"Testing statistical hypothesis on random trees"

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Running Title: Testing on random trees

Abstract

To distinguish between populations of trees, we consider the hypothesis test proposed recently by Balding, Ferrari, Fraiman and Sued (BFFS–test). A direct approach to calculate effectively the test statistic is quite difficult, since it is based on a supremum defined over the space of all trees, which grows exponentially fast. We show how to transform this problem into a max-flow over a network which can be solved using a Ford Fulkerson algorithm in polynomial time on the maximal number of vertices of the random tree. We also describe conditions that imply the characterization of the measure by the marginal distributions of each node of the random tree, which validate the use of the BFFS–test for measure discrimination. The performance of the test is studied via simulations on Galton-Watson processes.

Key words: Random trees, Galton–Watson process, Goodness–of–fit tests, Two–sample problem

AMS Subject Classification: Primary: 62G10, 60D05. Secondary: 60F17

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1 Introduction

Random trees have long been an important modeling tool. Trees are useful when a collection of observed objects are all descended from a common ancestral object via a process of duplication followed by gradual differentiation. There are two broad approaches to constructing random evolutionary trees: forwards in time “branching process” models, such as the Galton-Watson process, and backwards-in-time “coalescent” models such as Kingman’s coalescent model, Kingman (1982). In the statistics literature there are references to different kind of trees, like phylogenetic trees Holmes (1999), probabilistic trees Sturmfels and Patcher (2005), search trees and others, all of them with particularities related to the field of applications from whom they have arisen.

We consider trees that have a root and evolve forward in time in discrete generations, and each parent node (or vertex) having up to $m$ offspring nodes in the next generation, as in Balding et al. (2005), BFFS from now on. Given a suitable metric, BFFS prove law of large numbers for empiric samples of trees and an invariance principle on the space of continuous functions defined on the space of trees. They construct a Kolmogorov-Smirnov-type goodness-of-fit test (in what follows BFFS test) for the one-sample and two-sample problems.

The statistic for the BFFS test is a supremum over $t$ in the space of trees of $|g_T(t) - g_{T^*}(t)|$, the difference of the empiric mean distances of $t$ to each of the two samples (see (11)). This is a priori a difficult task; a naive search would involve an exponential complexity of the algorithm on the number of potential nodes. The main point of this paper is to show that the problem can be re-expressed as to find the maximal flow on a graph constructed as a function of the sample(s). The approach is inspired on the search of the Maximum a Posteriori in Bayesian image reconstruction using the Ising model, as proposed by Greig et al. (1989); see also Kolmogorov and Zahib (2004). The max-flow problem can be solved in a polynomial time on the number of vertices of the maximal tree, using Ford-Fulkerson type algorithms.

The test work for quite general distributions on the space of trees, but do not distinguish between measures with the same marginal distributions on each node. When the random trees have Markovian structure as defined in (14) we show that the marginals identify the measure. In this case the function $g$ defined in (5) that to each tree gives the mean distance to the random tree also identifies the measure. This is done in Section 3 where we also introduce the BFFS test for the one and two sample problem for random trees. In Section 4 we develop the algorithm to calculate the BFFS test statistic. In section 5 we try the test on several examples, in particular in the Galton-Watson process, an example of law determined by the expectation of the distance. The performance of the test is explored using Monte-Carlo methods. The proofs of selected results have been sent to the Appendix.
2 Trees, distances and tests

Start defining a full tree. Consider an alphabet $A = \{1, \ldots, m\}$, with $m \geq 2$ integer, representing the maximum number of children of a given node of the tree. Let $\tilde{V} = \{1, 11, 12, \ldots, 1m, 111, 112 \ldots\}$, the set of finite sequences of elements in $A$, all of them starting with the symbol 1. The word 1 represents the root of the tree. The full tree is the oriented graph $\tilde{t} = (\tilde{V}, \tilde{E})$ with edges $\tilde{E} \subset \tilde{V} \times \tilde{V}$ given by $\tilde{E} = \{(v, va) : v \in \tilde{V}, a \in A\}$, where $va$ is the sequence obtained by concatenation of $v$ and $a$. In the full tree each node (vertex) has exactly $m$ outgoing edges (to its offsprings) and one ingoing edge (from her father), except for the root who has only outgoing edges. The node $v = 1a_2 \ldots a_k$ is said to belong to the generation $k$; in this case we write $\text{gen}(v) = k$. Generation 1 has only one node, the root.

