Homework group number 0

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General description

Let's take a Markov discrete/continuous-time model which studies the deposition of particles that continuously perform random walks and interacts forming assorbing barriers via a fixed occupation criterion, inspired by the unidimensional-film growth model [1] [4].

The particles arrive in a random way on an unidimensional substrate $S_N = \{0, 1, \ldots, N+1\}$, then spread until $M \geq 2$ particles arrive at the same site, when they join together (nucleating) forming an island. Islands form absorbing barriers for the diffusion process of other particles. Assume that initially site 0 and $N+1$ are occupied by M particles (thus, they're already islands) but other sites are empty.

The Markov dynamics of the process is the following:

- At each site $x \in S_N$, new particles arrive indipendently at rate $\rho > 0$;
- If at a certain time a site is occupied by M or more particles, they all remain there and become inactive. Non-inactive particles are active;
- Each active particle takes (indipendently from the others) a simple simmetric random walk at rate 1: namely, each active particle jumps from x to $x+1$ or $x-1$ with equal probability $\frac{1}{2}$.

A certain state ω of the Markov process is a vector of occupancies for the sites $1, \ldots, N$ (it's not necessary to take into account the occupations of sites 0 and $N+1$): thereby $\omega(x)$ is the number of particles at site x.

Our idea is to find a suitable model of the problem at discrete time, aiming to find the quantities that characterize the dynamics (mean hitting times and their variances) for general M and N. We have to consider the presence of absorbing barriers. In Grinfield [3]'s *Mathematical tool for physicist* from which the problem on continuous time is inspired, some solutions for low M and N are sketched out, using also explicitly the resolvent matrix R. Many solutions are numerical, and can be studied only computationally. Furthermore, we could even simulate the dynamics of the process using *Gillespie*'s algorithm, in which exponentially-distributed random variables are generated and the destination of the jump is computed using the well-defined distribution for the associated jumping process (this is due to the indipencence between the holding time and the new jump destination).

A model for a continuous time Markov process

In order to build a consistent model we have to write the generation matrix Q of the Markov chain. We will use $T(\omega) = \sum_{x=1}^{N} \omega(x) \mathbb{1}_{\{\omega(x)<M\}}$, that is the number of active particles in the state ω. The waiting time in the state ω is exponential with parameter $T(\omega) + N\rho$: at the end of this time with probability $\frac{T(\omega)}{T(\omega)+N\rho}$ one of the active particles will jump (choosen uniformly from all active particles, and with equal probability to jump to the right or to the left), or a new particle will arrive in a random site $\{1, \dots, N\}$. We observe that the choice of having chosen a rate equal to 1 for the diffusion of the particle is not so restricted: we can assign an arbitrary rate σ to random walk process, but it is easy to show that a convenient rescaling of all the times can be done in order to set $\sigma = 1$. In other words, the ratio $\frac{\rho}{\sigma}$ is what matters. In an intuitive way, therefore, the vector of states $\omega(x)$ can be explicitly written for the cases of N, M fixed as

N	**M**	$\omega(x)$
1	2	$\{0,1,2\}$
2	2	$\{\{0,0\},\{0,1\},\{1,0\},\{1,1\},\{2,0\},\{0,2\},\{2,1\},\{1,2\}\}$
2	3	$\{\{0,0\},\{0,1\},\{1,0\},\{1,1\},\{2,0\},\{0,2\},\{2,1\},\{1,2\},\{3,0\},$ $\{0,3\},\{2,2\},\{3,1\},\{1,3\},\{3,2\},\{2,3\}\}$
3	2	$\{\{0,0,0\},\{1,0,0\},\{0,1,0\},\{0,0,1\},\{1,1,0\},\{1,0,1\},\{0,1,1\},\{2,0,0\},$ $\{0,2,0\},\{0,0,2\},\{2,1,0\},\{1,2,0\},\{0,2,1\},\{0,1,2\},\{2,0,1\},\{1,0,2\},$ $\{1,1,1\},\{2,1,1\},\{1,2,1\},\{1,1,2\}\}$
3	3	$\{\{0,0,0\},\{1,0,0\},\{0,1,0\},\{0,0,1\},\{1,1,0\},\{1,0,1\},\{0,1,1\},\{2,0,0\},$ $\{0,2,0\},\{0,0,2\},\{2,1,0\},\{1,2,0\},\{0,2,1\},\{0,1,2\},\{2,0,1\},\{1,0,2\},$ $\{3,0,0\},\{0,3,0\},\{0,0,3\},\{1,1,1\},\{2,1,1\},\{1,2,1\},\{1,1,2\},\{3,1,0\},$ $\{1,3,0\},\{0,1,3\},\{0,3,1\},\{1,0,3\},\{3,0,1\},\{2,2,1\},\{2,1,2\},\{1,2,2\},$ $\{3,1,1\},\{1,3,1\},\{1,1,3\},\{2,2,2\},\{3,2,1\},\{3,1,2\},\{1,3,2\},\{2,3,1\},$ $\{1,2,3\},\{2,1,3\},\{3,2,2\},\{2,3,2\},\{2,2,3\}\}$

where we have ordered our states with an increasing number of particles. We observe that the particular dynamics of our process involve some type of symmetries, and led us to eliminate some redudant states in the case $N = 3$. For example the states $\{1,0,0\}$ e $\{0,0,1\}$ can be evidently joined into a single state simbolically written as $\{1,0,0\}$, as we can see directly from the Q matrix. Similar considerations hold for the general case with $N \geq 3$. Moreover for each N the absorbing states with a number M of particles in one or other sites can be gather together by considering intrinsic symmetries of the problem. The symbol $*$ stands for a number of particle stricly $< M$ in one of the sites. The following analysis of mean hitting times and their variances will then be simplified a lot. In particolar the new vector of states $\omega(x)$ will be

N	**M**	$\omega(x)$
1	2	$\{0,1,2\}$
2	2	$\{\{0,0\},\{0,1\},\{1,0\},\{1,1\},\{2,*\}\}$
2	3	$\{\{0,0\},\{0,1\},\{1,0\},\{1,1\},\{2,0\},\{0,2\},\{2,1\},\{1,2\},\{2,2\},\{3,*\}\}$
3	2	$\{\{0,0,0\},\{1,0,0\},\{0,1,0\},\{1,1,0\},\{1,0,1,\},\{1,1,1\}$ $\{2,*,*\},\{*,2,*\}\}$
3	3	$\{\{0,0,0\},\{1,0,0\},\{0,1,0\},\{1,1,0\},\{1,0,1\},\{2,0,0\},$ $\{0,2,0\},\{2,1,0\},\{1,2,0\},\{2,0,1\},\{1,1,1\},\{2,2,0\},$ $\{2,0,2\},\{2,1,1\},\{1,2,1\},\{2,2,1\},\{2,1,2\},\{2,2,2\},$ $\{3,*,*\},\{*,3,*\}\}$

At this point we can study the Q matrix for the previous cases. We already know that in the diagonal of Q matrix there will be the value $-N\rho - T(\omega)$. Moreover each active particle, chosen uniformly from the $T(\omega)$, will jump to the right or to the left with the rate $\frac{1}{2}$ whereas a new particle can arrive at a random site with a rate ρ. So it is easy to build the Q matrix for our model for low N and M:

- $N = 1$, $M = 2$

$$Q = \begin{pmatrix} -\rho & \rho & 0 \\ 1 & -1-\rho & \rho \\ 0 & 0 & 0 \end{pmatrix}$$

- $N = 2$, $M = 2$

$$Q = \begin{pmatrix} -2\rho & \rho & \rho & 0 & 0 \\ \frac{1}{2} & -1-2\rho & \frac{1}{2} & \rho & \rho \\ \frac{1}{2} & \frac{1}{2} & -1-2\rho & \rho & \rho \\ 0 & \frac{1}{2} & \frac{1}{2} & -2-2\rho & 1+2\rho \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

- $N = 2$, $M = 3$

$$Q = \begin{pmatrix} -2\rho & \rho & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & -2\rho-1 & \frac{1}{2} & \rho & \rho & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & -2\rho-1 & \rho & 0 & \rho & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & -2\rho-2 & 0 & 0 & \rho+\frac{1}{2} & \rho+\frac{1}{2} & 0 & 0 \\ 0 & 1 & 0 & 1 & -2\rho-2 & 0 & \rho & 0 & 0 & \rho \\ 0 & 0 & 1 & 1 & 0 & -2\rho-2 & 0 & \rho & 0 & \rho \\ 0 & 0 & 0 & 1 & \frac{1}{2} & 0 & -2\rho-3 & 1 & \rho & \rho+\frac{1}{2} \\ 0 & 0 & 0 & 1 & 0 & \frac{1}{2} & 1 & -2\rho-3 & \rho & \rho+\frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -2\rho-4 & 2+2\rho \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

- $N = 3$, $M = 2$

$$Q = \begin{pmatrix} -3\rho & 2\rho & \rho & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & -1-3\rho & \frac{1}{2} & \rho & \rho & 0 & \rho & 0 \\ 0 & 1 & -1-3\rho & 2\rho & 0 & 0 & 0 & \rho \\ 0 & 0 & \frac{1}{2} & -2-3\rho & \frac{1}{2} & \rho & \rho+\frac{1}{2} & \rho+\frac{1}{2} \\ 0 & 1 & 0 & 1 & -2-3\rho & \rho & 2\rho & 0 \\ 0 & 0 & 0 & 1 & 0 & -3-3\rho & 1+2\rho & 1+\rho \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

- $N = 3$, $M = 3$

$$
Q = \begin{pmatrix}
-3\rho & 2\rho & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & -3\rho-1 & \frac{1}{2} & \rho & \rho & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -3\rho-1 & 2\rho & 0 & 0 & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{2} & -3\rho-2 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \rho & \rho & 0 & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & -3\rho-2 & 0 & 0 & 2\rho & 0 & 0 & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & -3\rho-2 & 0 & \rho & 0 & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho & 0 \\
0 & 0 & 0 & 2 & 0 & 0 & -3\rho-2 & 0 & 2\rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \rho \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & -3\rho-3 & 1 & \frac{1}{2} & 0 & \rho & 0 & \rho & 0 & 0 & 0 & 0 & \rho+\frac{1}{2} & 0 \\
0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 1 & -3\rho-3 & 0 & 1 & \rho & 0 & 0 & \rho & 0 & 0 & 0 & 0 & \rho+\frac{1}{2} \\
0 & 0 & 0 & 0 & 1 & \frac{1}{2} & 0 & 0 & 0 & -3\rho-3 & \frac{3}{2} & 0 & \rho & \rho & 0 & 0 & 0 & 0 & \rho & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & -3\rho-3 & 0 & 0 & 2\rho & \rho+1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -3\rho-4 & 1 & 0 & 0 & \rho & 0 & 0 & \rho+1 & \rho+1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & -3\rho-4 & 2 & 0 & 0 & \rho & 0 & 2\rho & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 1 & \frac{1}{2} & \frac{1}{2} & -3\rho-4 & 1 & \rho & \rho & 0 & \rho+\frac{1}{2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 2 & -3\rho-4 & 2\rho & 0 & 0 & 0 & \rho+1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 1 & -3\rho-5 & 1 & \rho & \rho+1 & \rho+\frac{3}{2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & -3\rho-5 & \rho & 2\rho+1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & -3\rho-6 & 2\rho+2 & \rho+2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

An analytic treatment of absorption probabilities with stochastic methods

For the cases with low N and M we can find an analitic formula for the absorption probabilities: starting from a matrix Q, we can compute the resolvent $R(\lambda) \doteq (\lambda I - Q)^{-1}$ and obtain the absorption probabilities $p_{ij}(t)$ by using the inverse Laplace transform of the elements of the $R(\lambda)$ matrix. This works because we can identify a transition semigroup of operators of the continuous Markov process, due to Chapman-Kolmogorov relation. That semigroup can be recovered from $R(\lambda)$, since at an infinitesimal level the generator of the process is the Q matrix.

$$r_{ij}(\rho, \lambda) = (\mathcal{L} p_{ij})(\rho, \lambda) = \int_0^{+\infty} e^{-\lambda t} p_{ij}(\rho, t) dt \tag{1}$$

$$p_{ij}(\rho, t) = \left(\mathcal{L}^{-1} r_{ij}\right)(\rho, t) \tag{2}$$

Here we are interested only in transitions -in the $N = 1, N = 2, N = 3$ cases- between the states without particles, that are $\{0\}, \{0, 0\}, \{0, 0, 0\}$, and the absorbing states $\{2\}$,$\{2, *\}$,$\{2, *, *\}$ and $\{*, 2, *\}$ respectively. In other words we want to compute in these four cases the probabilities $p_{13}^{N=1}(\rho, t)$, $p_{15}^{N=2}(\rho, t)$, $p_{17}^{N=3}(\rho, t)$ and $p_{18}^{N=3}(\rho, t)$ analitically, or at least in some limits. The entries of our Q matrices are polynomial in ρ, therefore the entries of $R(\lambda)$ are ratio of polynomials in ρ and λ as we can easily seen from the formula of a inverse of a matrix. Explicit result for the four cases are collected in the following table.

