NOTES AND CORRESPONDENCE

Statistical Significance Test for Transition Matrices of Atmospheric Markov Chains

ROBERT VAUTARD

Laboratoire de Météorologie Dynamique, Paris, France

KINGTSE C. MO

Climate Analysis Center, NMC/NWS/NOAA, Washington, District of Columbia

MICHAEL GHIL

Climate Dynamics Center, Department of Atmospheric Sciences, and Institute of Geophysics and Planetary Physics, University of California, Los Angeles, California

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ABSTRACT

Low-frequency variability of large-scale atmospheric dynamics can be represented schematically by a Markov chain of multiple flow regimes. This Markov chain contains useful information for the long-range forecaster, provided that the statistical significance of the associated transition matrix can be reliably tested. Monte Carlo simulation yields a very reliable significance test for the elements of this matrix. The results of this test agree with previously used empirical formulae when each cluster of maps identified as a distinct flow regime is sufficiently large and when they all contain a comparable number of maps. Monte Carlo simulation provides a more reliable way to test the statistical significance of transitions to and from small clusters. It can determine the most likely transitions, as well as the most unlikely ones, with a prescribed level of statistical significance.

1. Introduction

Recurrent and persistent anomaly patterns in atmospheric circulations can be classified into distinct flow regimes by subjective criteria (Spekat et al. 1983), by cluster analysis (Mo and Ghil 1988, MG88 hereafter), by a systematic search for the local maxima of multivariate probability density functions (Kimoto 1989; Molteni et al. 1989) or by identifying minima in the tendency between successive flow fields (Legras and Ghil 1985, Vautard and Legras 1988). Once a reasonable classification of flow patterns is obtained, one can study the transitions among them using a Markov chain description (Fraedrich and Müller 1983; Ghil 1987; Mo and Ghil 1987; Spekat et al. 1983). It is not necessary to classify all the maps into regimes, and in fact MG88 have argued that it is preferable to allow a large fraction of maps to belong to a diffuse, trivial, thin "cloud" of points in phase space, in which the truly interesting, synoptically recognizable, high-density regimes are embedded.

An uninterrupted sequence of maps within a regime, preceded and succeeded by one or more maps outside that regime, will be called an *event* (Ghil 1987; Mo and Ghil 1987, MG87 hereafter). To estimate a transition probability one can simply count the number of times that the flow moves from one regime to another—passing in between through the diffuse "cloud"—and divide by the total number of transitions from that regime to any other, including re-entry into the same regime. Since the time series of atmospheric fields at our disposal is finite and usually short, it is difficult to distinguish reliably between the transitions that are more or less likely to occur than by mere chance.

One way to assess statistical significance of elements of a transition matrix is to assume equal probability of transition from one regime to all other regimes, including re-entry into the same regime. Let us assume that there are N regimes, $i = 1, \cdots, N$, and let $\mathbf{T}$ be the transition matrix. T_{ij} gives the number of transitions from regime i to j. If n_i is the total number of events in regime i, then

$$\sum_{j=1}^{N} T_{ij} = n_i \quad \text{or} \quad n_i - 1$$

depending on whether the last event is in regime i or not; T_{ij}/n_i is an estimate for the transition probability p_{ij}. The total number of events in the time series is

$$K = \sum_{j=1}^{N} n_i.$$

Corresponding author address: Dr. Michael Ghil, Dept. of Atmospheric Sciences, University of California, 405 Hilgard Avenue, Los Angeles, CA 90024-1565.

Assuming equal probability, $p_{ij} \equiv p = 1/N$ is the probability of transition from regime i to any regime j, including re-entry. This is the case of a fair coin, $N = 2$, or of a fair die, $N = 6$. The average number of transitions is $m_i = n_i p = n_i/N$, and the associated standard deviation is $\sigma_i = (n_i pq)^{1/2}$, where $q = 1 - p$; the values m_i and σ_i correspond to the distribution of independent Bernoulli trials being binomial (e.g., Bajpai et al. 1978). For a sufficiently large number of trials, this can be approximated by a normal distribution; hence the element T_{ij} has to be larger than $m_i + 1.96\sigma_i$, $m_i + 1.64\sigma_i$, $m_i + 1.28\sigma_i$, and $m_i + \sigma_i$ in order to be statistically significant at the 95%, 90%, 80%, and 70% confidence level, respectively.

