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Efficient simulation of individual-based population models

The R package IBMPopSim

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Abstract

The R Package IBMPopSim aims to simulate the random evolution of heterogeneous populations using stochastic Individual-Based Models (IBMs). The package enables users to simulate population evolution, in which individuals are characterized by their age and some characteristics, and the population is modified by different types of events, including births/arrivals, death/exit events, or changes of characteristics. The frequency at which an event can occur to an individual can depend on their age and characteristics, but also on the characteristics of other individuals (interactions). Such models have a wide range of applications in fields including actuarial science, biology, ecology or epidemiology. IBMPopSim overcomes the limitations of time-consuming IBMs simulations by implementing new efficient algorithms based on thinning methods, which are compiled using the Rcpp package while providing a user-friendly interface.

Keywords: Individual-based models, stochastic simulation, population dynamics, Poisson measures, thinning method, actuarial science, insurance portfolio simulation

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1 Introduction

In various fields, advances in probability have contributed to the development of a new mathematical framework for so-called individual-based stochastic population dynamics, also called stochastic Individual-Based Models (IBMs).

Stochastic IBMs allow the modeling in continuous time of populations dynamics structured by age and/or characteristics. In the field of mathematical biology and ecology, a large community has used this formalism for the study of the evolution of structured populations (see e.g. (Ferrière and Tran 2009; Collet, Méléard, and Metz 2013; Bansaye and Méléard 2015; Costa et al. 2016; Billiard et al. 2016; Lavallée et al. 2019; Méléard, Rera, and Roget 2019; Calvez et al. 2020)), after the pioneer works (Fournier and Méléard 2004; Tran 2008; Méléard and Tran 2009).

IBMs are also useful in demography and actuarial sciences, for the modeling of human populations dynamics (see e.g. (Bensusan 2010; Boumezoued 2016; El Karoui, Hadji, and Kaakai 2021)). They allow the modeling of heterogeneous and complex population dynamics, which can be used to compute demographic indicators or simulate the evolution of insurance portfolios in order to study the basis risk, compute cash flows for annuity products or pension schemes, or for a fine assessment of mortality models (Barrieu et al. 2012). There are other domains in which stochastic IBMs can be used, for example in epidemiology with stochastic compartmental models, neurosciences, cyber risk, or Agent-Based Models (ABMs) in economy and social sciences, which can be seen as IBMs. Many mathematical results have been obtained in the literature cited above, for quantifying the limit behaviors of IBMs in long time or in large population. In particular, pathwise representations of IBMs have been introduced in (Fournier and Méléard 2004) (and extended to age-structured populations in (Tran 2008; Méléard and Tran 2009)), as measure-valued pure jumps Markov processes, solutions of SDEs driven by Poisson measures. These pathwise representations are based on the *thinning* and projection of Poisson random measures defined on extended spaces. However, the simulation of large and interacting populations is often referred as computationally expensive.

The aim of the R package `IBMPopSim` is to meet the needs of the various communities for efficient tools in order to simulate the evolution of stochastic IBMs. `IBMPopSim` provides a general framework for the simulation of a wide class of IBMs, where individuals are characterized by their age and/or a set of characteristics. Different types of events can be included in the modeling by users, depending on their needs: births, deaths, entry or exit in/to the population and changes of characteristics (swap events). Furthermore, the various events that can happen to individuals in the population can occur at a non-stationary frequency, depending on the individuals' characteristics and time, and also including potential interactions between individuals.

We introduce a unified mathematical and simulation framework for this class of IBMs, generalizing the pathwise representation of IBMs by thinning of Poisson measures, as well as the associated population simulation algorithm, based on an acceptance/rejection procedure. In particular, we provide general sufficient conditions on the event intensities under which the simulation of a particular model is possible.

We opted to implement the algorithms of the `IBMPopSim` package using the `Rcpp` package, a tool facilitating the seamless integration of high-performance C++ code into easily callable R functions (Eddelbuettel and Francois 2011). With just a few lines of C++ code, `IBMPopSim` offers user-friendly R functions for defining IBMs. Once events and their associated intensities are specified, an automated procedure creates the model. This involves integrating the user's source code into the primary C++ code using a template mechanism. Subsequently, `Rcpp` is invoked to compile the model and integrate it into the R session. Following this process, the model becomes callable with varying parameters, enabling the generation of diverse population evolution scenarios. Combined with the design of the simulation algorithms, the package structure yields very competitive simulation runtimes for IBMs, while staying user-friendly for R users. Several outputs function are also implemented in `IBMPopSim`. For instance the package allows the construction and visualization of age pyramids, as well as the construction of death and exposures table from the censored individual data, compatible with R packages concerned with mortality modelling, such as (Hyndman et al. 2023) or (A. Villegas, Millossovich, and Kaishev Hyndman 2018). Several examples are provided in the form of R vignettes

on the [website](#), and in recent works of (El Karoui, Hadji, and Kaakai 2021) and (Roget et al. 2022).

Designed for applications in social sciences, the R package `MicSim` (Zinn 2014) can be used for continuous time microsimulation. In continuous-time microsimulation, individual life-courses are usually specified by sequences of state transitions (events) and the time spans between these transitions. The state space is usually discrete and finite, which is not necessarily the case in `IBMPopSim`, where individuals can have continuous characteristics. But most importantly, microsimulation does not allow for interactions between individuals. Indeed, microsimulation produces separately the life courses of all individuals in the populations, based on the computation of the distribution functions of the waiting times in the distinct states of the state space, for each individual (Zinn 2014). This can be slow in comparison to the simulation by thinning of event times occurring in the population, which is based on selecting event times among some competing proposed event times. Finally, `MicSim` simplifies the `Mic-Core` microsimulation tool implemented in Java (Zinn et al. 2009). However, the implementation in R of simulation algorithms yields longer simulation run times than when using `Rcpp`. To the best of our knowledge, there are no other R packages currently available addressing the issue of IBMs efficient simulation.

In Section 2, we introduce the mathematical framework that characterizes the class of Stochastic Individual-Based Models (IBMs) that can be implemented in the `IBMPopSim` package. In particular, a general pathwise representation of IBMs is presented. The population dynamics is obtained as the solution of an SDE driven by Poisson measures, for which we obtain existence and uniqueness results in Theorem 2.1. Additionally, a succinct overview of the package is provided. In Section 3 the two main algorithms for simulating the population evolution of an IBM across the interval $[0, T]$ are detailed. In Section 4 we present the main functions of the `IBMPopSim` package, which allow for the definition of events and their intensities, the creation of a model, and the simulation of scenarios. Two examples are detailed in Section 5 and Section 6, featuring applications involving an heterogeneous insurance portfolio characterized by entry and exit events, and an age and size-structured population with intricate interactions.

2 Stochastic Individual-Based Models (IBMs) in `IBMPopSim`

Stochastic Individual-Based Models (IBMs) represent a broad class of random population dynamics models, allowing the description of populations evolution on a microscopic scale. Informally, an IBM can be summarized by the description of the individuals constituting the population, the various types of events that can occur to these individuals, along with their respective frequencies. In `IBMPopSim`, individuals can be characterized by their age and/or a collection of discrete or continuous characteristics. Moreover, the package enables users to simulate efficiently populations in which one or more of the following event types may occur:

- **Birth event:** addition of an individual of age 0 to the population.
- **Death event:** removal of an individual from the population.
- **Entry event:** arrival of an individual in the population.
- **Exit (emigration) event:** exit from the population (other than death).
- **Swap event:** an individual changes characteristics.

Each event type is linked to an associated event kernel, describing how the population is modified following the occurrence of the event. For some event types, the event kernel requires explicit specification. This is the case for entry events when a new individual joins the population. Then, the model should specify how the age and characteristics of this new individual are chosen. For instance, the characteristics of a new individual in the population can be chosen uniformly in the space of all characteristics, or can depend on the distribution of his parents or those of the other individuals composing the population.

The last component of an IBM are the event intensities. Informally, an event intensity is a function $\lambda_t^e(I, Z)$ describing the frequency at which an event e can occur to an individual I in a population Z at a time t . Given a history of the population (\mathcal{F}_t), the probability of event e occurring to individual I during a small interval of time $(t, t + dt]$ is proportional to $\lambda_t^e(I, t)$:

$$\mathbb{P}(\text{event } e \text{ occurring to } I \text{ during } (t, t + dt] | \mathcal{F}_t) \simeq \lambda_t^e(I, Z) dt.$$

The intensity function λ^e can include dependency on the individual's I age and characteristics, the time t , or the population composition Z in the presence of interactions.

2.1 Brief package overview

Prior to providing a detailed description of an Individual-Based Model (IBM), we present a simple model of birth and death in an age-structured *human* population. We assume no interactions between individuals, and individuals are characterized by their gender, in addition to their age. In this simple model, all individuals, regardless of gender, can give birth when their age falls between 15 and 40 years, with a constant birth rate of 0.05. The death intensity is assumed to follow a Gompertz-type intensity depending on age. The birth and death intensities are then given by

$$\lambda^b(t, I) = 0.05 \times \mathbf{1}_{[15, 40]}(a(I, t)), \quad \lambda^d(t, I) = \alpha \exp(\beta a(I, t)),$$

with $a(I, t)$ the age of individual I at time t . Birth events are also characterized with a kernel determining the gender of the newborn, who is male with probability p_{male} .

2.1.1 Model creation

To implement this model in IBMPopSim, it is necessary to individually define each event type. In this example, the `mk_event_individual` function is used. The creation of an event involves a few lines of cpp instructions defining the intensity and, if applicable, the kernel of the event. For a more in depth description of the event creation step and its parameters, we refer to Section 4.2.

The events of this simple model are for example defined through the following calls.

```
birth_event <- mk_event_individual(
  type = "birth",
  intensity_code = "result = birth_rate(I.age(t));",
  kernel_code = "newI.male = CUnif(0,1) < p_male;")

death_event <- mk_event_individual(
  type = "death",
  intensity_code = "result = alpha * exp(beta * I.age(t));")
```

In the cpp codes, the names `birth_rate`, `p_male`, `alpha` and `beta` refer to the model parameters defined in the following list.

```
params <- list(
  "alpha" = 0.008, "beta" = 0.02,
  "p_male" = 0.51,
  "birth_rate" = stepfun(c(15, 40), c(0, 0.05, 0)))
```

In a second step, the model is created by calling the function `mk_model`. A cpp source code is automatically created through a template mechanism based on the events and parameters, subsequently compiled using the `sourceCpp` function from the `Rcpp` package.

```

birth_death_model <- mk_model(
  characteristics = c("male" = "bool"),
  events = list(death_event, birth_event),
  parameters = params)

```

2.1.2 Simulation

Once the model is created and compiled, the `popsim` function is called to simulate the evolution of a population according to this model. To achieve this, an initial population must be defined. In this example, we extract a population from a dataset specified in the package (a sample of 100 000 individuals based on the population of England and Wales in 2014). It is also necessary to set bounds for the events intensities. In this example, they are obtained by assuming that the maximum age for an individual is 115 years.

```

a_max <- 115
events_bounds = c(
  "death" = params$alpha * exp(params$beta * a_max),
  "birth" = max(params$birth_rate))

```

The function `popsim` can now be called to simulate the population starting from the initial population `population(EW_pop_14$sample)` up to time $T = 30$.

```

sim_out <- popsim(
  birth_death_model,
  population(EW_pop_14$sample),
  events_bounds,
  parameters = params, age_max = a_max,
  time = 30)

```

The data frame `sim_out$population` contains the information (birth, death, gender) on individuals who lived in the population over the period $[0, 30]$. Functions of the package allows to provide aggregated information on the population.

In the remainder of this section, we define rigorously the class of IBMs that can be simulated in `IBMPopSim`, along with the assumptions that are required in order for the population to be simulatable. The representation of age-structured IBMs based on measure-valued processes, as introduced in Tran (2008), is generalized to a wider class of abstract population dynamics. The modeling differs slightly here, since individuals are *kept in the population* after their death (or exit), by including the death/exit date as an individual trait.

2.2 Population

2.2.1 Notations

In the remainder of the paper, the filtered probability space is denoted by $(\Omega, \{\mathcal{F}_t\}, \mathbb{P})$, under the usual assumptions. All processes are assumed to be càdlàg and adapted to the filtration $\{\mathcal{F}_t\}$ (for instance the history of the population) on a time interval $[0, T]$. For a càdlàg process X , we denote $X_{t-} := \lim_{s \rightarrow t} X_s$.

2.2.2 Individuals

An individual is represented by a triplet $I = (\tau^b, \tau^d, x) \in \mathcal{I} = \mathbb{R} \times \bar{\mathbb{R}} \times \mathcal{X}$ with:

- $\tau^b \in \mathbb{R}$ the date of birth,

- $\tau^d \in \bar{\mathbb{R}}$ the death date, with $\tau^d = \infty$ if the individual is still alive,
- a collection $x \in \mathcal{X}$ of characteristics where \mathcal{X} is the space of characteristics.

Note that in IBMs, individuals are usually characterized by their age $a(t) = t - \tau^b$ instead of their date of birth τ^b . However, using the latter is actually easier for the simulation, as it remains constant over time.

2.2.3 Population process

The population at a given time t is a random set

$$Z_t = \{I_k \in \mathcal{I}; k = 1, \dots, N_t\},$$

composed of all individuals (alive or dead) who have lived in the population before time t . As a random set, Z_t can be represented by a random counting measure on \mathcal{I} , that is an integer-valued measure $Z : \Omega \times \mathcal{I} \rightarrow \bar{\mathbb{N}}$ where for $A \in \mathcal{I}$, $Z(A)$ is the (random) number of individuals I in the subset A . With this representation:

$$Z_t(d\tau^b, d\tau^d, dx) = \sum_{k=1}^{N_t} \delta_{I_k}(\tau^b, \tau^d, x),$$

$$\text{with } \int_{\mathcal{I}} f(\tau^b, \tau^d, x) Z_t(d\tau^b, d\tau^d, dx) = \sum_{k=1}^{N_t} f(I_k).$$

The number of individuals present in the population *before time* t is obtained by taking $f \equiv 1$:

$$N_t = \int_{\mathcal{I}} Z_t(d\tau^b, d\tau^d, dx) = \sum_{k=1}^{N_t} \mathbf{1}_{\mathcal{I}}(I_k).$$

Note that $(N_t)_{t \geq 0}$ is an increasing process since dead/exited individuals are kept in the population Z . The number of alive individuals in the population at time t is:

$$N_t^a = \int_{\mathcal{I}} \mathbf{1}_{\{\tau^d > t\}} Z_t(d\tau^b, d\tau^d, dx) = \sum_{k=1}^{N_t} \mathbf{1}_{\{\tau_k^d > t\}}. \quad (1)$$

Another example is the number of alive individuals of age over a is

$$N_t([a, +\infty)) := \int_{\mathcal{I}} \mathbf{1}_{[a, +\infty)}(t - \tau^b) \mathbf{1}_{[t, \infty)}(\tau^d) Z_t(d\tau^b, d\tau^d, dx) = \sum_{k=1}^{N_t} \mathbf{1}_{\{t - \tau_k^b \geq a\}} \mathbf{1}_{\{\tau_k^d \geq t\}}.$$

2.3 Events

The population composition changes at random dates following different types of events. IBMPopSim allows the simulation of IBMs with the following events types:

- A **birth** event at time t is the addition of a new individual $I' = (t, \infty, X)$ of age 0 to the population. Their date of birth is $\tau^b = t$, and characteristics is X , a random variable of distribution defined by the birth kernel $k^b(t, I, dx)$ on \mathcal{X} , depending on t and its parent I . The population size becomes $N_t = N_{t-} + 1$, and the population composition after the event is

$$Z_t = Z_{t-} + \delta_{(t, \infty, X)}.$$

- An **entry** event at time t is also the addition of an individual I' in the population. However, this individual is not of age 0. The date of birth and characteristics of the new individual $I' = (\tau^b, \infty, X)$ are random variables of probability distribution defined by the entry kernel $k^{en}(t, ds, dx)$ on $\mathbb{R} \times \mathcal{X}$. The population size becomes $N_t = N_{t^-} + 1$, and the population composition after the event is:

$$Z_t = Z_{t^-} + \delta_{(\tau^b, \infty, X)}.$$

- A **death** or **exit** event of an individual $I = (\tau^b, \infty, x) \in Z_{t^-}$ at time t is the modification of its death date τ^d from $+\infty$ to t . This event results in the simultaneous addition of the individual (τ^b, t, x) and removal of the individual I from the population. The population size is not modified, and the population composition after the event is

$$Z_t = Z_{t^-} + \delta_{(\tau^b, t, x)} - \delta_I.$$

- A **swap** event (change of characteristics) results in the simultaneous addition and removal of an individual. If an individual $I = (\tau^b, \infty, x) \in Z_{t^-}$ changes of characteristics at time t , then it is removed from the population and replaced by $I' = (\tau^b, \infty, X)$. The new characteristics X is a random variable of distribution $k^s(t, I, dx)$ on \mathcal{X} , depending on time, the individual's age and previous characteristics x . In this case, the population size is not modified and the population becomes:

$$Z_t = Z_{t^-} + \delta_{(\tau^b, \infty, X)} - \delta_{(\tau^b, \infty, x)}.$$

To summarize, the space of event types is $E = \{b, en, d, s\}$, and the jump $\Delta Z_t = Z_t - Z_{t^-}$ (change in the population composition) generated by an event of type $e \in \{b, en, d, s\}$ is denoted by $\phi^e(t, I)$. We thus have the following rules summarized in Table 1.

