Approximate Bayesian Computation (ABC)

Theory 0000 Numerical Experiments

Approximate MCMC for Approximate Bayesian Methods

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Approximate Bayesian Computation (ABC)

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Outline

Introduction & Motivation Introduction

Motivation

Approximate Bayesian Computation (ABC)

Vanilla version ABC-MCMC Recycler ABC-MCMC Bayesian Synthetic Likelihood (BSL)

Theory

Vanishing TV distance Vanishing MSE

Numerical Experiments

Ricker's Model Stochastic Volatility

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A Bayesian's Best Friend: MCMC

- Due to MCMC developments, for 30+ years Bayesian statisticians were *computationally liberated* when thinking about a statistical model.
- Large data and/or intractable likelihoods have brought Bayesian computation at a crossroads.

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A Bayesian's Best Friend: MCMC

- Consider observed data y₀ ∈ 𝒱 and likelihood function L(θ|y) (or sampling distribution f(y|θ)) where θ ∈ R^d.
- For a prior $p(\theta)$ the posterior is $\pi(\theta|\mathbf{y}_0) \propto f(\mathbf{y}_0|\theta)p(\theta)$.
- The Metropolis-Hastings sampler is one of the most used algorithms in MCMC. It operates as follows:
 - Given the current state of the chain θ , draw $\xi \sim q(\xi|\theta)$.
 - Accept ξ with probability min $\left\{1, \frac{\pi(\xi|\mathbf{y}_0)q(\theta|\xi)}{\pi(\theta|\mathbf{y}_0)q(\xi|\theta)}\right\}$.
 - If ξ is accepted, the next state is ξ , otherwise it is (still) θ .
- Note that π(θ|y₀) ∝ p(θ)L(θ|y₀) needs to be computed at each iteration. (hence L(θ|y₀) must also be computable)

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Massive data set

- $L(\theta|\mathcal{D})$ is computable, but data is massive.
- Possible remedies: divide and conquer, sequential processing, pseudomarginal, precomputing, etc
- ► D &C: Divide data into batches, y⁽¹⁾ ∪ ... y^(K), distribute the sampling from the K sub-posteriors

$$\pi_j(heta) \propto [L_k(heta|\mathbf{y}^{(j)})]^a [p_j(heta)]^b$$

among K processing units

- Depending on a, b values, design recombination strategies for the π_j-samples to recover the characteristics of the full posterior distribution.
- Entezari et al (2018) applied D&C to BART.

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Motivation for ABC

When the likelihood L(θ|y) is not computable but one can sample from p(y|θ) for all θ's....

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Motivation for ABC

- When the likelihood L(θ|y) is not computable but one can sample from p(y|θ) for all θ's....
- Approximate Bayesian Computation (ABC Marin et al., Comp & Stat. 2012) or Bayesian Synthetic Likelihood (BSL -Price et al, JCGS 2018) methods can be used.

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A remarkable algorithm- ABC

► ABC:

- Sample $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$ and $\mathbf{y} \sim p(\mathbf{y}|\boldsymbol{\theta})$;
- Compute distance:

$$\delta(\mathbf{y}) := \|\mathbf{S}(\mathbf{y}), \mathbf{S}(\mathbf{y}_0)\| = \sqrt{[\mathbf{S}(\mathbf{y}) - \mathbf{S}(\mathbf{y}_0)]^T A [\mathbf{S}(\mathbf{y}) - \mathbf{S}(\mathbf{y}_0)]}$$

• If
$$\delta(\mathbf{y}) < \epsilon$$
 retain $(\boldsymbol{\theta}, \mathbf{y})$ as a draw from

$$\pi_\epsilon(oldsymbol{ heta}, \mathbf{y} | \mathbf{y}_0) \propto p(oldsymbol{ heta}) f(\mathbf{y} | oldsymbol{ heta}) \mathbf{1}_{\{\delta(\mathbf{y}) < \epsilon\}}$$

