Appendix: On the discrimination of Markov chains through their empirical transition matrices

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Introduction

We consider irreducible Markov chains on a finite number $k$ of states, with transition matrix $q$ and stationary distribution $p$. The number $\ell$ of edges used by the chain is the number of couples of states $(x, y)$ such that $q(x, y) > 0$, hence $k \leq \ell \leq k^2$. When $\ell = k$, the chain moves deterministically on an oriented discrete circle, hence one can exclude this case if necessary. On the contrary, as soon as $\ell \geq k + 1$, several trajectories are possible and the chain is truly random. Finally, $\ell = k^2$ means that all the transitions are allowed, hence the chain moves on the complete graph with loops. The dimension $D(q)$ of the chain is

$$D(q) := \ell - k,$$

This the number of free parameters among the nonzero coefficients of $q$, that is, the dimension of the simplex formed by the transition matrices subordinated to $q$, in the sense that the coefficients corresponding to coefficients of $q$ equal to 0 have to be equal to 0 too.

The maximum likelihood estimator $\hat{q}$ of $q$ uses countings along a trajectory of length $n$ and is a consistent estimator of $q$ when $n$ goes to infinity. The relation

$$\hat{q}(x, y) = q(x, y) + \frac{z_{xy}}{\sqrt{n}} + o(1/\sqrt{n}),$$

defines a Gaussian centered vector $(z_{xy})_{xy}$, indexed by the edges $(x, y)$, and whose covariance matrix is an explicit function of $p$ and $q$. 

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We consider the relative entropy of the empirical measure, given by the observed trajectory, with respect to the theoretical measure, given by \( p \) and \( q \). This random entropy is defined by

\[
H(\hat{q}, q) := \sum_{(x,y)} \hat{p}_x \hat{q}(x,y) \log(\hat{q}(x,y)/q(x,y)),
\]

where the sum indexed by \((x,y)\) has \( \ell \) terms and \( \hat{p} \) denotes the stationary distribution of \( \hat{q} \). One can also consider the entropy

\[
H(q, \hat{q}) := \sum_{(x,y)} p_x q(x,y) \log(q(x,y)/\hat{q}(x,y)).
\]

Using second-order Taylor series approximations of the logarithm function, one sees that both \( H(\hat{q}, q) \) and \( H(q, \hat{q}) \) are such that, when \( n \) becomes large,

\[
H = h/(2n) + o(1/n), \quad h := \sum_{(x,y)} z^2_{xy} p_x / q(x,y).
\]

In this appendix we show that the reduced relative entropy \( h \) follows a quite simple \( \chi^2 \) distribution and we draw some statistical consequences from this result.

**Convergence in distribution**

Let \( N_x \), respectively \( N_{xy} \), denote the number of times the vertex \( x \), respectively the edge \((x,y)\), is visited up to time \( n \). Consider

\[
\xi_{xy} := (N_{xy} - q(x,y)N_x)/\sqrt{N_x}.
\]

According to [P. Billingsley (1960). Statistical Inference in Markov Chain. The Stanford meetings of the Institute of Mathematical Statistics. Statistical Research Monographs, Vol. II. The University of Chicago Press, Chicago, Ill. 1961], the matrices \((\xi_{xy})_{xy}\) converge in distribution, when \( n \) goes to infinity, to a Gaussian centered matrix \((g_{xy})_{xy}\) distributed as follows. The vectors \((g_{xy})_y\) are independent for different states \( x \), hence the covariance of \( g_{xy} \) and \( g_{zt} \) is 0 for every \( x \neq z \) and every \( y \) and \( t \). Finally, for every \( x, y \) and \( z \),

\[
E(g_{xy}g_{xz}) = -q(x,y)q(x,z) \quad (y \neq z), \quad E(g^2_{xy}) = q(x,y)(1 - q(x,y)).
\]

Since \( N_x/n \) converges almost surely to \( p_x \), one can replace the factor \( 1/\sqrt{N_x} \) by \( 1/\sqrt{np_x} \). This remark yields the following convergence in distribution:

\[
np_x(\hat{q}(x,y) - q(x,y))^2 \rightarrow g^2_{xy}.
\]
In addition, we recall that, if one observes an i.i.d. sequence with theoretical distribution \( p \) on \( k \) states, then the empirical distribution \( \hat{p} \) is such that \( 2nH(\hat{p}, p) \) converges in distribution to a \( \chi^2 \) distribution with \( k - 1 \) degrees of freedom.

