

Characterizing Branching Processes from Sampled Data

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ABSTRACT

Branching processes model the evolution of populations of agents that randomly generate offspring (children). These processes, more patently Galton-Watson processes, are widely used to model biological, social, cognitive, and technological phenomena, such as the diffusion of ideas, knowledge, chain letters, viruses, and the evolution of humans through their Y-chromosome DNA or mitochondrial RNA. A practical challenge of modeling real phenomena using a Galton-Watson process is the choice of the offspring distribution, which must be measured from the population. In most cases, however, directly measuring the offspring distribution is unrealistic due to lack of resources or the death of agents. So far, researchers have relied on informed guesses to guide their choice of offspring distribution. In this work we propose two methods to estimate the offspring distribution from real sampled data. Using a small sampled fraction of the agents and instrumented with the identity of the ancestors of the sampled agents, we show that accurate offspring distribution estimates can be obtained by sampling as little as 14% of the population.

Categories and Subject Descriptors

G.3 [Probability and Statistics]: Probabilistic algorithms; I.6.8 [Simulation and Modeling]: Types of Simulation—*Monte Carlo*; G.2.2 [Discrete Mathematics]: Graph Theory—*trees*

Keywords

Branching processes; graph characterization; sampling and estimation; MCMC

1. INTRODUCTION

Branching processes, more markedly Galton-Watson (GW) processes, have been used to model a variety of phenomena, ranging from human Y-chromosome DNA and mitochondrial RNA evolution [5], to epidemics on complex networks [6], to block dissemination in peer-to-peer networks [8]. The GW process can be represented as a growing tree, where agents are nodes connected to their offspring (children) by edges. The number of offspring is a random variable associated with a distribution function. A GW process is completely characterized by its offspring distribution, assumed to be i.i.d. for all nodes. A practical challenge when modeling real world systems from a GW process is knowing the offspring distribution of the process, which must be measured from the population.

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In most applications, however, directly measuring the offspring distribution is unrealistic due to the lack of resources or the inaccessibility of agents (e.g. death). It is not reasonable to assume that one can collect genetic material from the entire human population or that in the branching process of chain letter signatures (see Chierichetti et al. [3] for further details), one may collect all possible branches of the chain letter created by forwarding the letter. So far, researchers have relied on informed guesses to guide their choice of offspring distribution.

In this work we propose two methods to estimate the offspring distribution from real sampled data. Our goal is to accurately estimate the offspring distribution by sampling and collecting ancestors ids of a small fraction of the agents. We study the case where a sampled agent reveals the identity of its ancestors and the trees are generated in the supercritical regime (i.e., average offspring > 1), assuming that the maximum offspring number is upperbounded by a (possibly large) constant and that tree has spanned over a finite number of generations and hence, is finite.

We show that accurate offspring distribution estimates can be obtained by sampling as little as 14% of the population. The first estimation method we propose consists of the exact computation of the likelihood function, whereas the second approximates this function via Metropolis–Hastings with importance sampling.

A related problem is characterizing graphs using traceroute sampling. Traceroute sampling from a single source can be thought as sampling a tree where nodes have different offspring (degree) distributions depending on their position with respect to the source. This is an important well known hard problem [1, 4] and it remains open to date. Our results have the added benefit of shedding some light also into the traceroute problem.

The outline of this work is as follows. Section 2 describes the network and sampling models. In Section 3 we first show how to estimate the offspring distribution through exact inference, showing it does not scale. We then propose an Markov Chain Monte Carlo (MCMC) method of performing approximate inference that works for small and medium sized trees (up to 2,000 nodes). In Section 4 we evaluate both methods using a set of 900 synthetic datasets, comprising small and medium trees. For small trees, exact inference yielded accurate estimates and outperforms the approximate estimator. On the other hand, approximate inference can handle larger trees, while obtaining significant improvement over more naïve approaches. Finally Section 5 presents our conclusions and future work.

2. MODEL

We assume that the underlying tree comes from a Galton-Watson (GW) process. The GW process models the growth of a population of individuals that evolves in discrete-time ($n = 0, 1, 2, \dots$)

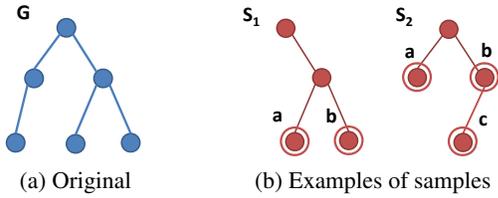


Figure 1: (a) Branching process tree. (b) Samples with 2 and 3 targets, respectively.

as follows. The population starts with one individual at the 0-th generation ($n = 0$). Each individual i at the n -th generation produces a random number $Y_i^{(n)}$ of individuals at the $(n + 1)$ st generation, called offspring. The offspring counts of all individuals are assumed to be i.i.d. random variables. An instance of the GW process is therefore described by a sequence of integers $\{X_n\}$ which denotes the number of individuals at each generation.

