# Asymptotic variance estimation for Adaptive MCMC

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Work partly supported by NSF grant DMS 0906631.

Based in part on collaborative work with Matias Cattaneo, University of Michigan.

January 4, 2011

# Outline of the talk

- Variance estimation is an important aspect of Monte Carlo simulation.

$$\sigma^2(h) = \lim_{n\to\infty} \mathrm{Var}\left(n^{-1/2}\sum_{k=1}^{n} h(X_k)\right) = \mathrm{Var}_\pi\left(h(X_0)\right) + \sum_{j\geq 1} \mathrm{Cov}_\pi\left(h(X_0), h(X_j)\right),$$

  for Markov chains.

- We focus on the so-called lag-window estimator or kernel estimators:

$$\Gamma_n^2(h) = \sum_{k=-n}^{n} w(kb_n)\gamma_n(k),$$

- For various class of processes, including Markov chains, It is known that when $nb_n \to \infty$, under regularity conditions, $\Gamma_n^2(h) \to \sigma^2(h)$.

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- For AMCMC, the behavior of $\Gamma_n^2(h)$ is similar. But we have to be careful when the limiting distribution in the CLT is a mixture of Gaussians.
- The analysis of $\Gamma_n^2(h)$ is related to the asymptotics of quadratic forms of Markov chains

$$\sum_{1 \le \ell \le j \le n} w_n(\ell, j) h_n(X_\ell, X_j),$$

  which has many applications in nonparametric time-series.
- We will also introduce a "small bandwidth" version of $\Gamma_n^2(h)$ where $b_n = 1/n$. $\Gamma_n^2(h)$ is then inconsistent, but as we will see, valid and much improved confidence intervals can still constructed.

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# Asymptotic variance estimation for MCMC

- Let $\{X_n,\ n \geq 0\}$ be a Markov chain with invariant distribution $\pi$ and transition kernel $P$.
- If $P^n$ converges to $\pi$ fast enough and under appropriate moment condition on $h$, then

$$\sigma^2(h) = \mathrm{Var}_\pi\left(h(X_0)\right) + 2\sum_{j\geq 1} \mathrm{Cov}_\pi\left(h(X_0), h(X_j)\right) < \infty,$$

  and

$$n^{-1/2}\sum_{i=1}^{n}\left(h(X_i) - \pi(h)\right) \xrightarrow{w} N(0, \sigma^2(h)),$$

- We call $\sigma^2(h)$ the asymptotic variance of $h$.

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# Asymptotic variance estimation for MCMC

- There are many Markov chain CLT results.
- See example Meyn & Tweedie (2009), Maxwell & Woodroofe (AP 2000).
- G. Jones (EJP 2006) gathers together many sets of assumptions under which the Markov chain CLT holds.

# Asymptotic variance estimation for MCMC

- The CLT naturally leads to an asymptotically valid confidence interval for $\pi(h)$:

$$\hat{\pi}_n(h) \pm z \frac{\hat{\sigma}_n(h)}{\sqrt{n}},$$

  for appropriate Gaussian quantile $z$, provided we have a consistent estimate $\hat{\sigma}_n(h)$ of $\sigma(h)$.

# Asymptotic variance estimation for MCMC

- There are many such estimators: Batch Means, overlapping Batch Means, regenerative simulations ( G. Jones et al. (2009), A. Tan (2009)). A popular estimator is the lag-window/kernel estimator,

$$\Gamma_n^2 = \sum_{k=-n}^{n} w(kb_n)\gamma_n(k),$$

- $\gamma_n(k) = n^{-1} \sum_{j=1}^{n-k} (h(X_j) - \pi_n(h)) (h(X_{j+k}) - \pi_n(h))$, $\gamma_n(-k) = \gamma_n(k)$, and $b_n^{-1}$ is the truncation point. I'll refer to $b_n$ as "bandwidth".
- $w : \mathbb{R} \to [0, 1]$ has support $[-1, 1]$, $w(-x) = w(x)$, $w(1) = 0$, and $w(0) = 1$.
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$$\Gamma_n^2(h) = \gamma_n(0) + 2 \sum_{k=1}^{b_n^{-1}-1} w(kb_n)\gamma_n(k).$$

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# Asymptotic variance estimation for MCMC

- The kernel estimator is well known estimator with a rich literature. Parzen (1960), Priestley (1981), Brockwell & Davis (1991)).
- A large literature in Econometrics as well: Andrews (1991); Hansen (1992); de Jong & Davidson (2000) and their references.
- Operation research: H. Damerdji (1991,1994).
- Most of the work impose some fairly strong mixing conditions.
- Jones et al. (2006, 2009) studies the Markov chain case where $P$ is geometrically ergodic.

