Sequentially guided MCMC proposals for synthetic likelihoods and correlated synthetic likelihoods.

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- Umberto Simola (Uni. Helsinki);
- Jukka Corander (Uni Oslo; Uni. Helsinki).

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Umberto Picchini[†], Umberto Simola[‡], and Jukka Corander[§]

Also in the Wednesday poster session.

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What is the **synthetic likelihood methodology**?

It is a simulation-based inference approach for models with intractable likelihoods.

Just like Approximate Bayesian Comutation (ABC), synthetic likelihood (SL) uses the output of a computer simulator to substitute the unavailable data likelihood $p(y|\theta)$ with an approximation based on informative summary statistics of the data:

$$p(y|\theta) \approx p(s_y|\theta).$$

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For observed data y, parameters θ and an intractable likelihood $p(y|\theta)$, simulate many (M) times from the stochastic model simulator $\mathcal{S}(\theta)$:

- given θ^*, independently simulate M datasets $y_1^*, ..., y_M^*$, using $\mathcal{S}(\theta^*) \to y_m^*$, $m = 1, ..., M$;
- compute finite-dimensional summary statistics $s_m^* = T(y_m^*)$, $m = 1, ..., M$;
- compute sample mean and covariance matrix

$$\hat{\mu}_{M,\theta^*} = \frac{\sum_{m=1}^{M} s_m^*}{M}, \qquad \hat{\Sigma}_{M,\theta^*} = \frac{\sum_{m=1}^{M}(s_m^* - \hat{\mu}_{\theta^*})(s_m^* - \hat{\mu}_{\theta^*})'}{M-1},$$

- for data y get $s_y = T(y)$ and approximate $p(y|\theta) \approx p(s_y|\theta) \approx \mathcal{N}(s_y; \hat{\mu}_{M,\theta}, \hat{\Sigma}_{M,\theta}) \equiv p_M(s_y|\theta)$.

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Synthetic likelihood (SL) is a methodology initially proposed by Wood (2010) and later studied by Price et al. (2018) in a purely Bayesian context.

- The SL $p_M(s_y|\theta)$ is typically plugged into a Metropolis-Hastings sampler in place of $p(y|\theta)$;
- so we obtain a Markov chain with stationary distr.

$$\pi_M(\theta|s_y) \propto p_M(s_y|\theta)\pi(\theta).$$

MCMC via SL often expensive: for each proposed θ it may need $M = 10^3$ or more.

It is especially difficult to initialize SL at some arbitrary initial θ_0 (very large variability in the SL and non-positive definite covariances).

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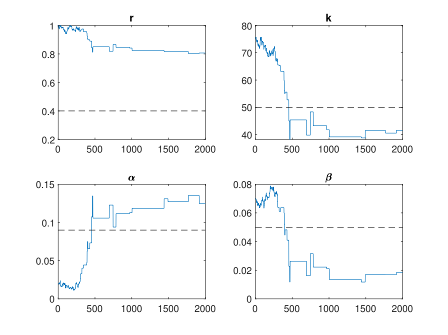
When θ_0 is far from the bulk of the posterior the chain may fail to mix.

This is due to high-variance in the estimated $\hat{\mu}_{M,\theta_0}$ and $\hat{\Sigma}_{M,\theta_0}$ causing unwanted overestimations of the $p(s_y|\theta_0)$ resulting in many rejections.



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In the figure we even used the robustified semiBSL of An et al (2020)

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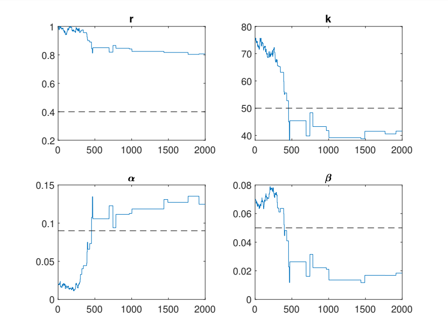

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Most of literature for synthetic likelihood focusses on how to robustify the inference (eg relax the Gaussianity assumption or deal with model misspecification) or reduce the computational cost by regularizing the covariance matrix.

However not much is available in terms of how to help the sampler to more rapidly reach the bulk of the posterior.