Formally, the GW branching process is a discrete-time Markov Chain $\{X_n\}_{n=1}^L$, where L is the number of generations, given by the following recursion

$$X_{n+1} = \sum_{i=1}^{X_n} Y_i^{(n)},$$

with $X_0 = 1$, where the $Y_i^{(n)} \geq 0$ are i.i.d. random variables with multinomial distribution $\theta = (\theta_0, \dots, \theta_W)$, $\forall i \geq 1, n \geq 0$, where W is the maximum number of offspring of an agent. The GW process can be seen as a generative process of a tree $G = (V, E)$, where X_n is the number of nodes at the n th generation and $Y_i^{(n)}$ is the offspring count of the i th node at the n th generation. For simplicity, we assume that $\theta_0 = 0$ and that the number of generations is fixed, so that all tree leaves sit exactly at generation L . Assuming finite L is a better mapping to real populations, which have grown over a finite period of time. On the other hand, our results can be easily adapted to the case where $\theta_0 > 0$ and the leaves are located at different levels.

Since the numbers of offspring are mutually independent, the probability of a given tree G is

$$P(G|\theta) = \prod_{j=1}^W \theta_j^{c_j(G)}, \quad (1)$$

where $c_j(G) = \sum_{i,n} \mathbf{1}\{Y_i^{(n)} = j\}$ is the number of nodes with offspring count j . Fig. 1a depicts an example of tree generated from $\theta = (0.3, 0.6, 0.1)$ with $L = 2$. In this case, $P(G|\theta) = 0.3^1 \cdot 0.6^2 = 0.108$.

Sampling Model

A node is said to be *observed* when the sampling process explicitly reveals its presence in the original graph (e.g. node look up is performed or node spontaneously advertise its presence). The *observed path*, however, consists of the observed node and its path to the root. A *sample* is a set of observed paths.

Let V be the set of nodes of the unlabeled graph G and $V' \subset V$ a set of randomly observed nodes. Let S be the sampled tree formed by the union of the paths from all nodes $v \in V'$ to the root of G . For instance, Fig. 1b shows sampled trees S_1 formed by $V' = \{a, b\}$ and S_2 formed by $V' = \{a, b, c\}$. We assume that nodes in V' are sampled from V with probability p . Although p may be unknown in some settings, it can be approximated as

$|V'|/|V''|$ from any subset of nodes V'' obtained via another independent sampling process.

We now show how to compute $P(S|G)$, assuming that V' is known, i.e., we know which nodes in S are observed. However, it is easy to modify the following analysis to the cases where (1) we only know $|V'|$ or (2) we know the topology of S , but not which or how many nodes are observed. Let $C_{G,S}$ be the number of ways in which S can be mapped onto G . Clearly, $C_{G,S} = 0$ if S is not a subgraph of G . Conditioning on a given mapping, we must have exactly $|V'|$ nodes chosen as targets and $|V| - |V'|$ not chosen as so. Therefore,

$$P(S|G) = C_{G,S} \cdot p^{|V'|} \cdot (1-p)^{|V|-|V'|}. \quad (2)$$

Consider an arbitrary ordering of the subtrees connected to the root of a tree, whether it is G or S . Orderings of G and S do not need to have any correspondence. Computing $C_{G,S}$ can be done recursively by first computing c_{ij} , the number of ways the i -th subtree connected to the root of S can be mapped to the j -th subtree connected to the root of G , for all i, j . For instance, in Fig. 1, the second subtree of S_2 can be mapped to the first subtree of G in a unique way, but in two different ways to the second subtree of G . Now consider the matrix $\mathbf{C} = [c_{ij}]_{n \times m}$. If we define the operator

$$|\mathbf{C}_{n \times m}| = \begin{cases} \sum_{j=1}^m c_{1j} |\mathbf{C}_{1j}|, & n \geq 1 \\ \sum_{j=1}^m c_{1j}, & n = 1, \end{cases} \quad (3)$$

where \mathbf{C}_{1j} is \mathbf{C} after removal of the 1st row and j th column, then we can show that $C_{G,S} = |\mathbf{C}|$. In the simple case of G and S_2 shown in Fig. 1b, we have $\mathbf{C} = \begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix}$ and hence, $|\mathbf{C}| = 1 \cdot 1 + 1 \cdot 2 = 3$. We can visually check that this is indeed the number of ways to map S_2 onto G . Therefore, $P(S_2|G) = 3p^3(1-p)^3$.

Inference on the structure of the tree G from the partial observation S is possible because we can compute $P(S|G')$ for any G' . This, in turn, allows us to do inference on the offspring distribution by considering how likely G' is to be generated from θ by using $P(G'|\theta)$ and weighting by how likely S is to be sampled given G' . In the next section we propose two estimation methods based on this idea.

3. ESTIMATORS

We consider the problem of estimating the offspring distribution θ of the GW process that generates a tree G given a sample S consisting of the union of random observed paths when nodes are observed with probability p .