We define tree as a function $t : \tilde{V} \rightarrow \{0, 1\}$ satisfying

$$t(v) \geq t(va).$$

(1)

for all $v \in \tilde{V}$ and $a \in A$. If $t(1) = 0$ we get the empty tree. Let $\mathcal{T}$ be the set of trees. Abusing notation, a tree $t$ is identified with the graph

$t = (V, E)$ with $V = \{v \in \tilde{V} : t(v) = 1\}$ and $E = \{(v, va) \in \tilde{E} : t(v) = t(va) = 1\}$

(2)

Let $\phi : \tilde{V} \rightarrow \mathbb{R}^+$ be a strictly positive function such that $\sum_{v \in \tilde{V}} \phi(v) < \infty$ and consider the distance

$$d(t, y) = \sum_{v \in \tilde{V}} \phi(v)(t(v) - y(v))^2.$$  

(3)

With this distance $(\mathcal{T}, d)$ becomes a compact metric space. We denote $\mathcal{B}$ the $\sigma$-field of Borel subsets of $\mathcal{T}$, induced by the metric $d$.

**Random trees** A random tree with distribution $\nu$ is a measurable function

$$T : \Omega \rightarrow \mathcal{T} \text{ such that } \mathbb{P}(T \in A) = \int_A \nu(dt).$$

(4)

for any Borel set $A \in \mathcal{B}$, where $(\Omega, \mathcal{F}, \mathbb{P})$ is a probability space and $\nu$ a probability on $(\mathcal{T}, \mathcal{B})$.

**Expected value** The expected distance from a tree $t$ to a random tree $T$ is defined by

$$g_T(t) := \mathbb{E}(d(T, t)) = \int_T d(y, t) \nu(dy).$$

(5)

The set $\mathbb{E}_d T$ is not empty Balding et al. (2005). Any element of the set $\mathbb{E}_d T$ is also called a $d$-mean or $d$-center. Since $\mathbb{E}_d T$ depends only on the distribution $\nu$ induced by $T$ on $\mathcal{T}$, it may also be denoted as $\mathbb{E}_d(\nu)$. 
**Empiric mean trees** Let \( T = (T_1, \ldots, T_n) \) be a random sample of \( T \) (independent random trees with the same law as \( T \)). The empiric expected distance of a tree \( t \) to the sample is defined by
\[
g_T(t) := \frac{1}{n} \sum_{i=1}^{n} d(T_i, t) \tag{6}\]

**Marginal expected values and variances** Let \( T \) be a random tree. We denote by \( \mu_T(v) \) and \( \sigma_T^2(v) \) the mean and variance of \( T(v) \),
\[
\mu_T(v) = \mathbb{E}[T(v)] = \mathbb{P}(T(v) = 1), \tag{7}
\]
\[
\sigma_T^2(v) = \mu_T(v)(1 - \mu_T(v)). \tag{8}
\]
When \( T = (T_1, \ldots, T_n) \) is a random sample with distribution \( \nu \) on \( T \), we denote by \( \overline{T} \) the empiric mean of the sample
\[
\overline{T}(v) = \frac{1}{n} \sum_{i=1}^{n} T_i(v). \tag{9}\]
Notice that \( \overline{T} \) is not a tree. But, considering the lexicographic order in \( \overline{V} \), \( \overline{T} \) is an increasing function on the nodes.

**Testing differences of populations** We consider measures \( \nu \in Q_f \), the space of probability measures that concentrate mass on trees with a finite number of nodes. We describe the two-sample problem. The one-sample problem could be addressed in a similar way.

