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Joint statistics of space and time exploration of $1d$ random walks

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The statistics of first-passage times of random walks to target sites has proved to play a key role in determining the *kinetics* of space exploration in various contexts. In parallel, the number of distinct sites visited by a random walker and related observables have been introduced to characterize the *geometry* of space exploration. Here, we address the question of the *joint* distribution of the first-passage time to a target and the number of distinct sites visited when the target is reached, which fully quantifies the coupling between kinetics and geometry of search trajectories. Focusing on 1-dimensional systems, we present a general method and derive explicit expressions of this joint distribution for several representative examples of Markovian search processes. In addition, we obtain a general scaling form, which holds also for non Markovian processes and captures the general dependence of the joint distribution on its space and time variables. We argue that the joint distribution has important applications to various problems, such as a conditional form of the Rosenstock trapping model, and the persistence properties of self-interacting random walks.

Quantifying the efficiency of space exploration by random walkers is a key issue involved in a variety of situations. Applications range from reactive particles diffusing in the presence of catalytic sites, living organisms looking for resources, to robots cleaning or demining a given area [1–3]. In this context, two important classes of observables have been considered.

First, the statistics of first-passage times (FPTs) to target sites of interest has proved to play a key role in determining the *kinetics* of space exploration [4–6]. The case of first-passage times in confined domains was found to be particularly relevant to assess the efficiency of target search processes, and has led to an important activity [7–10]. Related observables, such as the cover time of a domain [11–13] or the occupation time of a sub domain have also been considered in this context [14–17].

A second class of observables has been introduced to characterize the *geometry* of the territory explored by random walkers. In particular, the number of distinct sites visited (or the so called Wiener sausage in a continuous setting) by a random walker after n step, which quantifies the overall territory swept by the random walker, has been the focus of many studies with a broad range of applications [1, 18–20]. Notable extensions include the number of distinct sites visited by p independent walkers [19], the case of fractal geometries [21, 22], or the case of random stopping times [23–26].

Even if it is clear that both classes of observables are coupled, so far kinetic and geometric properties of exploration have been mainly discussed independently, with the notable exception of [27]. Qualitatively, the first-passage time to a target of a generic stochastic process carries information about the territory visited before hitting the target: large values of the first-passage time imply large values of the visited territory. However, the quantitative determination of this coupling is still lacking.

Here, we address the question of the *joint* distribution of the first-passage time to a target and the number of

distinct sites visited when the target is reached, which fully quantifies this coupling and gives access to a refined characterization of search trajectories. To the best of our knowledge, this quantity has never been studied so far. The joint law provides two conditional distributions, which allow to answer quantitatively the following questions: (Q_1) What is the territory visited by a random walker knowing that it reached a target (and stopped or exited the domain) after a given time? (Q_2) How long does it take a random walker to reach a target knowing that it has visited a given number of distinct sites before? We anticipate that these quantities could have applications in various situations where only partial information – either kinetic or geometric – on trajectories is accessible.

Summary of the results. We tackle this general question in the case of 1-dimensional processes, and determine the joint distribution $\sigma(s, n|s_0)$ of the FPT n at the target site 0 and the number s of distinct sites visited by a random walker starting from s_0 (see Fig. 1(a), where x, t are the continuous counterparts of s, n) [52]. Our approach applies to general (space and time) discrete or continuous random walkers, evolving in a semi infinite or finite domain, and yields fully explicit expressions of $\sigma(s, n|s_0)$ for several representative examples of Markovian processes, such as simple symmetric and biased random walks, persistent random walks [1, 18] or resetting random walks [28, 29], whose definitions are recalled below. In addition, we derive a general scaling form of $\sigma(s, n|s_0)$ in the large s, n regime, which holds also for non Markovian processes and captures the general dependence on s_0, s, n . Several applications of these central results are then discussed. First, we determine the efficiency of a schematic catalytic reaction [30] by deriving the probability that a diffusing particle has reacted in a domain with Poisson distributed targets before exiting the domain, knowing the exit time (see Fig. 1(b)). Second, we show that the knowledge of the joint distribution $\sigma(s, n|s_0)$ for simple random walks is actu-

