Recovering the past states of growing trees

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In principle one can reconstruct the past states of a growing network from only its current state. In practice, however, the extent to which this can be done is severely limited since existing methods are either inexact, inefficient, or both. Here we present methods for temporal reconstruction that are both exact and efficient on trees. We derive analytic expressions for the number of possible histories in which each node arrived at each time, and we present a Monte Carlo method to sample full histories in \(O(n \log \log n)\) operations for networks with \(n\) nodes. We demonstrate the use of these methods with a series of applications: seed finding, network interpolation, full history reconstruction, and model fitting. With these new tools one can directly fit growth models such as preferential attachment to static network data—testing models directly at the level of mechanism with only a single network snapshot.

A detailed description of the history of a complex network is highly informative. For example, epidemic forecasting [1], structural inference [2] or growth modeling [3] all benefit from complete temporal descriptions. Unfortunately, such complete descriptions are often unavailable [4].

In some cases the temporal descriptions will be missing because the information cannot be directly observed—for instance the networks of ancient civilizations [5] or present day biological networks that have undergone evolution [6, 7]—but limitations in our temporal knowledge also arise for other reasons. Examples include ecosystems that cannot be sampled in real time [8], or large scale networks where full temporal descriptions are too costly to track [9].

Realizing that temporal descriptions are useful but rarely available leads to the problem of temporal reconstruction. Can we infer the past states of a network from a few static snapshots? Or, perhaps harder still: can we infer the past states of a network from only its final state? Recent research shows that when a network is generated by a growth model, reconstruction is indeed often possible [10–18].

Existing methods that tackle the problem fall into three categories. First, and simplest, are the methods that exploit correlations between the age of nodes and their properties (degree, centrality, etc.) [11, 18]. Second, and more sophisticated, are methods that use combinatorial techniques to identify the initial graph or seed, a form of partial temporal reconstruction [12, 13]. And third, there are Monte Carlo methods that rely on indirect sampling to reconstruct the complete history of statically observed networks [14–18]. All of these approaches achieve some form of temporal reconstruction, but they are also all imperfect: inferences based on correlations are imprecise [18], the combinatorial methods do not yield complete reconstructions, and indirect sampling is not scalable [17, 18]. Our own methods, introduced below, address all of these problems simultaneously for the case of trees.

We consider growth models—models in which one node arrives at each discrete time step and attaches itself to the extant graph with an edge. The history of a graph is the sequence of sub-graphs that describe its state at each previous time. Our goal is to make rigorous inferences about these past states given only partial information, such as the final state of the graph.

A large number of different possible histories are typically consistent with the final state of a network. Our analytic calculations will directly compute averages within the set of all consistent histories. Effectively, our calculations assume a uniform distribution over all possible histories and in this sense they are model agnostic. However, two of the most well established growth models—uniform and preferential attachment—both entail an exactly uniform posterior distribution over consistent histories [18, 19] and so our calculations also correspond to exact computations in the posterior distributions of these models. For more complicated models with non-uniform distributions our Monte Carlo method can be applied using standard reweighting techniques.

So, how do we tackle temporal reconstruction? Naturally we start at the beginning and determine which node appeared first. If most of the possible histories put, for example, node \(i\) first, then it is likely that node \(i\) was first in the true history. Our first goal then will be to compute \(p_i\), the proportion of possible histories in which node \(i\) appeared first. As it turns out, there is already an algorithm that computes \(p_i\), although it was introduced for a different purpose [10]. The algorithm proceeds as follows.

Suppose we have a tree, \(G\), with \(n\) nodes. First, arbitrarily root \(G\) at any node. For simplicity, pick node 0 to obtain the rooted tree \(G_0\)—a directed graph with the same edges as \(G\) but with each edge directed to point away from node 0. Next, for each directed edge \(i \rightarrow j\) in...
which completes the calculation. Computed for all edges in linear time using recursion.

of the procedure alone it is not immediately obvious why

\[ h_i = (n-1)! \prod_{j} \frac{h_{i \rightarrow j}}{n_{i \rightarrow j}}! \]  

where the product is over children of \( i \).