Let \( \nu, \nu^* \) be distributions in \( Q_f \). The goal is to test
\[
H_0 : \nu = \nu^* \quad H_A : \nu \neq \nu^* \tag{10}\]
using i.i.d. random samples \( T = (T_1, \ldots, T_n) \) and \( T^* = (T_1^*, \ldots, T_m^*) \) with distribution \( \nu \) and \( \nu^* \) respectively.

**The BFFS test** BFFS have proposed the statistic
\[
\sup_{t \in \overline{T}} |W_{T,T^*}(y)| = \sup_{t \in \overline{T}} \sqrt{n} |g_T(t) - g_{T^*}(t)| \tag{11}\]
whose asymptotic law under \( H_0 \) is known to be Gaussian with zero mean and the same covariance function of the process \( X(t) = d(T(t), T) - \mathbb{E}(d(T(t))) \). Determining the quantiles \( q_\alpha \) using the asymptotic law, the null hypothesis is rejected at level \( \alpha \) when
\[
\sup_{t \in \overline{T}} |W_{T,T^*}(t)| > q_\alpha
\]
When there is no knowledge of the population distributions \( \nu \) and \( \nu^* \), a Monte Carlo integration simulation may be devised to obtain the quantiles, using bootstrap techniques to “sample from the samples”. In order to assess the performance of the tests, we work some examples with known distributions.
3 Does the mean distances determine a measure?

When the mean distances \( g_T \) determine univocally the probability \( \nu \) we can use \( g_T \) for statistical tests comparing measures. In this section we give a set of sufficient conditions on \( \nu \) under which \( g_T \) determines \( \nu \). We show in Lemma 3.1 that the knowledge of \( g_T \) is equivalent to the knowledge of the marginals \( (T(v), v \in \tilde{V}) \). Proposition 3.2 says that, under Markov type hypotheses, the marginal distributions determine the measure. The usual processes satisfy the Markov hypotheses.

Equivalence between \( g_T \) and \( \mu_T \)

**Lemma 3.1** Let \( T \) and \( T' \) be random trees. Then, \( g_T(t) = g_{T'}(t) \) for all \( t \in T \) if and only if \( \mu_T(v) = \mu_{T'}(v) \) for all \( v \in \tilde{V} \).

The proof is given in Appendix A. Different measures may have the same \( g_T \). For instance consider \( A = \{1, 2\} \) and \( \nu_1, \nu_2 \) defined by:

\[
\begin{align*}
\nu_1(\emptyset) &= \frac{1}{5}, \quad \nu_1(\{1\}) = \nu_1(\{1, 11\}) = \nu_1(\{1, 12\}) = \nu_1(\{1, 11, 12\}) = \frac{1}{8}; \\
\nu_2(\emptyset) &= \frac{1}{2}, \quad \nu_2(\{1\}) = \nu_2(\{1, 11, 12\}) = \frac{1}{4}.
\end{align*}
\]

(12) (13)

Then, if \( T \sim \nu_1 \) and \( T' \sim \nu_2 \), the marginals \( \mu_T(v) = \mu_{T'}(v) \) for all \( v \in \tilde{V} \). Lemma 3.1 implies that the functions \( g_T \) and \( g_{T'} \) will not help to solve the discrimination problem.

Some families where \( \mu_T \) determines the measure

Let \( T \) be a tree and let \( I \) be some set of nodes. We denote \( T_I \) the restriction of \( T \) to \( I \). Thus, \( T_I = 1 \) means that \( T(v) = 1 \) for all \( v \in I \), while \( T_I = 0 \), means that \( T(v) = 0 \) for all \( v \in I \).

Family relations

Let \( v \) be a node, and \( a, b \in A \). We shall call \( v \) father of \( va \), \( va \) son of \( v \), and \( va \) brother of \( vb \).

