COVARIANCE AND RELAXATION TIME IN FINITE MARKOV CHAINS

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The relaxation time T_{REL} of a finite ergodic Markov chain in continuous time, i.e., the time to reach ergodicity from some initial state distribution, is loosely given in the literature in terms of the eigenvalues λ_j of the infinitesimal generator $\underline{Q}$. One uses $T_{REL} = \theta^{-1}$ where $\theta = \min_{\lambda_j \neq 0} \{\operatorname{Re} \lambda_j[-\underline{Q}]\}$. This paper establishes for the relaxation time θ^{-1} the theoretical solidity of the time reversible case. It does so by examining the structure of the quadratic distance $d(t)$ to ergodicity. It is shown that, for any function $f(j)$ defined for states j , the correlation function $\rho_f(\tau)$ has the bound $|\rho_f(\tau)| \leq \exp[-\theta|\tau|]$ and that this inequality is tight. The argument is almost entirely in the real domain.

Key words: Finite Markov Chains, Covariance, Relaxation Time.

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1. Introduction

Let $J(t)$ be any ergodic Finite Markov Chain in continuous time with generator $\underline{Q}$. A single underscore will be used to denote vectors and a double underscore will be used for matrices. Let $\underline{p}^T(t) = \underline{p}^T(0)e^{\underline{tQ}}$ be the state probability vector so that

$$\lim_{t \rightarrow \infty} \underline{p}^T(t) = \underline{e}^T = (e_n)_1^K > \underline{0}^T; \quad \underline{e}^T \underline{Q} = \underline{0}^T.$$

We are interested in the relaxation time of $J(t)$. For time-reversible chains where all eigenvalues of $\underline{Q}$ are real the relaxation time is well understood (cf. Keilson [1]). For more general chains with real eigenvalues and eigenvalues occurring in complex conjugate pairs, all eigenvalues $\lambda_j[\underline{Q}]$ other than zero have $\operatorname{Re} \lambda_j[\underline{Q}] < 0$ (see appendix). Let $\theta = \min_{\lambda_j \neq 0} \{\operatorname{Re} \lambda_j[-\underline{Q}]\}$. The value $T_{REL} = \theta^{-1}$ is employed loosely for the relaxation time in the literature. This paper establishes for the relaxation time

θ^{-1} the theoretical solidity of the time reversible case.

Let $\underline{e}_D = \text{diag}(e_n)$. Recall that $\sqrt{\underline{x}^T \underline{U} \underline{x}}$ is a vector norm when $\underline{U}$ is positive definite. The scalar function

$$d(t) = \sqrt{(\underline{p}^T(t) - \underline{e}^T) \underline{e}_D^{-1} (\underline{p}^T(t) - \underline{e}^T)} \quad (1)$$

is then a vector norm and a distance to ergodicity.

It has been shown by D.G. Kendall [3] that the distance $d(t)$ is monotone decreasing for time reversible chains. It has also been shown by Keilson and Vasicek [2] that this distance decreases to zero for all ergodic chains. An independent proof will be given in this paper.

2. The Structure of the Distance to Ergodicity

The structure of $d(t)$ for all finite ergodic chains is examined more deeply here. This structure is used to establish the relaxation time θ^{-1} entirely in the real domain without any reference to complex eigenvalues until the end. We use the following notation:

Definitions:

$$\begin{array}{ll} 2a) & \underline{e}_D = \text{diag}(e_n) \\ 2b) & \underline{\nu}^T(t) = (\underline{p}^T(t) - \underline{e}^T) \underline{e}_D^{-1/2} \\ 2c) & w(t) = \underline{\nu}^T(t) \underline{\nu}(t) \\ 2d) & d(t) = \sqrt{w(t)} \\ 2e) & \underline{Q}^R = \underline{e}_D^{-1} \underline{Q}^T \underline{e}_D \\ 2f) & \underline{Q}^\# = \frac{1}{2} [\underline{Q} + \underline{Q}^R] \\ 2g) & \underline{B} = \underline{e}_D^{1/2} \underline{Q} \underline{e}_D^{-1/2} \\ 2h) & \underline{C} = \frac{1}{2} [\underline{B} + \underline{B}^T] = \underline{e}_D^{1/2} \underline{Q}^\# \underline{e}_D^{-1/2} \end{array}$$

The superscript R refers to the reverse chain. Note that $\underline{Q}$, $\underline{Q}^R$, and $\underline{Q}^\#$ all generate chains which have the same ergodic vector $\underline{e}^T$.

