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Random jumps with free partially deterministic coalescence

Abstract The aim of this paper is to discuss a special case of a coalescing random jumps model of infinitely many jumping individuals. Jumps are embedded with repulsion at the target point and coalescence kernel is defined in such a way that for two coalescing individuals the result is deterministically defined. A possible approach to study the dynamics of the system numerically is discussed. It is based on a Poisson approximation of states of the system. Some interesting results of simulations are showed.

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1. Introduction. Individual-based (or agent-based) models are focusing increased attention in the recent years. They usually describe phenomena at the microscopic scale, distinguishing between individuals that form bigger systems (populations) and taking into account interactions between those individuals, which lead to higher-level properties. The subject of this paper is a model of coalescing random jumps of infinitely many individuals. The random motion on the real line of particles that merge after collision was introduced in [1] and studied e.g. in [3, 6]. Evolution of the system is described there in terms of stochastic differential equations. In the model discussed in this work the statistical approach (see e.g. [2, 5]) is used, in which the evolution of states is described by means of correlation functions.

Considering infinite systems, it is easy to maintain locality of interactions by imposing compact support, which is easily distinguishable from the unbounded whole. In the case of finite systems, such a distinction is not that obvious, as the whole population belongs to a compact set. Additionally, working with an infinite system allows one to release from inconveniences of boundary conditions and focus on the essential properties of the system that comes from the rules imposed on the individuals. Usually, individuals are described by some properties that make each of them a separate entity. The considered

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model is very simple, as only one such property is introduced – the spatial location of the individual, represented by a vector from Euclidean space $\mathbb{R}^d$. It is possible to interpret this property differently. For example, taking $d = 1$ it can be understood as a logarithm of the mass of an individual.

2. The model. The discussed model is a special case of the model introduced by Kozitsky and Pilorz(2018) and its more general version considered by Pilorz(2016). It can also be seen as an extension of the model under study by Berns et al.(2013). The phase space is a configuration space Γ of all locally finite subsets of $\mathbb{R}^d$. The model is described by the operator L on the right-hand side of the corresponding Kolmogorov equation (see e.g. [4] and references therein)

$$\frac{d}{dt}F_t = LF_t, \qquad F_{t=0} = F_0, \tag{1}$$

where F_t are observables – appropriate real-valued functions on Γ. For the considered free coalescing random jumps, while coalescence is dependent on the configuration only through the merging individuals and hence called "free", the jumps are equipped with repulsion, which depends on the population structure around the target of a jump. Hence, the operator L takes the following form:

$$(LF)(\gamma) = \sum_{\{x,y\}\subset\gamma} c_c(x-y)\Big(F\big(\gamma\backslash\{x,y\}\cup z(x,y)\big) - F(\gamma)\Big)$$
$$+\sum_{x\in\gamma}\int_{\mathbb{R}^d} c_j(x-y)\prod_{u\in\gamma\backslash x} e^{-\phi(y-u)}\Big(F\big(\gamma\backslash\{x\}\cup\{y\}\big) - F(\gamma)\Big)dy.$$

The function c_c is a coalescence intensity, c_j a jump kernel and ϕ a repulsion potential. The individuals within this model are able to perform two actions – they can jump and coalesce. The jump is an action of changing the property of one individual (from x to y). Its intensity is altered by the repulsion described by the function ϕ. It lowers the intensity of jumps depending on the position of the target point with respect to the configuration. The coalescence is an action of merging two individuals into one (individuals with properties x and y respectively, merge into one individual with property $z(x,y)$). The coalescence can be used for modeling predation. The similar death by competition can be described more adequatly by the competition term of the death rate, as in [4].