Table 1: Action in the population for a given event name

| Event | Type | $\phi^e(t, I)$ | New individual |
|------------|------|---|--------------------------------------|
| Birth | b | $\delta_{(t, \infty, X)}$ | $\tau^b = t, X \sim k^b(t, I, dx)$ |
| Entry | en | $\delta_{(\tau^b, \infty, X)}$ | $(\tau^b, X) \sim k^{en}(t, ds, dx)$ |
| Death/Exit | d | $\delta_{(\tau^b, t, x)} - \delta_{(\tau^b, \infty, x)}$ | $\tau^d = t$ |
| Swap | s | $\delta_{(\tau^b, \infty, X)} - \delta_{(\tau^b, \infty, x)}$ | $X \sim k^s(t, I, dx)$ |

Remark 2.1 (Composition of the population).

- At time T , the population Z_T contains all individuals who lived in the population before T , including dead/exited individuals. If there are no swap events, or entries, the population state Z_t for any time $t \leq T$ can be obtained from Z_T . Indeed, if $Z_T = \sum_{k=1}^{N_T} \delta_{I_k}$, then the population at time $t \leq T$ is simply composed of the individuals born before t :

$$Z_t = \sum_{k=1}^{N_T} \mathbf{1}_{\{\tau_k^b \leq t\}} \delta_{I_k}.$$

- In the presence of entries (open population), a characteristic x can track the individuals' entry dates. Then, the previous equation can be easily modified in order to obtain the population Z_t at time $t \leq T$ from Z_T .

2.4 Events intensity

Once the different event types have been defined in the population model, the frequency at which each event occur in the population e have to be specified. Informally, the intensity $\Lambda_t^e(Z_t)$ at which an event e can occur is defined by

$$\mathbb{P}(\text{event } e \text{ occurs in the population } Z_t \in (t, t + dt] | \mathcal{F}_t) \simeq \Lambda_t^e(Z_t) dt.$$

For a more formal definition of stochastic intensities, we refer to (Brémaud 1981) or (Kaakai and El Karoui 2023). The form of the intensity function ($\Lambda_t^e(Z_t)$) determines the population simulation algorithm in IBMPopSim:

- When the event intensity does not depend on the population state,

$$(\Lambda_t^e(Z_t))_{t \in [0, T]} = (\mu^e(t))_{t \in [0, T]}, \quad (2)$$

with μ^e a deterministic function, the events of type e occur at the jump times of an inhomogeneous Poisson process of intensity function $(\mu^e(t))_{t \in [0, T]}$. When such an event occurs, the individual to whom the event happens to is drawn uniformly among alive individuals in the population. In a given model, the set of events $e \in E$ with Poisson intensities will be denoted by \mathcal{P} .

- Otherwise, we assume that the global intensity $\Lambda_t^e(Z_t)$ at which the events of type e occur in the population can be written as the sum of individual intensities $\lambda_t^e(I, Z_t)$:

$$\Lambda_t^e(Z_t) = \sum_{k=1}^{N_t} \lambda_t^e(I_k, Z_t),$$

$$\text{with } \mathbb{P}(\text{event } e \text{ occurs to an individual } I \in (t, t + dt] | \mathcal{F}_t) \simeq \lambda_t^e(I, Z_t) dt.$$

Obviously, nothing can happen to dead or exited individuals, i.e. individuals $I = (\tau^b, \tau^d, x)$ with $\tau^d \leq t$. Thus, individual event intensities are assumed to be null for dead/exited individuals:

$$\lambda_t^e(I, Z_t) = 0, \text{ if } \tau^d \leq t, \text{ so that } \Lambda_t^e(Z_t) = \sum_{k=1}^{N_t^a} \lambda_t^e(I_k, Z_t),$$

with N_t^a the number of alive individuals at time t .

The event's individual intensity $\lambda_t^e(I, Z_t)$ can depend on time (for instance when there is a mortality reduction over time), on the individual's age $t - \tau^b$ and characteristics, but also on the population composition Z_t . The dependence of λ^e on the population Z models interactions between individuals in the populations. Hence, two types of individual intensity functions can be implemented in IBMPopSim:

1. *No interactions*: The intensity function λ^e does not depend on the population composition. The intensity at which the event of type e occur to an individual I only depends on its date of birth and characteristics:

$$\lambda_t^e(I, Z_t) = \lambda^e(t, I), \quad (3)$$

where $\lambda^e : \mathbb{R}_+ \times \mathcal{I} \rightarrow \mathbb{R}^+$ is a deterministic function. In a given model, we denote by \mathcal{E} the set of event types with individual intensity Equation 3.

2. *"Quadratic" interactions*: The intensity at which an event of type e occurs to an individual I depends on I and on the population composition, through an interaction function W^e . The quantity $W^e(t, I, J)$ describes the intensity of interactions between two alive individuals I and J at time t , for instance in the presence of competition or cooperation. In this case, we have

$$\lambda_t^e(I, Z_t) = \sum_{j=1}^{N_t} W^e(t, I, I_j) = \int_{\mathcal{I}} W^e(t, I, (\tau^b, \tau^d, x)) Z_t(d\tau^b, d\tau^d, dx), \quad (4)$$

where $W^e(t, I, (\tau^b, \tau^d, x)) = 0$ if the individual $J = (\tau^b, \tau^d, x)$ is dead, i.e. $\tau^d \leq t$. In a given model, we denote by \mathcal{E}_W the set of event types with individual intensity Equation 4.

To summarize, an individual intensity in IBMPopSim can be written as:

$$\lambda_t^e(I, Z_t) = \lambda^e(t, I) \mathbf{1}_{\{e \in \mathcal{E}\}} + \left(\sum_{j=1}^{N_t} W^e(t, I, I_j) \right) \mathbf{1}_{\{e \in \mathcal{E}_W\}}. \quad (5)$$

Example 2.1.

1. An example of death intensity without interaction for an individual $I = (\tau^b, \tau^d, x)$ alive at time t , $t < \tau^d$, is:

$$\lambda_t^d(I) = \alpha_x \exp(\beta_x a(I, t)), \text{ where } a(I, t) = t - \tau^b$$

is the age of the individual I at time t . In this classical case, the death rate of an individual I is an exponential (Gompertz) function of the individual's age, with coefficients depending on the individual's characteristics x .

2. In the presence of competition between individuals, the death intensity of an individual I also depend on other individuals J in the population. For example, if $I = (\tau^b, \tau^d, x)$, with x its size, then we can have:

$$W^d(t, I, J) = (x_J - x)^+ \mathbf{1}_{\{\tau_J^d > t\}}, \quad \forall J = (\tau_J^b, \tau_J^d, x_J). \quad (6)$$

This can be interpreted as follows: if the individual I meets randomly an individual J alive at time t , and of bigger size $x_J > x$, then he can die at the intensity $x_J - x$. If J is smaller than I , then he cannot kill I . The bigger is the size x of I , the lower is his death intensity $\lambda_t^d(I, Z_t)$ defined by

$$\lambda_t^d(I, Z_t) = \sum_{\substack{J \in Z_t \\ x_J > x}} (x_J - x) \mathbf{1}_{\{\tau_J^d > t\}}.$$

3. IBMPopSim can simulate IBMs that include intensities expressed as a sum of Poisson intensities and individual intensities of the form $\Lambda^e(Z_t) = \mu_t^e + \sum_{k=1}^{N_t} \lambda^e(I_k, Z_t)$. Other examples are provided in Section 5 and Section 6. Finally, the global intensity at which an event can occur in the population is defined by:

$$\Lambda_t(Z_t) = \sum_{e \in \mathcal{P}} \mu^e(t) + \sum_{e \in \mathcal{E}} \left(\sum_{k=1}^{N_t} \lambda^e(t, I_k) \right) + \sum_{e \in \mathcal{E}_W} \left(\sum_{k=1}^{N_t} \sum_{j=1}^{N_t} W^e(t, I_k, I_j) \right). \quad (7)$$

An important point is that for events $e \in \mathcal{E}$ without interactions, the global event intensity $\Lambda_t^e(Z_t) = \sum_{k=1}^{N_t} \lambda^e(t, I_k)$ is of order N_t^a defined in Equation 1 (number of alive individuals at time t). On the other hand, for events $e \in \mathcal{E}_W$ with interactions, $\Lambda_t^e(Z_t) = \sum_{k=1}^{N_t} \sum_{j=1}^{N_t} W^e(t, I_k, I_j)$ is of order $(N_t^a)^2$. Informally, this means that when the population size increases, events with interaction are more costly to simulate. Furthermore, the numerous computations of the interaction kernel W^e can also be quite costly. The randomized Algorithm Algorithm 3, detailed in Section 2.3, allows us to overcome these limitations.

2.4.1 Events intensity bounds

The simulation algorithms implemented in IBMPopSim are based on an acceptance/rejection procedure, which requires to specify bounds for the various events intensities $\Lambda_t^e(Z_t)$. These bounds are defined differently depending on the expression of the intensity.

Assumption 2.1. For all events $e \in \mathcal{P}$ with Poisson intensity Equation 2, the intensity is assumed to be bounded on $[0, T]$:

$$\forall t \in [0, T], \quad \Lambda_t^e(Z_t) = \mu^e(t) \leq \bar{\mu}^e.$$

When $e \in \mathcal{E} \cup \mathcal{E}_W$, $\Lambda_t^e(Z_t) = \sum_{k=1}^{N_t} \lambda_t^e(I_k, Z_t)$, assuming that $\Lambda_t^e(Z_t)$ is uniformly bounded is too restrictive since the event intensity depends on the population size. In this case, the assumption is made on the individual intensity λ^e or on the interaction function W^e , depending on the situation.

Assumption 2.2. For all event types $e \in \mathcal{E}$, the associated individual event intensity λ^e with no interactions, i.e. λ^e verifies Equation 3, is assumed to be uniformly bounded:

$$\lambda^e(t, I) \leq \bar{\lambda}^e, \quad \forall t \in [0, T], \quad I \in \mathcal{I}.$$

In particular,

$$\forall t \in [0, T], \quad \Lambda_t^e(Z_t) = \sum_{k=1}^{N_t} \lambda^e(t, I) \leq \bar{\lambda}^e N_t. \quad (8)$$

Assumption 2.3. For all event types $e \in \mathcal{E}_W$, the associated interaction function W^e is assumed to be uniformly bounded:

$$W^e(t, I, J) \leq \bar{W}^e, \quad \forall t \in [0, T], \quad I, J \in \mathcal{I}.$$

In particular, $\forall t \in [0, T]$,

$$\lambda_t^e(I, Z_t) = \sum_{j=1}^{N_t} W^e(t, I, I_j) \leq \bar{W}^e N_t, \quad \text{and} \quad \Lambda_t^e(Z_t) \leq \bar{W}^e (N_t)^2.$$

Assumption 2.1, Assumption 2.2 and Assumption 2.3 yield that events in the population occur with the global event intensity $\Lambda_t(Z_t)$, given in Equation 7, which is dominated by a polynomial function in the population size:

$$\Lambda_t(Z_t) \leq \bar{\Lambda}(N_t), \quad \text{with} \quad \bar{\Lambda}(n) = \sum_{e \in \mathcal{P}} \bar{\mu}^e + \sum_{e \in \mathcal{E}} \bar{\lambda}^e n + \sum_{e \in \mathcal{E}_W} \bar{W}^e n^2. \quad (9)$$

This bound is linear in the population size if there are no interactions, and quadratic if there at least is an event including interactions. This assumption is the key to the algorithms implemented in IBMPopSim. Before presenting the simulation algorithm, we close this section with a rigorous definition of an IBM, based on the pathwise representation of its dynamics a Stochastic Differential Equation (SDE) driven by Poisson random measures.

2.5 Pathwise representation

Since the seminal paper of (Fournier and Méléard 2004), it has been shown in many examples that a stochastic IBM dynamics can be defined rigorously as the unique solution of an SDE driven by Poisson measures, under reasonable non explosion conditions. In the following, we introduce a unified framework for the pathwise representation of the class of stochastic IBMs introduced above. Some recalls on Poisson random measures are presented in the Appendix Section 7.1, and for more details on these representations on particular examples, we refer to the abundant literature on the subject.

In the following we consider an individual-based stochastic population $(Z_t)_{t \in [0, T]}$, keeping the notations introduced in Section 2.3 and Section 2.4 for the events and their intensities. In particular, the set of events types that define the population evolution is denoted by $\mathcal{P} \cup \mathcal{E} \cup \mathcal{E}_W \subset E$, with \mathcal{P} the set of events types with Poisson intensity verifying Assumption 2.1, \mathcal{E} the set of events types with individual intensity and no interaction, verifying Assumption 2.2 and finally \mathcal{E}_W the set of event types with interactions, verifying Assumption 2.3.

2.5.1 Non explosion criterion

First, one has to ensure that the number of events occurring in the population will not explode in finite time, leading to an infinite simulation time. Assumption 2.2 and Assumption 2.3 are not sufficient to guarantee the non explosion of the event number, due to the potential explosion of the population size in the presence of interactions. An example is the case when only birth events occur, with an intensity $\Lambda_t^b(Z_t) = C_b(N_t^a)^2$ ($W^b(t, I, J) = C_b$). Then, the number of alive individuals $(N_t^a)_{t \geq 0}$ is a well-known pure birth process of intensity function $g(n) = C_b n^2$ (intensity of moving from state n to $n + 1$). This process explodes in finite time, since g does not verify the necessary and sufficient non explosion criterion for pure birth Markov processes: $\sum_{n=1}^{\infty} \frac{1}{g(n)} = \infty$ (see e.g. Theorem 2.2 in (Bansaye and Méléard 2015)). There is thus an explosion in finite time of birth events.

This example shows that the important point for non explosion is to control the population size. We give below a general sufficient condition on birth and entry event intensities, in order for the population size to stay finite in finite time. This ensures that the number of events does not explode in finite time. Informally, the idea is to control the intensities by a pure birth intensity function verifying the non-explosion criterion.

Assumption 2.4. *Let $e = b$ or en , a birth or entry event type. If the intensity at which the events of type e occur in the population are not Poissonian, i.e. $e \in \mathcal{E} \cup \mathcal{E}_W$, then there exists a function $f^e : \mathbb{N} \rightarrow (0, +\infty)$, such that*

$$\sum_{n=1}^{\infty} \frac{1}{n f^e(n)} = \infty,$$

and for all individual $I \in \mathcal{I}$ and population measure $Z = \sum_{k=1}^n \delta_{I_k}$ of size n ,

$$\lambda_t^e(I, Z) \leq f^e(n), \quad \forall 0 \leq t \leq T.$$

If $e \in \mathcal{E}$, $\lambda_t^e(I, Z) = \lambda^e(t, I) \leq \bar{\lambda}^e$ by the domination Assumption 2.3, then Assumption 2.4 is always verified with $f^e(n) = \bar{\lambda}^e$.

Assumption 2.4 yields that the global intensity $\Lambda_t^e(\cdot)$ of event e is bounded by a function g^e only depending on the population size:

$$\Lambda_t^e(Z) \leq g^e(n) := n f^e(n), \quad \text{with} \quad \sum_{n=1}^{\infty} \frac{1}{g^e(n)} = \infty.$$

If $e \in \mathcal{P}$ has a Poisson intensity, then $\Lambda_t^e(Z) = \mu_t^e$ always verifies the previous equation with $g^e(n) = \bar{\mu}^e$.