The equiprobability model does not distinguish between the fairness of the generalized die with N faces, i.e., the equal likelihood of each face i being the outcome of a given trial k, on the one hand, and the equidistribution of the transitions from any given face i upon trial k to face j (including re-entry, $j = i$) upon trial $k + 1$, on the other. In practice, the number of events n_i within each regime is not the same. This number, divided by the total number of events K, approximates the *absolute*, or *unconditional* probability of occurrence of that regime, p_i. The absolute probabilities for the occurrence of the seven regimes detected in the Northern Hemisphere (NH) data by MG88, and of the five regimes in the Southern Hemisphere (SH) data of MG87 are obviously significantly different. For instance, Cluster 7 in the NH data has about twice as many events as Cluster 4 (MG88, Table 7), and the range of sizes is even larger for the SH data (MG87, Table 8).

Thus the long-range forecaster could "guess," on any day of a given winter, that the next persistent pattern to set in is the unconditionally most probable one. This, however, is not the best guess one can make. The point of the Markov-chain approach is, in agreement with physical intuition and long-range forecasting experience, that there is some additional information to be extracted from the present state of the system. For this information to be useful, it is necessary to evaluate the statistical significance of the transition probabilities, i.e. the *conditional* probabilities p_{ij} of occurrence of regime j after a realization of (i.e., an event in) regime i.

It is in this evaluation that the equiprobability model runs into trouble. Since it *assumes* that all regimes are *unconditionally* equiprobable, $p_j = K/N$, it is biased in assigning significantly higher conditional probabilities p_{ij} to transitions occurring towards regimes that actually contain a larger number of events, $p_j \gg K/N$. In other words, the equiprobability model does not allow one to compare the conditional probability p_{ij} of going from regime i to regime j with the absolute probability p_j of occurrence of j.

To take into account the disparity in the size of regimes, we designed a nonparametric method based on Monte Carlo simulation to assess the statistical significance of a transition matrix. Asymptotic methods, based on parameter-dependent probability models, for testing the adequacy of Markov chain fits to time series data have been known for some time (Anderson and Goodman 1957, and further references therein). These methods, however, require a large number of data points for their reliable application, while the number of events in both NH and SH datasets is rather small. Hence, the need for the computer-intensive but relatively-straightforward nonparametric method presented here.

This method is outlined in section 2, and an illustrative example using synthetic data is given. We apply the method in section 3 to the transition matrix of NH flow regimes given by MG88, and to the transition matrix of SH flow regimes given by MG87. A summary and discussion follow in section 4.

2. Method and example

We generate a time series $R(t; \omega)$ of numbers from 1 to N randomly and independently. $R(t; \omega)$ represents the regime that the system is in at the time t for realization ω. Each realization of $R(t; \omega)$ is generated subject to the constraint that the number of elements in each regime is prescribed and equal to n_i, so the total number of elements K is also a constant—i.e. the time series is K long for each ω. A Monte Carlo ensemble of 100 realizations of 320 random numbers has also been used by Hansen and Sutera (1986) in testing the bimodality of the time series of NH 500 mb heights with respect to a planetary-wave activity index.

We calculate the transition matrix $B_{ij}(\omega)$ for $R(t; \omega)$ and repeat the process 10 000 times. We then compare each B_{ij} with the original transition matrix T_{ij}, and count the number C_{ij} of the times when $B_{ij} \geqslant T_{ij}$, and the number D_{ij} of times when $B_{ij} \leqslant T_{ij}$ out of 10 000. For the transition $i \rightarrow j$ to be more likely than due to pure chance at a significance level of 95%, 90%, and 80%, C_{ij} has to be smaller than 500, 1000, and 2000 respectively. For the same transition to be less likely than due to pure chance at the 95%, 90%, and 80% confidence level, D_{ij} has to be smaller than 500, 1000, and 2000 respectively.

