Globally-centered autocovariances in MCMC

Medha Agarwal
Department of Mathematics and Statistics
IIT Kanpur
medhaaga@iitk.ac.in

Dootika Vats
Department of Mathematics and Statistics
IIT Kanpur
dootika@iitk.ac.in

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Abstract

Autocovariances are the fundamental quantity in many features of Markov chain Monte Carlo (MCMC) simulations with autcorrelation function (ACF) plots being often used as a visual tool to ascertain the performance of a Markov chain. Unfortunately, for slow mixing Markov chains, the empirical autocovariance can highly underestimate the truth. For multiple chain MCMC sampling, we propose a globally-centered estimate of the autocovariance that pools information from all Markov chains. We show the impact of these improved estimators in three aspects: (1) acf plots, (2) estimates of the Monte Carlo asymptotic covariance matrix, and (3) estimates of the effective sample size.

Main things to change

- I don't want to call this "Replicated autocovariance" or "Replicated spectral variance". I think "Globally-centered autocovariance" is more appropriate and self-explanatory. So we will have to go over the whole document and change this.
- The contents are a bit messy right now, and I am having trouble organizing my thoughts.

A rough outline of the organization

1. Introduction, with a sneak peak at new plots. Change this example to a univariate mixture of Gaussians.:

Here, we will just explain the problem with the old ACF and what happens by using the new ACF. We will show a plot to illustrate the impact. Then we will summarize the three places this will have an impact: (1) ACF plots (2) estimators of the asymptotic variance-covariance matrix (3) estimating effective sample size.

2. Globally-centered autocovariance
   - Theoretical soundness
3. Variance of Monte Carlo averages

   Describe MC averages and CLT here and not before
   - Globally-centered Spectral variance estimators
     - Theoretical results
     - Fast implementation
4. Effective sample size
5. Examples
6. Discussion
   - All plots have been made using the package:(name). The package can be found on GitHub.
   - One thing to discuss is that the new autocovariances can be used in the initial sequence estimators as well.
7. Appendix
   - Proofs
   - ACF plots for other examples.

1 Introduction

Markov chain Monte Carlo (MCMC) is a sampling method used to obtain correlated realizations from a stochastic process. Due to this serial correlation in observations, a large number of MCMC samples are required to estimate features of the target distribution as compared to the independent ones. Therefore, it becomes imperative for an MCMC practitioner to have an idea about underlying dependence structure in the Markov chains. Autocovariance function (ACF) characterizes this dependence for a stationary Markov chain. A famous sample autovariance function is the empirical estimator, which unfortunately comes with its drawbacks. Firstly, it is not immune to outliers (see

Ma and Genton (2000)) and secondly, it is usually non-informative in case of slowly mixing Markov chains for decently finite samples. We address the second issue in this paper by using multiple representative samples of the target distribution via parallel Markov chains.

Calculation of exact theoretical ACF has been done for simple models like autoregressive (AR), moving average (MA) (Quenouille (1947)), and autoregressive-moving-average (ARMA) (Box et al. (2015)) models. However, for most of the complex processes, we rely on sample ACF to understand the correlation in the chain at a particular lag. For a slowly mixing Markov chain or a multi-modal target distribution, Markov chains explore the sample space only partially for even high sample size. In such situations, single chain empirical ACF will underestimate the autocovariance giving misleading inferences. With convenient multi-core computation resources, it is possible to get multiple Markov chains for a target distribution. We propose a new autocovariance estimator called replicated autocovariance function (R-ACF) with a simple fix in centering a chain about the overall mean. An important application of ACF is in calculating the asymptotic variance in the CLT of a Markov chain process.

In the next section we introduce the new sample autocovariance estimator and calculate its bias for finite samples. We observe that the bias term for R-ACF is similar to the bias of empirical ACF except for a few small order end-effect terms that vanish as $n \to \infty$. In section 3, we introduce three estimators for Σ and study the properties of RSV estimator through proof of strong consistency, bias, and variance calculations. We will elaborate on the estimator for ESS using RSV in section 4. Section 5 gives a simulation study on three different examples for the proposed estimators. There are only a handful of stochastic processes where the true autocovariance and Σ are known. To compare the estimators when the truth is known, we use a slowly mixing vector autoregressive process of order 1 (VAR(1)). We successfully show in section 5.1 that our estimators yield better results as compared to the classical sample ACF and SVE. A more promising advantage of our estimators is observed when the target distribution is multi-modal. For this purpose we use a bivariate bi-modal probability distribution introduced by Gelman and Meng (1991) in section 5.2. All the important proofs are given in the Appendix.

Dootika: The introduction above needs some rewrite based on my pointers in blue above. We should introduce the definition of autocovariance here and present the old and the new estimators of Γ here. So take some of the details out of the next section and put them here.

Example 1 (Demonstrative example). We demonstrate the striking difference in the ACF plots through mixture of Gaussian target density using a random-walk Metropolis-Hastings sampler.

Dootika: add new plots here when available for this target density.

2 Globally-centered autocovariance

For a stationary stochastic process $\{X_t\}_{t\geq 1}$, let $\Gamma(k)$ denote the lag -k autocovariance. In time series literature, we generally encounter the following estimator for autocovariance.

$$\hat{\Gamma}(k) = \frac{1}{n}\sum_{t=1}^{n-|k|}(X_t - \bar{X})(X_{(t+|k|)} - \bar{X})^T$$

Priestley (1981) shows that this estimator is biased with the main bias term equal to $|k|\,\Gamma(k)/n$, ignoring the small order terms arising due to estimation of μ. An unbiased estimator with a divisor of $n - |k|$ instead of n exists, say $\Gamma^*(k)$. Nevertheless, the biased estimator is preferred for its lower mean square error (Priestley (1981)). For a small k relative to n, the two estimators are almost the same. However, for larger relative k the variance of $\hat{\Gamma}(k)$ compensates for larger bias rendering a smaller mean square error than $\Gamma^*(k)$.

A commonly faced problem with the MCMC algorithms is the slow mixing property. In case of multi modal target distributions, it has been observed that even decently mixing Markov chains fail to explore the sample space for the first few thousand observations. This leads to underestimation of autocovariance for a single Markov chain. We propose a simple and neat fix for estimating ACF while dealing with slow convergence. Suppose we have m replications of Markov chains for same target distribution, the overall mean $\bar{\bar{X}} = \sum_{i=1}^{m}\bar{X}_i/m$ provides a better estimate for the expectation value when the number of simulation per chain are not sufficient for the convergence to kick in. The replicated autocovariance estimator or s^{th} Markov chain is given by:

$$\hat{\Gamma}_{RAC,s}(k) = \frac{1}{n}\sum_{t=1}^{n-k}(X_{st} - \bar{\bar{X}})(X_{s(t+k)} - \bar{\bar{X}})^T$$

If the starting points of these parallel Markov chains are sufficiently dispersed, R-ACF provides more realistic estimation of lag covariances. It is a known problem that getting true autocovariance in closed form for non-simple problems is difficult. In Figure **??**, we will illustrate the comparison between ACF and R-ACF for a slowly mixing VAR-1 example, where the truth is known. We wish to make two points here: firstly, for small sample size, we observe that ACF gives extremely misleading estimates of autocovariance whereas R-ACF is very close to reality. Figure **??** depicts the scenario where the convergence is not achieved yet. Secondly, for a large sample size , the estimates from R-ACF as well as ACF are equivalent. Figure **??** depicts the scenario when convergence is achieved. This shows that R-ACF is at least as good as ACF; hence safe to use in any setting.

2.1 Theoretical results

The bias for R-ACF is similar to the bias of sample autocovariance estimator in case of single chain except for a few small order terms that shall be later addressed in theorem 1. Before getting to the bias results for $\hat{\Gamma}_{RAV}(k)$ for any lag k, we introduce an additional notation. For $q \geq 1$, we define

$$\Phi^{(q)} = \sum_{-\infty}^{\infty} |k|^q \left\| \Gamma(k) \right\|$$

We denote $\Phi^{(1)}$ by Φ.

Theorem 1.

$$\mathbb{E}[\hat{\Gamma}_{RAC}(k)] = \left(1 - \frac{|k|}{n}\right) \left(\Gamma(k) - \frac{\Sigma}{mn} - \frac{\Phi}{mn^2}\right) + \frac{2(m-1)}{m} \frac{|k|}{n^2} \left(\Sigma - \sum_{h=0}^{n-1} \Gamma(h)\right) + o(n^{-2})$$

Proof. The estimator for autocovariance with divisor n is suggested by Parzen et al. (1961) for its lesser mean square error despite having greater bias than the unbiased estimator with an $n - |k|$ divisor. We know that $\hat{\Gamma}_s(k)$ is asymptotically unbiased with a $o(1)$ bias term that remains fixed for any k. The bias term is given by Priestley (1981) as

$$\mathbb{E}[\hat{\Gamma}(k)] = \left(1 - \frac{|k|}{n}\right) \left(\Gamma(k) - \text{Var}(\bar{X})\right) \tag{1}$$

By proposition 1 in Song and Schmeiser (1995)

$$\text{Var}(\bar{X}) = \frac{\Sigma}{n} + \frac{\Phi}{n^2} + o(n^{-2}) \tag{2}$$

As a consequence, if $\text{Var}(\bar{X})$ is finite, then $\text{Var}(\bar{X}) \to 0$ as $n \to \infty$. We can break $\hat{\Gamma}_{RAC}$ into four parts for all $k \geq 1$ as:

$$\hat{\Gamma}_{RAC} = \frac{1}{m} \sum_{s=1}^{m} \hat{\Gamma}_s(k) - \frac{1}{mn} \sum_{s=1}^{m} \sum_{t=1}^{|k|} A_{st}^T - \frac{1}{mn} \sum_{s=1}^{m} \sum_{t=n-|k|+1}^{n} A_{st} + \frac{n-|k|}{mn} \sum_{s=1}^{m} (\bar{X}_s - \bar{\bar{X}})(\bar{X}_s - \bar{\bar{X}})^T,$$

where $A_{st} = (X_{st} - \bar{X}_s)(\bar{X}_s - \bar{\bar{X}})^T$
The expectation value of the first term is given by equation 1 and 2 while the other three terms contribute $o(1)$ terms. The complete proof evaluating the expectation values of last three terms can be found in Appendix subsection B.1. □

Remark 1. Using theorem 1 and equation 1,

$$\mathbb{E}[\hat{\Gamma}_{RAC}(k) - \hat{\Gamma}(k)] = \frac{|k|}{n}\left(1 - \frac{1}{m}\right)\left(\frac{\Sigma}{n} + \frac{\Phi}{n^2}\right) + \frac{2(m-1)}{m}\frac{|k|}{n^2}\left(\Sigma - \sum_{h=0}^{n-1}\Gamma(h)\right) + o(n^{-2})$$

We know that the sample autocovariance $\hat{\Gamma}(k)$ underestimates the truth due to a negative bias of $|k|\,\Gamma(k)/n$ for finite n. However, in practice, it is preferred to overestimate the autocovariance for finite n than to underestimate it in order to have a more realistic idea about the correlation in a Markov chain at a particular lag. Note that the RHS in the above expression is positive. As a consequence, R-ACF will counter this negative bias and give more reliable estimates for ACF.

Corollary 1.

$$\mathbb{E}[\hat{\Gamma}_{RAC}(0)] = \Gamma(0) + \frac{\Sigma}{mn} + \frac{\Phi}{mn^2} + o(n^{-2})$$

Proof. The proof is in Appendix subsection B.1. □

3 Variance Estimators for multiple Markov chains

Dootika: this section here needs to be much tighter in its presentation. We will need to remember that the paper is no longer about the SV estimators but about autocorrelations. So will have to present the discussion similarly.