Let \( f : \tilde{V} \setminus \{1\} \to \tilde{V} \) be a function such that for each \( v \neq 1 \), \( f(v) \) is father or brother of \( v \), and \( f^n(v) = 1 \) for some \( n = n(v) \in \mathbb{N} \). Notice that, in this case, \( f^{-1}(v) \) is empty or formed up by brothers and sons of \( v \). We call such a function a tree-shift. Consider for instance the function \( f \) that assigns to a node its father.

Markov hypotheses

Let \( T \) be a random tree with discrete distribution \( \nu \) (i.e. \( \sum_{t \in T} \nu(t) = 1 \)). We say that \( T \) satisfies a Markov hypotheses if there exists a tree-shift \( f \) such that if \( v = f(w) \), then

(a) \( 0 < \mu_T(w) < \mu_T(v) < 1 \)
(b) $\mathbb{P}(T(w) = 1 | T(v) = 0) = 0$

(c) Let $I, J \subset \tilde{V}$ be such that if $v \in I$, $w \notin I \cup J$ and $\mathbb{P}(T_I = 1, T_J = 0) > 0$, then
\[
\mathbb{P}(T(w) = 1 | T_I = 1, T_J = 0) = \mathbb{P}(T(w) = 1 | T(v) = 1)
\] (14)

**Proposition 3.2** Under the Markov hypotheses, the marginals $(\mu_T(v), v \in \tilde{V})$ determine the probabilities $(\nu(t), t \in T)$.

The proof is given in the Appendix A.

**Examples of measures satisfying the Markov hypotheses** The alphabet for the following examples is $A = \{1, \ldots, m\}$.

1. Let $f$ be defined by $f(va) = v$, $a \in A$. Let $k(v)$ be such that $f^{k(v)-1}(v) = 1$, for $v \in \tilde{V}$. If $\mu_T(v) = p^{k(v)}$ ($0 < p < 1$), we obtain a tree with $\nu(\{1\}) = p$, and when $T(v) = 1$, $T(va)$ is Bernoulli with parameter $p$, for $a \in A$. We call such tree distributions pseudo Galton-Watson processes.

2. Let $f$ be defined by $f(v1) = v$, and $f(v(a+1)) = va$ for $1 \leq a < m$. That is $v = f(w)$ if $w$ is the eldest brother and $v$ is the father of $w$, or if $v$ is the nearest older brother of $v$. Let now $p_0, \ldots, p_m$ be given probabilities, with $p_0 > 0$ and $p_0 + \cdots + p_m = 1$. If
\[
\mu_T(v1) = (p_1 + \cdots + p_m)\mu_T(v)
\]
\[
\mu_T(v(a+1)) = \frac{p_{a+1} + \cdots + p_m}{p_a + \cdots + p_m} \mu_T(va) \quad (1 \leq a \leq m - 1)
\]

we obtain the classical Galton-Watson process, with parameter probabilities $p_0, \ldots, p_m$.

4 **Network formulation of the variational problem**

Let $M$ be a nonnegative integer and $\tilde{V}_M = \{v \in \tilde{V} : \text{gen}(v) \leq M\}$. In the sequel we consider measures with support in $T_M$, the set of trees all whose vertices are in $\tilde{V}_M$. Abusing of notation we write $\tilde{V}$ instead of $\tilde{V}_M$.

We look for sets of trees at which the supremum (11) is attained:
\[
\arg \max_{t \in T} |g_T(t) - g^{\ast_T}(t)|,
\] (15)

for the two sample problem and
\[
\arg \max_{t \in T} |g_T(t) - g_T(t)|,
\] (16)
for the one-sample problem, where $T$ is a random tree with distribution $\nu_0$ and $g_T(t) = \mathbb{E}[d(T,t)]$.

