Approximate Computation for Approximate Bayesian Models

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MCMC at the crossroads

- Large data and/or intractable likelihoods have brought Bayesian computation at a crossroads.
- Consider observed data $\mathbf{y}_0 \in \mathcal{Y}$, likelihood function $L(\boldsymbol{\theta}|\mathbf{y}_0)$ (or sampling distribution $f(\mathbf{y}|\boldsymbol{\theta})$), prior $p(\boldsymbol{\theta})$ with $\boldsymbol{\theta} \in \mathbf{R}^d$.
- Focus is on $\pi(\boldsymbol{\theta}|\mathbf{y}_0) \propto f(\mathbf{y}_0|\boldsymbol{\theta})p(\boldsymbol{\theta})$.
- The Metropolis-Hastings sampler is one of the most used algorithms in MCMC.
  - 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 $\pi(\boldsymbol{\theta}|\mathbf{y}_0) \propto p(\boldsymbol{\theta})L(\boldsymbol{\theta}|\mathbf{y}_0)$ needs to be computed at each iteration. (hence $L(\theta|\mathbf{y}_0)$ must also be computable)

Massive data set

- $L(\theta|\mathcal{D})$ is computable, but data is massive.
- Possible remedies:
  - precomputing (Boland et al., EJS, 2018)
  - sequential processing (Bardenet et el. 2014; Korratikara et al. 2014)
  - divide and conquer (Neiswanger et al. 2013; Wang and Dunson 2013; Scott et al. 2016; Entezari et al. 2018; Nemeth and Sherlock 2018; Changye and Robert 2019)
  - subsampling (Quiroz et al. 2018; Campbell and Broderick 2019)

Divide and conquer

- D &C: Divide data into batches, $\mathbf{y}^{(1)} \cup \ldots \mathbf{y}^{(K)}$, distribute the sampling from the K sub-posteriors

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

  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.
- Challenge: provide theoretical guarantees or assess approximation errors beyond the Gaussian case.

Subsampling for MCMC - Quiroz et al. 2018

- Pseudo-marginal idea (Andrieu and Roberts 2009): Replace $L(\theta|\mathbf{y}_0)$ by an unbiased estimator.
- Let $\mathbf{u} = \{u_1, \dots, u_m\}$ be iid random variables uniformly distributed over $\{1, \dots, N\}$ and $\mathbf{y_u} = \{y_{u_1}, \dots, y_{u_m}\}$.
- Then $l_m(\boldsymbol{\theta}|\mathbf{y_u}) = \frac{1}{m}\sum_{k=1}^{m} l_{u_k}(\boldsymbol{\theta}|y_{u_k})$, is unbiased for the average log-likelihood $\frac{1}{N}\sum_{k=1}^{N} l_k(\boldsymbol{\theta}|y_k)$
- Introduce control variates to reduce variance of l_m
- Adjust the estimator $\exp[l_m(\boldsymbol{\theta}|\mathbf{y_u})]$ to be unbiased for $L(\theta|\mathbf{y}_0)$

Motivation for ABC

- When the likelihood $L(\theta|\mathbf{y}_0)$ is not computable but one can sample from $f(\mathbf{y}|\theta)$ for all θ's....

Motivation for ABC

- When the likelihood $L(\theta|\mathbf{y}_0)$ is not computable but one can sample from $f(\mathbf{y}|\theta)$ for all θ's....
- Approximate Bayesian Computation (ABC)
- Bayesian Synthetic Likelihood (BSL)

Double jeopardy: Large data and Intractable Likelihood

- The generation of pseudo-data can be expensive, e.g. climate change scenarios (Oyebamiji et al. 2015) or hurricane surges (Plumlee et al. 2021)
- Most of methods that address the challenge of large data cannot be used directly for intractable models.
- Today: discuss an approach that can be used with ABC and BSL.

A remarkable algorithm- ABC

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

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

- The marginal target (in $\boldsymbol{\theta}$) is

$$\begin{aligned} \pi_\epsilon(\boldsymbol{\theta}|\mathbf{y}_0) &= \int_{\mathcal{Y}} \pi_\epsilon(\boldsymbol{\theta}, \mathbf{y}|\mathbf{y}_0) d\mathbf{y} \propto \\ &\propto p(\boldsymbol{\theta}) \underbrace{\int_{\mathcal{Y}} f(\mathbf{y}|\boldsymbol{\theta}) \mathbf{1}_{\{\delta(\mathbf{y}) \le \epsilon\}} d\mathbf{y}}_{\text{approximate likelihood}} = p(\boldsymbol{\theta}) \underbrace{\Pr(\delta(\mathbf{y}) \le \epsilon | \boldsymbol{\theta}, \mathbf{y}_0)}_{:= h(\boldsymbol{\theta})} \end{aligned}$$

Vanilla ABC

- 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 $q(\theta|\theta_t)$ and they are accepted or rejected based on a MH-type rule.

