How to generate the tip of branching random walks evolved to large times

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Abstract – In a branching process, the number of particles increases exponentially with time, which makes numerical simulations for large times difficult. In many applications, however, only the region close to the extremal particles is relevant (the "tip"). We present a simple algorithm which allows to simulate a branching random walk in one dimension, keeping only the particles that arrive within some distance of the rightmost particle at a predefined time T. The complexity of the algorithm grows linearly with T. We can furthermore choose to require that the realizations have their rightmost particle arbitrarily far on the right from its typical position. We illustrate our algorithm by evaluating an observable for which no other practical method is known.

Introduction. – The branching Brownian motion (BBM) [1] and branching random walks (BRW) are stochastic processes [2] describing the time evolution of increasingly many particles characterized by their spatial positions [3]. These processes, supplemented or not by some selection mechanism [4], can model a range of phenomena in different fields of science, including physics [5], biology [6] and chemistry [7], computer science [8], and even economics [9].

In many applications of these branching processes in one space dimension, it is important to characterize the "tip" of the process, *i.e.*, the distribution of particles close to the rightmost particle, in typical and in rare events [10–12]. Many properties of the tip can be deduced from solutions to nonlinear evolution equations; in the case of the BBM, the relevant equation [13] is a partial differential equation named after Fisher, Kolmogorov, Petrovsky, Piscounov [14,15] (FKPP):

$$\partial_t u = \frac{1}{2}\partial_x^2 u + u - u^2. \tag{1}$$

For instance, the quantity $\mathbb{P}(R_t \geq x)$, with R_t the position of the rightmost particle at time t, is given by the solution to (1) for a step initial condition $u(0, x) = \mathbb{1}_{\{x \leq 0\}}$. More sophisticated observables can also be expressed; for example, if n is the number of particles at time T on the right of $R_T - a$, then one can show [10] that $\langle e^{-\lambda n} \rangle = 1 - \int \mathrm{d}x\, \partial_a u(T, x)$, where $u(t, x)$ is the solution to (1) with initial condition $u(0, x) = \mathbb{1}_{\{x \leq 0\}} + (1 - e^{-\lambda})\mathbb{1}_{\{x \in (0,a]\}}$.

This method has however some limitations: obtaining the tail of the distribution of n is impractical; other observables, such as the genealogical tree of the rightmost particles [16] cannot be obtained in this way.

Because the number of particles in a branching process increases exponentially fast with time, direct Monte Carlo simulations are ill-suited except for small times. Furthermore, they would not allow to study rare events in which the rightmost particle sits at a position very different from its expected position.

In this letter, we present an algorithm designed to only generate the particles ending in an interval $[X - \Delta, +\infty)$ at time T, in unbiased realizations conditioned to either possess at least one particle to the right of X, or to have their rightmost particle at position X exactly. This algorithm allows to study the properties of the

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tip in rare or typical realizations evolved to very large times.

While reminiscent of the classical spinal decomposition of the BBM [17,18], our method is actually quite different as we follow a tree of "special" particles.

We shall start by exposing the algorithm in the case of a particular BRW which is easy to implement numerically. In a second section, we provide a formulation for the BBM. A third section exposes briefly a variant of our algorithm, and we conclude by showing the numerical calculation of an observable for which the algorithm is especially efficient.

Generating realizations of a BRW with a particle beyond a given point. – We consider a branching random walk (BRW) on a spatial lattice with step δx, and in discrete time with step δt. The system starts at time $t = 0$ with one single particle at the origin. During each time step, a particle in the system evolves with the following rules: it can

$$
\begin{cases}
\llcorner\!\bullet\!\widehat{~} & \text{jump from } x \text{ to } x + \delta x, & \text{probability } p_r, \\
\widehat{~}\!\bullet\!\lrcorner & \text{jump from } x \text{ to } x - \delta x, & \text{probability } p_l, \\
\bullet\!\prec^{\bullet}_{\bullet} & \text{duplicate without moving,} & \text{probability } r,
\end{cases}
$$

with $p_l + p_r + r = 1$. When a particle duplicates (or branches), it is replaced by two particles at the same position which evolve independently afterwards.