The introduced Kolmogorov equation defines the rules that must be followed by individuals. It makes the evolution of the system Markovian in a sense that the future of the system is dependent on the current state only and independent from the past. The defined rules are stochastic in their nature. Even possessing the full knowledge of the system (exact properties of each individual) in a given moment of time, one cannot describe the future of the system in a deterministic way. Additionally, one should take into account that

even in the laboratory conditions it is impossible to have such knowledge of the studied system. Considering the above, the adequate mathematical object representing the state of the system is a probability measure. One can write an equation dual to (1) describing evolution of states, which is called Fokker-Planck or Forward Kolmogorov Equation:

$$\frac{d}{dt}\mu_t = L^*\mu_t, \qquad \mu_{t=0} = \mu_0. \tag{2}$$

When dealing with infinite populations, the above equation is not treatable directly, but there is a way to study it by employing the correlation functions, with the assumption that the initial state is a sub-Poissonian measure (see e.g. [4]). The scheme is following: first derive an equation dual to (2) that describes evolution of correlation functions with an initial condition being a correlation function of measure μ_0, say

$$\frac{d}{dt}k_t(\eta) = L^{\Delta}k_t(\eta), \qquad k_{t=0} = k_0. \tag{3}$$

Then, derive the unique solution for this dual equation. Finally, show that it is a correlation function for a unique sub-Poissonian measure μ_t. In this way one obtains a solution to (2) in a weak sense.

Even though the considered model is rather simple, applying the above scheme is not a trivial task. The author is able to obtain the result for a finite time horizon, proving the following Theorem 1, a reformulation of results obtained in a more general case in [5]. The assumptions used therein are sub-Poissonity of the initial state and positiveness, boundedness and integrability of functions c_c, c_j and ϕ. First, introduce appropriate Banach spaces for correlation functions.

Definition 1 For a given parameter $\theta \in \mathbb{R}$ we define

$$\mathcal{K}_\theta = \{k : \Gamma_0 \to \mathbb{R} : ||k||_\theta < \infty\},$$

with Γ_0 being a set of all finite subsets of $\mathbb{R}^d$ and

$$||k||_\theta = \operatorname*{ess\,sup}_{\eta\in\Gamma_0} \left(e^{-\theta|\eta|}|k(\eta)| \right).$$

For each sub-Poissonian measure there exists a parameter θ such that the correlation function of this measure lies in $\mathcal{K}_\theta$.

Theorem 1 *Choose $\alpha_0 \in \mathbb{R}$ such that the correlation function k_0 of initial state μ_0 lies in $\mathcal{K}_{\alpha_0}$. Then, for any $\alpha_* > \alpha_0$ there exists $T > 0$ (dependent on α_0 and α_*) such that the equation (3) has a unique classical solution $k_t \in \mathcal{K}_{\alpha_*}$ on $[0, T)$. Moreover, k_t is a correlation function of a unique sub-Poissonian state μ_t.* □

PROOF (SKETCH) We construct k_t in the form $Q(t)k_0$, where each $Q(t) : \mathcal{K}_{\alpha_0} \to \mathcal{K}_{\alpha_*}$ is a series of operators dependent on t and convergent for $t < T$. It is defined in such a way that $\frac{d}{dt}Q(t) = L^{\Delta}Q(t)$, recall (3). The operator L^{Δ} can be split into two parts, a multiplication operator and a perturbation. The latter, when considered as acting from $\mathcal{K}_\theta$ to $\mathcal{K}_{\theta'}$ with $\theta' > \theta$, undergoes a convenient norm estimation of the form $||B_{\theta'\theta} \leq \frac{\beta(\theta)}{e(\theta'-\theta)}||$. Each summand of the mentioned series is an alternating composition of operators based on those two parts. The convergence of the series is showed by the means of the above estimation and Stirling inequality.

The more demanding part is to show that k_t is a correlation function of a unique sub-Poissonian measure. In order to do that, we need to prove that $k(\emptyset) = 1$ (which follows easily from the fact that k_0 is a correlation function), that there exists some real constant C such that n-th order component of k_t is boundend by C^n in $L^\infty((\mathbb{R}^d)^n)$ (which is satisfied due to the choice of underlying Banach spaces $\mathcal{K}_\theta$) and finally that it fulfills a special positivity property (see e.g. Proposition 2.3 in [4]), which is the main technical difficulty. In order to prove that this property holds, we introduce an auxiliary model. We show the desired property first for its local evolution, then for the auxiliary model itself and finally for the original model. The detailed proof can be found in [5]. ■

Theorem 1 gives a weak solution to (2). While the result is quite demanding to prove and satisfactory from the athematical point of view, it does not provide much information about the behaviour of the system, giving only rough estimation for correlation functions.