N	**Element** $r(\rho, \lambda)$
1	$r_{13}^{N=1} = \frac{\rho^2}{\lambda(\lambda+(\lambda+\rho)^2)}$
2	$r_{15}^{N=2} = \frac{4\rho^2(3+\lambda+4\rho)}{\lambda(2(2+\lambda)(1+2\lambda)+4\lambda\rho(4+3\lambda)+12(1+2\rho)\rho^2+\rho^3)}$
3	$r_{17}^{N=3} = \frac{2\rho^2(114+4\lambda^4+\lambda^3(38+64\rho)+\lambda^2(133+16\rho(29+24\rho))+\rho(842+\rho(2153+4\rho(593+243\rho)))+\lambda(203+2\rho(549+\rho(923+504\rho))))}{\lambda(\lambda(3+\lambda)(1+2\lambda(2+\lambda))(7+2\lambda(4+\lambda))+4\lambda(118+\lambda(346+\lambda(334+\lambda\ (131+18\lambda))))\rho+2(207+2\lambda(873+\lambda(1390+3\lambda(254+45\lambda))))\rho^2+24(120+\lambda(427+9\lambda(41+10\lambda)))\rho^3+36(7+9\lambda)(28+15\lambda)\rho^4+324(23+18\lambda)\rho^5+2916\rho^6)}$
3	$r_{18}^{N=3} = \frac{2\rho^2(93+\lambda(151+2\lambda(44+\lambda(11+\lambda)))+598\rho+2\lambda(354+\lambda(133+16\lambda))\rho+(1375+2\lambda(527+96\lambda))\rho^2+2(677+252\lambda)\rho^3+486\rho^4))}{(\lambda(\lambda(3+\lambda)(1+2\lambda(2+\lambda))(7+2\lambda(4+\lambda))+4\lambda(118+\lambda(346+\lambda(334+\lambda(131+18\lambda))))\rho+2(207+2\lambda(873+\lambda(1390+3\lambda(254+45\lambda))))\rho^2+24(120+\lambda(427+9\lambda(41+10\lambda)))\rho^3+36(7+9\lambda)(28+15\lambda)\rho^4+324(23+18\lambda)\rho^5+2916\rho^6)}$

Once we obtain $R(\lambda)$, or at least the element we are interested in, we have to compute inverse Laplace transform. The general formula for inverting the Laplace transform is the Bromwich integral:

$$p_{ij}(\rho, t) = \left(\mathcal{L}^{-1} r_{ij}\right)(\rho, t) = \frac{1}{2\pi i} \int_{s-i\infty}^{s+i\infty} e^{\lambda t} r_{ij}(\rho, \lambda) \tag{3}$$

where $r_{ij}(\rho, \lambda)$ is treated as a complex function in the space $\{\Re\lambda, \Im\lambda\}$, s is a real positive number that is larger that the real parts of all the singularities of $e^{\lambda t} r_{ij}(\rho, \lambda)$. In practice, the integral must be performed along the infinite line L, parallel to the imaginary axis, at a distance s from the origin. At this point, a curve must be chosen in order to close the contour C. Possible completion paths are for instance the curves Γ_1 or Γ_2, the half-circles with radius R on the left and on the right of L, respectively. For $R \to +\infty$ these curves make with L a closed contour and the Bromwich integral can be evaluated by means of the residue theorem provided that the integral of the function $e^{\lambda t} r_{ij}(\rho, \lambda)$ tends to zero for R (radius of the chosen half-circle) tending to infinity.

We mentioned this formula because, computationally, it is simpler to find directly the poles of $r(\rho, \lambda)$ since it a ratio of polynomials in ρ and λ: there exists some methods already developed in software like mathematica ("TransferFunctionPoles") to find easily this kind of poles. By residue theorem, we can then get the final result by simply adding the residues of $e^{\lambda t} r(\rho, \lambda)$ for each pole.

Let's analyze the case $N = 1$ in great detail, since it is simpler to compute and to interpret explicitly.

$$p_{13}^{N=1}(\rho, t) = 1 - e^{\frac{-(1+2\rho)t}{2}} \left(\cosh\left(\frac{t\sqrt{1+4\rho}}{2}\right) + \frac{1+2\rho}{\sqrt{1+4\rho}} \sinh\left(\frac{t\sqrt{1+4\rho}}{2}\right)\right) \tag{4}$$

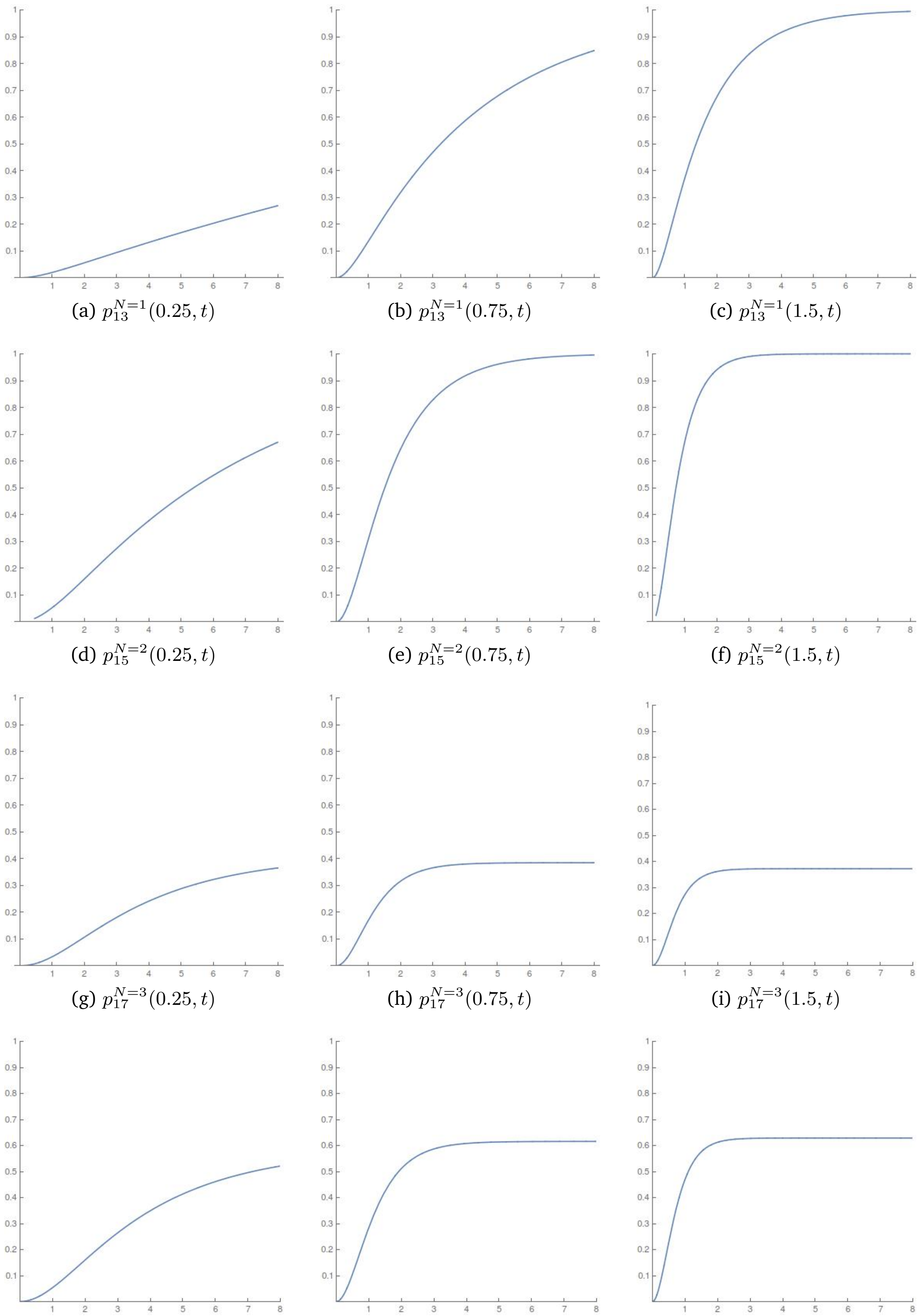
We can see that $\lim_{t\to+\infty} p_{13}^{N=1}(\rho, t) = 1$ if $\rho > 0$, that is physically correct (if we wait enough time, we can reach the absorbing state $\{2\}$); also it holds that $\lim_{\rho\to+\infty} p_{13}^{N=1}(\rho, t) = 1$ and $\lim_{\rho\to 0} p_{13}^{N=1}(\rho, t) = 0$ (the rate of incoming particles ρ control the velocity in which $p_{13}^{N=1}(\rho, t)$ grows in time). We can get a feeling with the analytical result by choosing a particular value of ρ, e.g. $\rho = \frac{1}{2}$.

$$p_{13}^{N=1}(t) = 1 - e^{\left(\frac{\sqrt{3}}{2}-1\right)t} \left(\frac{1}{2} + \frac{\sqrt{3}}{3}\right) + e^{-\left(\frac{\sqrt{3}}{2}+1\right)t} \left(\frac{\sqrt{3}}{3} - \frac{1}{2}\right) \tag{5}$$

The solution is thus a sum of exponential in the variable t (growth and decay) with positive and negative coefficients. Moreover the solution is monotone increasing in time when ρ is fixed: clearly the more time goes fast, the more it is likely that we reach an absorbing state. Now let's consider the other cases $N = 2$ and $N = 3$. These solutions are a lot more difficult and more computationally expensive (this is due also to the huge number of terms involved). Since it is impossible to condense the solutions in this page, we rely on the plotting of solutions in order to get some insight into the dynamics of our Markov chain. We have plotted $p_{13}^{N=1}(t)$, $p_{15}^{N=2}(t)$, $p_{17}^{N=3}(t)$ and $p_{18}^{N=3}(t)$ for three values of ρ, namely $\rho = 0.25$, $\rho = 0.75$ and $\rho = 1.5$.

As in the case $N = 1$, with ρ fixed all functions plotted in Fig.1 are monotone increasing in the t variable. We can make also the limit in which $\rho \to +\infty$ after the limit $t \to +\infty$: is not too difficult to get $\lim_{\rho\to+\infty} \lim_{t\to+\infty} p_{15}^{N=2}(\rho, t) = 1$, $\lim_{\rho\to+\infty} \lim_{t\to+\infty} p_{17}^{N=3}(\rho, t) = \frac{2}{3}$ and $\lim_{\rho\to+\infty} \lim_{t\to+\infty} p_{18}^{N=3}(\rho, t) = \frac{1}{3}$. For the case $N = 2$ this is obvious since there is only one absorbing state $\{2, *\}$. Clearly this is the result that we expected also in the case $N = 3$: since the rate is uniform, we guess that on the average the absorbing state $\{2, *, *\}$ (remember symmetry, this includes also $\{*, *, 2\}$) is two time more probable than the other $\{*, 2, *\}$. We can see also that for the same value of ρ in the case $N = 3$ the sum of $p_{17}^{N=3}(\rho, t)$ and $p_{18}^{N=3}(\rho, t)$ tends to 1 for $t \to \infty$, that is $\lim_{t\to\infty}(p_{17}^{N=3}(\rho_{fixed}, t) + p_{18}^{N=3}(\rho_{fixed}, t)) = 1$. There are many other things that we can note, like the velocity of approaching the limit $t \to \infty$ with ρ fixed: this increases with N, with the same $M = 2$. If instead N and M are fixed, that velocity clearly increases with ρ. This means that mean hitting times (and also their variances), at fixed ρ, decreases with N for the associate discrete time Markov process with the jump matrices: physically, this is due to the fact the rate is uniform for each site but the random walk of particles from nearby sites can lead to reach the absorbing states some time before. After the simulation with Gillespie's algorithm, then we will be able to compare the results with this plots in Fig.1.