We let R_t be the position of the rightmost particle at time t, and we introduce $u(t, x) = \mathbb{P}(R_t \geq x)$. The probability u satisfies the following discretization of (1):

$$
\begin{aligned}
u(t + \delta t, x) = {}& p_r u(t, x - \delta x) + p_l u(t, x + \delta x) \\
& + r u(t, x)[2 - u(t, x)],
\end{aligned} \tag{2}
$$

with initial condition $u(0, x) = \mathbb{1}_{\{x \leq 0\}}$.

From standard results on FKPP [19], u evolves at large time as a front centered around position $m_t = \langle R_t \rangle$. (We use $\langle \cdot \rangle$ to denote expectations.) When t is large, $m_t = v_0 t - \frac{3}{2\gamma_0} \log t + \text{const} + o(1)$, where v_0 and γ_0 are given by $v_0 = v(\gamma_0) = \min_\gamma v(\gamma)$, with $v(\gamma) = \frac{1}{\gamma \, \delta t} \log(p_r e^{\gamma \, \delta x} + p_l e^{-\gamma \, \delta x} + 2r)$; for a review see [20].

Pick a time horizon T and a target X. We introduce "red particles" in the BRW in the following way:

Definition 1. *A particle is red if its rightmost offspring at time T lies in $[X, \infty)$.*

A first goal of the algorithm is to follow the trajectories of all the red particles in the BRW conditioned on the event that the initial particle is red. The algorithm works for typical realizations if $X - m_T = \mathcal{O}(1)$ or for rare events if $X - m_T \gg 1$.

Introduce $U(t, x)$ as the probability that a given particle at (t, x) is red. By definition of u:

$$
U(t, x) := \mathbb{P}(\bullet \text{ is red}) = u(T - t, X - x). \tag{3}
$$

The probability that a particle at (t, x) is red and jumps to the lattice site on its right is

$$
\mathbb{P}(\llcorner\!\bullet\!\widehat{~}; \bullet \text{ is red}) = p_r U(t + \delta t, x + \delta x).
$$

(We write $\mathbb{P}(A; B)$ to mean $\mathbb{P}(A \text{ and } B)$.) Then, the probability that the particle at (t, x) jumps right given that it is red can be written as

$$
\mathbb{P}(\llcorner\!\bullet\!\widehat{~} \mid \bullet \text{ is red}) = p_r \frac{U(t + \delta t, x + \delta x)}{U(t, x)}. \tag{4}
$$

(We write $\mathbb{P}(A \mid B) = \mathbb{P}(A; B)/\mathbb{P}(B)$ for the conditional probability of A given that B is realized.) Similarly, the conditional probability of jumping left is

$$
\mathbb{P}(\widehat{~}\!\bullet\!\lrcorner \mid \bullet \text{ is red}) = p_l \frac{U(t + \delta t, x - \delta x)}{U(t, x)}. \tag{5}
$$

We now turn to branching. Consider a particle branching at (t, x), being thus replaced by two children at $(t + \delta t, x)$. The probability that both these children are red is $U(t + \delta t, x)^2$ and the probability that exactly one of them is red is $2U(t + \delta t, x)[1 - U(t + \delta t, x)]$. Thus, the probability to be red and branch into two red is

$$
\mathbb{P}\left(\bullet\!\prec^{\bullet \text{red}}_{\bullet \text{red}}; \bullet \text{ is red}\right) = r U(t + \delta t, x)^2,
$$

and the conditional probability is

$$
\mathbb{P}\left(\bullet\!\prec^{\bullet \text{red}}_{\bullet \text{red}} \mid \bullet \text{ is red}\right) = r \frac{U(t + \delta t, x)^2}{U(t, x)}. \tag{6}
$$

Similarly, the conditional probability, given that it is red, that a particle branches into one red and one non-red is

$$
\mathbb{P}\left(\bullet\!\prec^{\bullet \text{red}}_{\bullet \text{non-red}} \mid \bullet \text{ is red}\right) =
$$
$$
r \frac{2U(t + \delta t, x)[1 - U(t + \delta t, x)]}{U(t, x)}. \tag{7}
$$

One checks with (2) that the sum of the conditional probabilities in (4), (5), (6) and (7) is 1. With these equations, it is possible to generate realizations of the trajectories of all the red particles given that the initial particle is red: we simply start with a red particle at $x = 0$; then, any red particle can either jump right or left with probabilities (4) and (5), branch into two red with probability (6) or do nothing with probability (7). (In the latter case, the particle is actually branching into a red particle and a non-red particle that we ignore.) The price to be paid is that the probabilities of the different events are now time- and space-dependent.