Suppose F is the target distribution on support $\chi \subseteq \mathbb{R}^d$. For $g : \chi \longrightarrow \mathbb{R}^p$ be an F-integrable function. We are interested in

$$\mu_g = \mathbb{E}_F[g(X)] = \int_\chi g(x)F(dx)$$

Suppose we have m replications of Markov chains with n samples in each chain. Let $\{X_{st}\}_{t\geq 1}$ denote the s^{th} Harris ergodic (aperiodic, F-irreducible, and positive Harris recurrent) Markov chain having invariant distribution F. We will use the following Monte Carlo estimator in order to estimate μ for the s^{th} chain

$$\hat{\mu}_s = \frac{1}{n}\sum_{i=1}^{n} g(X_{si}) \xrightarrow{a.s.} \mu \text{ as } n \to \infty$$

Throughout this paper, we will deal with the function $g(X) = X$. We denote the sample mean of s^{th} Markov chain by $\bar{X}_s$ and the overall mean by $\bar{\bar{X}} = \sum_{s=1}^{m} \bar{X}_s/m$. We are interested in Monte Carlo error, i.e. $\bar{\bar{X}} - \mu$ to assess the reliability of simulations. The sampling distribution for Monte Carlo error of s^{th} chain is available via Markov chain CLT (Jones et al. (2004)) if there exists a positive definite matrix Σ such that

$$\sqrt{n}(\bar{X}_s - \mu) \xrightarrow{d} N(0, \Sigma)$$

With m i.i.d. samples of $\bar{X}_s,\ s \in \{1, ..., m\}$, the MCSE is given by Σ/mn. We are interested in consistent estimates of Σ for two reasons. Firstly, to construct asymptotically valid confidence intervals and secondly, to determine when to stop the simulations. For this purpose, we use the class of Multivariate Spectral Variance Estimators (MSVE) wherein we use R-ACF to estimate the autocovariance. We call this replicated spectral variance (RSV) estimator (see Argon and Andradóttir (2006) for replicated batch means).

MCMC ensures asymptotic convergence, however this is not practically very useful where the number of samples is finite. There are many criteria for terminating simulation like fixed-time rule, sequencial fixed-volume rule (see Glynn et al. (1992)), and using Gelman Rubin diagnostics (Gelman et al. (1992)). The relative fixed-volume rule has been thoroughly discussed for MCMC by Flegal and Gong (2015) and Gong and Flegal (2016). We will use method of effective sample size (ESS) defined by Vats et al. (2019) for terminating the simulations. The quality of estimation of Σ is critical in determining that the simulations are not stopped prematurely.

Markov chains are serially correlated and therefore $\mathrm{Var}_F(X)$ is non-informative about the correlatons in Markov chain. It is important to construct an estimator for Σ which is very close to underlying reality. There are many techniques for estimating Σ like batch means (BM), overlapping bath means (OBM), and spectral variance estimator (SVE). Due to their highly accurate results, we will only focus on SV estimates in this paper. Strong consistency for MSVE has been addressed by Vats et al. (2018). Bias and variance calculations for a variant of SV estimator with known mean is done by Hannan (2009). In this paper, we will address the asymptotic properties (basically strong consistency), bias and variance calculations for RSV estimator.

The most common practice would be to combine the SVE from m chains by averaging over them. We call this technique average spectral variance (ASV) estimator. We will address the issue of slowly mixing Markov chains and show that RSV performs better than ASV. Whereas on one side RSV gives better estimates than ASV for a poor Markov chain, it is as good as ASV for a good Markov chain. We will exemplify this property of RSV for a bi-modal target distribution in subsection 5.2. This appeals intuitively because for a fast mixing Markov chain, all the chains will give almost same estimates for mean.

3.1 Globally-centered spectral variance estimators

Let $\{X_t\}_{t\geq 1}$ be a stochastic process. Denote lag-k autocovariance matrix by $\Gamma(k)$, which is given by,

$$\Gamma(k) = \Gamma(-k) = \mathbb{E}[(X_t - \mathbb{E}[X])(X_{t+k} - \mathbb{E}[X])^T]$$

Recall that $\hat{\Gamma}(k)$ is the empirical autocovariance function given by

$$\hat{\Gamma}(k) = \frac{1}{n}\sum_{t=1}^{n-|k|}(X_t - \bar{X})(X_{t+|k|} - \bar{X})^T$$

The spectral variance estimator is the weighted and truncated sum of lag-k autocovariances, given by:

$$\hat{\Sigma}_{SV} = \sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\hat{\Gamma}_n(k)$$

where $w(.)$ is the lag window and b_n is the truncation point.
Consider m Markov chains where $\bar{X}_s$, $\hat{\Gamma}_s(k)$ and $\hat{\Sigma}_{SV,s}$ are the sample mean, sample lag-k autocovariance and spectral variance estimators respectively for s^{th} Markov chain, $s \in 1, ..., m$. We will consider two estimators for spectral variance calculations using multiple Markov chains.
Now we introduce the Replicated Spectral Variance Estimator (RSV). $\hat{\Gamma}_{RAC,s}(k)$ is the sample replicated lag-k autocovariance estimator for the s^{th} MC using overall mean ($\bar{\bar{X}}$) instead of $\bar{X}_s$ for centering. We construct an RSV estimator $\hat{\Sigma}_{RSV}$ using this replicated version of autocovariance estimator. Consider,

$$\hat{\Sigma}_{RSV,s} = \sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\hat{\Gamma}_{RAC,s}(k)$$

$$\hat{\Sigma}_{RSV} = \frac{1}{m}\sum_{s=1}^{m}\hat{\Sigma}_{RSV,s}$$

3.1.1 Theoretical results

The RSV estimator centers the data around the global mean. We are interested in proving the strong consistency, finding the bias and variance of RSV.

Assumption 1 (Strong Invariance Principle (SIP)). We assume the SIP holds for the Markov chain. Here $\{X_t\}_{t\geq 1}$ is the stochastic process that follows SIP with mean $\mu = \mathbb{E}[X]$. Let $\|.\|$ denote the Euclidean norm. Through SIP, there exists a $p \times p$ lower triangular matrix L, an increasing function ψ on the integers, a finite random variable D, and a sufficiently rich probability space such that, with probability 1,

$$\left\|\sum_{t=1}^{n} X_t - n\mu - LB(n)\right\| < D\psi(n)$$

Let $\{B(n)\}_{n\geq 0}$ denotes a standard p-dim Brownian motion and $B^{(i)}$ denotes its i^{th} component. As shown in the results Kuelbs and Philipp (1980), SIP will hold for $\psi(n) = n^{1/2-\lambda,\, \lambda>0}$ for Markov chains commonly encountered in MCMC settings. We know that $\psi(n)$ is an inherent property of the stochastic process that satisfies the CLT. This implies that $\psi(n)$ is at least $o(\sqrt{n})$. Using Law of Iterative Logarithms (LIL), a tighter bound for $\psi(n)$ is given by Strassen (1964) as $\mathcal{O}(\sqrt{n \log\log n})$.

Assumption 2. We assume that all the conditions given by Vats et al. (2018) for strong consistency of the spectral variance estimator hold true. As a consequence,

$$\hat{\Sigma}_{SV,s} \xrightarrow{a.s.} \Sigma \text{ as } n \to \infty \;\; \forall s \in \{1, ..., m\}$$

Theorem 2. *Let the Assumptions 1,2 hold and $n^{-1} b_n \log\log n \to 0$ as $n \to \infty$, then $\hat{\Sigma}_{RSV} \to \Sigma$ with probability 1, as $n \to \infty$.*

Proof. We complete the proof by showing that $\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}$ converges to 0 almost surely for all $i, j \in \{1, ..., p\}$ and $\tilde{\Sigma}^{ij} \to \Sigma^{ij}$ with probability 1 as $n \to \infty$. We will show that

$$\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij} = g_1(n)D^2 + g_2(n)D + g_3(n)$$

where D is the finite random variable associated with SIP. We will show that

$$\begin{aligned}
g_1(n) &= (4 + C_1)\frac{b_n \psi^2(n)}{n^2} - 4\frac{\psi^2(n)}{n^2} \\
g_2(n) &= 2\sqrt{2}\|L\| p^{1/2}(1+\epsilon)\left[(4 + C_1)\frac{b_n \psi(n)\sqrt{n\log\log n}}{n^2} - 4\frac{\psi(n)\sqrt{n\log\log n}}{n^2}\right] \\
g_3(n) &= \|L\|^2 p(1+\epsilon)^2\left[(4 + C_1)\frac{b_n \log\log n}{n} - 4\frac{\log\log n}{n}\right]
\end{aligned}$$

Using $\psi(n) = \mathcal{O}(\sqrt{n\log\log n})$, $b_n = o(n)$, and $b_n \log\log n = o(n)$, we will finally we prove that $g_1(n), g_2(n), g_3(n) \to 0$ with probability 1, as $n \to \infty$. The proof is in Appendix subsection B.2 $\square$

We are interested in the finding the bias for RSV estimator as a function of n. The proof below applies to all the important range of lag windows $w(x)$; where $w(x)$ is a continuous, even fnction with $w(0) = 1, |w(x)| < c$, and $\int_{-\infty}^{\infty} w^2(x)dx < \infty$. Define

$$W_n = \frac{1}{2\pi}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)$$

We have $W_n < \infty$ for all the important lag windows.

Assumption 3. Let $\Gamma_s(k)$ be the lag-k autocovariance for s^{th} Markov chain and $w(x)$ be the lag window. We assume that there exists a $q \geq 0$ such that

a. $\sum_{-\infty}^{\infty} |k|^q \|\Gamma(k)\| < \infty$

b. $\lim_{x\to 0} \dfrac{1-w(x)}{|x|^q} = k_q < \infty$

c. $\dfrac{b_n^q}{n} \to 0$ as $n \to \infty$

If k_q is finite for some q_o, then it is zero for $q < q_0$. q is taken to be the largest number satisfying the first two conditions above.

Theorem 3. *The limiting bias of replicated spectral variance is given by:*

$$\lim_{n\to\infty} b_n^q \mathbb{E}\left[\hat{\Sigma}_{RSV} - \Sigma\right] = -k_q \Phi^{(q)}$$

Proof.

$$\mathbb{E}\left[\hat{\Sigma}_{RSV} - \Sigma\right] = \sum_{k=-b_n+1}^{b_n-1} w\left(\frac{|k|}{b_n}\right) \mathbb{E}\left[\hat{\Gamma}_{RAC}(k)\right] - \sum_{k=-\infty}^{\infty} \Gamma(k)$$

Using theorem 1, we can write the expectation of $\hat{\Gamma}_{RAC}$ as a sum of equation 1 and some small order terms. The proof is given in the Appendix subsection B.1. □

Assumption 4. Let $\{X_{st}\}_{t\geq 1}$ be the s^{th} Markov chain for which SIP holds.

a. $\mathbb{E}[D^4] < \infty$ where D is a finite random variable associated with the SIP

b. $\mathbb{E}[X^4] < \infty$ where $\{X\}$ is the stochastic process

Theorem 4. *If Assumption 4 hold,* $b_n^{-1} n \, Var\left(\hat{\Sigma}_{RSV}^{ij}\right) = [\Sigma_{ii}\Sigma_{jj} + \Sigma_{ij}^2] \int_{-\infty}^{\infty} w(x)^2 dx + o(1)$.

Proof. Recall that $\tilde{\Sigma}$ is the averaged pseudo spectral variance estimator which uses the unobserved mean. Further, let $\tilde{\Sigma}^{ij}$ be the $(i,j)^{th}$ element of this matrix. We will prove that the variance of $\hat{\Sigma}_{RSV}$ and $\tilde{\Sigma}$ are equivalent for large sample sizes. The proof is in Appendix subsection B.4 □

3.1.2 Fast implementation

4 Effective sample size

Estimating the MCSE is crucial for determining when to terminate the simulations. The existing stopping rules rely on the strong consistency of the estimator of Σ. We will use the *relative standard deviation fixed-volume sequential stopping rule* proposed in Vats et al. (2019) when multivariate Markov chain central limit theorem holds. This stopping rule terminates the simulations on the basis of size of confidence interval relative to inherent variability in the target distribution. It terminates after the total number of samples, i.e. mn exceed some pre-specified n^* iterations to prevent pre-mature termination due to bad estimates of Σ and Λ. The rule is given by

$$\text{Volume of confidence region}^{1/p} + n^{-1} < \epsilon |\Lambda_n|^{1/2p}$$

where ϵ is the tolerance level, $|.|$ denotes the determinant and Λ_n is the sample covariance matrix given by

$$\frac{1}{mn-1}\sum_{s=1}^{m}\sum_{t=1}^{n}(X_{st} - \bar{\bar{X}})(X_{st} - \bar{\bar{X}})^T$$

The determinant of Monte Carlo standard error is called generalized variance in Wilks (1932) and gives a metric for volume of confidence interval. Vats et al. (2019) showed that if the estimator for Σ is strongly consistent, the stopping rule is asymptotically valid, in that the confidence regions created at termination have the right coverage probability as $\epsilon \to 0$. Since $\hat{\Sigma}_{RSV}$ is a strongly consistent estimator of Σ, w

$$\left|\hat{\Sigma}_{RSV}\right|^{1/p} + (mn)^{-1} < \epsilon |\Lambda_{mn}|^{1/2p}$$

Another way to get more accurate stopping rule is to use RSV estimator for estimating Effective Sample Size (ESS) in multivariate settings. RSV estimator better captures the standard error of target distribution by considering the global sample mean across the Markov chains; which might otherwise get lost when considering a single localized slowly mixing Markov chain. We therefore define our ESS rule as

$$\text{ESS} = mn\left(\frac{|\Lambda_{mn}|}{\left|\hat{\Sigma}_{RSV}\right|}\right)^{1/p}$$

When there is no correlation in Markov chain $\hat{\Sigma}_{RSV} = \Lambda_{mn}$ and therefore, ESS $= n$. Both the rules involve the ratio of generalized variances and therefore the relative standard deviation fixed-volume sequential stopping rule is asymptotically equivalent to stopping when ESS is greater than $W_{p,\alpha,\epsilon}$ which depends on dimension of state-space, level of confidence of the confidence region, and the relative precision required.