Figure 1: Explicit solution for absorption probabilities



(a) $p_{13}^{N=1}(0.25,t)$ (b) $p_{13}^{N=1}(0.75,t)$ (c) $p_{13}^{N=1}(1.5,t)$

(d) $p_{15}^{N=2}(0.25,t)$ (e) $p_{15}^{N=2}(0.75,t)$ (f) $p_{15}^{N=2}(1.5,t)$

(g) $p_{17}^{N=3}(0.25,t)$ (h) $p_{17}^{N=3}(0.75,t)$ (i) $p_{17}^{N=3}(1.5,t)$

(j) $p_{18}^{N=3}(0.25,t)$ (k) $p_{18}^{N=3}(0.75,t)$ (l) $p_{18}^{N=3}(1.5,t)$

Gillespie's algorithm

Taken a generator matrix Q, we can always associate a jump matrix J and simulate the behaviour of the system using a Montecarlo approach. We can thereby estimate the hitting times and their variances in a numerical way, and then compare the results with the continuous and discrete time analysis.

Let's denote with "i" a specific site, and with "n" the istant when a transition from a state to another occurs. Let "q_{ij}" be the elements of the matrix Q. The algorithm used is then the following:

(a) Take $\mathcal{U}_n([0,1])$ and generate for each site the $Y_n = \frac{\log(\mathcal{U}_n)}{q_i}$, in a way that each $Y_n \sim \text{Exp}\,(q_i)$, where $q_i = -\sum_{i\neq j} q_{ij}$;

(b) Generate the new waiting time T_{n+1} with the ricursive formula $T_{n+1} = T_n + Y_n$, $T_0 = 0$;

(c) Let $X(T_n) = i$ be the state of the system at time T_n. The new state $X(T_{n+1}) = j$ will be chosen with probability $\Pr[X(T_{n+1}) = j] = \frac{q_{ij}}{q_i}$, namely according to the distribution $\frac{q_{ij}}{q_i}$.

Using *R* language, we have written a function that simulates a continuous-time process, given a matrix Q in input (the `Q` argument) with a certain rate ρ and a vector of IDs for the states (the `state` argument), which are assumed to be integer numbers in N, starting from 1.

The code and simulations are the following:

```
markovSimulation <- function(Q, state){

  # absState will be the vector of IDs for the absorbent states of the chain.
  # We detect an absorbent state i as one with q_{ii} = 0.
  absState <- state[diag(Q) == 0]

  # Output of the function will be a list with two vectors:
  # - tao: a vector containing the jumping times of the chain.
  # We assume, without specific restrictions, that the chain starts at time 0;
  # - xTao: a vector containing the states crossed by the chain.
  # The chain starts at state 1, namely the state where system is empty of particles.
  tao <- 0
  xTao <- 1

  while(!(xTao[length(xTao)] %in% absState)){

    # Last state assumed by the chain:
    lastXTao <- xTao[length(xTao)]

    # New stopping time defined by the Gillespie algorithm:
    tao <- c(tao, tao[length(tao)] + (-1)/(-diag(Q)[lastXTao]) * log(runif(1)))

    # The distribution for the jumping time is:
    probIJ <- Q[lastXTao, ]/(-diag(Q)[lastXTao])
    probIJ[lastXTao] <- 0
```

```r
    # The new state is sampled from the distribution probIJ defined before:
    xTao <- c(xTao, sample(x = state,
                           prob = probIJ,
                           size = 1)
              )
  }

  # Output of the function
  out <- list()
  out$tao <- tao
  out$xTao <- xTao

  return(out)
}
```

Once defined the function, we can do some simulations in the cases listed before:

- $N = 1, M = 2$:

```r
# Initialization of the Q-matrix as a function of rho:
Q <- function(rho){
  QMatrix <- matrix(c(-rho, rho, 0, 1, -1-rho, rho, 0, 0, 0), 3, 3, byrow = T )
  return(QMatrix)
}
```

Just as a helpful example for the next pages, we fix $\rho = 1/2$ and show how the function works. Given a fixed ρ, we can create the Q-matrix for the Markov Chain as follows:

```r
QMatrix <- Q(1/2)
QMatrix
```

```
##      [,1] [,2] [,3]
## [1,] -0.5  0.5  0.0
## [2,]  1.0 -1.5  0.5
## [3,]  0.0  0.0  0.0
```

Given a fixed Q-matrix and considered $|S| = 3$, we can simulate a Markov Chain as follows:

```r
markovSimulation(QMatrix, 1:3)
```

```
## $tao
## [1] 0.000000 2.538457 3.038332
##
## $xTao
## [1] 1 2 3
```

We see the function returns a vector of the jumping-times, and a vector with all the states crossed by the simulated Markov Chain. There is a one-to-one correspondence between states' ID $(1, 2, 3)$ and states' names $(S = 1, 2, 3)$, so it's really easy to reconstruct the path followed by the Markov Chain.

A basic Montecarlo simulation of the mean hitting time and the variance hitting time with $B = 100000$ replications can be done as following:

```r
B <- 100000
n <- rep(NA, B)
for(i in 1:B){
  n[i] <- length(markovSimulation(QMatrix, 1:3)$tao) - 1
}
mean(n)
```

```
## [1] 5.96946
```

```r
var(n)
```

```
## [1] 23.44142
```

We can also see how the mean and hitting times varies with change of ρ:

```r
rhos <- c(0.1, 0.2, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 5, 10, 15) # Defined rhos
means <- rep(NA, length(rhos))
variances <- rep(NA, length(rhos))
B <- 100000

for (j in 1:length(rhos)){
  QMatrix <- Q(rhos[j]) # Creating the Q-matrix for a fixed value of rho
  n <- rep(NA, B)

  # MonteCarlo simulation:
  for(i in 1:B){
    n[i] <- length(markovSimulation(QMatrix, 1:3)$tao) - 1
  }

  means[j] <- mean(n)
  variances[j] <- var(n)
}

means
```

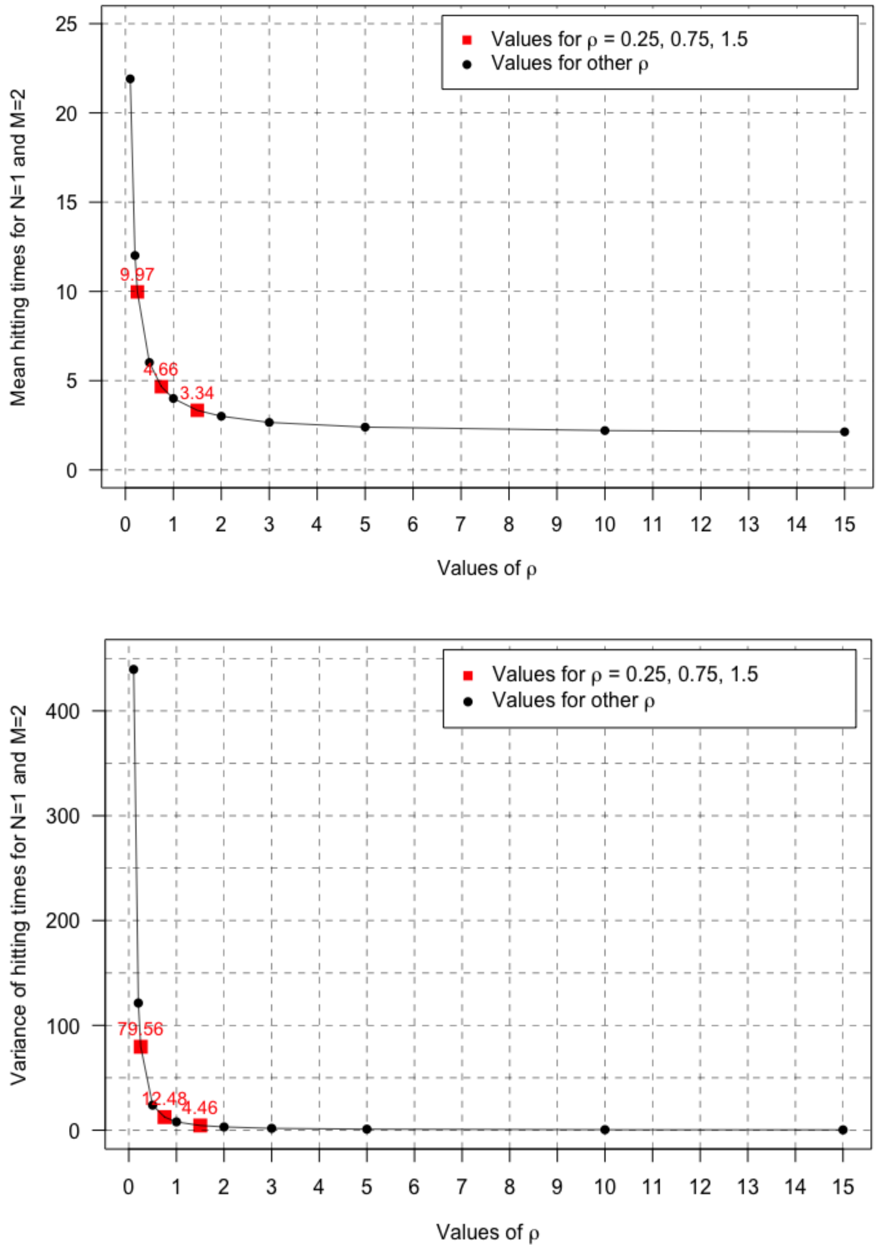
```
##  [1] 21.93900 11.97944  9.98792  6.01210  4.65658  4.00602  3.32734
##  [8]  2.99776  2.66294  2.39806  2.20250  2.13368
```

```r
variances
```

```
##  [1] 439.5415544 119.4619719  80.0984151  24.0818144  12.1797045
##  [6]   8.0544843   4.4686532   2.9957049   1.7902485   0.9574378
## [11]   0.4494382   0.2838925
```

We can even plot the values taken by the estimated mean hitting time and variance of hitting time, varying the values of ρ:

Figure 2: Estimated mean hitting time and variance of hitting time as a function of ρ, $N = 1$, $M = 2$



- $N = 2, M = 2$:

In this case, we can initialize the specific Q-matrix (dependent on a certain fixed value ρ) as following:

```
Q <- function(rho){
  QMatrix <- matrix(c(-2*rho, rho, rho, 0, 0,
                      1/2, -1-2*rho, 1/2, rho, rho,
                      1/2, 1/2, -1-2*rho, rho, rho,
                      0, 1/2, 1/2, -2-2*rho, 1+2*rho,
                      0, 0, 0, 0, 0),
                    5, 5, byrow = T)
  return(QMatrix)
}
```

As the previous case, we can simulate a certain Markov Chain (considering $|S| = 5$) for a certain rate ρ (fixed, for example, equal to $\rho = 1/2$):

```
QMatrix <- Q(1/2)
markovSimulation(QMatrix, 1:5)
```

```
## $tao
## [1] 0.0000000 0.6987638 1.1243798 1.2860175 1.4281583 2.1115038 3.1521159
##
## $xTao
## [1] 1 2 3 1 2 4 5
```

We can even perform a Montecarlo simulation of the mean hitting time and the variance of hitting time with $B = 100000$ replications, varying the value of ρ:

```
rhos <- c(0.1, 0.2, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 5, 10, 15) # Defined rhos
means <- rep(NA, length(rhos))
variances <- rep(NA, length(rhos))
B <- 100000

for (j in 1:length(rhos)){
  QMatrix <- Q(rhos[j]) # Creating the Q-matrix for a fixed value of rho
  n <- rep(NA, B)

  # MonteCarlo simulation:
  for(i in 1:B){
    n[i] <- length(markovSimulation(QMatrix, 1:5)$tao) - 1
  }

  means[j] <- mean(n)
  variances[j] <- var(n)
}

means
```