The mechanism can be extended to furthermore follow the trajectories of all the particles arriving in $[X - \Delta, X)$ for some length Δ. Introduce orange and blue particles:

Definition 2. *A particle is orange if its rightmost offspring at time T lies in $[X - \Delta, X)$.*

Definition 3. *A particle is blue if its rightmost offspring at time T lies in $(-\infty, X - \Delta)$.*

(Then, all non-red particles are either orange or blue.) Introduce $V_\Delta(t, x)$ as the probability that a particle at
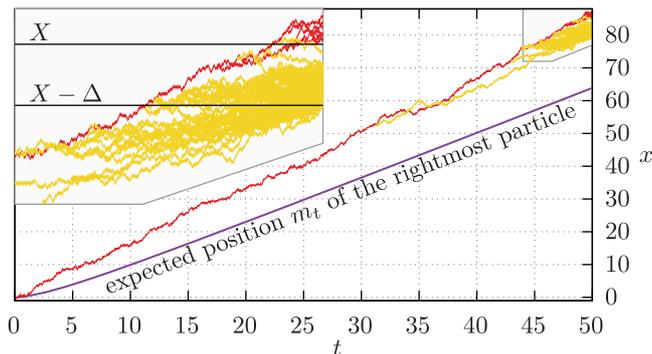
Fig. 1: A realization of the red (dark) and orange (light) particles in the BRW up to $T = 50$ with $X = 85.1 \simeq m_T + 3\sqrt{T}$ and $\Delta = 5$, compared to the curve m_t. The inset is a zoom of the final times.

(t, x) is orange. By definition of u and U, one has

$$V_\Delta(t, x) := \mathbb{P}(\bullet \text{ is orange}) = U(t, x + \Delta) - U(t, x).$$

An orange particle can be created by the branching of a red particle: we replace (7) by the probability for a red to branch into a red and an orange

$$\mathbb{P}\left(\bullet\kern-0.3em\raise0.5ex\hbox{$\scriptstyle\diagup$}\kern-0.5em\lower0.5ex\hbox{$\scriptstyle\diagdown$}\begin{matrix}\bullet\text{red}\\ \bullet\text{orange}\end{matrix} \;\middle|\; \bullet \text{ is red}\right) = r\frac{2U(t + \delta t, x)V_\Delta(t + \delta t, x)}{U(t, x)}, \tag{8}$$

and the probability to branch into a red and a blue

$$\mathbb{P}\left(\bullet\kern-0.3em\raise0.5ex\hbox{$\scriptstyle\diagup$}\kern-0.5em\lower0.5ex\hbox{$\scriptstyle\diagdown$}\begin{matrix}\bullet\text{red}\\ \bullet\text{blue}\end{matrix} \;\middle|\; \bullet \text{ is red}\right) =$$
$$r\frac{2U(t + \delta t, x)[1 - U(t + \delta t, x + \Delta)]}{U(t, x)}. \tag{9}$$

Once orange particles are created, we need to follow their trajectories. Conditioned on the event that a particle is orange, the probabilities that it jumps right, jumps left or branches into two orange particles are given, respectively, by (4), (5) and (6) with U replaced by V_Δ. The probability that an orange branches into one orange and one blue is, similarly to (9), $r \times 2V_\Delta(t + \delta t, x)[1 - U(t + \delta t, x + \Delta)]/V_\Delta(t, x)$.

To implement our algorithm, we represent the state of the system at a given time t by two arrays indexed by x containing the numbers of red and orange particles. To forward the system to time $t + \delta t$, one observes that on each site in each set, the numbers of particles undergoing the different possible events obey multinomial laws with parameters that we can compute from $u(t, x)$. This requires to integrate numerically (2) before the event generation begins.

