

Improved estimators for constrained Markov chain models

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Received February 2001; received in revised form April 2001

Abstract

Suppose we observe an ergodic Markov chain and know that the stationary law of one or two successive observations fulfills a linear constraint. We show how to improve the given estimators exploiting this knowledge, and prove that the best of these estimators is efficient. © 2001 Elsevier Science B.V. All rights reserved

MSC: primary 62M05; secondary 62G05; 62G20

Keywords: Empirical estimator; Asymptotically linear estimator; Influence function; Regular estimator; Markov chain model; Reversible chain; Symmetric chain; Linear autoregression

1. Introduction

To begin let X_1, \dots, X_n be *independent* with distribution P . Let $t(P)$ be a real-valued functional, and \hat{t} an estimator with influence function b in $L_2(P)$,

$$n^{1/2}(\hat{t} - t(P)) = n^{-1/2} \sum_{i=1}^n b(X_i) + o_p(1),$$

with $Pb = Eb(X) = 0$. If the distribution fulfills a constraint $Pv = 0$ for a known vector-valued function v with components in $L_2(P)$, we can introduce new estimators for $t(P)$,

$$\hat{t}(c) = \hat{t} - c^T \frac{1}{n} \sum_{i=1}^n v(X_i)$$

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¹ Supported in part by NSF Grant DMS0072174.

with influence function $b - c^T v$ and asymptotic variance $P[(b - c^T v)^2]$. If $P[vv^T]$ is invertible, then by the Schwarz inequality the asymptotic variance is minimized by $c = c_b$ with

$$c_b = (P[vv^T])^{-1}P[vb].$$

The constant c_b depends on the unknown distribution and must be estimated, say by

$$\hat{c}_b = \left(\sum_{i=1}^n v(X_i)v(X_i)^T \right)^{-1} \sum_{i=1}^n v(X_i)\hat{b}(X_i),$$

leading to the estimator $\hat{t}(\hat{c}_b)$. It is easily seen to be efficient if all we know about the distribution is that it fulfills the constraint $Pv = 0$. If $t(P)$ is linear, say $t(P) = Pf$, then estimation of $t(P)$ and c_b is particularly easy. A simple estimator of $t(P)$ is the empirical estimator $\hat{t} = (1/n) \sum_{i=1}^n f(X_i)$, with influence function $b(x) = f(x) - Pf$. Then $P[vb] = P[vf]$, and a consistent estimator of $P[vb]$ is the empirical estimator $(1/n) \sum_{i=1}^n v(X_i)f(X_i)$. We refer to Levit (1975), Haberman (1984) and the monograph of Bickel et al. (1998, Section 3.2, Example 3).

In Section 2 we extend the results from the i.i.d. case to Markov chains X_0, \dots, X_n with transition distribution Q and invariant distribution π . We consider constraints $\pi \otimes Qv = \int \int \pi(dx)Q(x, dy)v(x, y) = 0$ for vector-valued functions v , now of two arguments. Our estimators can be further improved if the chain is known to be reversible. In Section 3 we illustrate our results with a simple example, estimating the variance of the invariant distribution when the mean is known to be zero. The efficient estimator simplifies for the linear autoregressive model. In Remarks 1 and 2 we show how reversibility and symmetry can be described by linear constraints $\pi \otimes Qv = 0$ with infinite-dimensional v . We also construct efficient estimators for these models.

2. Results

Let X_0, \dots, X_n be observations from a positive Harris recurrent and V^2 -uniformly ergodic Markov chain on an arbitrary state space S with countably generated σ -field, with transition distribution Q and invariant distribution π . See e.g. Meyn and Tweedie (1993) for these concepts. We use the notation $\pi \otimes Q(dx, dy) = \pi(dx)Q(x, dy)$ and $Q_x w = \int Q(x, dy)w(y)$.

Let v be a k -dimensional measurable function defined on S^2 such that the constraint $\pi \otimes Qv = 0$ holds for all transition distributions Q in the model. Fix the true transition distribution Q , and let W be the set of all real-valued measurable functions w on S^2 such that $Q_x|w|/V(x)$ is bounded in x . Assume that v is in W . We refer to Schick and Wefelmeyer (2000a) for a discussion of this assumption. Set

$$H = \{h \in L_2(\pi \otimes Q): Qh = 0\}.$$

Then $h(X_{i-1}, X_i)$ is a martingale increment.

