Path storage in the particle filter

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Received: date / Accepted: date

Abstract This article considers the problem of storing the paths generated by a particle filter and more generally by a sequential Monte Carlo algorithm. It provides a theoretical result bounding the expected memory cost by $T + CN \log N$, where $T$ is the time horizon, $N$ is the number of particles and $C$ is a constant, as well as an efficient algorithm to realise this. The theoretical result and the algorithm are illustrated with numerical experiments.

Keywords Sequential Monte Carlo, particle filter, memory cost, parallel computation

1 Introduction

Consider the problem of filtering in state-space models (Cappé et al. 2005) defined by $X_0 \sim \mu(\cdot)$ and for $t = 1, \ldots, T$

$X_t | X_{t-1} = x_{t-1} \sim f(\cdot | x_{t-1})$, 

$Y_t | X_t = x_t \sim g(\cdot | x_t)$.

Here $X_{0:T}$ is a hidden Markov chain in some space $\mathcal{X}$ with initial distribution $\mu$ and transition density $f$. The observations $Y_{1:T}$ in space $\mathcal{Y}$ are conditionally independent given $X_{1:T}$, with measurement density $g$. For any vector $v$, introduce the notation $v_1:n = (v_1, \ldots, v_n)$ and $v^{1:n} = (v^1, \ldots, v^n)$.

We denote by $p_t$ the distribution of the path $X_{0:t}$ given the observations $Y_{1:t}$ available at time $t$, from which the filtering distribution of $X_t$ given $Y_{1:t}$, denoted by $p_t$, is a marginal. The bootstrap particle filter (Gordon et al., 1993), described in Algorithm 1, recursively approximates the distributions $p_{1:T}$, and has borne various other sequential Monte Carlo methods (Doucet et al., 2001; Doucet and Johansen, 2011).

In Algorithm 1 the resampling step relies on some distribution $\mathcal{R}$ on $\{1, \ldots, N\}^N$ taking normalized weights as parameters.

At each time $t$, Algorithm 1 approximates $p_t$ and $p_t$ by the empirical distributions

$p_N^n(dx_0) = w^n_1 \delta_{x_0^n}(dx_0) + \cdots + w^n_N \delta_{x_0^n}(dx_0)$

and

$p_N^n(dx_t) = w^n_1 \delta_{x_t^n}(dx_t) + \cdots + w^n_N \delta_{x_t^n}(dx_t)$.

It has been shown in Whiteley (2011); Douc et al. (2012); van Handel (2009), and in Theorem 7.4.4 in Del Moral (2004) that $\pi_N$ converges to $\pi$ with $N$ under mild conditions on the model laws $(\mu, f, g)$, and that the Monte Carlo error is constant with respect to $t$. However it is also well-known that
the path measures $p_t^N$, while converging to $p_t$ with $N$, have a Monte Carlo error typically exploding at least quadratically with the time $t$ (Del Moral and Doucet, 2003; Poyiadjis et al., 2011). Indeed the paths quickly coalesce due to the resampling steps, thus providing a poor approximation of the marginal distributions $p(dx_t|y_1:t)$ for large values of $t-s$. In the following we refer to the collection of paths $\bar{x}_t^N$ as the ancestry tree, to each $\bar{x}_t^k$ (for $k = 1, \ldots, N$ and $s = 0, \ldots, t$) as a node, to each $\bar{x}_t^N$ more specifically as a leaf node, and to paths as branches.

Figure 1 might help to visualise the typical shape of the ancestry tree generated by a particle filter. The time at which all the branches coalesce, denoted by $c_T$, separates the “trunk” made of a unique branch from $t = 0$ to $t = c_T - 1$ from the “crown” made of all the branches from $t = c_T$ to $t = T$. Despite its negative consequence on the estimation of filtering quantities, the particle degeneracy phenomenon results in crowns of small sizes, allowing full trees to be stored at low memory cost. This can be beneficial whenever full paths of the particle filter are required, such as for the conditional sequential Monte Carlo and particle Gibbs algorithms first described in Andrieu et al (2010), studied in Chopin and Singh (2013), and used extensively in Chopin et al (2013) and Lindsten et al (2012). Another instance of sequential Monte Carlo method requiring path storage is presented in Wang et al (2014) in the context of computational biology. In the present article algorithms and results are presented in the filtering terminology, however they immediately extend to any sequential Monte Carlo method for Feynman-Kac models (Del Moral, 2004).

In Section 2 we present an efficient algorithm to store ancestry trees recursively during the run of a particle filter. In Section 3 we present new theoretical results bounding the size of ancestry trees, in order to bound the expected memory requirements of the storage algorithm. Finally the theoretical results and the algorithmic performance are tested numerically in Section 4.

2 Algorithms

This section introduces a memory-efficient data structure and associated algorithms for storing only those paths with support at time $t$. The algorithms are designed for parallel execution, in keeping with the general parallelisability of other components of sequential Monte Carlo samplers (Lee et al., 2010; Murray, 2013).