Zooming in on the target

- We consider building a chain with target $\pi_\epsilon(\boldsymbol{\theta}|\mathbf{y}_0)$.
- Consider proposal $\tilde{\boldsymbol{\theta}} \sim q(\boldsymbol{\theta}|\boldsymbol{\theta}_t)$
- A Metropolis-Hastings sampler requires calculating

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

A marginal yet important target

- Lee et al (2012) propose to use $\tilde{\mathbf{y}}_1, \ldots, \tilde{\mathbf{y}}_J \sim f(\mathbf{y}|\tilde{\boldsymbol{\theta}})$ to estimate
$$\widehat{h}(\tilde{\boldsymbol{\theta}}) = J^{-1} \sum_{j=1}^{J} \mathbf{1}_{\{\delta(\tilde{\mathbf{y}}_j) < \epsilon\}}$$
- 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 $h(\tilde{\boldsymbol{\theta}})$.

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 $\delta_n = \delta(\mathbf{w}_n)$ are available for $0 \leq n \leq N-1$.
- This is the history, denoted $\mathcal{Z}_{N-1}$, of the chain.

A selective memory helps

- Given a new proposal $\zeta^* \sim q(|\theta^{(t)})$, we generate $\mathbf{w}^* \sim f(\cdot|\zeta^*)$ and compute $\delta^* = \delta(S(\mathbf{w}^*))$. Set $\zeta_N = \zeta^*$, $\mathbf{w}_N = \mathbf{w}^*$, $\mathcal{Z}_N = \mathcal{Z}_{N-1} \cup \{(\zeta_N, \delta_N)\}$ and estimate $h(\zeta^*)$ using

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

  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 $\mathcal{Z}_N$

Good news

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

$$\tilde{h}(\zeta^*) = \frac{1}{K}\sum_{j=1}^{K} \mathbf{1}_{\{\tilde{\delta}_j < \epsilon\}} \quad \Rightarrow \quad \text{unbiased}$$

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

- When K is small - reduce variability.
- When K is large - reduce costs.

Complications

- If the past samples are used to modify the kernel $\Rightarrow$ 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:
  - We use the Independent Metropolis sampler, i.e. $q(\zeta|\theta^{(t)}) = q(\zeta)$
  - Generate two independent samples

$$\{(\zeta_{t+1}, \mathbf{w}_{t+1}), (\tilde{\zeta}_{t+1}, \tilde{\mathbf{w}}_{t+1})\} \overset{\text{iid}}{\sim} q(\zeta) f(\mathbf{w}|\zeta)$$

  - Set $\mathcal{Z}_{N+1} = \mathcal{Z}_N \cup \{(\tilde{\zeta}_{N+1}, \tilde{\delta}_{N+1})\}$

Friendly neighbors

- The k-Nearest-Neighbor (kNN) regression approach has a property of uniform consistency
- Set $K = \sqrt{N}$ and relabel history so that $(\tilde{\zeta}_1, \tilde{\delta}_1)$ and $(\tilde{\zeta}_N, \tilde{\delta}_N)$ corresponds to the smallest and largest among all distances $\{\|\tilde{\zeta}_j - \zeta^*\| : \ 1 \leq j \leq N\}$
- 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 $W_{Nn}(\zeta^*) = W(\|\tilde{\zeta}_n - \zeta^*\|) = 1 - \|\tilde{\zeta}_n - \zeta^*\| / \|\tilde{\zeta}_K - \zeta^*\|$ for $n \leq K$ so that the weight decreases from 1 to 0 as n increases from 1 to K.

Indirect inference - A David and Goliath story

- Indirect inference (Gourieroux et al. 1993; Smith Jr 1993)
- Complex model: $f(\mathbf{y}|\boldsymbol{\theta})$ with intractable f
- Simpler model $g(\mathbf{y}|\phi(\boldsymbol{\theta}))$ approximates well $f(\mathbf{y}|\boldsymbol{\theta})$, with $\dim(\phi) > \dim(\boldsymbol{\theta})$, g is tractable and $\phi : \Theta \to \Phi$ is unknown
- We can estimate $\hat{\phi}(\boldsymbol{\theta})$ by sampling $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$, $\mathbf{y}_j \sim f(\mathbf{y}|\boldsymbol{\theta})$, $1 \leq j \leq K$ and estimate ϕ from $\mathbf{y}_1, \ldots, \mathbf{y}_K$ using g - repeat
- Posterior $\pi_f(\boldsymbol{\theta}|\mathbf{y}_0) \propto p(\boldsymbol{\theta}) f(\mathbf{y}_0|\boldsymbol{\theta})$ is then approximated by