The quantity \( h_{i \rightarrow j} \) can be computed in the same manner, but in the sub-tree with node \( j \) as its root,

\[ h_{i \rightarrow j} = (n_{i \rightarrow j} - 1)! \prod_{j} \frac{h_{j \rightarrow k}}{n_{j \rightarrow k}}! \]  

where the product is now over children of \( j \). Equation (4) defines a set of self-consistent equations that can be solved directly using recursion and then substituted into Eq. (3). However, to find \( p_i \) this is actually unnecessary. If nodes \( i \) and \( j \) are neighbors then from Eqs. (3) and (4)

\[ h_j = h_{i \rightarrow j} h_{j \rightarrow t} \frac{(n-1)!}{(n_{i \rightarrow j} - 1)! n_{i \rightarrow j}!} \]  

and from the equivalent expression for \( h_i \) we see that

\[ \frac{p_j}{p_i} = \frac{h_j}{h_i} = \frac{n_{i \rightarrow j}}{n_{i \rightarrow i} n_{i \rightarrow j}} = \frac{n_{i \rightarrow j}}{n - n_{i \rightarrow j}}. \]  

This completes the proof that Eq. (2) is indeed correct.

This procedure is an important first step but we are a long way from temporal reconstruction—we can currently only predict one step of the history. So, we now derive exact expressions for \( p_i(t) \), the proportion of histories in which node \( i \) arrives at time \( t \), making use of the quantities \( n_{i \rightarrow j} \) and \( h_{i \rightarrow j} \) already defined in Eqs. (1) and (4).

If node \( i \) arrives at time \( t \) then precisely one of its immediate neighbors must have arrived before time \( t \). Suppose, for the sake of argument, that it was node \( j \). We imagine cutting the network in two by severing edge \( i, j \). Let \( g_{i \rightarrow j}(t) \) be the number of histories in the subtree containing \( j \) in which node \( j \) arrives before \( t \). The total number of histories in which \( j \) arrives before \( t \), and \( i \) arrives at exactly \( t \) can again be computed by interlacing each of the \( g_{i \rightarrow j}(t) \) histories with the \( h_{j \rightarrow i} \) histories in the branch containing \( i \). The first \( t + 1 \) steps, however, will be fixed—the first \( t \) must occur in \( j \)'s branch, and the \( (t + 1) \)th is \( i \) itself arriving. Interlacing the remaining steps we see there are \( g_{i \rightarrow j}(t) h_{j \rightarrow i} (n_{i \rightarrow j} - 1) \) histories in which \( j \) arrives before \( t \), and \( i \) at exactly \( t \). To compute \( p_i(t) \) we sum this quantity over all neighbors \( j \),

\[ p_i(t) = \frac{1}{Z} \sum_j g_{i \rightarrow j}(t) h_{j \rightarrow i} \left( \frac{n - t - 1}{n_{i \rightarrow j} - t} \right), \]
where $Z$ is the total number of consistent histories.

Our calculation is currently incomplete since we do not yet know $g_{i\rightarrow j}(t)$, but we are almost there. The number of histories in which node $j$ arrives at exactly time $t$ in its sub-tree is $g_{i\rightarrow j}(t+1) - g_{i\rightarrow j}(t)$. For these histories, we know that exactly one of the neighbors of $j$ (excluding $i$) must have arrived before $t$. Suppose for now that this neighbor is $k$. There are $g_{j\rightarrow k}(t)$ histories where this happens and again, each of these histories will be interlaced with one of $h_{i,k\rightarrow j}$ histories starting at $j$, with $i$ and $k$ both removed. Hence,

$$g_{i\rightarrow j}(t+1) - g_{i\rightarrow j}(t) = \sum_{k \in N_{j} \setminus i} g_{j\rightarrow k}(t)h_{i,k\rightarrow j}\left(\frac{n_{i\rightarrow j} - t - 1}{n_{j\rightarrow k} - t}\right).$$  \hspace{1cm} (8)

where the sum is over the neighbors of $j$ except $i$, and the quantity $h_{i,k\rightarrow j}$ is calculated similarly to Eq. (4),

$$h_{i,k\rightarrow j} = (n_{k\rightarrow j} - 1)! \prod_{l \in N_{j} \setminus i,k} \frac{h_{j\rightarrow l}}{n_{j\rightarrow l}!} = \frac{h_{k\rightarrow j}n_{j\rightarrow i}[(n_{k\rightarrow j} - 1 - n_{j\rightarrow i})]}{h_{j\rightarrow i}(n_{k\rightarrow j} - 1)!}. \hspace{1cm} (9)$$

These expressions only depend on $n_{i\rightarrow j}$ and $h_{i\rightarrow j}$, which as discussed previously are easy to compute. The result is that we now have a complete set of self-consistent equations for $p_{i}(t)$, for all $i$ and $t$.

