Variable Order Fractional Fokker-Planck Equations derived from Continuous Time Random Walks

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Abstract

We propose a universal "Semi-Markov algorithm" for the computation of probability distributions of Continuous Time Random Walk (CTRW) scaling limits. It applies to fractional diffusion, tempered fractional diffusion, as well as their distributed-order and variable-order (in space) extensions. Drift and diffusivity may be space- and time-dependent, and the waiting times space-dependent.

The algorithm is based on the following assumptions only: i) a CTRW process is renewed after each jump-waiting time pair; ii) waiting times depend on space but not on time; iii) all coefficients can be evaluated numerically. We then show that the Semi-Markov algorithm shares the same properties as the recent "Discrete Time Random Walk" algorithm: it is consistent, conserves mass, generates strictly non-negative solutions, and has the same computational complexity. To highlight the applicability of our algorithm, we calculate probability densities of variable order fractional diffusion as well as fractional diffusion with spatially varying tempering.

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1. Introduction

Continuous Time Random Walks (CTRWs) (Scher and Montroll, 1975) generalize random walks by introducing heavy-tailed waiting times between jumps, and thus model "subdiffusion" via a sub-linear growth of the mean squared displacement (Henry et al., 2010b). A large number of experiments have reproduced subdiffusive processes (see e.g. Metzler and Klafter (2000), Tolić-Nørrelykke et al. (2004), Wong et al. (2004), Banks and Fradin (2005), Santamaria et al. (2006), Berkowitz et al. (2008), Höfling et al. (2012), Regner et al. (2013)), which has stimulated further research in the modelling of subdiffusion via CTRWs in the last two decades. Since the introduction of the Fractional Fokker-Planck Equation (FFPE) by Barkai et al. (2000), a powerful tool for the study of probability distributions of random walkers has become available. The FFPE has then been extended to include space- and time-dependent drift (Henry et al., 2010a), to model *tempered* (or transient) fractional diffusion (Gajda and Magdziarz, 2010, Straka, 2011, Zhang et al., 2015, Sabzikar et al., 2015) and to model fractional diffusion of spatially varying order (Chechkin et al., 2005, **?**).

Parallel to the theoretical advancement of fractional Fokker-Planck equations, numerous methods for the computation of solutions to FFPEs have been developed, among them explicit methods (Yuste and Acedo, 2005), implicit methods (Langlands and Henry, 2005), spectral methods (Li and Xu, 2009) and Galerkin methods (Mustapha and McLean, 2011). Hanert and Piret (2014) have generalized the spectral method to the tempered fractional setting. Chen et al. (2010), among others, have developed computational methods to compute solutions of *variable order* FFPEs; however, only their equation is consistent with a CTRW scaling limit representation (**?**).

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The recent Discrete Time Random Walk (DTRW) method (Angstmann et al., 2015b, 2016) calculates the probability distributions of a discrete stochastic process which approximates the continuum limit process whose distributions solve a FFPE. The advantage of this approach is that mass is necessarily conserved in each timestep, and that solutions are guaranteed to be nowhere negative. Its premise is the usage of Shibuya-distributed (discrete and power-law tailed) waiting times, which allow for the calculation of a discrete memory kernel via a Z-transform.

The Semi-Markov algorithm developed in this article generalizes the DTRW approach and at the same time maintains the advantageous properties "conservation of mass" and "positivity of solutions". It avoids the use of a Z-transform and is thus applicable to any conceivable scaling limit of waiting time distributions. What scaling limits of waiting time distributions are conceivable has been shown by **?** and Baeumer and Straka (2016): First, the observation is made that from the bivariate process (Y_u, Z_u) denoting a scaling limit of the cumulative sums of jumps and waiting times, the trajectory of a CTRW can be reconstructed. From the single assumption that the Markov property applies at each jump time, it follows that (Y_u, Z_u) must be a Langevin process driven by Lévy noise. Thus (Y_u, Z_u) is locally a Lévy process governed by a local coefficient triple

$$[a(y,t), \quad [b(y,t), d(y)], \quad \nu(w|y)] \tag{1.1}$$

of diffusivity, drift and Lévy jump measure; recall that a Lévy measure must satisfy

$$\int_0^\infty (1 \wedge w)\nu(w|y)\, dw < \infty \tag{1.2}$$

where $a \wedge b := \min\{a, b\}$.

In (Baeumer and Straka, 2016), probability densities $P(y,t)$ of CTRW limits with a general representation as above were shown to be unique solutions to a FFPE

$$\frac{\partial P(y,t)}{\partial t} = \mathcal{L}^*(y,t)\left[\frac{\partial}{\partial t}\int_0^t P(y,t-s)V(y,s)\, ds\right] + h(y,t), \tag{1.3}$$

in which $a(y,t)$ and $b(y,t)$ appear in the Fokker-Planck operator $\mathcal{L}^*$ as

$$\mathcal{L}^* g(y,t) = -\frac{\partial}{\partial y}[b(y,t)g(y,t)] + \frac{1}{2}\frac{\partial^2}{\partial y^2}[a(y,t)g(y,t)] \tag{1.4}$$

and where the memory kernel $V(y,t)$ is derived from $d(y)$ and $\nu(w|y)$ via its Laplace transform

$$\hat{V}(y,\lambda) = \int_0^\infty e^{-\lambda t} V(y,t)\, dt = \frac{1}{d(y)\lambda + \int_0^\infty (1 - e^{-\lambda w})\nu(w|y)\, dw}. \tag{1.5}$$

In (**?**), exact conditions on the distribution of jumps and waiting times were given under which a sequence of CTRWs converges to a limit whose distributions $P(y,t)$ solve (1.3). We give a short account of these results and their relevance for this article in Section 2.