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

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 $S(\mathbf{y})$ given θ is Gaussian with parameters $\phi(\boldsymbol{\theta}) = (\mu_\theta, \Sigma_\theta)$
- The Synthetic Likelihood (SL) procedure assigns to each θ the likelihood $SL(\theta) = \mathcal{N}(s_0; \mu_\theta, \Sigma_\theta)$, where $s_0 = S(\mathbf{y}_0)$.
- The BSL posterior is $\pi_{BSL}(\theta|s_0) \propto p(\theta)\mathcal{N}(s_0; \mu_\theta, \Sigma_\theta)$.
- Acceptance ratios for a MH sampler are estimated from m statistics $(s_1, \cdots, s_m)$ sampled from their conditional distribution given θ.

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

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

- An MCMC sampler designed for $\pi_{BSL}(\theta|s_0) \propto p(\theta) SL(\theta|s_0)$ requires

$$\min\left\{1, \frac{p(\theta) SL(\theta|s_0) q(\theta_t)}{p(\theta_t) SL(\theta_t|s_0) q(\theta)}\right\}$$

A different POV: Precomputation

- Given a proposal q, precompute $\mathcal{Z} = \{(\xi_h, s_h = (s_h^{(1)}, \ldots, s_h^{(m)})^T) : 1 \leq h \leq H\}$ where ξ_h q, $\mathbf{w}_h^{(1)}, \ldots, \mathbf{w}_h^{(m)} \overset{iid}{\sim} f(\mathbf{w}|\xi_h)$ and set $s_h^{(j)} = S(\mathbf{w}_h^{(j)})$ for all $1 \leq j \leq m$.
- Given a proposal $\boldsymbol{\theta}^*$ at t-th iteration

$$\tilde{\mu}(\boldsymbol{\theta}^*) = \frac{\sum_{h=1}^{K}[W_h(\boldsymbol{\theta}^*)\frac{1}{m}\sum_{j=1}^{m} s_h^{(j)}]}{\sum_{h=1}^{K} W_h(\boldsymbol{\theta}^*)},$$
$$\tilde{\Sigma}(\boldsymbol{\theta}^*) = \frac{\sum_{h=1}^{K}[W_h(\boldsymbol{\theta}^*)\frac{1}{m}\sum_{j=1}^{m}(s_h^{(j)} - \hat{\mu}_{\boldsymbol{\theta}^*})(s_h^{(j)} - \hat{\mu}_{\boldsymbol{\theta}^*})^T]}{\sum_{h=1}^{K} W_h(\boldsymbol{\theta}^*)}. \tag{2}$$

- We use $m = 1$.

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.

Some comfort

- Let $P(\cdot, \cdot)$ denote the transition kernel of our AABC sampler, if $h(\boldsymbol{\theta})$ were computed exactly.
- The stationary distribution of a chain with kernel $P(\cdot, \cdot)$ is μ
- The approximate kernel at time t is denoted $\hat{P}_t$
- The distribution of $\boldsymbol{\theta}_t$ is denoted $\mu_t := \nu \hat{P}_1 \ldots ... \hat{P}_t$

Some comfort

Vanishing TV Theorem

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

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

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

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

Numerical Experiments: Ricker's Model

- A particular instance of hidden Markov model:

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

  where $Pois(\lambda)$ is Poisson distribution

- Only $\mathbf{y} = (y_1, \cdots, y_n)$ sequence is observed, because the first 50 values are ignored.

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 $\mathbf{y}$, $\bar{y}$,

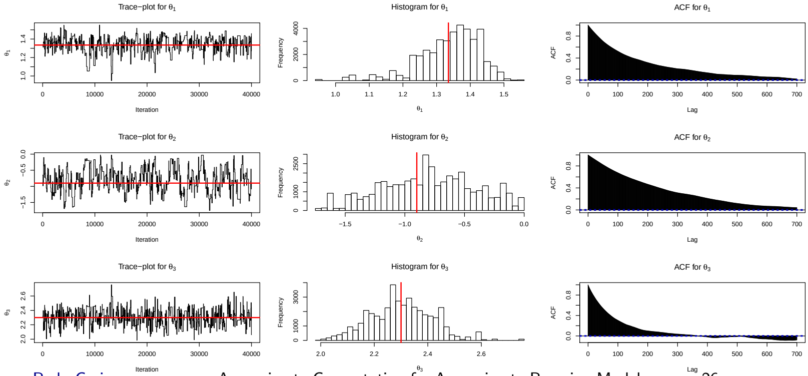
(C3:C7) Sample auto-correlations at lags 1 through 5,

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

(C12-C14) Coefficients $\beta_0, \beta_1, \beta_2$ of quadratic regression $y_i^{0.3} = \beta_0 + \beta_1 y_{i-1}^{0.3} + \beta_2 y_{i-1}^{0.6} + \epsilon_i$, $i = 2, \ldots, n$.