2.1. Asymptotic linearity

Let $t(Q)$ be a real-valued functional of the transition distribution. Following the approach outlined in the introduction for the i.i.d. case, call an estimator \hat{t} *asymptotically linear* with influence function b if $b \in H$

and \hat{t} admits the martingale approximation

$$n^{1/2}(\hat{t} - t(Q)) = n^{-1/2} \sum_{i=1}^n b(X_{i-1}, X_i) + o_p(1).$$

By a martingale central limit theorem, see Meyn and Tweedie (1993, Theorem 17.4.4), \hat{t} is asymptotically normal with variance $\pi \otimes Qb^2$. From the constraint $\pi \otimes Qv = 0$ we obtain new estimators

$$\hat{t}(c) = \hat{t} - c^T \frac{1}{n} \sum_{i=1}^n v(X_{i-1}, X_i). \quad (2.1)$$

By the martingale approximation of Gordin (1969), see Meyn and Tweedie (1993, Section 17.4), we have

$$n^{-1/2} \sum_{i=1}^n (v(X_{i-1}, X_i) - Av(X_{i-1}, X_i)) = o_p(1) \quad (2.2)$$

with

$$Av(x, y) = v(x, y) - Q_x v + \sum_{i=1}^n (Q_y^i - Q_x^{i+1})v.$$

From (2.1) and (2.2),

$$n^{1/2}(\hat{t}(c) - t(Q)) = n^{-1/2} \sum_{i=1}^n (b(X_{i-1}, X_i) - c^T Av(X_{i-1}, X_i)) + o_p(1).$$

By construction, $Av(X_{i-1}, X_i)$ is a martingale increment. Hence $\hat{t}(c)$ is asymptotically linear with influence function $b - c^T Av$. Again by the martingale central limit theorem, $\hat{t}(c)$ is asymptotically normal with variance $\sigma^2 = \pi \otimes Q[(b - c^T Av)^2]$. Assume that $\pi \otimes Q[Av \cdot Av^T]$ is invertible. By the Schwarz inequality, the variance is minimized for $c = c_b$ with

$$c_b = (\pi \otimes Q[Av \cdot Av^T])^{-1} \pi \otimes Q[Av \cdot b].$$

The minimal asymptotic variance is

$$\sigma_b^2 = \pi \otimes Qb^2 - \pi \otimes Q[bAv^T](\pi \otimes Q[Av \cdot Av^T])^{-1} \pi \otimes Q[Av \cdot b].$$

The optimal vector c_b depends on the unknown transition distribution and must be replaced by a consistent estimator \hat{c}_b . The estimator $\hat{t}(\hat{c}_b)$ has the same asymptotic variance as $\hat{t}(c_b)$. We arrive at the following result.

Theorem 1. *If \hat{c}_b is consistent for c_b , then the estimator $\hat{t}(\hat{c}_b)$ is asymptotically linear for $t(Q)$ with influence function $b - c_b^T Av$ and asymptotic variance σ_b^2 .*

2.2. Efficiency

We show now that if \hat{t} is asymptotically linear and regular, then $\hat{t}(\hat{c}_b)$ is regular and efficient in the sense of Hájek's convolution theorem. The set H introduced above consists of the functions h on S^2 for which one

can construct Hellinger differentiable perturbations of Q of the form

$$Q_{nh}(x, dy) \doteq Q(x, dy)(1 + n^{-1/2}h(x, y))$$

that are again transition distributions. This means that H is the *tangent space* of the full nonparametric model. By Kartashov (1985), see also Kartashov (1996) and Greenwood and Wefelmeyer (1999), we have the perturbation expansion

$$n^{1/2}(\pi_{nh} \otimes Q_{nh}v - \pi \otimes Qv) \rightarrow \pi \otimes Q[hAv]. \quad (2.3)$$