Note that, in general, $C_{ij} + D_{ij} \geqslant 10\,000$, and that the use of weak inequalities, $B_{ij} \geqslant T_{ij}$ for C and $B_{ij} \leqslant T_{ij}$ for D, provides a more stringent significance criterion than the use of the corresponding strict inequalities, $B_{ij} > T_{ij}$ and $B_{ij} < T_{ij}$. In particular, the former will eliminate as not significant any transition from or to a regime comprised of a single event.

We give now an artificially generated but illustrative example to show that the equiprobability model is biased toward transitions leading to large regimes, and against transitions toward regimes having a relatively small number of maps. The system we choose has three regimes, say "zonal flow" with $n_1 = 52$ events, "blocked flow" in the Atlantic with $n_2 = 37$ events, and blocked flow in the Pacific with $n_3 = 18$ events. The chronology of the events in the example is generated at random. The transition matrix and statistical significance limits estimated using the equiprobability method are given in Table 1a.

Table 1a shows that all the transitions to the largest cluster, $j = 1$, from other clusters are declared significant by this method at the 95% confidence level, while transitions $1 \rightarrow 3$ and $3 \rightarrow 3$ to the smallest cluster, $j = 3$, are declared unlikely at the 95% level. The matrices C_{ij} and D_{ij} for the Monte Carlo method are given in Table 1b. No transition is found significant even at the 80% level: Since the chronology is random, there is no useful forecasting information p_{ij} in the realization at any given time of regime i, distinct from and in addition to the absolute probability of occurrence p_j of regime j.

3. Application to hemispheric Markov chains

a. Northern Hemisphere

Mo and Ghil (1988) applied cluster analysis to a time series of 2400 daily observed 500 mb low-pass filtered height anomaly maps for 20 NH winters (1963–1982) of 120 days each (15 November–15 March). They projected the dataset onto its seven leading EOFs, which together make up more than 50% of the total variance (MG88, p. 10 939 and their Table 1), and obtained seven statistically significant clusters; the same clusters were obtained when working in the subspace spanned by the nine leading EOFs, with about 60% of the variance (MG88, p. 10 940 and their Table 1).

The total number of events in the seven clusters is 145, where an event is defined as passage of the NH map sequence through one of the clusters. Each event lasts on average six to seven days, so the clusters contain about 40% of the total number of maps available. The diffuse cluster of nonrecurrent maps, in which the seven stable ones are embedded, is not meteorologically significant and was omitted from the classification in order to accelerate and stabilize the clustering algorithm. The detailed description of the seven significant clusters appears in section 5 of MG88.

The dominant cluster, $i = 1$, is characterized by a zonal wavenumber 3 (W3), with the Pacific/North American (PNA) anomaly pattern of Wallace and Gutzler (1981) most prominent. The second cluster, $i = 2$, has a reverse wavenumber 3 structure (RW3), and is characterized by a wave train extending from the eastern United States over Greenland to northern Europe. The third cluster, $i = 3$, is dominated by a wavenumber 2 (W2) pattern, with a positive anomaly over the northern Soviet Union (NSU: Dole 1986) and zonal flow over the Pacific. The fourth cluster, $i = 4$, exhibits a North–South oscillation (NSO) in both the Pacific and the Atlantic sectors; the two features correspond roughly to the Western Pacific teleconnection pattern of Wallace and Gutzler (1981) and the Greenland–northern European seesaw of van Loon and Rogers (1978). A wave train (WT) starting off the southeastern coast of the United States across Eurasia to eastern Siberia characterizes the fifth cluster, $i = 5$. The sixth cluster, $i = 6$, is dominated by a reverse PNA pattern (RNA). The seventh cluster lies close to the time mean (TM) of the map sequence. The anomaly maps of the centers of each cluster (except the seventh, for obvious reasons) are shown in Figs. 10a–f of MG88.