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# Asymptotic variance estimation for AMCMC

We consider the adaptive MCMC case.

- Let $\{P_\theta, \ \theta \in \Theta\}$ be a family of TK. $P_\theta$ is inv. wrt $\pi$ for any $\theta \in \Theta$.
- Define $\{(X_n, \theta_n), \ n \geq 0\}$ a stoch. process s.t.

$$\theta_n \in \mathcal{F}_n, \quad \mathbb{P}\left(X_n \in A | \mathcal{F}_{n-1}\right) = P_{\theta_{n-1}}(X_{n-1}, A).$$

- $\{X_n, \ n \geq 0\}$ is an adaptive Markov chain (no longer Markov).

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# Central limit theorem

- Throughout, we assume diminishing adaptation:

$$D(\theta_n, \theta_{n-1}) \leq \gamma_n, \quad \text{where } \gamma_n \to 0.$$

- What can we say about $\Gamma_n^2(h)$ when $\{X_n,\ n \geq 0\}$ is an adaptive MCMC process?
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- Assume $\pi(h) = 0$ and for simplicity assume that $\gamma_n(k) = n^{-1} \sum_{j=1}^{n-k} h(X_j)h(X_{j+k})$. Define

$$g_\theta(x) := \sum_{j \geq 0} P_\theta^j h(x), \quad G_\theta(x, y) = g_\theta(y) - P_\theta g_\theta(x).$$

- Define $G_k = G_{\theta_{k-}}(X_{k-1}, X_k)$. $\mathbb{E}\left(G_k | \mathcal{F}_{k-1}\right) = 0$. We know from Andrieu & Moulines (06) that:

$$\sum_{k=1}^{n} h(X_k) = \sum_{k=1}^{n} G_k + R_n,$$

where $R_n = o_P(n^{1/2})$.

- The same martingale difference sequence $\{G_k\}$ can be used to decompose $\Gamma_n^2(h)$.

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# Ingredients of the Proof

## Theorem

*Under appropriate moments and ergodicity conditions,*

$$\sum_{\ell=1}^{n} h(X_\ell) = \sum_{\ell=1}^{n} G_\ell + R_n$$

$$\Gamma_n^2(h) = n^{-1} \sum_{\ell=1}^{n} G_\ell^2 + \frac{2}{n} \sum_{\ell=1}^{n} \sum_{j=1}^{\ell-1} w\left((\ell - j) b_n\right) G_\ell G_j + \zeta_n.$$

*where for* $p > 1$*,*

$$\mathbb{E}\left(|\zeta_n|^p\right) \leq C \left(n^{-1} + b_n + b_n^{1-\frac{1}{2} \vee \frac{1}{p}}\right)^p, \quad \textit{and}$$

$$\mathbb{E}\left(\left|\frac{1}{n} \sum_{\ell=1}^{n} \sum_{j=1}^{\ell-1} w\left((\ell - j) b_n\right) G_\ell G_j\right|^p\right) \leq C \left(n b_n\right)^{-\frac{p}{2}} n^{-\frac{p}{2}+1 \vee \frac{p}{2}}.$$

# Asymptotic variance estimation

## Corollary

$$\lim_{n\to\infty}\left(\Gamma_n^2(h)-\frac{1}{n}\sum_{k=1}^{n}G^2_{\theta_{k-1}}\left(X_{k-1},X_k\right)\right)=0,\quad \textit{in probab.},\qquad (1)$$

*provided* $nb_n \to \infty$*.*

The main condition is:

$$\sup_{\theta\in\Theta}|g_\theta(x)|\le W(x),\quad \text{where}\quad \sup_{n\ge 0}\mathbb{E}\left(W^{2p}(X_n)\right)<\infty.$$

# Few remarks

- The results says nothing about the CLT for the partial sum $\sum_{k=1}^{n} h(X_k)$.
- When $\frac{1}{n}\sum_{k=1}^{n} G^2_{\theta_{k-1}}(X_{k-1}, X_k)$ converges to a deterministic limit $\sigma^2(h)$, say, then $\Gamma^2_n(h)$, also converges to $\sigma^2(h)$.
- Of course, under our moments conditions, this implies that $n^{-1/2}\sum_{k=1}^{n} h(X_k) \xrightarrow{w} \mathcal{N}(0, \sigma^2(h))$.
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- But if the average square variation $n^{-1}\sum_{k=1}^{n} G^2_{\theta_{k-1}}(X_{k-1}, X_k)$ converges n probability to a stochastic limit $\Gamma^2(h)$, then of course $\Gamma^2_n(h)$ also converges in probability to $\Gamma^2(h)$ and

$$n^{-1/2}\sum_{k=1}^{n} h(X_k) \xrightarrow{w} \sqrt{\Gamma^2(h)}Z,$$

  where $Z \sim N(0,1)$ independent of $\Gamma^2(h)$ (Hall & Heyde (80), Theorem 3.2).