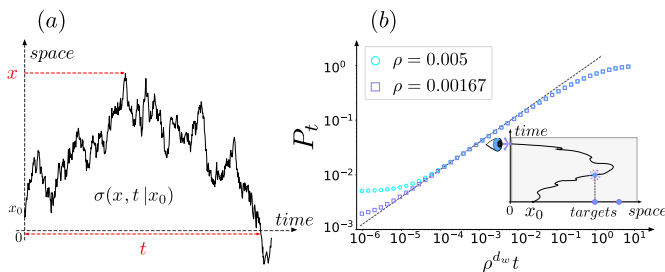


FIG. 1: (a) Starting from x_0 , the random walker crosses 0 for the first time at time t , having explored up to a distance x from the origin. The joint law $\sigma(x, t | x_0)$ is the density probability function of such joint events. (b) Consider a random searcher evolving in a (greyed out) domain, filled with Poisson distributed targets. Having as only information the time t of exit from the domain, we display the probability P_t of encounter with at least one target in terms of the rescaled variable $\rho^{d_w} t$ in the case of a Brownian searcher of diffusion coefficient $D = 1/2$. Numerical integration of the exact result (13) (symbols) and asymptotic scaling form (15) (dashed line) are shown.

ally required for determining first-passage properties of a class of strongly non Markovian processes, namely self-interacting random walks [31–35]. More precisely, with the help of the joint distribution, we derive exactly the full large time behavior of the FPT density of the so-called self-attracting walk (SATW) [36], which has been studied in the context of random search processes as a prototypical example of processes with long-range memory [37–40] and has important applications in the theoretical description of the trajectories of living organisms such as cells [41].

Discrete processes. We first consider the case of a general Markovian discrete (in space and time) process, which leaves no holes in its trajectory; in other words, the set of visited sites is assumed to be at all times the finite range $[[s_{\min}, s_{\max}]]$ defined by the min (s_{\min}) and max (s_{\max}) values of the random walker’s positions. This last hypothesis will hold for all processes presented in what follows. Denoting by $s_0 > 0$ the starting site, n the step at which the walker reaches the target 0 for the first time and s the number of distinct sites visited up to this random stopping time, we derive a systematic procedure to obtain the joint law $\sigma(s, n | s_0)$. In turn, this joint law gives immediate access to the conditional probabilities mentioned above, *ie* (i) the distribution of the number s of distinct sites visited before reaching 0 knowing that the random walker has reached 0 at step n :

$$G_{sp}(s | n, s_0) = \frac{\sigma(s, n | s_0)}{\sum_{s'=s_0}^{\infty} \sigma(s', n | s_0)} \equiv \frac{\sigma(s, n | s_0)}{F_{\underline{0}}(n | s_0)}, \quad (1)$$

where $F_{\underline{0}}(n | s_0)$ is the usual FPT distribution to 0 and (ii) the distribution of the FPT to 0 knowing that s distinct sites have been visited before reaching 0 :

$$G_{tm}(n | s, s_0) = \frac{\sigma(s, n | s_0)}{\sum_{n'=0}^{\infty} \sigma(s, n' | s_0)} \equiv \frac{\sigma(s, n | s_0)}{\mu_0(s | s_0)}, \quad (2)$$

where $\mu_0(s | s_0)$ is the distribution of the maximum s before reaching 0.

Let us denote $F_{\underline{0},s}(n | s_0)$ the probability that the walker reaches zero for the first time at step n , without ever reaching s , and make a partition over the rightmost site s' visited before reaching zero. Because the walker reaches 0 before s , one necessarily has $s' \in [[s_0, s - 1]]$, which yields $F_{\underline{0},s}(n | s_0) = \sum_{s'=s_0}^{s-1} \sigma(s', n | s_0)$. Note that this relation still holds for non Markovian processes. Equivalently, we obtain the key relation

$$\sigma(s, n | s_0) = F_{\underline{0},s+1}(n | s_0) - F_{\underline{0},s}(n | s_0) \equiv D_s F_{\underline{0},s}(n | s_0), \quad (3)$$

which allows one to write the joint law σ explicitly in terms of the quantity $F_{\underline{0},s}(n | s_0)$.