We have set the probabilities of the elementary processes to $r = \delta t$, $p_r = p_l = \frac{1}{2}(1 - \delta t)$, and the lattice sizes to $\delta t = 0.01$ and $\delta x = 0.1$; with this choice of parameters, the BRW is a discretized version of the BBM. A realization of this conditioned BRW is displayed in fig. 1.

In order to validate our algorithm and its implementation, we have measured the expected number of particles
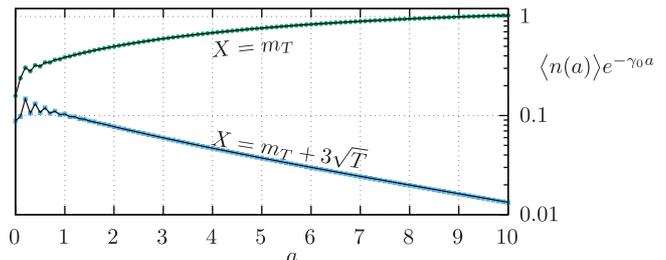

Fig. 2: The expected number $\langle n(a) \rangle$ of particles at site $R_T - a$, multiplied by $e^{-\gamma_0 a}$ (where $\gamma_0 = 1.43195\ldots$ in the model used here), as a function of a, for $T = 400$ and two values of X. The dots are obtained from $3\,10^6$ realizations of the algorithm outlined in this letter. The lines are from a numerical integration following the methods of [10]. For $a = 0$, we have removed 1 to the count of particles.

at distance a from the lead particle, because this quantity can also be evaluated from the formalism developed in [10] by solving numerically an equation related to (2). (See also the discussion in the introduction.) The results displayed in fig. 2 show a perfect agreement between both methods within statistical uncertainties.

Continuous limit: conditioning the BBM. – The branching Brownian motion (BBM) is the continuous version of the BRW. The particles in a BBM perform independent Brownian motions and branch with rate 1 (so that during each infinitesimal time dt, each particle is replaced by two particles with probability dt).

The method described in the previous section can be adapted to the BBM; the goal is not necessarily to generate realizations, but to offer a starting point to analytical studies of the tip in typical and extreme events.

Introduce as before $u(t, x) = \mathbb{P}(R_t \geq x)$ as the probability that the rightmost particle at time t is on the right of x. It satisfies the FKPP equation (1) with initial condition $u(0, x) = \mathbb{1}_{\{x \leq 0\}}$. Introduce also red particles in the BBM, as in the BRW. The probability that a particle is red is still $U(t, x) = u(T - t, X - x)$. We first consider the probability that a particle, conditioned to be red, branches into two red particles between t and $t + \delta t$. The reasoning leading to (6) is still valid and gives, to leading order in δt,

$$\mathbb{P}\left(\bullet\kern-0.3em\raise0.5ex\hbox{$\scriptstyle\diagup$}\kern-0.5em\lower0.5ex\hbox{$\scriptstyle\diagdown$}\begin{matrix}\bullet\text{red}\\ \bullet\text{red}\end{matrix} \;\middle|\; \bullet \text{ is red}\right) = \delta t\, U(t, x) + \mathcal{O}(\delta t^2). \tag{10}$$

(Compare to (6) with $r = \delta t$.) Similarly, the conditional probability for branching into a red and a non-red is

$$\mathbb{P}\left(\bullet\kern-0.3em\raise0.5ex\hbox{$\scriptstyle\diagup$}\kern-0.5em\lower0.5ex\hbox{$\scriptstyle\diagdown$}\begin{matrix}\bullet\text{red}\\ \bullet\text{non-red}\end{matrix} \;\middle|\; \bullet \text{ is red}\right) = \delta t\, 2[1 - U(t, x)] + \mathcal{O}(\delta t^2).$$