The constraints $\pi \otimes Qv = 0$ and $\pi_{nh} \otimes Q_{nh}v = 0$ now lead to a constraint on h , namely $\pi \otimes Q[hAv] = 0$. Hence the tangent space of the constrained model consists of all functions h orthogonal to Av ,

$$H_* = \{h \in H : \pi \otimes Q[hAv] = 0\}.$$

The functional $t(Q)$ is called *differentiable* at Q with *gradient* g if $g \in H$ and

$$n^{1/2}(t(Q_{nh}) - t(Q)) \rightarrow \pi \otimes Q[hg] \quad \text{for } h \in H_*. \quad (2.4)$$

The *canonical gradient* is the projection g_* of g onto H_* . The estimator \hat{t} is called *regular* at Q with *limit* L if

$$n^{1/2}(\hat{t} - t(Q_{nh})) \Rightarrow L \quad \text{under } P_{nh} \quad \text{for } h \in H_*.$$

Here P_{nh} is the law of X_0, \dots, X_n when Q_{nh} is the true transition distribution.

We recall two characterizations from the theory of efficient estimation; for appropriate versions see e.g. Wefelmeyer (1999, Sections 3 and 5). (1) *An asymptotically linear estimator is regular if and only if its influence function is a gradient.* (2) *A regular estimator is efficient if and only if it is asymptotically linear with influence function equal to the canonical gradient.*

By definition, H has the orthogonal decomposition $H = H_* \oplus [Av]$, where $[Av]$ is the linear span of Av . Hence the canonical gradient, the projection g_* of g onto H_* , can be written $g_* = g - g_v$, where g_v is the projection of g onto $[Av]$, i.e. $g_v = c_*^T Av$ with

$$c_* = (\pi \otimes Q[Av \cdot Av^T])^{-1} \pi \otimes Q[Av \cdot g].$$

Now let \hat{t} be a regular and asymptotically linear estimator for $t(Q)$. By characterization (1), its influence function is a gradient, say g . By Theorem 1, the estimator $\hat{t}(\hat{c}_*)$ has influence function $g - c_*^T Av = g_*$. From characterization (2) we obtain the following result.

Theorem 2. *If \hat{t} is a regular and asymptotically linear estimator for $t(Q)$, and \hat{c}_* is consistent for c_* , then $\hat{t}(\hat{c}_*)$ is regular and efficient for $t(Q)$ in the model constrained by $\pi \otimes Qv = 0$.*

Note that for the improvement $\hat{t}(c)$ we needed the constraint $\pi \otimes Qv = 0$ only for the true Q , while for efficiency of $\hat{t}(\hat{c}_*)$ we needed the constraint also for perturbations Q_{nh} , at least in the direction of the canonical gradient.

2.3. Reversible chains

Suppose we know, in addition to $\pi \otimes Qv=0$, that the Markov chain is *reversible*, $\pi(dx)Q(x,dy)=\pi(dy)Q(y,dx)$. By Greenwood and Wefelmeyer (1999), this puts the following additional constraint on the tangent space:

$$H_*^{\text{rev}} = \{h \in H_* : Bh \text{ symmetric}\}.$$

Here B is the *adjoint* of A in the sense that for $h \in H$ and $w \in W$,

$$\pi \otimes Q[hAw] = \pi \otimes Q[Bh \cdot w].$$

Let $t(Q)$ be differentiable at Q with gradient $g \in H$ in this doubly constrained model in the sense that (2.4) holds for $h \in H_*^{\text{rev}}$. As in the proof of Theorem 2 of Greenwood and Wefelmeyer (1999), the projection g_*^{rev} of g onto H_*^{rev} is obtained by symmetrizing g_* ,

$$g_*^{\text{rev}}(x, y) = \frac{1}{2}(g(x, y) + g(y, x)) - c_*^{\text{rev}} \frac{1}{2}(v(x, y) + v(y, x)),$$

$$c_*^{\text{rev}} = (E[Av(X_0, X_1) \cdot Av(X_0, X_1)^T])^{-1} \frac{1}{2} E[Av(X_0, X_1)(g(X_0, X_1) + g(X_1, X_0))].$$

Here and in the following, expectations are taken with respect to the *stationary* law of the chain. Note that if \hat{t} has influence function $g \in H$, then the symmetrized estimator

$$\frac{1}{2}(\hat{t}(X_0, \dots, X_n) + \hat{t}(X_n, \dots, X_0))$$

has influence function $\frac{1}{2}(g(x, y) + g(y, x))$. We arrive at the following result.