3. Poisson approximation. In order to understand the nature of the dynamics of the considered system, one can perform numerical simulations. One possible approach is to simulate the solution of the kinetic equation for densities of Poisson measures approximating the states of the considered system.

Definition 2 We say that a sub-Poissonian state μ is Poisson-approximable by a Poisson measure π_ρ with density ρ if there exists $\theta \in \mathbb{R}$ such that:

a) the correlation functions of both μ and π_ρ belong to $\mathcal{K}_\theta$,
b) there exists a continuous mapping $Q : [0,1] \to \mathcal{K}_\theta$ with $Q(0)$ being a correlation function of π_ρ and $Q(1)$ a correlation function of μ. □

One can obtain such an approximation of the equation (2) in a spirit of Vlasov mean-field scaling, see [7]. The corresponding kinetic equation for the

density ρ_t of approximating Poisson measures is of the following form:

$$\begin{aligned}\frac{d}{dt}\rho_t(x) &= \frac{1}{2}\int\limits_{(\mathbb{R}^d)^2} c_c(y_1-y_2)\delta(z(y_1,y_2)-x)\rho_t(y_1)\rho_t(y_2)dy_1dy_2 \\ &- \frac{1}{2}\int\limits_{\mathbb{R}^d}\Big(c_c(x-y_1)+c_c(y_1-x)\Big)\rho_t(x)\rho_t(y_1)dy_1 \\ &+ \int\limits_{\mathbb{R}^d} c_j(y_1-x)\exp\Big(-\int\limits_{\mathbb{R}^d}\phi(x-u)\rho_t(u)du\Big)\rho_t(y_1)dy_1 \\ &- \int\limits_{\mathbb{R}^d} c_j(x-y_1)\exp\Big(-\int\limits_{\mathbb{R}^d}\phi(y_1-u)\rho_t(u)du\Big)\rho_t(x)dy_1, \\ \rho_{t=0} &= \rho_0.\end{aligned} \tag{4}$$

Theorem 2 *Suppose that the initial state μ_0 is Poisson-approximable by π_{ρ_0}. Then, state μ_t described in Theorem 1 is Poisson-approximable by π_{ρ_t}, where ρ_t is the solution to (4).* □

Proof (Sketch) The assumption implies existence of $\theta_* \in \mathbb{R}$ and continuous $Q_0 : [0,1] \to \mathcal{K}_{\theta_*}$ such that $Q_0(0) = q_0$ (correlation function of π_{ρ_0}) and $Q_0(1) = k_0$ (correlation function of μ_0). We show continuity of $Q_t : [0,1] \to \mathcal{K}_{\theta^*}$ with $\theta^* > \theta_*$, where $Q_t(0) = q_t$ (correlation function of π_{ρ_t}) and $Q_t(\epsilon) = S_t^\epsilon Q_0(\epsilon)$ for $\epsilon \in (0,1]$ – the solution of problem

$$\frac{d}{dt}Q_t(\epsilon) = L_\epsilon^{\mathrm{ren}} Q_t(\epsilon), \quad Q_{t=0}(\epsilon) = Q_0(\epsilon),$$

obtained in a similar way to the one in the first part of Theorem 1 (see proof of Theorem 3.2 in [5] for details) with $L_\epsilon^{\mathrm{ren}}$ defined analogously as in [7], Chapter 4.1. $L_\epsilon^{\mathrm{ren}}$ is defined in such a way that $Q_t(1) = k_t$. The proof is split into two parts: first we show the continuity at $\epsilon = 0$ and then for $\epsilon \in (0,1]$. First, we observe that

$$Q_t(\epsilon) - q_t = S_t^\epsilon(Q_0(\epsilon) - q_0) + \int\limits_0^t S_s^\epsilon(L_\epsilon^{\mathrm{ren}} - V)q_{t-s}ds,$$

