithm to search for all possible generators of P, as follows.[1] (Ideas that are very similar in spirit to ours but somewhat different in precise detail, especially

[1] We have written a Maple program to carry out this search, available on the web at http://www.math.ubc.ca/~israel/irw/

regarding the eigenvalue ranges considered, are discussed by Singer and Spilerman 1976, Sec. 3.3a.)

The idea is to use Lagrange interpolation. If P is $n \times n$ with distinct eigenvalues $r_1, r_2, \ldots, r_n$, and f is any function that is analytic in a neighborhood of each eigenvalue, then $f(P) = g(P)$ where g is the polynomial of degree $n-1$ such that $g(r_j) = f(r_j)$ for each j. The Lagrange interpolation formula (or, Sylvester's formula, cf. Singer and Spilerman 1976, p. 18) says that

$$g(x) = \sum_j \prod_{k \neq j} \frac{x - r_k}{r_j - r_k} f(r_j); \tag{6.1}$$

here the sum is over all eigenvalues r_j, and the product is over all eigenvalues r_k except r_j. (If P has repeated eigenvalues, this must be modified to require some derivatives to agree: $g^{(m)}(r_j) = f^{(m)}(r_j)$ for $m <$ (multiplicity of r_j).)

To search for generators, each of the unknown values $f(r_j)$ can be equal to any branch of the logarithm of r_j. In general r_j may be a complex number, and the values $f(r_j)$ must satisfy

$$f(r_j) = \log |r_j| + i(\arg(r_j) + 2\pi k_j),$$

for any integers k_j subject to the condition of Theorem 6.1. (Here $|r| = \sqrt{\mathrm{Re}(r)^2 + \mathrm{Im}(r)^2}$ and $\arg(r) = \arctan(\mathrm{Im}(r)/\mathrm{Re}(r))$.) The search would be carried out by using Lagrange interpolation to compute $f(P)$ for each possible choice of $k_1, k_2, \ldots, k_n$, and checking the nonnegative off-diagonal condition for each possible $f(P)$ that arises.

We note that many symbolic calculation packages contain functions for computing such matrices $g(P)$ (e.g. "`linalg/matfunc(P, g(z), z)`" in Maple, or "`(funm×(P,'g'))`" in Matlab).

We summarize the above algorithm as follows:

Step 1. Compute the eigenvalues $r_1, r_2, \ldots, r_n$ of P, and verify that they are all distinct.
Step 2. For each eigenvalue r_j, choose an integer k_j such that $\lambda \equiv \log |r_j| + i(\arg(r_j) + 2\pi k_j)$ satisfies the restriction of Theorem 6.1—in other words, such that $|\mathrm{Im}\,\lambda| = |\arg(r_j) + 2\pi k_j| \leq |\ln(\det(P))|$.
Step 3. For the collection of integers $k_1, k_2, \ldots, k_n$, set $f(r_j) = \log |r_j| + i(\arg(r_j) + 2\pi k_j)$, and let $g(x)$ be the function given in (6.1).
Step 4. For this function $g(x)$, compute the matrix $Q = g(P)$, and see if it is a valid generator.
Step 5. Return to Step 2, modifying one or more of the integers k_j. Continue until all allowable collections $k_1, k_2, \ldots, k_n$ have been considered.

In practice, the credit rating transition matrices would most likely have distinct eigenvalues, and the above procedure is adequate. In the rare cases where repeated eigenvalues are present, the search would be much more involved. (For some guidance in this case, see, e.g., Singer and Spilerman 1976, Sec. 3.3b.)

7. DISCUSSIONS

As we have seen in Section 4, most of the empirical annual transition matrices are "sparse" in that the probabilities of remote migrations are mostly zero. As a result, almost all matrices would fail the test of Theorem 3.1(c), which renders a simple resolution: A true generator does not exist; that is, the empirical transition matrix is not compatible with a continuous Markov process. In such a case, a finance researcher has two choices. One is to opt for the simplest way out: to compute the series in (2.1) (since by Theorem 2.2 the convergence is guaranteed for most matrices in practice) and make adjustments (when necessary) as outlined in Section 3. The other is to make certain adjustment to the transition matrix first so that there are no obvious violations of, for example, Lemma 4.1 and Theorem 3.1(c), and then proceed to search for a valid generator. If multiple generators are obtained via the procedures in Section 6, then the "quick and dirty" selection rule in Section 5 can be used to choose the "correct" generator. Based on our limited experiments in Section 3, it appears that the series method works well for all practical purposes.

