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A practical introduction to butterfly and adaptive resampling in Sequential Monte Carlo

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Abstract: Parallel and distributed computing technologies offer great potential for speed-up of Monte Carlo algorithms. However, in the development of most existing algorithms it has been implicitly assumed that implementation would be on a serial machine, so algorithm structure is often not well-suited to parallel architectures. In recent work the authors have studied the theoretical properties of Sequential Monte Carlo algorithms involving a “butterfly” resampling method, whose conditional independence structure is intended to better match parallel and distributed architectures, with resampling broken down into stages, allowing sampling tasks for subsets of the particles to be handled concurrently. This paper provides a more practical overview of these methods, including consideration of adaptive resampling schemes, numerical results and an accessible account of theoretical properties.

Keywords: Particle filters, parallelization.

1. INTRODUCTION

Monte Carlo (MC) numerical methods are popular in a broad spectrum of applications across various applied fields, and Sequential Monte Carlo (SMC) methods in particular (Gordon et al., 1993; Doucet et al., 2001) are prominent due to their ease of implementation and wide applicability to inferential computation involving non-linear, non-Gaussian dynamical models. Historically, SMC methods, also known as particle filters, have been developed and analysed without much attention paid to the architecture of the computer systems on which they are implemented, the implicit assumption being that these algorithms would be deployed on a single processor system.

The modern picture is somewhat different: due to physical barriers and energy consumption, it is becoming increasingly difficult to design and develop processors with a faster central clock rate. Hence, the natural tendency for improved performance has been in moving towards parallel and distributed computation, realizing algorithms on systems consisting of slower but a very large number processing units. Many logical and physical arrangements for these very large number of processing units have been realized. However, traditional analysis of SMC methods has been focused on the behaviour of the error and does not provide any guidance for practical implementations on these modern architectures.

In modern parallel and distributed architectures, respecting data locality and avoiding unnecessary data movement is the key ingredient in the design of efficient algorithms. Here, consideration of the communication pattern - the structure via which computational elements exchange information, synchronize, balance computational load or access global memory - is crucial, as otherwise the potential benefits of parallel processing are easily lost (Lee et al., 2010; Suchard et al., 2010). The communication pattern of a SMC algorithm is naturally connected to the conditional independence structure of the stochastic process it simulates.

In this paper, we will focus on a new class of resampling algorithms called butterfly resampling, which the authors have recently proposed (Heine et al., 2014). The “butterfly” name reflects the fact that the conditional independence structure of the algorithm matches the pattern of the computation graphs of Cooley-Tukey Fast Fourier Transform, where each computation stage is called a butterfly. However, there several important practical and methodological issues which the theoretical work of Heine et al. (2014) does not address.

We present a practical overview of butterfly resampling algorithms with reference to their implementations on graphical processing units (GPUs). We also discuss their adaptive implementation based on monitoring the effective sample size. The performance of a practical implementation on a given system such as a such as a cluster, multicore processor or GPU’s will depend on the details of a careful implementation. We provide simulation results on a GPU which are indicative of some of the key computation speed, stochastic and numerical error behaviours of but-
Resampling is a key operation in the design of stable SMC algorithms and its somewhat collective nature hinders the parallelization of the particle filters. There are various existing works on parallel implementations of SMC. Amongst several others Brun et al. (2002) considered particle filters in a distributed computing setting, Bolić et al. (2005) devised algorithms in which interaction occurs occasionally between blocks of particles, Hendeby et al. (2007) considered a GPU implementation, Vergé et al. (2013) have suggested algorithms with resampling on two hierarchical levels, and Murray et al. (2014) outlines some different approaches to parallel implementation of various existing resampling techniques and compares their efficiencies. Paige et al. (2014) propose an algorithm substantially different from any 

2. RESAMPLING IN SMC

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2.1 Augmented resampling

In this paper we present resampling in terms of a set of input particles \( x_{in} = (x_{in}^{i})_{i=1}^{N} \), their weights \( w_{in} = (w_{in}^{i})_{i=1}^{N} \), and the corresponding output quantities, \( w_{out} = (w_{out}^{i})_{i=1}^{N} \). From henceforth for any integer \( n \geq 1 \), we write \( [n] := \{1, \ldots, n\} \).

