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IMPLEMENTATION OF POLYNOMIAL IDENTITIES FROM THE CHAIN RULE IN PROBABILITY GENERATING FUNCTIONS FOR BRANCHING PROCESSES

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Abstract. In this paper, the Bienaymé-Galton-Watson process is used to model in a stochastic sense the spreading of a disease over time. This is a type of stochastic process, which belongs to the class of branching processes. They can also be employed in other propagation phenomena, such as spam, fake news, innovation adoption and market value. Uncertainty is introduced in the way a single individual interacts with others. This is modeled as discrete random variable. Specifically for this work, it is treated as a Binomial distribution and named contagion. As a consequence, the number of subsequent people infected at a specific time is also a discrete random variable, named generation's size. A fundamental aspect to understand the evolution of the disease in this perspective is to find the mass function of such generations' size. A classical technique to do this is manipulating probability generating functions. This technique works well for early generations. However, it turns very time consuming as the generation number increases, becoming non-feasible for higher generations. The reason is that higher-order derivatives of more complex functions are tackled as the generation number increases. Therefore, a novelty in here is introducing a polynomial identity based on the chain rule approach to relieve the computational costs to perform the necessary derivatives. These two techniques are in here compared in terms of runtime and mathematical implications to find the mass functions for higher generations' size. Results show that the runtime spent for the probability generating function's technique in the absence of polynomial identities is smaller for the early generations. Moreover, analytical expressions relating the random variables of the contagion and the generation's size for different generations are preserved. On the other hand, as the generation number increases, the use of polynomial identities becomes advantageous to decrease the runtime spent and to cover a larger interval from the support of the mass functions.

1 INTRODUCTION

Many are the phenomena that propagate over time, such as epidemics, cell division, spam, malwares, fake news, innovation adoption and market value. Despite their heterogeneous subject, they follow some similar underlying principles, which are well discussed in Kucharski (2020). All of them have in general spark, growth, peak and decline. More specifically for the perspective of epidemic's spreading, modeling its temporal evolution dynamic is a challenging task, because a lot of different variables are presented and most of them are hardly traceable, e.g., human behavior facing epidemics, healthy conditions from exposed people and environmental aspects.

Verelst et al. (2016) provide a systematic review of models used to model the spread of a infectious. One of the most traditional and well-studied group of models are the compartmental ones, which are for instance explored in Martcheva (2015); Li (2018); Brauer et al. (2019). They belong to the population-level classification. The main idea behind them is to organize the population studied into different groups, as known as compartments, and an initial value problem characterizes the evolution of the number of individuals between them. A fundamental parameter related to the group transitions is the basic reproduction number. It represents an important property from epidemiology defined by Leung (2021) as transmissibility, which describes how easy or not an infected person spreads the disease to others.

However, a questionable assumption is made in these sort of models. The basic reproduction number is considered a discrete parameter despite the variability and uncertainty inherent in its physical representation. This is the reason why nowadays individual-level models are getting more attention. Stochastic outbreaks are instead captured on them for example through demographic stochasticity, which according to Haccou et al. (2005) is when the population's size randomness is a consequence of the uncertainty inherent in the individual.

A reasonable way to incorporate the demographic stochasticity is to model the number of new people infected per infector as a discrete random variable, which in this work is modeled as a Binomial family. Then, the evolution of the disease over time is considered a stochastic process and in this paper the Bienaymé-Galton-Watson (BGW) process is chosen to model it just like Borges et al. (2021a,b). It is a discrete time and state branching process, which its history is found in Bacaër (2011) and was initially proposed to explain why population of countries were growing exponentially, whilst family names were disappearing. But its use has extended this purpose and besides the propagation phenomena showed at the beginning, it is also used in the context of biochemical processes, genetics and actuarial sciences as cited in González et al. (2021). Each random variable attached to the BGW process represent in the proposed epidemiological context a generation's size of infected members.