Theorem 3. *If \hat{t} is a regular and asymptotically linear estimator for $t(Q)$, and \hat{c}_*^{rev} is consistent for c_*^{rev} , then*

$$\frac{1}{2}(\hat{t}(X_0, \dots, X_n) + \hat{t}(X_n, \dots, X_0)) - \hat{c}_*^{\text{rev}} \frac{1}{2n} \sum_{i=1}^n (v(X_{i-1}, X_i) + v(X_i, X_{i-1}))$$

is regular and efficient for $t(Q)$ in the model constrained by $\pi \otimes Qv=0$ and reversibility.

2.4. Linear functionals

In this subsection we treat the problem of estimating c_* for linear functionals $t(Q) = \pi \otimes Qf$ with f in W , and constraint $\pi \otimes Qv = Ev(X_0, X_1) = 0$. In the i.i.d. case, c_* was easy to estimate. For Markov chains, c_* involves the operator A , and estimation is less straightforward. By the martingale approximation (2.2), the empirical estimator

$$\hat{t} = \frac{1}{n} \sum_{i=1}^n f(X_{i-1}, X_i)$$

is asymptotically linear with influence function $b = Af$ in H . By the perturbation expansion (2.3), Af is a gradient of $\pi \otimes Qf$. Hence the empirical estimator is regular by characterization (1). If nothing is known

about Q , the empirical estimator is efficient: see Penev (1991) and Bickel (1993) for functions f of one argument, and Greenwood and Wefelmeyer (1995) for functions f of two arguments; or simply note that H is the tangent space of the full nonparametric model, and hence Av is the canonical gradient of $\pi \otimes Qf$.

For $t(Q) = \pi \otimes Qf$ we have

$$c_* = c_f = (\pi \otimes Q[Av \cdot Av^T])^{-1} \pi \otimes Q[Av \cdot Af] = \Sigma^{-1}F,$$

say. One checks that for vectors w and z with components in W ,

$$\begin{aligned} \pi \otimes Q[Aw \cdot Az^T] &= E[(w(X_0, X_1) - Ew(X_0, X_1))z(X_0, X_1)^T] \\ &\quad + \sum_{j=1}^{\infty} (E[(w(X_0, X_1) - Ew(X_0, X_1))z(X_j, X_{j+1})^T] \\ &\quad + E[(w(X_j, X_{j+1}) - Ew(X_0, X_1))z(X_0, X_1)^T]). \end{aligned}$$

For functions of *one* argument compare Meyn and Tweedie (1993, Section 17.4.3). Now we use the constraint $Ev(X_0, X_1) = 0$ to estimate $\Sigma = \pi \otimes Q[Av \cdot Av^T]$ by

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n v(X_{i-1}, X_i) v(X_{i-1}, X_i)^T + \sum_{j=1}^{m(n)} \frac{2}{n-j} \sum_{i=1}^{n-j} v(X_{i-1}, X_i) v(X_{i+j-1}, X_{i+j})^T$$

and $F = \pi \otimes Q[Av \cdot Af]$ by

$$\begin{aligned} \hat{F} &= \frac{1}{n} \sum_{i=1}^n v(X_{i-1}, X_i) f(X_{i-1}, X_i) \\ &\quad + \sum_{j=1}^{m(n)} \frac{1}{n-j} \sum_{i=1}^{n-j} (v(X_{i-1}, X_i) f(X_{i+j-1}, X_{i+j}) + v(X_{i+j-1}, X_{i+j}) f(X_{i-1}, X_i)). \end{aligned}$$

Since the chain is assumed V^2 -uniformly ergodic, it is V^2 -uniformly mixing by Meyn and Tweedie (1993, Theorem 16.1.5). To prove consistency of \hat{F} , set $v_K = -K \vee v \wedge K$ and write \hat{F}_K for the corresponding estimator with truncated v . Since $\sum_{j=1}^{\infty} Q^j f$ converges in $L_2(\pi)$, we obtain from the Cauchy–Schwarz inequality that for each $\varepsilon > 0$ there is a K such that

$$E|\hat{F}_K - \hat{F}| \leq \varepsilon, \quad |\pi \otimes Q[Av_K \cdot Af] - \pi \otimes Q[Av \cdot Af]| \leq \varepsilon.$$

Furthermore, by straightforward calculation, for $m(n)$ tending to infinity more slowly than n ,

$$E[\hat{F}_K - \pi \otimes Q[Av_K \cdot Af]]^2 \rightarrow 0.$$

Hence \hat{F} is consistent. In practice $m(n)$ will be taken small. Consistency of $\hat{\Sigma}$ is proved similarly. We arrive at the following result.