It should be pointed out that our research focuses on the compatibility of an empirical transition matrix with a continuous Markov process. When the underlying process is discrete, the research problem becomes one of identifying the one-step transition matrix given a multistep matrix—that is, it becomes a problem of taking the root of a matrix. Unfortunately, as pointed out by Singer and Spilerman (1976), none of the difficulties encountered in the continuous time setting would go away. Just as a logarithm is multivalued, so is a root operation. Therefore, switching the modeling framework to a discrete setting would not avoid the fundamental difficulties.

Lastly, as pointed out by Singer and Spilerman (1976) and readily intuitive to most researchers, if we could empirically estimate two transition matrices $P(t_1)$ and $P(t_2)$ such that $t_2 > t_1 > 0$ but t_2/t_1 is not rational, then the generator can be uniquely identified if it does exist. Alternatively, one could directly estimate the generator using transition data as outlined by Jarrow et al. (1997, p. 504). To make these approaches empirically feasible, we need time-stamped transitions for a universe of bonds. This type of data does appear to be available from Moody's or Standard and Poor's. Our future research endeavor will be to develop estimation procedures to directly extract a generator from such rating migration data.

8. CONCLUSIONS

Credit risk modeling and credit derivatives pricing have become a mainstream research subject in finance. A key building block for this line of research is the rating transition matrix. Given that empirically estimated matrices are mostly for a one-year period, there is a need to recover a matrix generator so that one can obtain a transition matrix for any arbitrary period of time, as often dictated by a valuation problem such as pricing a default swap. This paper identifies conditions under which a true generator does or does not exist.

It is shown that most of the observed average annual transition matrices would not be compatible with a continuous Markov process—that is, they do not admit a valid generator. Therefore a researcher is left with two options: either to obtain an approximate generator for the observed transition matrix or to modify the transition matrix first (to make it compatible with an underlying Markov process) and then search for true generators. Our limited experiments point to the choice of the first option.

We have presented a collection of theorems and propositions to help determine if and when a generator exists. The results, by their nature of generality, will have applications beyond research in finance.

APPENDIX: THEOREM PROOFS

In this Appendix, we provide proofs of all the theorems in the text (including, for completeness, those theorems previously proved elsewhere as indicated).

We begin with some standard facts from the functional calculus, which we shall use (explicitly or implicitly) in many of our proofs.

Standard Results. Let A be any $n \times n$ matrix. Let $H(A)$ be the algebra of functions that are analytic in a neighborhood of the set $\sigma(A)$ of eigenvalues of A. There is a mapping $f \mapsto f(A)$ from H to $n \times n$ complex matrices such that

(1) $f \mapsto f(A)$ is an algebra homomorphism.
(2) If $f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n$ is a Taylor series converging in a neighborhood of $\sigma(A)$, then $f(A) = \sum_{n=0}^{\infty} a_n (A - z_0 I)^n$. In particular, $f(A) = \exp(A)$ (as previously defined) for $f = \exp$.
(3) $\sigma(f(A)) = f(\sigma(A))$.
(4) $f(A)$ commutes with every $n \times n$ matrix that commutes with A.
(5) $f(A) = g(A)$ if $f - g$ is divisible (as a member of $H(A)$) by the characteristic polynomial of A.
(6) If $g \in H(f(A))$ then $g(f(A)) = (g \circ f)(A)$.
(7) If A has distinct eigenvalues then $f(A) = g(A)$ if and only if $f(r) = g(r)$ for each eigenvalue r of A.
(8) If A has distinct eigenvalues then every $n \times n$ matrix that commutes with A is $f(A)$ for some f.
(9) If A is a real matrix and $f(\bar{z}) = \overline{f(z)}$ in a neighborhood of $\sigma(A)$, then $f(A)$ is real.
(10) If $\mathbf{v}$ is an eigenvector of A for eigenvalue r, then $f(A)\mathbf{v} = f(r)\mathbf{v}$.