Now let \( m \geq 1 \) and \( A_{k} \), \( k = 1, \ldots, m \) be non-negative matrices, each of size \( N \times N \). We shall assume that

A1 each \( A_{k} \) is doubly stochastic,

A2 \( (A_{m}A_{m-1} \cdots A_{1})^{ij} = 1/N, \quad \forall i, j \in [N] \).

The starting point for butterfly resampling is the following augmented resampling procedure, which introduces \( m \) steps between the input and output.

\[
\begin{align*}
  &\text{for } i \in [N], \quad \text{set } w_{0}^{i} = w_{in}^{i}, \quad \xi_{0}^{i} = x_{in}^{i}, \\
  &\text{for } k \in [m], i \in [N], \quad \text{set } w_{k}^{i} = \sum_{j} A_{k}^{ij} w_{k-1}^{j}, \\
  &\quad \text{and sample } \xi_{k}^{i} \sim \frac{\sum_{j} A_{k}^{ij} w_{k-1}^{j} \delta_{\xi_{k-1}}} {\sum_{j} A_{k}^{ij} w_{k-1}^{j}}, \\
  &\text{for } i \in [N], \quad \text{set } w_{out}^{i} = w_{m}^{i}, \quad x_{out}^{i} = \xi_{m}^{i}.
\end{align*}
\]

Our interest in this procedure is that the matrices \( A_{k} \) can be used to impose constraints on the conditional independence structure of random variables it involves. The specifics of these constraints are discussed a little later, in Section 3. However, introducing those details requires us to bring in another layer of notation, so before doing that we establish some important regularity and lack-of-bias properties of augmented resampling, in the sense of the following Lemma.

Lemma 1. For any \( k \in [m], \)

\[
\begin{align*}
  \max_{i} w_{k}^{i} \leq \max_{i} w_{in}^{i},
\end{align*}
\]

and for any integrable \( \varphi, \)

\[
\begin{align*}
  \mathbb{E} \left[ \frac{1}{N} \sum_{i} w_{k}^{i} \varphi(\xi_{k}^{i}) \middle| x_{in}, w_{in} \right] = \frac{1}{N} \sum_{i} w_{in}^{i} \varphi(x_{in}^{i}),
\end{align*}
\]

and

\[
\begin{align*}
  \mathbb{E} \left[ \frac{1}{N} \sum_{i} \varphi(x_{out}^{i}) \middle| x_{in}, w_{in} \right] = \frac{\sum_{i} w_{in}^{i} \varphi(x_{in}^{i})} {\sum_{i} w_{in}^{i}}.
\end{align*}
\]

Proof. The first claim follows from the row-stochasticity of the \( A_{k} \) and the fact that

\[
\begin{align*}
  w_{k}^{i} &= \sum_{j} (A_{k}A_{k-1} \cdots A_{1})^{ij} w_{in}^{j}.
\end{align*}
\]

For the second claim, using the column-stochasticity of each \( A_{k} \), or equivalently \( \frac{1}{N} \sum_{i} A_{k}^{ij} = \frac{1}{N} \), we have

\[
\begin{align*}
  \frac{1}{N} \sum_{i} w_{k}^{i} \varphi(\xi_{k}^{i}) &= \frac{1}{N} \sum_{i} w_{in}^{i} \varphi(x_{in}^{i}) \\
  &= \sum_{ij} A_{k}^{ij} \sum_{i} w_{k}^{i} \varphi(\xi_{k-1}^{i}) - \frac{1}{N} \sum_{i} \sum_{j} A_{k}^{ij} \sum_{i} w_{k-1}^{i} \varphi(\xi_{k-1}^{i}) \\
  &= \sum_{ij} A_{k}^{ij} \sum_{i} w_{k}^{i} \Delta_{k}^{i}.
\end{align*}
\]

From the “sample” part of the procedure, we have

\[
\begin{align*}
  \mathbb{E} \left[ w_{k}^{i} \Delta_{k}^{i} \middle| x_{in}, w_{in} \right] &= \mathbb{E} \left[ w_{in}^{i} \mathbb{E} \left[ \Delta_{k}^{i} \middle| x_{in}, w_{in}, (\xi_{k}^{i}) \in [N] \right] \middle| x_{in}, w_{in} \right] \\
  &= 0,
\end{align*}
\]

hence (1) holds.