TABLE 1a. Transition matrix for a synthetic example.

From/To	1	2	3	Sum	Ave.	S.D.
1	**24**	19	*08*	51	17.0	3.37
2	**18**	12	07	37	12.3	2.87
3	**10**	05	*03*	18	6.0	1.15
Sum	52	36	18	106		

Boldface and italics indicate most and least likely transitions, respectively, from the equiprobability model; confidence level used is 95%.

TABLE 1b. Matrices **C** and **D** calculated by the Monte Carlo method.

	C			**D**		
	1	2	3	1	2	3
1	6859	4196	7346	4647	7273	4545
2	5880	6504	4314	5786	5198	7558
3	3488	8298	5767	8202	3453	6933

The transition matrix and statistical significance estimated by the equiprobability model are given in Table 2a. The ratio of number of events in the smallest regime to that in the largest regime is $14/28 = 1/2$ vs. $18/52 \approx 1/3$ in the example. The matrices C_{ij} and D_{ij} calculated from the Monte Carlo method are given in Table 2b. Transitions significant at the 95% confidence level are $4 \rightarrow 1$ and $6 \rightarrow 6$. Additional transitions, significant at the 90% confidence level, are $1 \rightarrow 3$, $2 \rightarrow 7$, $5 \rightarrow 2$ and $7 \rightarrow 3$. At the 95% significance level, the most unlikely paths are $2 \rightarrow 3$, $4 \rightarrow 7$ and $6 \rightarrow 5$.

Figure 1 provides the statistical confidence limits, based on Table 2b, for all paths given in MG88. The figure is schematic: the locations of the clusters correspond approximately, but not exactly, to the position of their centers in a reduced, three-dimensional phase space, shown in an axionometric representation with origin near TM, the first empirical orthogonal function (EOF 1) of the dataset pointing along the bisector of the third quadrant (at 7:30 on a dial), EOF 2 to the right (at 3:00), and EOF 3 up (at 12:00) (compare Fig. 14 of MG88). Note that the confidence level used in MG88 was only 70%. At this level, of all the transitions in Fig. 1, only $6 \rightarrow 7$ is not found significant by the Monte Carlo method. This exception reflects the bias discussed in the present note, since Cluster 7 is the largest one. The otherwise rather good agreement

TABLE 2a. Transition matrix between regimes in the NH data (after MG88).

From/To	1	2	3	4	5	6	7	Sum	Ave.	S.D.
1	1	3	6	2	6	1	4	23	3.3	1.71
2	5	2	0	0	4	3	7	21	3.0	1.61
3	4	2	2	1	2	2	**6**	19	2.7	1.50
4	**6**	1	1	3	3	0	0	14	1.9	1.36
5	1	6	1	3	2	4	6	23	3.3	1.68
6	1	2	2	2	0	**6**	4	17	2.4	1.44
7	5	5	7	2	6	1	2	28	4.0	1.85
Sum	23	21	19	13	23	17	29	145		

Boldface and italics indicate most and least likely transitions, at the 95% level, for the equiprobability model.

between the two methods is due to the relatively small variation in the size of the clusters.

b. Southern Hemisphere

Mo and Ghil (1897) calculated the transition matrix between regimes obtained from the EOF analysis of 981 maps of 500 mb height for eleven 92-day SH winters between June 1972 and July 1983. This time series is much shorter than the NH one, and hence smaller statistical significance is expected. But the results of the EOF analysis, at least, have been confirmed and refined, using slightly different and improved data handling procedures, by Farrara et al. (1989).

There are five regimes obtained in MG87 by a pattern correlation method and only 22 events. The regimes are described in detail in section 5 of MG87. The first two flow regimes show a large zonal wavenumber 3 component, but differ in the meridional position and zonal phase of this component, and in the amplitude of the wavenumber 1 component. The third flow regime is dominated by a zonal wavenumber 4 component. The fourth regime lies close to the time mean, and the fifth regime groups persistent events of differing patterns, too small in number to be further subdivided. The ratio of the number of events in the smallest regime to that in the largest regime is 1:8.