Theorem A: For any finite ergodic Markov chain $J(t)$:

- (a) $\underline{Q}^\#$ is the Q -matrix of an ergodic chain;
- (b) $\underline{C} = \underline{e}_D^{1/2} \underline{Q}^\# \underline{e}_D^{-1/2}$ is symmetric and negative-semidefinite with eigenvalues $\lambda_1 = 0, \lambda_j < 0, j \neq 1$.
- (c) The stationary chain generated by $\underline{Q}^\#$ is time-reversible.

Proof: $\underline{Q}$ and $\underline{Q}^R = \underline{e}_D^{-1} \underline{Q}^T \underline{e}_D$ have the zero structure needed to be an ergodic Q matrix as does $\underline{Q}^\# = \frac{1}{2} [\underline{Q} + \underline{Q}^R]$. The matrices $\underline{Q}$, $\underline{Q}^R$ and $\underline{Q}^\#$ all have row sum zero. Also $2\underline{e}_D^{1/2} \underline{Q}^\# \underline{e}_D^{-1/2} = \underline{e}_D^{1/2} \underline{Q} \underline{e}_D^{-1/2} + \underline{e}_D^{1/2} \underline{Q}^R \underline{e}_D^{-1/2} = \underline{e}_D^{1/2} \underline{Q} \underline{e}_D^{-1/2} + \underline{e}_D^{-1/2} \underline{Q}^T \underline{e}_D^{1/2}$ is symmetric. Hence $\underline{e}_D \underline{Q}^\# = \underline{e}_D^{1/2} [\underline{e}_D^{1/2} \underline{Q}^\# \underline{e}_D^{-1/2}] \underline{e}_D^{1/2}$ is symmetric and $J^\#(t)$ governed by $\underline{Q}^\#$ is time-reversible (cf. Keilson [1]). $\square$

Theorem B: Let $\theta = \min_{\lambda_j \neq 0} \{\lambda_j[-\underline{C}]\} = \min_{\lambda_j \neq 0} \{\lambda_j[-\underline{Q}^\#]\}$. $T_{REL}^\# = \theta^{-1}$ is then the relaxation time of the ergodic time reversible chain $J^\#(t)$. For any finite ergodic Markov chain, it has been shown in [4] that

$$\frac{d(t)}{d(0)} = \sqrt{\frac{w(t)}{w(0)}} \leq e^{-\theta t}. \quad (3)$$

The rate θ will be called the *global decay rate* of $d(t) = \sqrt{w(t)}$. The proof is given here.

Proof: From the definitions, one has at once $\frac{d}{dt}\underline{\nu}^T(t) = \underline{\nu}^T(t)\underline{B}$ and $\frac{d}{dt}\underline{\nu}(t) = \underline{B}^T\underline{\nu}(t)$. Hence $\frac{d}{dt}w(t) = \frac{d}{dt}[\underline{\nu}^T(t)\underline{\nu}(t)] = \underline{\nu}^T(t)\underline{B}\underline{\nu}(t) + \underline{\nu}^T(t)\underline{B}^T\underline{\nu}(t)$. This implies

$$\frac{d}{dt}w(t) = 2 \left[\underline{\nu}^T(t)\underline{C}\underline{\nu}(t) \right]. \quad (4)$$