The vectors \((g_{xy})_{xy}\) are independent. Furthermore, for each fixed \( x \), \((g_{xy})_{y}\) admits the same covariances that the limit gaussian distribution obtained for an i.i.d. sequence of distribution \( q(x, \cdot) \). In addition, the random variable

\[
H_x := \sum_y q(x, y) \log(q(x, y)/\tilde{q}(x, y))
\]

corresponds to the observation of this i.i.d. process during a time which corresponds to the number of visits of \( x \) before \( n \), that is, a random number of visits which is \( np_x + o(n) \). Hence, \( 2(np_x)H_x \) converges in distribution to the \( \chi^2 \) distribution with \( D_x(q) \) degrees of freedom, where \( D_x(q) + 1 \) is equal the number of \( y \) such that \( q(x, y) > 0 \). By independence of the limits in distribution of the \( 2np_xH_x \), their sum \( 2nH \) converges in distribution to the \( \chi^2 \) distribution with \( D(q) \) degrees of freedom, where \( D(q) \) is the sum indexed by \( x \) of the \( D_x(q) \).

In conclusion, \( h \) follows the \( \chi^2 \) distribution with \( D(q) \) degrees of freedom.

**Statistical applications**

Assume that one has two independent sequences of observations of the same Markov chain with transition matrix \( q \). This yields two estimators \( \hat{q}_1 \) and \( \hat{q}_2 \) of \( q \), based respectively on the countings \( N^{(1)} \) and \( N^{(2)} \). We proved the relations

\[
\hat{q}_i(x, y) = q(x, y) + z^{(i)}_{xy}/\sqrt{n} + o(1/\sqrt{n}), \quad i = 1, 2,
\]

where the two families \((z^{(1)}_{xy})_{xy}\) and \((z^{(2)}_{xy})_{xy}\) are independent and follow the distribution of \((z_{xy})_{xy}\) described in the previous section. The reduced relative entropy between the two sequences of observations is asymptotically equal to

\[
h(\hat{q}_1, \hat{q}_2) := \sum_{(x, y)} (z^{(1)}_{xy} - z^{(2)}_{xy})^2 \alpha_{xy},
\]

where \( \alpha_{xy} \) can be indifferently \( p^{(1)}_x/q_1(x, y) \) or \( p^{(2)}_x/q_2(x, y) \) or \( p_x/q(x, y) \). If one uses \( \alpha_{xy} = p_x/q(x, y) \), then \( h(\hat{q}_1, \hat{q}_2) \) follows exactly the distribution of \( 2h(\hat{q}, q) \), and the same result holds asymptotically for the other choices of \( \alpha_{x,y} \). Hence, to determine whether \( \hat{q}_1 \) and \( \hat{q}_2 \) correspond to the same Markov chain or not, one can use the fact that, if they do, \( nH(\hat{q}_1, \hat{q}_2) \) is asymptotically \( \chi^2 \) with \( D(q) \) degrees of freedom. In particular,

\[
E(H(\hat{q}_1, \hat{q}_2)) \sim D(q)/n.
\]
If one wishes to work instead with the symmetrized form of the relative entropy, one can use
\[ \zeta := n(H(\hat{q}_1, \hat{q}_2) + H(\hat{q}_2, \hat{q}_1)) = \sum_{(x,y)} (N^{(1)}_{xy} - N^{(2)}_{xy}) \log \left( \frac{N^{(1)}_{xy}}{N^{(1)}_{y}} \cdot \frac{N^{(2)}_{xy}}{N^{(2)}_{y}} \right) . \]

Since \( \zeta \) is asymptotically twice a \( \chi^2 \) with \( D(q) \) degrees of freedom, one can compute the \( p \)-value of the event \( \{ \zeta \geq t \} \) for every \( t \geq 2D(q) \).

To compute upper bounds of the \( p \)-values of \( \chi^2 \) distributions of large dimension \( d \), one can use exponential Cramer bounds. This yields that, for every \( t \geq d \), the probability that a \( \chi^2 \) distribution with \( d \) degrees of freedom is greater than \( t \) is at most
\[ e^{-t/2}(tc/d)^{d/2} . \]

This approximation yields for instance that, if \( d = 400 - 20 = 380 \), the \( p \)-value for \( t = 460 \) is less than 2.47 % and the \( p \)-value for \( t = 480 \) is less than 0.04 %, to be compared to the true \( p \)-values 0.3% and 0.03% respectively.