When dealing with stochastic models, the most complete information comes from the probability mass function (pmf) or its continuous counterpart probability density function (pdf) of the random variables presented. Lima and Sampaio (2018) discuss how these entities remain the best option in uncertainty quantification. Therefore, finding the mass function of generations' size is valuable to understand the stochastic evolution of the disease over time. Moreover, it allows us to evaluate statistics, check the influence of the contagion's random variable, obtain the extinction probability of the disease and it also provides useful mechanisms to work with bayesian approaches.

A classical analytical technique to achieve this goal is to manipulate probability generating functions (pgfs). However, the computational costs associated to the extensive use of symbolic computation turn it into a non-feasible technique as the generation number increases. Then,

a novelty introduced in here is the implementation and discussion of polynomial identities for the chain rule to relieve the higher-order derivatives involved in the pgf technique. The comparison between these two techniques in this paper takes into account runtimes, mathematical implications and the capacity to cover the support from the mass function for generations' size.

2 DISEASE PROPAGATION MODELED AS A BGW PROCESS

We assume that initially there is only an individual somehow sick, who belongs to the so-called 0th generation of infected members. Fig. 1 shows one possible evolution of how the disease could have spread. The first infector is represented in the ramification tree of Fig. 1 as individual number 1. Only another person was infected by infector number 1 according to this digraph, which is the individual number 2. This time, individual number 2 spread the disease to two people. They are indicated as individuals number 3 and 4 and form the 2nd generation. Therefore, the size of this generation is two. The remain network displays the relation of infections up to the 5th generation.

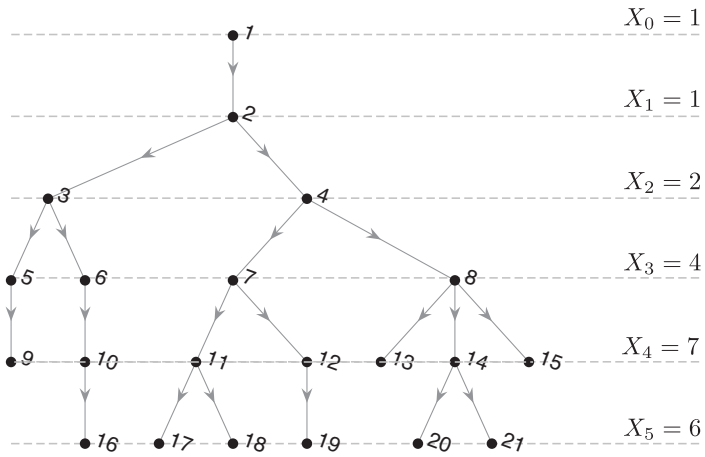

Figure 1: Realization of the BGW process up to the fifth generation of infected members

The directed graph in Fig. 1 is a realization of the BGW process. Each random variable from the family of random variables of this stochastic process $\mathcal{X} = \{X_t\}$ models the generation's size of infected members attached to the index t. At $t = 0$, it is always assumed that there is just a single initial infector, i.e., $X_0 = 1$. Since it is dealt with population sizes per generation, the state space $\mathbb{S}$ of this branching process is also discrete. The generation's size can take any non-negative value, then $\mathbb{S} = \mathbb{N}^0$, where $\mathbb{N}^0$ represents the set of the natural numbers including zero.

The key factor that rules the branching process is the number of successful infections per infector. This aspect is modeled in here also as a discrete random variable that assumes non-negative values. It is named as the contagion random variable C. For instance, in the example of Fig. 1, for the individual number 6 and number 7 from the 3rd generation, each realization of the contagion resulted in respectively one and two members infected that belongs to the 4th generation. It is important to highlight that in the BGW process, the contagions are independent and identically distributed (i.i.d.) random variables. This means in the current context that the transmissibility does not rely on the population size of the generation nor on the evolution of the disease over time and reflects the demographic stochasticity.