Before introducing the IBM SDE, let us give an idea of the equation construction. Between two successive events, the population composition Z_t stays constant, since the population process $(Z_t)_{t \geq 0}$ is a pure jump process. Furthermore, since each event type is characterized by an intensity function, the jumps occurring in the population can be represented by restriction and projection of a Poisson measure defined on a larger state space. More precisely, we introduce a random Poisson measure Q on $\mathbb{R}^+ \times \mathcal{J} \times \mathbb{R}^+$, with $\mathcal{J} = \mathbb{N} \times (\mathcal{E} \cup \mathcal{E}_W)$. Q is composed of random quadruplets (τ, k, e, θ) , where τ represents a potential event time for an individual I_k and event type e . The last variable θ is used to accept/reject this proposed event, depending on the event intensity. Hence, the Poisson measure is restricted to a certain random set and then projected on the space of interest $\mathbb{R}^+ \times \mathcal{J}$. If the event is accepted, then a jump $\phi^e(\tau, I_k)$ occurs.

Theorem 2.1 (Pathwise representation). *Let $T \in \mathbb{R}^+$ and $\mathcal{J} = \mathbb{N} \times (\mathcal{E} \cup \mathcal{E}_W)$. Let Q be a random Poisson measure on $\mathbb{R}^+ \times \mathcal{J} \times \mathbb{R}^+$, of intensity $dt \delta_{\mathcal{J}}(dk, de) \mathbf{1}_{[0, \bar{\lambda}^e]}(\theta) d\theta$, with $\delta_{\mathcal{J}}$ the counting measure on \mathcal{J} . Finally, let $Q^{\mathcal{P}}$ be a random Poisson measure on $\mathbb{R}^+ \times \mathcal{P} \times \mathbb{R}^+$, of intensity $dt \delta_{\mathcal{P}}(de) \mathbf{1}_{[0, \bar{\mu}^e]}(\theta) d\theta$, and*

386 $Z_0 = \sum_{k=1}^{N_0} \delta_{I_k}$ an initial population. Then, under Assumption 2.4, there exists a unique measure-valued
 387 population process Z , strong solution on the following SDE driven by the Poisson measure Q :

$$\begin{aligned} Z_t = Z_0 &+ \int_0^t \int_{\mathcal{I} \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{k \leq N_{s-}\}} \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_{s-})\}} Q(ds, dk, de, d\theta) \\ &+ \int_0^t \int_{\mathcal{P} \times \mathbb{R}^+} \phi^e(s, I_{s-}) \mathbf{1}_{\{\theta \leq \mu^e(s)\}} Q^{\mathcal{P}}(ds, de, d\theta), \quad \forall 0 \leq t \leq T, \end{aligned}$$

388 and where I_{s-} is an individual, chosen uniformly among alive individuals in the population Z_{s-} .

389 The proof of Theorem 2.1 is detailed in the Appendix, Section 7.2.2. Note that Equation 10 is an SDE
 390 describing the evolution of the IBM, the intensity of the events in the right hand side of the equation
 391 depending on the population process Z itself. The main idea of the proof of Theorem 2.1 is to use
 392 the non explosion property of Lemma 2.1, and to write the r.h.s of Equation 10 as a sum of simple
 393 equations between two successive events, solved by induction.

394 **Lemma 2.1.** *Let Z be a solution of Equation 10 on \mathbb{R}^+ , with $(T_n)_{n \geq 0}$ its jump times, $T_0 = 0$. If*
 395 *Assumption 2.4 is satisfied, then*

$$\lim_{n \rightarrow \infty} T_n = \infty, \quad \mathbb{P}\text{-a.s.}$$

396 The proof of Lemma 2.1, detailed in Appendix Section 7.2.3 is more technical and rely on pathwise
 397 comparison result, generalizing those obtained in (Kaakai and El Karoui 2023). An alternative
 398 pathwise representation of the population process, inspired by the randomized Algorithm 3 is given
 399 as well in Proposition 3.3.

400 3 Population simulation

401 We now present the main algorithm for simulating the evolution of an IBM over $[0, T]$. The algorithm
 402 implemented in `IBMPopSim` allows the exact simulation of Equation 10, based on an acceptance/reject
 403 algorithm for simulating random times called *thinning*. The exact simulation of event times with
 404 this acceptance/reject procedure is closely related to the simulations of inhomogeneous Poisson
 405 processes by the so-called thinning algorithm, often attributed to Lewis and Shedler (1979). The
 406 simulation methods for inhomogeneous Poisson processes can be adapted to IBMs, and we introduce
 407 in this section a general algorithm extending those by Fournier and Méléard (2004) (see also Ferrière
 408 and Tran (2009), Bensusan (2010)).

409 The algorithm is based on exponential “candidate” event times, chosen with a (constant) intensity
 410 which must be greater than the global event intensity $\Lambda_t(Z_t)$ (Equation 3). Starting from time t , once a
 411 candidate event time $t + \tilde{T}_\ell$ has been proposed, a candidate event type e (birth, death,...) is chosen with
 412 a probability p^e depending on the event intensity bounds $\bar{\mu}^e$, $\bar{\lambda}^e$ and \bar{W}^e , as defined in Assumption 2.2
 413 and Assumption 2.3. An individual I is then drawn from the population. Finally, it remains to accept
 414 or reject the candidate event with a probability $q^e(t, I, Z_t)$ depending on the true event intensity. If
 415 the candidate event time is accepted, then the event e occurs at time $t + \tilde{T}_\ell$ to the individual I . The
 416 main idea of the algorithm implemented can be summarized as follows:

- 417 1. Draw a candidate time $t + \tilde{T}_\ell$ and candidate event type e .
- 418 2. Draw a uniform variable $\theta \sim \mathcal{U}([0, 1])$ and individual I .
- 419 3. **If** $\theta \leq q^e(t, I, Z_t)$ **then** event e occur to individual I , **else** Do nothing and start again from $t + \tilde{T}_\ell$.

420 Before introducing the main algorithms in more details, we recall briefly the thinning procedure
 421 for simulating inhomogeneous Poisson processes, as well as the links with pathwise representa-
 422 tions. Some recalls on Poisson random measures are presented in Section 7.1. For a more general

presentation of thinning of a Poisson random measure, see (Devroye 1986; Çinlar 2011; Kallenberg 2017).

3.1 Thinning of Poisson measure

Let us start with the simulation and pathwise representation of an inhomogeneous Poisson process on $[0, T]$ with intensity $(\Lambda(t))_{t \in [0, T]}$. The thinning procedure is based on the fundamental assumption that $\Lambda(t) \leq \bar{\Lambda}$ is bounded on $[0, T]$. In this case, the inhomogeneous Poisson can be obtained from an homogeneous Poisson process of intensity $\bar{\Lambda}$, which can be simulated easily.

First, the Poisson process can be extended to a Marked Poisson measure $\bar{Q} := \sum_{\ell \geq 1} \delta_{(\bar{T}_\ell, \bar{\Theta}_\ell)}$ on $(\mathbb{R}^+)^2$, defined as follow:

- The jump times of $(\bar{T}_\ell)_{\ell \geq 1}$ of \bar{Q} are the jump times of a Poisson process of intensity $\bar{\Lambda}$.
- The marks $(\bar{\Theta}_\ell)_{\ell \geq 1}$ are *i.i.d.* random variables, uniformly distributed on $[0, \bar{\Lambda}]$.

By Proposition 7.3, \bar{Q} is a Poisson random measure with mean measure

$$\bar{\mu}(dt, d\theta) := \bar{\Lambda} dt \frac{\mathbf{1}_{[0, \bar{\Lambda}]}(\theta)}{\bar{\Lambda}} d\theta = dt \mathbf{1}_{[0, \bar{\Lambda}]}(\theta) d\theta.$$

In particular, the average number of atoms $(\bar{T}_\ell, \bar{\Theta}_\ell)$ in $[0, t] \times [0, h]$ is

$$\mathbb{E}[Q([0, t] \times [0, h])] = \mathbb{E}\left[\sum_{\ell} \mathbf{1}_{[0, t] \times [0, h]}(\bar{T}_\ell, \bar{\Theta}_\ell)\right] = \int_{(\mathbb{R}^+)^2} \bar{\mu}(dt, d\theta) = t(\bar{\Lambda} \wedge h).$$

The thinning is based on the restriction property for Poisson measure: for a measurable set $\Delta \subset \mathbb{R}^+ \times \mathbb{R}^+$, the restriction $Q^\Delta := \mathbf{1}_\Delta \bar{Q}$ of \bar{Q} to Δ (by taking only atoms in Δ) is also a Poisson random measure of mean measure $\mu^\Delta(dt, d\theta) = \mathbf{1}_\Delta(t, \theta) \bar{\mu}(dt, d\theta)$.

In order to obtain an inhomogeneous Poisson measure of intensity $(\Lambda(t))$, the “good” choice of Δ is the hypograph of Λ : $\Delta = \{(t, \theta) \in [0, T] \times [0, \bar{\Lambda}]; \theta \leq \Lambda(t)\}$ (see Figure 1). Then,

$$Q^\Delta = \sum_{\ell \geq 1} \mathbf{1}_{\{\bar{\Theta}_\ell \leq \Lambda(\bar{T}_\ell)\}} \delta_{(\bar{T}_\ell, \bar{\Theta}_\ell)},$$

and since $\Lambda(t) \leq \bar{\Lambda}$, on $[0, T]$:

$$\mu^\Delta(dt, d\theta) = \mathbf{1}_{\{\theta \leq \Lambda(t)\}} dt \mathbf{1}_{[0, \bar{\Lambda}]}(\theta) d\theta = \mathbf{1}_{\{\theta \leq \Lambda(t)\}} dt d\theta.$$

Finally, the inhomogeneous Poisson process is obtained by the projection Proposition 7.2, which states that the jump times of Q^Δ are the jump times of an inhomogeneous Poisson process of intensity $(\Lambda(t))$.

Proposition 3.1. *The counting process N^Λ , projection of Q^Δ on the time component and defined by,*

$$N_t^\Lambda := Q^\Delta([0, t] \times \mathbb{R}^+) = \int_0^t \int_{\mathbb{R}^+} \mathbf{1}_{\{\theta \leq \Lambda(s)\}} \bar{Q}(ds, d\theta) = \sum_{\ell \geq 1} \mathbf{1}_{\{\bar{T}_\ell \leq t\}} \mathbf{1}_{\{\bar{\Theta}_\ell \leq \Lambda(\bar{T}_\ell)\}}, \quad \forall t \in [0, T], \quad (10)$$

is an inhomogeneous Poisson process on $[0, T]$ of intensity function $(\Lambda(t))_{t \in [0, T]}$. The thinning Equation 10 is a pathwise representation of N^Λ by restriction and projection of the Poisson measure Q on $[0, T]$.

The previous proposition yields a straightforward thinning algorithm to simulate the jump times $(T_k)_{k \geq 1}$ of an inhomogeneous Poisson process of intensity $\Lambda(t)$, by selecting jump times \bar{T}_ℓ such that $\bar{\Theta}_\ell \leq \Lambda(\bar{T}_\ell)$.

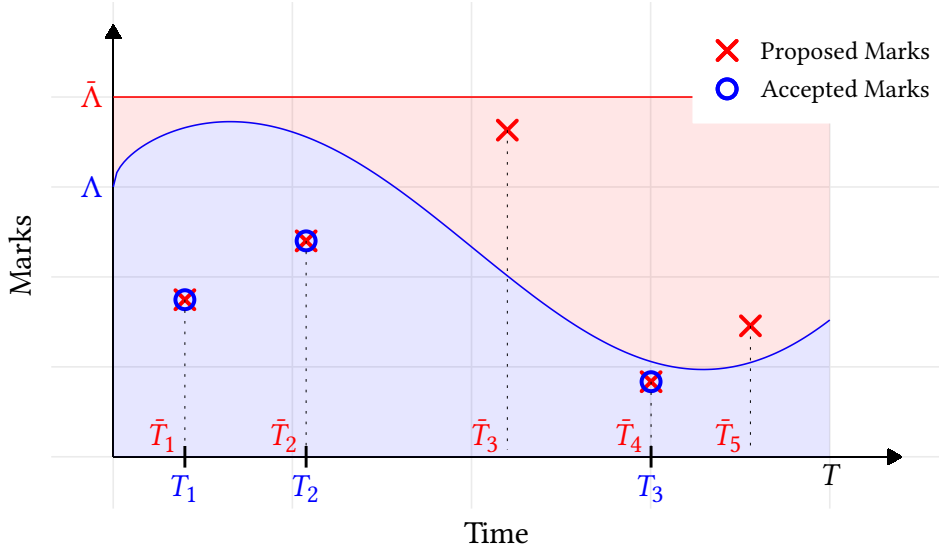


Figure 1: Realization of a Marked Poisson measure \bar{Q} on $[0, T]$ with mean measure $\bar{\mu}(dt, d\theta) = dt \mathbf{1}_{[0, \bar{\Lambda}]}(\theta) d\theta$ (red crosses), and realization of the restriction \bar{Q}^Δ where $\Delta = \{(t, \theta) \in [0, T] \times [0, \bar{\Lambda}], \theta \leq \Lambda(t)\}$ (blue circles). The projection of \bar{Q}^Δ on first component is an inhomogeneous Poisson process on $[0, T]$ of intensity $(\Lambda(t))$ and jump times $(T_k)_{k \geq 1}$.

3.1.1 Multivariate Poisson process

This can be extended to the simulation of multivariate inhomogeneous Poisson processes, which is an important example before tackling the simulation of an IBM.

Let $(N^j)_{j \in \mathcal{J}}$ be a (inhomogeneous) multivariate Poisson process indexed by a finite set \mathcal{J} , such that $\forall j \in \mathcal{J}$, the intensity $(\lambda_j(t))_{t \in [0, T]}$ of N_j is bounded on $[0, T]$:

$$\sup_{t \in [0, T]} \lambda_j(t) \leq \bar{\lambda}_j, \text{ and let } \bar{\Lambda} = \sum_{j \in \mathcal{J}} \bar{\lambda}_j.$$

Recall that such multivariate counting process can be rewritten as a Poisson random measure $N = \sum_{k \geq 1} \delta_{(T_k, J_k)}$ on $\mathbb{R}^+ \times \mathcal{J}$ (see e.g. Sec. 2 of Chapter 6 in (Çinlar 2011)), where T_k is the k th jump time of $\sum_{j \in \mathcal{J}} N^j$ and J_k corresponds to the component of the the vector which jumps. In particular, $N_t^j = N([0, t] \times \{j\})$.

Once again the simulation of such process can be obtained from the simulation of a (homogeneous) multivariate Poisson process of intensity vector $(\bar{\lambda}_j)_{j \in \mathcal{J}}$, extended into a Poisson measures by adding marks on \mathbb{R}^+ . Thus, we introduce the Marked Poisson measure $\bar{Q} = \sum \delta_{(\bar{T}_\ell, \bar{J}_\ell, \bar{\Theta}_\ell)}$ on $\mathbb{R}^+ \times \mathcal{J} \times \mathbb{R}^+$, such that:

- The jump times (\bar{T}_ℓ) of \bar{Q} are the jump times of a Poisson measure of intensity $\bar{\Lambda}$.
- The variables (\bar{J}_ℓ) are *i.i.d.* random variables on \mathcal{J} , with $p_j = \mathbb{P}(\bar{J}_1 = j) = \bar{\lambda}_j / \bar{\Lambda}$ and representing the component of the vector which jumps.
- The marks $(\bar{\Theta}_\ell)$ are independent variables with $\bar{\Theta}_\ell$ a uniform random variable on $[0, \bar{\lambda}_{\bar{J}_\ell}]$, $\forall \ell \geq 1$.