Let $\varphi : \tilde{V} \to \mathbb{R}$ be a real function and $t_{\varphi} : \tilde{V} \to \{0, 1\}$ be the function defined by $t_{\varphi}(v) = 1\{\varphi(v) < 0\}$ Define the family of Hamiltonians

$$
\mathcal{H}_{\beta,\varphi}(t) = \sum_{v \in \tilde{V}} |\varphi(v)|1\{t(v) \neq t_{\varphi}(v)\} + \beta \sum_{v \in \tilde{V}} \sum_{v' \sim v} 1\{t(v) \neq t(v')\}
$$

(17)

To maximize (15) is equivalent to minimize $\mathcal{H}_{\beta,\varphi}$ for two specific $\varphi$. The same is valid for (16). This is the main point in this section:

**Proposition 4.1** Let $\beta > \sum_{v \in \tilde{V}} \phi(v)$ and define

$$
\varphi^\pm(v) = \beta \gamma(v) \pm 2\phi(v)\Delta(v)
$$

(18)

where $\gamma(v)$ is the number of parents of $v$ minus the number of children of $v$ (see (57)). Then the set

$$
\text{arg min}_{t \in T}(\text{min}\{\mathcal{H}_{\beta,\varphi^+}(t), \mathcal{H}_{\beta,\varphi^-}(t)\})
$$

is equal to (15) when $\Delta(v) = \overline{T}(v) - \overline{T^*}(v)$ and it is equal to (16) when $\Delta(v) = \overline{T}(v) - \mu_T(v)$.

The proof of Proposition 4.1 is given in Appendix B.

**Associated Network**

In analogy with Greig et al. (1989), the network associated to a finite tree $(\tilde{V}, \sim)$ and the Hamiltonian $\mathcal{H}_{\beta,\varphi}$ given in (17) is the following:

- the set of nodes includes the ones of $\tilde{V}$ plus two extra nodes denoted by $s$ (source) and $b$ (sink)

$$
\tilde{V} \cup \{s\} \cup \{b\},
$$

(19)

- the set of edges is

$$
E = \left( \bigcup_{v \in \tilde{V}} \{(s, v)\} \right) \cup \left( \bigcup_{v \in \tilde{V}} \{(v, b)\} \right) \cup \left( \bigcup_{v' \sim v} \{(v, v')\} \right).
$$

(20)

- the capacities of the network are defined as: If $\varphi(v) > 0$ let $c(s, v) = |\varphi(v)|$; otherwise let $c(v, b) = |\varphi(v)|$; to each edge $e = (v, v')$ of neighbor nodes in $(\tilde{V}, \sim)$ let be $c(e) = \beta$. All other edges have zero capacity.
**Cuts** For $t \in T$ let

\[
S(t) = \{s\} \cup \{v \in \tilde{V} : t(v) = 1\}, \\
B(t) = \{b\} \cup \{v \in \tilde{V} : t(v) = 0\}
\]

These two sets define a cut of the network

\[
C(t) = \{(v, v') \in E : v \in S(t), v' \in B(t)\},
\]

whose capacity $c(t)$ is

\[
c(t) = \sum_{(v, v') \in C(t)} c(v, v') \tag{21}\]

The next result has been proven in Greig et al. (1989); we include a short proof for completeness.

**Proposition 4.2** It holds that $c(t) = \mathcal{H}_{\beta, \varphi}(t)$.

**Proof.** In the cut $C(t)$ we find two type of edges: external and internal. The external edges are of two types: one with the form $(s, v)$ where $v$ is such that $t(v) = 0$ and the others with the form $(v, b)$ where $v$ is such that $t(v) = 1$. In the first case, the associated capacity is

\[
c(e) = \begin{cases} 
|\varphi(v)| & \text{if } \varphi(v) > 0, \\
0 & \text{in other case}
\end{cases} = |\varphi(v)|1 \{t(v) \neq t_\varphi(v)\}, \tag{22}\]

while in the second case

\[
c(e) = \begin{cases} 
0 & \text{if } \varphi(v) > 0, \\
|\varphi(v)| & \text{if } \varphi(v) < 0
\end{cases} = |\varphi(v)|1 \{t(v) \neq t_\varphi(v)\}. \tag{23}\]

For the internal edges we have

\[
c(e) = m1 \{t(v) \neq t(v')\}. \tag{24}\]

The result follows from (22), (23) and (24).