The transition matrix and statistical significance estimated by the equiprobability model are given in Table 3a. Transitions 4 → 1 and 5 → 1 appear to be significant at 95%, but the entries in the transition matrix, T_{41} in particular, are very low, due to the shortness of the time series. The statistical significance level assessed by this crude method may thus not be meaningful, since the number of transitions is unlikely to follow closely a normal distribution.

The matrices **C** and **D** calculated from the Monte Carlo method are given in Table 3b. We find no significant transition at the 95% confidence level. Only the transition 5 → 1 is significant at the 90% level. The next transition in order of significance is 3 → 5, at 73%. The path 1 → 1, classified as likely at 80% by the equiprobability method, is only significant at 53%. Transitions 2 → 1, 3 → 1, and 5 → 5 are unlikely, but their significance does not exceed 90%. These results show clearly that longer time series are required for the analysis of the transitions.

4. Concluding remarks

A coarse-grained description of large-scale atmospheric dynamics in terms of multiple flow regimes was advocated by Ghil (1987, 1988), based on pertinent ideas from dynamical systems theory (Eckmann and Ruelle 1985; Guckenheimer and Holmes 1983). Such a description lends itself well to the purposes of 30–90 day (intraseasonal) long-range forecasting (LRF). From the point of view of practical LRF, the

TABLE 2b. Matrices **C** and **D** calculated by the Monte Carlo method.

	C							**D**						
	1	2	3	4	5	6	7	1	2	3	4	5	6	7
1	9835	6833	551	6915	1216	9560	7170	960	5729	9855	6206	9559	2096	5027
2	2180	8278	10000	10000	4274	4487	900	9135	4185	*393*	1042	7836	7945	9713
3	3463	8061	7129	8718	8399	6842	1458	8497	4623	5830	4373	3926	6158	9495
4	**105**	8953	8702	1182	3781	10000	10000	9982	3798	4282	9737	8475	1634	*375*
5	9844	820	9678	3797	9030	2732	2931	887	9754	1634	8469	2735	8953	8618
6	9546	7443	6803	5083	10000	**38**	4408	2068	5416	6189	7866	*450*	9994	7798
7	4985	4116	518	8115	2800	9792	9885	7128	7844	9856	4466	8672	1053	502

Transitions occurring more and less likely than by mere chance at the 95% level are indicated by boldface and italics, respectively.

TABLE 3a. Same as Table 2a for the SH data (after MG87).

From/To	1	2	3	4	5	Sum	Ave.	S.D.
1	3	1	1	1	2	8	1.6	1.13
2	0	1	1	0	1	3	0.6	0.69
3	0	1	1	0	2	4	0.8	0.80
4	**1**	0	0	0	0	1	0.2	0.40
5	**4**	1	1	0	0	6	1.2	0.98
Sum	8	4	4	1	5	22		

key ingredient is the transition matrix associated with the Markov chain defined by the regimes.

Given a currently observed flow regime, the LRF forecaster can use the most likely transition from that regime in his 30 day forecast to indicate, after the collapse or "break" of the current pattern, what other pattern is most likely to affect the next monthly anomaly map. The mean duration of NH events is only 6 days, and that of sequences of unclassified maps within the thinly populated portions of phase space are about 9.5 days (Mo and Ghil 1988, MG88 in the main text). Thus, one or two classifiable events will occur within the next month, affecting its mean anomaly pattern. Statistical confidence in the elements of the transition matrix is, therefore, of considerable importance to intraseasonal LRF.

MG88 used an equiprobability model in order to evaluate the statistical significance of the transitions they determined. We have shown in sections 2 and 3 that this model is biased in favor of transitions to large clusters and against transitions to small ones (Tables 1a, 2a, and 3a). This was fortunately not too deleterious for the estimate of confidence limits for NH transitions, since the ratio of the largest to the smallest cluster identified by MG88 was no larger than 2:1. It is only for ratios as large as 3:1 that serious distortions in the confidence estimates occur (Table 1b).