• The marginal target (in θ) is

$$\pi_{\epsilon}(\boldsymbol{\theta}|\mathbf{y}_{0}) = \int_{\mathcal{Y}} \pi_{\epsilon}(\boldsymbol{\theta}, \mathbf{y}|\mathbf{y}_{0}) d\mathbf{y} \propto$$

$$\propto p(\boldsymbol{\theta}) \underbrace{\int_{\mathcal{Y}} f(\mathbf{y}|\boldsymbol{\theta}) \mathbf{1}_{\{\delta(\mathbf{y}) \leq \epsilon\}} d\mathbf{y}}_{\text{approximate likelihood}} = p(\boldsymbol{\theta}) \Pr(\delta(\mathbf{y}) \leq \epsilon | \boldsymbol{\theta}, \mathbf{y}_{0})$$

Vanilla ABC

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- Sampling candidate θ's from the prior is inefficient, especially if the prior is in conflict with the data (Evans and Moshonov, 2006).
- ► Marjoram et al (2003) propose an ABC-MCMC in which candidate moves are generated using a proposal q(θ|θ_t) and they are accepted or rejected based on a MH-type rule.

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Marjoram's ABC-MCMC

- Consider the joint target distribution in $(\boldsymbol{\theta}, \mathbf{y})$: $\pi_{\epsilon}(\boldsymbol{\theta}, \mathbf{y} | \mathbf{y}_0)$.
- A proposal (θ, y) ~ q(θ|θ_t) × f(y|θ) is accepted using the Metropolis-Hastings acceptance ratio

$$\begin{aligned} \alpha &= \min\left\{1, \frac{\pi_{\epsilon}(\theta, \mathbf{y}|\mathbf{y}_{0}) \times q(\theta_{t}|\theta)f(\mathbf{y}_{t}|\theta_{t})}{\pi_{\epsilon}(\theta_{t}, \mathbf{y}_{t}|\mathbf{y}_{0}) \times q(\theta|\theta_{t})f(\mathbf{y}|\theta)}\right\} \mathbf{1}_{\{\delta(\mathbf{y}) \leq \epsilon\}} \\ &= \min\left\{1, \frac{p(\theta)q(\theta_{t}|\theta)}{p(\theta_{t})q(\theta|\theta_{t})}\right\} \mathbf{1}_{\{\delta(\mathbf{y}) \leq \epsilon\}} \end{aligned}$$

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Zooming in on the target

- We consider building a chain with target $\pi_{\epsilon}(\boldsymbol{\theta}|\mathbf{y}_0)$.
- Set $h(\theta) = \Pr(\delta(\mathbf{y}) < \epsilon | \theta, \mathbf{y}_0)$ and proposal $\tilde{\theta} \sim q(\theta | \theta_t)$
- A Metropolis-Hastings sampler requires

 $\frac{p(\tilde{\theta})h(\tilde{\theta})q(\theta_t|\tilde{\theta})}{p(\theta_t)h(\theta_t)q(\tilde{\theta}|\theta_t)}$

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A marginal yet important target

Lee et al (2012) propose to use $\tilde{\mathbf{y}}_1, \dots, \tilde{\mathbf{y}}_J \sim f(\mathbf{y}|\tilde{\theta})$ to estimate

$$\widehat{h}(\widetilde{ heta}) = J^{-1} \sum_{j=1}^J \mathbf{1}_{\{\delta(\widetilde{ extbf{y}}_j) < \epsilon\}}$$

- ▶ Wilkinson (2013) generalizes to smoothing kernels
- Bornn et al (2014) make the case of using J = 1.
- Idea in this talk: Recycle past proposals to estimate $h(\tilde{\theta})$.

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History repeating itself

- At time *n* the proposal is $(\zeta_{n+1}, \mathbf{w}_{n+1}) \sim q(\zeta | \theta^{(n)}) f(\mathbf{w} | \zeta)$
- At iteration N, all the proposals ζ_n, the accepted and rejected ones, along with corresponding distances δ_n = δ(w_n) are available for 0 ≤ n ≤ N − 1.
- This is the history, denoted Z_{N-1} , of the chain.