Theorem 4. *If $m(n)$ tends to infinity more slowly than n , then $\hat{c}_f = \hat{\Sigma}^{-1} \hat{F}$ is consistent for c_f .*

3. Applications

Example 1. If the function v is constant in one argument, say $v(x, y) = v_1(y)$, then the constraint is $\pi \otimes Qv = \pi v_1 = 0$. In particular, for real state space $S = \mathbb{R}$ and constraint $\pi v = 0$ with $v(x, y) = y$, the chain has mean zero. A natural estimator for the variance $t(Q) = E(X - EX)^2$ of the invariant distribution is the empirical estimator $(1/n) \sum_{i=1}^n X_i^2 - ((1/n) \sum_{i=1}^n X_i)^2$. Since $EX = 0$, we have $E(X - EX)^2 = EX^2$, and an asymptotically equivalent estimator is the empirical second moment $(1/n) \sum_{i=1}^n X_i^2$. By Theorem 2, a better estimator is

$$\hat{t}(\hat{c}_f) = \frac{1}{n} \sum_{i=1}^n X_i^2 - \hat{c}_f \frac{1}{n} \sum_{i=1}^n X_i,$$

with \hat{c}_f a consistent estimator of $(\pi \otimes Q[(Av)^2])^{-1} \pi \otimes Q[Av \cdot Af]$ for $v(x, y) = y$ and $f(x, y) = y^2$.

Example 2. Consider the linear autoregressive model of order one, $X_i = \rho X_{i-1} + \varepsilon_i$, where the innovations ε_i are i.i.d. with mean zero, finite variance σ^2 , finite fourth moment and $|\rho| < 1$. Then the invariant distribution π has mean zero. This is a submodel of Example 1. For this submodel, the operator A and the estimator for c_f simplify. Let us again consider the problem of estimating the variance $t(Q) = E(X - EX)^2 = EX^2$ of the invariant distribution. For $w \in L_2(\pi)$,

$$Q_y^j w = Ew \left(\sum_{k=0}^{j-1} \rho^k \varepsilon_{i-k} + \rho^j y \right).$$

In particular, for $v(x, y) = y$ and $f(x, y) = y^2$,

$$Av(x, y) = \frac{1}{1 - \rho} (y - \rho x), \quad Af(x, y) = \frac{1}{1 - \rho^2} (y^2 - \rho^2 x^2 - \sigma^2).$$

Hence

$$\pi \otimes Q[(Av)^2] = \frac{\sigma^2}{(1 - \rho)^2}, \quad \pi \otimes Q[Av \cdot Af] = \frac{\alpha_3}{(1 - \rho)(1 - \rho^2)},$$

where $\alpha_3 = E\varepsilon^3$ is the third moment of the innovation distribution.

Estimate the autoregression coefficient ρ by the least squares estimator

$$\hat{\rho} = \frac{\sum_{i=1}^n X_{i-1} X_i}{\sum_{i=1}^n X_{i-1}^2},$$

the innovations ε_i by $\hat{\varepsilon}_i = X_i - \hat{\rho} X_{i-1}$, and σ^2 and α_3 by the empirical moments based on the estimated innovations,

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n \hat{\varepsilon}_i^2, \quad \hat{\alpha}_3 = \frac{1}{n} \sum_{i=1}^n \hat{\varepsilon}_i^3.$$

We obtain

$$\hat{t}(\hat{c}_f) = \frac{1}{n} \sum_{i=1}^n X_i^2 - \frac{\hat{\alpha}_3}{(1 + \hat{\rho}) \hat{\sigma}^2} \frac{1}{n} \sum_{i=1}^n X_i.$$

We note that for $\rho=0$ the observations are $X_i = \varepsilon_i$ and i.i.d., and the estimator $\hat{t}(\hat{c}_f)$ is asymptotically equivalent to the estimator obtained in the i.i.d. case.