By Proposition 7.3 and Proposition 7.2, each measure $\bar{Q}_j(dt, d\theta) = \bar{Q}(dt, \{j\}, d\theta) = \sum_{\ell \geq 1} \mathbf{1}_{\{\bar{J}_\ell = j\}} \delta_{(\bar{T}_\ell, \bar{\Theta}_\ell)}$ is a marked Poisson measure of intensity

$$\bar{\mu}_j(dt, d\theta) = \bar{\Lambda} p_j dt \frac{\mathbf{1}_{\{\theta \leq \bar{\lambda}_j\}}(\theta)}{\bar{\lambda}_j} d\theta = dt \mathbf{1}_{\{\theta \leq \bar{\lambda}_j\}}(\theta) d\theta.$$

As a direct application of Proposition 3.1, the inhomogeneous multivariate Poisson process is obtained by restriction of each measures \bar{Q}_j to $\Delta_j = \{(t, \theta) \in [0, T] \times [0, \bar{\lambda}_j]; \theta \leq \lambda_j(t)\}$ and projection.

Proposition 3.2. *The multivariate counting process $(N_t^j)_{j \in \mathcal{J}}$, defined for all $j \in \mathcal{J}$ and $t \in [0, T]$ by thinning and projection of \bar{Q} :*

$$N_t^j := \int_0^t \int_{\mathbb{R}^+} \mathbf{1}_{\{\theta \leq \lambda_j(s)\}} \bar{Q}(ds, \{j\}, d\theta) = \sum_{\ell \geq 1} \mathbf{1}_{\{\bar{T}_\ell \leq t\}} \mathbf{1}_{\{\bar{J}_\ell = j\}} \mathbf{1}_{\{\bar{\Theta}_\ell \leq \lambda_j(\bar{T}_\ell)\}},$$

is an inhomogeneous Poisson process of intensity vector $(\lambda_j(t))_{j \in \mathcal{J}}$ on $[0, T]$.

Proposition 3.2 yields the following simulation Algorithm 1 for multivariate Poisson processes.

Algorithm 1 Thinning algorithm for multivariate inhomogeneous Poisson processes.

```

1: Input: Functions  $\lambda_j : [0, T] \rightarrow [0, \bar{\lambda}]$  and  $\bar{\lambda}_j, \bar{\Lambda} = \sum_{j \in \mathcal{J}} \bar{\lambda}_j$ 
2: Output: Points  $(T_k, J_k)$  of Poisson measure  $N$  on  $[0, T] \times \mathcal{J}$ 
3: Initialization  $T_0 \leftarrow 0, \bar{T}_0 \leftarrow 0$ 
4: while  $T_k < T$  do
5:   repeat
6:     increment iterative variable  $\ell \leftarrow \ell + 1$ 
7:     compute next proposed time  $\bar{T}_\ell \leftarrow \bar{T}_{\ell-1} + S_\ell$  with  $S_\ell \sim \mathcal{G}(\bar{\Lambda})$ 
8:     draw  $\bar{J}_\ell \sim \mathcal{U}\{\bar{\lambda}_j/\bar{\Lambda}, j \in \mathcal{J}\}$  i.e.  $\mathbb{P}(\bar{J}_\ell = j) = \bar{\lambda}_j/\bar{\Lambda}$ 
9:     draw  $\bar{\Theta}_\ell \sim \mathcal{U}([0, \bar{\lambda}_{\bar{J}_\ell}])$ 
10:    until accepted event  $\bar{\Theta}_\ell \leq \lambda_{\bar{J}_\ell}(\bar{T}_\ell)$ 
11:    record  $(T_k, J_k) \leftarrow (\bar{T}_\ell, \bar{J}_\ell)$  as accepted point
12: end while

```

Remark 3.1. The acceptance/rejection Algorithm 1 can be efficient when the functions λ_j are of different order, and thus bounded by different $\bar{\lambda}_j$. However, it is important to note that the simulation of the discrete random variables (\bar{J}_ℓ) can be costly (compared to a uniform law) when \mathcal{J} is large, for instance when an individual is drawn from a large population. In this case, an alternative is to choose the same bound $\bar{\lambda}_j = \bar{\lambda}$ for all $j \in \mathcal{J}$. Then the marks $(\bar{J}_\ell, \bar{\Theta}_\ell)$ are *i.i.d.* uniform variables on $\mathcal{J} \times [0, \bar{\lambda}]$, faster to simulate.

3.2 Simulation algorithm

Let us now come back to the simulation of the IBM introduced in Section 2. For ease of notations, we assume that there are no event with Poisson intensity ($\mathcal{P} = \emptyset$), so that all events that occur are of type $e \in \mathcal{E} \cup \mathcal{E}_W$, with individual intensity $\lambda_t^e(I, Z_t)$ depending on the population composition Z_t ($e \in \mathcal{E}_W$) or not ($e \in \mathcal{E}$), as defined in Equation 5 and verifying either Assumption 2.2 or Assumption 2.3. The global intensity Equation 7 at time $t \in [0, T]$ is thus

$$\Lambda_t(Z_t) = \sum_{e \in \mathcal{E}} \left(\sum_{k=1}^{N_t} \lambda_t^e(t, I_k) \right) + \sum_{e \in \mathcal{E}_W} \left(\sum_{k=1}^{N_t} \sum_{j=1}^{N_t} W^e(t, I_k, I_j) \right) \leq \bar{\Lambda}(N_t), \quad (11)$$

with $\bar{\Lambda}(n) = (\sum_{e \in \mathcal{E}} \bar{\lambda}^e) n + (\sum_{e \in \mathcal{E}_W} \bar{W}^e) n^2$.

One of the main difficulty is that the intensity of events is not deterministic as in the case of inhomogeneous Poisson processes, but a function $\Lambda_t(Z_t)$ of the population state, bounded by a function which also depends on the population size. However, the Algorithm 1 can be adapted to simulate the IBM. The construction is done by induction, by conditioning on the state of the population Z_{T_k} at the k th event time T_k ($T_0 = 0$).

We first present the construction of the first event at time T_1 .

3.2.1 First event simulation

Before the first event time, on $\{t < T_1\}$, the population composition is constant : $Z_t = Z_0 = \{I_1, \dots, I_{N_0}\}$. For each type of event e and individual I_k , $k \in \{1, \dots, N_0\}$, we denote by $N^{k,e}$ the counting process of intensity $\lambda_t^e(I_k, Z_t)$, counting the occurrences of the events of type e happening to the individual I_k . Then, the first event T_1 is the first jump time of the multivariate counting vector $(N^{(k,e)})_{(k,e) \in \mathcal{J}_0}$, with $\mathcal{J}_0 = \{1, \dots, N_0\} \times (\mathcal{E} \cup \mathcal{E}_W)$.

Since the population composition is constant before the first event time, each counting process N^j coincides on $[0, T_1[$ with an inhomogeneous Poisson process, of intensity $\lambda_t^e(I_k, Z_0)$. Thus (conditionally to Z_0), T_1 is also the first jump time of an inhomogeneous multivariate Poisson process $N^0 = (N^{0,j})_{j \in \mathcal{J}_0}$ of intensity function $(\lambda_j)_{j \in \mathcal{J}_0}$, defined for all $j = (k, e) \in \mathcal{J}_0$ by:

$$\lambda_j(t) = \lambda_t^e(I_k, Z_0) \leq \bar{\lambda}_0^e \quad \text{with} \quad \bar{\lambda}_0^e = \bar{\lambda}^e \mathbf{1}_{e \in \mathcal{E}} + \bar{W}^e N_0 \mathbf{1}_{e \in \mathcal{E}_W},$$

by Assumption 2.2 and Assumption 2.3. In particular, the jump times of N^0 occur at the intensity

$$\Lambda(t) = \sum_{j \in \mathcal{J}_0} \lambda_j(t) = \sum_{e \in \mathcal{E} \cup \mathcal{E}_W} \sum_{k=1}^{N_0} \lambda_t^e(I_k, Z_0) \leq \bar{\Lambda}(N_0) = N_0 \sum_{e \in \mathcal{E} \cup \mathcal{E}_W} \bar{\lambda}_0^e.$$

By Proposition 3.2, N^0 can be obtained by thinning of the marked Poisson measure $\bar{Q}^0 = \sum_{\ell \geq 1} \delta_{(\bar{T}_\ell, (\bar{K}_\ell, \bar{E}_\ell), \bar{\Theta}_\ell)}$ on $\mathbb{R}^+ \times \mathcal{J}_0 \times \mathbb{R}^+$, with:

- $(\bar{T}_\ell)_{\ell \in \mathbb{N}^*}$ the jump times of a Poisson process of rate $\bar{\Lambda}(N_0)$.
- $(\bar{K}_\ell, \bar{E}_\ell)_{\ell \in \mathbb{N}^*}$ discrete *i.i.d.* random variables on $\mathcal{J}_0 = \{1, \dots, N_0\} \times (\mathcal{E} \cup \mathcal{E}_W)$, with \bar{K}_ℓ representing the index of the chosen individual and \bar{E}_ℓ the event type for the proposed event, such that:

$$\mathbb{P}(\bar{K}_1 = k, \bar{E}_1 = e) = \frac{\bar{\lambda}_0^e}{\bar{\Lambda}(N_0)} = \frac{1}{N_0} \frac{\bar{\lambda}_0^e N_0}{\bar{\Lambda}(N_0)},$$

i.e. (\bar{K}_1, \bar{E}_1) are distributed as independent random variables where $\bar{K}_1 \sim \mathcal{U}(\{1, \dots, N_0\})$ and \bar{E}_1 such that

$$p_e := \mathbb{P}(\bar{E}_1 = e) = \frac{\bar{\lambda}_0^e N_0}{\bar{\Lambda}(N_0)}.$$

- $(\bar{\Theta}_\ell)_{\ell \in \mathbb{N}^*}$ are independent uniform random variables, with $\bar{\Theta}_\ell \sim \mathcal{U}([0, \bar{\lambda}^{\bar{E}_\ell}])$.

Since the first event is the first jump of N^0 , by Proposition 3.2 and Algorithm 1, the first event time T_1 is the first jump time \bar{T}_ℓ of \bar{Q}^0 such that $\bar{\Theta}_\ell \leq \lambda_{\bar{T}_\ell}^{\bar{E}_\ell}(I_{\bar{K}_\ell}, Z_0)$.

At $T_1 = \bar{T}_\ell$, the event \bar{E}_ℓ occurs to the individual $I_{\bar{K}_\ell} = (\tau^b, \infty, x)$. For instance, if $\bar{E}_\ell = d$, a death/exit event occurs, so that $Z_{T_1} = Z_0 + \delta_{(\tau^b, T_1, x)} - \delta_{I_{\bar{K}_\ell}}$ and $N_{T_1} = N_0$. If $\bar{E}_\ell = b$ or en , a birth or entry event occurs, so that $N_{T_1} = N_0 + 1$, and a new individual I_{N_0+1} is added to the population, chosen as described in Table 1. Finally, if $\bar{E}_\ell = s$, a swap event occurs, the population size stays constant and $I_{\bar{K}_\ell}$ is replaced by an individual $I'_{\bar{K}_\ell}$, chosen as described in Table 1.

The steps for simulating the first event in the population can be iterated in order to simulate the population. At the k th step, the same procedure is repeated to simulate the k th event, starting from a population $Z_{T_{k-1}}$ of size $N_{T_{k-1}}$.

Theorem 3.1. A population process $(Z_t)_{t \in [0, T]}$ simulated by the Algorithm 2 is an exact solution of the SDE Equation 10.

The proof of Theorem 3.1 is detailed in the Appendix Section 7.3.

Algorithm 2 IBM simulation algorithm (without events of Poissonian intensity)

```

1: Input: Initial population  $Z_0$ , horizon  $T > 0$ , and events described by:
2: - Intensity functions and bounds  $(\lambda^e, \bar{\lambda}^e)$  for  $e \in \mathcal{E}$  and  $(W^e, \bar{W}^e)$  for  $e \in \mathcal{E}_W$ 
3: - Event action functions  $\phi^e(t, I)$  for  $e \in \mathcal{E} \cup \mathcal{E}_W$ 
4: Output: Population  $Z_T$ 
5: Initialization  $T_0 \leftarrow 0, \bar{T}_0 \leftarrow 0$ 
6: while  $T_k < T$  do
7:   repeat
8:     increment iterative variable  $\ell \leftarrow \ell + 1$ 
9:     compute next proposed time  $\bar{T}_\ell \leftarrow \bar{T}_{\ell-1} + \mathcal{E}(\bar{\Lambda}(N_{T_k}))$ 
10:    draw a proposed event  $\bar{E}_\ell \sim \mathcal{U}\{p_e\}$  with  $p_e = \frac{\bar{\lambda}^e \mathbf{1}_{e \in \mathcal{E}} + \bar{W}^e N_{T_k} \mathbf{1}_{e \in \mathcal{E}_W}}{\sum_{e \in \mathcal{E}} \bar{\lambda}^e + \sum_{e \in \mathcal{E}_W} \bar{W}^e N_{T_k}}$ 
11:    draw an individual index  $\bar{K}_\ell \sim \mathcal{U}(\{1, \dots, N_{T_k}\})$ 
12:    draw  $\bar{\Theta}_\ell \sim \mathcal{U}([0, \bar{\lambda}^{\bar{E}_\ell}])$  if  $\bar{E}_\ell \in \mathcal{E}$  or  $\bar{\Theta}_\ell \sim \mathcal{U}([0, \bar{W}^{\bar{E}_\ell} N_{T_k}])$  if  $\bar{E}_\ell \in \mathcal{E}_W$ 
13:    until accepted event  $\bar{\Theta}_\ell \leq \lambda_{\bar{T}_\ell}^{\bar{E}_\ell}(I_{\bar{K}_\ell}, Z_{T_k})$ 
14:    increment iterative variable  $k \leftarrow k + 1$ 
15:    record  $(T_k, E_k, I_k) \leftarrow (\bar{T}_\ell, \bar{E}_\ell, I_{\bar{K}_\ell})$  as accepted time, event and individual
16:    update the population  $Z_{T_k} = Z_{T_{k-1}} + \phi^{E_k}(T_k, I_k)$ 
17:  end while

```

Remark 3.2. The population Z_{T_k} includes dead/exited individuals before the event time T_k . Thus, $N_{T_k} > N_{T_k}^a$ is greater than the number of alive individuals at time T_k . When a dead individual $I_{\bar{K}_\ell}$ is drawn from the population during the rejection/acceptance phase of the algorithm, the proposed event $(\bar{T}_\ell, \bar{E}_\ell, I_{\bar{K}_\ell})$ is automatically rejected since the event intensity is $\lambda_{\bar{T}_\ell}^{\bar{E}_\ell}(I_{\bar{K}_\ell}, Z_{T_k}) = 0$ (nothing can happen to a dead individual). This can slow down the algorithm, especially when the proportion of dead/exited individuals in the population increases. However, the computational cost of keeping dead/exited individuals in the population is much lower than the cost of removing an individual from the population at each death/exit event, which is linear in the population size.

Actually, dead/exited individuals are regularly removed from the population in the IBMPopSim algorithm, in order to optimize the trade-off between having too many dead individuals and removing dead individuals from the population too often. The frequency at which dead individuals are “removed from the population” can be chosen by the user, as an optional argument of the main function `popsim` (see details in Section 3).

Remark 3.3. In practice, the bounds $\bar{\lambda}^e$ and \bar{W}^e should be chosen as sharp as possible. It is easy to see that conditionally to $\{\bar{E}_\ell = e, \bar{T}_\ell = t, \bar{K}_\ell = l\}$ the probability of accepting the event is, depending if there are interactions,

$$\mathbb{P}(\bar{\Theta}_\ell \leq \lambda_t^e(I_l, Z_{T_k}) | \mathcal{F}_{T_k}) = \frac{\lambda^e(t, I_l)}{\bar{\lambda}^e} \mathbf{1}_{e \in \mathcal{E}} + \frac{\sum_{j=1}^{N_{T_k}} W^e(t, I_l, I_j)}{\bar{W}^e N_{T_k}} \mathbf{1}_{e \in \mathcal{E}_W}.$$

The sharper the bounds $\bar{\lambda}^e$ and \bar{W}^e are, the higher is the acceptance rate. For even sharper bounds, an alternative is to define bounds $\bar{\lambda}^e(I_l)$ and $\bar{W}^e(I_l)$ depending on the individuals’ characteristics. However, the algorithm is modified and the individual I_l is not chosen uniformly in the population anymore. Due to the population size, this is way more costly than choosing uniform bounds, as explained in Remark 3.1.