2.1 Proposed scheme

Up to time $t$, the particle filter produces particles $x_t^1:N$ and ancestors $a_t^1:N$. From $a_t^1:N$ offspring counts $o_t^1:N$ are readily obtained (Murray et al., 2013), where $o_t^i$ represents the number of children at generation $i$ of particle $x_{t-1}^i$. Let $x_t^1:M$ represent $M$ slots in memory for storing particles. At any time, some of these slots are empty, while others store the nodes of the tree. Let $a_t^1:M$ be an ancestry vector, where $a_t^i = 0$ if $x_t^i$ is empty or a root node, and otherwise $a_t^i = j$ to indicate that the particle in $x_t^i$ is the parent of the particle in $x_t^j$. Let $a_t^1:M$ be the offspring vector corresponding to $a_t^1:M$, where $o_t^i = n$ indicates that $x_t^i$ has $n$ children. Finally, let $l_t^1:N$ give the numbers of the $N$ slots in $x_t^1:M$ that store the particles of the youngest generation; these are the leaf nodes of the tree.

Basic operations on the tree are its initialisation, the insertion of a new generation of particles, and the pruning just before a new generation is inserted.

Algorithm 2 Parallel algorithms for basic operations on an ancestry tree: initialising from the first generation of particles, inserting a new generation of particles, and pruning just before a new generation is inserted.

| Operation | Description |
|-----------|-------------|
| INIT($x_t^1:N$) | For each $i \in \{1, \ldots, M\}$ |
| | $a_t^i := 0$ |
| | $o_t^i := 0$ |
| | For each $i \in \{1, \ldots, N\}$ |
| | $x_t^i := x_0^i$ |
| | $l_t^i := i$ |
| INSERT($x_t^1:N$, $a_t^1:M$) | $b_t := \text{GATHER}(l_t, a_t)$ |
| | $z_t := \text{TRANSFORM-PREFIX-SUM}(o_t, 1_0)$ |
| | $l_t := \text{LOWER-BOUND}(z_t, (1, \ldots, N))$ |
| | $a_t := \text{SCATTER}(b_t, l_t)$ |
| | $x_t := \text{SCATTER}(x_t, l_t)$ |
| PRUNE($o_t^1:N$) | For each $i \in \{1, \ldots, N\}$ |
| | $j := l_t^i$ |
| | While $j > 0$ and $o_t^j = 0$ |
| | $j := a_t^j$ |
| | If $j > 0$ |
| | $o_t^j := o_t^j - 1$ |

To begin, the first of the $M$ empty slots of the tree are initialised with the first generation of $N$ particles as in the INIT procedure of Algorithm 2. We assume, for now, that $M$ is sufficiently large to accommodate all subsequent operations on the tree, but see remarks in Section 2.2 below.

Each new generation is inserted as in the INSERT procedure of Algorithm 2. The procedure searches for nodes with no offspring in the current generation, and replaces them...
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Algorithm 3 Primitives used in pseudocode.

\begin{algorithm}
\caption{Primitives used in pseudocode.}
\begin{algorithmic}
\STATE \textsc{Gather}(p^{1:P}, q^{1:Q}) \rightarrow r^{1:Q}
\FOR {each \(i \in \{1, \ldots, P\}\)}
\STATE \(r^i \leftarrow p^i\)
\ENDFOR
\STATE \textsc{Scatter}(p^{1:P}, q^{1:Q}) \rightarrow r^{1:Q}
\FOR {each \(i \in \{1, \ldots, P\}\)}
\STATE \(r^i \leftarrow p^i\)
\ENDFOR
\STATE \textsc{Transform-Prefix-Sum}(p^{1:P}, f) \rightarrow r^{1:P}
\FOR {each \(i \in \{1, \ldots, P\}\)}
\STATE \(r^i \leftarrow \sum_{j=1}^i f(p^j)\)
\ENDFOR
\STATE \textsc{Lower-Bound}(p^{1:P}, q^{1:Q}) \rightarrow r^{1:Q}
\FOR {each \(i \in \{1, \ldots, Q\}\)}
\STATE \(r^i \leftarrow \min\{f : q^j \leq p^i\}\)
\ENDFOR
\end{algorithmic}
\end{algorithm}

with the new leaf nodes. The vector \(z_s\) is introduced, where \(z^T_s\) is equal to the number of nodes between 1 and \(i\) with no offspring. Nodes to replace are then located by searching for the increments in \(z_s\). The new generation is inserted at these locations.

Finally, the tree is pruned before the insertion of each new generation \(t\), using the \textsc{Prune} procedure of Algorithm 2. This requires the offspring vector, \(o_s\), of the new generation. The algorithm determines which of the current leaf nodes have no offspring in the new generation, decrements the offspring counts of their parent nodes, and proceeds recursively up the tree for cases where the parent has no remaining offspring either. Each non-leaf node \(i\) is considered pruned if \(o_s^i = 0\), and may be overwritten by future calls to \textsc{Insert}.

2.2 Remarks and improvements

The \textsc{Insert} procedure of Algorithm 2 assumes that there are at least \(N\) free slots in which to place the latest nodes. If this is not true, the buffer can be enlarged by allocating a larger block of memory, copying the contents of the ancestry tree across, and filling the new regions of the \(o_s\) and \(a_s\) vectors with zeros. Various heuristics can be used to set the new size \(M\), aiming to reduce fragmentation and the chance of future increases. Because memory reallocations involve an expensive copy, it is worth increasing \(M\) more than strictly necessary to postpone additional reallocations. For instance, implementations of the C++ Standard Template Library typically double the storage capacity of a vector that is extended by just one element, anticipating further extensions. A more conservative strategy is to start with a value of \(M\) equal to a small multiple of \(N\), and enlarge by \(N\) slots whenever necessary. Ultimately, we have not found that the particular enlargement strategy affects execution time a great deal, particularly since, as in the proceeding theoretical results, the size of the ancestry tree crown is independent of \(T\), so that the need for reallocations diminishes as \(t\) increases.