To estimate c_f , we have used the information that the Markov chain is an AR(1) model. This information simplifies \hat{c}_f but does not improve the estimator $\hat{t}(\hat{c}_f)$ asymptotically. We refer to Schick and Wefelmeyer (2000b, Section 6) for better estimators of EX^2 , and to Schick and Wefelmeyer (2000c) for efficient estimators of general linear functionals of invariant laws of linear time series.

Remark 1. Constraints $\pi \otimes Qv = 0$ for functions $v(x, y) = u(x)w(y) - u(y)w(x)$ describe symmetries of the joint law of two successive observations with respect to time reversal. If such constraints hold for a sufficiently large class of functions, e.g., in the case of real state space, for all indicators $u(x) = 1_{(-\infty, a]}(x)$ and $w(y) = 1_{(-\infty, b]}(y)$ with $a, b \in \mathbb{R}$, then the chain is reversible. Let $t(Q)$ be differentiable, and let $\hat{t} = \hat{t}(X_0, \dots, X_n)$ be an asymptotically linear estimator for $t(Q)$. By the arguments in Section 2.3 the symmetrized estimator

$$\frac{1}{2}(\hat{t}(X_0, \dots, X_n) + \hat{t}(X_n, \dots, X_0))$$

is efficient for $t(Q)$ if the chain is known to be reversible.

Remark 2. For real state space, constraints $\pi \otimes Qv = 0$ for functions $v(x, y) = z(x, y) - z(-x, -y)$ describe symmetries of the joint law of two successive observations with respect to reflection at zero. If such constraints hold for a sufficiently large class of functions, e.g. for all functions $z(x, y) = 1_{(-\infty, a]}(x)1_{(-\infty, b]}(y)$ with $a, b \in \mathbb{R}$, then

$$\pi(dx)Q(x, dy) = \pi(-dx)Q(-x, -dy)$$

and therefore $\pi(dx) = \pi(-dx)$ and $Q(x, dy) = Q(-x, -dy)$. In this case, we do not need the results of Section 2. Note also that the condition $Q(x, dy) = Q(-x, -dy)$ implies

$$\int \pi(-dx)Q(x, dy) = \int \pi(-dx)Q(-x, -dy) = \pi(-dy)$$

and hence $\pi(dx) = \pi(-dx)$ holds automatically. The tangent space of the model constrained by symmetry of the transition distribution, $Q(x, dy) = Q(-x, -dy)$, is

$$H_* = \{h \in H: h(x, y) = h(-x, -y)\}.$$

Write $f^-(x, y) = f(-x, -y)$. It is straightforward to check that $Af^- = (Af)^-$. For $h \in H_*$ we have $h = h^-$ and

$$\pi \otimes Q[hAf] = \pi \otimes Q[h^-(Af)^-] = \frac{1}{2}\pi \otimes Q[h(Af + (Af)^-)] = \frac{1}{2}\pi \otimes Q[hA(f + f^-)].$$

Hence the projection of Af onto H_* is $\frac{1}{2}A(f + f^-)$. By the martingale approximation (2.2), this is the influence function of the symmetrized empirical estimator

$$\hat{t}_* = \frac{1}{2n} \sum_{i=1}^n (f(X_{i-1}, X_i) + f(-X_{i-1}, -X_i)),$$

which is therefore efficient for $\pi \otimes Qf$ under the constraint $Q(x, dy) = Q(-x, -dy)$.

Similarly as in Remark 1, the result generalizes to arbitrary differentiable functionals $t(Q)$ with gradient $g \in H$. Let \hat{t} be an asymptotically linear estimator for $t(Q)$ with influence function g . Then the symmetrized estimator

$$\hat{t}_* = \frac{1}{2}(\hat{t}(X_0, \dots, X_n) + \hat{t}(-X_0, \dots, -X_n))$$

is efficient for $t(Q)$ if the chain is known to be symmetric.

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