In Section 3 we construct a sequence $X_t^{(c)}$ of DTRWs (i.e. CTRWs with discrete jumps and waiting times) which converges as $c \to \infty$ to a CTRW limit process X_t given in its most general form by (1.1). The stochastic process convergence guarantees the convergence of the probability distributions of X_t to the solutions $P(y,t)$ of (1.3), which translates into the consistency of the algorithm.

In Section 4 we calculate the probability distributions of the DTRW $X_t^{(c)}$, by utilizing the Semi-Markov property: If the age $V_t^{(c)}$ (i.e. the time since the last jump) is tracked, then $(X_t^{(c)}, V_t^{(c)})$ is a Markov process, and its joint probability distributions $\xi(i,j,k)$ can be calculated iteratively via master equations; the distribution of $X_t^{(c)}$ is then simply obtained by marginalizing. We also give details of boundary conditions on the space-time lattice.

In Section 5 we compute probability distributions for two examples: a spatially variable order FFPE, and a FFPE with spatially varying tempering. Section 6 concludes.

2. Stochastic solutions to Fokker-Planck equations with memory

2.1. Assumptions

The FPE with spatially varying memory in its general form (1.3) was derived from CTRW limits in Baeumer and Straka (2016). We make the following assumptions on the CTRWs and the FPE (1.3) in this article:

1. The variance of the jumps is (uniformly) bounded. This means that the CTRW limit X_t has continuous sample paths[1].
2. The waiting times are strictly positive, and their distribution depends on space and not on time.
3. The coefficient functions $a(y,t)$, $b(y,t)$, $d(y) \geq 0$ and $\nu(w|y)$ must be Lipschitz continuous and satisfy a linear growth condition. A sufficient condition is easily expressed in the case of spatially varying tempered subdiffusion, i.e. when
$$\nu(w|y) = \frac{\beta(y)}{\Gamma(1-\beta(y))} w^{-1-\beta(y)} e^{-\theta(x)w}, \quad w > 0, \quad \theta(x) \geq 0, \quad \beta(y) \in (\varepsilon, 1-\varepsilon) \tag{2.1}$$
for some $\varepsilon > 0$: All of the functions a, b, d, β and θ are continuously differentiable with bounded derivatives.
4. The tail function
$$\overline{\nu}(w|y) = \int_w^\infty \nu(w'|y)\, dw', \quad w > 0 \tag{2.2}$$
of the Lévy measure is weakly singular at 0, that is
$$\overline{\nu}(w|y) \sim C w^{-\beta(y)}, \quad w \downarrow 0, \quad \beta(y) \in (0,1). \tag{2.3}$$
for some constant $C > 0$.

The technical Condition 3 is needed for the existence of a unique solution to the Langevin equation defining (Y_u, Z_u), see **?**. Condition 4 ensures that the Lévy measure is infinite; if it wasn't, the CTRW limit could be an uninteresting CTRW process with finite numbers of steps in finite time intervals. Moreover, it simplifies our analysis further below for (3.8).

2.2. CTRWs as random walks in space-time

CTRWs are renewed after each jump: The next waiting time w and the next jump z are, given the current location x and the current time s, independent of the past trajectory. This means that the entire dynamics of a CTRW $X_t^{(c)}$ are captured in a space-time transition kernel
$$K^{(c)}(z, w|x, s), \tag{2.4}$$
which is a bivariate probability density in $(z,w) \in \mathbb{R} \times [0,\infty)$ for every $(x,s) \in \mathbb{R} \times [0,\infty)$. We assume the scaling parameter c to be such that
$$K^{(c)}(z, w|x, s) \to \delta_{(0,0)}(z, w), \quad c \to \infty, \tag{2.5}$$
where $\delta_{(0,0)}$ denotes the Dirac delta function at $(0,0)$. For more details, see **?**.

[1] An extension of the theory in this article to infinite variance jumps is feasible: Lévy noise would also enter the spatial component and an integral term would enter in the Fokker-Planck operator $\mathcal{L}^*$.

2.3. Conditions for convergence of CTRWs

Conditions for the convergence of $X_t^{(c)}$ to a limit X_t whose probability distributions $P(y,t)$ solve (1.3) were given in **?**:

$$\lim_{\epsilon\downarrow 0}\lim_{c\to\infty} c \iint\limits_{|z|<\epsilon,\, 0<w<\epsilon} zK^{(c)}(z,w|x,s)\,dz\,dw = b(x,s) \tag{2.6}$$

$$\lim_{\epsilon\downarrow 0}\lim_{c\to\infty} c \iint\limits_{|z|<\epsilon,\, 0<w<\epsilon} z^2K^{(c)}(z,w|x,s)\,dz\,dw = a(x,s) \tag{2.7}$$

$$\lim_{\epsilon\downarrow 0}\lim_{c\to\infty} c \iint\limits_{|z|<\epsilon,\, 0<w<\epsilon} wK^{(c)}(z,w|x,s)\,dz\,dw = d(x) \tag{2.8}$$

$$\lim_{c\to\infty} c \iint\limits_{|z|\geq\varepsilon \text{ or } w\geq 0} g(z,w)K^{(c)}(z,w|x,s)\,dz\,dw = \int g(0,w)\nu(w|x)\,dw, \quad \varepsilon>0, \tag{2.9}$$

where $g(z,w)$ is any bounded measurable function which vanishes in a neighbourhood of the origin.