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A selective memory helps

Given a new proposal ζ* ~ q(|θ^(t)), we generate w* ~ f(·|ζ*) and compute δ* = δ(S(w*)). Set ζ_N = ζ*, w_N = w*, Z_N = Z_{N-1} ∪ {(ζ_N, δ_N)} and estimate h(ζ*) using

$$\hat{h}(\zeta^*) = \frac{\sum_{n=1}^{N} W_{Nn}(\zeta^*) \mathbf{1}_{\delta_n < \epsilon}}{\sum_{n=1}^{N} W_{Nn}(\zeta^*)},$$
(1)

where $W_{Nn}(\zeta^*) = W(||\zeta_n - \zeta^*||)$ are weights and $W : \mathbf{R} \to [0, \infty)$ is a decreasing function.

• An alternative to (1) is to use a subset of size K of Z_N

Good news

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- If $\delta^* > \epsilon \Rightarrow$ rejection for ABC-MCMC
- But if $\exists \zeta^*$ with a corresponding $\delta < \epsilon$ then $h(\zeta^*) \neq 0$

Compare

$$ilde{h}(\zeta^*) = rac{1}{\mathcal{K}} \sum_{j=1}^{\mathcal{K}} \mathbf{1}_{\{ ilde{\delta}_j < \epsilon\}} \hspace{2mm} \Rightarrow \hspace{2mm} \mathsf{unbiased}$$

$$\hat{h}(\zeta^*) = \frac{\sum_{n=1}^{N} W_{Nn}(\zeta^*) \mathbf{1}_{\{\tilde{\delta}_n < \epsilon\}}}{\sum_{n=1}^{N} W_{Nn}(\zeta^*)} \Rightarrow \text{ consistent}$$

- ► When *K* is small reduce variability.
- ▶ When *K* is large reduce costs.

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Complications

- ► If the past samples are used to modify the kernel ⇒ Adaptive MCMC
- In order to avoid AMCMC conditions for validity, we separate the samples used as proposals from those used to estimate h
- At each time t:
 - Generate two independent samples

$$\{(\zeta_{t+1}, \mathsf{w}_{t+1}), (\tilde{\zeta}_{t+1}, \tilde{\mathsf{w}}_{t+1})\} \stackrel{\mathsf{iid}}{\sim} q(\zeta|\theta^{(t)})f(\mathsf{w}|\zeta)$$

- Set $\mathcal{Z}_{N+1} = \mathcal{Z}_N \cup \{(\tilde{\zeta}_{N+1}, \tilde{\delta}_{N+1})\}$
- We use the Independent Metropolis sampler, i.e. q(ζ|θ^(t)) = q(ζ) so that the chain's trajectory is independent of Z

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Friendly neighbors

- The k-Nearest-Neighbor (kNN) regression approach has a property of uniform consistency
- Set K = √N and relabel history so that (ζ̃₁, δ̃₁) and (ζ̃_N, δ̃_N) corresponds to the smallest and largest among all distances { ||ζ̃_j − ζ^{*}|| : 1 ≤ j ≤ N}
- Weights are defined as:
 - $W_n = 0$ for n > K
 - (U) The uniform kNN with $W_{Nn}(\zeta^*) = 1$ for all $n \leq K$;
 - (L) The *linear* kNN with
 - $W_{Nn}(\zeta^*) = W(\|\tilde{\zeta}_n \zeta^*\|) = 1 \|\tilde{\zeta}_n \zeta^*\| / \|\tilde{\zeta}_K \zeta^*\| \text{ for } n \le K \text{ so that the weight decreases from 1 to 0 as } n \text{ increases from 1 to } K.$

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Indirect inference - A David and Goliath story

- Indirect inference (Gallant and McCulloch, 2009)
- Complex model: $f(\mathbf{y}|\boldsymbol{\theta})$ with intractable f
- Simpler model g(y|φ(θ)) approximates well f(y|θ), with dim(φ) > dim(θ), g is tractable and φ : Θ → Φ is unknown
- ▶ We can estimate $\hat{\phi}(\theta)$ by sampling $\theta \sim p(\theta)$, $\mathbf{y}_j \sim f(\mathbf{y}|\theta), \ 1 \leq j \leq K$ and estimate ϕ from $\mathbf{y}_1, \ldots, \mathbf{y}_K$ using g - repeat
- Posterior $\pi_f(\theta|\mathbf{y}_0) \propto p(\theta) f(\mathbf{y}_0|\theta)$ is then approximated by