5 Examples

In the following examples we compare the performance of asymptotic variance estimators (ASVE and RSVE) for Markov chain CLT. We will successfully illustrate that the replicated spectral variance estimator performs better than the average spectral variance estimator in terms of ESS calculations, coverage probabilities , and sample distribution of Σ. We will also show that in case of nicely mixing Markov chains, these estimators give almost equivalent results. As a consequence, while out replicated version of variance estimator is better in cases where the Markov chains do not explore the entire sample space in finite time, it is harmless to be used in cases where they do. about this new FFT based method for faster RSVE calculations

5.1 Vector Autoregressive Process

We examine the vector autoregressive process of order 1 (VAR(1)) where the true autocovariance in known in closed form. We have already illustrated the better performance of R-ACF over traditional ACF on a slowly mixing VAR(1) process in Figure **??**. Here we will examine the performance of RSV estimator on the same process. Consider a p-dimensional VAR(1) process $\{X_t\}_{t\geq 1}$ such that

$$X_t = \Phi X_{t-1} + \epsilon_t$$

where $X_t \in \mathbb{R}^p$, Φ is a $p \times p$ matrix, $\epsilon_t \overset{i.i.d.}{\sim} N(0, \Omega)$, and Ω is a positive definite $p \times p$ matrix. The invariant distribution for this Markov chain is $N(0, \Psi)$ where $\vec{\Psi} = (I_{p^2} - \Phi \otimes \Phi)\vec{\Omega}$. The lag-k autocovariance can be calculated easily for $k > 0$ as

$$\Gamma(k) = \Phi^k \Psi$$
$$\Gamma(-k) = \Psi(\Phi^T)^k$$

The Markov chain is geometrically ergodic when the spectral norm of Φ is less than 1 (Tjstheim (1990)). The CLT holds for the invariant distribution, therefore, Σ exists and is given by

$$\Sigma = (1 - \Phi)^{-1}\Psi + \Psi(1 - \Phi^T)^{-1} - \Psi$$

Let ϕ_{max} be the largest absolute eigenvalue of Φ such that $|\phi_{max}| < 1$. The larger it is, the slower the Markov chain mixes. For our case, we require a slowly mixing VAR(1) process. We consider a bivariate example with $\phi_{max} = 0.9999$. We run five parallel Markov chains with their starting points evenly distributed about the center of invariant distribution. Figure **??** shows that for the first 500 samples, the chains have not explored the sample space well unlike Figure **??** with $5 \cdot 10^4$ samples.

5.2 Boomerang Distribution

We will use a bivariate bi-modal distribution introduced by Gelman and Meng (1991) which has Gaussian conditional distributions in both directions. This allows us to sample parallel Markov chains using the Gibbs sampler. Let x and y be two random variable that are jointly distributed as

$$f(x, y) \propto \exp\left(-\frac{1}{2}[Ax^2y^2 + x^2 + y^2 - 2Bxy - 2C_1x - 2C_2y]\right)$$

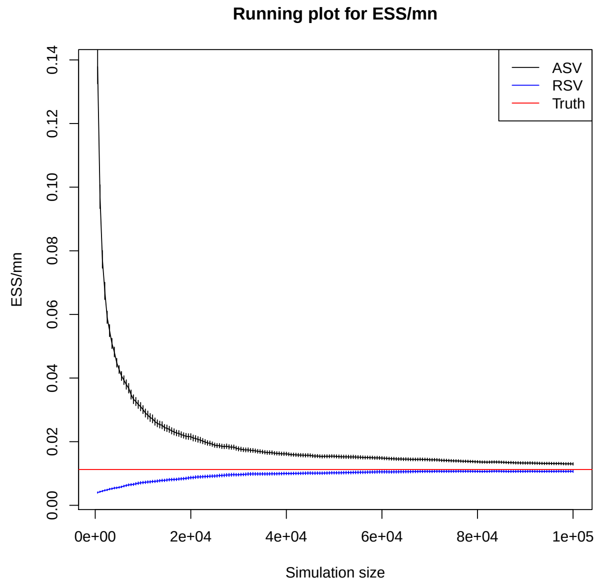


Figure 1: Running plots for $E\hat{S}S/mn$ calculated using ASV (black) and RSV (blue). The true ESS/mn (red) is known.

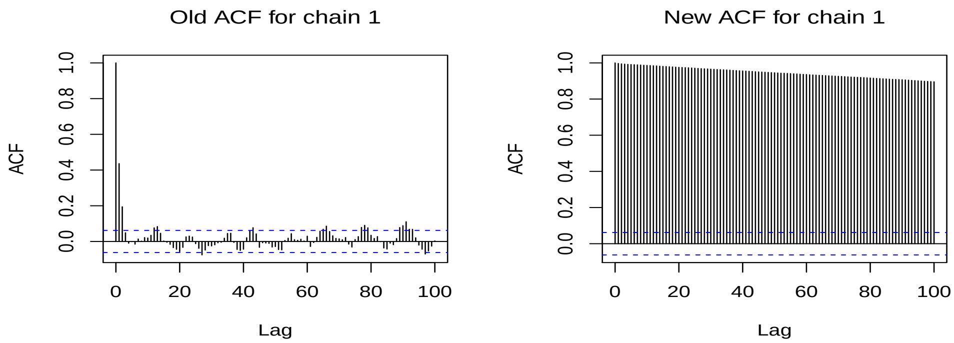
The conditional distribution of x given y and vice versa is a normal distribution given by:

$$x_1 \mid x_2 \sim N\left(\frac{Bx_2 + C_1}{Ax_2^2 + 1}, \frac{1}{Ax_2^2 + 1}\right)$$
$$x_2 \mid x_1 \sim N\left(\frac{Bx_1 + C_2}{Ax_1^2 + 1}, \frac{1}{Ax_1^2 + 1}\right)$$

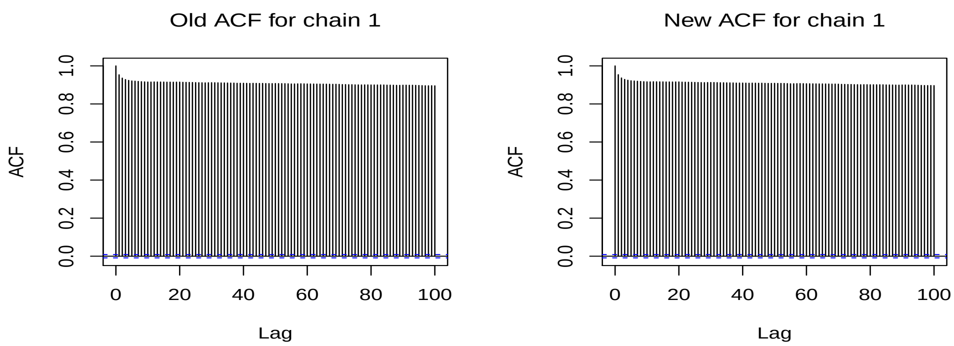
We use a carefully chosen parameterization of $A = 1,\ B = 3,\ C = 8$ which ensures bimodality for our purpose. Let n be the number of samples in each chain and m be the number of Markov chain replications. Finding the actual mean of this distribution in closed form is difficult. Therefore, we use numerical integration with fine tuning to calculate it. We sample two parallel Markov chains with well-separated starting values.

In Figure **??**, we demonstrate the "sticky" nature of the Markov chains. For the first thousand samples, both the chains are oblivious of the existence of another mode. By ten thousand samples, both the Markov chains have explored the two modes. This property will affect the single chain estimators like ACF. In Figure 2a, the ACF is severely underestimated because the chain-1 has not jumped to the other mode. Whereas, in Figure 2b, both ACF and R-ACF give almost similar results indicating that both modes have been explored by chain-1.

We also run five parallel Markov chains with well-separated starting points. In Table 1, we give the coverage probabilities for 95% confidence interval for both the estimator. We can see that the RSVE



(a) $n = 1000$



(b) $n = 50000$

Figure 2: ACF and R-ACF for component-1 of chain-1 at two different number of Monte Carlo samples.

gives better coverage probabilities for all the n. For smaller sample size, the coverage probability of RSVE is significantly higher than ASVE. As the number of samples per chain increases, they start coming closer due to the strong consistency of both the estimators.

A good estimate of ESS is crucial to determine when to stop the simulations. We can see in Figure 3 that for the first few thousand samples, ASVE gives misleadingly higher $E\hat{S}S/mn$ than RSVE. This can cause us to stop the sampling before the sample space has been explored by the chains. The inferences derived from this chain would then be severely non-informative.

To examine the performance of RSV for a nicely mixing Markov chain, we use the parametrization of $A = 1,\ B = 10,\ C = 7$. This is also a bimodal distribution, however, the two modes interact well with each other (Figure **??**). In Figure 4, we observe that both RSV and ASV give almost the same estimates for ESS. Similar is the case with coverage probabilities in Table 2 for a 95% confidence region.

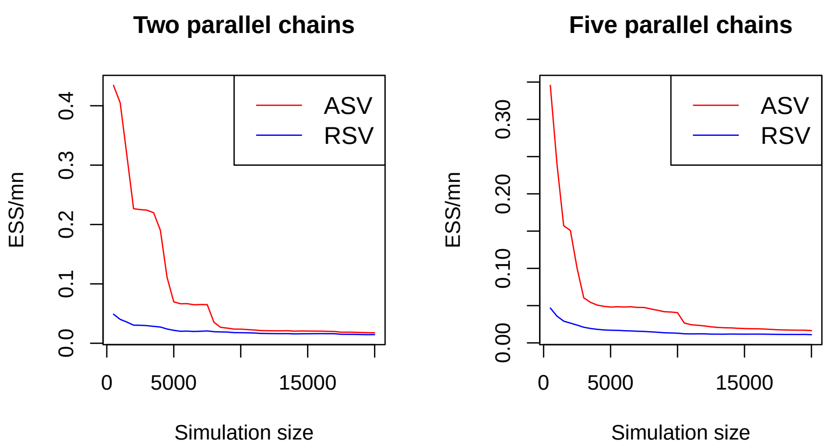


Figure 3: Running plot for $E\hat{S}S/mn$ using ASV and RSV calculated for two chains (left) and five chains (right). The parameters for target distribution are $A == 1,\ B = 3,\ C = 8$.

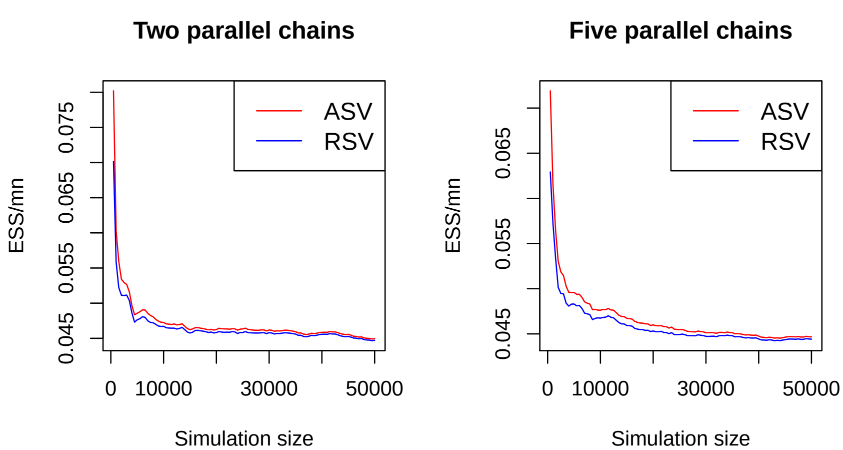


Figure 4: Running plot for $E\hat{S}S/mn$ using ASV and RSV calculated for two chains (left) and five chains (right). The parameters of target distribution are $A = 1,\ B = 10,\ C = 7$

n	$m=2$		$m=5$	
	ASV	RSV	ASV	RSV
10^3	0.612	0.689	0.602	0.753
$2 \cdot 10^3$	0.693	0.751	0.735	0.827
$5 \cdot 10^3$	0.826	0.854	0.847	0.880
10^4	0.862	0.868	0.884	0.907
$2 \cdot 10^4$	0.899	0.906	0.922	0.934

Table 1: Coverage probabilities for parameter values $A = 1,\ B = 3,\ C = 8$.

n	$m=2$		$m=5$	
	ASV	RSV	ASV	RSV
10^3	0.873	0.884	0.875	0.898
$2 \cdot 10^3$	0.881	0.888	0.897	0.914
$5 \cdot 10^3$	0.902	0.908	0.919	0.929
10^4	0.923	0.927	0.925	0.926
$5 \cdot 10^4$	0.951	0.952	0.939	0.939

Table 2: Coverage probabilities for parameter values $A = 1,\ B = 10,\ C = 7$.