We next provide a procedure based on backward equations to derive the probability $F_{\underline{0},s}(n | s_0)$ in presence of two absorbing sites 0 and s for a given Markovian stochastic process. In this case, the propagator $P(s, n | s_0)$, *ie* the probability for the walker to be at site s after n steps, obeys the backward equation $P(s, n + 1 | s_0) = \mathcal{L}_{s_0} [P(s, n | s_0)]$ [1, 42], obtained by partitioning over the first step of the walk, where \mathcal{L}_{s_0} is a linear operator acting on s_0 . For instance, in the case of a simple random walk, $\mathcal{L}_{s_0} [P(s, n | s_0)] = \frac{1}{2} P(s, n | s_0 + 1) + \frac{1}{2} P(s, n | s_0 - 1)$. It is easily seen that $F_{\underline{0},s}(n | s_0)$ obeys the same backward equation for $0 < s_0 < s$ and, introducing the generating function $\tilde{F}_{\underline{0},s}(\xi | s_0) = \sum_{n=0}^{\infty} \xi^n F_{\underline{0},s}(n | s_0)$, we obtain:

$$\tilde{F}_{\underline{0},s}(\xi | s_0) = \xi \mathcal{L}_{s_0} [\tilde{F}_{\underline{0},s}(\xi | s_0)]. \quad (4)$$

Reminding that both 0 and s are absorbing boundaries, we have that, for any $n > 0$, $F_{\underline{0},s}(n | 0) = 0$ whereas $F_{\underline{0},s}(0 | 0) = 1$ and $F_{\underline{0},s}(0 | s) = 0$. In terms of generating functions, we obtain the following boundary conditions:

$$\tilde{F}_{\underline{0},s}(\xi | 0) = 1 ; \tilde{F}_{\underline{0},s}(\xi | s) = 0. \quad (5)$$

Eq. (4), completed by (5), fully determines $\tilde{F}_{\underline{0},s}(\xi | s_0)$. Making use of (3), we then derive the generating function of the joint law σ .

As an illustration, we obtain in the case of a simple random walk (see supplementary material (SM))

$$\tilde{\sigma}(s, \xi | s_0) = \frac{r_+ - r_-}{r_+^s - r_-^s} \frac{r_+^{s_0} - r_-^{s_0}}{r_+^{s+1} - r_-^{s+1}} \quad (6)$$

where $r_{\pm} = \frac{1}{\xi} (1 \pm \sqrt{1 - \xi^2})$. Further illustration is provided in SM, where explicit expressions of $\tilde{\sigma}(s, \xi | s_0)$ are determined for the important examples of biased random walks (for which a step is taken to the right with probability p , and to the left with probability $1 - p$), persistent random walks (for which each step is taken identical to the previous one with probability p) [43, 44] and resetting random walks (for which at each step the walker has a probability λ to jump back to its initial position) [28, 29, 45, 46]. Finally, in each case, a series expansion

with respect to ξ gives access to an exact determination of $\sigma(s, n|s_0)$ (see SM for validation by numerical simulations), which constitutes the main result of this section; its physical implications are commented below (see *discussion* and *applications*).

Continuous space and time. This method is easily adapted to continuous space and time (x, t) Markovian processes. Defining $F_{0,x}(t|x_0)$ as the probability density to reach 0 before x at time t , the continuous counterpart of Eq. (3) reads:

$$\sigma(x, t|x_0) = D_x F_{0,x}(t|x_0) \quad (7)$$

where here D_x is the differential operator with respect to x , and the Laplace transform $\tilde{F}_{0,x}(p|x_0) = \int_0^\infty e^{-pt} F_{0,x}(t|x_0) dt$ satisfies the continuous counterpart of Eq (4), (5) (see SM). As an explicit example, for Brownian diffusion with diffusion coefficient D , it is found that the joint law is given by

$$\begin{aligned} \sigma(x, t|x_0) = \frac{2D\pi}{x^3} \sum_{k=1}^{\infty} e^{-(k\pi)^2 D\tau} k \sin(k\pi\tilde{x}_0) \times \\ \times \left[2(k\pi)^2 D\tau - 2 - \frac{k\pi\tilde{x}_0}{\tan(k\pi\tilde{x}_0)} \right], \end{aligned} \quad (8)$$

where $\tilde{x}_0 = \frac{x_0}{x}$ and $\tau = \frac{t}{x^2}$. Explicit expressions of $\tilde{\sigma}$ for other continuous Markov processes (biased diffusion and continuous resetting) are presented in SM. Importantly, it is also shown in SM that our approach can be further extended to the case of continuous space but discrete time processes, also known as jump processes, as well as Markovian processes in confined domains.