In particular, if f is any branch of the logarithm that is analytic in a neighborhood of $\sigma(P)$ then by (6), $\exp(f(P)) = P$. On the other hand, if P has distinct eigenvalues then by (4) every matrix Q such that $\exp(Q) = P$ must commute with P, and therefore by (8) $Q = g(P)$ for some $g \in H(P)$. By (6), $P = \exp(g(P)) = (\exp \circ g)(P)$, so by (7) $r = \exp(g(r))$ for each eigenvalue r of P; in other words, $g(r)$ is one of the values of $\log r$. There is a branch of the logarithm, f, that is analytic in a neighborhood of $\sigma(P)$ with $f(r) = g(r)$ for each r, and so, by (7) again, $Q = f(P)$.

Suppose P has row-sums 1; that is, the vector $\mathbf{1}$ whose entries are all 1 is an eigenvector of P with eigenvalue 1. Then by (10), $f(P)$ has row-sums $f(1)$.

Recall that we will use log to denote the principal branch of the logarithm—that is, for any nonzero complex number z, $\log(z)$ is the unique complex number w such that $\exp(w) = z$ and $-\pi < \mathrm{Im}\ w \leq \pi$. This is analytic in the complex plane except for the branch cut $(-\infty, 0]$. Thus $\log(P)$ is defined whenever P has no eigenvalues in $(-\infty, 0]$, and is a real matrix.

We now proceed to the proofs of the theorems from the text.

Proof of Theorem 2.1. Note first that the quantity S is simply the square of the numerical radius of $P - I$. Hence, by the *spectral radius formula* (see, e.g., Rudin 1991, Thm. 10.13), the norm of $(P - I)^k$ is asymptotic (as $k \to \infty$) to $S^{k/2}$. Hence, if $S < 1$, then the series (2.1) converges geometrically quickly as claimed, and in fact converges absolutely.

Furthermore, recall the expansion

$$\log(x) = (x-1) - (x-1)^2/2 + (x-1)^3/3 - (x-1)^4/4 + \dots$$

for real numbers x, provided that the series converges absolutely. This also applies to matrices, with 1 replaced by I. It follows that the definition (1) ensures that $\widetilde{Q} = \log(P)$—in other words, that $P = \exp(\widetilde{Q})$.

All that remains to prove is that $\widetilde{Q}$ has row-sums 0. For this we use the following lemma.

LEMMA A1. *Let A and B be $N \times N$ matrices. Suppose that A has row-sums α, and B has row-sums β. Set $C = AB$. Then C has row-sums $\alpha\beta$.*

Proof of Lemma A1. We compute that

$$\sum_j c_{ij} = \sum_j \sum_k a_{ik} b_{kj} = \sum_k a_{ik} \left(\sum_j b_{kj} \right) = \sum_k a_{ik}(\beta) = \beta \left(\sum_k a_{ik} \right) = \beta(\alpha),$$

thus proving Lemma A1. □

Now, since $P - I$ has row-sums 0, the lemma proves that $(P - I)^k$ has row-sums 0 for all positive integers k. Since the series (2.1) for $\widetilde{Q}$ is a limit of linear combinations of different $(P - I)^k$, it follows that $\widetilde{Q}$ also has row-sums 0. This completes the proof of Theorem 2.1. □

REMARK A1. If, instead, $S > 1$ then the series (2.1) will never converge. This is not surprising. For example, if P is self-adjoint (e.g., symmetric), then $S > 1$ if and only if the matrix P has negative eigenvalues; and it is well known that in this case there does not exist a generator for P.

Proof of Theorem 2.2. Let $m = \min\{p_{ii}\}$. Then $m > \frac{1}{2}$ by assumption. Write

$$P = mI + (1-m)R,$$

where $R = \frac{1}{1-m}(P - mI)$. Then R is also a Markov transition matrix. Now we compute that

$$P - I = (1-m)(R - I).$$

Since R is a transition matrix, we have $\|R\| \le 1$ (where $\|\cdots\|$ is the usual operator norm), so that $\|R - I\| \le 2$ by the triangle inequality, and $\|(R - I)^k\| \le 2^k$. Hence, $\|(P - I)^k\| \le (2 - 2m)^k$. But then, by the spectral radius formula again,

$$\sqrt{S} = \lim_{k\to\infty} \|(P-I)^k\|^{1/k} \le \lim_{k\to\infty} \left((2-2m)^k\right)^{1/k} = 2 - 2m.$$