According to the results of Section 3, the expectation of the size of the tree grows linearly with \(T\), but this is only due to the trunk. The size of the crown is independent of \(T\). It may be possible to improve the algorithms by identifying the nodes along the trunk and storing them separately, as these nodes will never be overwritten by subsequent insertions. Under this modified scheme a separate, single growing trunk needs to be stored but not searched, while the nodes of the crown need to be stored and searched at every time step. The number of nodes in the crown is of constant expectation according to Theorem 1 of Section 3. Hence this modification induces a scheme of constant expected computational cost in \(T\), which could be relevant in applications where the time horizon is very long, although there will be overhead in identifying the trunk. See Fig. 3(b) in Section 4 for a report on the computational cost of the proposed method. Memory reallocation is also reduced by storing the trunk separately.

We establish in Section 3 that the size of the tree is expected to be bounded by \(T + 2\Delta_s N \log N\) for some constant \(\Delta_s\). The size of the data structure, \(M\), must be at least as large as this. We assume that, with a sensible enlargement strat-
3 Size of the ancestry tree

3.1 Results

From a theoretical point of view, similar random trees have been studied in population genetics Del Moral et al. (2009); Möhle (2004) in a setting that corresponds to a state-space model that assigns equal weights to all paths; these results do not apply directly here. In order to bound the expected number of nodes in an ancestry tree, we first study the distance \( d_T = T - c_T \) between the final time \( T \) and the full coalescence time \( c_T \) when all the paths merge. Theorem 1 proposes a bound on the expectation of \( d_T \), which is independent of \( T \) and explicit in \( N \).

**Assumption 1** There exists \( \varepsilon \in [0, 1] \) such that for all \( y \in \mathcal{Y} \) and for all \( x \in \mathcal{X} \):

\[
\sqrt{\varepsilon} \leq g(y \mid x) \leq \frac{1}{\sqrt{\varepsilon}}.
\]

**Theorem 1** Under Assumption 1 the distance to the most recent common ancestor \( d_T \) satisfies

\[
E[d_T] \leq \Delta_1 N \log N
\]

for some \( \Delta_1 > 0 \), which does not depend \( N \) nor \( T \).

The expected number of nodes in the tree can be bounded explicitly in \( N \) and \( T \), as in Theorem 2.

**Theorem 2** We suppose here that \( N \geq 3 \). Under Assumption 1 the number of nodes, denoted by \( n_T \) at time \( T \), satisfies

\[
E[n_T] \leq T + \Delta_2 N \log N
\]

for some \( \Delta_2 > 0 \) that does not depend on \( N \) nor \( T \).

These results quantify the practical difference between storing all the generated particles (for a deterministic cost of \( T \times N \) memory units) and storing only the surviving particles (for a random cost expected to be bounded by \( T + \Delta_2 N \log N \)).

Assumption 1 is very strong outside compact spaces, and for instance does not even cover the linear-Gaussian case, although the experiments of Section 4 indicate that similar results might hold for non-linear and non-Gaussian cases. The numerical experiments show that the bound is accurate as a function of \( N \), so that even if some inequalities used in the proofs appear quite crude, the overall result is precise. However the results do not capture the shape of the tree as a function of \( \varepsilon \), which is why we write the constants \( \Delta_1 \) and \( \Delta_2 \) without making their dependency on \( \varepsilon \) explicit. Consider for example Theorem 1, where \( \Delta_1 \) can be defined by \( \Delta_1 = 1 + 8/\varepsilon \), as will be proven in Section 3.3. If the bound was sharp as a function of \( \varepsilon \), it would mean that the time to full coalescence increases to infinity when \( \varepsilon \) goes to zero. However path degeneracy is expected be more acute for smaller \( \varepsilon \), since more variability in the particle weights is then allowed. The dependency on \( \varepsilon \) in \( \Delta_1 \) is thus not realistic. We believe the bounds could in fact be independent of \( \varepsilon \), by considering \( \varepsilon = 1 \) as the case corresponding to the largest expectations of \( d_T \) and \( n_T \); a claim not proven here.

Moreover, the proposed proof relies on the multinomial resampling scheme, while most practitioners favour more sophisticated schemes (Carpenter et al., 1999; Liu and Chen, 1998; Kitagawa, 1998; Doucet and Johansen, 2011). Figure 3(a) of Section 4 indicates that similar results hold for these other resampling schemes. There are some obvious counter-examples, for instance when the measurement density is constant, leading to equal weights at each step (equivalently \( \varepsilon = 1 \)). Then the results above hold for multinomial resampling but systematic resampling would completely obviate the path degeneracy phenomenon. Describing features of ancestry trees corresponding to general resampling schemes would constitute an interesting avenue of research.

The rest of the section is devoted to proving Theorem 1 and Theorem 2.
3.2 From non-uniform weights to uniform weights

We first relate the ancestry process associated with particle filters using multinomial resampling, with the ancestry process associated with the neutral case, where all the weights would be equal to $N^{-1}$ at every time step. To do so we introduce various intermediate processes, starting with the exact multinomial resampling process denoted by $(A_i)_{i \geq 0}$, then an approximation represented by $(A_i')_{i \geq 0}$ which provides an almost sure upper bound and eventually a process $(Z_k)_{k \geq 0}$ counting the number of nodes at generation $T - k$ in the neutral case, for a fixed time horizon $T$.