Two approaches to this problem based on Maximum Likelihood Estimation are proposed in this paper. While the former consists of the exact computation of the likelihood function $P(S|\theta)$, the latter approximates this function via Metropolis-Hastings with importance sampling.

3.1 Exact inference

The graphical model in Fig. 2 depicts the statistical relationship between S , θ and G . The shaded node, S , is the only observable variable, while the white nodes, θ and G are unobservable. This figure shows that to find the relationship between S and θ , we have to sum over the variable G , i.e., over all possible trees given the number of generations L and the maximum degree W . Let $\mathcal{G}_{L,W}$



Figure 2: Graphical model representing network generation and sampling. White nodes are unobservable and shaded node is observable.

Table 1: Growth of the space of trees as a function of L , for $W = 3$.

L	1	2	3	4	5
$ \mathcal{G}_{L,3} \approx$	3	39	6×10^4	2.3×10^{14}	1.2×10^{43}
$ \mathcal{G}_{L,3}^{\text{non-iso}} \approx$	3	19	1.5×10^3	6.1×10^8	3.8×10^{25}

be the set of all possible trees given L and W . It follows that

$$\begin{aligned}
P(S|\theta) &= \sum_{G \in \mathcal{G}_{L,W}} P(S, G|\theta) \\
&= \sum_{G \in \mathcal{G}_{L,W}} P(S|G, \theta) P(G|\theta) \\
&= \sum_{G \in \mathcal{G}_{L,W}} P(S|G) P(G|\theta), \quad (4)
\end{aligned}$$

where from line 2 to line 3 we use the fact that S is conditionally independent on θ given G (see Fig. 2). However, $|\mathcal{G}_{L,W}|$ grows exponentially both in L and W , which limits this approach to very small trees. In fact, we can show that

$$|\mathcal{G}_{L,W}| = \begin{cases} W, & L = 1 \\ \sum_{i=1}^W |\mathcal{G}_{L-1,W}|^i > |\mathcal{G}_{L-1,W}|^W, & L > 1. \end{cases}$$

Solving the recursion yields $\log^{(L-1)} |\mathcal{G}_{L,W}| = O(W)$, where $\log^{(\cdot)}$ is the repeated logarithm. Note however that isomorphic trees are being counted more than once. Therefore, we can reduce the computational cost by counting only non-isomorphic trees (appropriately weighted by their multiplicity).

Let $\mathcal{G}_{L,W}^{\text{non-iso}}$ be the set of non-isomorphic trees of $\mathcal{G}_{L,W}$. It is possible to show that

$$|\mathcal{G}_{L,W}^{\text{non-iso}}| = \begin{cases} W, & L = 1 \\ \frac{(W+1)^{\binom{W+|\mathcal{G}_{L-1,W}^{\text{non-iso}}}{W+1}}}{|\mathcal{G}_{L-1,W}^{\text{non-iso}}|} - 1, & L > 1. \end{cases}$$

Table 3.1 illustrates some values of $|\mathcal{G}_{L,W}|$ and $|\mathcal{G}_{L,W}^{\text{non-iso}}|$ for $W = 3$ and $L = 1, \dots, 5$. As we can see, counting only non-isomorphic trees reduces significantly the state space, but it is still not feasible to compute eq. (4) except for rather small numbers such as $W = 3$ and $L = 4$. Nevertheless, we utilize this approach to perform inference more efficiently. In the following, we explain how to enumerate trees in $\mathcal{G}_{L,W}^{\text{non-iso}}$ and how to compute their multiplicities.

Counting only non-isomorphic trees

Once again consider the tree in Fig. 1a. Despite of the fact that by swapping the two subtrees directly connected to the root of G we obtain another tree G' , both G and G' contribute with the same amount to (4) since they are isomorphic and hence, $P(S|G) = P(S|G')$ and $P(G|\theta) = P(G'|\theta)$. Ideally, we would like to avoid generating isomorphic trees when enumerating $G \in \mathcal{G}_{L,W}$ in the computation of $P(S|\theta)$.

A straightforward way to enumerate all trees in $\mathcal{G}_{L,W}^{\text{non-iso}}$ is: (1) to enumerate non-isomorphic trees in $\mathcal{G}_{L-1,W}^{\text{non-iso}}$ and assign a numeric id to each of them; and (2) construct trees in $\mathcal{G}_{L,W}^{\text{non-iso}}$ by attaching to a root node trees from $\mathcal{G}_{L-1,W}^{\text{non-iso}}$ where ids are in non-increasing order. Note that two trees are isomorphic in this construction if the sets of ids of the subtrees connected to the root node are permutations of each other, which cannot occur due to the ordering.