For the third claim, note that property A2 of the matrices implies that for all \( i \in [N], \)

\[
\begin{align*}
  w_{in}^{i} &= \sum_{j} (A_{m}A_{m-1} \cdots A_{1})^{ij} w_{in}^{j} = \frac{1}{N} \sum_{j} w_{in}^{j}, \quad (2)
\end{align*}
\]

then re-arrange (1) with \( k = m. \) \( \square \)

2.2 Adaptive strategies

In standard SMC algorithms, one may choose to perform resampling at only certain time steps, determined as the algorithm runs by monitoring the Effective Sample Size (ESS) and triggering resampling when the ESS falls below some chosen threshold, see (Whiteley et al., 2014) and references therein for background information and analysis of this approach. One can employ a similar strategy within the augmented resampling procedure outlined in the previous section. For instance with

\[
\begin{align*}
  \xi_{k}^{N} = \left( \frac{1}{N} \sum_{i} w_{k}^{i} \right)^{2} = \frac{1}{N} \sum_{i} (w_{k}^{i})^{2},
\end{align*}
\]

and \( \tau \in (0, 1] \) a constant, define \( k^{*} := \min\{0 \leq k \leq m : \xi_{k}^{N} \geq \tau\}. \) Note that as per (2), \( w_{in}^{i} \) is in fact constant across \( i \), so \( \xi_{m}^{N} = 1 \) always. Thus \( k^{*} \) is well defined.

An alternative to the procedure of the previous section is then:
3. BUTTERFLY RESAMPLING

3.1 Definition and properties

Let \( N = r_1 r_2 \cdots r_m \) be a factorization of \( N \) with \( r_k \geq 2 \) for all \( k = 1, \ldots, m \) and then let \( A_1, \ldots, A_m \) be the family of matrices defined for \( k = 1, \ldots, m \) as

\[
A_k = I_{r_k} \otimes \cdots \otimes I_{r_{k-1}} \otimes 1_{r_k} \otimes I_{r_{k-1}} \otimes \cdots \otimes I_{r_1},
\]

where \( \otimes \) denotes Kronecker product and for any positive integer \( n \), we write \( 1_n \) for the \( n \times n \) matrix which has 1/n as every entry.

It follows by elementary properties of the Kronecker product that: \( A1 \) is satisfied, each \( A_k \) is symmetric, \( A_k A_l \) for any \( 1 \leq k < l \leq m \), \( A_m \cdots A_1 = 1_N \) so \( A2 \) is satisfied, and each \( A_k \) matrix has exactly \( r_k \) non-zero elements on each row for \( k = 1, \ldots, m \).

It can also be shown using elementary properties of the Kronecker product that the nonzero entries of the matrices \( A_k, k = 1, \ldots, m \) be characterized by the following modular congruence relations:

\[
A^j_k > 0 \iff \left\lfloor \frac{j-1}{r_1 \cdots r_{k-1}} \right\rfloor = \left\lfloor \frac{j-1}{r_1 \cdots r_k} \right\rfloor
d\]

\[
(i - 1) \mod (r_1 \cdots r_{k-1}) = (j - 1) \mod (r_1 \cdots r_k).
\]

These relations are important because it is the zero entries of the matrices \( A_k \) which determine the conditional independence structure of the random variables in the augmented resampling scheme and influence which elements can be implemented algorithmically in parallel.

A specific instance of this setup is the case in which \( r_1 = \cdots = r_m = r \), and the directed acyclic graph in Figure 1 shows the conditional independence structure of the resulting instance of augmented resampling when \( N = 8 \) and \( r = 2 \). The corresponding graph for multinomial resampling is also shown.