Finally, since $m > \frac{1}{2}$, we have $2 - 2m < 1$, so that $\sqrt{S} < 1$, and hence also $S < 1$. This completes the proof. □

Proof of Theorem 3.1. For part (a), we recall the well-known formula that

$$\det(\exp(Q)) = \exp(\operatorname{trace}(Q)). \tag{A.1}$$

(To see this, first transform into a basis where Q is upper-triangular.) Hence, if $P = \exp(Q)$ for some matrix Q (whether a generator or not), then we must have $\det(P) = \det(\exp(Q)) > 0$.

For part (b), suppose to the contrary that P had a generator Q. Let $R(t) = \exp(tQ)$. Then $R'_{ii}(t) \geq Q_{ii}R_{ii}(t)$ and $R_{ii}(0) = 1$, so $R_{ii}(t) \geq \exp(tQ_{ii})$. Hence, $p_{ii} = R_{ii}(1) \geq \exp(Q_{ii})$. Hence, using (A.1), we have

$$\prod_i p_{ii} \geq \prod_i \exp(Q_{ii}) = \exp\Big(\sum_i Q_{ii}\Big) = \exp(\operatorname{trace}(Q)) = \det(P),$$

contradicting condition (b). Hence, assuming condition (b), there is no such generator Q.

Part (c) follows from the Lévy Dichotomy, which states that if P has a proper generator Q then for each pair (i, j) of states we must have either $p_{ij}(t) > 0$ for all $t > 0$ or $p_{ij}(t) = 0$ for all $t > 0$ (where $p_{ij}(t)$ is the ij entry of P_t).

To prove the Lévy Dichotomy, suppose that P did have a generator. Then for each state k we would have $p_{kk}(s) \to 1$ as $s \searrow 0$, so that for sufficiently small s we have $p_{kk}(s) > 0$ for all states k. (In fact, it then follows that this condition holds for all $s > 0$.) Hence, if $p_{ij}(t) = 0$ for some $t > 0$, then we must have $p_{ij}(t/n) = 0$ for all sufficiently large integers n (otherwise we would have $p_{ij}(t) \geq p_{ij}(t/n)(p_{jj}(t/n))^{n-1} > 0$). That is, the set of zeros of the function $p_{ij}(s)$ would have a limit point (i.e., 0). But $p_{ij}(s)$ is an analytic function of s. Hence, it must be that $p_{ij}(s) = 0$ for all $s > 0$, contradicting our assumption that $p_{ij}(t) = 0$ for some $t > 0$. This proves the Lévy Dichotomy.

To complete the proof of Theorem 3.1(c), suppose that j is accessible from i. Then we have $p_{ij}(m) > 0$ for appropriate positive integer m. Hence, we must have $p_{ij}(t) > 0$ for all t, and in particular $p_{ij}(1) = p_{ij} > 0$, as claimed. □

Proof of Theorem 5.1. We claim that exp is one-to-one on $\{Q : \|Q\| < \ln 2\}$. To see this, note that if $\|Q_1\| \leq r$ and $\|Q_2\| \leq r$ with $0 < r < \ln 2$,

$$\begin{aligned}
\|\exp(Q_1) - \exp(Q_2) - (Q_1 - Q_2)\| &\leq \sum_{n=2}^{\infty} \|Q_1^n - Q_2^n\|/n! \\
&\leq \sum_{n=2}^{\infty}\sum_{j=0}^{n-1} \|Q_2^j(Q_1 - Q_2)Q_1^{n-1-j}\|/n! \\
&\leq \|Q_1 - Q_2\| \sum_{n=2}^{\infty} nr^{n-1}/n! \\
&= \|Q_1 - Q_2\|(e^r - 1) < \|Q_1 - Q_2\|,
\end{aligned}$$

so $\|\exp(Q_1) - \exp(Q_2)\| > 0$.

Since $\det(\exp(Q)) = \exp(\operatorname{trace} Q)$, if Q is a generator for a transition matrix P with $\det(P) > 1/2$, we have $\operatorname{trace} Q > -\ln 2$. Now if we use the L^1-norm on vectors, $\|Q\| \leq \max_j \sum_i |Q_{ij}|$. But for a generator, $|Q_{ij}| \leq -Q_{ii}$ so $\|Q\| \leq -\sum_i Q_{ii} = -\operatorname{trace} Q < \ln 2$. Therefore there can be at most one generator. This proves (a).