3.3 Simulation algorithm with randomization

Let $e \in E_W$ be an event with interactions. In order to evaluate the individual intensity $\lambda_t^e(I, Z_t) = \sum_{j=1}^{N_t} W^e(t, I, I_j)$ one must compute $W^e(t, I, I_j)$ for all individuals in the population. This step can be computationally costly, especially for large populations. One way to avoid this summation is to use randomization (see also Fournier and Méléard (2004) in a model without age). The randomization consists in replacing the summation by an evaluation of the interaction function W^e using an individual J drawn uniformly from the population.

More precisely, if $J \sim \mathcal{U}(\{1, \dots, N_{T_k}\})$ is independent of $\bar{\Theta}_\ell$, we have

$$\mathbb{P}\left(\bar{\Theta}_\ell \leq \sum_{j=1}^{N_{T_k}} W^e(t, I, I_j) \middle| \mathcal{F}_{T_k}\right) = \mathbb{P}(\bar{\Theta}_\ell \leq N_{T_k} W^e(t, I, I_J) \middle| \mathcal{F}_{T_k}). \quad (12)$$

Equivalently, we can write this probability as $\mathbb{P}(\bar{\Theta}_\ell \leq W^e(t, I, I_J))$ where $\bar{\Theta}_\ell = \frac{\bar{\Theta}_\ell}{N_{T_k}} \sim \mathcal{U}([0, \bar{W}^e])$ is independent of $J \sim \mathcal{U}(\{1, \dots, N_{T_k}\})$.

The efficiency of the randomization procedure increases with the population homogeneity. If the function W^e varies little according to the individuals in the population, the randomization approach is very efficient in practice, especially when the population is large.

We now present the main algorithm implemented in the `popsim` function of the `IBMPopSim` package in the case where events arrive with individual intensities, but also with interactions (using randomization) and Poisson intensities. In this general case, $\bar{\Lambda}(n)$ is defined by Equation 9.

Proposition 3.3. *The population processes $(Z_t)_{t \in [0, T]}$ simulated by the Algorithm 2 and Algorithm 3 have the same law.*

Proof. The only difference between Algorithm 2 and Algorithm 3 is in the acceptance/rejection step of proposed events, in the presence of interactions. In Algorithm 3, a proposed event $(\bar{T}_\ell, \bar{E}_\ell, \bar{K}_\ell)$, with $\bar{E}_\ell \in \mathcal{E}_W$ an event with interaction, is accepted as a true event in the population if

$$\bar{\Theta}_\ell \leq W^{\bar{E}_\ell}(\bar{T}_\ell, I_{\bar{K}_\ell}, I_{\bar{J}_\ell}), \text{ with } (\bar{\Theta}_\ell, \bar{J}_\ell) \sim \mathcal{U}([0, \bar{W}^{\bar{E}_\ell}] \times \{1, \dots, N_{T_k}\}).$$

By Equation 12, the probability of accepting this event is the same than in Algorithm 2, which achieves the proof. \square

4 Model creation and simulation with IBMPopSim

The use of the `IBMPopSim` package is mainly done in two steps: a first model creation followed by the simulation of the population evolution. The creation of a model is itself based on two steps: the description of the population Z_t , as introduced in Section 2.2, and the description of the events types, along with their associated intensities, as detailed in Section 2.3 and Section 2.4. A model is compiled by calling the `mk_model` function, which internally uses a template mechanism to generate automatically the source code describing the model, which is subsequently compiled using the `Rcpp` package to produce the object code.

After the compilation of the model, the simulations are launched by calling the `popsim` function. This function depends on the previously compiled model and simulates a random trajectory of the population evolution based on an initial population and on parameter values, which can change from a call to another.

Algorithm 3 Randomized IBM simulation algorithm.

```
1: Input: Initial population  $Z_0$ , horizon  $T > 0$ , and events described by
2: Intensity functions and bounds  $(\lambda^e, \bar{\lambda}^e)$  for  $e \in \mathcal{E}$ ,  $(W^e, \bar{W}^e)$  for  $e \in \mathcal{E}_W$  and  $(\mu^e, \bar{\mu}^e)$  for  $e \in \mathcal{P}$ 
3: Event action functions  $\phi^e(t, I)$  for  $e \in \mathcal{E} \cup \mathcal{E}_W \cup \mathcal{P}$ 
4: Output: Population  $Z_T$ 
5: Initialization  $T_0 \leftarrow 0, \bar{T}_0 \leftarrow 0$ 
6: while  $T_k < T$  do
7:   repeat
8:     increment iterative variable  $\ell \leftarrow \ell + 1$ 
9:     compute next proposed time  $\bar{T}_\ell \leftarrow \bar{T}_{\ell-1} + \mathcal{E}(\bar{\Lambda}(N_{T_k}))$ 
10:    draw an individual index  $\bar{K}_\ell \sim \mathcal{U}(\{1, \dots, N_{T_k}\})$ 
11:    draw a proposed event  $\bar{E}_\ell \sim \mathcal{U}\{p_e\}$  with  $p_e = \frac{\bar{\mu}^e \mathbf{1}_{e \in \mathcal{P}} + \bar{\lambda}^e N_{T_k} \mathbf{1}_{e \in \mathcal{E}} + \bar{W}^e(N_{T_k})^2 \mathbf{1}_{e \in \mathcal{E}_W}}{\bar{\Lambda}(N_{T_k})}$ 
12:    if  $\bar{E}_\ell \in \mathcal{E}$  (without interaction) then
13:      draw  $\bar{\Theta}_\ell \sim \mathcal{U}([0, \bar{\lambda}^{\bar{E}_\ell}])$ 
14:       $accepted \leftarrow \bar{\Theta}_\ell \leq \lambda^{\bar{E}_\ell}(\bar{T}_\ell, I_{\bar{K}_\ell})$ 
15:    end if
16:    if  $\bar{E}_\ell \in \mathcal{E}_W$  (with interaction) then
17:      draw  $(\bar{\Theta}_\ell, J_\ell) \sim \mathcal{U}([0, \bar{W}^{\bar{E}_\ell}] \times \{1, \dots, N_{T_k}\})$ 
18:       $accepted \leftarrow \bar{\Theta}_\ell \leq W^{\bar{E}_\ell}(\bar{T}_\ell, I_{\bar{K}_\ell}, I_{J_\ell})$ 
19:    end if
20:    if  $\bar{E}_\ell \in \mathcal{P}$  (Poissonian intensity) then
21:      draw  $\bar{\Theta}_\ell \sim \mathcal{U}([0, \bar{\mu}^{\bar{E}_\ell}])$ 
22:       $accepted \leftarrow \bar{\Theta}_\ell \leq \mu^{\bar{E}_\ell}(\bar{T}_\ell)$ 
23:    end if
24:    until accepted
25:    increment iterative variable  $k \leftarrow k + 1$ 
26:    record  $(T_k, E_k, I_k) \leftarrow (\bar{T}_\ell, \bar{E}_\ell, \bar{I}_{\bar{K}_\ell})$  as accepted time, event and individual
27:    update the population  $Z_{T_k} = Z_{T_{k-1}} + \phi^{E_k}(T_k, I_k)$ 
28: end while
```

583 In this section, we take a closer look at each component of a model in IBMPopSim. We also refer to
584 the [IBMPopSim website](#) and to the vignettes of the package for more details on the package and
585 various examples of model creation.

586 4.1 Population

587 A population Z is represented by an object of class `population` containing a data frame where each
588 row corresponds to an individual $I = (\tau^b, \tau^d, x)$, and which has at least two columns, `birth` and `death`,
589 corresponding to the birth date τ^b and death/exit date τ^d (τ^d is set to NA for alive individuals). The data
590 frame can contain more than two columns if individuals are described by additional characteristics
591 $x = (x_1, \dots, x_n)$.

592 If entry events can occur in the population, the population shall contain a characteristic named
593 `entry`. This can be done by setting the flag `entry=TRUE` in the `population` function, or by calling the
594 `add_characteristic` function on an existing population. During the simulation, the date at which
595 an individual enters the population is automatically recorded in the variable `I.entry`. If exit events
596 can occur, the population shall contain a characteristic named `out`. This can be done by setting the
597 flag `out=TRUE` in the `population` function, or by calling the `add_characteristic` function. When

an individual I exits the population during the simulation, $I.out$ is set to TRUE and its exit time is recorded as a “death” date.

In the example below, individuals are described by their birth and death dates, as well a Boolean characteristics called male, and the entry characteristic. For instance, the first individual is a female whose age at $t_0 = 0$ is 107 and who was originally in the population.

```
pop_init <- population(EW_pop_14$sample, entry=TRUE)
str(pop_init)
```

```
Classes 'population' and 'data.frame': 100000 obs. of 4 variables:
 $ birth: num -107 -107 -105 -104 -104 ...
 $ death: num NA NA NA NA NA NA NA NA NA NA ...
 $ male : logi FALSE FALSE TRUE FALSE FALSE FALSE ...
 $ entry: logi NA NA NA NA NA NA ...
```

4.1.1 Individual

In the C++ model which is automatically generated and compiled, an individual I is an object of an internal class containing some attributes (birth_date, death_date and the characteristics), and some methods including:

- $I.age(t)$: a const method returning the age of an individual I at time t ,
- $I.set_age(a, t)$: a method to set the age a at time t of an individual I (set birth_date at $t-a$),
- $I.is_dead(t)$: a const method returning true if the individual I is dead at time t .

Remark 4.1. A characteristic x_i must be of atomic type: logical, integer, double or character. The function `get_characteristic` allows to easily get characteristics names and their types from a population data frame. We draw the attention to the fact that some names for characteristics are forbidden, or reserved to specific cases : this is the case for birth, death, entry, out, id.

4.2 Events

The most important step of the model creation is the events creation. The call to the function creating an event is of form

```
mk_event_CLASS(type="TYPE", name="NAME", ...)
```

where CLASS is replaced by the class of the event intensity, described in Section 2.4 , and type corresponds to the event type, described in Section 2.3. Table 2a and Table 2b summarize the different possible choices for intensity classes and types of event. The optional argument name gives a name to the event. If not specified, the name of the event is its type, for instance death. However, a name must be specified if the model is composed of several events with the same type (for instance when there are multiple death events corresponding to different causes of death). The other arguments depend on the intensity class and on the event type.

The intensity function and the kernel of an event are defined through arguments of the function `mk_event_CLASS`. These arguments are strings composed of few lines of code. Since the model is compiled using Rcpp, the code should be written in C++. However, thanks to the functions/variables of the package, even the non-experienced C++ user can define a model quite easily. To facilitate the implementation, the user can also define a list of **model parameters**, which can be used in the event and intensity definitions. These parameters are stored in a named list and can be of various types: atomic type, numeric vector or matrix, predefined function of one variable (`stepfun`, `linfun`, `gompertz`, `weibull`, `piecewise_x`), piecewise functions of two variables (`piecewise_xy`). We refer

Table 2: Choices of CLASS and TYPE arguments for an event creation.

| (a) Intensity Classes | | | (b) Event Types | |
|-----------------------|-----------------|-----------------------|-----------------|-------|
| Intensity class | Set | CLASS | Event type | TYPE |
| Individual | \mathcal{E} | individual | Birth | birth |
| Interaction | \mathcal{E}_W | interaction | Death | death |
| Poisson | \mathcal{P} | poisson | Entry | entry |
| Inhomogeneous Poisson | \mathcal{P} | inhomogeneous_poisson | Exit | exit |
| | | | Swap | swap |

to the `vignette(IBMPopSim_cpp)` for more details on parameters types and basic C++ tools. Another advantage of the model parameters is that their value can be modified from a simulation to another without changing the model.

4.2.1 Intensities

In IBMPopSim, the intensity of an event can belong to three classes Section 2.4: individual intensities without interaction between individuals, corresponding to events $e \in \mathcal{E}$, individual intensities with interaction, corresponding to events $e \in \mathcal{E}_W$, and Poisson intensities (homogeneous and inhomogeneous), corresponding to events $e \in \mathcal{P}$.

Event creation with individual intensity

An event $e \in \mathcal{E}$ (see Equation 3) has an intensity of the form $\lambda^e(t, I)$ which depends only on the individual I and time. Events with such intensity are created using the function

```
mk_event_individual(type = "TYPE",
                    name = "NAME",
                    intensity_code = "INTENSITY", ...)
```

The `intensity_code` argument is a character string containing few lines of C++ code describing the intensity function $\lambda^e(t, I)$. The intensity value has to be stored in a variable called `result` and the available variables for the intensity code are given in Table 3.

Table 3: C++ variables available for intensity code

| Variable | Description |
|------------------|---|
| Variable | Description |
| I | Current individual |
| J | Another individual in the population (only for interaction) |
| t | Current time |
| Model parameters | Depends on the model |

For instance, the intensity code below corresponds to an individual death intensity $\lambda^d(t, I)$ equal to $d_1(a(I, t)) = \alpha_1 \exp(\beta_1 a(I, t))$ for males and $d_2(a(I, t)) = \alpha_2 \exp(\beta_2 a(I, t))$ for females, where $a(I, t) = t - \tau^b$ is the age of the individual $I = (\tau^b, \tau^d, x)$ at time t . In this case, the intensity function depends on the individuals' age, gender, and on the model parameters $\alpha = (\alpha_1, \alpha_2)$ and $\beta = (\beta_1, \beta_2)$.

```
death_intensity <- "
  if (I.male) result = alpha_1 * exp(beta_1 * I.age(t));
```

```

else result = alpha_2 * exp(beta_2 * I.age(t));
"

```

656 *Event creation with interaction intensity*

657 An event $e \in \mathcal{E}_W$ is an event which occurs to an individual at a frequency which is the result of
658 interactions with other members of the population (see Equation 4), and which can be written as
659 $\lambda_t^e(I, Z_t) = \sum_{J \in Z_t} W^e(t, I, J)$ where $W^e(t, I, J)$ is the intensity of the interaction between individual I
660 and individual J .

661 An event $e \in \mathcal{E}_W$ with such intensity is created by calling the function

```

mk_event_interaction(type = "TYPE",
                    name = "NAME",
                    interaction_code = "INTERACTION_CODE",
                    interaction_type = "random", ...)

```

662 The `interaction_code` argument contains few lines of C++ code describing the interaction function
663 $W^e(t, I, J)$. The interaction function value has to be stored in a variable called `result` and the available
664 variables for the intensity code are given in Table 3. For example, if we set

```

death_interaction_code <- "result = max(J.size - I.size, 0.);"

```

665 the death intensity of an individual I is the result of the competition between individuals, depending
666 on a characteristic named `size`, as defined in Equation 6.

667 The argument `interaction_type`, set by default at `random`, is the algorithm choice for sim-
668 ulating the model. When `interaction_type=full`, the simulation follows Algorithm 2 ,
669 `interaction_type=random` it follows Algorithm 3 . In most cases, the random algorithm is much
670 faster than the full algorithm, as we illustrate for instance in Section 6 , where we observe the
671 gain of a factor of 40 between the two algorithms, on a set of standard parameters. This allows in
672 particular to explore parameter sets that give larger population sizes, without reaching computation
673 times that explode.

674 *Events creation with Poisson and Inhomogeneous Poisson intensity*

675 For events $e \in \mathcal{P}$ with an intensity $\mu^e(t)$ which does not depend on the population, the event intensity
676 is of class `inhomogeneous_poisson` or `poisson` depending on whether or not the intensity depends
677 on time (in the second case the intensity is constant).

678 For Poisson (constant) intensities the events are created with the function

```

mk_event_poisson(type = "TYPE",
                 name = "NAME",
                 intensity = "CONSTANT", ...)

```

679 The following example creates a death event, where individuals die at a constant intensity `lambda`
680 (which has to be in the list of model parameters):

```

mk_event_poisson(type = "death",
                 intensity = "lambda")

```

681 When the intensity ($\mu^e(t)$) depends on time, the event can be created similarly by using the function

```

mk_event_inhomogeneous_poisson(type = "TYPE",
                                name = "NAME", intensity = "CONSTANT", ...)

```


4.2.2 Event kernel code

When an event occurs, the events kernels k^e specify how the event modifies the population. The events kernels are defined in the `kernel_code` parameter of the `mk_event_CLASS(type = "TYPE", name = "NAME", ...)` function. The `kernel_code` is NULL by default and doesn't have to be specified for death, exit events and birth events, but mandatory for entry and swap events. Recall that the `kernel_code` argument is a string composed of a few lines of C++ code, characterizing the individual characteristics following the event. Table 4 summarizes the list of available variables that can be used in the `kernel_code`.