To sum up, the epidemic always begins only with a single infector from the 0th generation. A subsequent size generation X_{t+1} depends on a quantity of realizations of the contagion random variable. This quantity is the population size of the most previous generation X_t. Notice that there is no way to ensure this value at first, unless a realization of X_t is done. Except for the first generation, in which $X_1 = C$, since the previous generation's size is unitary from the deterministic statement. Generally speaking, the size X_{t+1} is determined according to Schinazi (2014) as

$$X_{t+1} = \sum_{k=0}^{X_t} C,\ t \in \mathbb{N}^0. \tag{1}$$

This stochastic process ends when the size of any generation $X_k, k \in \mathbb{N}$ is zero. In this situation, for any further value $t > k$, X_t is also zero, which means the extinction of the disease in the epidemiological context. Next, probability generating function itself and in the presence of polynomial identities are presented to find the mass function for any further generation X_{t+1}.

3 PROBABILITY GENERATING FUNCTIONS

The probabilities $p_k = \mathbb{P}(X = k)$, $k \in \mathbb{S}$, for a non-negative integers-valued random variable X can be rewritten uniquely in a power series configuration of increasing values of k: $p_0 + p_1 s + p_2 s^2 + \ldots$. One way to generate this sequence is with the help of its probability generating function (pgf). The pgf of a random variable X is the function $G_X(s)$ defined by

$$G_X(s) := \sum_{x=0}^{\infty} s^x \, \mathbb{P}(X = x) = p_0 + p_1 s + p_2 s^2 + \ldots. \tag{2}$$

The pgf can be related to an expectation value using the law of subconscious statistician, which is enunciated in Theorem 2.29 of Grimmett and Welsh (2014),

$$G_X(s) = \sum_{x=0}^{\infty} s^x \, \mathbb{P}(X = x) = \mathbb{E}\left(s^X\right). \tag{3}$$

A really common pgf is the one related to the $Binomial(m, p)$. This distribution models in this context an infector who contacts with m infectees at most and the probability of infection is p for each of them. Its pgf is given as

$$G_X(s) = \sum_{x=0}^{\infty} \binom{m}{x} p^x (1-p)^{m-x} s^x = [(1-p) + p\,s]^m. \tag{4}$$

A useful property coming from the pgfs is the possibility to build a pgf for the sum of a random quantity of i.i.d. random variables, such as the case in Eq. (1). As a consequence, it enables to rewrite the probabilities related to X_{t+1} in a sequential way. The key aspect is to describe the pgf $G_{X_{t+1}}(s)$ as a function of $G_C(s)$, which is known, once the contagion's probabilistic model is completely previously defined. This relation is represented in Eq. (5).

$$
\begin{aligned}
G_{X_{t+1}}(s) &= \sum_{x=0}^{\infty} s^x \, \mathbb{P}(X_{t+1}=x) = \mathbb{E}\left(s^{X_{t+1}}\right) = \sum_{i=0}^{\infty} \mathbb{E}\left(s^{X_{t+1}} \mid X_t = i\right) \mathbb{P}(X_t = i) \\
&= \sum_{i=0}^{\infty} \mathbb{E}\left(s^{\underbrace{C+C+\ldots+C}_{X_t \text{ times}}} \right) \mathbb{P}(X_t = i) = \sum_{i=0}^{\infty} \underbrace{G_C(s)}_{\text{argument}}^{i} \mathbb{P}(X_t = i) \qquad (5) \\
&= G_{X_t}(G_C(s)), \text{ as result of the definition in Eq. (2).} \\
&= G_C(G_C(\ldots(G_C(s)))), \text{ recurrence happens } t \text{ times.}
\end{aligned}
$$

Once the pgf of X_{t+1} is described in terms of the pgf of C, it is possible to evaluate the probabilities $\mathbb{P}(X_{t+1}=k), k \in \mathbb{S}$. In order to do that, it is necessary to take the k-th derivative of $G_{X_{t+1}}(s)$, divide it for the factorial of k and then evaluate the analytical expression in $s=0$. These operations are summed up in Eq. (6)

$$
\mathbb{P}(X_{t+1}=k) = \frac{1}{k!} \left. \frac{d^{(k)}\left[G_C(G_C(\ldots(G_C(s))))\right]}{ds^{(k)}} \right|_{s=0}. \qquad (6)
$$