Let us introduce an alternative representation of the multinomial resampling scheme. For each particle index $j = 1, \ldots, N$ at time $t$, draw $V^j_t$ uniformly in $[0,1]$. If $V^j_t \leq \varepsilon$, draw $U^j_t \sim \mathcal{U}([0,1])$ and set $a^j_t = k$ for $k$ such that $U^j_t \in ([k-1]/N,k/N]$. If however $V^j_t > \varepsilon$, draw $a^j_t$ from $\sum_{1 \leq i \leq N}(w^j_{i-1} - \varepsilon/N)(1 - \varepsilon)^{-1}$ $\delta_i(\cdot)$. One can check that Assumption 1 ensures that $w^j_{i-1} - \varepsilon/N \geq 0$ for each $1 \leq i \leq N$ and that the scheme described above leads to $P(a^j_t = k) = w^j_{k-1}$ as in multinomial resampling. The alternative representation amounts to a mixture of two steps: one step that does not take the weights into account, applied if $V^j_t \leq \varepsilon$, and another step that uses the weights, applied if $V^j_t \geq \varepsilon$. This perspective allows to introduce an approximate resampling scheme represented by the process $(A_i')_{i \geq 0}$ described below.

For each time $t$, define $A_t : j \in \{1, \ldots, N\} \mapsto a^j_t \in \{1, \ldots, N\}$ and then $A_t' : \{1, \ldots, N\} \rightarrow \{1, \ldots, N\}$ as follows. For all $j$ in $C_t = \{k \in \{1, \ldots, N\} : V^k_t \leq \varepsilon\}$, set $A_t'(j) = a^j_t$. Order the $p$ remaining indices of the set $\{j \in \{1, \ldots, N\} : V^j_t > \varepsilon\}$ into $\{j_1 < \cdots < j_p\}$, set $A_t'(j_i) = \inf(\{1, \ldots, N\} \backslash A_t(C_t))$ and then recursively $A_t'(j_k) = \inf(\{1, \ldots, N\} \backslash A_t'(C_t) \cup A_t'(j_1, \ldots, A_t'(j_{k-1})))$.

Such a function $A_t'$ almost surely maps to more unique values than $A_t$ by construction. It can be seen as a mixture of two steps, as described for $A_t$ above, but this time neither step relies on the values of the weights.

We write $|a|$ for the cardinal of the image of a function $a : \{1, \ldots, N\} \rightarrow \{1, \ldots, N\}$. In terms of the functions $(A_k)_{k \leq T-1}$, the full coalescence time $c_T$ can be defined as $c_T = \sup\{0 \leq k \leq T-1 : | A_k \circ A_{k+1} \cdots \circ A_{T-1} | = 1\}$, with the convention $c_T = 0$ in the event $| A_k \circ A_{k+1} \cdots \circ A_{T-1} | > 1$ for each $0 \leq k \leq T-1$, which almost surely satisfies $c_T \geq c_T'$ with $c_T' = \sup\{k \leq T-1 : | A'_k \circ A'_1 \circ \cdots \circ A'_{T-1} | = 1\}$.

Indeed since $A_t'$ maps to more unique values than $A_t$ at each time $t$, the quantity $| A'_k \circ \cdots \circ A'_{T-1} |$, counting the unique ancestors from generation $k$ of the particles at time $T$ when using the resampling scheme $A'$, is almost surely larger than $| A_k \circ \cdots \circ A_{T-1} |$ for any $k$, and hence it takes longer to reach the full coalescence time when using $A'$ compared to $A$.

Following Del Moral et al. (2009), Section 4 and Möhle (2004), the sequence $(K_k)_{k \geq 0} = (| A'_{T-k} \circ \cdots \circ A'_{T-1} |)_{k \geq 0}$ is a Markov chain in the filtration $(\mathcal{F}_k)_{k \geq 0}$ with

$$\mathcal{F}_k = \sigma(V^j_{1:N}, U^j_{1:N})_{T-k \leq t < T-1},$$

with the convention $K_0 = N$. For all $n \geq 0, q \in \{1, \ldots, N\}$ and $p < q$ its transition law verifies

$$p_{n,q} = P(K_{n+1} = q | K_n = q) = \frac{\sum_{q'=q-p+1}^{q} \binom{q}{q'} \varepsilon^q (1-\varepsilon)^{q'-q} \binom{n}{q'-q} \binom{q}{q'} \frac{(N)^{q-q+p}}{N^n}}$$

and $p_{n,q} = P(K_{n+1} = q | K_n = q)$

$$= \frac{\sum_{q'=0}^{q} \binom{q}{q'} \varepsilon^q (1-\varepsilon)^{q'-q} \binom{n}{q'-q} \binom{q}{q'} \frac{(N)^{q-q+p}}{N^n}}$$

(2)

where $\binom{q}{q'}$ is the Stirling number of the second kind giving the number of ways of partitioning the set $\{1, \ldots, q\}$ into $p$ non-empty blocks and where $(N)^p = N!/(N-p)!$. Note that Eq. (2) is a special case of Eq. (1).