- **Death/Exit event** If the user defines a death event, the death date of the current individual `I` is set automatically to the current time `t`. Similarly, when an individual `I` exits the population, `I.out` is set automatically to TRUE and his exit time is recorded as a "death" date. For these events types, the `kernel_code` doesn't have to be specified by the user.
- **Birth event** The default generated event kernel is that an individual `I` gives birth to a new individual `newI` of age 0 at the current time `t`, with same characteristics than the parent `I`. If no kernel is specified, the default generated C++ code for a birth event is:

```
individual newI = I;
newI.birth_date = t;
pop.add(newI);
```

The user can modify the birth kernel, by specify the argument `kernel_code` of `mk_event_CLASS`. In this case, the generated code is

```
individual newI = I;
newI.birth_date = t;
_KERNEL_CODE_
pop.add(newI);
```

where `_KERNEL_CODE_` is replaced by the content of the `kernel_code` argument.

- **Entry event** When an individual `I` enters the population, `I.entry` is set automatically as the date at which the individual enters the population. When an entry occurs the individual entering the population is not of age 0. In this case, the user must specify the `kernel_code` argument indicating how the age and characteristics of the new individual are chosen. For instance, the code below creates an event of type `entry`, named `ev_example`, where individuals enter the population at a Poisson constant intensity. When an individual `newI` enters the population at time `t`, his age is chosen as a normally distributed random variable, with mean 20 and variance 4.

```
mk_event_poisson(
    type = "entry",
    name = "ev_example",
    intensity = "lambda",
    kernel_code = "
        double a_I = max(CNorm(20, 2), 0.);
        newI.set_age(a_I, t);
    ")
```

- **Swap event** The user must specify the `kernel_code` argument indicating how the characteristics of an individual are modified following a swap.

Table 4: C++ variables available for events kernel code

| Variable | Description |
|------------------|---|
| Variable | Description |
| I | Current individual |
| J | Another individual in the population (only for interaction) |
| t | Current time |
| pop | Current population (vector) |
| newI | Available only for birth and entry events. |
| Model parameters | Depends on the model |

710 When there are several events of the same type, the user can identify which events generated a
711 particular event by adding a characteristic to the population recording the event name/id when it
712 occurs. See e.g. vignette(IBMPopSim_human_pop) for an example with different causes of death.

713 4.3 Model creation

714 Once the population, the events, and model parameters are defined, the IBM model is created using
715 the function `mk_model`.

```
model <- mk_model(characteristics = get_characteristics(pop_init),
                  event = events_list,
                  parameters = model_params)
```

716 During this step which can take a few seconds, the model is created and compiled using the Rcpp
717 package. The model structure in IBMPopSim is that the model depends only on the population
718 characteristics' and parameters names and types, rather than their values. This means that once
719 the model has been created, various simulations can be done with different initial populations and
720 different parameters values.

721 **Example 4.1.** Here is an example of model with a population structured by age and gender, with
722 birth and death events. The death intensity of an individual of age a is $d(a) = \alpha \exp(\beta a)$, and females
723 between 15 and 40 can give birth with birth intensity $b(a) = \bar{\lambda}^b \mathbf{1}_{[15,40]}$. The newborn is a male with
724 probability p_{male} .

```
params <- list("p_male" = 0.51,
              "birth_rate" = stepfun(c(15,40),c(0,0.05,0)),
              "death_rate" = gompertz(0.008,0.02))

death_event <- mk_event_individual(type = "death", name = "my_death_event",
                                   intensity_code = "result = death_rate(age(I,t));")

birth_event <- mk_event_individual( type = "birth",
                                   intensity_code = "if (I.male)
                                                         result = 0;
                                                         else
                                                         result=birth_rate(age(I,t));",
                                   kernel_code = "newI.male = CUnif(0, 1) < p_male;")

pop <- population(EW_pop_14$sample)
```

```

model <- mk_model(characteristics = get_characteristics(pop),
                  events = list(death_event, birth_event),
                  parameters = params)

```

4.4 Simulation

The simulation of the IBM is based on the algorithms presented in Section 3.2 and Section 3.3. The user has first to specify bounds for the intensity or interaction functions of each event type. The random evolution of the population can then be simulated over a period of time $[0, T]$ by calling the function `popsim`.

4.4.1 Events bounds

Since the IBM simulation algorithm is based on an acceptance-rejection method for simulating random times, the user has to specify bounds for the intensity (or interaction) functions of each event (see Assumption 2.2 and Assumption 2.3). These bounds should be stored in a named vector, where for event e , the name corresponding to the event bound $\bar{\mu}^e$, $\bar{\lambda}^e$ or \bar{W}^e is the event name defined during the event creation step.

In Example 4.1 from previous section the intensity bound for birth events is $\bar{\lambda}_b$. Since the death intensity function is not bounded, the user will have to specify a maximum age a_{\max} in `popsim` (all individuals above a_{\max} die automatically). Then, the bound for death events is $\bar{\lambda}_d = \alpha \exp(\beta a_{\max})$. In the example, the death event has been named `my_death_event`. No name has been specified for the birth event which thus has the default name `birth`. Then,

```

a_max <- 120 # maximum age
events_bounds <- c("my_death_event" = params$death_rate(a_max),
                  "birth" = max(params$birth_rate))

```

Once the model and events bounds have been defined, a random trajectory of the population can be simulated by calling

```

sim_out <- popsim(model, pop, events_bounds, params,
                  age_max = a_max, time = 30)

```

Optional parameters

5 Insurance portfolio

This section provides an example of how to use the `IBMPopSim` package to simulate a heterogeneous life insurance portfolio (see also `vignette(IBMPopSim_insurance_portfolio)`).

We consider an insurance portfolio consisting of male policyholders, of age greater than 65. These policyholders are characterized by their age, assumed to be less than $a_{\max} = 110$, and risk class $x \in \mathcal{X} = \{1, 2\}$.

Entries in the portfolio New policyholders enter the population at a constant Poisson rate $\mu^{en} = \lambda$, which means that on average, λ individuals enter the portfolio each year. A new individual enters the population at an age a that is uniformly distributed between 65 and 70, and is in risk class 1 with probability p .

Death events A baseline age and time specific death rate is first calibrated on “England and Wales (EW)” males mortality historic data^[1], and projected for 30 years using the Lee-Carter model with

the package StMoMo (see (A. M. Villegas, Kaishev, and Millossovich 2018)). The forecasted baseline death intensity is denoted by $d(t, a)$, defined by:

$$d(t, a) = \sum_{k=0}^{29} \mathbf{1}_{\{k \leq t < k+1\}} d_k(a), \quad \forall t \in [0, 30] \text{ and } a \in [65, a_{\max}], \quad (13)$$

with $d_k(a)$ the point estimate of the forecasted mortality rate for age a and year k . Individuals in risk class 1 are assumed to have mortality rates that are 20% higher than the baseline mortality (for instance, the risk class could refer to smokers), while individuals in risk class 2 are assumed to have mortality rates that are 20% lower than the baseline (non smokers). The death intensity of an individual $I = (\tau_b, \infty, x)$, of age $a(I, t) = t - \tau_b$ at time t and in risk class $x \in \{1, 2\}$ is thus the function

$$\lambda^d(t, I) = \alpha_x d(t, a(I, t)), \quad \alpha_1 = 1.2, \quad \alpha_2 = 0.8.$$

In particular, the death intensity verifies Assumption 2.3 since:

$$\lambda^d(t, I) \leq \bar{d} := \alpha_1 \sup_{t \in [0, 30]} d(t, a_{\max}). \quad (14)$$

Exits from the portfolio Individuals exit the portfolio at a constant (individual) rate $\lambda^{ex}(t, I) = \mu^i$ only depending on their risk class $i \in \{1, 2\}$.

5.1 Population

We start with an initial population of 30 000 males of age 65, distributed uniformly in each risk class. The population data frame has thus the two (mandatory) columns `birth` (here the initial time is $t_0 = 0$) and `death` (NA if alive), and an additional column `risk_cls` corresponding to the policyholders risk class. Since there are entry and exit events, the entry and out flags of the population constructor are set to TRUE.

```
N <- 30000
pop_df <- data.frame("birth" = rep(-65, N), "death" = rep(NA, N),
                    "risk_cls" = rep(1:2, each=N/2))
pop_init <- population(pop_df, entry=TRUE, out=TRUE)
```

5.2 Events

5.2.0.1 Entry events

The age of the new individual is determined by the `kernel_code` argument in the `mk_event_poisson` function.

```
entry_params <- list("lambda" = 30000, "p" = 0.5)
entry_event <- mk_event_poisson(
  type = "entry",
  intensity = "lambda",
  kernel_code = "if (CUnif() < p) newI.risk_cls = 1;
                else newI.risk_cls = 2;
                double a = CUnif(65, 70);
                newI.set_age(a, t);")
```

Note that the variables `newI` and `t`, as well as the function `CUnif()`, are implicitly defined and usable in the `kernel_code`. The field `risk_cls` comes from the names of characteristics of individuals in

779 the population. The names `lambda` and `p` are parameter names that will be specified in the R named
780 list `params`.

781 Here we use a constant λ as the event intensity, but we could also use a rate $\lambda(t)$ that depends on
782 time, using the function `mk_event_poisson_inhomogeneous`.

783 5.2.0.2 Death and exit events

784 The baseline death intensity defined in Equation 13 and obtained with the package `StMoMo` is stored
785 in the variable `death_male`.

```
# StMoMo death rates
library('StMoMo')
library('reshape2')
EWStMoMoMale <- StMoMoData(EWdata_hmd, series = "male")
LC <- lc()
ages.fit <- 65:100
years.fit <- 1950:2016
LCfitMale <- fit(LC, data = EWStMoMoMale, ages.fit = ages.fit, years.fit = years.fit)

786 StMoMo: Start fitting with gnm
787 Initialising
788 Running start-up iterations..
789 Running main iterations.....
790 Done
791 StMoMo: Finish fitting with gnm

t <- 30
LCforecastMale <- forecast(LCfitMale, h = t)
d_k <- apply(LCforecastMale$rates, 2, function(x) stepfun(66:100, x))
breaks <- 1:29
death_male <- piecewise_xy(breaks, d_k)

death_max <- max(sapply(d_k, function(x) { max(x) }))

death_params <- list("death_male" = death_male, "alpha" = c(1.2, 0.8))
death_event <- mk_event_individual(
  type = "death",
  intensity_code = "result = alpha[I.risk_cls-1] * death_male(t, I.age(t));")

792 The death and exit intensities are of class individual (see Table 2a). Hence, the death and exit events
793 are created with the mk_event_individual function.

death_params <- list("death_male" = death_male, "alpha" = c(1.2, 0.8))
death_event <- mk_event_individual(
  type = "death",
  intensity_code = "result = alpha[I.risk_cls-1] * death_male(t, I.age(t));")

exit_params = list("mu" = c(0.001, 0.06))
exit_event <- mk_event_individual(
  type = "exit",
  intensity_code = "result = mu[I.risk_cls-1]; ")
```

5.3 Model creation and simulation

The model is created from all the previously defined building blocks, by calling the `mk_model`.

```
model <- mk_model(  
  characteristics = get_characteristics(pop_init),  
  events = list(entry_event, death_event, exit_event),  
  parameters = c(entry_params, death_params, exit_params))
```

Once the model is compiled, it can be used with different parameters and run simulations for various scenarios. Similarly, the initial population (here `pop_df`) can be modified without rerunning the `mk_model` function. The bounds for entry events is simply the intensity λ . For death events, the bound is given by \bar{d} defined in Equation 14, which is stored in the `death_max` variable.

```
bounds <- c("entry" = entry_params$lambda,  
  "death" = death_max,  
  "exit" = max(exit_params$mu))  
  
sim_out <- popsim(  
  model = model,  
  initial_population = pop_init,  
  events_bounds = bounds,  
  parameters = c(entry_params, death_params, exit_params),  
  time = 30,  
  age_max = 110,  
  multithreading = TRUE)
```

5.4 Outputs

The data frame `sim_out$population` consists of all individuals present in the portfolio during the period of $[0, 30]$, including the individuals in the initial population and those who entered the portfolio. Each row represents an individual, with their date of birth, date of death (NA if still alive at the end of the simulation), risk class, and characteristics entry and out. Recall that if an individual enters the population at time t , his entry characteristic is automatically set up to be equal to t . The characteristics out is set to TRUE for individuals who left the portfolio due to an exit event.

In this example, the simulation time over 30 years, starting from an initial population of 30 000 individuals is of 2×10^{-4} seconds, for an acceptance rate of proposed event of approximately 25%. At the end of the simulation, the number of alive individuals is approximately 430 000.

Initially in the portfolio (at $t = 0$), there is the same number of 65 years old policyholders in each risk class. However, policyholders in the risk class 2 with lower mortality rates leave the portfolio at higher rate than policyholders in the risk class 1 : $\mu^2 > \mu^1$. Therefore, the heterogeneous portfolio composition changes with time, including more and more individuals in risk class 1 with higher mortality rates, but with variations across age classes. To illustrate the composition of the total population at the end of the simulation ($t = 30$), we present in Figure 2 the age pyramid of the final composition of the portfolio obtained with the `age_pyramid` and `plot` function of the `pyramid` class.

IBMPopSim also allows the fast computation of exact life tables from truncated and censored individual data (due to entry and exit events), using the functions `death_table` and `exposure_table`. These function are particularly efficient, since the computations are made using the `Rccp` library.

In Figure 3, we illustrate the central death rates in the simulated portfolio at final time. Due to the mortality differential between risk class 1 and 2, one would expect to observe more individuals in

risk class 2 at higher ages. However, due to exit events, a higher proportion of individuals in risk class 1 exit the portfolio over time, resulting in a greater proportion of individuals in risk class 1 at higher ages than what would be expected in the absence of exit events. Consequently, the mortality rates in the portfolio are more aligned with those of risk class 1 at higher ages. This is a simple example of how composition changes in the portfolio can impact aggregated mortality rates and potentially compensate or reduce an overall mortality reduction (see also (Kaakai et al. 2019)).

```
[1] 427741      5
[1] 0.1932777
[1] 0.2474907
```

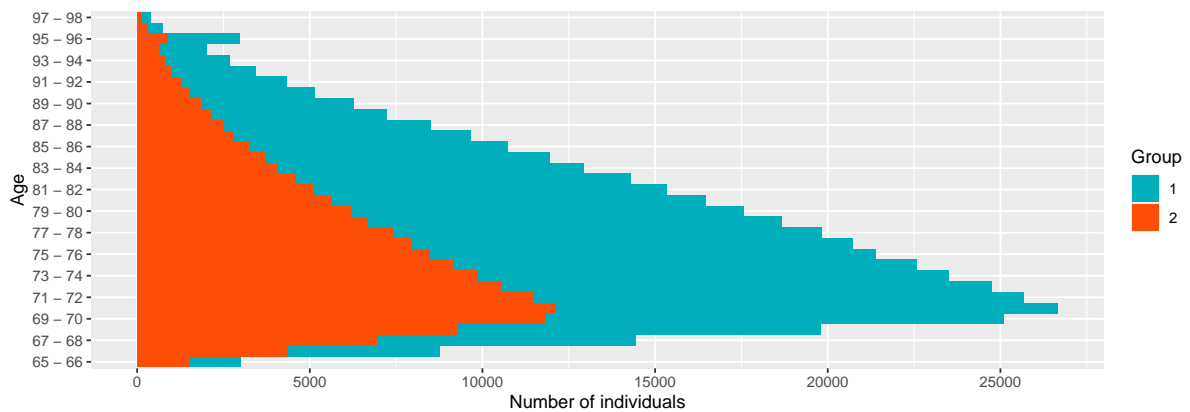


Figure 2: Portfolio age pyramid at t = 30 for individuals in risk class 1 (blue) and 2 (red).

```
StMoMo: The following cohorts have been zero weighed: -93 -92 -91 -90 -89 -88 -
87 -86 -85 -84 -83 -82 -81 -80 -79 -78 -77 -76 -75 -74 -73 -72 -71 -70
StMoMo: Start fitting with gnm
Initialising
Running start-up iterations..
Running main iterations.....
Done
StMoMo: Finish fitting with gnm
```

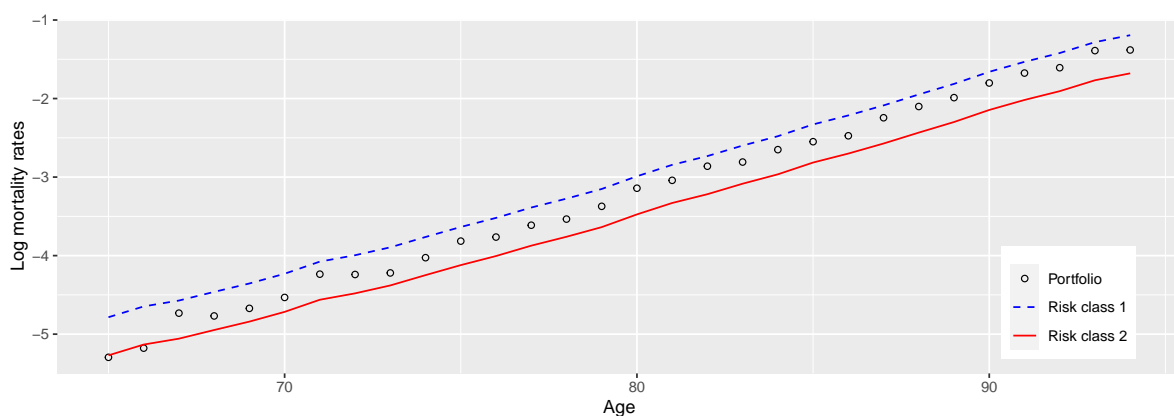


Figure 3: Portfolio central death rates at t = 30 (black).