This approach provides a piecewise function with analytical expressions per generation and state. They map the contagion random variable, through its pgf, with any generation's size probability. There is no need in this technique to find probabilities of previous generations to get values of the mass function for further ones. This property is so-called time-independency. Moreover, the probabilities of states of the same generation are evaluated individually, which means this methodology is a local one. In terms of computational aspects, an extensive use of symbolic computation is required to find the analytical multicomposition function of the pgfs and take their derivatives.

4 POLYNOMIAL IDENTITIES FOR THE CHAIN RULE

The task of evaluating directly the derivative in Eq. (6) may not be feasible. As the generation number increases, the corresponding function of the pgf gets more complex, since the number of recurrences in the multicomposition function increases. Another crucial aspect is that the order of the derivative also increases accordingly to the number of infectors desired. Instead of taking this straight approach, the chain rule could be applied and then the derivatives are done individually for each function that composes the multicomposition pgf. For instance, suppose the 1st and 2nd derivatives of the composition function $\Phi(b) = f(g(b))$ are sought. From the chain rule,

$$
\begin{aligned}
\frac{d^{(1)}[\Phi(b)]}{db^{(1)}} &= \left. \frac{d^{(1)}[f(a)]}{da^{(1)}} \right|_{a=g(b)} \frac{d^{(1)}[g(b)]}{db^{(1)}} \\
\frac{d^{(2)}[\Phi(b)]}{db^{(2)}} &= \left. \frac{d^{(1)}[f(a)]}{da^{(1)}} \right|_{a=g(b)} \frac{d^{(2)}[g(b)]}{db^{(2)}} + \left. \frac{d^{(2)}[f(a)]}{da^{(2)}} \right|_{a=g(b)} \left[\frac{d^{(1)}[g(b)]}{db^{(1)}} \right]^2.
\end{aligned}
$$

Notice that the chain rule gives an identity in which derivatives are done individually for the functions $f(a)$ and $g(b)$. In order to explain how these identities are generated, some definitions are introduced.

$$
\Phi_k := D^{(k)}\Phi(b), \quad f_k := D^{(k)} f(a)\big|_{a=g(b)}, \quad g_k := D^{(k)} g(b).
$$

The derivatives above are then rewritten in a polynomial structure,

$$\underbrace{\frac{d^{(1)}\left[\Phi\left(b\right)\right]}{db^{(1)}}}_{\Phi_1} = \underbrace{\left.\frac{d^{(1)}\left[f\left(a\right)\right]}{da^{(1)}}\right|_{a=g(b)}}_{f_1} \underbrace{\frac{d^{(1)}\left[g\left(b\right)\right]}{db^{(1)}}}_{g_1}$$

$$\Phi_1 = f_1\, g_1$$

$$\underbrace{\frac{d^{(2)}\left[\Phi\left(b\right)\right]}{db^{(2)}}}_{\Phi_2} = \underbrace{\left.\frac{d^{(1)}\left[f\left(a\right)\right]}{da^{(1)}}\right|_{a=g(b)}}_{f_1} \underbrace{\frac{d^{(2)}\left[g\left(b\right)\right]}{db^{(2)}}}_{g_2} + \underbrace{\left.\frac{d^{(2)}\left[f\left(a\right)\right]}{da^{(2)}}\right|_{a=g(b)}}_{f_2} \left[\underbrace{\frac{d^{(1)}\left[g\left(b\right)\right]}{db^{(1)}}}_{g_1}\right]^2$$

$$\Phi_2 = f_1\, g_2 + f_2\, g_1^2.$$

The k-th derivative of a composition, Φ_k, is then related to a k-th polynomial $\mathcal{B}_k$ composed by the monomials $f_1, f_2, \ldots, f_k, g_1, g_2, \ldots, g_k$:

$$\Phi_k = \mathcal{B}_k\left(f_1, g_1, f_2, g_2, \ldots, f_k, g_k\right) := \mathcal{B}_k\left(\left\{f_k\right\}, \left\{g_k\right\}\right). \tag{7}$$