Since $\underline{x}^T\underline{C}\underline{x} < 0$, for all real $\underline{x} \neq \underline{0}$, $\frac{d}{dt}w(t) \leq 0$ and $w(t)$ decreases in t . The matrix $\underline{C}$ has principal left eigenvector $\underline{e}_C^T = (e_n^{1/2})$ corresponding to eigenvalue 0 and $\underline{\nu}^T(t)\underline{e}_C = (\underline{p}^T t) - \underline{e}^T \underline{1} = 0$. Thus $\underline{\nu}^T(t)$ is orthogonal to the principal rank one eigenspace of $\underline{C}$. When $\underline{p}^T(0) \neq \underline{e}^T$, $\underline{\nu}^T(t)$ moves in this space, and does not vanish. One has from the Rayleigh-Ritz principal

$$\frac{d}{dt}\log w(t) = 2 \frac{\underline{\nu}^T(t)\underline{C}\underline{\nu}(t)}{\underline{\nu}^T(t)\underline{\nu}(t)} \leq -2 \min_{\lambda_j > 0} \{\lambda_j[-\underline{C}]\} = -2\theta.$$

If one integrates from 0 to t , Theorem B follows. $\square$

Convexity Lemma: *The function $w(t)$ is convex and*

$$\frac{d^2}{dt^2}w(t) = 4\underline{\nu}^T(t)\underline{C}^2\underline{\nu}(t) \geq 0. \quad (5)$$

Proof: From $\frac{d}{dt}w(t) = \frac{d}{dt}[\underline{\nu}^T(t)\underline{\nu}(t)] = 2\underline{\nu}^T(t)\underline{C}\underline{\nu}(t)$ one has

$$\frac{d^2}{dt^2}w(t) = \frac{d}{dt}[\underline{\nu}^T(t)\underline{C}\underline{\nu}(t)] = 2\underline{\nu}^T(t)[\underline{B}\underline{C} + \underline{C}\underline{B}^T]\underline{\nu}(t).$$

But

$$2[\underline{B}\underline{C} + \underline{C}\underline{B}^T] = \underline{B}[\underline{B} + \underline{B}^T] + [\underline{B} + \underline{B}^T]\underline{B}^T = (\underline{B} + \underline{B}^T)^2 + (\underline{B}\underline{B}^T - \underline{B}^T\underline{B})$$

and $(\underline{B}\underline{B}^T - \underline{B}^T\underline{B})$ is antisymmetric. The lemma then follows. $\square$

A stronger result is available.

Theorem C: *For any finite ergodic Markov chain, with $d(0) \neq 0$,*

- (a) $w(t)$ is convex and decreasing in t ;
- (b) $\log w(t)$ is convex in t , i.e. $\frac{w'(t)}{w(t)}$ increases with t ;
- (c) $\frac{w'(t)}{w(t)} \leq -2\theta$. This equality is tight, i.e., an initial state vector can be found for which $\frac{w'(t)}{w(t)} = -2\theta$ for all t .

Proof: From the proof of Theorem B, $w'(t) < 0$. We must show that $[\log w(t)]'' = \frac{w(t)w''(t) - [w'(t)]^2}{w^2} \geq 0$. Calculation gives

$$w(t)w''(t) - [w'(t)]^2 = 4 \left\{ [\underline{\nu}^T(t)\underline{\nu}(t)][\underline{\nu}^T(t)\underline{C}^2\underline{\nu}(t)] - [\underline{\nu}^T(t)\underline{C}\underline{\nu}(t)]^2 \right\}$$

where $\underline{C} = \underline{e}_D^{1/2} Q^\# \underline{e}_D^{-1/2}$. Moreover since $\underline{C}$ is symmetric, the Schwartz inequality

gives

$$\left| \underline{\nu}^T(t) \underline{C} \underline{\nu}(t) \right|^2 \leq \left| \underline{\nu}^T(t) \underline{C} \right|^2 \left[\underline{\nu}^T(t) \underline{\nu}(t) \right] = \left[\underline{\nu}^T(t) \underline{C}^2 \underline{\nu}(t) \right] \left[\underline{\nu}^T(t) \underline{\nu}(t) \right]$$

and $w(t)w''(t) - [w'(t)]^2 \geq 0$. This proves log-convexity.

For $\underline{p}^T(0) \neq \underline{e}^T$, the Schwartz inequality is strict and the convexity of $\log \frac{w(t)}{w(0)}$ is strict unless $\underline{\nu}^T(t) \underline{C} = K \underline{\nu}^T$ for some constant K . This can only happen when $\underline{\nu}^T(t)$ is an eigenvector of $\underline{C}$, i.e., when $(\underline{p}^T(t) - \underline{e}^T) \underline{e}_D^{-1/2} \underline{C} = \lambda_j [\underline{C}] (\underline{p}^T(t) - \underline{e}^T) \underline{e}_D^{-1/2}$.