Let us give more details on Eq. (1) and (2). First consider the expression of $p_{n,q}$. The index $q'$ represents the number of particles associated with realisations of $V_{T-k-1}$ being less than $\varepsilon$. Hence it is the number of particles of step $T-k-1$ for which the ancestor $A'_{T-k-1}$ was chosen according to the uniform distribution on $\{1, \ldots, N\}$; the remaining $q-q'$ ancestors are chosen deterministically; see the definition of $(A'_t)$. The term $\binom{q}{q'} \varepsilon^q (1-\varepsilon)^{q'-q}$ corresponds to the probability of obtaining $q'$ uniform draws of $V_{T-k-1}$ with values less than $\varepsilon$ among $q$ particles at time $T-k$. The term $(N)^{q-q+p} / N^n$ corresponds to the probability of these $q'$ ancestors, drawn uniformly on $\{1, \ldots, N\}$, landing on $q'$ unique values. Now consider the probability $P(K_{n+1} = p | K_n = q)$ for some $p < q$. For $K_n$ to fall from $q$ to $p$ at the next step, $q-p$ unique particles must disappear; since particles corresponding to $V_{T-k-1} > \varepsilon$ do not disappear, there must be at least $q-p+1$ particles corresponding to $V_{T-k-1} \leq \varepsilon$. Hence the index $q'$, still representing the number of particles with realisations of $V_{T-k-1}$ less than $\varepsilon$, now starts at $q-p+1$. The binomial term is similar to the case where $p = q$. Among the $q'$ particles with realisations of $V_{T-k-1}$ less than $\varepsilon$, $p' = p - (q-q')$ of them must choose unique ancestors and the other $q-p$ must coalesce. The Stirling number $\binom{q}{q'}$ indeed counts the number of partitions (groups of particles that will coalesce) of $\{1, \ldots, q'\}$ in $p'$ non-empty blocks (each corresponding to a unique ancestor).

Note that conditional upon $K_t = q$ there can be any number $I \in \{1, \ldots, q\}$ of variables $V^j_{1:T}$ falling under $\varepsilon$. We can write $E[K_{n+1} | K_n = q]$ as

$$\sum_{i=0}^{q} \sum_{j=0}^{q} \binom{q}{j} \varepsilon^j (1-\varepsilon)^{q-j} E[K_{n+1} | K_n = q, I = i]$$.
We now focus on $\mathbb{E}[K_{k+1} | K_k = q, I = i]$, the expected number of ancestors of $q$ different particles, given that $i$ of them choose their ancestors uniformly in $\{1, \ldots, N\}$ and that $q - i$ have a unique ancestor. Of course the difficulty comes from the random component, *id est* the $i$ particles that choose their ancestors uniformly. Introduce the process $(Z_k)_{k \geq 0}$ on $\mathbb{N}$ corresponding to the number of ancestors in a scheme using only those uniform selections, which is equivalent to a multinomial resampling scheme with uniform weights. More formally the transition of $(Z_k)_{k \geq 0}$ satisfies

$$
P(Z_{k+1} = p | Z_k = q) = \binom{N}{p} \frac{q}{N^q}, \quad (3)
$$

following the same reasoning as for the transition probabilities of $(K_k)_{k \geq 0}$. The initial distribution of $Z_0$ is not used in the following hence we do not need to specify it. The link between $(Z_k)_{k \geq 0}$ and $(K_k)_{k \geq 0}$ is explicitly given by

$$
\mathbb{E}[K_{k+1} | K_k = q, I = i] = (q - i) + \mathbb{E}[Z_{k+1} | Z_k = i],
$$

so that we have

$$
\mathbb{E}[K_{k+1} | K_k = q] = q(1 - q) + \sum_{i=0}^{q} \binom{q}{i} q^i (1 - q)^{q-i} \mathbb{E}[Z_{k+1} | Z_k = i]. \quad (4)
$$

Note that the process $(Z_k)_{k \geq 0}$ is not used in the proof of Theorem 1, where we start from $(K_k)_{k \geq 0}$ again, but is pivotal for the proof of Theorem 2.

### 3.3 Distance to the most recent common ancestor

We start with the proof of Theorem 1. We define a Markov chain $(L_k)_{k \geq 0}$ on $\mathbb{N}$ such that $L_0 = N$ and its transition satisfies

$$
P(L_{k+1} = q - 1 | L_k = q) = \sum_{p < q} \mathbb{P}(K_{k+1} = p | K_k = q)
$$

and thus for all $k \geq 0$ and $p \leq q$

$$
P(L_{k+1} = p | L_k = q) = \begin{cases} p_{N,q} & \text{if } p = q, \\ 1 - p_{N,q} & \text{if } p = q - 1, \end{cases}
$$

where $p_{N,q}$ is defined in Eq. (2). In addition we couple $(L_k)_{k \geq 0}$ and $(K_k)_{k \geq 0}$ by assuming

- $[L_k = K_k] \Rightarrow [L_{k+1} < L_k \Leftrightarrow K_{k+1} < K_k]$ (if the two chains are at the same point, then if one of them decreases, the other one decreases too)
- $[L_k \neq K_k] \Rightarrow K_{k+1}$ and $L_{k+1}$ are independent, conditionally upon $L_k, K_k$.

By construction $L_k \geq K_k$ for all $k \geq 0$ almost surely. Hence $c_T^k \geq T - \delta_T$ with $\delta_T = \inf\{k \geq 1 : L_k = 1\}$ and thus $d_T = T - c_T^k \leq T - c_T^k \leq \delta_T$ almost surely.