The Faà di Bruno's formula presented in Riordan (1958) gives an explicit expression to find the polynomial identities $\mathcal{B}_k$. However, a faster methodology in terms of runtime is the recursive fashion technique that replaces monomials' indexes from previous polynomials generated according to Natalini and Ricci (2004),

$$\mathcal{B}_{k+1}\left(f_1, g_1, f_2, g_2, \ldots, f_k, g_k\right) = \sum_{j=0}^{k} \binom{k}{j} \mathcal{B}_{k-j}\left(f_2, g_1, f_3, g_2, \ldots, f_{k-j+1}, g_{k-j}\right) g_{j+1}. \tag{8}$$

in which $\mathcal{B}_0 = f_1$.

It is important to highlight that the polynomial identities found are associated to derivatives of a function composition $\Phi\left(b\right) = f\left(g\left(b\right)\right)$. This is the case specifically for the 2nd generation, in which $\Phi\left(s\right) = G_C\left(G_C\left(s\right)\right)$. For any other multicomposition function, the polynomial identities for a composition function can be applied recurrently. For instance, suppose the 1st derivative of the multicomposition function $\Phi\left(c\right) = f\left(g\left(h\left(c\right)\right)\right)$ is sought. Firstly, $g\left(h\left(c\right)\right)$ is rewritten as $j\left(c\right)$. Then, from the polynomial identities

$$\Phi_1 = \mathcal{B}\left(\left\{f_1\right\}, \left\{j_1\right\}\right)$$
$$\Phi_1 = f_1\, j_1.$$

But j_1 itself is the first derivative of a composition function $g\left(h\left(c\right)\right)$. Applying again the first polynomial identity,

$$\Phi_1 = f_1\, \mathcal{B}\left(\left\{g_1\right\}, \left\{h_1\right\}\right)$$
$$\Phi_1 = f_1\, g_1\, h_1,$$

in which

$$f_1 = \left.\frac{d^{(1)}\left[f\left(a\right)\right]}{da^{(1)}}\right|_{a=g(h(c))}, \quad g_1 = \left.\frac{d^{(1)}\left[g\left(b\right)\right]}{db^{(1)}}\right|_{b=h(c)}, \quad h_1 = \frac{d^{(1)}\left[h\left(c\right)\right]}{dc^{(1)}}.$$

Eq. (6) can be then rewritten in terms of the polynomial identities for derivatives of composition functions when $k > 0$,

$$\mathbb{P}\left(X_{t+1}=k\right)=\frac{1}{k!}\,\mathcal{B}_k\left(\left\{G_C\left(s\right)_k\right\},\left\{\underbrace{G_C\left(G_C\left(\ldots\left(G_C\left(s\right)\right)\right)\right)_k}_{\text{t-1 recurrences}}\right\}\right)\Bigg|_{s=0}. \tag{9}$$

Next, an example showing the use of polynomial identities with the pgfs is presented to discuss some mathematical considerations of the approach taken in this work for its implementation. Suppose that $C \sim Binomial\left(3, 0.50\right)$ and the probability of two members infected from the third generation $\mathbb{P}\left(X_3=2\right)$ is sought.