2.4. Stochastic Process convergence

If the four conditions (2.6)–(2.9) are all satisfied, then the CTRW process $X_t^{(c)}$ converges to the CTRW limit X_t in the sense of stochastic processes; we write

$$\left\{X_t^{(c)}\right\}_{t\geq 0} \longrightarrow \{X_t\}_{t\geq 0} \quad \text{as } c\to\infty \quad \text{in } D(\mathbb{R}). \tag{2.10}$$

That is, $X_t^{(c)}$ and X_t are viewed as random elements in the space $D(\mathbb{R})$ of $\mathbb{R}$-valued trajectories with distributions $\mathbf{P}^{(c)}$ and $\mathbf{P}$, and $\mathbf{P}^{(c)}$ converges (weakly) to $\mathbf{P}$ as $c\to\infty$. This means that

$$\lim_{c\to\infty}\int f(\omega)\mathbf{P}^{(c)}(d\omega) = \int f(\omega)\mathbf{P}(d\omega), \tag{2.11}$$

for all real valued, bounded and continuous f defined on $D(\mathbb{R})$. The Skorokhod J_1 topology on $D(\mathbb{R})$ defines continuity on $D(\mathbb{R})$. For full details, see Whitt (2001). A consequence of the stochastic process convergence is the convergence of *finite-dimensional distributions*: For any $0\leq t_1<\ldots<t_n$, the distribution of the random vectors

$$(X_{t_1}^{(c)},\ldots,X_{t_n}^{(c)}) \to (X_{t_1},\ldots,X_{t_n}) \tag{2.12}$$

converges.

3. DTRW dynamics

Recall our general aim: given a general FFPE of the form (1.3), we would like to compute an approximation of the solution $P(y,t)$. In this section, we give a space-time kernel (2.4) which defines a *DTRW*, i.e. a CTRW with discrete jumps and waiting times, which converges to a CTRW limit X_t whose distributions $P(y,t)$ solve (1.3).

3.1. Waiting time distribution

The discrete waiting time distribution $\psi^{(c)}(w|x)$ we will define now will be supported on the points $\tau, 2\tau, 3\tau,\ldots$ where $\tau=1/c$. We use an upper bar for the tail functions of the Lévy measure (1.2) and the waiting time distribution $\psi^{(c)}(w|x)$:

$$\overline{\nu}(w|y) = \int_w^\infty \nu(w'|y)\,dw', \quad \overline{\psi}^{(c)}(w|x) = \sum_{w'=j\tau,\, w'>w} \psi^{(c)}(w'|x), \quad w>0. \tag{3.1}$$

For convenience, we use the convention that $\overline{\nu}(w|y) = \infty$ for $w \le 0$. We first define the tail function of a continuous probability measure via

$$H^{(c)}(w|y) := 1 \wedge [\tau \overline{\nu}(w - \tau d(y))], \quad w > 0. \tag{3.2}$$

For $w > 0$, let w_τ be the nearest lattice point which is not smaller; i.e.

$$w_\tau = j\tau \ge w > (j-1)\tau, \tag{3.3}$$

and take the piecewise constant, right-continuous and non-increasing function

$$\overline{\psi}^{(c)}(w|y) := H^{(c)}(w_\tau|y), \quad w \ge 0 \tag{3.4}$$

to be the tail probability function which defines $\psi^{(c)}(w|y)$. Equivalently, we have

$$\psi^{(c)}(j\tau|y) = H^{(c)}((j-1)\tau|y) - H^{(c)}(j\tau|y). \tag{3.5}$$

Note that $\psi^{(c)}(0\tau|y) = 0$, i.e. waiting times are strictly positive.

3.2. Preliminary calculations

We need to calculate two sums which will be useful for checking conditions (2.8) & (2.9) below.

Lemma 3.1. *The waiting time distribution* (3.5) *satisfies, as* $c \to \infty$,

$$\int f(w)\psi^{(c)}(w|y)\,dw = \sum_{j=1}^{\infty} f(j\tau)\psi^{(c)}(j\tau|y) \to f(0), \tag{3.6}$$

$$c\int g(w)\psi^{(c)}(w|y)\,dw = c\sum_{j\tau>0} g(j\tau)\psi^{(c)}(j\tau|y) \to \int g(w)\nu(w|y)\,dw, \tag{3.7}$$

$$c\int_0^\varepsilon w\psi^{(c)}(w|y)\,dw = c\sum_{0<j\tau\le\varepsilon} j\tau\psi^{(c)}(j\tau|y) \to d(y) + \mathcal{O}(\varepsilon^{1-\beta(y)}), \quad \varepsilon > 0. \tag{3.8}$$

where f *and* g *are bounded continuous, and where* g *vanishes in a neighbourhood of* 0.

Proof. (3.6) holds since $\psi^{(c)}(w|y)$ is a probability distribution on the positive numbers and $\overline{\psi}^{(c)}(w|y) \to 0$ as $c \to \infty$ for all $w > 0$. For (3.7), we first note that

$$c\overline{\psi}^{(c)}(w|y) = c \wedge [\overline{\nu}(w - \tau d(y))] \to \overline{\nu}(w).$$

If g is differentiable, we may calculate

$$\begin{aligned} c\int_0^\infty g(w)\psi^{(c)}(w|y)\,dw &= c\int_\varepsilon^\infty g(w)\psi^{(c)}(w|y)\,dw = c\int_\varepsilon^\infty g'(w)\overline{\psi}^{(c)}(w|y)\,dw \\ &\to \int_\varepsilon^\infty g'(w)\overline{\nu}(w|y)\,dw = \int_\varepsilon^\infty g(w)\nu(w|y)\,dw = \int_0^\infty g(w)\nu(w|y)\,dw \end{aligned}$$