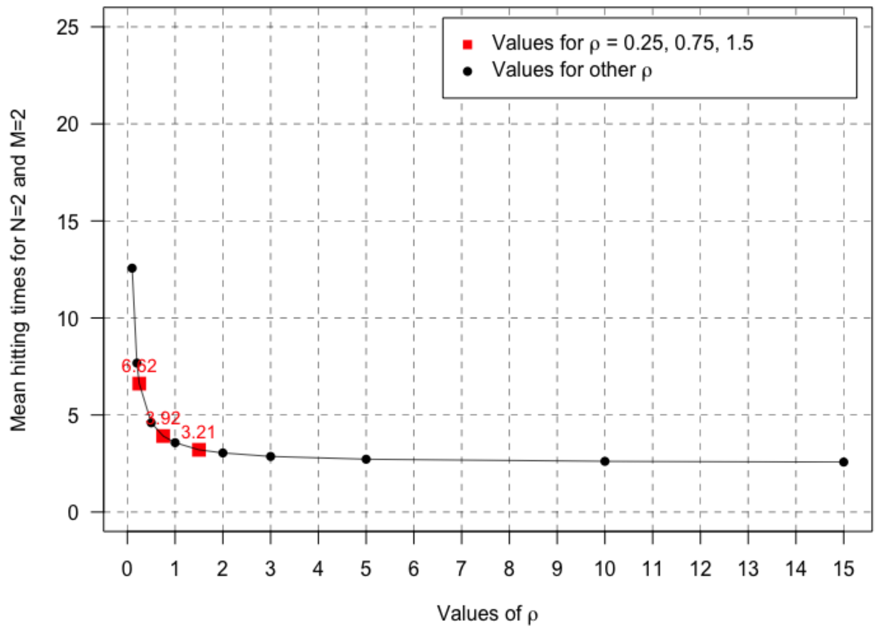
```
##  [1] 12.56541  7.67481  6.61748  4.60024  3.91604  3.57426  3.20614
##  [8]  3.04535  2.86471  2.72117  2.61193  2.57426
```

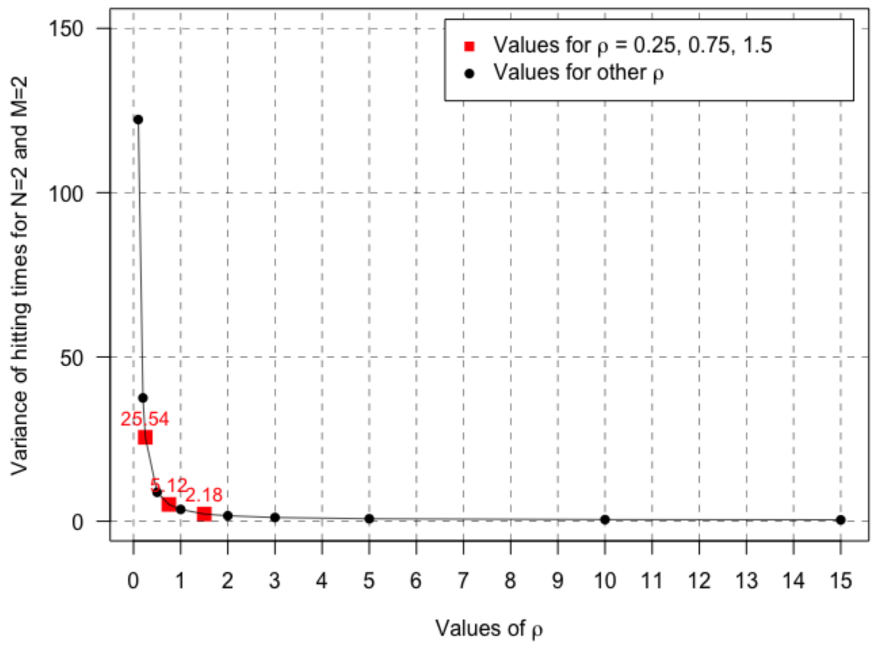
```
variances
```

```
##  [1] 122.2550641  37.5207567  25.5390338   8.7996599   5.1177819
##  [6]   3.5863813   2.1758481   1.6574300   1.1286979   0.7457313
## [11]   0.4824565   0.4052295
```

We can even plot the values taken by the estimated mean hitting time and variance of hitting time, varying the values of ρ:

Figure 3: Estimated mean hitting time and variance of hitting time as a function of ρ, $N = 2$, $M = 2$





- $N = 3, M = 2$:

As the previous case, we initially implement the Q-matrix varying in ρ:

```
Q <- function(rho){
  QMatrix <- matrix(c(-3*rho, 2*rho, rho, 0, 0, 0, 0, 0,
                      1/2, -1-3*rho, 1/2, rho, rho, 0, rho, 0,
                      0, 1, -1-3*rho, 2*rho, 0, 0, 0, rho,
                      0, 0, 1/2, -2-3*rho, 1/2, rho, rho+1/2, rho+1/2,
                      0, 1, 0, 1, -2-3*rho, rho, 2*rho, 0,
                      0, 0, 0, 1, 0, -3-3*rho, 1+2*rho, 1+rho,
                      rep(0, 8),
                      rep(0, 8)),
                    8, 8, byrow = TRUE)
  return(QMatrix)
}
```

Then, we study, via MonteCarlo simulation, how the mean hitting times and the variance of hitting times varies as ρ changes. In this case we must pay attention, as we have 2 distinct assorbing states instead of 1, namely distinguished with IDs 7 and 8. Thus, we need to split the two different hitting times:

```
rhos <- c(0.1, 0.2, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 5, 10, 15) # Defined rhos
means7 <- rep(NA, length(rhos))
means8 <- rep(NA, length(rhos))
variances7 <- rep(NA, length(rhos))
variances8 <- rep(NA, length(rhos))
B <- 100000

for (j in 1:length(rhos)){
  QMatrix <- Q(rhos[j]) # Creating the Q-matrix for a fixed value of rho
  n <- rep(NA, B)
  absorbedIn <- rep(NA, B)

  # MonteCarlo simulation:
  for(i in 1:B){
    simul <- markovSimulation(QMatrix, 1:8)$xTao # i-th simulation of the Markov Chain
    n[i] <- length(simul) - 1

    if(simul[length(simul)] == 7){
      absorbedIn[i] <- 7
    }
    else{
      absorbedIn[i] <- 8
    }
  }

  means7[j] <- mean(n[absorbedIn == 7])
  means8[j] <- mean(n[absorbedIn == 8])
  variances7[j] <- var(n[absorbedIn == 7])
  variances8[j] <- var(n[absorbedIn == 8])
```

```
}

means7
```

```
## [1] 9.782757 6.400161 5.753139 4.357584 3.879325 3.634900 3.397976
## [8] 3.269472 3.142864 3.038418 2.971938 2.942700
```

```
means8
```

```
## [1] 9.914682 6.583923 5.881008 4.491380 4.013338 3.753348 3.494271
## [8] 3.356078 3.205718 3.085573 2.995846 2.954857
```

```
variances7
```

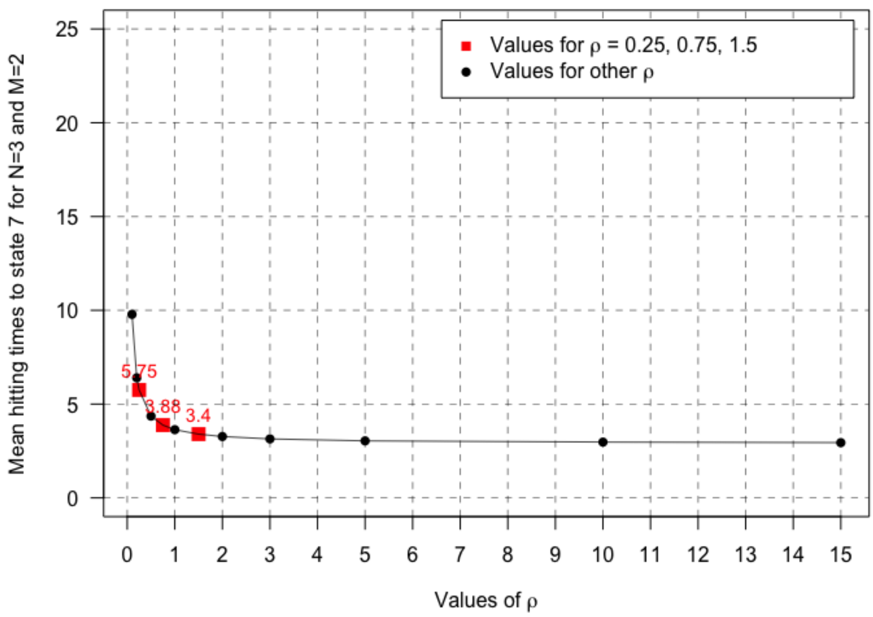
```
## [1] 62.9335923 20.1441332 14.7521246  5.8286706  3.6907660  2.7383723
## [7]  1.9512770  1.5404262  1.1825926  0.9159870  0.7272463  0.6657552
```

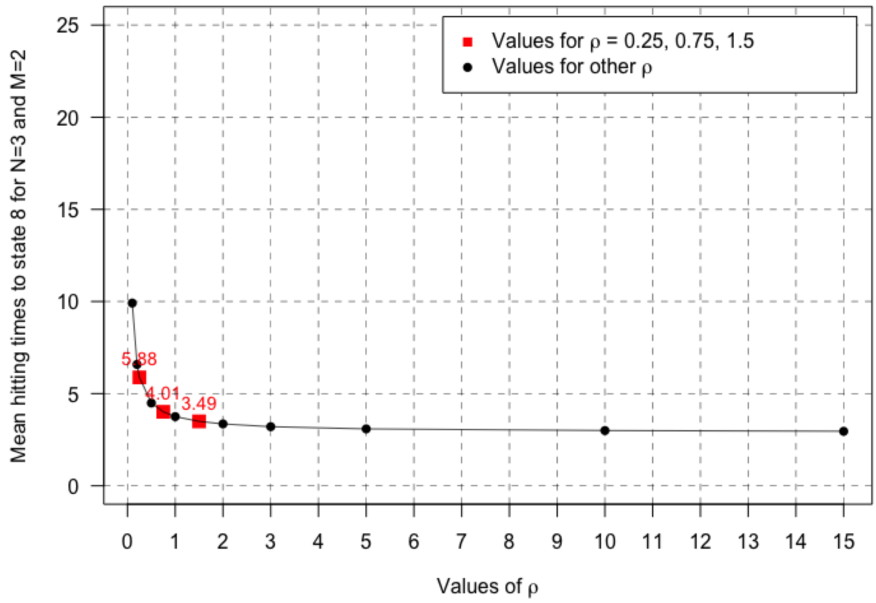
```
variances8
```

```
## [1] 60.5521003 20.0481894 14.2869693  5.8114904  3.7048264  2.8096435
## [7]  1.9874494  1.5623116  1.2302880  0.9459916  0.7441389  0.6808601
```

Then, we plot the values taken by the estimated mean hitting time varying the values of ρ, differentiating by the absorbing state (7 or 8):

Figure 4: Estimated mean hitting time as a function of ρ, $N = 3$, $M = 2$





- $N = 2, M = 3$:

```
Q <- function(rho){
  QMatrix <- matrix(c(-2*rho, rho, rho, 0, 0, 0, 0, 0, 0, 0,
                      1/2, -2*rho-1, 1/2, rho, rho, 0, 0, 0, 0, 0,
                      1/2, 1/2, -2*rho-1, rho, 0, rho, 0, 0, 0, 0,
                      0, 1/2, 1/2, -2-2*rho, 0, 0, rho+1/2, rho+1/2, 0, 0,
                      0, 1, 0, 1, -2-2*rho, 0, rho, 0, 0, rho,
                      0, 0, 1, 1, 0, -2-2*rho, 0, rho, 0, rho,
                      0, 0, 0, 1, 1/2, 0, -2*rho-3, 1, rho, rho+1/2,
                      0, 0, 0, 1, 0, 1/2, 1, -2*rho-3, rho, rho+1/2,
                      0, 0, 0, 0, 0, 0, 1, 1, -2*rho-4, 2+2*rho,
                      rep(0, 10)),
                    10, 10, byrow = TRUE)
  return(QMatrix)
}
```

```
rhos <- c(0.1, 0.2, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 5, 10, 15) # Defined rhos
means <- rep(NA, length(rhos))
variances <- rep(NA, length(rhos))
B <- 20000

for (j in 1:length(rhos)){
  QMatrix <- Q(rhos[j]) # Creating the Q-matrix for a fixed value of rho
  n <- rep(NA, B)

  # MonteCarlo simulation:
  for(i in 1:B){
    n[i] <- length(markovSimulation(QMatrix, 1:10)$tao) - 1
  }

  means[j] <- mean(n)
```

```
  variances[j] <- var(n)
}

means
```