General scaling form. Beyond the case of Markovian processes, we now show that the joint law σ assumes a general scaling form for symmetric processes, which holds even in the non Markovian case and elucidates its dependence on the parameters s, s_0, n . Because we are interested only in the large time and space limit, we adopt a continuous formalism and make use of the variables x, x_0, t . Extending an approach given in [47, 48], we derive below a general scaling form for $F_{0,x}(t|x_0)$, which leads to the asymptotic behavior of $\sigma(x, t, x_0)$.

First, note that walkers reaching x before 0 do not contribute to the probability $F_{0,x}(t|x_0)$. Hence, for times shorter than the typical time $T_{typ} \propto x^{d_w}$ needed to reach x (which defines the walk dimension d_w of the process), $F_{0,x}(t|x_0)$ behaves as the first-passage time density $F_0(t|x_0)$ in a semi-infinite domain, with a *single* target in 0. We now assume that this quantity has an algebraic decay with time for $t \rightarrow \infty$, quantified by the persistence exponent θ of the process: $F_0(t|x_0) \sim k(x_0)t^{-(\theta+1)}$, where $k(x_0) \propto x_0^{d_w\theta}$ for $x_0 \gg 1$ [6]. Because almost all random walkers have either reached 0 or x at times $t \gg x^{d_w}$, we write

$$F_{0,x}(t|x_0) \sim F_0(t|x_0)g\left(\frac{t}{x^{d_w}}\right) \sim k(x_0)t^{-(\theta+1)}g\left(\frac{t}{x^{d_w}}\right) \quad (9)$$

where g is a smooth cut-off function with $g(0) = 1$ and $g(y)$ vanishes for large y . Finally, with the help of (7), we obtain the general scaling form for the joint law in the scaling limit defined by $x \rightarrow \infty, t \rightarrow \infty$ with $\tau = t/x^{d_w}$ fixed :

$$\sigma(x, t|x_0) \sim \frac{h(x_0)}{x^{d_w(\theta+1)+1}} f(\tau) \quad (10)$$

where, defining $f_1(\tau) = -d_w g'(\tau)\tau^{-\theta}$ and $\mathcal{N} = \int_0^\infty f_1(\tau)d\tau$, we have $h(x_0) = k(x_0)\mathcal{N}$ and $f = f_1/\mathcal{N}$. In addition, $h(x_0) \propto x_0^{d_w\theta}$ for $x_0 \gg 1$, and $f(\tau)$ is a normalized process dependent function.

Of note, integrating equation (10) over t recovers the distribution of the maximum $\mu_0(x|x_0) = h(x_0)x^{-(d_w\theta+1)}$ before reaching 0, in agreement with known results [47]. In turn, this provides a simple physical interpretation of $f(\tau)$. Making use of (2), we obtain the conditional density $G_{tm}(t|x, x_0) \sim \frac{1}{x^{d_w}} f(\tau)$. Thus, $f(\tau)$ is the density of the rescaled variable τ conditioned by the value of the maximum x . In particular, we stress that f is independent of x_0 .

The general relation (10) is confirmed in Fig 2 by numerical simulations for representative examples of both Markovian processes (simple random walks and Riemann walks, *ie* discrete space and time Levy flights [1]), and non Markovian processes (Fractional Brownian Motion [49] and the Random Acceleration Process [50], see SM for definitions). Indeed, we find that the conditional density of the FPT knowing the territory covered, which a priori depends on the variables t, x, x_0 , can in fact be rewritten as the distribution $f(\tau)$ of the single reduced variable τ , as shown by the data collapse in the figure. Next, thanks to the exact Eq. (2), and the exact scaling of the distribution μ_0 of the maximum reminded above [47], this observed scaling of f directly confirms (10).