 $\pi_g(oldsymbol{ heta}|\mathbf{y}_0) \propto p(oldsymbol{ heta})g(\mathbf{y}_0|\hat{\phi}(oldsymbol{ heta}))$

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Bayesian Synthetic Likelihood (BSL)

- Alternative approach to bypass the intractability of the sampling distribution proposed by Wood (*Nature*, 2010).
- ► The simpler model (g): the conditional distribution for a user-defined statistic S(y) given θ is Gaussian with parameters φ(θ) = (μ_θ, Σ_θ)
- The Synthetic Likelihood (SL) procedure assigns to each θ the likelihood SL(θ) = N(s₀; μ_θ, Σ_θ).
- The BSL posterior is $\pi(\theta|s_0) \propto p(\theta)\mathcal{N}(s_0; \mu_{\theta}, \Sigma_{\theta})$.
- Acceptance ratios for a MH sampler are estimated from m statistics (s₁, · · · , s_m) sampled from their conditional distribution given θ.

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Bayesian Synthetic Likelihood (BSL)

- Generate $\mathbf{y}_i \sim f(\mathbf{y}|\theta)$ and set $s_i = S(\mathbf{y}_i), i = 1, \cdots, m$
- Estimate

$$\begin{aligned} \hat{\mu}_{\theta} &= \frac{\sum_{i=1}^{m} s_i}{m}, \\ \hat{\Sigma}_{\theta} &= \frac{\sum_{i=1}^{m} (s_i - \hat{\mu}_{\theta}) (s_i - \hat{\mu}_{\theta})^T}{m - 1}, \end{aligned}$$

The synthetic likelihood is

$$SL(\theta|\mathbf{y}_0) = \mathcal{N}(S(\mathbf{y}_0); \hat{\mu}_{\theta}, \hat{\Sigma}_{\theta}).$$
(2)

Acceptance probability requires repeated estimation of (2)

$$\min\left\{1, \frac{p(\theta)S(\theta|\mathbf{y}_0)q(\theta_t)}{p(\theta_t)S(\theta_t|\mathbf{y}_0)q(\theta)}\right\}$$

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A bit of theory

- (B1) Θ is a compact set.
- **(B2)** $q(\theta) > 0$ is a continuous density (proposal).
- **(B3)** $p(\theta) > 0$ is a continuous density (prior).
- **(B4)** $h(\theta)$ continuous function of θ .
- (B5) In kNN estimation assume that $K(N) = \sqrt{N}$ with uniform or linear weights.

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Some comfort

- Let P(·,·) denote the transition kernel of our AABC sampler, if h(θ) were computable exactly.
- The invariant distribution of $P(\cdot, \cdot)$ is denoted μ
- The approximate kernel at time t is denoted \hat{P}_t
- The distribution of θ_t is denoted $\mu_t := \nu \hat{P}_1 \dots \hat{P}_t$

Some comfort

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Vanishing TV Theorem

Suppose that (A1)- (A3) are satisfied . Let π denote the invariant measure of P and ν be any probability measure on (Θ, \mathcal{F}_0) , then

$$\left\|\mu - \frac{\sum_{t=0}^{M-1} \nu \hat{P}_1 \cdots \hat{P}_t}{M}\right\|_{TV} \leq O(M^{-1}) + O(M^{-1}\epsilon) + O(\epsilon),$$

More Comfort

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Vanishing MSE Theorem

Let π denote the invariant measure of *P*, $f(\theta)$ be a bounded function and $\theta^{(0)} \sim \nu$, where ν is a probability distribution. Then

$$E\left[\left(\mu f - \frac{1}{M}\sum_{t=0}^{M-1} f(\theta^{(t)})\right)^2\right] \le |f|^2 [O(M^{-1}) + O(\epsilon^2) + O(M^{-1}\epsilon)]$$

where $\mu f = E_{\mu}f$.