For $q = 2, \ldots, N$ denote by $J_q^{(N)}$ the time required for $(L_k)_{k \geq 0}$ to jump from $q$ to $q - 1$. Each $J_q^{(N)}$ follows a geometric law with parameter $(1 - p_{N,q})$ and $\mathbb{E}[\delta_T] = \sum_{q=2}^{N} p_{N,q} - 1$. To conclude, we manipulate this sum as follows. For any $k = 1, \ldots, N$ a crude bound on $(N)_k/N^k$ is given by $\exp(-k/2N)$, from which we obtain

$$
p_{N,q} \leq \left(1 - \frac{(1 - e^{-1/2N})^q}{q}\right).
$$

We have, for all $N$, $(8N)^{-1} \leq 1 - \exp(-1/2N)$ and for all $x \geq 1$ and $\epsilon \in (0, 1)$, $(1 - \epsilon/x)^x \leq \exp(-\epsilon)$; combining these inequalities we obtain

$$
\mathbb{E}[\delta_T] \leq \sum_{q=2}^{N} (1 - \alpha^{\alpha/N})^{-1}
$$

where $\alpha = \exp(-\epsilon/8)$. We can now bound this series by expanding $\alpha^{\alpha/N} = \exp\{(q/N) \log \alpha\}$ into an alternating series and by bounding the alternating series always by one of its partial sums:

$$
\sum_{q=2}^{N} (1 - \alpha^{\alpha/N})^{-1} \leq \sum_{q=2}^{N} \left(\frac{q}{N}(- \log \alpha) - \frac{1}{2!} \left(\frac{q}{N}\right)^2 (\log \alpha)^2\right)^{-1}
$$

$$
\leq - \frac{N}{\log \alpha} \log N + (N - 1) \leq \left(1 + \frac{8}{\epsilon}\right) N \log N,
$$

which concludes the proof of Theorem 1.

Note that bounding $(K_k)_{k \geq 0}$ by $(L_k)_{k \geq 0}$ almost surely seems very crude, since $K_0$ can possibly jump from $q$ to $p < q$ in one step whereas $L_k$ can only jump from $q$ to $q - 1$. However the time to coalescence is mostly dominated by the final jumps, because the probabilities $\mathbb{P}(K_{k+1} = p | K_k = q)$ are close to 0 when $N$ is large compared to $q$ and $p < q$. In other words after a few time steps, $q$ is small compared to $N$ and then $(K_k)_{k \geq 0}$ mostly jumps from $q$ to $q - 1$ if it jumps at all, so that $(L_k)$ provides an accurate bounding process. The additional approximations used to bound $p_{N,q}$ and thus $\mathbb{E}[\delta_T]$ are also to be considered in the regime of small $q$ compared to $N$, where they prove accurate enough to obtain the desired result in $N \log N$.

### 3.4 Number of nodes in the ancestry tree

We now proceed to the proof of Theorem 2. Denote by $m_T$ the number of nodes in the crown. The bound on $d_T$ from Theorem 1 gives a first crude bound

$$
\mathbb{E}[m_T] \leq \Delta_1 N^2 \log N
$$
which is obtained by bounding the size of every generation in the crown by $N$. However we can obtain a better bound, in $N \log N$, by the following arguments.

The process $(K_k)_{k \geq 0}$ was already introduced to bound $E[dt]$ but we can naturally use it to bound $E[mt]$ since

$$mt \leq \sum_{k=0}^{\tau_r} K_k$$

almost surely, where $\tau_r = \inf \{k \leq T : K_k = 1\}$; note that $\tau_r = T - c_r$. To bound $E[K_k]$ we use the chain $(Z_k)_{k \geq 0}$ defined by Eq. (3). By definition of $(Z_k)_{k \geq 0}$ and denoting by $(C_j)_{j=1}^N$ independent uniform variables in $\{1, \ldots, N\}$, we have

$$E[Z_{k+1} | Z_k = q] = E[N \sum_{j=1}^{N} \mathbb{I}_{\{k \in \{1, \ldots, q\}; C_k = j\}]$$

$$= N - N \sum_{j=1}^{N} E[\mathbb{I}_{\{k \in \{1, \ldots, q\}; C_k \neq j\}]}$$

$$= N - N \left(1 - \frac{1}{N}\right)^q$$

which, using Eq. (4), implies

$$E[K_{k+1} | K_k = q] = q(1 - \varepsilon) + N \left(1 - \left(\frac{1 - \varepsilon}{N}\right)^q\right).$$

By expanding $(1 - (1 - \varepsilon/N)^q)$ into its alternating series and bounding the series by its third partial sum, we obtain

$$E[K_{k+1} | K_k = q] \leq q - \frac{\varepsilon^2}{2N} q(q - 1) + \frac{\varepsilon^3}{6N^2} q(q - 1)(q - 2).$$

Now for $x \in [1, N]$ define the function $g_{N, \varepsilon}$ by:

$$g_{N, \varepsilon}(x) = x - \frac{\varepsilon^2}{2N} (x - 1) + \frac{\varepsilon^3}{6N^2} x(x - 1)(x - 2).$$

Noting that $g_{N, \varepsilon}$ is concave and using Jensen’s inequality, we obtain

$$E[K_{k+1}] = E[E[K_{k+1} | K_k]] \leq g_{N, \varepsilon}(E[K_k]).$$

Introduce the sequence $u_0 = N$, and $u_{n+1} = g_{N, \varepsilon}(u_n)$ for $n > 0$. By the above inequality and because $g_{N, \varepsilon}$ is nondecreasing, we have $E(K_k) \leq u_k$ for all $k$. We can finally bound the expected number of nodes in the crown as follows

$$E \left[ \sum_{k=0}^{\tau_r} K_k \right] = E \left[ \sum_{k=0}^{\tau_r} (K_k - 1) \right] + \tau_r$$

$$\leq \sum_{k=0}^{\tau_r} (u_k - 1) + \tau_r$$

using Theorem 1 to bound $E[\tau_r]$. We use the following technical lemma to bound $\sum_{k=0}^{\tau_r} (u_k - 1)$.