where V is a Vlasov operator analogous to the one in [7], Chapter 4.1. The desired continuity is obtained by means of assumed continuity of Q_0, estimation analogous to (4.16) in [5] and some technical estimations concerning $L_\epsilon - V$ (the most laborious part of the proof). The second part of the proof is based on the similar observation

$$Q_t(\epsilon) - Q_t(\epsilon') = S_t^\epsilon(Q_0(\epsilon) - Q_0(\epsilon')) + \int\limits_0^t S_s^\epsilon(L_\epsilon^{\mathrm{ren}} - L_{\epsilon'}^{\mathrm{ren}})Q_{t-s}(\epsilon')ds,$$

followed by analogous estimations. ■

4. Simulations. In order to reduce the amount of time required to simulate the behaviour of the system, we consider only the one-dimensional case ($d = 1$). Additionally, for the sake of simplicity, we choose $z(x, y) = \frac{x+y}{2}$, which means that during the act of coalescence of two individuals located respectively at x and y, the resulting individual appears at the midpoint.

One should notice that there are no straightforward methods to simulate the behaviour of a system with unbounded domain (at least up to the author's knowledge). In order to deal with this difficulty, we restrict the initial condition to some special cases. The first obvious choice is a homogeneous Poisson measure with density $\rho_0(x) = \rho_0$, but in this case the system can be reduced to a simple ODE with an explicit solution

$$\rho_t = \frac{\rho_0}{1 + \frac{<c_c>}{2}\rho_0 t}, \quad \text{where the } <c_c> = \int_{\mathbb{R}} c_c(x)dx.$$

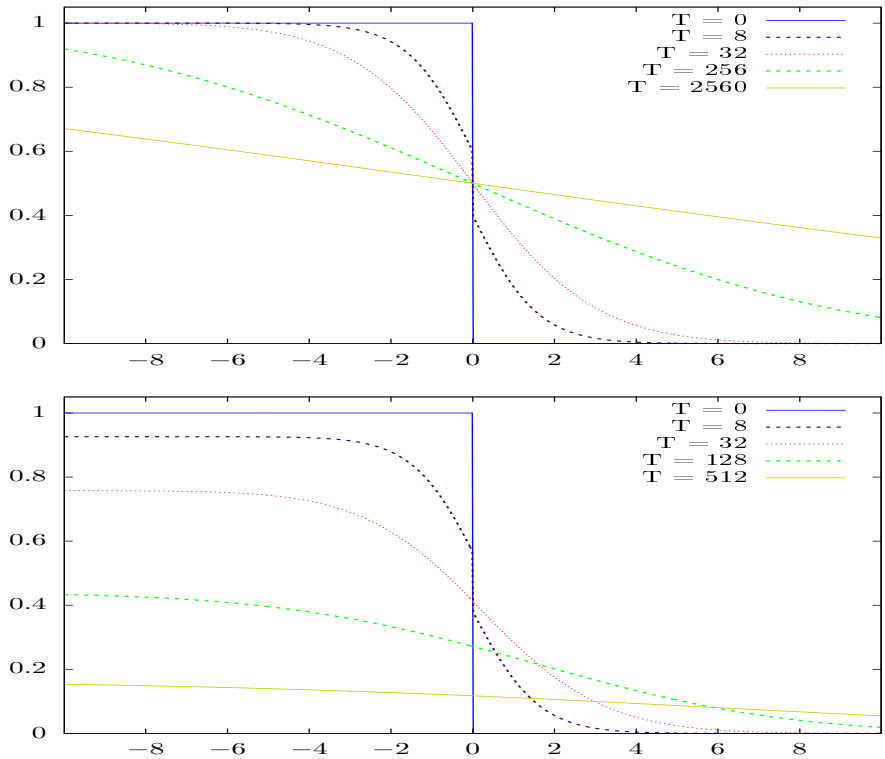
One can consider also a Poisson measure with density $\rho_0(x) = I_{(-\infty,0]}$, where I denotes an indicator function. With such a choice of the initial condition it is easy to deal with unboundedness of the domain. However, it introduces some interesting behaviour of the system that is worth a closer look. This choice can be interpreted as dealing with a big homogeneous population which is exposed to a sudden enlargment of habitable domain.