The Monte Carlo approach developed here is nonparametric and robust, since it makes no a priori assumptions about the transition probabilities. It takes into account the relative sizes of the regimes by using a sufficiently large number of realizations of the time series under consideration, subject to the constraint of the size of each regime being given. It provides a reliable estimate of the likelihood of a given transition being distinct from—i.e. above or below—that due to pure chance, for the given distribution of absolute probabilities of occurrence of the regimes. This likelihood can be determined for any given threshold, e.g., 80%, 90%, or 95%.

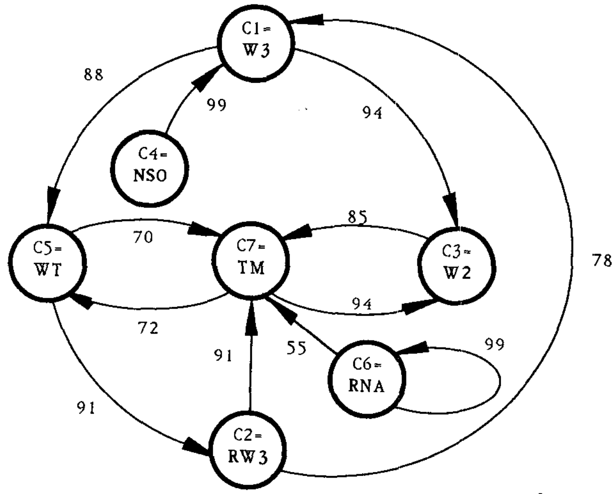

FIG. 1. Statistical confidence level for all paths given in MG88, by Monte Carlo method. The acronyms associated with each cluster stand for their characteristic features: 1) W3 for zonal wavenumber three, 2) RW3 for approximate reverse of the former, 3) W3 for zonal wavenumber two, 4) NSO for North–South oscillation, 5) WT for wave train, 6) RNA for reverse PNA, and, 7) TM for time mean (see text and MG88 for details).

With this Monte Carlo method, we have partially confirmed the previous results of MG88 for NH regimes (Table 2b and Fig. 1) and of Mo and Ghil (1987, MG87 in the main text) for SH regimes (Table 3b). The most reliably favored transitions for the NH Markov chain are 4 → 1 and 6 → 6, i.e. from NSO to W3 and from RNA to itself, at the 99% confidence level. These are followed by 1 → 3 and 7 → 3, i.e. W3 like to W2 and TM to W2 at 94%, and by WT to RW3 like RW3 to TM at 91% (see Fig. 1). In the SH winter, the only significant transition is from regime 5 to 1. No other conclusion can be drawn due to the shortness of the SH record under study.

The careful evaluation of statistical significance for transition matrices of observed atmospheric field sequences helps establish the practical credibility for LRF of the Markov chain method. But existing map sequences are still rather short, especially for the SH at-

TABLE 3b. Same as Table 2b for the SH data.

	1	2	3	4	5	1	2	3	4	5
1	4647	8395	8462	3486	7117	8500	5564	5591	10000	6699
2	10000	4518	5560	10000	7363	1490	9346	8787	8268	7324
3	10000	5557	4532	10000	2728	1525	8837	9344	8203	9573
4	3490	10000	10000	10000	10000	10000	8234	8291	10000	7396
5	837	7343	7411	10000	10000	9908	7275	7339	7431	1830

mosphere, and cannot be extended in practice as rapidly as we would wish. The only way of obtaining better, more reliable transition probabilities from flow regime to flow regime is by the use of general circulation models (GCMs) for LRF (Ghil 1987, section 4). A GCM has to be verified first, as to its own preferred regimes and transition probabilities, against existing atmospheric datasets. If and when the GCM passes this test, it can be run for much longer time intervals, of tens and hopefully hundreds of years, to yield more reliable transition matrices, as well as the dynamical and physical details of each transition.

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