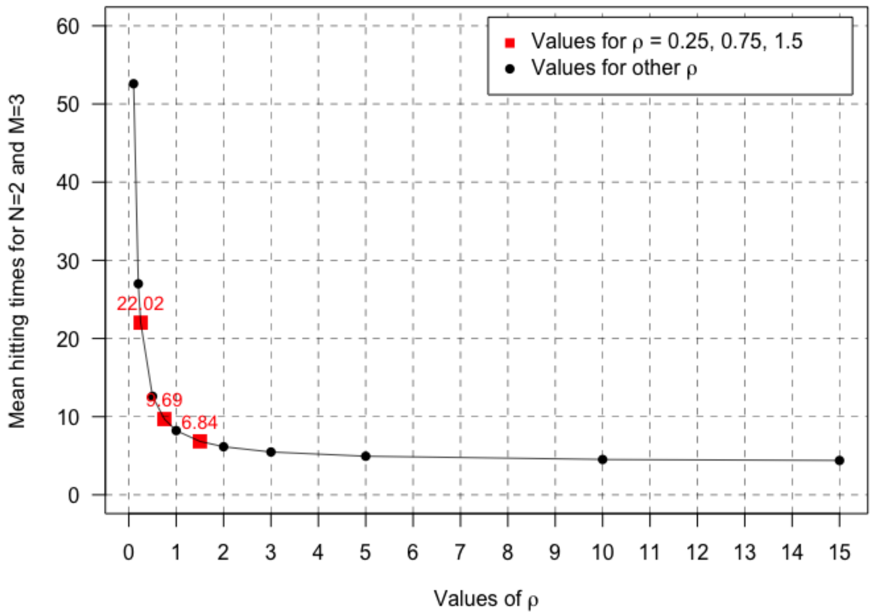
```
##  [1] 52.588695 26.934050 21.997865 12.611140  9.640520  8.240605  6.834575
## [12] 6.143460  5.457935  4.934045  4.525500 4.396045
```

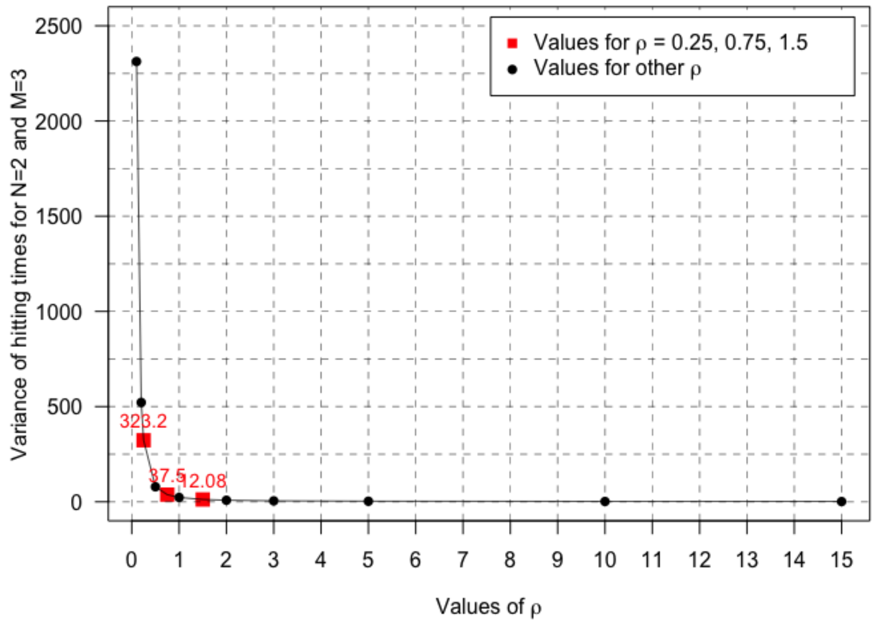
```
variances
```

```
##  [1] 2310.769907  517.603509  321.437618  79.893067   37.189540
##  [6]   22.830918   12.028980   8.041839   4.813725    2.838159
## [11]   1.599138    1.244370
```

Finally, we plot the values taken by the estimated mean hitting time varying the values of ρ: (7 or 8):

Figure 5: Estimated mean hitting time and variance of hitting time as a function of ρ, $N = 2$, $M = 3$





First, let's consider N and M fixed. From all plots it is clear that mean hitting times and their variances are monotonically decreasing with ρ, as it is expected from the physical intuition. Moreover they diverge when $\rho \to 0$, since in that case it becomes more and more difficult to approach the absorbing state.

In the following we consider instead ρ to be fixed, and N and M are free to change. We can see that, as N increases, the mean hitting times decreases as their variances, as expected. Also, from plots of Fig.1, we can see that a rough estimate of mean hitting time from the width of the interval $[0, \rho]$ in which $p_{ij}(\rho_{fixed}, t)$ reach its asymptotic value corresponds to our result with Montecarlo simulation. Also variances of these times, related to the velocity of approaching the limiting values, decrease with N as expected.

Regarding the influence of the threshold M, we clearly see that mean hitting times and their variances increase as M increases, as we could have guessed by intuition. Instead the shape of that functions remain nearly the same.

Before starting to analyze the discrete model and compare analytical formulas with the results of our simulations, we can make two summary plots regarding the behaviour of mean hitting times and their variances with respect to N and M. From Fig.6, where we have plotted mean hitting times for $N =$ 1,2,3 and $M = 2$, we can see an interesting feature of our Markov chain. There is an inversion phenomena: for small rates low N have higher mean hitting times, whereas for higher rates higher N have higher hitting times. This is because there is a "competition" between two processes, incoming of new particles and random walk of active particles already present. For low rate, it is more probable that particles already active would be absorbed outside on the barrier, and so for low N this process is dominant since there are few sites in which particles can move before being absorbed into the barriers. This means that mean hitting times are higher in this case. On the opposite, let's consider high rates. Then a lot of particles are incoming, and that process is dominant over random walk: for low N is it simpler to get faster to the absorbing state, since there are no high spreading of active particles into a lot of sites. The same line of reasoning can be applied for high N. This explains our results. In Fig.7 we have plotted mean hitting times for $N = 2$ and $M =$ 2,3: we clearly see that all values are on an higher level for higher M, as expected. Also the shape of the functions are similar.

Figure 6: Summary plots of variation of mean hitting times with respect to N

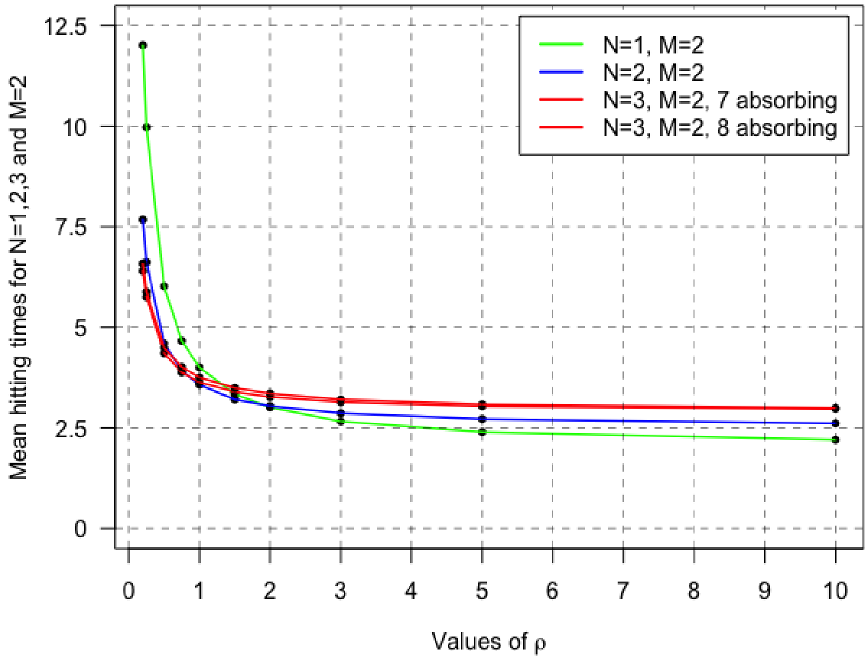
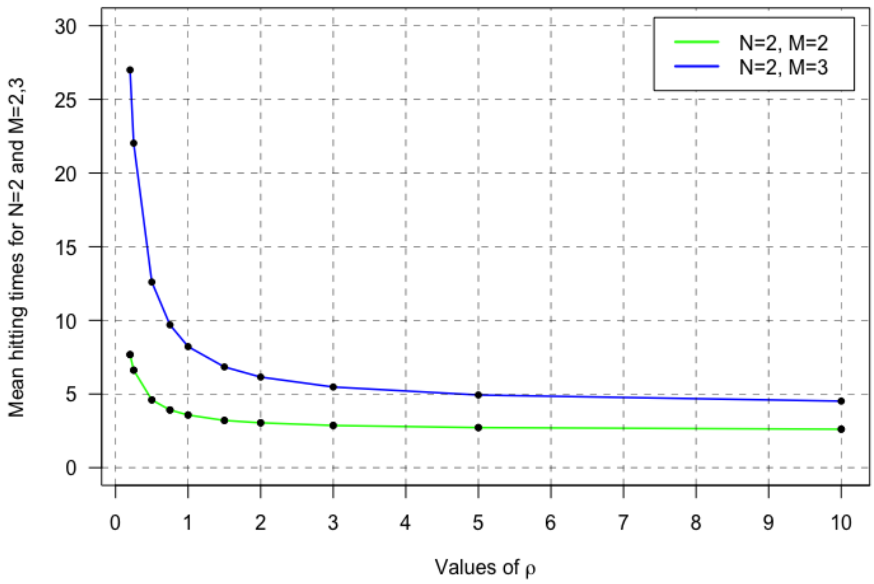


Figure 7: Summary plots of variation of mean hitting times with respect to M



A model for a discrete time Markov process

In the discrete time case, we have two possibilities. The first is to build the jump matrix that is directly related to the Q generating matrices written in the previous section. The second is to develop an indipendent model from scratch, taking advantage of the more “freedom” of the discrete time Markov chains. Let’s begin by computing the jump matrices for our remarkable cases:

- $N = 1$, $M = 2$

$$J = \begin{pmatrix} 0 & 1 & 0 \\ \frac{1}{1+\rho} & 0 & \frac{\rho}{1+\rho} \\ 0 & 0 & 1 \end{pmatrix}$$

- $N = 2$, $M = 2$

$$J = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2(1+2\rho)} & 0 & \frac{1}{2(1+2\rho)} & \frac{\rho}{(1+2\rho)} & \frac{\rho}{(1+2\rho)} \\ \frac{1}{2(1+2\rho)} & \frac{1}{2(1+2\rho)} & 0 & \frac{\rho}{(1+2\rho)} & \frac{\rho}{(1+2\rho)} \\ 0 & \frac{1}{2(2+2\rho)} & \frac{1}{2(1+2\rho)} & 0 & \frac{1+2\rho}{(2+2\rho)} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