(Compare to (7).) We now turn to the motion of one single red particle during a time $\delta t \ll 1$. As branching occurs with small probability of order δt, we ignore this possibility in the discussion below. The probability that a particle at (t, x) moves during δt by $\Delta x \in [\epsilon, \epsilon + d\epsilon]$ (which

we write for short $\Delta x \in \mathrm{d}\epsilon$) and is red is

$$\mathbb{P}(\Delta x \in \mathrm{d}\epsilon\,;\,\bullet \text{ is red}) = \frac{e^{-\frac{\epsilon^2}{2\delta t}}}{\sqrt{2\pi\,\delta t}}\,\mathrm{d}\epsilon \times U(t+\delta t, x+\epsilon).$$

Dividing by $U(t,x)$ gives $\mathbb{P}(\Delta x \in \mathrm{d}\epsilon \mid \bullet \text{ is red})$; then, multiplying by ϵ and integrating over ϵ, we obtain after changing variable $\epsilon = z\sqrt{\delta t}$ and expanding for small δt,

$$\langle \Delta x \mid \bullet \text{ is red}\rangle = \delta t\,\partial_x \ln U(t,x) + \mathcal{O}(\delta t^2). \tag{11}$$

With (11) and (10), we thus obtain the following result:

The trajectories of the particles in a BBM ending on the right of X at time T, conditioned on the event that there is at least one of them, is a BBM with a space- and time-dependent drift $\partial_x \ln U(t,x)$ and a space- and time-dependent branching rate $U(t,x)$.

If orange particles are needed, one checks that a red particle branches out an orange particle at rate $2V_\Delta(t,x)$, that an orange particle branches into two orange at rate $V_\Delta(t,x)$ and that orange particles have a drift $\partial_x \ln V_\Delta(t,x)$.

There is another way to construct the tree of red particles in the BBM. Consider a particle at (t,x) and call (τ_1,ξ_1) the time and place of the next branching event (so that $\tau_1 > t$). One has, for $x_1 \in \mathbb{R}$ and $t_1 > t$,

$$\mathbb{P}(\tau_1 \in \mathrm{d}t_1;\,\xi_1 \in \mathrm{d}x_1) = e^{-(t_1-t)}\mathrm{d}t_1 \times \frac{e^{-\frac{(x_1-x)^2}{2(t_1-t)}}}{\sqrt{2\pi(t_1-t)}}\mathrm{d}x_1.$$

For $t_1 < T$, the probability that the particle that just branched is furthermore red is obtained by multiplying the right hand side by $U(t_1,x_1)[2-U(t_1,x_1)]$, the probability that at least one of the two children is red. Then, dividing by $U(t,x)$ we obtain the conditional probability

$$\mathbb{P}(\tau_1 \in \mathrm{d}t_1;\,\xi_1 \in \mathrm{d}x_1 \mid \bullet \text{ is red}) = e^{-(t_1-t)}\mathrm{d}t_1$$
$$\times \frac{e^{-\frac{(x_1-x)^2}{2(t_1-t)}}}{\sqrt{2\pi(t_1-t)}}\mathrm{d}x_1 \times \frac{U(t_1,x_1)[2-U(t_1,x_1)]}{U(t,x)}. \tag{12}$$

Note that this probability is not normalized: the integral of (12) on $x_1 \in \mathbb{R}$ and on $t_1 \in [t,T]$ is smaller than 1, and the remaining probability corresponds to the event that the next branching occurs after the time horizon T. In that case, the trajectory up to time T of the red particle is simply a Brownian motion (no branching) conditioned to finish on the right of X.

With (12) one can draw the coordinates (τ_1,ξ_1) of the next branching event. The trajectory between t and τ_1 is then a Brownian motion conditioned to be at position (τ_1,ξ_1). It remains to determine the type of branching at time τ_1. With no conditioning, the probability to branch into two red is U^2, writing for short U instead of $U(\tau_1,\xi_1)$, and the probability to branch into one red and one non-red is $2U(1-U)$. Then, given that the branching particle is red, the probability that it branches into two red is $U/(2-U)$. With the complementary probability, only one red particle remains. In either case, the algorithm is restarted from (τ_1,ξ_1).