But differentiable functions lie dense in the space of bounded continuous functions, so (3.7) follows. For (3.8), first note that

$$1 = H^{(c)}(w|y) \iff w \le \overline{\nu}^{-1}(c|y) + d(y)\tau =: C(y,c).$$

Hence we have $j\tau \le C(y,c) \implies \psi^{(c)}(j\tau|y) = 0$. We let $n_1 = \lfloor C(y,c)/\tau \rfloor$ and $n_2 = \lfloor \varepsilon/\tau \rfloor$. Then by assumption (2.3),

$$\overline{\nu}(c|y)^{-1} \sim \Gamma(1-\beta(y))c^{-1/\beta}, \quad c \to \infty, \tag{3.9}$$

and hence

$$\lim_{c\to\infty} \tau n_1 c = \lim_{c\to\infty} \tau \overline{\nu}^{-1}(c|y) + d(y) = d(y) \tag{3.10}$$

Then the left side of (3.8) is

$$\begin{aligned} c \sum_{C(y,c)<j\tau\le\varepsilon} j\tau\psi^{(c)}(j\tau|y) &= c\sum_{j=n_1}^{n_2} j\tau\left[H^{(c)}(j\tau|y) - H^{(c)}((j+1)\tau|y)\right] \\ &= cn_1\tau H^{(c)}(n_1\tau|y) - c(n_2+1)\tau H^{(c)}((n_2+1)\tau|y) + \tau\sum_{j=n_1}^{n_2} cH^{(c)}(j\tau) \end{aligned}$$

where for the second equality sign, we have splitted the sum in two, shifted the index in the second resulting second sum, and simplified the result. In the first term of the result, we have $H^{(c)}(n_1\tau|y) = 1$ and (3.10). For the second term, note that $n_2\tau \to \varepsilon$, and $cH^{(c)}(w|y) \to \overline{\nu}(w)$ for every $w > 0$. And finally, the last term is seen to be the Riemann sum of an integral. Keeping in mind that as $c \to \infty$, $C(y,c) \downarrow 0$ and again that $cH^{(c)}(w|y) \to \overline{\nu}(w)$, the above converges to

$$d(y) - \varepsilon\overline{\nu}(\varepsilon|y) + \int_0^\varepsilon \overline{\nu}(w)\,dw,$$

which is $d(y) + \mathcal{O}(\varepsilon^{1-\beta(y)})$ due to (2.3). □

3.3. Jump distribution

We assume that the DTRW jumps can have one of the three values $\{-\chi, 0, +\chi\}$, where $\bar{a} = \sup\{a(x,t)\}$ and $\chi = (\bar{a}/c)^{1/2}$. The probabilities to jump left, to "self-jump" (i.e. jump back to the original location), and to jump right, are given by

$$\ell^{(c)}(x,t) = \frac{a(x,t) - \chi b(x,t)}{2\bar{a}}, \quad n(x,t) = 1 - a(x,t)/\bar{a}, \quad r^{(c)}(x,t) = \frac{a(x,t) + \chi b(x,t)}{2\bar{a}}.$$

where x is the location of the walker before the jump, and t is the time at which the jump occurs. In order for r, n and ℓ to be between 0 and 1, we need χ to be small enough so that

$$\chi|b(x,t)| \le a(x,t), \quad (x,t) \in \mathbb{R}\times[0,\infty). \tag{3.11}$$

For later use, we note that

$$c[-\chi\ell^{(c)}(x,t+w) + \chi r^{(c)}(x,t+w)] = b(x,t+w) \tag{3.12}$$

$$c\chi^2[\ell^{(c)}(x,t+w) + r^{(c)}(x,t+w)] = a(x,t+w) \tag{3.13}$$

$$\int_{\mathbb{R}} f(z)\left[r^{(c)}(x,t)\delta_\chi(z) + n(x,t)\delta_0(z) + \ell^{(c)}(x,t)\delta_{-\chi}(z)\right]\,dz \to f(0) \tag{3.14}$$

as $c \to \infty$ for all bounded continuous f.

3.4. Conditions (2.6) – (2.9)

Assume now that a jump happens at time t and the location of the walker immediately after the jump is (x,t). Then the next jump will happen at time $t+w$, where w is drawn from $\psi^{(c)}(w|y)$, and it is common to evaluate the probabilities to jump left/right/self-jump at time $t+w$. In this case the space-time transition kernel governing the DTRW is

$$K^{(c)}(z,w|x,t) = \left[r^{(c)}(x,t+w)\delta_{+\chi}(z) + n(x,t+w)\delta_0(z) + \ell^{(c)}(x,t+w)\delta_{-\chi}(z)\right]\psi^{(c)}(w|x). \tag{3.15}$$

Alternatively, one may assume that the bias to jump left/right/self-jump is evaluated at the *beginning* of a waiting time, which leads to

$$K^{(c)}(z,w|x,t) = \left[r^{(c)}(x,t)\delta_{+\chi}(z) + n(x,t)\delta_0(z) + \ell^{(c)}(x,t)\delta_{-\chi}(z)\right]\psi^{(c)}(w|x). \tag{3.16}$$

These dynamics were considered in Angstmann et al. (2015a), where it was already found that (3.15) and (3.16) yield the same CTRW limit process. Indeed, both kernels satisfy conditions (2.6)–(2.9).

To see that (2.6)–(2.7) hold, use (3.12)–(3.13) and (3.6). To see (2.8), use (3.8) and let $\varepsilon \downarrow 0$; and finally, to see (2.9), use (3.7) and (3.14).

4. Semi-Markov numeric scheme

4.1. Master equations

In the previous section, we have constructed a DTRW $X_t^{(c)}$ which converges to the CTRW limit X_t whose densities $P(y,t)$ solve (1.3). For large values of c, the probability densities of $X_t^{(c)}$ will hence be a good approximation of $P(y,t)$, see (4.8) below. In this section, we calculate the probability distributions of $X_t^{(c)}$.