Proposition 4.2 shows that the problem of minimizing $\mathcal{H}_{\beta, \varphi}(t)$ is equivalent to find a minimum cut in its associated network. This problem can be solved by means of the Ford-Fulkerson’s algorithm. In the examples of Section 5 we have used the variant of this algorithm proposed and implemented by Kolmogorov and Zahib (2004).
5 Numerical examples

In this section we check the performance of our approach for the problem of testing if two populations of trees are equally distributed (10).

Let \( \nu, \nu^* \) be distributions in \( Q_f \). The goal is to test

\[
H_0 : \nu = \nu^* \quad \text{\( H_A : \nu \neq \nu^* \)}
\]

using two i.i.d. random samples \( T = (T_1, \ldots, T_n) \) and \( T^* = (T_1^*, \ldots, T_m^*) \) with distribution \( \nu \) and \( \nu^* \) respectively. In section 2, we sketched the BFFS test, whose statistic is computed using the approach of Section 4. To study the performance of the test on a controlled environment we simulate several populations of trees using Galton-Watson processes and simple variations of it. We carefully choose the parameters to challenge the power of the tests.

It is important to note that we have chosen distributions over the space of trees which are determined by their matched \( g_T \) function, as the one induced by the pseudo Galton-Watson process with Binomial\((m, p)\) offspring distribution, \( p \in [0, 1] \), \( m \in \mathbb{N} \).

We study binary trees, \( m = 2 \), the extension to an arbitrary number of offsprings \( m \) being straightforward. In a binary binomial Galton-Watson model, the offspring number is 0, 1 or 2 with probabilities \((1 - p)^2, 2p(1 - p)\) and \( p^2 \).

Assume we have two random samples, each one from a Galton-Watson process with possibly different parameters \( p \) and \( p^* \), denoted \( GP(p) \) and \( GP(p^*) \). We would like to test if these samples come from the same process, that is,

\[
H_0 : T \sim GP(p), \ T^* \sim GP(p^*) \quad \text{\( p = p^* \)} \quad \text{\( H_A : T \sim GP(p), \ T^* \sim GP(p^*), \ p \neq p^* \)}
\]

The lack of knowledge of the distribution of the statistics is overcome estimating the quantiles with Monte Carlo simulation. We have followed the next steps to obtain the quantiles under the null hypothesis and assess the power of the test:

1. Quantile

(a) In practice, since the underlying distribution under the null hypothesis is unknown, we should bootstrap from the pooled sample to obtain each pair of bootstrap samples. However, in our simulation we already know the underlying distributions \( \nu \) and \( \nu^* \). Thus we sample trees from a mixture of both laws at random, until we reach the size of the first sample and label it sample 1. Then we continue selecting with the same mixture, until we reach the size of the second sample, and label it sample 2.

(b) We compute the test statistic using the samples.

(c) We repeat the above procedure a fixed number of times \( N \).
(d) We order the computed statistics values increasingly and define the quantile \( q(1 - \alpha) \) as the statistic in place \( (1 - \alpha)N \).

(e) We calculate the quantiles for several values of \( \alpha \) and sample sizes.

2. Power

(a) We generate sample 1 from the distribution \( \nu \), and sample 2 from the distribution \( \nu^* \), and calculate the test statistics using them.

(b) We compare the obtained value against the quantile, and reject the null hypothesis with level \( \alpha \) if \( W > q(1 - \alpha) \).

(c) We repeat the last two steps a fixed number of times and compute the percentage of rejections for each value of \( \alpha \) as a measure of the power of the test.

5.1 BFFS test

To perform the test, it is necessary to compute the statistic

\[
W = \sup_{y \in T} |g_T(y) - g_{T^*}(y)|
\]

which measures in a weak way the differences between the empirical distributions of the samples. The computation of the statistic is tricky when the distribution of the population gives mass to very large trees.