An exception is the use of a GP-based surrogate of the logdistances $\log ||s^* - s_y||$, as implemented in the `ELFI` Python package (Lintusaari et al 2018).[1] Then they rapidly find a minimizer of $\log ||s^* - s_y||$ via Bayesian optimization.

This minimizer could then be used to initialize SL.

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Initial idea to guide θ

In-nuce, here is the basic idea to construct a proposal sampler $g(\theta|s_y)$ which conditions on data summaries.

- At iteration k of Metropolis-Hastings say we collected M summaries $\{s_k^{*1}, ..., s_k^{*M}\}$ simulated using θ_k^*.
- Compute

$$\bar{s}_k^* = \frac{\sum_{m=1}^{M} s_k^{*m}}{M}.$$

- By CLT, for M large $\bar{s}_k$ is approximately Gaussian.
- After K iterations we have pairs $\{\theta_k^*, \bar{s}_k^*\}_{k=1}^{K}$.

Consider a proposal sampler for the pair $(\theta_k^*, \bar{s}_k^*)$ to be a d-dimensional Gaussian, with

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Set a d-dimensional mean vector $m \equiv (m_\theta, m_s)$ and the $d \times d$ covariance matrix

$$S \equiv \begin{bmatrix} S_\theta & S_{\theta s} \\ S_{s\theta} & S_s \end{bmatrix}.$$

We estimate m and S using $\{\theta_k^*, \bar{s}_k^*\}_{k=1}^K$ as follows.

Define $x_k := (\theta_k^*, \bar{s}_k^*)$ then

$$\hat{m} = \frac{\sum_{k=1}^K x_k}{K}, \quad \hat{S} = \frac{\sum_{k=1}^K (x_k - \hat{m})(x_k - \hat{m})'}{K-1}.$$

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$$\textbf{guided proposal } g(\theta|s_y) \equiv \mathcal{N}(\hat{m}_{\theta|s}, \hat{S}_{\theta|s})$$

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So what we described essentially is a way to **initialize a guided method**.

- We run a non-guided burnin using K iterations of our favourite MCMC sampler;
- we collect the K pairs $\{\theta_k^*, \bar{s}_k^*\}_{k=1}^{K}$;
- at iteration K+1 we build a first guided sampler $g(\theta|s_y) \equiv \mathcal{N}(\hat{m}_{\theta|s}, \hat{S}_{\theta|s})$ ad described.

And then?

How do we keep guiding our sampler for next iterations?

We got inspired by the *Sequential Neural Likelihood* method of Papamakarios-Sterratt-Murray (AISTATS 2019).

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Here is the SNL method of Papamakarios-Sterratt-Murray (AISTATS '19).

Input: observed data y, estimator $q_\phi(y^*|\theta)$, number of rounds R, simulations per round N
Set $\hat{\pi}_0(\theta|y) = \pi(\theta)$ and $\mathcal{D} = \{\emptyset\}$

for $r = 1 : R$ **do**
    for $n = 1 : N$ **do**
        sample $\theta_n^* \sim \hat{\pi}_{r-1}(\theta|y)$ with MCMC
        simulate $\mathcal{S}(\theta_n^*) \to y_n^*$ add (θ_n^*, y_n^*) into $\mathcal{D}$
    end for
    (re-)train $q_\phi(y^*\theta)$ on $\mathcal{D}$ and set $\hat{\pi}_r(\theta|y) \propto q_\phi(y|\theta)\pi(\theta)$
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Return $\hat{\pi}_R(\theta|y)$

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Notice SNL has nothing to do with synthetic likelihoods. It’s a generic method.

Input: K pairs $\{\theta_k^*, \bar{s}_k^*\}_{k=1}^K$ from burnin. Positive integers N and T. Initialize $\mathcal{D} := \{\theta_k^*, \bar{s}_k^*\}_{k=1}^K$.

Construct starting conditional Gaussian proposal g_0 using $\{\theta_k^*, \bar{s}_k^*\}_{k=1}^K$ as already shown. Set $\theta_0 := \theta_K^*$.

for $t = 1 : T$ **do**

  Starting at θ_{t-1} run N MCMC iterations (SL) using g_{t-1}, producing $\{\theta_n^*, \bar{s}_n^*\}_{n=1}^N$.