5.3 Sensor Network Localization

For our third example, we consider a real-life problem of sensor locations previously discussed by Ihler et al. (2005). The goal is to identify unknown sensor locations using noisy distance data. This problem is specifically interesting in our case because the joint posterior distribution for missing sensor locations is multi-modal.

Tak et al. (2018) modified the simulation settings of Lan et al. (2014) to include only six sensor locations (four unknown and two unknown) out of eleven locations (eight known and three unknown). Following Tak et al. (2018), we assume that there are six sensors scattered on a planar region where $x_i = (x_{i1}, x_{i2})^T$ denote the $2d$ coordinates of i^{th} sensor. Let $y_{ij} = (y_{ji})$ denote the distance between the sensors x_i and x_j. The distance between x_i and x_j is observed with probability $\pi(x_i, x_j) = \exp \|x_i - x_j\|^2/2R^2$ and with a Gaussian measurement error of σ^2. Let zij denote the indicator variable which is equal to 1 when the distance between x_i and x_j is observed. The probability model is then,

$$z_{ij}|x_1, ..., x_6 \sim Bernoulli\left(\exp\left(\frac{-\|x_i - x_j\|^2}{2R^2}\right)\right)$$

$$y_{ij}|w_{ij} = 1, x_1, ..., x_6 \sim N(\|x_i - x_j\|^2, \sigma^2)$$

Ahn et al. (2013) suggested the value of $R = 0.3$ and $\sigma = 0.02$. We use a Gaussian prior for the unknown locations with mean equal to $(0, 0)$ and covariance matrix equal to $100I_2$. y_{ij} is specified only if $w_{ij} = 1$. The likelihood function is then,

$$L(x_1, x_2, x_3, x_4) \propto$$
$$\prod_{j>i}\left[\left(\exp\left(\frac{-\|x_i - x_j\|^2}{2 \times 0.3^2}\right)\right)^{w_{ij}}\left(1 - \exp\left(\frac{-\|x_i - x_j\|^2}{2 \times 0.3^2}\right)\right)^{1-w_{ij}} \exp\left(-\frac{y_{ij} - \|x_i - x_j\|^2}{2 \times 0.02^2}\right)\right]$$

The full posterior distribution with Gaussian prior is given by,

$$\pi(x_1, x_2, x_3, x_4|y, w) \propto L(x_1, x_2, x_3, x_4) \times \exp\left(-\frac{\sum_{i=1}^{4} x_i^T x_i}{2 \times 0.02^2}\right) \tag{3}$$

where $y = (y_{ij}, j > i)$ and $w = (w_{ij}, j > i)$. We follow the Markov chain structure as described by Tak et al. (2018) and sample from the four bivariate conditionals for each sensor location using a Gibbs sampler. In their paper on Repelling Attractive Metropolis (RAM) algorithms, Tak et al. (2018) compare the performance of three different sampling techniques namely - Metropolis, RAM and Tempered Transitions (TT). RAM is shown to improve the acceptance rate by a factor of at least 5.5 over Metropolis using the same jumping scale. RAM algorithm supplies Markov chains with higher jumping frequency between the modes of a multimodal target distribution.

We will use the RAM algorithm with a jumping scale equal to 0.5 to sample five parallel Markov chains with well-separated starting points. The total simulation size for each chain is fixed at $100,000$. Figure 5 demonstrates the trace plots of the first chain for the x-component of all four unknown locations. We observe the bi-modal nature of the marginal distribution for each component. The Markov chains get stuck at a particular mode for a long time before jumping to the other mode. Figure 6 shows the effect of this "sticky" nature of Markov chains over the autocorrelations centered around the local and global mean. For a small sample size of 1000, it can be seen that the third chain has not explored the sample space well. As a consequence, the local mean differs a lot from the global mean (averaged over all five chains).

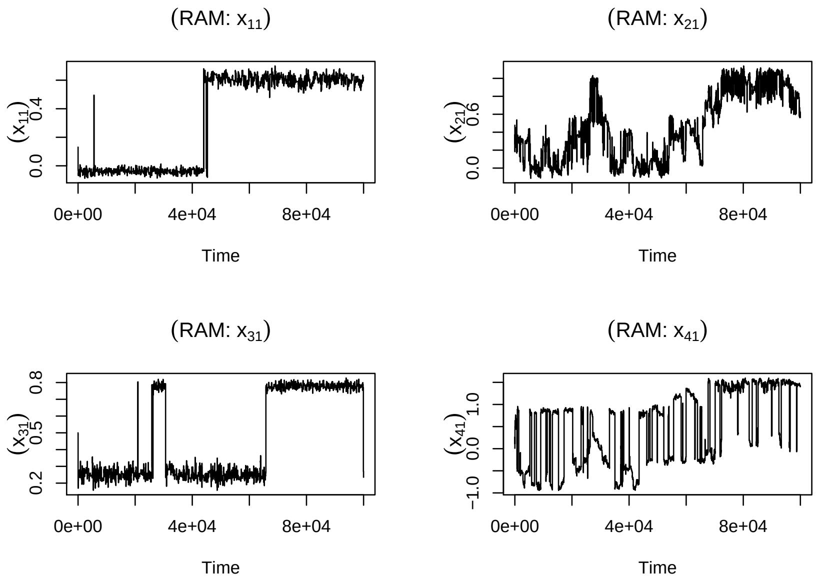


Figure 5: Trace plots for the x-component of all four locations of the third chain.

6 Discussion

A Preliminaries

Lemma 1. *(Csörgo and Révész (2014)). Suppose Assumption 1 holds, then for all $\epsilon > 0$ and for almost all sample paths, there exists $n_0(\epsilon)$ such that $\forall n \geq n_0$ and $\forall i = 1, ..., p$*

$$\sup_{0 \leq t \leq n-b_n} \sup_{0 \leq s \leq b_n} \left| B^{(i)}(t+s) - B^{(i)}(t) \right| < (1+\epsilon) \left(2b_n \left(\log \frac{n}{b_n} + \log \ \log \ n \right) \right)^{1/2},$$

$$\sup_{0 \leq s \leq b_n} \left| B^{(i)}(n) - B^{(i)}(n-s) \right| < (1+\epsilon) \left(2b_n \left(\log \frac{n}{b_n} + \log \ \log \ n \right) \right)^{1/2}, \text{ and}$$

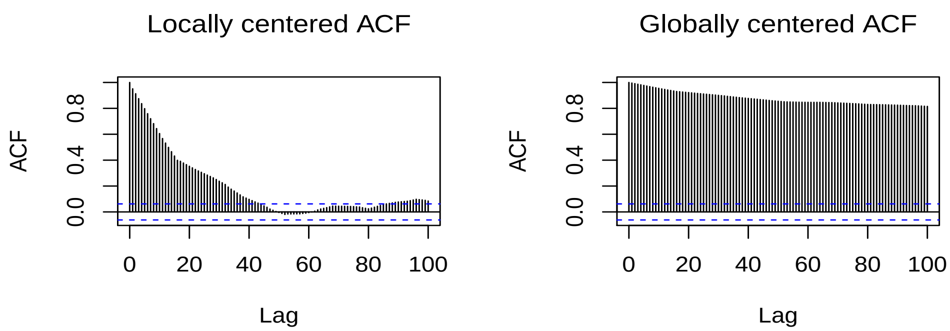
$$\left| B^{(i)}(n) \right| < (1+\epsilon) \sqrt{2n \ \log \log n} \,.$$

B Proof of Theorems

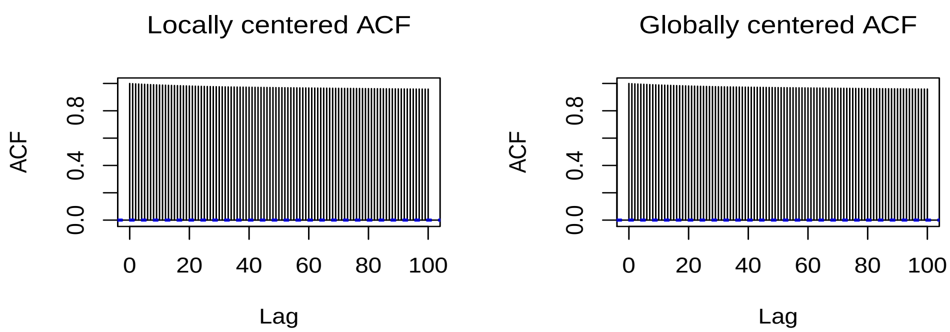
B.1 Bias of autocovariance

Proof of Theorem 1.

$$\hat{\Gamma}_{RAC,s}(k)$$



(a) $n = 10^3$



(b) $n = 10^5$

Figure 6: ACF and R-ACF for component-3 of chain-3 at two different number of Monte Carlo samples.

$$
\begin{aligned}
&= \frac{1}{n}\sum_{t=1}^{n-|k|}\left(X_{st} - \bar{\bar{X}}\right)\left(X_{s(t+k)} - \bar{\bar{X}}\right)^T \\
&= \left[\frac{1}{n}\sum_{t=1}^{n-|k|}\left(X_{st} - \bar{X}_s\right)\left(X_{s(t+k)} - \bar{X}_s\right)^T\right] + \left[\frac{1}{n}\sum_{t=1}^{|k|}\left(\bar{X}_s - \bar{\bar{X}}\right)\left(\bar{X}_s - X_{st}\right)^T\right] \\
&\quad + \left[\frac{1}{n}\sum_{t=n-|k|+1}^{n}\left(\bar{X}_s - X_{st}\right)\left(\bar{X}_s - \bar{\bar{X}}\right)^T\right] + \left[\frac{n-|k|}{n}\left(\bar{X}_s - \bar{\bar{X}}\right)\left(\bar{X}_s - \bar{\bar{X}}\right)^T\right] \\
&= \hat{\Gamma}_s(k) - \frac{1}{n}\sum_{t=1}^{|k|} A_{st}^T - \frac{1}{n}\sum_{t=n-|k|+1}^{n} A_{st} + \frac{n-|k|}{n}\left(\bar{X}_s - \bar{\bar{X}}\right)\left(\bar{X}_s - \bar{\bar{X}}\right)^T,
\end{aligned} \tag{4}
$$

where $A_{st} = (X_{st} - \bar{X}_s)(\bar{X}_s - \bar{\bar{X}})^T$. We will study the expectations of the each of the above terms. Without loss of generality, consider A_{11},