In what follows we compute the probability that sample S is observed given the offspring distribution θ through the enumeration of non-isomorphic trees. Let $m_i^{(L)}$ be the multiplicity of the i -th tree, say G_i , in the labeled space $\mathcal{G}_{L,W}^{\text{non-iso}}$. Eq. (4) is equivalent to

$$P(S|\theta) = \sum_{G_i \in \mathcal{G}_{L,W}^{\text{non-iso}}} m_i^{(L)} P(S|G_i) P(G_i|\theta). \quad (5)$$

The multiplicity $m_i^{(L)}$ can be calculated from the ids of subtrees directly connected to the root node in G_i and their multiplicities. More precisely, $m_i^{(L)}$ is simply the number of permutations of the ids multiplied by the product of the multiplicities of each subtree. For instance, if there are j subtrees connected to the root with distinct ids $(1, \dots, j)$, then $m_i^{(L)} = j! \times \prod_{k=1}^j m_{(k)}^{(L-1)}$. In the general case, where ids can appear more than once, we have

$$m_i^{(L)} = \frac{j! \times \prod_{k=1}^j m_{(k)}^{(L-1)}}{\prod_{id=1}^{|\mathcal{G}_{L-1,W}^{\text{non-iso}}|} \left(\sum_{k=1}^j \mathbf{1}\{id = k\} \right)!}$$

The first estimator we propose is

$$\hat{\theta}_{\text{Exact}} = \arg \max_{\theta} P(S|\theta), \quad (6)$$

where $P(S|\theta)$ is computed as in (5).

Maximum Likelihood Estimation

After obtaining a sample, we write the summation in Eq. (5) as a function of θ , say $\mathcal{L}(\theta) = P(S|\theta)$. Unfortunately, this likelihood function is a sum of a potentially enormous number of terms and using the log-likelihood is not helpful in this case. We apply several tricks to solve this optimization task.

One simple trick to reduce the number of terms consists of grouping together trees that have the same configuration in terms of offspring counts, i.e., that account for the same $P(G|\theta)$. Note that there are many such trees even when considering non-isomorphic trees only, although they correspond to different values of $P(S|G)$.

Also note that this is a constrained maximization problem. Since θ is a probability distribution, $0 \leq \theta_i \leq 1$ for $i \in \{1, \dots, W\}$ and $\sum_{i=1}^W \theta_i = 1$. We can turn it into a non-constrained maximization problem by replacing $\theta_i = \frac{e^{\alpha_i}}{Z}$ for $i \in \{1, \dots, W\}$ where $Z = \sum_{i=1}^W e^{\alpha_i}$, setting $\alpha_W = 1$ (for regularization purposes) and then maximizing w.r.t. α . Note that α_i can now assume any value in \mathbb{R} for $i \in \{1, \dots, W-1\}$. Nevertheless, one must be careful when using this parameter transformation since the products of the exponentials can quickly lead to overflows. Therefore, we use log representation and the *logsumexp* trick.

After this transformation, the maximization problem becomes

$$\arg \max_{\alpha} \mathcal{L}(\alpha) = \sum_j c_j \frac{e^{\sum_{i=1}^W x_{ji} \alpha_i}}{Z^{y_j}}$$

where c_j is the sum of the coefficients of the terms corresponding to the same j -th configuration of $P(G|\theta)$, x_{ji} is the number of nodes with offspring i in the j -th configuration and $y_j = \sum_{i=1}^W x_{ji}$. In

order to compute the likelihood function and its gradient more efficiently, we express them in matrix notation as

$$\mathcal{L}(\alpha) = \mathbf{c}^T \cdot (\exp(\mathbf{X}\alpha)/Z^{\mathbf{y}})$$

$$\nabla \mathcal{L}(\alpha) = \exp(\mathbf{X}\alpha)/Z^{\mathbf{y}} - \exp(\mathbf{X}\alpha)/Z^{\mathbf{y}+1}$$

where $\mathbf{c} = [c_j]$, $\mathbf{X} = [x_{ji}]$, $\alpha = [\alpha_i]$, $\mathbf{y} = [y_j]$, $Z^{\mathbf{y}} = [Z^{y_j}]$, the “/” symbol corresponds to division of two vectors element-wise and $\mathbf{1}$ is a column vector with all entries equal to 1.

The maximization then goes as follows. We sample 10,000 points uniformly from \mathbb{R}^{W-1} . The one with the maximum value of $l(\cdot)$ will be $\alpha^{(0)}$, the starting point to be used with the BFGS¹ (limited to 100 iterations, relative convergence tolerance of 10^{-8} , step size 10^{-3}). The estimate $\hat{\theta}$ can be obtained from $\hat{\alpha}$ by exponentiating and then normalizing the latter.

3.2 Approximate inference with MCMC

The previous approach only applies to small problems due to the enormous number of terms in the summation (5). To solve larger problems, we approximate eq. (4) using MCMC.

Let $h = P(S|G)$ and $f(G) = P(G|\theta)$. Since $f(G)$ defines a probability distribution on the space $\mathcal{G}_{L,W}$, it follows that

$$P(S|\theta) = \sum_G h f(G) = E_f[h]. \quad (7)$$

where $E_f[\cdot]$ denotes expectation w.r.t. distribution f .