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Numerical Experiments: General Setup

Efficiency measures

Diff in mean (DIM) = $Mean_{r,s}(|Mean_t(\theta_{rs}^{(t)}) - Mean_t(\tilde{\theta}_{rs}^{(t)})|),$ Diff in covariance (DIC) = $Mean_{r,s}(|Cov_t(\theta_{rs}^{(t)}) - Cov_t(\tilde{\theta}_{rs}^{(t)})|),$ Total Variation (TV) = $Mean_{r,s}\left(0.5\int |D_{rs}(x) - \tilde{D}_{rs}(x)|dx\right),$ Bias² = $Mean_s\left(\left(Mean_{tr}(\theta_{rs}^{(t)}) - \theta_s^{true}\right)^2\right),$ VAR = $Mean_s(Var_r(Mean_t(\theta_{rs}^{(t)}))),$ MSE = Bias² + VAR.

where r is the replicate and s is the parameter component.

We account for CPU time using

$$ESS = Mean_{rs}((M - B) / ACT_{rs}),$$

$$ESS/CPU = Mean_{rs}((M - B) / ACT_{rs} / CPU_{r}),$$
(3)

where M - B is the number of chain iterations.

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Numerical Experiments: Ricker's Model

• A particular instance of hidden Markov model:

$$\begin{aligned} x_{-49} &= 1; \quad z_i \stackrel{iid}{\sim} \mathcal{N}(0, \exp(\theta_2)^2); \quad i = \{-48, \cdots, n\}, \\ x_i &= \exp(\exp(\theta_1))x_{i-1}\exp(-x_{i-1} + z_i); \quad i = \{-48, \cdots, n\}, \\ y_i &= Pois(\exp(\theta_3)x_i); \quad i = \{-48, \cdots, n\}, \end{aligned}$$

where $Pois(\lambda)$ is Poisson distribution

► Only y = (y₁, · · · , y_n) sequence is observed, because the first 50 values are ignored.

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Numerical Experiments: Ricker's Model

Define summary statistics $S(\mathbf{y})$ as the 14-dimensional vector whose components are:

(C1)
$$\#\{i: y_i = 0\},\$$

(C2) Average of \mathbf{y} , \bar{y} ,

(C3:C7) Sample auto-correlations at lags 1 through 5,

(C8:C11) Coefficients $\beta_0, \beta_1, \beta_2, \beta_3$ of cubic regression $(y_i - y_{i-1}) = \beta_0 + \beta_1 y_i + \beta_2 y_i^2 + \beta_3 y_i^3 + \epsilon_i, i = 2, ..., n,$ (C12-C14) Coefficients $\beta_0, \beta_1, \beta_2$ of quadratic regression

 $y_i^{0.3} = \beta_0 + \beta_1 y_{i-1}^{0.3} + \beta_2 y_{i-1}^{0.6} + \epsilon_i, \ i = 2, \dots, n.$

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Numerical Experiments: Ricker's Model - ABC/RWM

Figure: Ricker's model: ABC-RW Sampler. Each row corresponds to parameters θ_1 (top row), θ_2 (middle row) and θ_3 (bottom row) and shows in order from left to right: Trace-plot, Histogram and Auto-correlation function. Red lines represent true parameter values.



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Numerical Experiments: Ricker's Model - BSL

Figure: Ricker's model: ABSL-U Sampler.



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Numerical Experiments: Ricker's Model - ABC

Figure: Ricker's model: AABC-U Sampler.



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Numerical Experiments: Ricker's Model - ABC

	Diff with exact			Diff with true parameter			Efficiency	
Sampler	DIM	DIC	ΤV	$\sqrt{\text{Bias}^2}$	\sqrt{VAR}	\sqrt{MSE}	ESS	ESS/CPU
SMC	0.152	0.0177	0.378	0.086	0.201	0.219	472	0.521
ABC-RW	0.135	0.0201	0.389	0.059	0.180	0.189	87	0.199
ABC-IS	0.139	0.0215	0.485	0.063	0.195	0.205	47	0.099
AABC-U	0.147	0.0279	0.402	0.076	0.190	0.204	3563	4.390
AABC-L	0.141	0.0258	0.392	0.070	0.189	0.201	4206	5.193
BSL-RW	0.129	0.0080	0.382	0.038	0.206	0.209	131	0.030
BSL-IS	0.122	0.0082	0.455	0.022	0.197	0.198	33	0.007
ABSL-U	0.103	0.0054	0.377	0.023	0.170	0.171	284	0.180
ABSL-L	0.106	0.0051	0.382	0.012	0.173	0.173	207	0.135