In the case of diffusive random walks, $f(\tau)$ can be determined explicitly by taking $x \rightarrow \infty$ and $t \rightarrow \infty$ with τ fixed in Eq. (8):

$$f_{BM}(\tau) = 2D\pi^2 \sum_{k=1}^{\infty} e^{-(k\pi)^2 D\tau} k^2 [2(k\pi)^2 D\tau - 3]. \quad (11)$$

Of note, this asymptotic conditional distribution holds for any symmetric Markovian random walk satisfying the central limit theorem.

Similarly (see SM), the other conditional distribution defined in (1) can be written from (10) as $G_{sp}(x|t, x_0) \sim \frac{1}{t^{1/d_w}} \phi(\chi)$ where the density of the rescaled variable $\chi = x/t^{1/d_w}$ is given in terms of f by :

$$\phi(\chi) = \frac{\chi^{-d_w(\theta+1)-1} f(\chi^{-d_w})}{\int_0^\infty u^{-d_w(\theta+1)-1} f(u^{-d_w}) du}. \quad (12)$$

The agreement of this result with numerical simulations is shown in SM.

Discussion. The above results yield both exact expressions of the joint law for Markovian processes, and

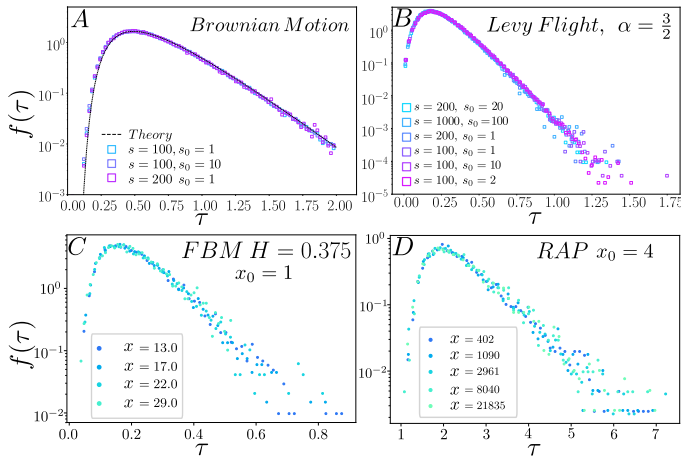


FIG. 2: Conditional distribution $f(\tau)$ of the rescaled variable τ (see text). Distributions are drawn for fixed s (discrete space) or x (continuous space) and collapse. **A,B** - Markovian Processes ; **C,D** Non Markovian Processes. See SM for details on simulations.

scaling forms for general non Markovian processes, and have important implications. (i) The joint law, because it gives access to all correlation functions $\langle x^n t^m \rangle$, fully quantifies the coupling between the kinetics of space exploration and the territory explored by a random walker. This coupling manifests itself in the dependence of σ on the rescaled variable $\tau = t/x^{d_w}$. (ii) The joint law yields the conditional distributions G_{sp} (see (1)) and G_{tm} (see (2)), which provide new insights in the quantification of space exploration, and in particular explicit answers to the questions Q_1, Q_2 raised in introduction. Below, we further illustrate the importance of the joint law and turn to examples of applications of our results.

Application - Conditional Rosenstock problem. The above results provide as a by product an explicit solution to a conditional version of the celebrated Rosenstock problem [1, 30]. We consider a reactive diffusing particle that enters a 1-dimensional chemical reactor at x_0 and leaves it at 0. The reactor contains Poisson distributed catalytic point-like sites of density ρ , which trigger a reaction upon encounter with the reactive particle (see Fig.1 (b)). The efficiency of such schematic catalytic reaction can be quantified by the probability P_t that the reactive particle has reacted with a catalytic site before exiting the domain, knowing the exit time t . This is readily obtained as

$$P_t = \int_0^\infty (1 - e^{-\rho x}) G_{sp}(x|t, x_0) dx. \quad (13)$$

The determination of P_t thus requires G_{sp} , and therefore the joint law. Making use of the general scaling (10), we obtain the large time scaling behaviour :

$$P_t \underset{t \rightarrow \infty}{\sim} \int_0^\infty (1 - e^{-\rho t^{1/d_w} u}) \phi(u) du; \quad (14)$$

this shows that P_t is asymptotically a function of the reduced variable $\rho t^{1/d_w}$ only, with $P_t \propto \rho t^{1/d_w}$ for $\rho t^{1/d_w} \rightarrow$