Monte Carlo simulation approximates expectations (integrals, more generally) by sampling from a desired distribution f [2]. The problem here is that we cannot sample from f because we don't know θ . However, we can sample from some other distribution g and compensate for the fact that in g some trees are more (or less) likely to appear than in f by using importance sampling. More precisely,

$$P(S|\theta) = \sum_G h f(G) = \sum_G h \frac{f(G)}{g(G)} g(G) = E_g \left[h \frac{f(G)}{g(G)} \right]. \quad (8)$$

Recall from Section 2 that we can generate trees using the GW process from a given offspring distribution θ_0 . Hence we can set

$$g(G) = \frac{1}{\mathcal{Z}} P(S|G) P(G|\theta_0), \quad (9)$$

where \mathcal{Z} is a normalizing constant². Substituting eq. (9) into (8) yields

$$P(S|\theta) = E_g \left[\frac{P(S|G) P(G|\theta)}{\frac{1}{\mathcal{Z}} P(S|G) P(G|\theta_0)} \right] \approx \frac{\mathcal{Z}}{m} \sum_{i=1}^m \frac{P(G_i|\theta)}{P(G_i|\theta_0)},$$

where $G_i \sim g(G)$. Note that $\frac{\mathcal{Z}}{m}$ is not a function of θ and do not need to be considered when maximizing θ . Therefore, the second estimator we propose is

$$\hat{\theta}_{\text{Approximate}} = \arg \max_{\theta} \sum_{i=1}^m \frac{P(G_i|\theta)}{P(G_i|\theta_0)}. \quad (10)$$

In order to draw $G_i \sim g(G)$, we use the Metropolis-Hastings algorithm where each state X_j of the Markov Chain is a tree. We start the chain in a state X_0 consistent with S , in particular, we set $X_0 = S$. The transition kernel $X_i \rightarrow X_{i+1}$ we use is shown in Algorithm 1. The new tree X_{i+1} is accepted with probability

¹We use R implementation in package **stats**.

²We could have set $g(G) = P(G|\theta_0)$ instead, but our approach restrict us to generating trees that are consistent with the sample and thus, is more efficient.

Algorithm 1 Transition Kernel(X_i, X_{i+1})

```

v ← internal node selected uniformly at random from Xi
dv ← degree(v)
if dv = 1 then
  action ← add
else if dv = W then
  action ← remove
else
  if U(0, 1) < 0.5 then
    action ← add
  else
    action ← remove
  end if
end if
if action = add then
  Tv ← GaltonWatson(θ0, L - l)
  v.child[dv + 1] ← Tv
  dv ← dv + 1
else if action = remove then
  shuffle(v.child)
  v.child[dv] ← nil
  dv ← dv - 1
end if

```

$$r = \min \left(1, \frac{P(S|X_{i+1})P(X_{i+1}|\theta_0)q(X_{i+1} \rightarrow X_i)}{P(S|X_i)P(X_i|\theta_0)q(X_i \rightarrow X_{i+1})} \right). \quad (11)$$

where $q(X_i \rightarrow X_j)$ is the probability that the transition kernel proposes transition $X_i \rightarrow X_j$. It is easy to include the calculation of $q(X_i \rightarrow X_{i+1})$ and $q(X_{i+1} \rightarrow X_i)$ in the transition kernel implementation. In particular, let N_i and L_i denote the number of nodes and leaves in X_i , respectively. Hence, if $action = add$,

$$q(X_i \rightarrow X_{i+1}) = \frac{0.5^{\mathbf{1}\{d_v > 1\}} \times P(T_v|\theta_0)}{N_i - L_i - 1},$$

$$q(X_{i+1} \rightarrow X_i) = \frac{0.5^{\mathbf{1}\{d_v + 1 < W\}} (d_v + 1)^{-1}}{N_{i+1} - L_{i+1} - 1},$$

otherwise,

$$q(X_i \rightarrow X_{i+1}) = \frac{0.5^{\mathbf{1}\{d_v < W\}} d_v^{-1}}{N_i - L_i - 1},$$

$$q(X_{i+1} \rightarrow X_i) = \frac{0.5^{\mathbf{1}\{d_v - 1 > 1\}} \times P(T_v|\theta_0)}{N_{i+1} - L_{i+1} - 1},$$

where $0.5^{\mathbf{1}\{d_v > 1\}}$ accounts for the fact that if v has degree > 1 , action *add* is chosen with probability 0.5, but when $d_v = 1$, *add* is always chosen. The case for *remove* is similar³.

Maximum Likelihood Estimation

After obtaining roughly independent samples $G_i \sim g(G)$, we write the summation in the RHS of eq. (8) and perform maximization as in the case of exact inference.

