Improved estimators for constrained Markov chain models

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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 given estimators exploiting this knowledge, and prove that the best of these estimators is efficient.

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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 $t(P)$,

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

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

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

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

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

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 $\hat{t} = \frac{1}{n}\sum_{i=1}^n f(X_i)$, with influence function $b(x) = f(x) - Pf$. Then $P[vb] = P[vf]$, and a consistent estimator of $P[vb]$ is the empirical estimator $\frac{1}{n}\sum_{i=1}^n v(X_i) f(X_i)$. We refer to Levit (1975), Haberman (1984) and the monograph of Bickel, Klaassen, Ritov and Wellner (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 $\pi \otimes Qv = \iint \pi(dx)Q(x, dy)v(x, y) = 0$ 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 $Q_x w = \int Q(x, dy)w(x, y)$.

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.

1. 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

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

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

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

with

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

From (2.1) and (2.2),

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

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

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

The minimal asymptotic variance is

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

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 $b - c_b^\top Av$ and asymptotic variance σ_b^2.*

2. 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

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

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

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

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

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

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. $g_v = c_*^\top Av$ with

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

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 $g - c_*^\top Av = g_*$. 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.

3. 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:

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

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 $h \in H_*^{\mathrm{rev}}$. 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_*,

$$\begin{aligned} g_*^{\mathrm{rev}}(x,y) &= \frac{1}{2}\big(g(x,y)+g(y,x)\big) - c_*^{\mathrm{rev}}\frac{1}{2}\big(v(x,y)+v(y,x)\big), \\ c_*^{\mathrm{rev}} &= \big(E[Av(X_0,X_1)\cdot Av(X_0,X_1)^\top]\big)^{-1} \\ &\quad \frac{1}{2}E\big[Av(X_0,X_1)\big(g(X_0,X_1)+g(X_1,X_0)\big)\big]. \end{aligned}$$

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

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

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

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

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

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

4. 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 Af is the canonical gradient of $\pi \otimes Qf$.

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

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

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

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

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 $\Sigma = \pi \otimes Q[Av \cdot Av^\top]$ by

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

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

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

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,

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

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 $S = \mathbf{R}$ 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 $\frac{1}{n}\sum_{i=1}^n X_i^2 - (\frac{1}{n}\sum_{i=1}^n X_i)^2$. Since $EX = 0$, we have $E(X - EX)^2 = EX^2$, and an asymptotically equivalent estimator is the empirical second moment $\frac{1}{n}\sum_{i=1}^n X_i^2$. 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 $w \in L_2(\pi)$,

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

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

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

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

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

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 $a,b\in\mathbf{R}$, 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 Subsection 3 of Section 2, the symmetrized estimator

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

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 $a, b \in \mathbf{R}$, 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

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

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

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

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

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