- $N = 2$, $M = 3$

$$J = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2(2\rho+1)} & 0 & \frac{1}{2(2\rho+1)} & \frac{\rho}{2\rho+1} & \frac{\rho}{2\rho+1} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2(2\rho+1)} & \frac{1}{2(2\rho+1)} & 0 & \frac{\rho}{2\rho+1} & 0 & \frac{\rho}{2\rho+1} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2(2\rho+2)} & \frac{1}{2(2\rho+2)} & 0 & 0 & 0 & \frac{1+2\rho}{2(2\rho+2)} & \frac{1+2\rho}{2(2\rho+2)} & 0 & 0 \\ 0 & \frac{1}{2\rho+2} & 0 & \frac{1}{2\rho+2} & 0 & 0 & \frac{\rho}{2\rho+2} & 0 & 0 & \frac{\rho}{2\rho+2} \\ 0 & 0 & \frac{1}{2\rho+2} & \frac{1}{2\rho+2} & 0 & 0 & 0 & \frac{\rho}{2\rho+2} & 0 & \frac{\rho}{2\rho+2} \\ 0 & 0 & 0 & \frac{1}{2\rho+3} & \frac{1}{2(2\rho+3)} & 0 & 0 & \frac{1}{2\rho+3} & \frac{\rho}{2\rho+3} & \frac{2\rho+1}{2(2\rho+3)} \\ 0 & 0 & 0 & \frac{1}{2\rho+3} & 0 & \frac{1}{2(2\rho+3)} & \frac{1}{2\rho+3} & 0 & \frac{\rho}{2\rho+3} & \frac{2\rho+1}{2(2\rho+3)} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\rho+4} & \frac{1}{2\rho+4} & 0 & \frac{2+2\rho}{2\rho+4} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

- $N = 3$, $M = 2$

$$J = \begin{pmatrix} 0 & \frac{2}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2(1+3\rho)} & 0 & \frac{1}{2(1+3\rho)} & \frac{\rho}{1+3\rho} & \frac{\rho}{1+3\rho} & 0 & \frac{\rho}{1+3\rho} & 0 \\ 0 & \frac{1}{1+3\rho} & 0 & \frac{2\rho}{1+3\rho} & 0 & 0 & 0 & \frac{\rho}{1+3\rho} \\ 0 & 0 & \frac{1}{2(2+3\rho)} & 0 & \frac{1}{2(2+3\rho)} & \frac{\rho}{2+3\rho} & \frac{1+2\rho}{2(2+3\rho)} & \frac{1+2\rho}{2(2+3\rho)} \\ 0 & \frac{1}{2+3\rho} & 0 & \frac{1}{2+3\rho} & 0 & \frac{\rho}{2+3\rho} & \frac{2\rho}{2+3\rho} & 0 \\ 0 & 0 & 0 & \frac{1}{3+3\rho} & 0 & 0 & \frac{1+2\rho}{3+3\rho} & \frac{1+\rho}{3+3\rho} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The other model is based upon the definition of two new probabilities p_1 e p_2, one related to the incoming rate of new particles for each site and the other one related to the diffusion of the particle with an asymmetric (in general) random walk. We define:

- p_1 probability for each site i that a new particle arrive
- p_2 probability for an active particle in the site i to jump to the right into the site $i+1$ (and thus $1-p_2$ probability for an active particle in the site i to jump into the site $i-1$)

With some effort we can give an example of this model for $N = 2$ and $M = 2$. We consider the states $\{0,0\}$,$\{1,0\}$,$\{0,1\}$,$\{1,1\}$,$\{2,*\} \cup \{*,2\}$ since there is no symmetry because of p_2.

$$P = \begin{pmatrix} (1-p_1)^2 & p_1(1-p_1) & p_1(1-p_1) & p_1^2 & 0 \\ (1-p_2)(1-p_1)^2 & (1-p_2)p_1(1-p_1) & (1-p_1)(p_1+p_2-p_1p_2) & p_1(p_1+p_2-p_1p_2) & p_1p_2 \\ p_2(1-p_1)^2 & (1-p_1)(1-p_1-p_2+2p_1p_2) & p_2p_1(1-p_1) & p_1(1-p_1-p_2+2p_1p_2) & p_1(1-p_2) \\ p_2(1-p_2)(1-p_1)^2 & (1-p_2)(1-p_1)(1-p_1-p_2+2p_1p_2) & p_2(1-p_1)(p_1+p_2-2p_1p_2) & (p_1+p_2-2p_1p_2)(1-p_1-p_2+2p_1p_2) & p_1(1-p_1p_2(p_2+1)) \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

This model is interesting because it allows to remain in the same state, since the diagonal is not zero. There is then the possibility that no new particles will arrive, differently from the jump matrix associated to the continuous Markov chain model for $N = 2$,$M = 2$. Here we will consider only jump matrices for the moment, in order to compare our results with those of the previous sections.

Analytical calculation of mean hitting times and their variances

We will analyze the first model with our jump matrices and we will compute the estimated hitting times $E(\rho)$(and their variances $V(\rho)$) for the absorbing states starting from the state with zero particles. We will then compare direcly on the following plots our analytical results with the previous results obtained by Gillespie's algorithm: these last values will be highlined with a red dot. Using MATLAB we can compute easily the theoretical values of mean and variance of the hitting time simply by solving a system of equations. We will write the full code only for the trivial case $N = 1$,$M = 2$ as an example of the procedure.

(a) $N = 1$ $M = 2$

```
#we introduce p as the rate of incoming particles in a generic site
#so we use it as a parameter, in order to get later functions
#E(p) and V(p), that are mean and variance of the hitting time
syms p
#we can now write down the sub matrix A of J, that will be used
in the computation
A=[0, 1; 1/(1+p),0]
#we also write some vectors and matrices that will be used in the computation
#the index will be replaced by the dimension of the submatrices in the other cases
x=ones(2,1)
I=eye(2)
#we use the following formulas
N=(I-A)^(-1)
E(p)=N*x
V(p) = (2*N-I)*(N*x) - (N*x).^2
```

Since we want to know only the hitting time of $\{2\}$ starting from $\{0\}$, we will always consider the first element of each vector. Then we obtain for this case the simple equations:

$$E(\rho) = \frac{2(\rho+1)}{\rho} \tag{6}$$

$$V(\rho) = \frac{4(\rho+1)}{\rho^2} \tag{7}$$

We note that $\lim_{\rho\to 0} E(\rho) = \lim_{\rho\to 0} V(\rho) = +\infty$, as expected naively from previous simulations. Also $\lim_{\rho\to\infty} E(\rho) = 2$ and $\lim_{\rho\to\infty} V(\rho) = 0$. Then we can plot our functions $E(\rho)$ and $V(\rho)$ in the domain $\rho \in [0, 15]$ with a blue smooth line:

Figure 8: Analytical and estimated mean hitting time as a function of ρ , $N = 1$, $M = 2$

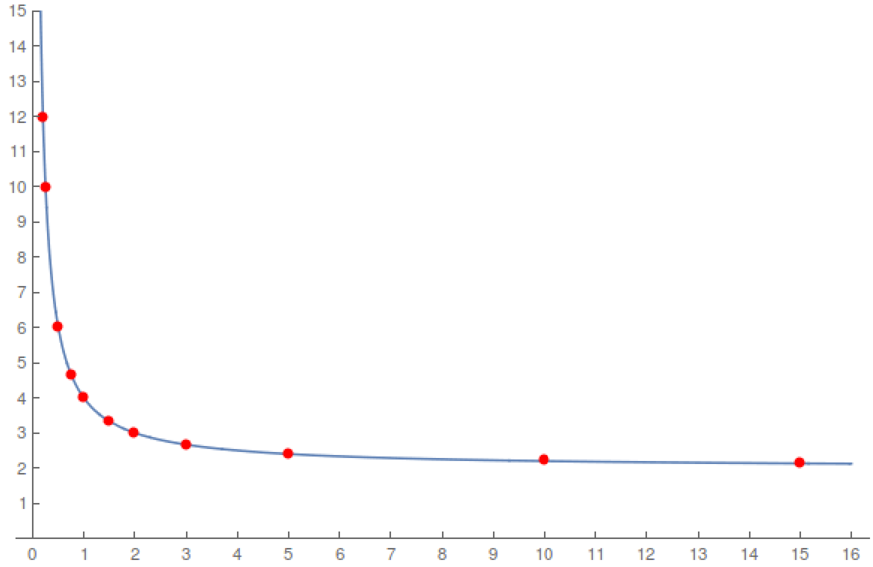
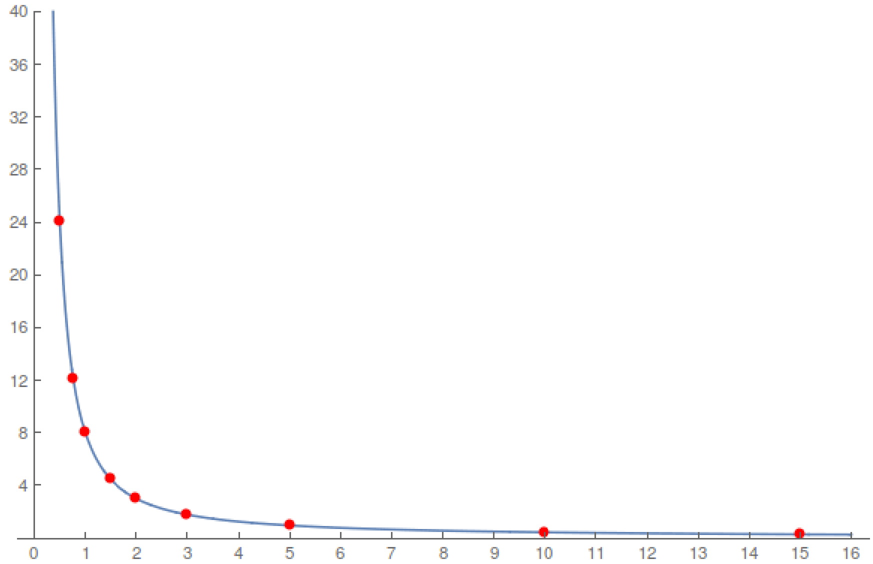


Figure 9: Analytical and estimated variance of mean hitting time as a function of ρ , $N = 1$, $M = 2$



We can check also explicitly for special fixed values of ρ how accurate is the agreement:

Table 1: Comparison between theory and simulation for mean hitting times

ρ	0.25	0.75	1.5
Mean	9.98792	4.65658	3.32734
$E(\rho)$	10	4.66667	3.33333
Absolute error	0.01208	0.01009	0.00599
Relative error	0.12%	0.22%	0.18%

Table 2: Comparison between theory and simulation for variances of mean hitting times

ρ	0.25	0.75	1.5
Variance	80.0984	12.1797	4.4686532
$V(\rho)$	80.0000	12.4444	4.4444
Absolute error	0.0984	0.2647	0.0243
Relative error	0.12%	2.13%	0.55%

(b) $N = 2$, $M = 2$
Using almost the same MATLAB code except for the following

```
x=ones(4,1)
I=eye(4)
```

we find the following expressions:

$$E(\rho) = \frac{3 + 12\rho + 10\rho^2}{3\rho + 4\rho^2} \tag{8}$$

$$V(\rho) = \frac{9 + 45\rho + 74\rho^2 + 42\rho^3 + 4\rho^4}{\rho^2(3 + 4\rho)^2} \tag{9}$$

We note that $\lim_{\rho\to 0} E(\rho) = \lim_{\rho\to 0} V(\rho) = +\infty$ also in this case. Also $\lim_{\rho\to\infty} E(\rho) = \frac{5}{2}$ and $\lim_{\rho\to\infty} V(\rho) = \frac{1}{4}$. In this case the variance $V(\rho)$ tends to a finite limit for $\rho \to \infty$, differently from the previous case $N = 1, M = 2$. Then we can plot our functions $E(\rho)$ and $V(\rho)$ in the domain $\rho \in [0, 15]$ with a blue smooth line:

Figure 10: Analytical and estimated mean hitting time as a function of ρ , $N = 2$, $M = 2$