We solve these equations as follows. First, set $g_{i\rightarrow j}(1) = h_{i\rightarrow j}$. Then, for each $t > 1$ use Eq. (8) to compute $g_{i\rightarrow j}(t+1)$ from $g_{i\rightarrow j}(t)$. Finally, set $p_{i}(0) = p_{i}$ and for each $t > 0$ set $p_{i}(t)$ using Eq. (7). The normalizing factor $Z$ is easily computed by requiring $\sum_{i} p_{i}(t) = 1$. Each iteration of Eq. (8) takes $O(qn)$ time where $q = (\langle k^{2} \rangle - \langle k \rangle)/\langle k \rangle$, the “excess degree”, with $\langle k \rangle$ being the average degree. The total run time is therefore $O(qn^{2})$.

This calculation is exact and reasonably efficient. We are computing $n^{2}$ quantities, and we take $qn^{2}$ time. However, for many purposes all $n^{2}$ values of $p_{i}(t)$ are more than we need. For example, we might simply wish to know the expected arrival times, $\langle t_{i} \rangle = \sum_{t} t p_{i}(t)$.

To complement our analytic method we now introduce an extremely efficient Monte Carlo procedure that samples exactly from the set of histories.

Since we can already compute the seed probability $p_{i}$ in linear time, we need to solve an interpolation problem. Namely, we need to find a method that can generate uniform samples from the set of histories that start at an initial graph $G_{I}$ and end at a final graph $G_{F}$, “bridging” between the two states [17]. Sampling uniformly from histories is then achieved by picking the seed proportional to $p_{i}$ and interpolating between this node and $G$.

For the class of growth processes we are considering all histories progress by attaching one node to the extant graph. As a result, when the graph has $t$ nodes, the next node to arrive must be directly attached to one of these $t$ nodes in the final graph. In other words, the next node must be chosen from the “boundary” set $B_{t}$, the set of all nodes that are not yet in the graph but in the final state are directly connected to one that is.

To generate a complete bridge between $G_{I}$ and $G_{F}$ we can, without loss of generality, root $G_{F}$ at any node in $G_{I}$ and compute $n_{j\rightarrow k}$ in the rooted tree. All nodes (except the root) will have an in-degree of 1 so for simplicity we write $n_{k} = n_{j\rightarrow k}$. Then, at each time we sample a node from the boundary set proportional to $n_{k}$. At time $t$ the probability of adding node $k \in B_{t}$ is

$$\frac{n_{k}}{\sum_{l \in B_{t}} n_{l}}. \hspace{1cm} (10)$$

Noting also that the denominator $\sum_{l \in B_{t}} n_{l}$ is equal to the number of nodes that are not yet in the graph, which is $n - t$, we see that node $k$ is added at time $t$ with probability $n_{k}/(n - t)$. A specific interpolation

$$H = v_{t+1}, v_{t+2}, \ldots, v_{F}$$

is generated with probability

$$P(H) = \prod_{t=t+1}^{F} \frac{n_{v_{t}}}{n - t}, \hspace{1cm} (11)$$

which is independent of $H$, and thus uniform over consistent histories. By using an efficient set sampling algorithm we can both update and sample from $B_{t}$ in $O(\log \log n)$ time [20]. The full procedure is thus close to linear—$O(n \log \log n)$.

Since our methods are efficient we can use them to tackle reconstruction tasks on large trees, opening up many applications. Figure 2 shows the outcome of a number of reconstruction experiments carried out on synthetic data: seed-finding [21], network archaeology [6, 18], network interpolation [4], and kernel inference [3, 22, 23].

Seed-finding (Fig. 2a) is the simplest task, with $p_{i}$ being equal to the proportion of histories in which each node was the seed. For models with uniform posteriors over histories, such as preferential attachment and uniform attachment [18, 19], $p_{i}$ is exactly equal to the posterior probability that node $i$ was the seed. In more complicated models with non-uniform posterior distributions over histories, one can compute the correct seed posterior by sampling uniformly and reweighting these samples by the posterior probabilities.