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Example: Stochastic Volatility

Stochastic volatility model with stable errors:

$$\begin{aligned} x_1 &\sim \mathcal{N}(0, 1/(1-\theta_1^2)); \quad v_i \stackrel{iid}{\sim} \mathcal{N}(0, 1); \quad w_i \stackrel{iid}{\sim} Stab(\theta_4, -1); \quad i = \{1, \cdots \\ x_i &= \theta_1 x_{i-1} + v_i; \quad i = \{2, \cdots, n\}, \\ y_i &= \sqrt{\exp(\theta_2 + \exp(\theta_3) x_i)} w_i; \quad i = \{1, \cdots, n\}. \end{aligned}$$

Here $St(\alpha, \beta)$ is a stable distribution with parameters $\theta_4 \in [0, 2]$ and skew parameter.

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Example: Stochastic Volatility

For summary statistics we use a 7-dimensional vector whose components are:

- (C1) $\#\{i: y_i^2 > \text{quantile}(\mathbf{y}_0^2, 0.99)\},\$
- (C2) Average of y^2 ,
- (C3) Standard deviation of y^2 ,

(C4) Sum of the first 5 auto-correlations of y^2 ,

- (C5) Sum of the first 5 auto-correlations of $\{\mathbf{1}_{\{y_i^2 < \text{quantile}(\mathbf{y}^2, 0.1)\}}\}_{i=1}^n$,
- (C6) Sum of the first 5 auto-correlations of $\{\mathbf{1}_{\{y_i^2 < \text{quantile}(\mathbf{y}^2, 0.5)\}}\}_{i=1}^n$,
- (C7) Sum of the first 5 auto-correlations of $\{\mathbf{1}_{\{y_i^2 < \text{quantile}(\mathbf{y}^2, 0.9)\}}\}_{i=1}^n$.

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Example: Stochastic Volatility cont..

Figure: First row compares SMC, ABC-RW and AABC-U samplers. Second row compares SMC, BSL-IS and ABSL-U. From left to right: θ_1 , θ_2 , θ_3 and θ_4 .



 $\mathsf{ESS}/\mathsf{CPU}$ shows 400-800% improvements over competitive algorithms (SMC, ABC-RWM)

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Example: Stochastic Volatility cont..

	Diff with SMC			Diff with true parameter			Efficiency	
Sampler	DIM	DIC	ΤV	$\sqrt{\text{Bias}^2}$	\sqrt{VAR}	\sqrt{MSE}	ESS	ESS/CPU
SMC	0.000	0.0000	0.000	0.221	0.201	0.299	468	0.267
ABC-RW	0.078	0.0126	0.205	0.248	0.198	0.317	24	0.069
ABC-IS	0.082	0.0151	0.306	0.232	0.221	0.320	26	0.071
AABC-U	0.069	0.0124	0.170	0.250	0.183	0.310	1303	1.617
AABC-L	0.069	0.0132	0.161	0.246	0.181	0.305	1256	1.546
BSL-RW	0.044	0.0116	0.122	0.225	0.181	0.289	123	0.037
BSL-IS	0.045	0.0103	0.125	0.226	0.177	0.287	285	0.084
ABSL-U	0.063	0.0133	0.228	0.225	0.181	0.289	832	0.735
ABSL-L	0.061	0.0140	0.230	0.236	0.183	0.299	757	0.671

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Conclusions

- ► ABC and BSL are useful when the likelihood is not tractable.
- The computational burden can prohibit the full reach for these approximate methods.
- Currently exploring links between ABC and divide-and-conquer MCMC for large data.

All papers available at:

http://www.utstat.toronto.edu/craiu/Papers/index.html