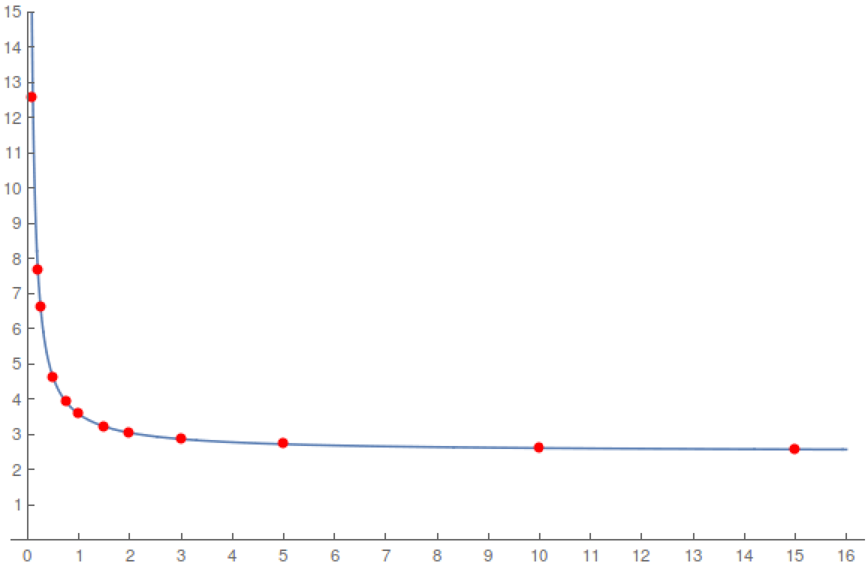
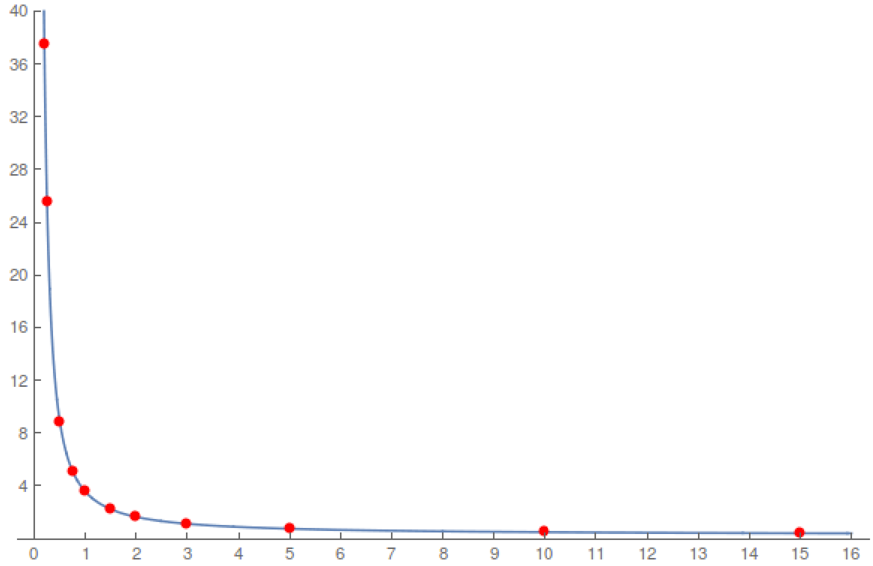


Figure 11: Analytical and estimated variance of mean hitting time as a function of ρ , $N=2$, $M=2$



We can check also explicitly for special fixed values of ρ how accurate is the agreement:

Table 3: Comparison between theory and simulation for mean hitting times

ρ	0.25	0.75	1.5
Mean	6.6175	3.9160	3.2061
$E(\rho)$	6.6256	3.9167	3.2222
Absolute error	0.0081	0.0007	0.0243
Relative error	0.12%	0.02%	0.50%

Table 4: Comparison between theory and simulation for variances of mean hitting times

ρ	0.25	0.75	1.5
Variance	25.5390	5.1178	2.1758
$V(\rho)$	25.5469	5.1042	2.2222
Absolute error	0.0079	0.0136	0.0464
Relative error	0.03%	0.27%	2.09%

(c) $N=2$, $M=3$

Using almost the same MATLAB code except for the following

```
x=ones(6,1)
I=eye(6)
```

we find the following expressions:

$$E(\rho)=\frac{66+525\rho+1470\rho^2+1896\rho^3+1148\rho^4+264\rho^5}{2\rho(1+\rho)(6+49\rho+76\rho^2+32\rho^3)} \tag{10}$$

$$V(\rho)=\frac{4356+61020\rho+348025\rho^2+1085250\rho^3+2078070\rho^4+2571500\rho^5}{4\rho^2(1+\rho)^2(6+49\rho+76\rho^2+32\rho^3)^2}+ \tag{11}$$

$$+\frac{2082480\rho^6+1079832\rho^7+334656\rho^8+52480\rho^9+2496\rho^{10}}{4\rho^2(1+\rho)^2(6+49\rho+76\rho^2+32\rho^3)^2} \tag{12}$$

We note that $\lim_{\rho\to 0} E(\rho) = \lim_{\rho\to 0} V(\rho) = +\infty$ also in this case. Also $\lim_{\rho\to\infty} E(\rho) = \frac{33}{4}$ and $\lim_{\rho\to\infty} V(\rho) = \frac{39}{16}$. Then we can plot our functions $E(\rho)$ and $V(\rho)$ in the domain $\rho \in [0, 15]$ with a blue smooth line:

Figure 12: Analytical and estimated mean hitting time as a function of ρ , $N = 2$, $M = 3$

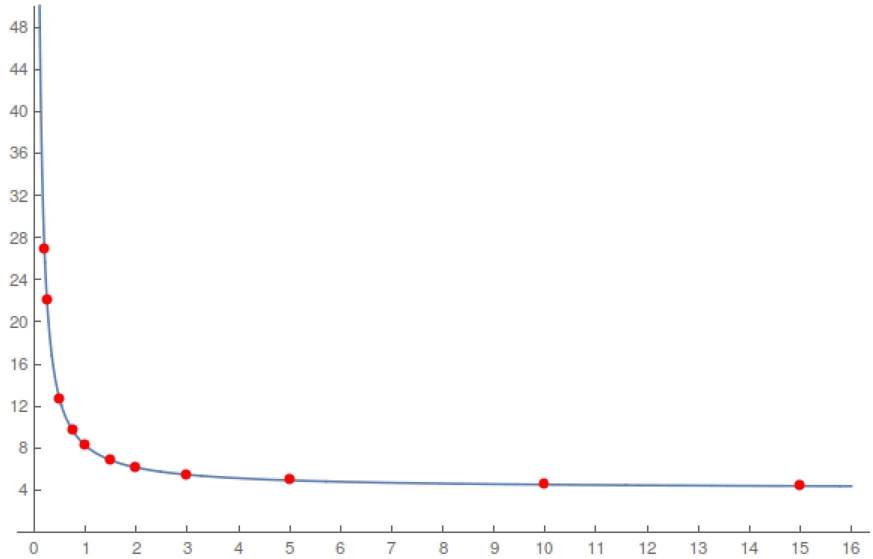
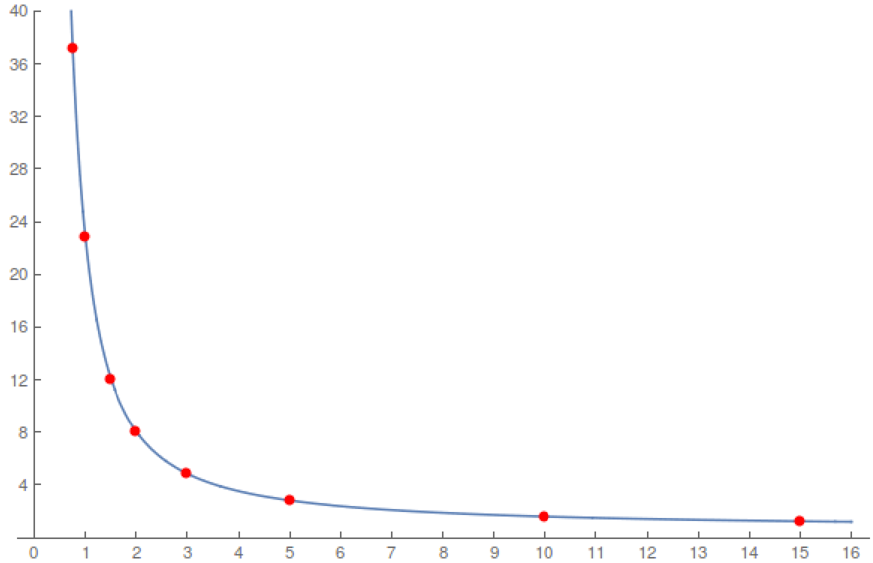


Figure 13: Analytical and estimated variance of mean hitting time as a function of ρ , $N = 2$, $M = 3$



We can check also explicitly for special fixed values of ρ how accurate is the agreement:

Table 5: Comparison between theory and simulation for mean hitting times

ρ	0.25	0.75	1.5
Mean	21.9979	9.6405	6.8346
$E(\rho)$	22.025	9.6133	6.8346
Absolute error	0.0271	0.0272	0
Relative error	0.12%	0.28%	0%

Table 6: Comparison between theory and simulation for variances of mean hitting times

ρ	0.25	0.75	1.5
Variance	321.4376	37.1895	12.0290
$V(\rho)$	322.3024	37.3707	12.1031
Absolute error	0.8648	0.1812	0.0741
Relative error	0.27%	0.48%	0.61%

(d) $N = 3$, $M = 2$

This case is a bit different from the previous ones because there are two absorbing states, $\{2, *, *\}$ and $\{*, 2, *\}$. For this reason we have to evaluate conditioned matrices before, and then apply the standard theory to find mean hitting times and their variances. We begin computing the probability to hit state $\{7\}$ (that is $\{2, *, *\}$):

```
#we define A as the upper left submatrice 6x6 of J
#then we define the vector x as a subcolumn of J
x=[0;p/(1+3*p);0;(1+2*p)/(2*(2+3*p));2*p/(2+3*p);(1+2*p)/(3+3*p)]
I=eye(6)
#we compute the probability resolving the system of equation
H=((I-A)^(-1))*x
#now we can compute the conditioned matrix B
B=zeros(6)
fori=[1:6]
forj=[1:6]
B(i,j)=A(i,j)*H(j)/H(i)
end
end
```

From the matrix B we can compute mean and variance of hitting times following our precedent method using almost the same MATLAB code except for the the sequent lines

```
x=ones(6,1)
I=eye(6)
```

we find the following expressions:

$$E^{\{7\}}(\rho) = \frac{31122 + 598890\rho + 4865549\rho^2 + 22044980\rho^3 + 61894556\rho^4}{18\rho(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)(114 + 842\rho + 2153\rho^2 + 2372\rho^3 + 972\rho^4} + \\ + \frac{112547304\rho^5 + 133422264\rho^6 + 99963720\rho^7 + 43127640\rho^8 + 8188128\rho^9}{18\rho(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)(114 + 842\rho + 2153\rho^2 + 2372\rho^3 + 972\rho^4} \quad (13)$$

$$V^{\{7\}}(\rho) = \frac{968578884 + 31674672000\rho + 481918755816\rho^2 + 4530486269460\rho^3 + 29485314955945\rho^4 + 141093138822494\rho^5}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(114 + 842\rho + 2153\rho^2 + 2372\rho^3 + 972\rho^4)^2} +$$
$$+ \frac{514632285055020\rho^6 + 1463609597009648\rho^7 + 3291634663469020\rho^8 + 5900025225324492\rho^9 + 8450551797553656\rho^{10}}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(114 + 842\rho + 2153\rho^2 + 2372\rho^3 + 972\rho^4)^2} +$$
$$+ \frac{9649146234092976\rho^{11} + 8716031641122912\rho^{12} + 6139859297596128\rho^{13} + 3294619994654784\rho^{14} + 1296630134570016\rho^{15}}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(114 + 842\rho + 2153\rho^2 + 2372\rho^3 + 972\rho^4)^2} +$$
$$+ \frac{351185634186048\rho^{16} + 58062335614848\rho^{17} + 4363904388096\rho^{18}}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(114 + 842\rho + 2153\rho^2 + 2372\rho^3 + 972\rho^4)^2} \tag{14}$$

We note that $\lim_{\rho\to 0} E^{\{7\}}(\rho) = \lim_{\rho\to 0} V^{\{7\}}(\rho) = +\infty$ also in this case. Also $\lim_{\rho\to\infty} E^{\{7\}}(\rho) = \frac{26}{9}$ and $\lim_{\rho\to\infty} V^{\{7\}}(\rho) = \frac{44}{81}$. Then we can plot our functions $E^{\{7\}}(\rho)$ and $V^{\{7\}}(\rho)$ in the domain $\rho \in [0, 15]$ with a blue smooth line:

Figure 14: Analytical and estimated mean hitting time as a function of ρ for state $\{2, *, *\}$, $N = 3$, $M = 2$