The performed simulations were based on Runge-Kutta method of the fourth order on a bounded segment $[-L, L]$ with asymptotic boundary condition on the left and Dirichlet boundary condition on the right. Additionally, an automatically adjustable system-size procedure was used. The asymptotic boundary condition on the left boundary was defined as the analytical solution to the homogeneous case. Whenever the simulated density function began to differ from the homogeneous solution in the neighbourhood of $-L$, the domain of the simulation was enlarged in order to avoid the influence of the boundary on the results. A similar procedure was used for the right boundary - the domain was automatically enlarged when nonzero values were approaching L. The author believes that the used mechanisms are sufficient to successfully imitate the considered infinite population.

First, consider the simplest case of jumps without coalescence and repulsion ($c_c = 0, \phi = 0$). The boundary condition on the left becomes Dirichlet, as without coalescence the homogeneous solution is just constant. Choose jump intensity to be a rescaled Gaussian $c_j(x) = \frac{0.2}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$ and set the initial size of the system to 20 ($L = 10$). As one should expect, the population starts to inhabit the unoccupied region. With the flow of density to the right, the initial discontinuity vanishes changing to less and less steep decreasing curve with values bigger than $\frac{1}{2}$ to the left and smaller than $\frac{1}{2}$ to the right from the initial discontinuity point (see Fig. 1, upper plot). One can expect that with $t \to \infty$ the density tends to homogeneous $\frac{1}{2}$.

In order to see how the coalescence affects the dynamics of the system,

Figure 1: Numerical solution to kinetic equation in the case of free jumps with gaussian intensities: density over [-10, 10] at the chosen time moments in the absence of coalescence (upper) and in the presence of coalescence (lower)



set coalescence intensity to be also a Gaussian, but weaker than jump kernel (strength factor 0.02 instead of 0.2). In the presence of coalescence, the asymptotic behaviour of the system is trivial, as the density tends to zero everywhere. It is worth taking a closer look at the short-time behaviour, though. The lower plot in Figure 1 shows the dynamics of the system. When comparing with the upper plot, homogeneity at the initial domain seems to be achieved faster than in the absence of coalescence. The density at the initial discontinuity point appears to take higher values than $\frac{1}{2}$ of the homogeneous solution.

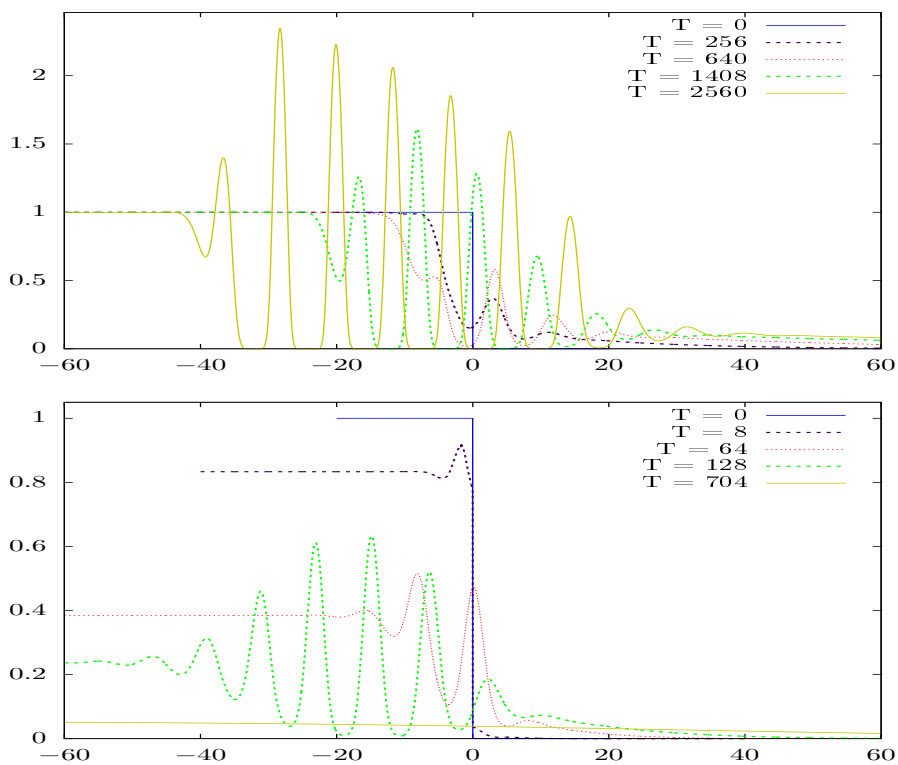
So far, in the discussed cases we were omitting the repulsion, which actually can drastically change the dynamics of the system. Consider the case of jumps with nonzero repulsion potential but without coalescence (setting $c_c = 0$). It appears that due to repulsion, the system can obtain interesting spatial heterogeneity. In order to see this, set both jump kernel and repulsion