Consider the space-time transition kernel (3.15) which defines the DTRW. Since all jumps are from $\{-\chi, 0, +\chi\}$, the walker will be hopping on a lattice embedded in $\mathbb{R}$. Recall that a waiting time W at a spatial lattice point $i\chi$ is drawn from $\psi^{(c)}(w|i\chi)$ and thus satisfies

$$\mathbf{P}(W > j\tau) = H^{(c)}(j\tau|i\chi) =: h_{i,j}. \tag{4.1}$$

Conditional on $W > j\tau$, the probability that $W > (j+1)\tau$ is

$$\mathbf{P}(W > (j+1)\tau | W > j\tau) = h_{i,j+1}/h_{i,j}.$$

We now write $(x_k, v_k) \in \mathbb{Z} \times (\mathbb{N} \cup \{0\})$ for the lattice coordinates of a walker's location and age at time $k\tau$. That is, $(x_k, v_k) = (i,j)$ means that at time $k\tau$, the walker is at $i\chi$, and has arrived there at time $(k-j)\tau$ (and not moved since). Now if $(x_k, v_k) = (i,j)$, then by time $(k+1)\tau$ either

- no jump has occured: then $(x_{k+1}, v_{k+1}) = (i, j+1)$, which happens with probability $h_{i,j+1}/h_{i,j}$. Or,
- a jump has occured: then $(x_{k+1}, v_{k+1}) = (i+z, 0)$, which happens with probability $1 - h_{i,j+1}/h_{i,j}$, and independently z equals $+1$, -1 or 0 with probabilities $r_i^k = r^{(c)}(i\chi, (k+1)\tau)$, $\ell_i^k = \ell^{(c)}(i\chi, (k+1)\tau)$ or $n_i^k = n(i\chi, (k+1)\tau)$, respectively.

The above dynamics uniquely determine the stepwise evolution of (x_k, v_k). We write $\xi_{i,j}^k = \mathbf{P}(x_k = i, v_k = j)$ for the probability distribution of (i,j) at time k. The master equations for $\xi_{i,j}^k$ then read:

$$\xi_{i,j}^{k+1} = \frac{h_{i,j}}{h_{i,j-1}}\,\xi_{i,j-1}^k, \quad 1 \le j < J-1, \tag{4.2}$$

$$\xi_{i,0}^{k+1} = \sum_{j=0}^{J}\left(1 - \frac{h_{i,j+1}}{h_{i,j}}\right)(\ell_{i+1}^k \xi_{i+1,j}^k + r_{i-1}^k \xi_{i-1,j}^k + n_{i,j}^k \xi_{i,j}^k) \tag{4.3}$$

The line (4.2) states that for a walker to have age $j \ge 1$, it must have had age $j-1$ in the previous time step, and not jumped. The line (4.3) states that for a walker to have age $j = 0$, it must have jumped to its location i in the previous time step, from a neighbouring lattice site or from i itself. The probability mass of all walkers jumping from site i during time step $k \to k+1$ is $\sum_{j=0}^{J}(1 - h_{i,j+1}/h_{i,j})\,\xi_{i,j}^k$, which is redistributed according to the probabilities $r_{i,j}^{k+1}$, $\ell_{i,j}^{k+1}$ and $c_{i,j}^{k+1}$. This interpretation shows that (4.2)–(4.3) **conserve probability mass**.

4.2. Boundary conditions

In practice, one can only allocate a finite number J of points to the lattice of ages. If we cannot allocate $\lfloor T/\tau \rfloor$ lattice points, where T is the largest time of interest, then it is possible that the age of walkers may reach the end of the lattice. In this case, and if the walker does not jump in the next time step, we do not increase its age any further, until it eventually does jump:

$$\xi_{i,J}^{k+1} = \frac{h_{i,J}}{h_{i,J-1}} \xi_{i,J-1}^{k} + \frac{h_{i,J+1}}{h_{i,J}} \xi_{i,J}^{k}. \tag{4.4}$$

Finally, assuming that the spatial coordinates of the lattice go from $-I$ to I, we implement Neumann boundary conditions by placing a walker back on the boundary whenever it would otherwise have jumped off the lattice, that is:

$$\ell_{-I}^{k} = 0, \qquad n_{-I}^{k} = \ell(-I\chi, k\tau) + n(-I\chi, k\tau), \qquad r_{-I}^{k} = r(-I\chi, k\tau), \tag{4.5}$$

$$\ell_{I}^{k} = \ell(I\chi, k\tau), \qquad n_{I}^{k} = n(I\chi, k\tau) + r(I\chi, k\tau), \qquad r_{I}^{k} = 0 \tag{4.6}$$

4.3. Properties of the algorithm

The main interest lies in the probability distribution of $X_t^{(c)}$. Since the temporal lattice $\{k\tau\}$ is embedded in $[0, \infty)$, we have $X_t^{(c)} = X_{t_\tau}^{(c)}$, where t_τ is defined exactly as w_τ in (3.3). By marginalizing over the age j, we thus find

$$\mathbf{P}(X_t^{(c)} = i\chi) =: \rho_i^k = \sum_{j=0}^{J} \xi_{i,j}^k, \quad k = \lfloor t/\tau \rfloor. \tag{4.7}$$

Positivity. From (4.2)–(4.3), it is evident that the $\xi_{i,j}^k$ are necessarily non-negative, and hence the solution ρ_i^k cannot be negative.