  Form $\mathcal{D} := \mathcal{D} \cup \{\theta_n^*, \bar{s}_n^*\}_{n=1}^N$, compute $(\hat{m}^{0:t}, \hat{S}^{0:t})$ on $\mathcal{D}$, update $(\hat{m}_{\theta|s}^{0:t}, \hat{S}_{\theta|s}^{0:t})$ to construct $g_t(\theta) = \mathcal{N}(\hat{m}_{\theta|s}^{0:t}, \hat{S}_{\theta|s}^{0:t})$ where

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  Set $\theta_t := \theta_N^*$.

end for

Return $\theta_1, ..., \theta_T$ to be provided as input to another adaptive MCMC algorithm for SL.

Best results with $N = 1$, i.e. we **immediately make use of each accepted draw towards guiding the algorithm to modal posterior regions.**

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I said *towards modal regions*, because this algorithm has no known stationary distribution.

So we will not use it to provide posterior sampling.

It will very rapidly guide the chain towards the mode of $\pi(\theta|s_y)$ with $T \approx 50$ iterations.

After its last iterations we can use the accepted draws to initialize another MCMC sampling with known ergodic properties.

In our example, we use our guided procedure to initialize the classic adaptive MCMC of Haario et al (Bernoulli 2001).

SL MCMC will run much faster after our procedure since we can reduce the number of model simulations M.

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Super-standard toy model in likelihood-free inference.

Its density is unavailable in closed form, but easy to sample from its quantiles function.

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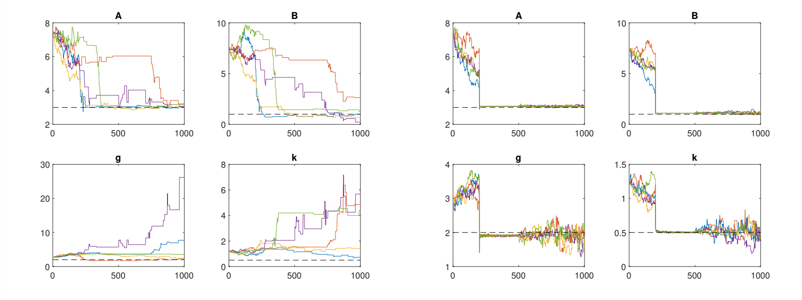

(a) non-guided approach **(b)** guided approach

Figure 2: (a) non-guided approach using the Haario et al 2001 sampler. (b) uses the guided sampler from iteration 200 to 500. We display the first 1,000 iterations to emphasize the effect of the guided sampler. The black dashed lines mark ground-truth parameters.

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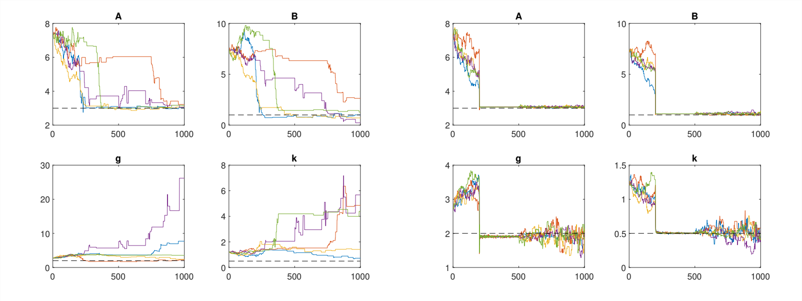

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Example: bimodal target

Here our likelihood is a 2 components bivariate Gaussian mixture *(way more complex case-studies are in the paper)*.

Of course we absolutely do not need synthetic likelihoods here, but it's a useful case study.

$$y \sim 0.5\mathcal{N}(\mu_1, \Sigma_1) + 0.5\mathcal{N}(\mu_2, \Sigma_2).$$

We wish to fit its mean values $\mu_1 = (\mu_{11}, \mu_{12})^{\mathrm{T}}$, $\mu_2 = (\mu_{21}, \mu_{22})^{\mathrm{T}}$.