potential to be rescaled, shifted and symmetrized Gaussians

$$c_j(x) = \frac{1}{2\sqrt{2\pi}}\left(e^{-\frac{(x-2)^2}{2}} + e^{-\frac{(x+2)^2}{2}}\right),$$
$$\phi(x) = \frac{5}{\sqrt{2\pi}}\left(e^{-\frac{(x-4)^2}{2}} + e^{-\frac{(x+4)^2}{2}}\right).$$

Additionally, change the initial domain to [-20, 20] and observe the dynamics at a little bigger domain [-60, 60]. The results of simulations (see Figure 2, upper plot) clearly shows an appearance of spatial heterogeneity that extends both to the left and to the right from the initial point of discontinuity. After a period of time, in regularly distributed regions, the density of population even exceeds the initial homogeneous value. The observed behaviour suggests existence of nontrivial stationary states that can be approached starting from a distant initial state.

Figure 2: Numerical solution to kinetic equation in the case of jumps with repulsion and symmetrized, shifted gaussian intensities: density over [-60, 60] at the chosen moments of time in the absence of coalescence (upper) and in the presence of coalescence (lower)



Consider addition of coalescence with relatively small intensity

$$c_c(x) = \frac{0.025}{\sqrt{2\pi}} \left(e^{-\frac{(x-2)^2}{2}} + e^{-\frac{(x+2)^2}{2}} \right).$$

Similarly as in the case of free jumps, the appearance of merging seems to speed up the dynamics, as the heterogeneity appears much more quickly. However, after some time it proves to also have a regulatory effect that counters propagation of heterogeneity and turns the system back homogeneous (see Figure 2, lower plot).

Please take into account that the showed behaviour of the system was obtained only for the chosen $z(x, y)$, kernels c_c, c_j, repulsion potential ϕ and most notably the initial density ρ_0. In the view of an immense number of possible choices of these functions, there is of course much more to show. For example, in the case of the system with lone coalescence, it is possible to choose intensity and the initial state that approaches a nontrivial stationary state or create different spatial heterogeneity. Hopefully, an article covering some more examples of interesting behaviour of the considered system will appear soon.

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Skoki z częściowo deterministycznym sklejaniem.

Krzysztof Pilorz

Streszczenie Celem niniejszego artykułu jest omówienie szczególnego przypadku modelu skoków z odpychaniem oraz ze sklejaniem opisującego dynamikę nieskończonej liczby agentów. Skoki są wyposażone w mechanizm odpychania oparty o punkt docelowy skoku. Jądro koalescencji jest zdefiniowane w taki sposób, że wynik sklejania dwóch agentów jest określony w sposób deterministyczny. Podany został przykład podejścia do badania numerycznego dynamiki tego modelu opierający się o przybliżanie stanów układu miarami Poissona. Pokazano kilka ciekawych rezultatów takich symulacji.

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[a] References to his research papers are found in MathSciNet under ID: 1170044 and the European Mathematical Society, FIZ Karlsruhe, and the Heidelberg Academy of Sciences bibliography database known as zbMath under ai:Pilorz.Krzysztof.

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