For (b), note that if $\|P - I\| = r < 1/2$ then the series (2.1) for $\log P$ converges, and $\|\log P\| \leq -\ln(1 - r) < \ln 2$. Thus $Q = \log P$.

For (c), note that if Q is a generator for P and $\det(P) > \exp(-\pi)$ then $0 \geq \operatorname{trace} Q > -\pi$. Let $r = -\operatorname{trace} Q$. Now $Q + rI$ is a matrix with nonnegative entries, and its maximum nonnegative eigenvalue is r. By the Perron–Frobenius Theorem, all eigenvalues of this matrix have absolute value at most r, and in particular the imaginary part of any eigenvalue of Q is in $[-r, r]$. But Q must be $f(P)$ for some branch of the logarithm, and the only one whose imaginary parts are all in $(-\pi, \pi)$ is log. □

Proof of Theorem 5.2. Suppose Q is a generator for P. Since $\sigma(\exp(Q)) = \exp(\sigma(Q))$, exp must be one-to-one on $\sigma(Q)$. Since Q is a real matrix, any nonreal eigenvalues come in complex-conjugate pairs. If r and $\bar{r}$ form such a pair, then $\exp(r)$ and $\exp(\bar{r})$ are eigenvalues of $P = \exp(Q)$. But $\exp(\bar{r}) = \overline{\exp(r)} = \exp(r)$ since the eigenvalues of P are real, so exp would not be one-to-one on $\sigma(Q)$. Thus Q must have all real eigenvalues. As remarked earlier, if P has distinct eigenvalues then $Q = f(P)$ where f is some branch of the logarithm. Thus for each eigenvalue r of P, $f(r)$ is real and thus must be $\log(r)$. Therefore $Q = \log(P)$. Moreover, P cannot have any negative eigenvalues because negative numbers have no real logarithms. □

Proof of Theorem 5.3. The key is to condition on the number of jumps N which the chain makes in a time interval of length 1. Now $N \leq N'$, where N' is a Poisson random variable with mean $\lambda \equiv \max_i(-Q_{ii})$. Let $R(t) = \exp(tQ)$ and $R_{i,j}(n, t) = \mathbf{Pr}(X(t) = j | X(0) = i, N = n)$. Then $R_{i,j}(n, t/2) \geq 2^{-n} R_{i,j}(n, t)$ (as can be seen by writing the probability of a given sequence of n transitions as an n-fold integral). So

$$R_{i,j}(s) \geq s^m \sum_{n \leq m} R_{i,j}(n, 1) \geq s^m (P_{i,j} - \mathbf{Pr}(N' > m)).$$

Therefore, if $\mathbf{Pr}(N' > m) = b_m$, $P_{i,j} > b_m$ and $P_{j,k} > b_r$ then we must have

$$P_{i,k} \geq R_{i,j}(s) R_{j,k}(1-s) \geq s^m (1-s)^r (P_{i,j} - b_m)(P_{j,k} - b_r)$$

for any $0 < s < 1$. This bound is maximized when $s = m/(m+r)$. Summing over all j with $P_{i,j} > b_m$ and $P_{j,k} > b_r$ then gives the result. □

Proof of Theorem 6.1. If P has all distinct eigenvalues, then any Q will be $f(P)$ where f is some branch of the logarithm, and thus will be determined by the values $f(r)$ for eigenvalues r of P, where $f(r) = \log(r) + 2\pi k(r) i$ for some integers $k(r)$. If Q cannot have eigenvalues with |imaginary part| $\geq \pi$ then uniqueness is established. Now if $\det(P) > \exp(-\pi)$, then $\operatorname{trace}(Q) > -\pi$, and (for some $\epsilon > 0$), $Q + (\pi - \epsilon)I$ is a matrix with all nonnegative entries and its largest real eigenvalue is $\pi - \epsilon$. By Perron–Frobenius, all eigenvalues of $Q + (\pi - \epsilon)I$ have absolute value $\leq \pi - \epsilon$, so the imaginary part of any eigenvalue of Q has absolute value $< \pi$. □

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