$$\begin{aligned}
\mathbb{P}\left(X_3=2\right) &= \frac{1}{2!}\,\mathcal{B}_2\left(\underbrace{\left\{G_C\left(s\right)_2\right\}}_{\{f_2\}},\underbrace{\left\{G_C\left(G_C\left(s\right)\right)_2\right\}}_{\{j_2\}}\right)\Bigg|_{s=0} \\
&= \frac{1}{2!}\,\left(f_1\,j_2+f_2\,j_1^2\right)\big|_{s=0} = \frac{1}{2!}\,\left(f_1|_{s=0}\;j_2|_{s=0}+f_2|_{s=0}\;{j_1|_{s=0}}^2\right) \\
&= \frac{1}{2!}\,\left[f_1|_{s=0}\;\mathcal{B}\left(\underbrace{\left\{G_C\left(s\right)_2\right\}}_{\{g_2\}},\underbrace{\left\{G_C\left(s\right)_2\right\}}_{\{h_2\}}\right)\Bigg|_{s=0}+f_2|_{s=0}\right. \\
&\quad \left.\mathcal{B}\left(\underbrace{\left\{G_C\left(s\right)_1\right\}}_{\{g_1\}},\underbrace{\left\{G_C\left(s\right)_1\right\}}_{\{h_1\}}\right)\Bigg|_{s=0}\right] \\
&= \frac{1}{2!}\,\left[f_1|_{s=0}\;\underbrace{\left(g_1\,h_2+g_2\,h_1^2\right)\big|_{s=0}}_{2!\,\mathbb{P}(X_2=2)}+f_2|_{s=0}\;\underbrace{{\left(g_1\,h_1\right)|_{s=0}}^2}_{1!\,\mathbb{P}(X_2=1)}\right] \\
&= \frac{1}{2!}\,\left(0.520\times 0.475+0.884\times 0.178^2\right)=0.138.
\end{aligned}$$

Notice that in order to calculate $\mathbb{P}\left(X_3=2\right)$, the probabilities $\mathbb{P}\left(X_2=2\right)$ and $\mathbb{P}\left(X_2=1\right)$ could have been used if their values are beforehand known. Instead of working with this technique with time-independency, it is chosen to embrace this time-dependency to avoid extra operations. It means that if $\mathbb{P}\left(X_{t+1}=k\right), t>1$ and $k>1$ is desired to be calculated, the probabilities $\mathbb{P}\left(X_t=k\right), k>1$ will be calculated before. It seems at first hand not a beneficial idea. However, when the aim is to find the whole mass function for subsequent further generations to see how the process develops in a stochastic sense, this option provides advantages in terms of runtime. On the other hand, the analytical expression relating the probability of any state from a further generation and the contagion random variable is partially suppressed and hence it does not provide likelihood functions to do bayesian inference studies.

5 COMPARISON BETWEEN THE METHODOLOGIES

The results presented in this text comes from codes that were written in MATLAB and they were run on a MacBook Air M2, 16 GB of RAM and 512 GB of storage. Before showing the comparsion in terms of runtime between the probability generating function technique itself and with the presence of the polynomial identities, it is necessary to get them. Fig. 2 displays the runtime spent to generate each polynomial identity according to Eq. (8).

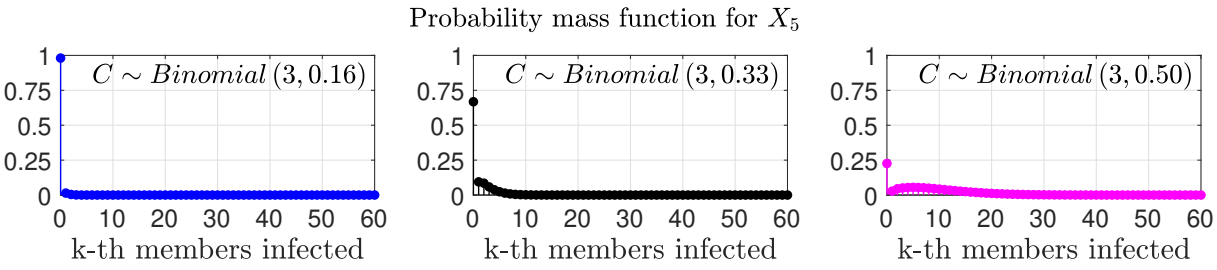

Figure 3: Probability mass functions for the 2nd up to the 5th generation.