Heine et al. (2014) established central limit theorems for various instances of butterfly resampling. A particularly unusual feature of these results is that they show that butterfly resampling exhibits non-standard scaling: under mild regularity assumptions on \( x_{in}, w_{in} \), the results of (Heine et al., 2014) can be applied in the case \( r_1 = \cdots = r_m = r \) to show that the output from the procedure in Section 2.1 with the matrices as in (3) has the property that for any bounded test function \( \varphi \),

\[
\sqrt{N} \log N \left[ \frac{1}{N} \sum \varphi(x_{out}^i) - \frac{1}{N} \sum w_{in}^i \varphi(x_{in}^i) \right] \Rightarrow \mathcal{N}(0, \sigma_r^2),
\]

where the convergence is in distribution as \( N \) tends to infinity along the sequence \( (r^m; m = 1, 2, \ldots) \). Thus depending on the choice of \( m \) and \( r_m \) butterfly resampling may converge more slowly than standard methods, which typically have \( \sqrt{N} \) scaling as opposed to \( \sqrt{N \log N} \). Thus speed-ups which butterfly resampling enjoys may trade off against loss in statistical performance.

In order to frame some of our considerations when implementing butterfly resampling, it’s convenient to first discuss some properties of the standard multinomial method, which one can obtain as a special case by setting \( m = 1 \) and \( A_1 = 1_N \).

Pseudocode for multinomial resampling is given in algorithm 1 and involves parallel calls of the INVERSIONSAMPLING procedure, which itself consists of the generation of a uniform random number \( u \) in the interval \([0, W^N]\) and a binary search within the cumulative weights vector \( W = (W_k = \sum_{n=1}^N w_{in}^n/N) \) to locate the subinterval \([W^{j-1}, W^j]\) such that \( u \in [W^{j-1}, W^j] \). It returns the index \( j \) such that \( u \in [W^{j-1}, W^j] \).

The pseudocode for butterfly resampling, which amounts to the augmented resampling procedure of Section 2.1 with the matrices (3), is given in algorithm 2, and expressed in terms of the following quantities:
We consider 4.1 Single Step of Resampling
CUDA Toolkit version 5.5. All simulations are run on a
synchronization and local memory for in-place propagation
to be carried out in shared memory and utilization of barrier
temporarily by the threads. This allows inversion sampling to
resampling operations are mapped to thread blocks and
several resampling operations on smaller particle sets that

The partitioning of the index set into equivalence classes

correspond to division of the resampling operation into
several resampling operations on smaller particle sets that
can be carried out in parallel. On a GPU, these smaller
resampling operations are mapped to thread blocks and
within a thread block resampling is performed cooperatively
by the threads. This allows inversion sampling to
be carried out in shared memory and utilization of barrier
synchronization and local memory for in-place propagation
of particles.

4. EXPERIMENTAL RESULTS

We implemented the algorithms in CUDA C/C++ using
CUDA Toolkit version 5.5. All simulations are run on a
NVIDIA GeForce GTX680 GPU with CUDA capability
3.0.

4.1 Single Step of Resampling

We consider \( x_{in} \) samples a distribution \( \pi_0 \) and \( w_{in} = g(x_{in}) \), for some non-negative function \( g \). For test function \( \varphi(x) = x \) we consider estimation of \( \tilde{\pi}_0(\varphi) = \int (\varphi(x)g(x)/\pi_0(g))\pi_0(dx) \) and measure performance in terms of numerical approximation of the MSE:

\[
\mathbb{E}\left[ \left( \sum_{i=1}^{N} \frac{w_{out}^i}{\sum_j w_{out}^j} \varphi(x_{out}^i) - \tilde{\pi}_0(\varphi) \right)^2 \right],
\]

obtained over 1000 algorithm runs.

We consider two scenarios:

1. \( \pi_0 \) is uniform distribution on \([-\sigma, \sigma] \) and \( g(x) = \exp(-x^2/2\sigma^2) \),
2. \( \pi_0 \) is Poisson distribution with parameter \( \lambda \) and \( g(x) = \lambda^x/x! \),

with \( \sigma = \lambda = 10 \).