4. EXPERIMENTS AND RESULTS

We first describe the experiments used to assess the performance of the two estimation methods, henceforth referred to as EXACT and APPROXIMATE, respectively. We then compare methods w.r.t. the distance between the estimated distribution and θ using the Kullback-Leibler (KL) divergence, which is a widely used way to measure distance between distributions. In addition, we show

³All calculations should be performed in log space.

some results in detail to illustrate the Mean Squared Error (MSE) per distribution parameter and how performance increases with the sampling probability. In general, EXACT performs best but is only feasible for small datasets. Nevertheless, APPROXIMATE exhibits comparable performance and can cope with larger datasets (up to 2,000 nodes).

4.1 Experiments description

Based on the size of $\mathcal{G}_{L,W}$, we define two classes of estimation problems: small and medium size problems. For medium size ones, we would like to compare the methods' performance for short and long tail offspring distributions, hereby represented by truncated⁴ Poisson and Zipf distributions, respectively. Parameters of these distributions were chosen so that their average is \bar{d} .

In what concerns the sampling process, we choose three sampling probabilities representing low, medium and high sampling rates for each class. The set of values of p has to be different for each class for two reasons. The practical reason is that as the tree size grows, the cost to sample it grows linearly on p and we may be limited by a budget. The second reason is that, if there is no such constraint, while values of p such as 0.5 are reasonable for small problems, they will likely reveal all nodes from the top levels for large problems. Hence, taking the empirical distribution from the first levels per se would be an accurate estimator. Inside each class, consider the following distributions and sampling probabilities:

1. Small size: $W = 3, L = 3, \bar{d} = 2.1$
 - $\theta^{(1)} = (0.2, 0.5, 0.3)$
 - $p \in \{0.1, 0.2, 0.5\}$
2. Medium size: $W = 10, L = 5, \bar{d} = 3.15$
 - $\theta^{(2)} \sim \text{truncated Poisson}(\lambda = 3)$
 - $\theta^{(3)} \sim \text{Zipf}(\alpha = 1.132, N = 10)$
 - $p \in \{0.5, 1.0, 5.0\} \times 10^{-2}$

Average tree sizes per class are ≈ 17 and ≈ 454 , respectively.

In order to test the inference methods, we build a set of estimation problems as follows. For each distribution $\theta^{(i)}$, $i = 1, \dots, 3$, we generate 10 trees t_{ij} , $j = 1, \dots, 10$ from a GW process with height $L + 1$ (30 trees in total). Next, for each of the 90 pairs (t_{ij}, p_{ik}) , $k = 1, 2, 3$, we generate 10 samples s_{ijkl} , $l = 1, \dots, 10$ (900 samples in total).

We assume each sample s_{ijkl} constitutes a separate estimation problem (also referred to as *dataset* to avoid confusion with MCMC samples). This can be interpreted as if we had one tree (originated from the GW process), and a single opportunity to sample it. No other samples can be obtained from the same tree, nor other trees are available for sampling. Ideally, we would like to try both methods with each problem, but EXACT is only feasible for small problems. Before presenting the results, we briefly discuss implementation issues related to APPROXIMATE.

4.2 Implementation issues of APPROXIMATE

The main difficulty in the APPROXIMATE method is knowing when to stop the approximation as, without knowing the true distribution, we need a mechanism that tells us how close we are to the steady state distribution of the Markov chain.

Recall that we use the Metropolis Hastings (MH) algorithm to sample graphs from $g(G)$ (see Eq. (8)). As with any MCMC method,

⁴Here truncated means that we took the original probability mass function for values between 1 and W and normalized by their sum, while setting the probability mass of other values to zero.

three questions must be addressed: (1) How long should the burn-in period be? (2) What should the thinning ratio be? (3) What is the minimum number of uncorrelated samples that we need? We use the Raftery-Lewis (RL) Diagnostic [7] to address these issues⁵.

The RL Diagnostic attempts to determine the necessary conditions to estimate a quantile q of the measure of interest, within a tolerance r with probability s . We take the likelihood of the MH samples as the measure of interest. The diagnostic was then applied individually to each dataset with default parameters ($q = 0.025$, $r = 0.005$ and $s = 0.95$). Results concerning the burn-in period and thinning ratio are subsumed by the required number of samples and hence will be omitted. The minimum number of MCMC samples for small datasets was less than 50,000 graphs and for medium datasets, less than 500,000, in summary. We conducted some experiments with more MCMC samples than those values, but there was no significant improvement w.r.t. the estimation accuracy. Therefore, the results described in the following refer to the minimum number of samples suggested by the Raftery-Lewis test.

Last, recall from Section 3.2 that θ_0 can be any distribution. However, the closer it is to θ , the better is the convergence of the MCMC. When estimating the offspring distribution in medium size problems, we will assume that θ_0 is binomial and set its parameters so that the average is \bar{d} . This implies assuming that the average number of offspring can be estimated, but in fact a rough estimate can be obtained by simply taking the average of the observed node degrees from the first generations in the sample, whose edges have a relatively high probability of being sampled. For small sized tree, we simply set θ_0 to be uniform.