**Lemma 1** Let $N \in \mathbb{N}$, $N \geq 6$ and $\varepsilon \in (0, 1)$. Consider the sequence $(u_k)_{k \geq 0}$ such that $u_0 = N$ and for $k \geq 1$

$$u_k = u_{k-1} - \frac{\varepsilon^2}{2N} u_{k-1}(u_{k-1} - 1) + \frac{\varepsilon^3}{6N^2} u_{k-1}(u_{k-1} - 1)(u_{k-1} - 2).$$

Then there exists $C > 0$ independent of $N$ such that

$$\sum_{k=0}^{\tau_r} (u_k - 1) \leq CN \log N.$$

The proof of Lemma 1, based on elementary real analysis, is given in Appendix A. Using Lemma 1 and Eq. (8) we obtain Theorem 2 with $\Delta_2 = C + \Delta_1$.

### 4 Numerical experiments

This section provides numerical experiments to illustrate the results of Section 3 and the efficiency of the algorithms presented in Section 2. The results summarise $K = 500$ independent runs, using $N = 128$ particles and $T \leq 1000$ time steps. For each run, a new synthetic dataset is generated and a different random seed is used. The default resampling scheme is the multinomial scheme, applied at every time step. The algorithms of Section 2 have been implemented in LibBi (Murray, 2013, www.libbi.org), which is used for the numerical results here.

We use the Phytoplankton-Zooplankton (PZ) model described in Jones et al (2010) and Murray et al (2012). Concentrations of phytoplankton ($P$) and zooplankton ($Z$), along with the stochastic growth rate of phytoplankton ($\alpha_t$), constitute the hidden state. The state follows the continuous-time dynamics $dP/dt = \alpha_t P - cPZ$ and $dZ/dt = eCZ - m_t Z - m_Z Z^2$, with $\alpha_t \sim \mathcal{N}(\mu, \sigma^2)$ drawn at every integer time $t$. The initial conditions are $log P_0 \sim \mathcal{N}(\log(2), 0.2)$, $log Z_0 \sim \mathcal{N}(\log(2), 0.1)$. The observations $(I_t)$ measure $(P, Z)$ with additive log-normal noise, that is $log Y_t \sim \mathcal{N}(log P_t, \sigma_t)$. The parameters are set to $\mu = 0.4$, $\sigma = 0.2$, $\varepsilon = 0.25$, $\epsilon = 0.3$, $m_t = m_q = 0.1$ and $\sigma_t = 0.2$.

Lemma 2 is illustrated by plots of the adjusted number of nodes defined by $\tilde{N} = (n_T - T)/N$ for various $N$ against $T$ on Fig. 2(a) and for various $T$ against $N$ on Fig. 2(b). The quantity is averaged over $K$ independent runs. According to the lemma $\tilde{N}$ should be uniformly bounded as a function of $T$ and should grow logarithmically as a function of $N$; this is confirmed by the graphs. Figure 3(a) shows that a similar behaviour is expected for other resampling schemes such as stratified and systematic, only with a different value for $\Delta_2$.

To illustrate the efficiency of the procedures presented in Section 2, Fig. 3(b) shows the combined time taken to execute the pruning and insertion algorithms at each time step, for various $T$ and $N$. The results suggest that the computational cost is not greatly influenced by $T$, and close to linear with respect to $N$: evidence of a practical implementation with comparable complexity to the particle filter itself.
Fig. 2 Adjusted number of nodes \( \tilde{n}_T = (n_T - T)/N \) against \( T \), for various methods.

5 Conclusion

We have presented a bound on the expected number of nodes in the ancestry tree produced by particle filters. The numerical experiments of Section 4 indicate that the result is accurate, even outside the scope of the assumptions made in the theoretical study, and that the proposed algorithm to store the tree is computationally efficient.

A Proof of Lemma 1

Let \( N \in \mathbb{N} \) and \( \varepsilon \in (0, 1) \), define \( (u_k)_{k \geq 0} \) as in the statement of the lemma and define \( g_{N, \varepsilon} \) as in Eq. (6). We are interested in \( \sum_{k \geq 0} u_k \). Note first that \( g_{N, \varepsilon} \) is contracting and is such that \( g_{N, \varepsilon}(1) = 1 \), so that \( u_k \) goes to 1 using Banach fixed-point theorem. The contraction coefficient of \( g_{N, \varepsilon} \) can be bounded by

\[
\sup_{x} |g'_{N, \varepsilon}(x)| \leq g_{N, \varepsilon}(1) = 1 - \frac{\varepsilon^2}{2N} < 1,
\]

however this contraction coefficient depends on \( N \) and a direct use of it yields a bound on \( \sum_{k \geq 0} u_k - 1 \) that is not in \( N \log N \).