Network archaeology (Fig. 2b) can be solved along the same lines. In this task the goal is to infer the past state of a graph given only its final state. To summarize all these possible states one can compute the expected arrival times, $\langle t_{i} \rangle$. This is easy to do analytically using $p_{i}(t)$ when the posterior is uniform over histories. For more complicated non-uniform models, one can use
FIG. 2. Example of temporal reconstruction problems solved by our methods. (a) Posterior seed probability $p_i$ of the nodes of a small artificial graph grown with the preferential attachment model [24]. Nodes are ordered from left to right by true time of arrival. (b) Inferred arrival time plotted against the true arrival time, for uniform attachment networks of 100 nodes. The black symbols show the exact estimators $\langle \tau_i \rangle$ calculated for a single network. Monte Carlo estimates ($N = 4000$) of these quantities are also shown, but they are visually indistinguishable from the exact values. Fluctuations in the graph structure rather than the sampling procedure explain the noise. They disappear once we average over networks, as shown by the solid line (3 000 networks). (c) Interpolation of the excess degree, calculated for a single preferential attachment network that is known at $t = 20$ and $t = 80$. Gray lines show how this quantity evolves for single bridges, while the orange line shows the average value from 100 interpolations. (d) Posterior distributions of $\gamma$ for networks generated with the generalized preferential attachment model [25]. Each posterior distribution $P(\gamma|G)$ is computed from 100 samples, and corresponds to a network of $n = 1000$ nodes with kernel exponent $\gamma = 0, 1/3, 2/3, 1$ (see main text).

Monte Carlo samples to estimate

$$\langle t_i \rangle = \sum_H \tau_i(H)P(H), \quad (12)$$

TABLE I. 95% credible interval on the value of the kernel exponent $\gamma$, obtained by fitting a static network to non-linear preferential attachment [25].

| Network                              | $n$  | 95% CI          |
|--------------------------------------|------|-----------------|
| Erdős number network [26]           | 6927 | [1.18, 1.21]    |
| Twitter reply tree                   | 748  | [0.89, 1.00]    |
| WNV phylogenetic tree [27]          | 4120 | [−0.52, −0.39] |

where $\tau_i(H)$ is the time of arrival of node $i$ in history $H$ and $P(H)$ is the probability of sequence $H$ under the chosen growth model.

Interpolation (Fig. 2c) is conceptually no different. One can use our sampling method to interpolate between an initial state and a final state, tracking the evolution of any network quantity of interest along the way. Non-uniform models can again be handled by computing average trajectories with reweighting.

Our final example (Fig. 2d) is a little different. In the previous examples we assumed that the posterior probability of a history is known—either by assuming a uniform distribution, or by assuming a precisely defined growth model. This is often an unrealistic assumption. A more common inference task supposes that a family of models is defined with unknown free parameters. For instance, one might consider a non-linear degree based attachment kernel—a rule to determine where incoming nodes attach [25]. Each time a new node is introduced it connects to an extant node proportional to that node’s degree, raised to the power $\gamma$. The probability that a new node $i$ attaches to node $j$ is thus

$$P[i \rightarrow j] = \frac{k_j^\gamma}{\sum_l k_l^\gamma}, \quad (13)$$

where $k_j$ is the degree of node $j$ and the sum is over all nodes already in $G$. Clearly $\gamma = 0$ corresponds to uniform attachment while $\gamma = 1$ corresponds to (linear) preferential attachment. This allows us to write $P(H|\gamma)$, the probability of any specific history given $\gamma$. Assuming a uniform prior on $\gamma$ we can further write

$$P(\gamma|G) \propto \sum_s P(G, H_s|\gamma), \quad (14)$$

which assigns a posterior probability to each choice of $\gamma$. Our Monte Carlo method can be used to generate samples and evaluate Eq. (14). Panel (d) of Fig. 2 shows how we are able to recover the attachment kernel, given only the final network as input.

Having confirmed that our methods work on artificial data, we conclude with a simple demonstration applying them to real data. The prevalence of the preferential attachment mechanism, and its relation to so-called “scale-free” networks, has been debated. One problem is that previous tests of the mechanism required accurately
time-resolved data [22, 23]. With our methods one can now rigorously test preferential attachment given only one snapshot of the network. Since summary statistics such as degree distributions are not sufficient to estimate the kernel [17, 28], our method is the correct approach for testing preferential attachment when temporal data is unavailable, whereas fitting degree distributions is not.

When applied to real trees without temporal metadata (Table I) our method finds that the co-authorship network centered on Paul Erdős [26] is plausibly grown by a super-preferential attachment mechanism [25], a network of re-tweets on Twitter is explained by a regular preferential attachment mechanism, and the phylogenetic tree of Western Nile Virus [27] certainly did not grow by this mechanism.

To conclude, we have developed analytic expressions and an efficient Monte Carlo method for temporal reconstruction problems on trees. We have derived expressions for the proportion of histories in which each node arrived at each time, and a Monte Carlo procedure to interpolate between any two states. In artificial and real-world networks we have used these methods to reconstruct the past states of statically observed networks.

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