For each number of particles \( N = 2^{11}, 2^{12}, \ldots, 2^{24} \), we took
\( m = \lceil \log_R N \rceil \) where \( R = 1024 \) is the maximum number of
threads per thread block and then selected the sequence
\( r_1, \ldots, r_m \) obeying \( N = r_1 \cdots r_m \) and giving the fastest
performance.

We ran experiments in both single and double precision
arithmetic. Results are plotted in figures 2 and 3. We see
that butterfly resampling algorithm provides up to
two times speed-up, since we utilized shared memory.
However, with double precision, if look at the MSE against
CPU time we do not see an improvement over standard
multinomial resampling, this stems from the difference in
the scaling factors of butterfly and standard multinomial
resampling algorithms. While computation time grows at
the order of \( \log N \) for both algorithms, MSE of butterfly
resampling decays at the order of \( \log N/N \) and MSE of
standard multinomial resampling decays at the order of
\( 1/N \).

On the other hand, in single precision implementations,
standard multinomial resampling exhibits numerically
instability for large numbers of particles whilst butterfly
resampling does not. We believe this is due the fact that
in butterfly resampling, the prefix sum operation is
applied to smaller subsets of the weights, which are in turn
“smoothed out” over the stages of the algorithm.
4.2 Experiments with Particle Filters

In our particle filter experiments, we estimate filtering expectations $\hat{\pi}_t(\varphi)$ for $t \geq 1$ and for some test function $\varphi$. We measure the Monte Carlo errors by numerically estimating the MSEs averaged over time (AMSE):

$$
\text{AMSE} = \frac{1}{T} \sum_{t=1}^{T} (\hat{\pi}_t^N(\varphi) - \hat{\pi}_t(\varphi))^2.
$$

We implement two different particle filtering scenarios:

1. resampling every time step, i) using multinomial and ii) butterfly resampling
2. resampling adaptively, i) using multinomial resampling whenever the ESS of the weights falls below a given threshold, $\tau$ and ii) using the method of Section 2.2.

We use the following state space model for the filtering recursions:

$$
x_{t+1} = f(x_t, \cdot) = N(x_t, \sigma_1),
$$

$$
g_t(x) = \{\exp((x - 0.5t)^2/2\sigma_2^2) + \exp((x + 0.5t)^2/2\sigma_2^2)\}/2.
$$

This is a synthetic model that admits closed form computation of expectations of the function $\varphi(x) = x$ under a multimodal filtering distribution.

We use the same settings for $m$ and $r_1, \ldots, r_m$ as in the previous experiments. Model parameters are set as $\sigma_1 = 0.1, \sigma_2 = 0.1$. We run each experiment for $M = 1000$ particle filter instances with $T = 100$ timestep and $\tau = 0.6$ for adaptive resampling, then compute AMSE for $\varphi(x) = x$.

MSE and speed results for bootstrap particle filters are shown in figure 4 and for adaptive resampling particle filters are shown in figure 5. As in single step resampling experiments, we see that butterfly resampling performs faster but produce more Monte Carlo error. In bootstrap PFs, butterfly resampling can provide up to 4 times speed-up but MSE per time does not differ substantially from standard multinomial resampling. However, in adaptive resampling PFs, butterfly resampling can provide up to 8 times speed-up and MSE difference is less than that of bootstrap case as a results of adaptivity, so we see an improvement over standard multinomial resampling in terms of MSE per time.