We next show that the inequality (3) in Theorem B is tight in that, for any ergodic chain one can always find a $\underline{p}^T(0)$ for which $\frac{w(t)}{w(0)} = \exp[-2\theta]t$. If $\frac{w'(0)}{w(0)} = -2\theta$, knowledge that $\frac{w'(t)}{w(t)}$ is increasing and $\frac{w'(t)}{w(t)} \leq -2\theta$ implies that $\frac{w'(t)}{w(t)} = -2\theta$ for all t . Let $\underline{u}_1^T$ be any real orthonormal eigenvector of $\underline{C}$ for the eigenvalue $-\theta$, and α be small and real. If $\underline{\nu}^T(0) = (\underline{p}^T(0) - \underline{e}^T) \underline{e}_D^{-1/2} = \alpha \underline{u}_1^T$, so that $\underline{\nu}^T(0) \underline{C} = -\alpha \theta \underline{u}_1^T$ then $\frac{w'(0)}{w(0)} = 2 \frac{\underline{\nu}^T(0) \underline{C} \underline{\nu}(0)}{\underline{\nu}^T(0) \underline{\nu}(0)} = -2\theta$ as needed. If one chooses $\underline{p}^T(0) = \underline{e}^T + \alpha \underline{u}_1^T \underline{e}_D^{1/2}$, one will have $\underline{p}^T(0) > \underline{0}^T$ for α sufficiently small. Moreover one will also have $\underline{p}^T(0) \underline{1} = 1$. For

$$(\underline{p}^T(0) - \underline{e}^T) \underline{1} = \alpha \underline{u}_1^T \underline{e}_D^{1/2} \underline{1} \text{ and } -\theta \underline{u}_1^T \underline{e}_D^{1/2} \underline{1} = \underline{u}_1^T \underline{C} \underline{e}_D^{1/2} \underline{1} = \underline{u}_1^T \underline{e}_D^{1/2} Q^\# \underline{1} = 0. \quad \square$$

Time-reversible case: When $J(t)$ governed by Q is time reversible, a special case of the above, $\underline{Q} = Q^R = Q^\#$ and θ is just the reciprocal of the relaxation time described in [1]. For this time reversible case, for any λ_j and real eigenvector $\underline{u}_j^T$ of $\underline{Q}$, one can find initial vectors $\underline{p}^T(0)$ for which $w(t)$ will have purely exponential decay at rate $2|\lambda_j|$ faster than 2θ . The global decay rate is still θ .

3. The Covariance Function

Let $J(t)$ be any finite ergodic Markov chain which is stationary. Let $f(j)$ be any real function of state j . The covariance function is $R_f(\tau) = \text{cov}[f(J(t)), f(J(t+\tau))]$ and (cf. [1]) $R_f(\tau) = \underline{f}^T \underline{e}_D [\underline{p}(\tau) - \underline{1} \underline{e}^T] \underline{f}$ for $\tau > 0$.

The correlation function is $\rho_f(\tau) = \frac{R_f(|\tau|)}{R_f(0)}$.

Theorem D: For any finite ergodic Markov chain $J(t)$ which is stationary, the correlation function satisfies

$$|\rho_f(\tau)| \leq \exp[-\theta |\tau|]$$

and the inequality is tight.