4.3 Results

The estimation results span over a number of dimensions equal to the number of parameters assumed in the multinomial distribution. We use the Kullback-Leibler (KL) divergence as an objective criterion to compare the estimation methods in a single dimension.

Let the estimated offspring distribution be $\hat{\theta} = (\hat{\theta}_1, \dots, \hat{\theta}_W)$. The KL-divergence of $\hat{\theta}$ from θ is defined by

$$D_{\text{KL}}(\theta || \hat{\theta}) = \sum_{i=1}^W (\log \theta_i - \log \hat{\theta}_i) \theta_i, \quad (12)$$

when $\hat{\theta}_i > 0$, $i = 1, \dots, W$. When this condition does not always hold, as in our case, absolute discounting is frequently used to smooth $\hat{\theta}$. Hence, we distribute $\epsilon = 10^{-7}$ of probability mass among the zero estimates, discounting this value equally from the non-zero estimates.

Table 2 shows the median KL-divergence obtained for each set of problems (indexed by $\theta^{(i)}$, $i = 1, \dots, 3$), for EXACT and APPROXIMATE, when the sampling probability p is medium. Dashes

	$\theta^{(1)}$	$\theta^{(2)}$	$\theta^{(3)}$
EXACT	1.86	-	-
APPROXIMATE	2.98	0.58	0.78

Table 2: Median KL-divergence of estimators

indicate that EXACT could not find estimates for medium size problems in a reasonable amount of time. However, it outperformed APPROXIMATE in the estimation of $\theta^{(1)}$. Note that although KL-divergence implies some ordering within each column in terms of accuracy, neither the relative ratios have a direct interpretation,

⁵We use the R implementation in package `coda`.

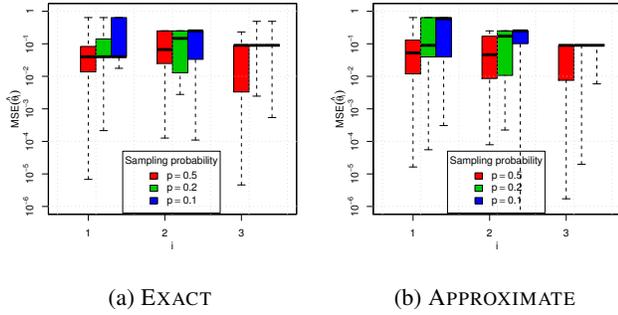


Figure 3: Boxplots of the MSE per parameter for $\theta^{(1)}$.

nor values across different columns can be compared. We will next evaluate the results w.r.t. the MSE of each parameter estimate, which will allow us to conclude that the performance of APPROXIMATE is in fact very close to the one of EXACT for small datasets.

The effect of the sampling probability p

As we increase p , we gather more information about the original graph and hence estimators will clearly perform better. We study the performance gains w.r.t. the MSE of the parameter estimates.

Figs. 3(a-b) show boxplots of the MSE of the estimates $\hat{\theta}_i$, $i = 1, \dots, W$ obtained by EXACT and APPROXIMATE, respectively, for datasets coming from $\theta^{(1)}$. Each boxplot shows minimum, 1st quartile, median, 3rd quartile and maximum values, computed over 100 estimates (10 samples for each of the 10 trees). Colors correspond to different sampling probabilities. In both cases, the median MSE increases as we decrease p , as expected.

Similarly, Fig. 4 shows the results obtained by APPROXIMATE for datasets that come from $\theta^{(2)}$. In general, increasing the sampling probability reduces the MSE, but not by a significant amount. Results for $\theta^{(3)}$ are similar and will be omitted.

We conjecture that most of the information that allows us to estimate θ comes from the top levels of the tree. As we increase p , we obtain many more observations from the bottom levels of the tree, but only a few new observations from the top levels. While edges closer to the root are observed with higher probability, edges from lower levels are more rarely sampled and there is much more uncertainty in those samples. This implies that increasing p should not improve the estimates significantly after a certain point.

This short digression might lead the reader wonder whether the values of p we use would sample so many edges from the top levels that would be enough to take the empirical distribution of the observed degrees at those levels as an estimate for θ . To show that this is not the case, we compare the MSE results for APPROXIMATE with the empirical distribution of the observed degrees from the top 1, 2 and 3 levels in a cumulative fashion. Intuitively, the empirical distribution is biased towards smaller degrees, especially if lower levels are taken into account, this being the reason why we stop at three levels. For instance, regarding datasets that come from $\theta^{(2)}$ when the sampling probability is small ($p = 5 \times 10^{-3}$), the fraction of sampled edges at the top three levels is 100%, 60% and 33%, respectively (relative to the number of edges from the root to those levels). Considering the entire trees, the average fraction of sampled edges is 2.3%. On the other hand, when the sampling probability is large ($p = 5 \times 10^{-2}$), the top three levels include re-