$\mathbb{E}\left[A_{11}\right]$

$$
\begin{aligned}
&= \mathbb{E}\left[\left(X_{11} - \bar{X}_1\right)\left(\bar{X}_1 - \bar{\bar{X}}\right)^T\right] \\
&= \mathbb{E}\left[X_{11}\bar{X}_1^T\right] - \mathbb{E}\left[X_{11}\bar{\bar{X}}^T\right] + \mathbb{E}\left[\bar{X}_1\bar{\bar{X}}^T\right] - \mathbb{E}\left[\bar{X}_1\bar{X}_1^T\right] \\
&= \mathbb{E}\left[X_{11}\bar{X}_1^T\right] - \frac{1}{m}\mathbb{E}\left[X_{11}\bar{X}_1^T\right] - \frac{m-1}{m}\mathbb{E}\left[X_{11}\bar{X}_2^T\right] + \frac{1}{m}\mathbb{E}\left[\bar{X}_1\bar{X}_1^T\right] + \frac{m-1}{m}\mathbb{E}\left[\bar{X}_1\bar{X}_2^T\right] - \mathbb{E}\left[\bar{X}_1\bar{X}_1^T\right] \\
&= \frac{m-1}{m}\left(\mathbb{E}\left[X_{11}\bar{X}_1^T\right] - \mathbb{E}\left[X_{11}\bar{X}_2^T\right] + \mathbb{E}\left[\bar{X}_1\bar{X}_2^T\right] - \mathbb{E}\left[\bar{X}_1\bar{X}_1^T\right]\right) \\
&= \frac{m-1}{m}\left(\frac{1}{n}\sum_{t=1}^{n}\mathbb{E}\left[X_{11}X_{1t}^T\right] - \mathbb{E}\left[X_{11}\right]\mathbb{E}\left[\bar{X}_2^T\right] + \mathbb{E}\left[\bar{X}_1\right]\mathbb{E}\left[\bar{X}_2^T\right] - \mathrm{Var}\left[\bar{X}_1\right] - \mathbb{E}\left[\bar{X}_1\right]\mathbb{E}\left[\bar{X}_1^T\right]\right) \\
&= \frac{m-1}{m}\left(\frac{1}{n}\sum_{k=0}^{n-1}\Gamma(k) + \mu\mu^T - \mu\mu^T + \mu\mu^T - \mathrm{Var}\left[\bar{X}_1\right] - \mu\mu^T\right) \\
&= \frac{m-1}{mn}\left(\sum_{k=0}^{n-1}\Gamma(k) - n\mathrm{Var}\left[\bar{X}_1\right]\right). \qquad (5)
\end{aligned}
$$

Similarly,

$$
\mathbb{E}\left[A_{11}^T\right] = \mathbb{E}\left[A_{11}\right]^T = \frac{m-1}{mn}\left(\sum_{k=0}^{n-1}\Gamma(k)^T - n\mathrm{Var}\left[\bar{X}_1\right]\right). \qquad (6)
$$

Further,

$$
\begin{aligned}
\mathbb{E}\left[\left(\bar{X}_s - \bar{\bar{X}}\right)\left(\bar{X}_s - \bar{\bar{X}}\right)^T\right] &= \mathbb{E}\left[\bar{X}_s\bar{X}_s^T - \bar{X}_s\bar{\bar{X}}^T - \bar{\bar{X}}\bar{X}_s^T + \bar{\bar{X}}\bar{\bar{X}}^T\right] \\
&= \mathbb{E}\left[\bar{X}_s\bar{X}_s^T - \bar{\bar{X}}\bar{\bar{X}}^T\right] \\
&= \left(\mathbb{E}\left[\bar{X}_1\bar{X}_1^T\right] - \mathbb{E}\left[\bar{\bar{X}}\bar{\bar{X}}^T\right]\right) \\
&= \left(\mathrm{Var}(\bar{X}_1) + \mu\mu^T - \mathrm{Var}(\bar{\bar{X}}) - \mu\mu^T\right) \\
&= \frac{m-1}{m}\mathrm{Var}(\bar{X}_1). \qquad (7)
\end{aligned}
$$

Using (1), (5), (6), and (7) in (4),

$$
\begin{aligned}
&\mathbb{E}\left[\hat{\Gamma}_{RAC,s}(k)\right] \\
&= \mathbb{E}\left[\hat{\Gamma}_s(k)\right] - \frac{1}{n}\left(\sum_{t=1}^{|k|}\mathbb{E}[A_{1t}^T] + \sum_{t=n-|k|+1}^{n}\mathbb{E}[A_{1t}]\right) + \left(1 - \frac{|k|}{n}\right)\left(1 - \frac{1}{m}\right)\mathrm{Var}(\bar{X}_1)
\end{aligned}
$$

$$= \mathbb{E}\left[\hat{\Gamma}_s(k)\right] - \frac{|k|}{n}\left(1 - \frac{1}{m}\right)\left(\frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h) + \frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h)^T - 2\text{Var}(\bar{X}_1)\right) + \left(1 - \frac{|k|}{n}\right)\left(1 - \frac{1}{m}\right)\text{Var}(\bar{X}_1)$$

$$= \left(1 - \frac{|k|}{n}\right)\Gamma(k) - \frac{|k|}{n}\left[\left(1 - \frac{1}{m}\right)\left(\frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h)^T + \frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h)\right) - \left(2 - \frac{1}{m}\right)\text{Var}(\bar{X}_1)\right] - \frac{\text{Var}(\overline{X}_1)}{m}.$$

We can use the results of Song and Schmeiser (1995) given in (2) to expand $\text{Var}(\bar{X}_1)$. Expectation of $\hat{\Gamma}_{RAC,s}(k)$ can then broken down as following,

$$\mathbb{E}\left[\hat{\Gamma}_{RAC}(k)\right] = \left(1 - \frac{|k|}{n}\right)\Gamma(k) + O_1 + O_2\,. \tag{8}$$

where,

$$\begin{aligned} O_1 &= -\frac{|k|}{n}\left[\left(1 - \frac{1}{m}\right)\left(\frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h)^T + \frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h)\right) - \left(2 - \frac{1}{m}\right)\left(\frac{\Sigma}{n} + \frac{\Phi}{n^2}\right)\right], \\ O_2 &= -\frac{1}{m}\left(\frac{\Sigma}{n} + \frac{\Phi}{n^2}\right) + o(n^{-2}) \end{aligned}$$

We observe that both O_1 and O_2 are small order terms that converge to 0 as $n \to \infty$. Here, $O_1 = (-|k|/n)\mathcal{O}(1/n)$ and $O_2 = \mathcal{O}(1/n)$. For a diagonal element of Γ,

$$\mathbb{E}\left[\hat{\Gamma}^{ii}_{RAC,s}\right]$$

$$= \mathbb{E}\left[\hat{\Gamma}^{ii}_s(k)\right] - \frac{|k|}{n}\left[\left(1 - \frac{1}{m}\right)\left(\frac{1}{n}\sum_{h=0}^{n-1}\Gamma^{ii}(h)^T + \frac{1}{n}\sum_{h=0}^{n-1}\Gamma^{ii}(h)\right) - \left(2 - \frac{1}{m}\right)\text{Var}(\overline{X}_1)^{ii}\right] - \frac{\text{Var}(\overline{X}_1)^{ii}}{m}.$$

In the presence of positive correlation, the leftover term is positive. □

Proof of corollary 1.

$$\begin{aligned} \hat{\Gamma}_{RAC}(0) &= \frac{1}{m}\sum_{s=1}^{m}\hat{\Gamma}_{RAC,s}(0) = \frac{1}{mn}\sum_{s=1}^{m}\sum_{t=1}^{n}\left(X_{st} - \bar{\bar{X}}\right)\left(X_{st} - \bar{\bar{X}}\right)^T \\ &= \left[\frac{1}{mn}\sum_{s=1}^{m}\sum_{t=1}^{n}\left(X_{st} - \bar{X}_s\right)\left(X_{st} - \bar{X}_s\right)^T\right] + \left[\frac{1}{m}\sum_{s=1}^{m}\left(\bar{X}_s - \bar{\bar{X}}\right)\left(\bar{X}_s - \bar{\bar{X}}\right)^T\right] \\ &= \frac{1}{m}\sum_{s=1}^{m}\hat{\Gamma}_s(0) + \frac{1}{m}\sum_{s=1}^{m}\left(\bar{X}_s - \bar{\bar{X}}\right)\left(\bar{X}_s - \bar{\bar{X}}\right)^T. \end{aligned}$$

Using (1) and (7) the expectation of $\hat{\Gamma}_{RAC}(0)$ can be written as

$$
\begin{aligned}
\mathbb{E}\left[\hat{\Gamma}_{RAC}(0)\right] &= \mathbb{E}\left[\hat{\Gamma}_1(0)\right] + \left(1 - \frac{1}{m}\right)\mathrm{Var}(\bar{X}_1) \\
&= \Gamma(k) - \frac{1}{m}\mathrm{Var}(\bar{X}_1)\,.
\end{aligned}
$$

$\square$

B.2 Strong consistency argument

We are going to consider a class of pseudo spectral variance estimator denoted by $\tilde{\Sigma}$ which uses data centered around the unobserved actual mean μ. Such pseudo covariance estimator and auto-covariance estimator for the j^{th} chain is denoted by $\tilde{\Sigma}_s$ and $\tilde{\Gamma}_s$ respectively.

$$
\begin{aligned}
\tilde{\Gamma}_s(k) &= \frac{1}{n}\sum_{t=1}^{n-|k|}(X_{st}-\mu)(X_{s(t+k)}-\mu)^T \\
\tilde{\Sigma}_s &= \sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\tilde{\Gamma}_s(k)\,.
\end{aligned}
$$

The average pseudo spectral variance estimator (APSVE) is given by

$$
\tilde{\Sigma} = \frac{1}{m}\sum_{s=1}^{m}\tilde{\Sigma}_s
$$

Further, let

$$
\begin{aligned}
M_1 &= \frac{1}{m}\sum_{s=1}^{m}\left\{\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\sum_{t=1}^{n-|k|}\frac{1}{n}\left[(X_{st}-\mu)_i\left(\mu-\bar{\bar{X}}\right)_j + \left(\mu-\bar{\bar{X}}\right)_i\left(X_{s(t+k)}-\mu\right)_j\right]\right\}, \\
M_2 &= \left(\mu-\bar{\bar{X}}\right)_i\left(\mu-\bar{\bar{X}}\right)_j\sum_{k=-b_n+1}^{b_n-1}\left(1-\frac{|k|}{n}\right)w\left(\frac{k}{b_n}\right)\,.
\end{aligned}
$$

Lemma 2. *For the RSV estimator* $\hat{\Sigma}^{ij}_{RSV} = \tilde{\Sigma}^{ij} + M_1 + M_2$ *and*

$$
|M_1 + M_2| \le D^2 g_1(n) + D g_2(n) + g_3(n)
$$

where

$$
g_1(n) = (4 + C_1)\frac{b_n\psi^2(n)}{n^2} - 4\frac{\psi^2(n)}{n^2} \to 0
$$

$$
\begin{aligned}
g_2(n) &= 2\sqrt{2}\|L\|p^{1/2}(1+\epsilon)\left[(4+C_1)\frac{b_n\psi(n)\sqrt{n\log\log n}}{n^2} - 4\frac{\psi(n)\sqrt{n\log\log n}}{n^2}\right] \to 0 \\
g_3(n) &= \|L\|^2 p(1+\epsilon)^2\left[(4+C_1)\frac{b_n \log\log n}{n} - 4\frac{\log\log n}{n}\right] \to 0\,.
\end{aligned}
$$

Proof. The proof follows from standard algebraic calculations and is presented here for completeness. Consider,

$$
\begin{aligned}
&\hat{\Sigma}^{ij}_{RSV} \\
&= \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left(X_{st}-\bar{\bar{X}}\right)_i\left(X_{s(t+k)}-\bar{\bar{X}}\right)_j \\
&= \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left\{(X_{st}-\mu)_i + \left(\mu-\bar{\bar{X}}\right)_i\right\}\left\{\left(X_{s(t+k)}-\mu\right)_j + \left(\mu-\bar{\bar{X}}\right)_j\right\}\right] \\
&= \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[(X_{st}-\mu)_i\left(X_{s(t+k)}-\mu\right)_j + (X_{st}-\mu)_i\left(\mu-\bar{\bar{X}}\right)_j\right. \\
&\quad \left. + \left(\mu-\bar{\bar{X}}\right)_i\left(X_{s(t+k)}-\mu\right)_j + \left(\mu-\bar{\bar{X}}\right)_i\left(\mu-\bar{\bar{X}}\right)_j\right] \\
&= \tilde{\Sigma}^{ij} + \left[(\mu-\bar{\bar{X}})_i(\mu-\bar{\bar{X}})_j\sum_{k=-b_n+1}^{b_n-1}\left(1-\frac{|k|}{n}\right)w\left(\frac{k}{b_n}\right)\right] \\
&\quad + \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\sum_{t=1}^{n-|k|}\left[\frac{1}{n}(X_{st}-\mu)_i\left(\mu-\bar{\bar{X}}\right)_j + \frac{1}{n}\left(\mu-\bar{\bar{X}}\right)_i\left(X_{s(t+k)}-\mu\right)_j\right] \\
&= \tilde{\Sigma}^{ij} + M_1 + M_2\,.
\end{aligned}
$$

Consequently

$$
\left|\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right| = |M_1 + M_2| \le |M_1| + |M_2|\,.
$$