Consistency of the algorithm. Due to (2.10), the convergence

$$\sum_{i=-I}^{I} f(i\chi)\rho_i^{\lfloor t/\tau \rfloor} = \langle f(X_t^{(c)}) \rangle \longrightarrow \langle f(X_t) \rangle \quad \text{as } c \to \infty, \tag{4.8}$$

holds for all bounded continuous real-valued f defined on $\mathbb{R}$. Now if X_t is Lebesgue absolutely continuous (has a density), then we may take f to be an indicator function of an interval (a, b), and (4.8) reads

$$\sum_{a<i\chi<b} \rho_i^{\lfloor t/\tau \rfloor} \longrightarrow \mathbf{P}(a < X_t < b) \quad \text{as } c \to \infty. \tag{4.9}$$

Equivalence with DTRW approach. The Discrete Time Random Walk algorithm by Angstmann et al. (2015b) assumes discrete waiting times with the Sibuya distribution, whose tail function $\Psi(n)$ has the asymptotics $\Psi(n) \sim n^{-\beta}$. In (4.3), see that we have $\xi_{i,j}^k = \xi_{i,0}^{k-j} h_{i,j}$, by telescoping (4.2) and $h_{i,0} = 1$. Hence (4.3) rewrites to

$$\xi_{i,0}^{k+1} = \sum_{j=0}^{J} (h_{i,j} - h_{i,j+1})(\ell_{i+1}^{k+1} \xi_{i+1,0}^{k-j} + r_{i-1}^{k+1} \xi_{i-1,0}^{k-j} + c_{i,j}^{k+1} \xi_{i,0}^{k-j}),$$

assuming that $h_{i,j}$ is constant in i (homogeneous waiting times). Since $h_{i,j} - h_{i,j+1}$ is the probability of a waiting time being $j + 1$, one sees the equivalence with Equation (16) in Angstmann et al. (2015b), if we choose $h_{i,j} = \Psi(j)$.

5. Examples

Within this semi-Markov framework, we may now implement the above numeric scheme to calculate approximations of the densities of a variety of CTRW limits. By allowing for various initial residence times Gill and Straka (2016), waiting time distributions $\psi(\omega|x)$ and spatially varying exponents $\beta(x)$ these are able to model a very wide set of subdiffusive systems.

Spatially varying exponent. For simplicity we let the coefficients $b \equiv 0$ and $d \equiv 0$. For the diffusivity we have $a(x) = T_0^{-\beta(x)}$ where T_0 is the time scale and waiting time distribution tail function $\Psi(x,t) = \frac{t^{-\beta(x)}}{\Gamma(1-\beta(x))}$. For the variable order $\beta(x)$ we consider a system where the subdiffusion slows down in one direction and speeds up in the other direction, defining $\beta(x) = 0.25 + 0.5/(1+e^{-x})$ so that $\lim_{x\to-\infty}\beta(x) = 0.25$ and $\lim_{x\to\infty}\beta(x) = 0.75$. Figure 1 shows the evolution of the density $P(x,t)$ at multiple times. The distinctive cusp shape of subdiffusion (with constant exponent) is present at small times, however the long-time behaviour shows the aggregation which begins to occur towards areas of smaller exponent $\beta(x)$ i.e. the particles aggregates towards and become trapped in the slower end of the system.

In Korabel and Barkai (2010), the authors modelled a subdiffusive system with $\beta = 0.3$ for $x < 0$ and $\beta = 0.75$ for $x > 0$, while at the interface ($x = 0$) the particles wait an exponentially distributed amount of time, and observed that in the long-time limit all particles end up in the left half. Here we consider a variable order system with $\beta(x) = 0.55e^{-x^2} + 0.15 + 0.5/(1+e^{-2x})$, noting that $\lim_{x\to-\infty}\beta(x) = 0.15$, $\lim_{x\to\infty}\beta(x) = 0.65$, while at the interface ($x = 0$) the system is near-diffusive with $\beta = 0.95$. Figure 2 shows the evolution of the density $P(x,t)$ of the system. At small times we observe two peaks reflecting the trapping that occurs either side of the interface, however in the long-time we can see the aggregation of all particles towards the left hand side ($x < 0$) which has lower exponent β.

Spatially varying Tempering. The tempered Tail function is obtained by multiplying it by an exponential term $e^{-\theta t}$. This yields the new Tail function $\Psi(x,t) = \frac{t^{-\beta(x)}e^{-\theta t}}{\Gamma(1-\beta(x))}$ where $\theta \geq 0$ and we can see that this Tail function will now be integrable. Note that for $\theta = 0$ this reduces to the original tail function, and observe that for small t and small θ dynamics of the system will still appear subdiffusive, while for large t they will approach diffusive. Here we are now able to generalize this to allow the tempering parameter $\theta(x) \geq 0$ to be spatially varying so that the effect of this tempering may not be homogeneous throughout the system. Taking the variable order to be the same as in Figure 1 $\beta(x) = 0.25 + 0.5/(1+e^{-x})$, we consider the inhomogeneous tempering $\theta(x) = 1/(1+e^{0.5x})$. Figure 3 illustrates the density $P(x,t)$ for this case, where we can see that particles begin to accumulate where tempering is low ($x > 0$). Noting that the variable exponent $\beta(x)$ is lower for $x < 0$, this suggests that the effect of the tempering parameter $\theta(x)$ is stronger than that of $\beta(x)$.