6 Population with genetically variable traits

This section provides an example of how to use the `IBMPopSim` package to simulate an age-structured population with interactions, based on the model proposed in Example 1 of Ferrière and Tran (2009) (see also Méléard and Tran (2009)).

In this model, individuals are characterized by their body size at birth $x_0 \in [0, 4]$ and by their physical age $a \in [0, 2]$. The body size of an individual $I = (\tau^b, \infty, x_0)$ at time t is a linear function of its age $a(I, t) = t - \tau^b$:

$$x(t) = x_0 + ga(I, t),$$

where g is a constant growth rate assumed to be identical for all individuals.

Birth events The birth intensity of each individual $I = (\tau^b, \infty, x_0)$ depends on a parameter $\alpha > 0$ and on its initial size, as given by the equation

$$\lambda^b(t, I) = \alpha(4 - x_0) \leq \bar{\lambda}^b = 4\alpha. \quad (15)$$

Thus, smaller individuals have a higher birth intensity. When a birth occurs, the new individual inherits the same birth size x_0 as its parent with high probability $1 - p$, or a mutation can occur with probability p , resulting in a birth size given by

$$x'_0 = \min(\max(0, x_0 + G), 4), \quad (16)$$

where G is a Gaussian random variable with mean 0 and variance σ^2 .

Death events Due to competition between individuals, the death intensity of an individual depends on the size of other individuals in the population. Bigger individuals have a better chance of survival. If an individual $I = (\tau^b, \infty, x_0)$ of size $x(t) = x_0 + ga(I, t)$ encounters an individual $J = (\tau^b_j, \infty, x'_0)$ of size $x'(t) = x'_0 + ga(J, t)$, then it can die with the intensity

$$W(t, I, J) = U(x(t), x'(t)),$$

where the interaction function U is defined by

$$U(x, y) = \beta \left(1 - \frac{1}{1 + c \exp(-4(x - y))} \right) \leq \bar{W} = \beta. \quad (17)$$

The death intensity of an individual I at time t and in a population Z is the result of interactions with all individuals in the population, including itself, and is given by

$$\lambda^d_t(I, Z) = \sum_{J=(\tau^b, \infty, x'_0) \in Z} W(x_0 + ga(I, t), x'_0 + ga(J, t)),$$

6.1 Population

We use an initial population of 900 living individuals, all of whom have the same size and ages uniformly distributed between 0 and 2 years.

```
N <- 900
x0 <- 1.06
agemin <- 0.
agemax <- 2.

pop_df <- data.frame(
  "birth" = -runif(N, agemin, agemax), # Uniform age in [0,2]
  "death" = as.double(NA), # All individuals are alive
  "birth_size" = x0) # All individuals have the same initial birth size x0
pop_init <- population(pop_df)
```

6.2 Events

6.2.1 Birth events

The parameters involved in a birth event are the probability of mutation p , the variance of the Gaussian random variable and the coefficient α of the intensity.

```
params_birth <- list("p" = 0.03, "sigma" = sqrt(0.01), "alpha" = 1)
```

The birth intensity Equation 15 is of class individual. Hence, the event is created by calling the `mk_event_individual` function. The size of the new individual is given in the kernel following Equation 16.

```
birth_event <- mk_event_individual(  
  type = "birth",  
  intensity_code = "result = alpha*(4 - I.birth_size);",  
  kernel_code = "if (CUnif() < p)  
    newI.birth_size = min(max(0.,CNorm(I.birth_size,sigma)),4.);  
  else  
    newI.birth_size = I.birth_size;"
```

6.2.2 Death events

The death intensity Equation 17 is of class interaction. Hence, the event is created by calling the `mk_event_interaction` function. The parameters used for this event are the growth rate g , the amplitude of the interaction function β , and the strength of competition c .

```
params_death <- list("g" = 1, "beta" = 2./300., "c" = 1.2)  
death_event <- mk_event_interaction(  
  type = "death",  
  interaction_code = "double x_I = I.birth_size + g * age(I,t);  
    double x_J = J.birth_size + g * age(J,t);  
    result = beta*(1.-1./(1.+c*exp(-4.*(x_I-x_J))));"
```

6.3 Model creation and simulation

The model is created using the `mk_model` function.

The simulation of one scenario can then be launched with the call of the `popsim` function, after computing the events bounds $\bar{\lambda}^b = 4\alpha$ and $\bar{W} = \beta$.

```
model <- mk_model(  
  characteristics = get_characteristics(pop_init),  
  events = list(birth_event, death_event),  
  parameters = c(params_birth, params_death))
```

The simulation of one scenario can then be launched with the call of the `popsim` function, after computing the events bounds $\bar{\lambda}^b = 4\alpha$ and $\bar{W} = \beta$.

```
sim_out <- popsim(model = model,  
  initial_population = pop_init,  
  events_bounds = c("birth" = 4 * params_birth$alpha,  
    "death" = params_death$beta),  
  parameters = c(params_birth, params_death),  
  age_max = 2,  
  time = 500)
```


Based on the results of a simulation, we can reproduce the numerical results of Ferrière and Tran (2009). In Figure 4, we draw a line for each individual in the population to represent their birth size during their lifetime.

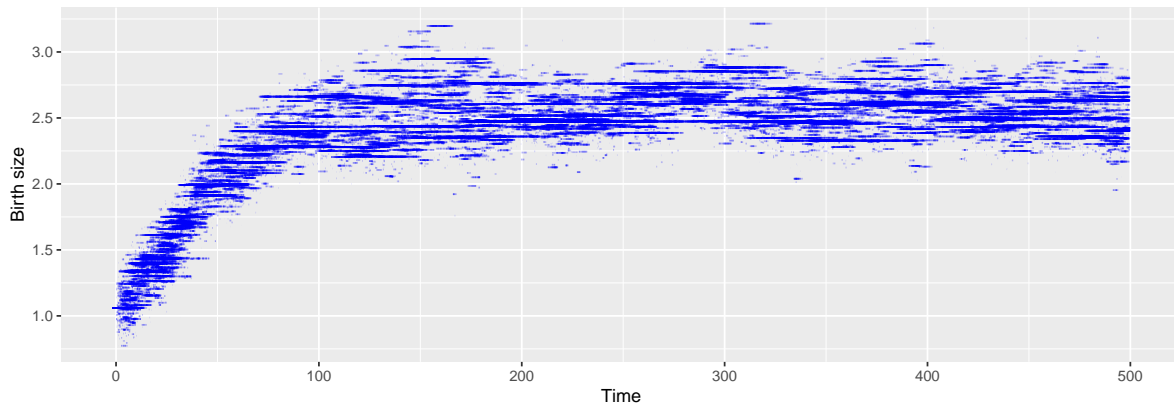


Figure 4: Evolution of birth size

In this example, the randomized Algorithm 3 allows for much faster computation times than the model implemented below with Algorithm 2 (“full” algorithm):

```
death_event_full <- mk_event_interaction(type = "death",
                                       interaction_type= "full",
                                       interaction_code = "double x_I = I.birth_size + g * age(I,t);
                                                         double x_J = J.birth_size + g * age(J,t);
                                                         result = beta * ( 1.- 1./(1. + c * exp(-4. * (x_I-x_J)))));"
)

model_full <- mk_model(characteristics = get_characteristics(pop_init),
                      events = list(birth_event, death_event_full),
                      parameters = c(params_birth, params_death))

sim_out_full <- popsim(model = model_full,
                     initial_population = pop_init,
                     events_bounds = c("birth" = 4 * params_birth$alpha,
                                       "death" = params_death$beta),
                     parameters = c(params_birth, params_death),
                     age_max = 2,
                     time = 500)
```

[1] "The full algorithm is 15.0644940357944 times slower than the randomized version"

In Figure 5, the two algorithms are compared for different population sizes.

We progressively decrease the value of the mortality rate parameter β and increase the birth rate parameter α . Starting with the values provided in Ferrière and Tran (2009), $\alpha = 1$ and $\beta = 2/300$, resulting in a stationary population size of approximately $N = 360$ individuals for a sample of 50 simulations, we can easily increase the stationary population size to approximately $N = 2600$ individuals with $\alpha = 2$ and $\beta = 1/300$.³ In the log-scaled figure, we can observe the trend of

³The choices $(\alpha, \beta) \in \{(1, 2/300), (1, 1/300), (1.5, 1/300), (2, 1/300)\}$ lead to the stationary population sizes $N \in \{360, 900, 1800, 2600\}$. For each set of parameters, we generated a new initial population, which was used for a benchmark of 50 simulations with both randomized and full algorithm. The simulations run on a Intel Core i7-8550U CPU 1.80GHz \times 8 processor, with 15.3 GiB of RAM, under Debian GNU/Linux 11.

computation time as a function of the population size N , which is linear for the randomized algorithm and quadratic for the full one (Algorithm 2). We can also see that the randomized version of the algorithm is between 17 to 100 times faster than the full one in this example, taking only 2 seconds in average for the randomized version versus 211 seconds for Algorithm 2 for the biggest population size ($N = 2600$) and $T = 500$.

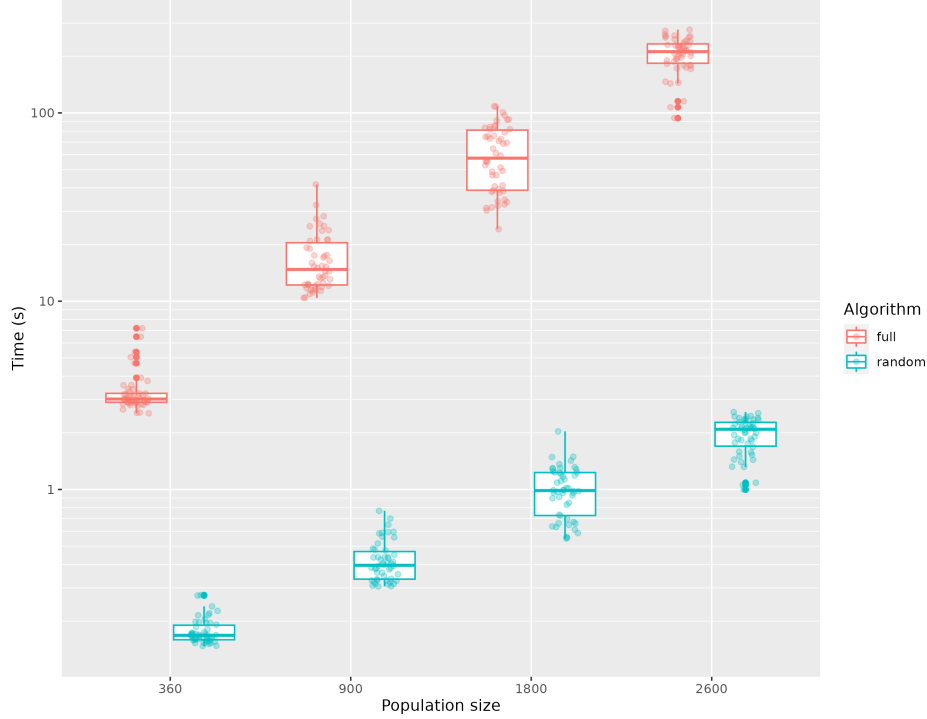


Figure 5: Full vs random algorithm computation time

7 Appendix

7.1 Recall on Poisson random measures

We recall below some useful properties of Poisson random measures, mainly following Chapter 6 of (Çınlar 2011). We also refer to (Kallenberg 2017) for a more comprehensive presentation of random counting measures.

Definition 7.1 (Poisson Random Measures). Let μ be a σ -finite diffuse measure on a Borel subspace (E, \mathcal{E}) of $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$. A random counting measure $Q = \sum_{k \geq 1} \delta_{X_k}$ is a Poisson (counting) random measure of mean measure μ if

1. $\forall A \in \mathcal{E}$, $Q(A)$ is a Poisson random variable with $E[Q(A)] = \mu(A)$.
2. For all disjoint subsets $A_1, \dots, A_n \in \mathcal{E}$, $Q(A_1), \dots, Q(A_n)$ are independent Poisson random variables.

Let us briefly recall here some simple but useful operations on Poisson measures. In the following, Q is a Poisson measure of mean measure μ , unless stated otherwise.

Proposition 7.1 (Restricted Poisson measure). If $B \in \mathcal{E}$, then, the restriction of Q to B defined by

$$Q^B = \mathbf{1}_B Q = \sum_{k \geq 1} \mathbf{1}_B(X_k) \delta_{X_k}$$

is also a Poisson random measure, of mean measure $\mu^B = \mu(\cdot \cap B)$.

Proposition 7.2 (Projection of Poisson measure). *If $E = F_1 \times F_2$ is a product space, then the projection*

$$Q_1(dx) = \int_{F_2} Q(dx, dy)$$

is a Poisson random measure of mean measure $\mu_1(dx) = \int_{F_2} \mu(dx, dy)$.

7.1.1 Link with Poisson processes

Let $Q = \sum_{k \geq 1} \delta_{T_k}$ a Poisson random measure on $E = \mathbb{R}^+$ with mean measure $\mu(dt) = \Lambda(t)dt$ absolutely continuous with respect to the Lebesgue measure, $\mu(A) = \int_A \Lambda(t)dt$. The counting process $(N_t)_{t \geq 0}$ defined by

$$N_t = Q([0, t]) = \sum_{k \geq 1} \mathbf{1}_{\{T_k \leq t\}}, \quad \forall t \geq 0, \quad (18)$$

is an inhomogeneous Poisson process with intensity function (or rate) $t \mapsto \Lambda(t)$. In particular, when $\Lambda(t) \equiv c$ is a constant, N is a homogeneous Poisson process with rate c . Assuming that the atoms are ordered $T_1 < T_2 < \dots$, we recall that the sequence $(T_{k+1} - T_k)_{k \geq 1}$ is a sequence of *i.i.d.* exponential variables of parameter c .

7.1.2 Marked Poisson measures on $E = \mathbb{R}^+ \times F$

We are interested in the particular case when E is the product space $\mathbb{R}^+ \times F$, with (F, \mathcal{F}) a Borel subspace of \mathbb{R}^d . Then, a random counting measure is defined by a random set $S = \{(T_k, \Theta_k), k \geq 1\}$. The random variables $T_k \geq 0$ can be considered as time variables, and constitute the jump times of the random measure, while the variables $\Theta_k \in F$ represent space variables.

We recall in this special case the Theorem VI.3.2 in (Çınlar 2011).