Both the techniques in here proposed were able to find the complete mass function for the 2nd and 3rd generation's size. However, there are only 60 polynomial identities generated and it is not enough to cover the entire for support for the 3rd generation and the further ones. But, none of the techniques could cover all the support from the 5th generation. In this situation, it is not feasible anymore to do it with the pgf itself technique, because the runtime spent increases a lot. Next, it is presented in Fig. 5, the runtime spent for both the techniques to find the mass functions presented.

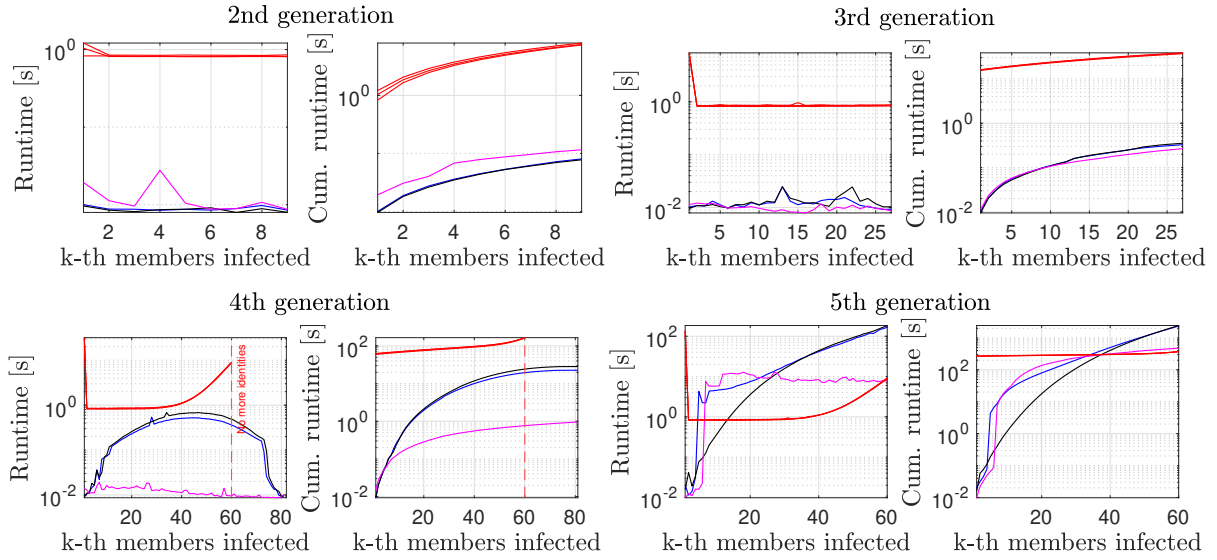

Figure 4: Runtimes to find probability mass functions for the 2nd up to the 5th generation. The solid blue, black and pink lines represent the cases of $C \sim Binomial(3, 0.16)$, $C \sim Binomial(3, 0.33)$ and $C \sim Binomial(3, 0.50)$ respectively. The solid red lines are related to the pfg with presence of polynomial identities and the dashed red line indicates no more polynomial identities available.

The runtime spent with polynomial identity remains the same regardless the contagion's law. Moreover, this technique is a time-dependent method and that's why the first infected member always started with a notable peak on runtime. Only from the 5th generation on, it presented lower values of runtime per number of members infected, reflecting ins a benefit in the cumulative runtime around 30 infectors. The times presented in here do not include the generation and loading time.

6 CONCLUSIONS

Despite the limited number of polynomial identities due RAM issues, it shows lower runtimes in further generations, where the pgf approach turns not feasible and cannot also cover

the entire supports. Runtimes in this technique do not change according to the parameters of the probabilistic model from the contagion. On the other hand, the decision of making this technique a time-dependent to improve runtime does not provide likelihood functions to do bayesian inference studies.

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