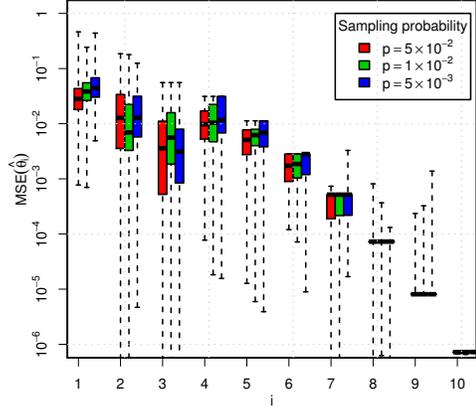


Figure 4: Boxplots of the MSE of APPROXIMATE for $\theta^{(2)}$.

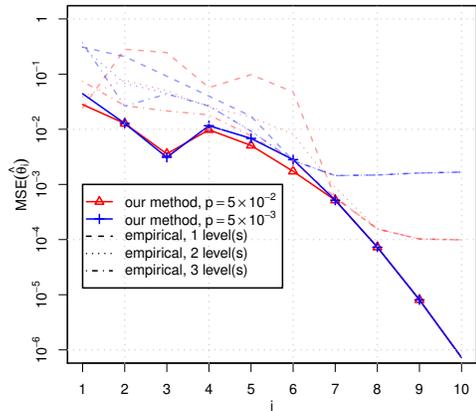


Figure 5: Median MSE of APPROXIMATE and empirical estimates for $\theta^{(2)}$.

spectively 100%, 97% and 85% of the total number of edges from the root to those levels. In this case, the overall average is 13.51%.

Fig. 5 shows the median values of the MSE (also seen in the previous figure), but only for “small” and “large” p values, for the sake of clarity. In addition, dashed lines display the median MSE obtained when the empirical distributions are used as estimators. Estimates for $p = 5 \times 10^{-3}$ exhibit a one-order magnitude gain in accuracy (for most parameters) relative to the best empirical estimate, but estimates for $p = 5 \times 10^{-2}$ only yield significant improvements at the tail of the distribution. In general, empirical distributions are not good estimates, especially for distribution tails due to its bias towards small degrees. One exception we found was in the case of $\theta^{(3)}$, where the probability mass at the tail is so large that high degree nodes are likely to be observed at the top levels. However, we observed in additional experiments that this is not the case for long tailed distributions with larger support, such as $W = 100$.

5. CONCLUSIONS

In this paper we propose and analyze two methods to estimate the offspring distribution of a branching process from a sample of random observed paths to the root. The former, based on exact inference, is limited to small problems since the number of terms to be computed in the likelihood function grows exponentially with the maximum degree and number of levels. The latter approximates the likelihood function using MCMC samples, and was able to handle both small and medium size problems. For small problems, its performance was similar to that of exact inference.

Finally, our experiments suggest that most of the information about the offspring distribution contained in the sample comes from the top levels, where nodes are observed with higher probability. This suggests the possibility of designing estimators for the degree distribution of a network sampled via traceroute from a single source where observations from top levels are given more weight. In particular, estimates from different levels could be combined with weights inversely proportional to their variances.

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7. REFERENCES

- [1] D. Achlioptas, A. Clauset, D. Kempe, and C. Moore. On the bias of traceroute sampling: Or, power-law degree distributions in regular graphs. *J. ACM*, 56(4):21:1–21:28, July 2009.
- [2] P. Beerli and J. Felsenstein. Maximum-Likelihood Estimation of Migration Rates and Effective Population Numbers in Two Populations Using a Coalescent Approach. *Genetics*, 152(2):763–773, June 1999.
- [3] F. Chierichetti, J. Kleinberg, and D. Liben-Nowell. Reconstructing patterns of information diffusion from incomplete observations. In *NIPS'11*, pages 792–800, 2011.
- [4] A. Lakhina, J.W. Byers, M. Crovella, and P. Xie. Sampling biases in ip topology measurements. In *INFOCOM 2003*, volume 1, pages 332 – 341 vol.1, march-3 april 2003.
- [5] A. Neves and C. Moreira. Applications of the galton-watson process to human dna evolution and demography. *Physica A*, 368(1):132 – 146, 2006.
- [6] R. Pastor-Satorras and A. Vespignani. *Evolution and Structure of the Internet: A Statistical Physics Approach*. Cambridge University Press, New York, NY, USA, 2004.
- [7] A. Raftery and S. Lewis. The number of iterations, convergence diagnostics and generic Metropolis algorithms. In *In Practical Markov Chain Monte Carlo (W.R. Gilks, D.J. Spiegelhalter and S. Richardson, eds.)*, pages 115–130, 1995.
- [8] X. Yang and G. de Veciana. Service capacity of peer to peer networks. In *INFOCOM*, pages 2242–2252 vol.4, march 2004.