4.3 Comparison of Resampling Strategies in a Practical Application

In our final experiment, we compare resampling strategies with constrained and full interactions within the context of a parameter estimation method that uses a particle filter as a subroutine. We have a family of state space models parameterized by some parameter vector $\theta \in \Theta$, where typically $\Theta = \mathbb{R}^d$, such that

$$
X_0 \sim \mu_\theta,
$$

$$
X_n | \{X_{n-1} = x_{n-1}\} \sim f_\theta(x_{n-1}, \cdot),
$$

$$
Y_n | \{X_n = x_n\} \sim g_\theta(x_n, \cdot),
$$

and a set of observations $y = \{y_n, \ldots\}$ and we perform maximum likelihood (ML) estimation of parameters $\theta$ to find the values of $\theta$ that maximize log-likelihood function defined as:

$$
\ell(\theta) = \log \left( \int \mu_\theta(x_0) \prod_{i=1}^{n} f_\theta(x_{i-1}, x_i) \prod_{i=0}^{n} g_\theta(x_i, y_i) dx_{0:n} \right),
$$

via sequential Monte Carlo expectation-maximization (SMCEM) algorithm (Olsson et al., 2008). SMCEM algorithm is based on expectation-maximization algorithm, a standard tool for ML estimation in the presence of intractable likelihoods, and uses particle filter as a subroutine.

In the experiments of this section, we follow example 4.2 of Olsson et al. (2008) and estimate parameters of the stochastic volatility model given as:

$$
X_0 \sim N(0, \sigma^2),
$$

$$
X_n \sim N(\alpha X_{n-1}, \sigma^2), n \geq 1,
$$

$$
Y_n \sim N(0, \beta^2 \exp(X_n)), n \geq 0.
We simulate $M = 10$ different observation sequences $(y^m_n, m = 1, \ldots, M)$ of length $n = 100$ using the above model with parameters $\theta^*_1 = \alpha^* = 0.975, \theta^*_2 = \beta^* = 0.63$ and $\theta^*_3 = \sigma^* = 0.16$. For each observation sequence $y^m, m = 1, \ldots, M$ we perform SMCEM algorithm to obtain $m$ parameter estimates $\hat{\theta}^m, m = 1, \ldots, M$ and compute MSE of the parameters given by the equations $\frac{1}{M} \sum_{m=1}^{M} (\hat{\theta}^m_i - \theta^*_i)^2, i = 1, 2, 3$.

We experiment with two different implementations of particle filter algorithms, one that uses standard multinomial resampling and another one that uses a special case of butterfly resampling algorithm. To simulate a situation with hard communication constraints and a fair comparison with standard multinomial resampling, we set the maximum radix sequence to 256 and we the following resampling strategy:

(1) for the particle filter with standard multinomial resampling, we perform at every $\lfloor \log_{256} N \rfloor$th timestep and defer resampling at other timesteps,

(2) for the particle filter with butterfly multinomial resampling, we perform one stage of butterfly resampling algorithm at every timestep by cyclically traversing the radix sequence.

For the choice of radix sequence we follow the guidelines we described in section 4.1.

We repeat this experiment for the particle numbers $\log N = 11, 13, \ldots, 21$ and plot the running time as a function of $\log N$ in figure 6. The accuracy of the parameter estimates, as measured by MSE, were omitted as they were qualitatively very similar. We observe that resampling under constrained interactions can provide up to three times speed-up over standard multinomial resampling while resulting effectively identical parameter estimates.

![Fig. 6. Speed comparison of resampling algorithms in SMCEM algorithm.](image)

5. CONCLUSIONS

Our goal was to investigate the tradeoff between particle interactions and estimation error, as well as how the reduced interaction structure can be used to obtain faster algorithms on standard hardware. We focused on the GPU implementations of the resampling algorithms, and we compared the performance of butterfly resampling algorithm to standard multinomial resampling in terms of speed and Monte Carlo error. In our experiments with the reference implementations, we see that butterfly resampling can provide up to eight times speed-up in an adaptive resampling scenario with a competitive level of Monte Carlo error and up to three times speed-up in a parameter estimation problem with a competitive level of estimation quality.

We believe that the constrained interaction structure of the butterfly resampling provides additional flexibility in the design of resampling algorithms. We speculate that this additional flexibility may be exploited on alternative platforms such as distributed computer clusters or configurable hardware devices (e.g. field-programmable gate array – FPGA) to obtain faster algorithms without compromising estimation quality. A particularly interesting scenario would be to use alternative sampling strategies, such as stratified and systematic sampling, within the butterfly method.

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