- $\sqrt{\Gamma^2(h)}Z$ is a mixture of Gaussians.

- But

$$\lim_{n\to\infty} \mathrm{Var}\left(n^{-1/2}\sum_{k=1}^{n} h(X_k)\right) = \mathbb{E}\left(\Gamma^2(h)\right) = \sigma^2(h).$$

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# Choice of the bandwidth

- One of the main limitations of this estimator is the difficulty in choosing the bandwidth $b_n$. Often $b_n = n^{-\rho}$, $\rho \in \{1/2, 2/3\}$ resulting in a slowly converging $\Gamma_n^2(h)$.
- Neave (Annals Math. Stat. 1970) criticized the assumption $nb_n \to \infty$ as "a mathematically convenient assumption to ensure consistency of the estimates, but which is unrealistic when such estimators are used in practice where the value $nb_n$ cannot be zero".
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# Small "bandwidth" asymptotics

- Neave (1970) suggested using $b_n = n^{-1}$ which is known to give an inconsistent estimator but still confidence intervals can be constructed.
- Kiefer & Vogelsang (2002,2005,2009) have recently further developed the idea in the Econometrics literature under some restrictive model assumptions.
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$$= \frac{1}{n}\sum_{\ell=1}^{n} G_\ell \sum_{j=0}^{n-1} w((\ell-1-j)b_n)G_{j+1} + \zeta_n.$$

- Define $W_{n,\ell} = \frac{G_\ell}{\sqrt{n}\sigma(h)}$, where $\sigma^2(h) = \mathbb{E}_\pi(G^2(X_0, X_1))$, the asymp. variance. And

$$B_n(t) = \sum_{\ell=1}^{\lfloor nt \rfloor} W_{n,\ell}, \quad 0 \le t \le 1$$

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$$= \frac{1}{n}\sum_{\ell=1}^{n} G_\ell \sum_{j=0}^{n-1} w((\ell - 1 - j)b_n)G_{j+1} + \zeta_n.$$

- Define $W_{n,\ell} = \frac{G_\ell}{\sqrt{n}\sigma(h)}$, where $\sigma^2(h) = \mathbb{E}_\pi(G^2(X_0, X_1))$, the asymp. variance. And

$$B_n(t) = \sum_{\ell=1}^{\lfloor nt \rfloor} W_{n,\ell}, \quad 0 \le t \le 1$$

# Small "bandwidth" asymptotics

Then

$$\sum_{\ell=1}^{n} \frac{h(X_\ell)}{\sqrt{n}\sigma(h)} = \sum_{\ell=1}^{n} W_{n,\ell} + \tilde{R}_n = B_n(1) + \tilde{R}_n,$$

and for $b_n = n^{-1}$,

$$\sum_{j=0}^{n-1} w((\ell - 1 - j)b_n) \frac{G_{j+1}}{\sigma(h)\sqrt{n}} = Z_n\left((\ell - 1)b_n\right).$$

where

$$Z_n(t) = \int_0^1 w(t-u) dB_n(u).$$

# Small "bandwidth" asymptotics

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$$\sum_{\ell=1}^{n} \frac{h(X_\ell)}{\sqrt{n}\sigma(h)} = B_n(1) + \tilde{R}_n$$

$$\Gamma_n^2(h) = \sigma^2(h)\sigma^2(h) \int_0^1 Z_n(t) dB_n(t) + \zeta_n.$$

- As $n \to \infty$, $\{B_n(t),\ 0 \leq t \leq 1\}$ converges weakly to $\{B(t),\ 0 \leq t \leq 1\}$ the standard Brownian motion.
- Then we use Kurtz & Protter (AP 1992) on the weak convergence of stochastic integrals to get.

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# Small "bandwidth" asymptotics

## Theorem

*Assume* $\{X_n,\ n \geq 0\}$ *is a Markov chain. Let* $\{B(t),\ 0 \leq t \leq 1\}$ *be the standard Brownian motion. If* $b_n = n^{-1}$, *then*

$$\Gamma_n^2(h) \xrightarrow{w} \sigma^2(h) \int_0^1 \int_0^1 w(t-s)dB(s)dB(t).$$

*Furthermore, assuming* $\Gamma_n^2(h) > 0$ *almost surely,*

$$\frac{n^{-1/2}\sum_{j=1}^n h(X_j)}{\sqrt{\Gamma_n^2(h)}} \xrightarrow{w} \frac{B(1)}{\sqrt{\int_0^1 \int_0^1 w(t-s)dB(s)dB(t)}}.$$