Proof: Without loss of generality, we may assume that $f_n > 0$ since a positive constant may always be added to f_n without altering the covariance. Let $\underline{p}(\tau) =$

$[p_{mn}(\tau)]$ be the transition probability matrix of $J(t)$. For $\underline{\nu}^T(\tau) = \frac{\underline{f}^T \underline{e}_D}{\underline{f}^T \underline{e}_D \underline{1}} [\underline{p}(\tau) - \underline{1} \underline{e}^T] \underline{e}_D^{-1/2}$, algebra gives

$$\begin{aligned} R_f(\tau) &= \underline{f}^T \underline{e}_D [\underline{p}(\tau) - \underline{1} \underline{e}^T] \underline{e}_D^{-1/2} \underline{e}_D^{-1/2} [\underline{e}_D \underline{f} - (\underline{f}^T \underline{e}_D \underline{1}) \underline{e}] \\ &= (\underline{f}^T \underline{e}_D \underline{1})^2 [\underline{\nu}^T(\tau) \underline{\nu}(0)]. \end{aligned}$$

From the Schwartz inequality,

$$\rho_f^2(\tau) = \frac{R_f^2(\tau)}{R_f^2(0)} = \frac{[\underline{\nu}^T(\tau) \underline{\nu}(0)]^2}{[\underline{\nu}^T(0) \underline{\nu}(0)]^2} \leq \frac{|\underline{\nu}(\tau)|^2}{|\underline{\nu}(0)|^2} = \frac{w(\tau)}{w(0)} \leq \exp[-2\theta\tau].$$

The tightness of the inequality follows from the tightness in Theorem C. This proves the theorem. $\square$

4. The Relaxation Time

In [1] the relaxation time was defined by $T_{REL} = \sup_f \int_0^\infty \rho_f(\tau) d\tau$. This was motivated by the similarity of $\rho_f(\tau)$ to a survival function. One then has at once from Theorem D, $T_{REL} = \theta^{-1}$.

One must finally relate the decay rate θ to the eigenvalues of $\underline{Q}$. Suppose that there are eigenvalues of $\underline{Q}$ with negative real part $-\zeta$ and that other eigenvalues have a more negative real part. Consider $w(t) = \underline{\nu}^T(t) \underline{\nu}(t) = (\underline{p}^T(t) - \underline{e}^T) \underline{e}_D^{-1} (\underline{p}(t) - \underline{e})$. $e^{2\zeta t} w(t) = [e^{\zeta t} (\underline{p}^T(t) - \underline{e}^T)] \underline{e}_D^{-1} [e^{\zeta t} (\underline{p}(t) - \underline{e})] = [e^{\zeta t} d(t)]^2$ and that this is log-convex in t , all ζ . For $\underline{p}^T(t) - \underline{e}^T \neq 0$, $\limsup_{t \rightarrow \infty} e^{2\zeta t} w(t) = 0$, when $\zeta < -\theta^*$ and $\limsup_{t \rightarrow \infty} e^{2\zeta t} w(t) = \infty$, when $\zeta > -\theta^*$. From the tightness in Theorem C, we must then identify θ^* with θ .

A calculation has been carried out using the symbolic and numerical power of Maple for the chain $J(t)$ starting in any state and generator

$$\underline{Q} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & 0 & -1 \end{bmatrix}.$$

The graph given by Maple is found to be log-convex as predicted. The symbolic expression for $w(t)$ has the asymptotic decay rate predicted.

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Appendix

Lemma: If $\lambda_j[\underline{Q}]$ is the eigenvalue of an ergodic finite Markov chain in continuous time with infinitesimal generator $\underline{Q}$, then apart from the principal eigenvalue at 0, all eigenvalues of $\underline{Q}$ have a strictly negative real part.

Proof: We may use uniformization [1] to write $\underline{Q} = -\nu[\underline{I} - \underline{a}_\nu]$ where ν is any positive rate exceeding the largest exit rate from a state and $\underline{a}_\nu$ is a stochastic ergodic (irreducible and aperiodic) matrix. Then $\lambda_j[\underline{Q}] = -\nu(1 - \lambda_j[\underline{a}_\nu])$ and $|\lambda_j[\underline{a}_\nu]| < 1$ for other than $\lambda_1[\underline{a}_\nu] = 1$. The lemma then follows.

Remark: One can have a stochastic matrix which is ergodic and has purely imaginary eigenvalues.

An example with eigenvalues 1, $-\frac{1}{2}$, $\frac{1}{2}i$, $-\frac{1}{2}i$ is

$$\begin{bmatrix} \frac{1}{8} & \frac{5}{8} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{5}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{5}{8} \\ \frac{5}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \end{bmatrix}.$$

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