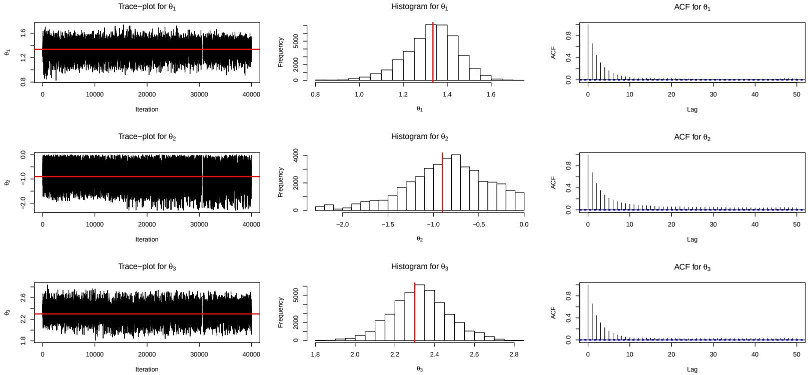
Numerical Experiments: Ricker's Model - ABC/RWM

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.



Numerical Experiments: Ricker's Model - ABC

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



Numerical Experiments: Ricker's Model - ABC

	Diff with exact			Diff with true parameter			Efficiency	
Sampler	DIM	DIC	TV	$\sqrt{\text{Bias}^2}$	$\sqrt{\text{VAR}}$	$\sqrt{\text{MSE}}$	ESS	ESS/CPU
ABC-RW	0.135	0.0201	0.389	0.059	0.180	0.189	87	0.199
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
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

Table: Summaries based on 40K samples

Example: Stochastic Volatility

- Stochastic volatility model with stable errors:

$$v_i \overset{iid}{\sim} \mathcal{N}(0,1);\ w_i \overset{iid}{\sim} Stab(\theta_4,-1);\ i=\{1,\cdots,500\}$$
$$x_1 \sim \mathcal{N}(0, 1/(1-\theta_1^2));$$
$$x_i = \theta_1 x_{i-1} + v_i; \quad i=\{2,\cdots,500\},$$

Observed data: $y_i = \sqrt{\exp[\theta_2 + \exp(\theta_3)x_i]}w_i; \quad i=\{1,\cdots,500\}.$

- Here $Stab(\theta_4,-1)$ is a stable distribution with parameters $\theta_4 \in [0,2]$ and skew parameter -1.
- True parameter values: $\theta_1 = 0.95$, $\theta_2 = -2$, $\theta_3 = -1$, and $\theta_4 = 1.8$.

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 $\mathbf{y}^2$,

(C3) Standard deviation of $\mathbf{y}^2$,

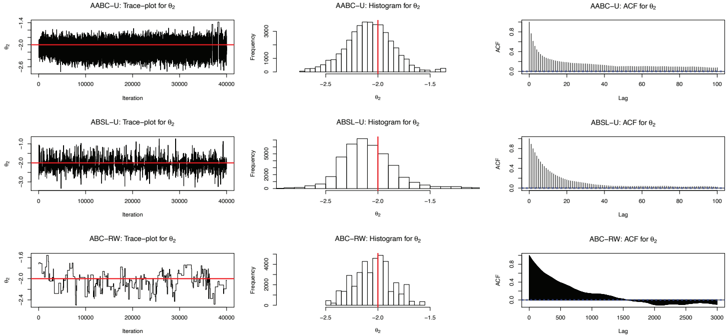
(C4) Sum of the first 5 auto-correlations of $\mathbf{y}^2$,

(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 $\{\mathbf{1}_{\{y_i^2 < \text{quantile}(\mathbf{y}^2, 0.9)\}}\}_{i=1}^n$.

Example: Stochastic Volatility cont..



Example: Stochastic Volatility cont..

	Diff with SMC			Diff with true parameter			Efficiency	
Sampler	DIM	DIC	TV	$\sqrt{\text{Bias}^2}$	$\sqrt{\text{VAR}}$	$\sqrt{\text{MSE}}$	ESS	ESS/CPU
ABC-RW	0.078	0.0126	0.205	0.248	0.198	0.317	24	0.069
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
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

Table: Summaries based on 40K samples

Concluding remarks

- Our methods show good results even if $q(\xi|\theta) = \mathcal{N}(\theta, \Sigma)$ but theory is not fully developed.
- Ideally we want to combine with adaptive MCMC.
- The computational burden can prohibit the full reach for these approximate methods so more solutions are needed.

All papers available at:
http://www.utstat.toronto.edu/craiu/Papers/index.html