We first present a result which will be useful to use later. For any Markov chain s,

$$
\begin{aligned}
\|\bar{X}_s - \mu\|_\infty \le \|\bar{X}_s - \mu\| &= \frac{1}{mn}\left\|\sum_{t=1}^{n} X_{st} - n\mu\right\| \\
&= \frac{1}{n}\left\|\sum_{t=1}^{n} X_{st} - n\mu \pm LB(n)\right\| \\
&\le \frac{1}{n}\left\|\sum_{t=1}^{n} X_{st} - n\mu - LB(n)\right\| + \frac{\|LB(n)\|}{n}
\end{aligned}
$$

$$
\begin{aligned}
&< \frac{D\psi(n)}{n} + \frac{\|LB(n)\|}{n} \\
&< \frac{D\psi(n)}{n} + \frac{1}{n}\|L\| \left(\sum_{i=1}^{p} |B^{(i)}(k)|^2 \right)^{1/2} \\
&\leq \frac{D\psi(n)}{n} + \frac{1}{n}\|L\| p^{1/2}(1+\epsilon)\sqrt{2n \log\log n}\,. \qquad (9)
\end{aligned}
$$

Similarly,

$$
\|\bar{\bar{X}} - \mu\|_\infty \leq \frac{D\psi(n)}{n} + \frac{1}{n}\|L\| p^{1/2}(1+\epsilon)\sqrt{2n \log\log n}\,. \qquad (10)
$$

Now consider,

$$
\begin{aligned}
&|M_1| \\
&= \left| \frac{1}{m}\sum_{s=1}^{m} \left\{ \sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right) \sum_{t=1}^{n-|k|} \frac{1}{n} \left[(X_{st}-\mu)_i \left(\mu - \bar{\bar{X}}\right)_j + \left(\mu - \bar{\bar{X}}\right)_i \left(X_{s(t+k)} - \mu\right)_j \right] \right\} \right| \\
&\leq \frac{1}{m}\sum_{s=1}^{m} \left\{ \sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right) \left[\frac{1}{n} \left| \sum_{t=1}^{n-|k|} (X_{st}-\mu)_i \left(\mu - \bar{\bar{X}}\right)_j \right| + \frac{1}{n} \left| \sum_{t=1}^{n-|k|} \left(\mu - \bar{\bar{X}}\right)_i \left(X_{s(t+k)} - \mu\right)_j \right| \right] \right\} \\
&\leq \frac{1}{m}\sum_{s=1}^{m} \left\{ \sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right) \left[\frac{1}{n} \left| \sum_{t=1}^{n-|k|} (X_{st}-\mu)_i \right| \left| (\mu - \bar{\bar{X}})_j \right| + \frac{1}{n} \left| (\mu - \bar{\bar{X}})_i \right| \left| \sum_{t=1}^{n-|k|} (X_{j(t+k)} - \mu)_j \right| \right] \right\} \\
&\leq \frac{\|(\bar{\bar{X}} - \mu)\|_\infty}{m} \sum_{s=1}^{m} \sum_{k=-b_n+1}^{b_n-1} \left[\frac{1}{n} \left\| \sum_{t=1}^{n-|k|} (X_{st}-\mu) \right\|_\infty + \frac{1}{n} \left\| \sum_{t=1}^{n-|k|} (X_{s(t+k)} - \mu) \right\|_\infty \right] \\
&\leq \frac{\|(\bar{\bar{X}} - \mu)\|_\infty}{m} \\
&\quad \times \sum_{s=1}^{m} \sum_{k=-b_n+1}^{b_n-1} \left[\frac{1}{n} \left\| \sum_{t=n-|k|+1}^{n} (X_{st}-\mu) - n(\bar{X}_s - \mu) \right\|_\infty + \frac{1}{n} \left\| \sum_{t=1}^{|k|} (X_{st}-\mu) - n(\bar{X}_s - \mu) \right\|_\infty \right] \\
&\leq \frac{\|(\bar{\bar{X}} - \mu)\|_\infty}{m} \sum_{s=1}^{m} \sum_{k=-b_n+1}^{b_n-1} \left[\frac{1}{n} \left\| \sum_{t=n-|k|+1}^{n} (X_{st}-\mu) \right\|_\infty + \frac{1}{n} \left\| \sum_{t=1}^{|k|} (X_{st}-\mu) \right\|_\infty + 2\|\bar{X}_s - \mu\|_\infty \right] \\
&\leq \frac{\|(\bar{\bar{X}} - \mu)\|_\infty}{m} \sum_{s=1}^{m} \sum_{k=-b_n+1}^{b_n-1} \frac{1}{n} \left[\left\| \sum_{t=n-|k|+1}^{n} (X_{st}-\mu) \right\|_\infty + \left\| \sum_{t=1}^{|k|} (X_{st}-\mu) \right\|_\infty \right] \\
&\quad + 2(2b_n - 1)\|\bar{\bar{X}} - \mu\|_\infty \|\bar{X}_1 - \mu\|_\infty\,.
\end{aligned}
$$

Using SIP on summation of k terms, we obtain the following upper bound for $|M_1|$

$$
\begin{aligned}
|M_1| &< 2\|(\bar{\bar{X}} - \mu)\|_\infty \sum_{k=-b_n+1}^{b_n-1} \left[\frac{D\psi(k)}{n} + \frac{\|L\| p^{1/2}(1+\epsilon)\sqrt{2k \log\log k}}{n} \right] \\
&\quad + 2(2b_n - 1)\|\bar{\bar{X}} - \mu\|_\infty \|\bar{X}_1 - \mu\|_\infty \\
&\leq 2(2b_n - 1)\|(\bar{\bar{X}} - \mu)\|_\infty \left[\frac{D\psi(n)}{n} + \frac{\|L\| p^{1/2}(1+\epsilon)\sqrt{n \log\log n}}{n} \right] \\
&\quad + 2(2b_n - 1)\|\bar{\bar{X}} - \mu\|_\infty \|\bar{X}_1 - \mu\|_\infty \\
&\leq 4(2b_n - 1) \left[\frac{D\psi(n)}{n} + \frac{\|L\| p^{1/2}(1+\epsilon)\sqrt{n \log\log n}}{n} \right]^2 \quad \text{(by (9) and (10))}. \qquad (11)
\end{aligned}
$$

For M_2,

$$
\begin{aligned}
|M_2| &= \left| \frac{1}{m} \sum_{s=1}^{m} \left\{ \left(\mu - \bar{\bar{X}}\right)_i \left(\mu - \bar{\bar{X}}\right)_j \sum_{k=-b_n+1}^{b_n-1} \left(1 - \frac{|k|}{n}\right) w\left(\frac{k}{b_n}\right) \right\} \right| \\
&\leq \|\bar{\bar{X}} - \mu\|_\infty^2 \left[\sum_{k=-b_n+1}^{b_n-1} \left(1 - \frac{|k|}{n}\right) w\left(\frac{k}{b_n}\right) \right] \\
&< \|\bar{\bar{X}} - \mu\|_\infty^2 \left[\sum_{k=-b_n+1}^{b_n-1} \left| w\left(\frac{k}{b_n}\right) \right| \right] \\
&= b_n \|\bar{\bar{X}} - \mu\|_\infty^2 \left[\frac{1}{b_n} \sum_{k=-b_n+1}^{b_n-1} \left| w\left(\frac{k}{b_n}\right) \right| \right] \\
&\leq b_n \|\bar{\bar{X}} - \mu\|_\infty^2 \int_{-\infty}^{\infty} |w(x)| dx \\
&\leq C b_n \left[\frac{D\psi(n)}{n} + \frac{\|L\| p^{1/2}(1+\epsilon)\sqrt{n \log\log n}}{n} \right]^2 \quad \text{(by (10))}. \qquad (12)
\end{aligned}
$$

Using (11) and (12),

$$
\begin{aligned}
&|M_1 + M_2| \\
&\leq |M_1| + |M_2| \\
&\leq 4(2b_n - 1) \left[\frac{D\psi(n)}{n} + \frac{\|L\| p^{1/2}(1+\epsilon)\sqrt{n \log\log n}}{n} \right]^2 + C b_n \left[\frac{D\psi(n)}{n} + \frac{\|L\| p^{1/2}(1+\epsilon)\sqrt{n \log\log n}}{n} \right]^2 \\
&= D^2 g_1(n) + D g_2(n) + g_3(n)
\end{aligned}
$$

where

$$
\begin{aligned}
g_1(n) &= (8+C)\frac{b_n\psi^2(n)}{n^2} - 4\frac{\psi^2(n)}{n^2} \\
g_2(n) &= 2\sqrt{2}\|L\|p^{1/2}(1+\epsilon)\left[(8+C)\frac{b_n\psi(n)\sqrt{n\log\log n}}{n^2} - 4\frac{\psi(n)\sqrt{n\log\log n}}{n^2}\right] \\
g_3(n) &= \|L\|^2 p(1+\epsilon)^2\left[(8+C)\frac{b_n\log\log n}{n} - 4\frac{\log\log n}{n}\right].
\end{aligned}
$$

Under our assumptions, $b_n \log\log n/n \to 0$ and $\psi(n) = o(\sqrt{n\log\log n})$. Consequently, $b_n\psi^2(n)/n^2 \to 0$, $\psi^2(n)/n^2 \to 0$, $b_n\psi(n)\sqrt{n\log\log n}/n^2 \to 0$, and $\psi(n)\sqrt{n\log\log n}/n^2 \to 0$. Thus, $g_1(n), g_2(n)$ and $g_3(n) \to 0$ as $n \to \infty$.

□

Proof of theorem 2. We have the following decomposition,

$$
\begin{aligned}
&\tilde{\Sigma}^{ij} \\
&= \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}(X_{st}-\mu)_i\left(X_{s(t+k)}-\mu\right)_j \\
&= \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}(X_{st}\pm\bar{X}_s-\mu)_i\left(X_{s(t+k)}\pm\bar{X}_s-\mu\right)_j \\
&= \hat{\Sigma}^{ij}_{SV} + \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left(X_{st}-\bar{X}_s\right)_i\left(\bar{X}_s-\mu\right)_j + \left(\bar{X}_s-\mu\right)_i\left(X_{s(t+k)}-\bar{X}_s\right)_j\right] \\
&\quad + \left[\frac{1}{m}\sum_{s=1}^{m}\left(\bar{X}_s-\mu\right)_i\left(\bar{X}_s-\mu\right)_j\right]\left[\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\left(1-\frac{|k|}{b_n}\right)\right] \\
&= \hat{\Sigma}^{ij}_{SV} + N_1 + N_2\,,
\end{aligned}
$$

where

$$
\begin{aligned}
N_1 &= \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left(X_{st}-\bar{X}_s\right)_i\left(\bar{X}_s-\mu\right)_j + \left(\bar{X}_s-\mu\right)_i\left(X_{s(t+k)}-\bar{X}_s\right)_j\right] \\
N_2 &= \left[\frac{1}{m}\sum_{s=1}^{m}\left(\bar{X}_s-\mu\right)_i\left(\bar{X}_s-\mu\right)_j\right]\left[\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\left(1-\frac{|k|}{b_n}\right)\right].
\end{aligned}
$$

Using the above and Lemma 2,

$$
\left|\hat{\Sigma}^{ij}_{RSV} - \Sigma^{ij}\right| = \left|\hat{\Sigma}^{ij}_{SV} - \Sigma^{ij} + N_1 + N_2 + M_1 + M_2\right|
$$

$$\leq \left|\hat{\Sigma}^{ij}_{SV} - \Sigma^{ij}\right| + |N_1| + |N_2| + |M_1 + M_2| \tag{13}$$

By Assumption 2, the first term goes to with probability 1 and by Lemma 2, the third term goes to 0 with probability 1 as $n \to \infty$. What is left to show is that $|N_1| \to 0$ and $|N_2| \to 0$ with probability 1

$$\begin{aligned}
|N_1| &= \left| \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left(X_{st}-\bar{X}_s\right)_i\left(\bar{X}_s-\mu\right)_j + \left(\bar{X}_s-\mu\right)_i\left(X_{s(t+k)}-\bar{X}_s\right)_j\right]\right| \\
&\leq \left| \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left(X_{st}-\bar{X}_s\right)_i\left(\bar{X}_s-\mu\right)_j\right]\right| \\
&\quad + \left| \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left(\bar{X}_s-\mu\right)_i\left(X_{s(t+k)}-\bar{X}_s\right)_j\right]\right|
\end{aligned}$$