Variant: fixing the exact position of the rightmost particle. – We briefly present a variant of our algorithm. The idea is to condition the red particles at time T to be *exactly* at position X, rather than in $[X,\infty)$. In the BRW, the probability for a particle at (t,x) to have its rightmost offspring at time T exactly on lattice site X is

$$\tilde{U}(t,x) := u(T-t, X-x) - u(T-t, X-x+\delta x).$$

Compare to (3). Then, following the same argument as above, the evolution probabilities for these "new red" particles are given by (4), (5), (6) and (8) with U replaced by $\tilde{U}$ and by (9) with the two U outside the square brackets replaced by $\tilde{U}$. With these new equations, one can follow the "new red" (and the orange) particles.

This variant is a bit more difficult to implement correctly, because it is harder to obtain a good numerical precision for $\tilde{U}$ than for U. Its advantage is that it allows to generate unbiased realizations of all the particles on the right of $R_T - \Delta$ in a BRW. To do this, for each realization, we first draw the value of R_T; as we need anyway to compute $u(T,x) = \mathbb{P}(R_T \geq x)$, this operation is easy. Then, we run the variant of our algorithm with $X = R_T$ to generate the "new red" particles (ending at X) and the orange particles (ending in $[X-\Delta, X)$). The resulting particles form an unbiased realization of the tip of the BRW.

For the BBM, the same variant can also be used; the probability of ending in $\mathrm{d}X$ is $\partial_x U(t,x)\,\mathrm{d}X$, and one finds that the "new red" particle follows a Brownian motion with drift $\partial_x \ln[\partial_x U(t,x)]$, compare to (11). This particle branches out particles conditioned to end to the left of X with rate $2[1-U(t,x)]$. (More precisely, it branches orange particles with rate $2V_\Delta(t,x)$ and blue particles with rate $2[1-U(t,x)-V_\Delta(t,x)] = 2[1-U(t,x+\Delta)]$.) It cannot branch into two "new red" particles, because there is a probability zero that a second particle ends up exactly at position X. This description of the BBM, with exactly one marked particle branching BBMs conditioned to not overtake it, is the same as the spine description [17].

Conclusion and outlook. – We have presented a simple algorithm to generate only the tip (the rightmost particles) in realizations of BRW in which the rightmost particle is constrained to be on the right of an arbitrary position X at an arbitrary time T or, in a variant, to be exactly at X. We have validated it by comparing Monte Carlo calculations obtained with this algorithm to predictions obtained by a different method.

When X is large compared to the expected position m_T of the rightmost particle at time T, our algorithm allows to study rare realizations. When X is close to m_T, it allows to generate more typical realizations.

Our algorithm enables the study of observables of the tip region of the BRW for which no other method is available to date. For example, we have measured numerically the distribution of the number of particles at distance a to
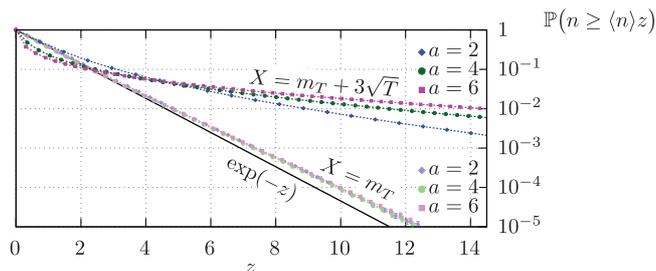
Fig. 3: Rescaled tail distribution $\mathbb{P}(n \geq \langle n \rangle z)$ as a function of z for the number n of particles at position $R_T - a$ with $T = 400$, for two values of X and three values of a. These probabilities were measured from the same realizations as for fig. 2. The distribution of n is roughly exponential for $X = m_T$, but it exhibits a much fatter tail when $X = m_T + 3\sqrt{T}$.

the left of the rightmost, in typical and rare realizations, see fig. 3, and this will allow to check a recent heuristic calculation in [21].

Among the further developments made possible by this algorithm, we intend to investigate observables such as the distribution of the genealogical tree of the particles in the tip [16,22].

While our main focus has been the BRW, we have also given a theoretical description of the conditioned BBM which may be useful to give a mathematical description of the tip along lines similar to [11].

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