0. Equation (14) provides, thanks to (12), an explicit determination of P_t for all processes for which σ (and thus f) is known, and in particular elucidates its dependence on the exit time t from the domain (see Fig.1(b)). On the example of Brownian motion, one obtains (for $x_0^2/D \ll t \ll 1/(D\rho^2)$):

$$P_t \sim \sqrt{\pi} \rho (Dt)^{\frac{1}{2}}. \quad (15)$$

Application - Self-interacting walkers. Next, we show that the joint law can be needed to obtain the first-passage time distribution. This is the case of self-interacting random walks, which are defined generically as random walks whose jump probabilities at time n depend on the full set of visited sites at earlier times $n' < n$. We focus on the example of the 1d self-attracting walk (SATW) [36], which has been studied in the context of random search processes as a prototypical example of process with long-range memory, and has recently proved to be relevant to describe the dynamics of motile cells [41]. At each time step, if both its neighboring sites have already been visited, the random walker hops on either of them with probability 1/2. However, if one of them has never been visited, it is chosen with probability β . Note that this can either be an attractive effect ($\beta < 1/2$) or a repulsive one ($\beta > 1/2$). Since the dynamics of the walk is completely determined by the location of unvisited sites, the determination of the first-passage time distribution requires the knowledge of all times at which unvisited sites have been discovered. Denoting here $F_{0,\underline{s}}(n|s_0)$ the probability to reach s before 0 for the first time at step n , knowing that the sites $\llbracket 1, s-1 \rrbracket$ have already been visited, the generating function of $\sigma(s, n|1)$ can be written as :

$$\tilde{\sigma}(s, \xi|1) = \frac{\xi}{2} \left(\prod_{s'=3}^s \tilde{F}_{0,\underline{s}'}(\xi|s' - 1) \right) \tilde{F}_{0,\underline{s}+1}(\xi|s) \quad (16)$$

Solving for $\tilde{F}_{0,\underline{s}}(\xi|s_0)$ yields an explicit expression of $\tilde{\sigma}$ (see SM). For large s and n , with $\tau = \frac{n}{s^2}$ fixed, this yields $\sigma(s, n|s_0) = h(s_0) s^{-\frac{1-\beta}{\beta}-3} f_{SATW}(\tau)$ where $h(1) = \frac{\Gamma(-2+2/\beta) \Gamma(1-\beta)}{\Gamma(-1+1/\beta) \Gamma(\beta)}$ and $h(s_0) \propto s_0^{\frac{1-\beta}{\beta}}$ for large s_0 [53]. Finally, the conditional distribution f_{SATW} is defined by its strikingly simple Laplace transform:

$$\tilde{f}_{SATW}(p) = \int_0^\infty e^{-pu} f_{SATW}(u) du = \left(\frac{\sqrt{2p}}{\sinh(\sqrt{2p})} \right)^{\frac{1}{\beta}}. \quad (17)$$

The FPT distribution is finally deduced from $\sigma(s, n|1)$ and yields the following exact asymptotics (see SM):

$$F_{0,\underline{s}}(n|s_0 = 1) \underset{n \rightarrow \infty}{\sim} \frac{\Gamma(\frac{2}{\beta} - 1)}{\Gamma(\frac{1}{2\beta} - \frac{1}{2})} 2^{-\frac{1+\beta}{2\beta}} n^{-\frac{1-\beta}{2\beta}-1}. \quad (18)$$

While the n decay is in agreement with the recent determination of the persistent exponent of the SATW relying on a different approach [51], this formalism based on the

joint law gives access to the explicit expression of the prefactor for this strongly non Markovian process.

Conclusion. We have proposed a general method to derive explicit expressions of the joint distribution of the first-passage time to a target and the number of distinct sites visited when the target is reached for $1d$ random walks. This method yields explicit expressions for several representative examples of Markovian search processes. Furthermore, we showed that the dependence of the joint

distribution on its space and time variables is captured by a general scaling form, which holds even for non Markovian processes. We argue that the joint distribution could have applications in various situations where only partial information – either kinetic or geometric – on trajectories is accessible ; in addition, it appears to be a useful technical tool that for instance can give access to persistence properties of self interacting random walks.

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