Both terms are similar and we will show that the first term goes to 0. The proof for the second term is similar. Consider

$$\begin{aligned}
&\left| \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left(X_{st}-\bar{X}_s\right)_i\left(\bar{X}_s-\mu\right)_j\right]\right| \\
&\leq \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1}\left|w\left(\frac{k}{b_n}\right)\right|\frac{\left|\left(\bar{X}_s-\mu\right)_j\right|}{n}\left[\left|\sum_{t=1}^{|k|}\left(\bar{X}_s-X_{st}\right)_i\right|\right] \\
&\leq \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1}\left|w\left(\frac{k}{b_n}\right)\right|\frac{\left|\left(\bar{X}_s-\mu\right)_j\right|}{n}\left[\left|\sum_{t=1}^{|k|}\left(\mu-X_{st}\right)_i\right| + |k|\left|\left(\bar{X}_s-\mu\right)_i\right|\right] \\
&\leq \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1}\left|w\left(\frac{k}{b_n}\right)\right|\frac{\|\bar{X}_s-\mu\|_\infty}{n}\left\|\sum_{t=1}^{|k|}\left(\mu-X_{st}\right) + |k|\left(\bar{X}_s-\mu\right)\right\|_\infty \\
&\leq \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1}\left|w\left(\frac{k}{b_n}\right)\right|\frac{\|\bar{X}_s-\mu\|_\infty}{n}\left(\left\|\sum_{t=1}^{|k|}\left(X_{st}-\mu\right)\right\|_\infty + |k|\,\|\bar{X}_s-\mu\|_\infty\right) \\
&\leq \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1}\frac{\|\bar{X}_s-\mu\|_\infty}{n}\left\|\sum_{t=1}^{|k|}\left(X_{st}-\mu\right)\right\| + \frac{1}{m}\sum_{s=1}^{m}\frac{b_n(b_n-1)}{n}\left\|\bar{X}_s-\mu\right\|_\infty^2 .
\end{aligned}$$

Using SIP on the summation of k terms,

$$\left| \frac{1}{m}\sum_{s=1}^{m}\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\frac{1}{n}\sum_{t=1}^{n-|k|}\left[\left(X_{st}-\bar{X}_s\right)_i\left(\bar{X}_s-\mu\right)_j\right]\right|$$

$$
\begin{aligned}
&< \frac{1}{m}\sum_{s=1}^{m}\|\bar{X}_s-\mu\|_\infty \sum_{k=-b_n+1}^{b_n-1}\left[\frac{D\psi(k)}{n}+\frac{\|L\|p^{1/2}(1+\epsilon)\sqrt{2k\log\log k}}{n}\right]+\frac{1}{m}\sum_{s=1}^{m}\frac{b_n(b_n-1)}{n}\|\bar{X}_s-\mu\|_\infty^2 \\
&< \frac{(2b_n-1)}{m}\sum_{s=1}^{m}\|\bar{X}_s-\mu\|_\infty\left[\frac{D\psi(n)}{n}+\frac{\|L\|p^{1/2}(1+\epsilon)\sqrt{2n\log\log n}}{n}\right]+\frac{1}{m}\sum_{s=1}^{m}\frac{b_n(b_n-1)}{n}\|\bar{X}_s-\mu\|_\infty^2 \\
&\leq \left(2b_n-1+\frac{b_n^2}{n}-\frac{b_n}{n}\right)\left[\frac{D\psi(n)}{n}+\frac{\|L\|p^{1/2}(1+\epsilon)\sqrt{2n\log\log n}}{n}\right]^2 \quad \text{(by (9))} \\
&\to 0\,.
\end{aligned}
$$

Similar to the above proof, second part of N_1 can also be written as a summation of k terms and the proof follows exactly as the first part. Now we prove that $N_2 \xrightarrow{a.s.} 0$ as $n \to \infty$. Following the steps in (12), we get

$$
|N_2| \leq Cb_n\left[\frac{D\psi(n)}{n}+\frac{\|L\|p^{1/2}(1+\epsilon)\sqrt{2n\log\log n}}{n}\right]^2 \to 0\,.
$$

Thus, in (13), each of the terms goes to 0 with probability 1, and $\hat{\Sigma}^{ij}_{RSV} \to \Sigma^{ij}$ with probability 1 as $n \to \infty$. □

B.3 RSV Bias

Proof of theorem 3. The convoluted end effect terms in theorem 1 are all essentially $\mathcal{O}(1/n)$. We are interested in finding the asymptotic bias here. Therefore we can write the expectation of replicated autocovariance in form of equation 8 as,

$$
\begin{aligned}
&\mathbb{E}\left[\hat{\Gamma}_{RAC}(k)\right] \\
&= \left(1-\frac{|k|}{n}\right)\Gamma(k)-\frac{|k|}{n}\left[\left(1-\frac{1}{m}\right)\left(\frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h)^T+\frac{1}{n}\sum_{h=0}^{n-1}\Gamma(h)\right)-\left(2-\frac{1}{m}\right)\mathrm{Var}(\bar{X}_1)\right]-\frac{\mathrm{Var}(\overline{X}_1)}{m} \\
&= \left(1-\frac{|k|}{n}\right)\Gamma(k)+O_1+O_2\,. \qquad (14)
\end{aligned}
$$

where both O_1 and O_2 are the small order terms. By our assumptions, $\sum_{h=-\infty}^{\infty}\Gamma(h) < \infty$, so $O_1 = o(1/n)$ and $O_2 = o(1/n)$. Consider the RSV estimator,

$$
\begin{aligned}
&\mathbb{E}\left[\hat{\Sigma}_{RSV}-\Sigma\right] \\
&= \sum_{k=-n+1}^{n-1} w\left(\frac{k}{b_n}\right)\mathbb{E}\left[\hat{\Gamma}_{RAC}(k)\right]-\sum_{k=-\infty}^{\infty}\Gamma(k)
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{k=-n+1}^{n-1} w\left(\frac{k}{b_n}\right)\left[\left(1-\frac{|k|}{n}\right)\Gamma(k)+O_1+O_2\right]-\sum_{k=-\infty}^{\inf}\Gamma(k) \\
&= \sum_{k=-n+1}^{n-1}\left[w\left(\frac{k}{b_n}\right)\left(1-\frac{|k|}{n}\right)\Gamma(k)\right]-\sum_{k=-\infty}^{\infty}\Gamma(k)+\sum_{k=-n+1}^{n-1}\left[w\left(\frac{k}{b_n}\right)(O_1+O_2)\right] \\
&= P_1+o\left(\frac{1}{n}\right)
\end{aligned}
$$

where

$$
P_1=\sum_{k=-n+1}^{n-1}\left[w\left(\frac{k}{b_n}\right)\left(1-\frac{|k|}{n}\right)\Gamma(k)\right]-\sum_{k=-\infty}^{\infty}\Gamma(k)\,.
$$

We first solve for term P_1 by breaking it into three parts as in Hannan (2009). Note that notation $A=o(z)$ for matrix A implies $A^{ij}=o(z)$ for each element of the matrix A. Consider,

$$
P_1=-\sum_{|k|\geq n}\Gamma(k)-\sum_{k=-n+1}^{n-1} w\left(\frac{|k|}{n}\right)\frac{|k|}{n}\Gamma(k)-\sum_{k=-n+1}^{n-1}\left(1-w\left(\frac{|k|}{n}\right)\right)\Gamma(k)\,. \tag{15}
$$

We deal with the three subterms of term P_1 individually. First,

$$
-\sum_{|k|\geq n}\Gamma(k)\leq\sum_{|k|\geq n}\left|\frac{k}{n}\right|^q\Gamma(k)=\frac{1}{b_n^q}\left|\frac{b_n}{n}\right|^q\sum_{|k|\geq n}|k|^q\Gamma(k)=o\left(\frac{1}{b_n^q}\right)\,, \tag{16}
$$

since $\sum_{|k|\geq n}|k|^q\Gamma(k)<\infty$. Next,

$$
\sum_{k=-n+1}^{n-1} w\left(\frac{k}{n}\right)\frac{|k|}{n}\Gamma(k)\leq\frac{C}{n}\sum_{k=-n+1}^{n-1}|k|\Gamma(k)\,.
$$

For $q\geq 1$,

$$
\frac{C}{n}\sum_{k=-n+1}^{n-1}|k|\Gamma(k)\leq\frac{C}{n}\sum_{k=-n+1}^{n-1}|k|^q\Gamma(k)=\frac{1}{b_n^q}\frac{b_n^q}{n}C\sum_{k=-n+1}^{n-1}|k|^q\Gamma(k)=o\left(\frac{1}{b_n^q}\right)\,.
$$

For $q<1$,

$$
\frac{C}{n}\sum_{k=-n+1}^{n-1}|k|\Gamma(k)\leq C\sum_{k=-n+1}^{n-1}\left|\frac{k}{n}\right|^q\Gamma(k)=\frac{1}{b_n^q}\frac{b_n^q}{n^q}C\sum_{k=-n+1}^{n-1}|k|^q\Gamma(k)=o\left(\frac{1}{b_n^q}\right)\,.
$$

So,

$$\sum_{k=-n+1}^{n-1} w\left(\frac{|k|}{n}\right)\frac{|k|}{n}\Gamma(k) = o\left(\frac{1}{b_n^q}\right) \tag{17}$$

Lastly, by our assumptions, for $x \to 0$

$$\frac{1-w(x)}{|x|^q} = k_q + o(1)\,.$$

For $x = k/b_n$, $\left|k/b_n\right|^{-q}(1-w(k/b_n))$ converges boundedly to k_q for each k. So,

$$\begin{aligned}
\sum_{k=-n+1}^{n-1}\left(1-w\left(\frac{k}{b_n}\right)\right)\Gamma(k) &= -\frac{1}{b_n^q}\sum_{k=-n+1}^{n-1}\left(\frac{|k|}{b_n}\right)^{-q}\left(1-w\left(\frac{|k|}{b_n}\right)\right)|k|^q\Gamma(k) \\
&= -\frac{1}{b_n^q}\sum_{k=-n+1}^{n-1}\left[k_q + o(1)\right]|k|^q\Gamma(k) \\
&= -\frac{k_q\Phi^{(q)}}{b_n^q} + o\left(\frac{1}{b_n^q}\right)\,.
\end{aligned} \tag{18}$$

Using (16), (17), and (18) in (15), we get

$$\mathbb{E}\left[\hat{\Sigma}_{RSV} - \Sigma\right] = -\frac{k_q\Phi^{(q)}}{b_n^q} + o\left(\frac{1}{b_n^q}\right)\,,$$

which completes the result. □

B.4 Variance Calculation

Proof of Theorem 4. Due to the strong consistency proof from theorem 2, as $n \to \infty$,

$$\left|\hat{\Sigma}_{RSV} - \tilde{\Sigma}\right| \to 0 \text{ with probability } 1\,. \tag{19}$$

Further, we have defined $g_1(n), g_2(n), g_3(n)$ such that as $n \to \infty$,

$$\begin{aligned}
g_1(n) &= (4+C_1)\frac{b_n\psi^2(n)}{n^2} - 4\frac{\psi^2(n)}{n^2} \to 0 \\
g_2(n) &= 2\sqrt{2}\|L\|p^{1/2}(1+\epsilon)\left[(4+C_1)\frac{b_n\psi(n)\sqrt{n\log\log n}}{n^2} - 4\frac{\psi(n)\sqrt{n\log\log n}}{n^2}\right] \to 0 \\
g_3(n) &= \|L\|^2 p(1+\epsilon)^2\left[(4+C_1)\frac{b_n\log\log n}{n} - 4\frac{\log\log n}{n}\right] \to 0
\end{aligned}$$

We have shown from the proof of strong consistency that,

$$
\begin{aligned}
&\left|\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right| \\
&\leq \frac{1}{m}\sum_{s=1}^{m}\left|\sum_{k=-b_n+1}^{b_n-1} w\left(\frac{k}{b_n}\right)\sum_{t=1}^{n-|k|}\left[\left(\frac{(X_{st}-\mu)_i(\mu-\bar{\bar{X}})_j}{n}\right) + \left(\frac{(\mu-\bar{\bar{X}})_i(X_{s(t+k)}-\mu)_j}{n}\right)\right]\right. \\
&\qquad \left. +(\mu-\bar{\bar{X}})(\mu-\bar{\bar{X}})^T\sum_{k=-b_n+1}^{b_n-1}\left(\frac{n-|k|}{n}\right) w\left(\frac{k}{n}\right)\right| \\
&< D^2 g_1(n) + Dg_2(n) + g_3(n)\,.
\end{aligned}
$$