6. Conclusion

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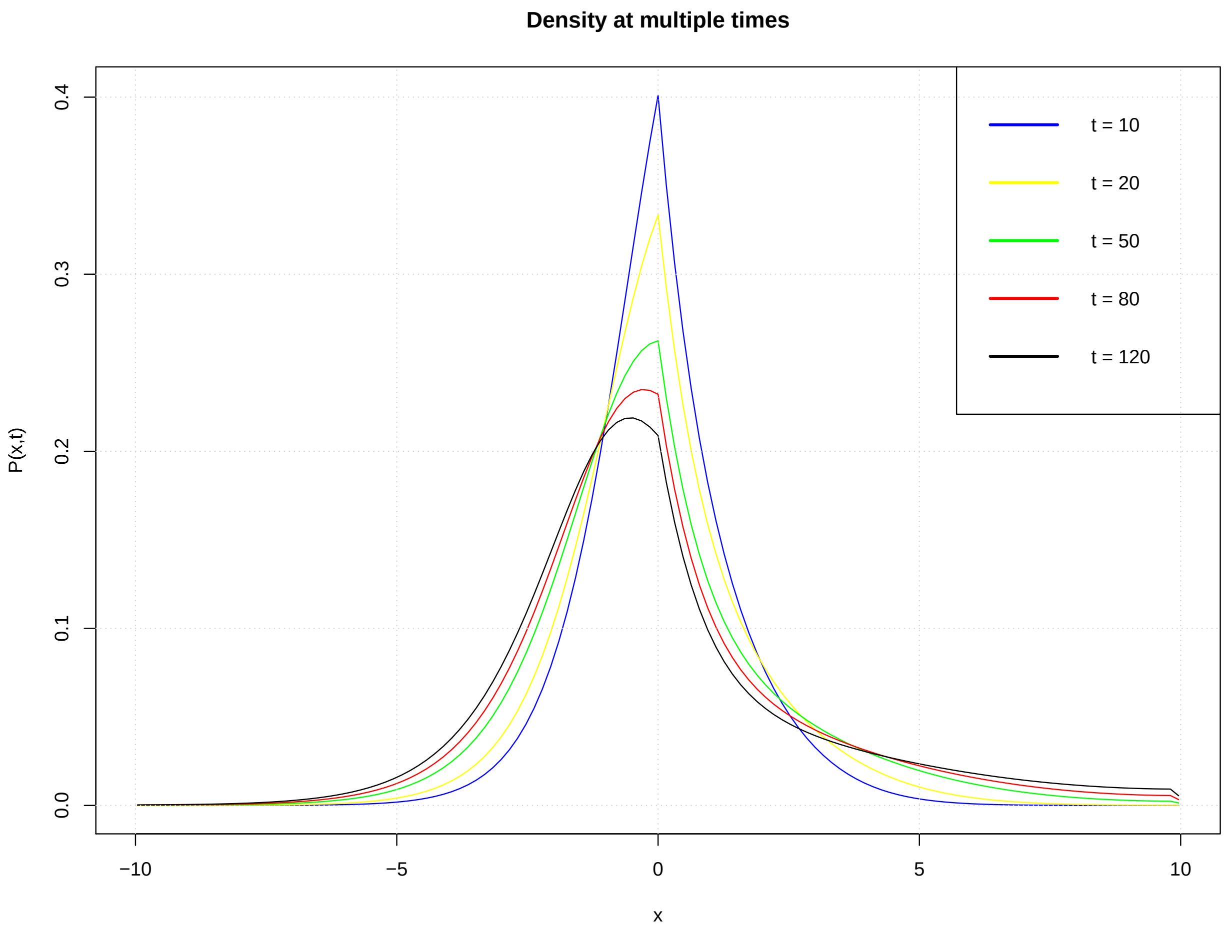

Figure 1: Density $P(x,t)$ at multiple times of a variable order subdiffusive system with $\beta(x) = 0.25 + 0.5/(1 + e^{-x})$. The time scale $T_0 = 2$ and $c = 40$.

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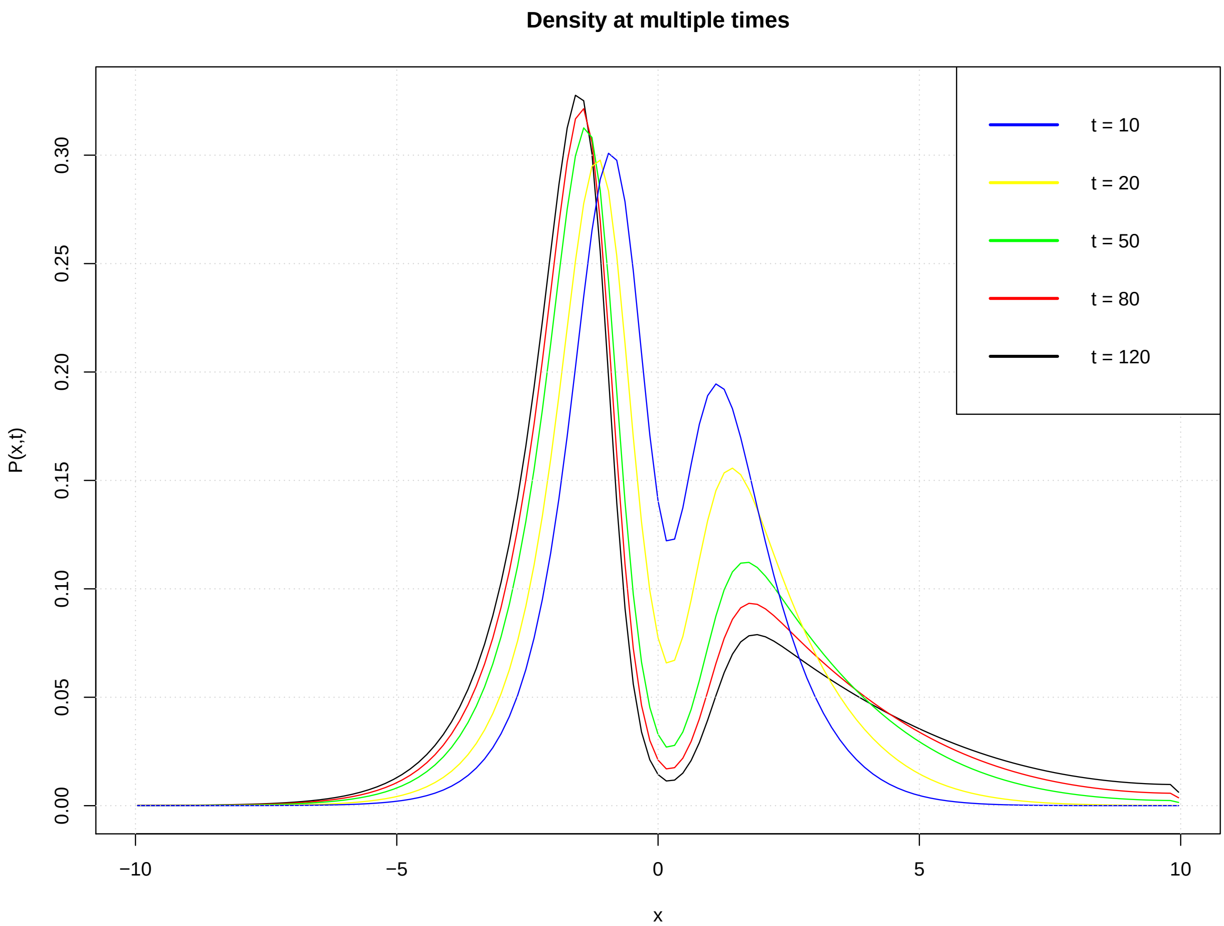