Note also that even though \( u_k \) goes to 1, we can focus on the partial sum \( \sum_{k=0}^{n} u_k - 1 \) where \( \sigma_2 = \inf \{ k : u_k \leq 2 \} \), because \( \sum_{k=\sigma_2}^{n} u_k - 1 \) is essentially bounded by \( N \). Indeed note that for \( 1 \leq u \leq 2 \) we have

\[
(u^3/6N^2)u(u-1)(u-2) \leq 0 \quad \text{so that}
\]

\[
u_k - 1 \leq u_{k-1} - 1 - \frac{u^3}{2N}u_{k-1}(u_k - 1) \leq (u_{k-1} - 1)(1 - \frac{\varepsilon^2}{2N}),
\]

hence \( \sum_{k=0}^{\sigma_2} (u_k - 1) \leq (2N/\varepsilon^2) \). Therefore we can focus on bounding \( \sum_{k=\sigma_2}^{m} (u_k - 1) \) by \( N \log N \). Let us split this sum into partial sums, where the first partial sum is over indices \( k \) such that \( N/2 \leq u_k \leq N \); the second is over indices \( k \) such that \( N/4 \leq u_k \leq N/2 \), etc. More formally, we introduce \( (k_j)_{j=0} \) such that \( k_0 = 0 \), \( k_1 = \inf \{ k : u_k \leq N/2 \} \), \ldots , \( k_j = \inf \{ k : u_k \leq N/2^j \} \) or equivalently \( \log N/\log 2^j \leq k_j \leq j \). For instance we take \( J = \lfloor \log N/\log 2 \rfloor \). Thus we have split \( \sum_{k=0}^{m} (u_k - 1) \) into \( J \) partial sums of the form \( \sum_{k=0}^{k_j-1} (u_k - 1) \) and we are now going to bound each of these partial sum by the same quantity \( C(e)N \) for some \( C(e) \) that depends only on \( e \).

To do so, we consider the time needed by \( (u_k)_{k \geq 0} \) to decrease from a value \( N/m_j \) to a value \( N/m_{j+1} \), with \( m_j > m_{j+1} \); we will later take \( m_j = 2^j \) and \( m_{j+1} = 2^{j+1} \). Note that for any \( m \) we have

\[
\sum_{k=0}^{N/m} \frac{N}{m} \left( 1 - \frac{1}{m} \left[ \frac{e^3}{2N} + \frac{me}{6m} + \frac{e^3}{2N} + \frac{me^3}{3N^2} \right] \right).
\]

Define

\[
\beta(N, m, e) = \frac{e^3}{2N} + \frac{me}{6m} + \frac{e^3}{2N} + \frac{me^3}{3N^2}.
\]
and note that for any $N \geq 6$ and $m \leq N/2$ we have
\[
\beta(x) := \frac{e^x}{4} \leq \beta(N, m, \epsilon),
\]
which is clear upon noticing that $\beta(N, m, \epsilon)$ as a function of $m$ on $[1, N/2]$ is concave and thus reaches its minimum in 1 or $N/2$ (and this minimum is greater than $e^x/4$, provided $N \geq 6$). For any $x \geq N/m_{j+1}$ we can check that
\[
g_{N, x}(x) \leq \frac{g_{N,x}(N/m_{j+1})}{N/m_{j+1}} \times x
\]
by noticing that $g_{N, x}$ is concave and that $g_{N, x}(x) \leq N$ for all $x \in [0, N]$. Hence for $k \geq 0$ such that $u_{k-1} \geq N/m_{j+1}$, we have
\[
u_k \leq \left(1 - \frac{1}{m_{j+1}} \beta(x)\right) u_{k-1}.
\]
Now suppose that for some $k_j \geq 0$ we have $u_{k_j} \leq N/m_j$. Then let us find $K$ such that $u_{k_j+K} \leq N/m_{j+1}$. It is sufficient to find $K$ such that
\[
\left(1 - \frac{1}{m_{j+1}} \beta(x)\right) \frac{N}{m_j} \leq \frac{N}{m_{j+1}}
\]
\[
\Leftrightarrow K \geq \log \frac{m_{j+1}}{m_j} \left(-\log \left(1 - \frac{1}{m_{j+1}} \beta(x)\right)\right)^{-1}.
\]
Finally by using
\[
\forall x \in (0, 1) \quad \frac{1}{x} - 1 \leq -\log(1-x) \leq \frac{1}{x}
\]
we conclude that $K$ defined as
\[
K = \left[\log \frac{m_{j+1}}{m_j} \frac{m_{j+1}}{\beta(x)}\right]
\]
guarantees the inequality $u_{k_j+K} \leq N/m_{j+1}$. In other words $(u_k)_{k \geq 0}$ needs less than $K$ steps to decrease from $N/m_j$ to $N/m_{j+1}$. Summing the terms between $k_j$ and $k_j + K$, we obtain
\[
\sum_{k=k_j}^{k_j+K} u_k \leq K \frac{N}{m_j} \leq \left[\log \frac{m_{j+1}}{m_j} \frac{m_{j+1}}{\beta(x)} + 1\right] \frac{N}{m_j}.
\]
Taking $m_j = 2^j$ and $m_{j+1} = 2^{j+1}$, we have $k_j + K \leq k_j + K$ and thus obtain
\[
\sum_{k=k_j}^{k_j+K} u_k \leq \left(2 \log \frac{2}{\beta(x)} + 1\right) N = C(\epsilon)N
\]
with $C(\epsilon)$ independent of $N$. We have thus bounded the full sum by
\[
\sum_{k=0}^{k_j} (u_k - 1) \leq \sum_{k=0}^{k_j} (u_k - 1) \leq \sum_{k \geq 0} \rho_k (u_k - 1) \leq \log N \log 2 \leq D(\epsilon) N \log N
\]
for some $D(\epsilon)$ independent of $N$.

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