# Small "bandwidth" asymptotics

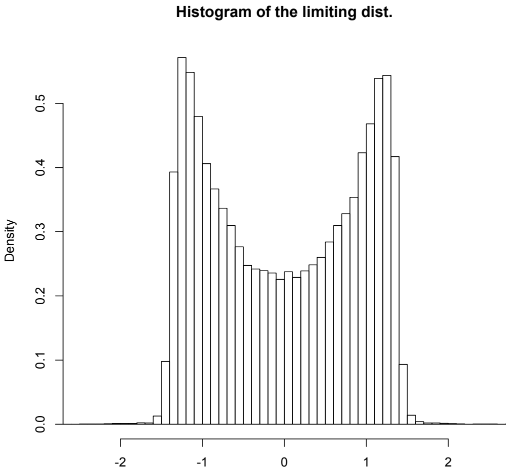
- We can then still construct a valid confidence interval for 0:

$$n^{-1}\sum_{\ell=1}^{n} h(X_\ell) \pm \bar{z}\frac{\sqrt{\Gamma_n^2(h)}}{\sqrt{n}}.$$

- $\bar{z}$ is the appropriate quantile of the distribution of $\frac{B(1)}{\sqrt{\int_0^1\int_0^1 w(t-s)dB(s)dB(t)}}$.
- We approximate this by Monte Carlo.

# Small "bandwidth" asymptotics

For the Parzen kernel, the distribution of $\frac{B(1)}{\sqrt{\int_0^1 \int_0^1 w(t-s)dB(s)dB(t)}}$.



# Small "bandwidth" asymptotics

- The 97.5% quantile is estimated at 1.360.
- When $\pi(h) \neq 0$ and we use $\gamma_{n,k} = n^{-1} \sum_{j=1}^{n-k} (h(X_j) - \hat{\pi}_n(h)) (h(X_{j+k}) - \hat{\pi}_n(h))$ instead of $\gamma_n(k) = n^{-1} \sum_{j=1}^{n-k} h(X_j)h(X_{j+k})$, a similar result holds.
- But the limiting distribution is different from $\frac{B(1)}{\sqrt{\int_0^1 \int_0^1 w(t-s)dB(s)dB(t)}}$.

# $AR(1)$ example

- For $\rho = 0.95$ and $\{\epsilon_n, \ n \geq 1\}$ is an iid $N(0,1)$

$$X_0 = 0, \quad \text{and} \quad X_n = \rho X_{n-1} + \epsilon_n$$

.

- For $|\rho| < 1$, the chain is geometrically ergodic with target distribution $N(0,(1-\rho^2)^{-1})$. We estimate $\mu = \int x\pi(x)dx = 0$.
- We build a confidence interval for $\mu$ comparing the regular bandwidth $b_n = n^{-1/2}$ with the small bandwidth $b_n = n^{-1}$.

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# An example

| | $b_n = n^{-1/2}$ | $\mathrm{b}_n = n^{-1}$ |
|---|---|---|
| $N = 1000$ | 0.83% | 0.96 |
| $N = 5000$ | 0.86% | 0.97 |
| $N = 10,000$ | 0.865% | 0.935 |
| $N = 20,000$ | 0.928% | 0.950 |

# An example

$$\ell(\beta|X) = \sum_{i=1}^{n} y_i x_i \beta - \log\left(1 + e^{x_i \beta}\right).$$

We assume a Gaussian prior distribution $\pi(\beta) \propto e^{-\|\beta\|^2/c}$. Posterior distribution:

$$\pi\left(\beta|X\right) \propto e^{\ell(\beta|X)} e^{-\|\beta\|^2/c}.$$

# An example

We build a Random Walk Metropolis to sample fom the posterior distribution:

## Algorithm

- *Given* $\beta_n$*: propose* $\beta' \sim N(\beta_n, \Sigma)$*.*
- *Set* $\beta_{n+1} = \beta'$ *with prob.* $\min\left(1, \frac{\tilde{\pi}(\beta'|X)}{\tilde{\pi}(\beta_n|X)}\right)$*. Otherwise, set* $\beta_{n+1} = \beta_n$*.*

We compare two choices of: $\Sigma = \sigma_\star \Sigma_\pi$ and $\Sigma = 0.0005 \times \mathcal{I}^{-1}$.

# An example

| | $b_n = n^{-1/2}$ | $b_n = n^{-1}$ |
|---|---|---|
| $\Sigma = \sigma_\star \Sigma_\pi$ | 0.940 | 0.942 |
| $\Sigma = 0.0005 \times I_d$ | 0.63 | 0.96 |

$N = 20,000$