By (19), there exists an N_0 such that

$$
\begin{aligned}
\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)^2 &= \left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)^2 I(0 \leq n \leq N_0) + \left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)^2 I(n > N_0) \\
&\leq \left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)^2 I(0 \leq n \leq N_0) + \left(D^2 g_1(n) + Dg_2(n) + g_3(n)\right)^2 I(n > N_0) \\
&:= g^*_n(X_{11}, \dots, X_{1n}, \dots, X_{m1}, \dots, X_{mn})\,.
\end{aligned}
$$

But since by assumption $\mathbb{E}D^4 < \infty$ and the fourth moment is finite,

$$
\mathbb{E}\left|g^*_n\right| \leq \mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}_{A}\right)^2\right] + \mathbb{E}\left[\left(D^2 g_1(n) + Dg_2(n) + g_3(n)\right)^2\right] < \infty\,.
$$

Thus, $\mathbb{E}\left|g^*_n\right| < \infty$ and further as $n \to \infty$, $g_n \to 0$ under the assumptions. Since $g_1, g_2, g_3 \to 0$, $\mathbb{E}g^*_n \to 0$. By the majorized convergence theorem (Zeidler, 2013), as $n \to \infty$,

$$
\mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)^2\right] \to 0\,. \tag{20}
$$

We will use (20) to show that the variances are equivalent. Define,

$$
\xi\left(\hat{\Sigma}^{ij}_{RSV}, \tilde{\Sigma}^{ij}\right) = \operatorname{Var}\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right) + 2\mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)\left(\tilde{\Sigma}^{ij} - \mathbb{E}\left(\tilde{\Sigma}^{ij}\right)\right)\right]
$$

We will show that the above is $o(1)$. Using Cauchy-Schwarz inequality followed by (20),

$$
\begin{aligned}
\left|\xi\left(\hat{\Sigma}^{ij}_{RSV}, \tilde{\Sigma}^{ij}\right)\right| &\leq \left|\operatorname{Var}\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)\right| + \left|2\mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)\left(\tilde{\Sigma}^{ij} - \mathbb{E}\left(\tilde{\Sigma}^{ij}\right)\right)\right]\right| \\
&\leq \mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)^2\right] + 2\left|\left(\mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)^2\right]\operatorname{Var}\left(\tilde{\Sigma}^{ij}\right)\right)^{1/2}\right|
\end{aligned}
$$

$$
\begin{aligned}
&= o(1) + 2\left(o(1)\left(O\left(\frac{b_n}{n}\right) + o\left(\frac{b_n}{n}\right)\right)\right) \\
&= o(1)\,.
\end{aligned}
$$

Finally,

$$
\begin{aligned}
&\mathrm{Var}\left(\hat{\Sigma}^{ij}_{RSV}\right) \\
&= \mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \mathbb{E}\left[\hat{\Sigma}^{ij}_{R}\right]\right)^2\right] \\
&= \mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} \pm \tilde{\Sigma}^{ij} \pm \mathbb{E}\left[\tilde{\Sigma}^{ij}\right] - \mathbb{E}\left[\hat{\Sigma}^{ij}_{RSV}\right]\right)^2\right] \\
&= \mathbb{E}\left[\left(\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right) + \left(\tilde{\Sigma}^{ij} - \mathbb{E}\left[\tilde{\Sigma}^{ij}\right]\right) + \left(\mathbb{E}\left[\tilde{\Sigma}^{ij}\right] - \mathbb{E}\left[\hat{\Sigma}^{ij}_{RSV}\right]\right)\right)^2\right] \\
&= \mathbb{E}\left[\left(\tilde{\Sigma}^{ij} - \mathbb{E}\left[\tilde{\Sigma}^{ij}\right]\right)^2\right] + \mathbb{E}\left[\left(\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right) + \left(\mathbb{E}\left[\tilde{\Sigma}^{ij}\right] - \mathbb{E}\left[\hat{\Sigma}^{ij}_{RSV}\right]\right)\right)^2\right] \\
&\quad + 2\mathbb{E}\left[\left(\tilde{\Sigma}^{ij} - \mathbb{E}\left[\tilde{\Sigma}^{ij}\right]\right)\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)\right] + 2\mathbb{E}\left[\left(\tilde{\Sigma}^{ij} - \mathbb{E}\left[\tilde{\Sigma}^{ij}\right]\right)\left(\mathbb{E}\left[\tilde{\Sigma}^{ij}\right] - \mathbb{E}\left[\hat{\Sigma}^{ij}_{RSV}\right]\right)\right] \\
&= \mathrm{Var}\left(\tilde{\Sigma}^{ij}\right) + \mathrm{Var}\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right) + 2\mathbb{E}\left[\left(\hat{\Sigma}^{ij}_{RSV} - \tilde{\Sigma}^{ij}\right)\left(\tilde{\Sigma}^{ij} - \mathbb{E}\left(\tilde{\Sigma}^{ij}\right)\right)\right] + o(1) \\
&= \mathrm{Var}\left(\tilde{\Sigma}^{ij}\right) + o(1)
\end{aligned}
$$

Hannan (2009) has given the calculations for variance of $\tilde{\Sigma}$ as

$$
\frac{n}{b_n}\mathrm{Var}(\tilde{\Sigma}^{ij}) = [\Sigma^{ii}\Sigma^{jj} + \left(\Sigma^{ij}\right)2]\int_{-\infty}^{\infty} w^2(x)dx + o(1) \tag{21}
$$

Plugging (21) into variance of $\hat{\Sigma}_{RSV}$ gives the result of the theorem.

□

C Additional Examples

We have established that estimating autocovariance is crucial to estimate the Markov chain standard error. In this section we will use two real-life datsets to exemplify the better performance of our replicated autocovariance estimator for multiple Markov chains. R packages already exist to create Markov chains for these examples. However, when these chains are started from different points, we will observe that they do not represent the target distribution well for finite samples. The traditional empirical ACF estimator fails in these cases, whereas our estimator shows promising results. We will not engage into full error analysis for these examples due to computational restrictions posed by high dimensional sample space.

C.1 Bayesian Poisson Change Point Model

Pollins (1996) theorizes a cyclical pattern in the number of international conflicts. Four core theories by Gilpin (1981), Wallerstein (1983), Goldstein (1988), and Modelski and Thompson (1988) put different weights on the role of global economic and political order in explaining this cyclical pattern. See Martin et al. (2011) for detailed discussion on the effect of these theories on the cyclic behavior of international disputes.

In this example, we will fit a Poisson change-point model on the annual number of military conflicts from the militarized interstate dispute (MID) data. We wish to detect the number and timings of the cyclic phases in the international conflicts. Chib (1998) describes the Poisson change-point as a Markov mixture model where observations are assumed to be drawn from latent states. Following Martin et al. (2011), we will use `MCMCpoissonChange` from `MCMCpack` to fit the model which samples the latent states based on the algorithm in Chib (1998). The Poisson change-point model in `MCMCpoissonChange` uses conjugate priors and can be written as:

$$\begin{aligned} y_t &\sim Poisson(\lambda_i), \qquad i = 1, ..., k \\ \lambda_i &\sim Gamma(c_o, d_o), \qquad i = 1, ..., k \\ p_{ii} &\sim Beta(\alpha, \beta), \qquad i = 1, ..., k \end{aligned}$$

The results of model comparison by Martin et al. (2011) showed that the ratio of maximum likelihood for six change-point model is favored over the alternatives. We will use this information and present the ACF results for a six change-points model only. We will use the hyperparameters values $c_o = 13$ and $d_o = 1$ because the mean of MID is around 13.

We run two parallel Markov chains starting from random poits. In Figure 7, it is evident that the chains have not explored the sample space well. Hence for 10^3 samples ACF severely underestimates the autocorrelations whereas R-ACF gives more realistic estimates. For a large sample size of 10^5, the Markov chains have mixed properly and therefore, both the estimators are approximately alike.

C.2 High School Social Network

Handcock et al. (2008) implemented an exponential-family random graph modelling (ERGM) on network data in the package `ergm`. The `faux.magnolia.high` dataset available in the package

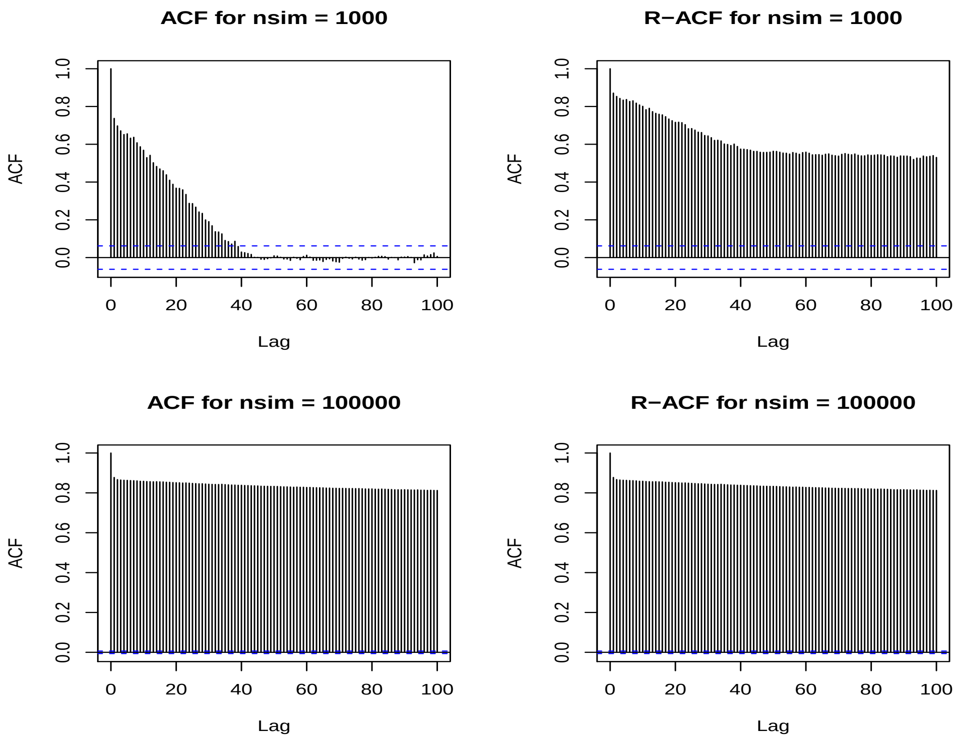


Figure 7: ACF and R-ACF for first component of first chain. ACF underestimates the autocorrelations for 10^3 samples (top) whereas R-ACF gives more realistic estimates. They perform alike for 10^5 samples (bottom).

represents a simulated within school friendship network based on Ad-Health data (Resnick et al. (1997)). The school communities represented by the network data are located in the southern United States. Each node represents a student and each edge represents a friendship between the nodes it connects. Nilakanta et al. (2019) modified the data by removing 1,022 out of 1,461 nodes to obtain a well-connected graph. This resulting social network has 439 nodes and 573 edges.

Let V denote the non-empty set of countable nodes, $E \subseteq V \times V$ denote the set of edges, and $G = (V, E)$ denote the network. We are interested in exploring all the nodes uniformly, i.e. sample from a uniform distribution over V. Let λ denote a uniform distribution over V let $h : V \to \mathbb{R}^p$ map each node to certain features of interest. If $X \sim \lambda$, we wish to calculate the expected value of $h(X)$ with respect to λ given by

$$\mathbb{E}[h(X)]_\lambda = \frac{1}{n} \sum_{x \in V} h(x).$$

Here n is the set cardinality of V. We use a Metropolis-Hastings algorithm with a simple random-walk (SRW) proposal suggested by Gjoka et al. (2011). The stationary distribution for this algorithm is a uniform distribution over V, i.e. $\lambda(i) = 1/n$ for all $i \in V$. The Metropolis-Hastings transition kernel for this method is

$$P(i,j) = \begin{cases} \dfrac{1}{d_i} min\left(1, \dfrac{d_i}{d_j}\right) & \text{if j is a neighbor of i} \\ 1 - \sum_{k \neq i} \dfrac{1}{d_i} min\left(1, \dfrac{d_i}{d_k}\right) & \text{if } j = i \\ 0 & \text{otherwise.} \end{cases}$$

Table (blah) shows the population parameters we are interested in estimating using MCMC methods. The race and sex parameters are estimated as proportion of whites and females in the sample respectively. We start two parallel Markov chains from two students belonging to different races and study its impacts on the average features of their immediate social group. It is hypothesized that students from certain communities tend to engage more with students of same or other marginally represented communities. We believe that this "selective networking" might cause formation of clusters in the network wherein students within a cluster engage more with each other than with the students outside it. Given that the graph is well-connected, the Markov chains will eventually explore all the nodes.

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