Proposition 7.3 (Marked Poisson measure). *Let m be a σ -finite diffuse measure on \mathbb{R}^+ , and K a transition probability kernel from $(\mathbb{R}^+, \mathcal{B}(\mathbb{R}^+))$ into (F, \mathcal{F}) . Assume that the collection $(T_k)_{k \geq 1}$ forms a Poisson process $(N_t) = (\sum_{k \geq 1} \mathbf{1}_{\{T_k \leq t\}})$ with mean $m(dt) = \Lambda(t)dt$, and that given $(T_k)_{k \geq 1}$, the variables Θ_k are conditionally independent and have the respective distributions $K(T_k, \cdot)$.*

1. *Then, $\{(T_k, \Theta_k); k \geq 1\}$ forms a Poisson random measure $Q = \sum_{k \geq 1} \delta_{(T_k, \Theta_k)}$ on $(\mathbb{R}^+ \times F, \mathcal{B}(\mathbb{R}^+) \otimes \mathcal{F})$, called a Marked point process, with mean μ defined by*

$$\mu(dt, dy) = \Lambda(t)dt K(t, dy).$$

2. *Reciprocally let Q be a Poisson random measure of mean measure $\mu(dt, dy)$, admitting the following disintegration with respect to the first coordinate: $\mu(dt, dy) = \tilde{\Lambda}(t)dt v(t, dy)$, with $v(t, F) < \infty$. Let $K(t, dy) = \frac{v(t, dy)}{v(t, F)}$ and $\Lambda(t) = v(t, F)\tilde{\Lambda}(t)$. Then, $Q = \sum_{k \geq 1} \delta_{(T_k, \Theta_k)}$ is a marked Poisson measure with $(T_k, \Theta_k)_{k \in \mathbb{N}^*}$ defined as above. In particular, the projection $N = (N_t)_{t \geq 0}$ of the Poisson measure on the first coordinate,*

$$N_t = Q([0, t] \times F) = \sum_{k \geq 1} \mathbf{1}_{[0, t] \times F}(T_k, \Theta_k) = \sum_{k \geq 1} \mathbf{1}_{\{T_k \leq t\}}, \quad \forall t \geq 0,$$

is an inhomogeneous Poisson process of rate $\Lambda(t) = v(t, F)\tilde{\Lambda}(t)$.

When the transition probability kernel K does not depend on the time: $K(t, A) = v(A)$ for some probability measure v , then the marks $(\Theta_k)_{k \geq 1}$ form an *i.i.d.* sequence with distribution v , independent of $(T_k)_{k \geq 1}$.

The preceding proposition thus yields a straight forward iterative simulation procedure for a Marked Poisson process on $[0, T] \times F$ with mean measure $\mu(dt, dy) = c dt K(t, dy)$ and $c > 0$. The procedure is described in Algorithm ?? .

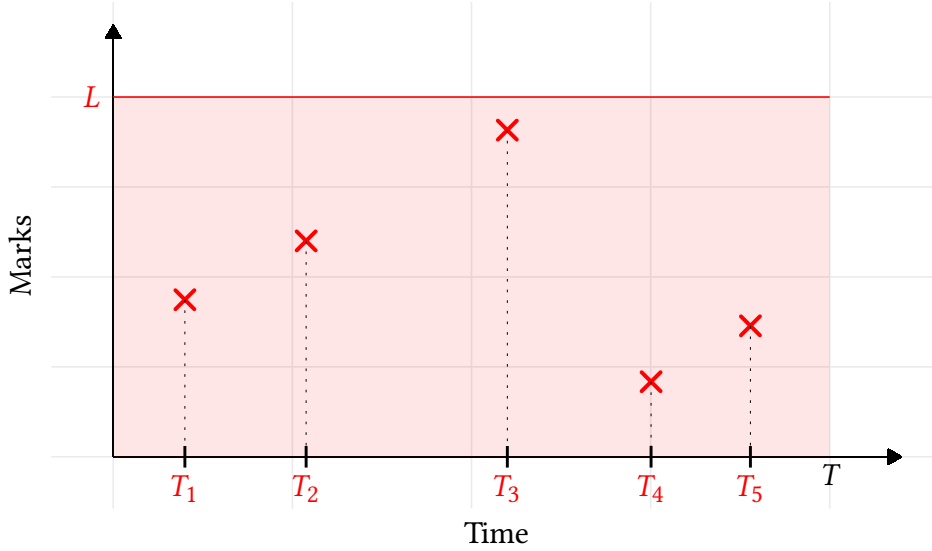


Figure 6: Example of Marked Poisson measure on $[0, T]$ with $m(dt) = Ldt$ (jump times occur at Poisson arrival times of rate L) and with $\nu(dy) = \frac{1}{L}\mathbf{1}_{[0,L]}(y)dy$ (marks are drawn uniformly on $[0, L]$). The mean measure is then $\mu(dt, dy) = dt\mathbf{1}_{[0,L]}(y)dy$.

7.2 Pathwise representation of IBMs

7.2.1 Notation reminder

The population's evolution is described by the measure valued process $(Z_t)_{t \geq 0}$. Several types of events e can occur to individuals denoted by I . In an event of type e occur to the individual I at time t , then the population state Z_{t-} is modified by $\phi^e(t, I)$. If $e \in \mathcal{E} \cup \mathcal{E}_W$, then events of type e occur with an intensity $\sum_{k=1}^{N_t} \lambda_t^e(I, Z_t)$, with $\lambda_t^e(I, Z_t)$ defined by Equation 5. If $e \in \mathcal{P}$, then events of type e occur in the population at a Poisson intensity of (μ_t^e) .

7.2.2 Proof of Theorem 2.1

Proof. For ease of notation, we prove the case when $\mathcal{P} = \emptyset$ (there are no events with Poisson intensity).

- Step 1. The existence of a solution to Equation 10 is obtained by induction. Let Z^1 be the unique solution the thinning equation:

$$Z_t^1 = Z_0 + \int_0^t \int_{\mathcal{J} \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{k \leq N_0\}} \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_0)\}} Q(ds, dk, de, d\theta), \quad \forall 0 \leq t \leq T.$$

Let T_1 be the first jump time of Z^1 . Since $Z_{s-}^1 = Z_0$ and $N_{s-} = N_0$ on $[0, T_1]$, Z^1 is solution of Equation 10 on $[0, T_1]$.

Let us now assume that Equation 10 admits a solution Z^n on $[0, T_n]$, with T_n the n -th event time in the population. Let Z^{n+1} be the unique solution of the thinning equation:

$$Z_t^{n+1} = Z_{t \wedge T_n}^n + \int_{t \wedge T_n}^t \int_{\mathcal{J} \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_{T_n}^n)\}} \mathbf{1}_{\{k \leq N_{T_n}^n\}} Q(ds, dk, de, d\theta).$$

First, observe that Z^{n+1} coincides with Z^n on $[0, T_n]$. Let T_{n+1} be the $(n+1)$ -th jump of Z^{n+1} . Furthermore, $Z_{s-}^{n+1} = Z_{s-}^n$ and $N_{s-}^{n+1} = N_{s-}^n$ on $[T_n, T_{n+1}]$ (nothing happens between two successive

event times), Z^{n+1} verifies for all $t \leq T_{n+1}$:

$$Z_t^{n+1} = Z_{t \wedge T_n}^n + \int_{t \wedge T_n}^t \int_{\mathcal{J} \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_s^{n+1})\}} \mathbf{1}_{\{k \leq N_s^{n+1}\}} Q(ds, dk, de, d\theta).$$

Since, Z^n is a solution of Equation 10 on $[0, T_n]$ coinciding with Z^{n+1} , this achieves to prove that Z^{n+1} is solution of Equation 10 on $[0, T_{n+1}]$. Finally, let $Z = \lim_{n \rightarrow \infty} Z^n$. For all $n \geq 1$, T_n is the n -th event time of Z , and Z is solution of Equation 10 on all time intervals $[0, T_n \wedge T]$ by construction.

By Lemma 2.1 $T_n \xrightarrow{n \rightarrow \infty} \infty$. Thus, by letting $n \rightarrow \infty$ we can conclude that Z is a solution of Equation 10 on $[0, T]$.

- Step 2. Let \tilde{Z} be a solution of Equation 10. Using the same arguments than in Step 1, it is straight forward to show that \tilde{Z} coincides with Z^n on $[0, T_n]$, for all $n \geq 1$. Thus, $\tilde{Z} = Z$, with achieves to prove uniqueness.

□

7.2.3 Proof of Lemma 2.1

The proof is obtained using pathwise comparison result, generalizing those obtained in (Kaakai and El Karoui 2023).

Proof. TODO

□

7.2.4 Alternative pathwise representation

TODO

7.3 Proof of Theorem 3.1

For ease of notation, we prove the case when $\mathcal{P} = \emptyset$ (there are no events with Poisson intensity). Let Z be the population process obtained by Algorithm 2, and $(T_n)_{n \geq 0}$ the sequence of its jump times ($T_0 = 0$).

Step 1 Let T_1 be the first event time in the population, with its associated marks defining the type E_1 of the event and the individual I_1 to which this event occurs. By construction, (T_1, E_1, I_1) is characterized by the first jump of:

$$Q^0(dt, dk, de) = \int_{\mathbb{R}^+} \mathbf{1}_{\{\theta \leq \lambda_t^e(I_k, Z_0)\}} \bar{Q}^0(dt, dk, de, d\theta),$$

with \bar{Q}^0 the Poisson measure introduced in the first step of the algorithm described in Section 3.2.

Since T_1 is the first event time, the population composition stays constant, $Z_t = Z_0$, on $\{t < T_1\}$. In addition, recalling that the first event has the action $\phi^{E_1}(T_1, I_1)$ (see Table 1) on the population Z , we obtain that:

$$\begin{aligned} Z_{t \wedge T_1} &= Z_0 + \mathbf{1}_{\{t \geq T_1\}} \phi^{E_1}(T_1, I_1) \\ &= Z_0 + \int_0^{t \wedge T_1} \int_{\mathcal{J}_0} \phi^e(s, I_k) Q^0(ds, dk, de) \\ &= Z_0 + \int_0^{t \wedge T_1} \int_{\mathcal{J}_0} \int_{\mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_0)\}} \bar{Q}^0(ds, dk, de, d\theta). \end{aligned}$$

991 Since $Z_{s^-} = Z_0$ on $\{s \leq T_1\}$, the last equation can be rewritten as

$$Z_{t \wedge T_1} = Z_0 + \int_0^{t \wedge T_1} \int_{\mathcal{J}_0} \int_{\mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_{s^-})\}} \bar{Q}^0(ds, dk, de, d\theta).$$

992 **Step 2** The population size at the n -th event time T_n is N_{T_n} . The $(n+1)$ -th event type and the
 993 individual to which this event occur are thus chosen in the set

$$\mathcal{J}_n := \{1, \dots, N_{T_n}\} \times (\mathcal{E} \cup \mathcal{E}_W).$$

994 Conditionally to \mathcal{F}_{T_n} , let us first introduce the marked Poisson measure \bar{Q}^n on $[T_n, \infty) \times \mathcal{J}_n \times \mathbb{R}^+$, of
 995 intensity:

$$\begin{aligned} \bar{\mu}^n(dt, dk, de, d\theta) &:= \mathbf{1}_{\{t > T_n\}} \bar{\Lambda}(N_{T_n}) dt \frac{\bar{\lambda}^e}{\bar{\Lambda}(N_{T_n})} \delta_{\mathcal{J}_n}(dk, de) \frac{1}{\bar{\lambda}^e} \mathbf{1}_{[0, \bar{\lambda}^e]}(\theta) d\theta, \\ &= \mathbf{1}_{\{t > T_n\}} dt \delta_{\mathcal{J}_n}(dk, de) \mathbf{1}_{[0, \bar{\lambda}^e]}(\theta) d\theta. \end{aligned}$$

996 By definition, \bar{Q}^n has no jumps before T_n .

997 As for the first event, the triplet $(T_{n+1}, E_{n+1}, I_{n+1})$ is determined by the first jump of the measure
 998 $\bar{Q}^n(ds, dk, de) := \int_{\mathbb{R}^+} \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_{T_n})\}} \bar{Q}^n(ds, dk, de, d\theta)$, obtained by thinning of \bar{Q}^n . Finally, since the
 999 population composition is constant on $[T_n, T_{n+1}[$, $Z_t = Z_{T_n}$, the population on $[0, T_{n+1}]$ is defined by:

$$\begin{aligned} Z_{t \wedge T_{n+1}} &= Z_{t \wedge T_n} + \mathbf{1}_{\{t \geq T_{n+1}\}} \phi^{E_{n+1}}(T_{n+1}, I_{n+1}), \\ &= Z_{t \wedge T_n} + \int_{t \wedge T_n}^{t \wedge T_{n+1}} \int_{\mathcal{J}_n \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, Z_{s^-})\}} \bar{Q}^n(ds, dk, de, d\theta). \end{aligned}$$

1000 Applying n times Equation 19 yields that:

$$Z_{t \wedge T_{n+1}} = Z_0 + \sum_{l=0}^n \int_{t \wedge T_l}^{t \wedge T_{l+1}} \int_{\mathcal{J}_l \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, \tilde{Z}_{s^-})\}} \bar{Q}^l(ds, dk, de, d\theta).$$

1001 **Step 3** Finally, let \tilde{Z} be the solution of Equation 10, with $(\tilde{T}_n)_{n \geq 0}$ the sequence of its event times.
 1002 Then, we can write similarly for all $n \geq 0$:

$$\begin{aligned} \tilde{Z}_{t \wedge \tilde{T}_{n+1}} &= Z_0 + \sum_{l=0}^n \int_{t \wedge \tilde{T}_l}^{t \wedge \tilde{T}_{l+1}} \int_{\mathcal{J} \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, \tilde{Z}_{s^-})\}} \mathbf{1}_{\{k \leq \tilde{N}_{s^-}\}} Q(ds, dk, de, d\theta), \\ &= Z_0 + \sum_{l=0}^n \int_{t \wedge \tilde{T}_l}^{t \wedge \tilde{T}_{l+1}} \int_{\mathcal{J} \times \mathbb{R}^+} \phi^e(s, I_k) \mathbf{1}_{\{\theta \leq \lambda_s^e(I_k, \tilde{Z}_{s^-})\}} \mathbf{1}_{\{k \leq \tilde{N}_{\tilde{T}_l}\}} Q(ds, dk, de, d\theta), \end{aligned}$$

1003 since $\tilde{N}_{s^-} = \tilde{N}_{\tilde{T}_l}$ on $[\tilde{T}_l, \tilde{T}_{l+1}]$.

1004 For each $l \geq 0$, let

$$\tilde{Q}^l(dt, dk, de, d\theta) = \mathbf{1}_{\{t > \tilde{T}_l\}} \mathbf{1}_{\{1, \dots, \tilde{N}_{\tilde{T}_l}\}}(k) Q(dt, dk, de, d\theta).$$

1005 By Proposition 7.1, \tilde{Q}^l is, conditionally to $\mathcal{F}_{\tilde{T}_l}$, a Poisson measure of intensity

$$\mathbf{1}_{\{t > \tilde{T}_l\}} dt \mathbf{1}_{\{1, \dots, \tilde{N}_{\tilde{T}_l}\}}(k) \delta_{\mathcal{J}}(dk, de) d\theta.$$

1006 Noticing that $\mathbf{1}_{\{1, \dots, \tilde{N}_{\tilde{T}_l}\}}(k) \delta_{\mathcal{J}}(dk, de) = \delta_{\mathcal{J}_l}(dk, de)$, this shows that \tilde{Q}^l has the conditional intensity $\bar{\mu}^l$
 1007 defined in Equation 19 and has thus the same distribution than \bar{Q}^l . Thus, Z in an exact simulation of
 1008 Equation 10.

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Session information

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Running under: Debian GNU/Linux trixie/sid

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BLAS: /usr/lib/x86_64-linux-gnu/blas/libblas.so.3.11.0
LAPACK: /usr/lib/x86_64-linux-gnu/lapack/liblapack.so.3.11.0

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 [4] LC_COLLATE=C.UTF-8    LC_MONETARY=C.UTF-8    LC_MESSAGES=C.UTF-8
 [7] LC_PAPER=C.UTF-8      LC_NAME=C              LC_ADDRESS=C
[10] LC_TELEPHONE=C        LC_MEASUREMENT=C.UTF-8 LC_IDENTIFICATION=C

time zone: Europe/Paris
tzcode source: system (glibc)

attached base packages:
[1] stats      graphics  grDevices  utils      datasets  methods   base

other attached packages:
[1] reshape2_1.4.4 StMoMo_0.4.1   forecast_8.21.1 gnm_1.1-5
[5] IBMPopSim_1.0.0 ggplot2_3.4.4

loaded via a namespace (and not attached):
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