Figure 2: Density $P(x,t)$ at multiple times of a variable order subdiffusive system with $\beta(x) = 0.55e^{-x^2} + 0.15 + 0.5/(1+e^{-2x})$. The time scale $T_0 = 2$ and $c = 40$.

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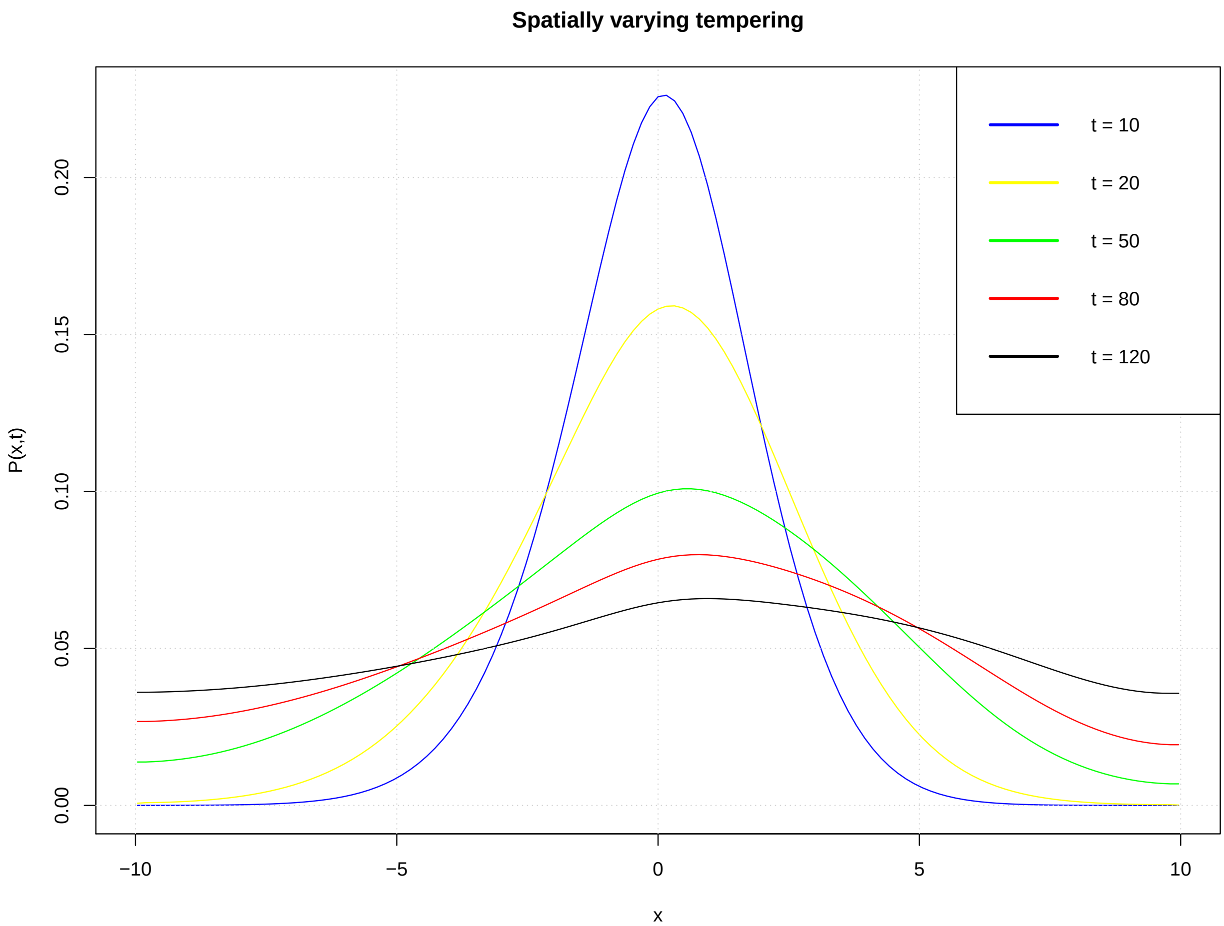

Figure 3: Density $P(x,t)$ at multiple times of a variable order subdiffusive system with spatially varying tempering. We set $\beta(x) = 0.25 + 0.5/(1 + e^{-x})$ and $\theta(x) = 1/(1 + e^{0.5x})$. The time scale $T_0 = 2$ and $c = 40$.

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