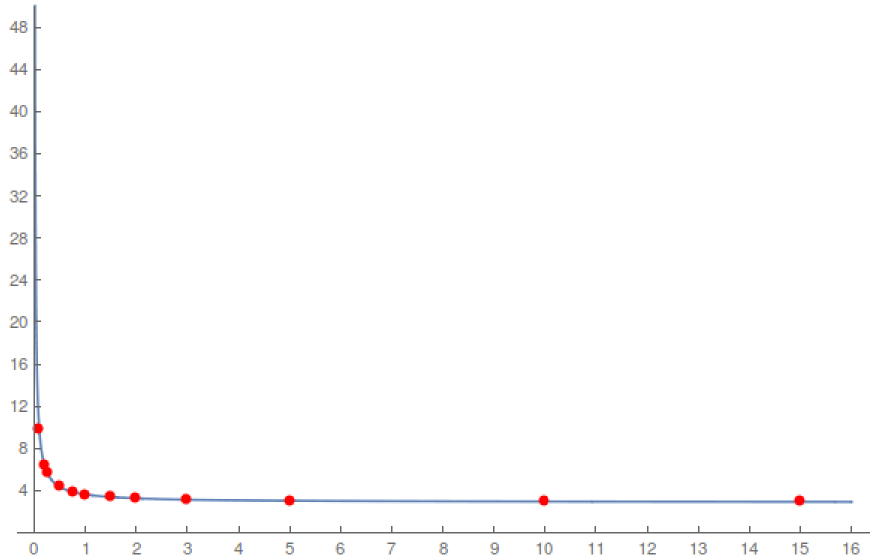
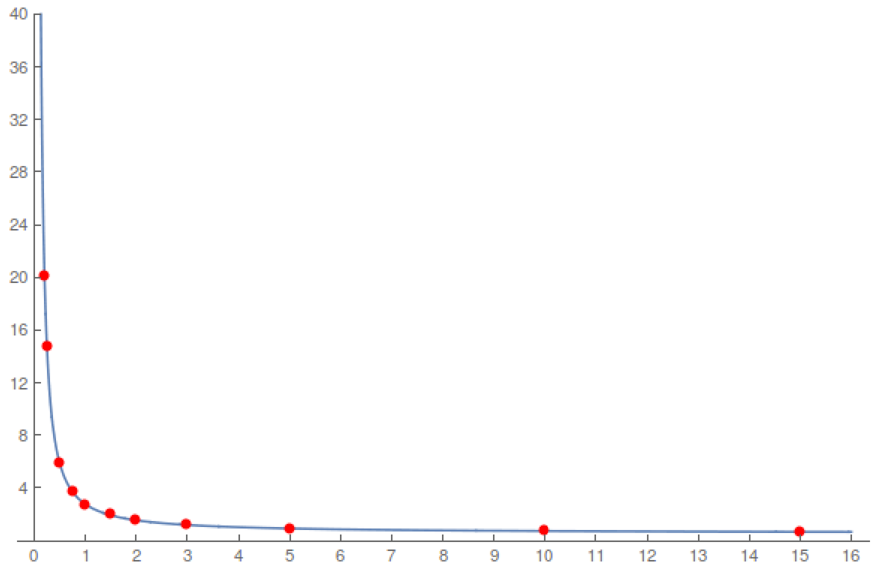


Figure 15: Analytical and estimated variance of mean hitting time as a function of ρ for state $\{2,*,*\}$, $N=3$, $M=2$



We can check also explicitly for special fixed values of ρ how accurate is the agreement:

Table 7: Comparison between theoretical and simulation values of hitting times $E^{\{7\}}(\rho)$ for for state $\{2,*,*\}$,$N=3$,$M=2$

ρ	0.25	0.75	1.5
Mean	5.7531	3.8793	3.3980
$E^{\{7\}}(\rho)$	5.7346	3.8814	3.3953
Absolute error	0.0185	0.1812	0.0027
Relative error	0.32%	0.05%	0.08%

Table 8: Comparison between theoretical and simulation values of variance of hitting times $V^{\{7\}}(\rho)$ for for state $\{2,*,*\}$,$N=3$,$M=2$

ρ	0.25	0.75	1.5
Variance	14.7521	3.6908	1.9513
$V^{\{7\}}(\rho)$	14.6039	3.6894	1.9244
Absolute error	0.1482	0.0014	0.0027
Relative error	1.01%	0.05%	0.04%

Now we compute the probability to hit state $\{8\}$ (that is $\{*,2,*\}$):

```
#we define A as the upper left submatrice 6x6 of J
#then we define the vector x as a subcolumn of J
x=[0;0;p/(1+3*p);(1+2*p)/(2*(2+3*p));0;(1+p)/(3+3*p)]
I=eye(6)
#we compute the probability risolving the system of equation
H=((I-A)^(-1))*x
#now we can compute the conditioned matrix B
B=zeros(6)
```

```
fori=[1:6]
forj=[1:6]
B(i,j)=A(i,j)*H(j)/H(i)
end
end
```

From the matrix B we can compute mean and variance of hitting times following our precedent method using almost the same MATLAB code except for the the sequent lines

```
x=ones(6,1)
I=eye(6)
```

we find the following expressions:

$$
\begin{aligned}
E^{\{8\}}(\rho) = & \frac{25389 + 473190\rho + 3671599\rho^2 + 15860410\rho^3 + 42449518\rho^4}{18\rho(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)(93 + 598\rho + 1375\rho^2 + 1354\rho^3 + 486\rho^4} \\
& + \frac{73434744\rho^5 + 82437984\rho^6 + 58079592\rho^7 + 23357160\rho^8 + 4094064\rho^9}{18\rho(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)(93 + 598\rho + 1375\rho^2 + 1354\rho^3 + 486\rho^4}
\end{aligned}
\tag{15}
$$

$$
\begin{aligned}
V^{\{8\}}(\rho) = & \frac{644601321 + 19847595186\rho + 284787963126\rho^2 + 2527182651180\rho^3 + 15538659524209\rho^4 + 70322606450870\rho^5}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(93 + 598\rho + 1375\rho^2 + 1354\rho^3 + 486\rho^4)^2} + \\
& + \frac{242911365278412\rho^6 + 655260705627440\rho^7 + 1400138071702768\rho^8 + 2388452515918452\rho^9 + 3260731008119544\rho^{10}}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(93 + 598\rho + 1375\rho^2 + 1354\rho^3 + 486\rho^4)^2} + \\
& + \frac{3552989210183088\rho^{11} + 3064426972833456\rho^{12} + 2060584958474352\rho^{13} + 1053921210848640\rho^{14} + 394179532312608\rho^{15}}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(93 + 598\rho + 1375\rho^2 + 1354\rho^3 + 486\rho^4)^2} + \\
& + \frac{100953144580032\rho^{16} + 15660282308544\rho^{17} + 1090976097024\rho^{18}}{324\rho^2(23 + 160\rho + 392\rho^2 + 414\rho^3 + 162\rho^4)^2(93 + 598\rho + 1375\rho^2 + 1354\rho^3 + 486\rho^4)^2}
\end{aligned}
\tag{16}
$$

We note that $\lim_{\rho\to 0} E^{\{8\}}(\rho) = \lim_{\rho\to 0} V^{\{8\}}(\rho) = +\infty$ also in this case. Also $\lim_{\rho\to\infty} E^{\{8\}}(\rho) = \frac{26}{9}$ and $\lim_{\rho\to\infty} V^{\{8\}}(\rho) = \frac{44}{81}$ as in the previous case, since the situation is symmetric. Then we can plot our functions $E^{\{8\}}(\rho)$ and $V^{\{8\}}(\rho)$ in the domain $\rho \in [0, 15]$ with a blue smooth line:

Figure 16: Analytical and estimated mean hitting time as a function of ρ for state $\{*, 2, *\}$, $N = 3$, $M = 2$

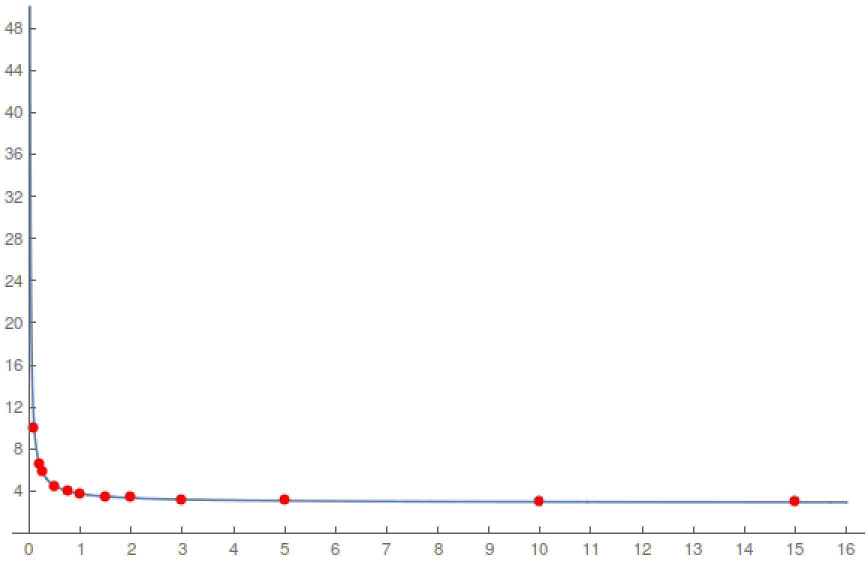
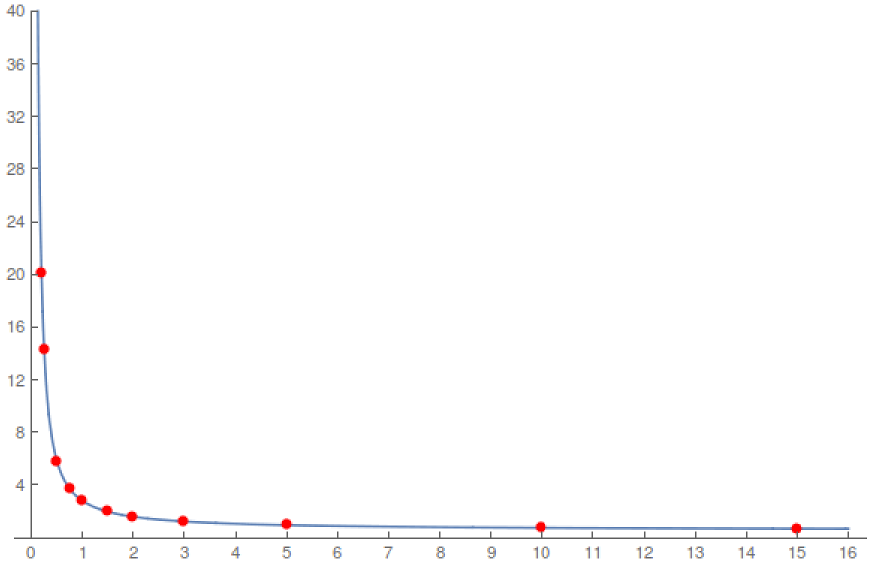


Figure 17: Analytical and estimated variance of mean hitting time as a function of ρ for state $\{*, 2, *\}$, $N = 3$, $M = 2$



We can check also explicitly for special fixed values of ρ how accurate is the agreement:

Table 9: Comparison between theoretical and simulation values of hitting times $E^{\{8\}}(\rho)$ for for state $\{2, *, *\}$,$N = 3$,$M = 2$

ρ	0.25	0.75	1.5
Mean	5.8810	4.0133	3.4943
$E^{\{8\}}(\rho)$	5.8981	4.0085	3.4912
Absolute error	0.0171	0.0048	0.0031
Relative error	0.29%	0.12%	0.09%

Table 10: Comparison between theoretical and simulation values of variance of hitting times $V^{\{8\}}(\rho)$ for for state $\{2, *, *\}$,$N = 3$,$M = 2$

ρ	0.25	0.75	1.5
Variance	14.2870	3.7048	1.9874
$V^{\{8\}}(\rho)$	14.5697	3.7117	1.9645
Absolute error	0.2827	0.0069	0.229
Relative error	1.94%	0.19%	1.17%

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[4] Grinfeld M. Lamb W. O'Neill K.P. and P.A. Mulheran Gap-size and capture-zone distributions in one-dimensional point-island nucleation and growth simulations: Asymptotics and models. in: *Phys. Rev.E*, **85**: (2012) doi: 10.1103/PhysRevE.85.021601 (see p. 2)