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At each proposed $\theta = (\mu_1, \mu_2)$:

- we simulate 5,000 data points from the mixture;
- we fit the 5,000 points with a bivariate 2-components Gaussian mixture: the fitted means are used as summary statistics.

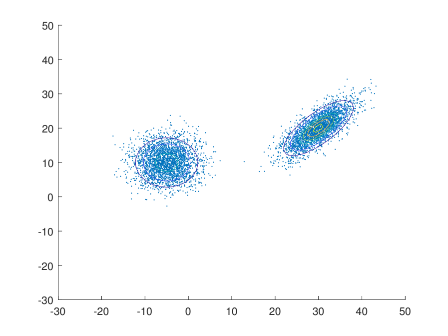
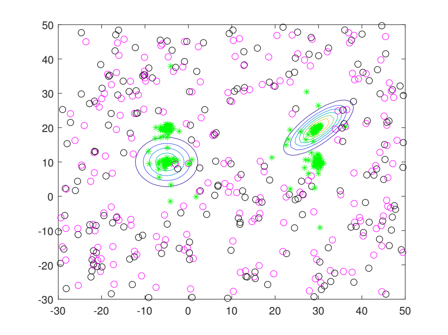


Figure 3: Data

We pick 100 starting values for $\mu_1 = (\mu_{11}, \mu_{12})^{\mathrm{T}}$, $\mu_2 = (\mu_{21}, \mu_{22})^{\mathrm{T}}$, randomly and uniformly in the square below and run 100 MCMC chains.



Starting values are the black circles. After 49 iterations of random walk proposals we get the circles in magenta. These are followed by a single guided iteration in green.

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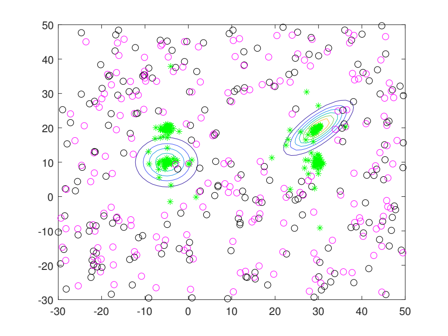

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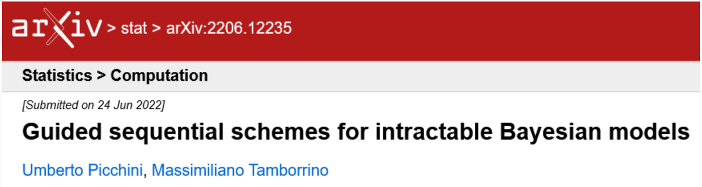
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Appendix

Correlated synthetic likelihoods

Denote with U the vector of all "auxiliary variables", i.e. pseudorandom numbers (typically standard Gaussian or uniform) that are necessary to produce a non-negative likelihood approximation $\hat{p}(s_y|\theta, \mathrm{U})$ at a given parameter θ.

In Tran et al. (2016) the set U is divided into G blocks $U = (U_{(1)}, ..., U_{(G)})$, and one of these blocks is updated jointly with θ in each MCMC iteration.

We can write the acceptance probability as

$$\alpha = \min\left\{1, \frac{p_M\left(s|\theta^p, \mathrm{U}^c_{(1)}, ..., \mathrm{U}^c_{(k-1)}, \mathrm{U}^p_{(k)}, \mathrm{U}^c_{(k+1)}, ..., \mathrm{U}^c_{(G)}\right)\pi\left(\theta^p\right)}{p_M\left(s|\theta^c, \mathrm{U}^c_{(1)}, ..., \mathrm{U}^c_{(k-1)}, \mathrm{U}^c_{(k)}, \mathrm{U}^c_{(k+1)}, ..., \mathrm{U}^c_{(G)}\right)\pi\left(\theta^c\right)} \frac{g\left(\theta^c|\theta^p\right)}{g\left(\theta^p|\theta^c\right)}\right\} \tag{1}$$

which we therefore call "correlated synthetic likelihood" (CSL) approach.

If we take p_M to be the unbiased SL of Price et al (2018), then we are still targeting the exact $\pi(\theta|s_y)$ (Tran et al. 2016).

Left: standard SL.

Right: correlated SL.