We consider two examples. In the first one we just consider the two sample problem when the underlying distributions are given by two Galton-Watson processes with Binomial offspring distributions, for different values of the parameters \( p^* \).

In the second example we consider a branching process with offspring distribution given by a mixture of two Binomial distributions; \( Bi(2, p_1) \) with probability \( q \), and \( Bi(2, p_2) \) with probability \( (1 - q) \). We have chosen \( p_1 \) and \( p_2 \) to add the same value \( \bar{p} < 1 \), under the null hypothesis and the alternative, so each node has the same expected number of children. This constraint rules out simpler tests based on differences in the expected number of children per node.

Example 1: Binomial. Suppose that the number of children in a given node has Binomial distribution \( Bi(m, p) \) and consider the following hypothesis

\[
H_0 : T \sim GP(p), \ T^* \sim GP(p^*) \quad p = p^* \quad \quad H_A : T \sim GP(0.5), \ T^* \sim GP(p^*), \quad p^* \neq 0.5
\]

We have computed the percentage of rejection over 1000 tests of level \( \alpha = 0.10, 0.05, 0.01 \), when \( T_{k,1}, \ldots, T_{k,n}^* \) is \( GP(p^*) \), with \( p^* = 0.6, 0.7, 0.8 \), for sample sizes \( n = 31, 51, 125 \). The results are reported on Table 1.

Observe that the results are quite encouraging for the BFFS test, which is consistent for alternatives with any value of \( p \neq 0.5 \) (the value under the null hypothesis).
Table 1: Power of the tests with $p = 0.5$ and $p^* = 0.6, 0.7, 0.8$, sample size $n=31, 51, 125$

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</table>

**Example 2: Mixture of Binomials.** Suppose that the number of children in a given node follows a mixture of Binomials. We observe a Binomial distribution with parameter $(m, p_1)$ if we have success with an independent Bernoulli variable of parameter $q$. If we fail (with probability $1-q$), we observe a Binomial with parameters $(m, p_2)$.

Let us denote by $MB(m, q, p_1, p_2)$ the distribution of a branching process for which the number of children at a given node is a mixture of Binomials, independently of the past.

We consider two populations of trees with laws $MB(2, 0.5, p_1, p_2)$ and $MB(2, 0.5, p_3, p_4)$ respectively, and want to test the null hypothesis $\{p_1, p_2\} = \{p_3, p_4\}$.

To make the problem harder, for the null and the alternative distribution we choose values of $p_1, p_2, p_3, p_4$ such that the mean value of the number of children at each node is the same under both models.

The first pair, $p_1 = 0.45$, $p_2 = 0.5$, $p_3 = 0.1$ and $p_4 = 0.85$, produce an example of the most different distributions this model can allow, and the second pair, $p_1 = 0.3$, $p_2 = 0.65$, $p_3 = 0.45$ and $p_4 = 0.5$ one of the closest. Both models are difficult, so we may expect low power with small sample sizes.

We also set the parameter $z$ of the distance as 0.36 and 0.49. Recall that for infinite trees, the majorizing measure condition stated in BFFS required

$$\frac{1}{\sqrt{m^3}} < z < \frac{1}{m}$$

so, if $m = 2$, $z$ must be between 0.35 and 0.5.

The results of our simulation are summarized in Table 2 and Figures 1 and 2, while Figures 3 and 4 corresponds to the second pair of values $p_1 = 0.3$, $p_2 = 0.65$, $p_3 = 0.45$ and $p_4 = 0.5$.

The model chosen rules out any simple statistic we could be tempted to use to discriminate between the populations, like distance of empiric mean trees or the sample mean at each node (the expected mean at each node is the same since $p_1 + p_2 = p_3 + p_4$). Also, the distributions chosen per population, even different, remain close to each other, but the BFFS test statistic needs only a moderate sample size to give high power to the test.
Figure 1: Histogram of the test statistic under null hypothesis (red plot) and alternative (blue plot), with parameters $z = 0.36$ (left column) and $z = 0.49$ (right column), with $p_1 = 0.45$, $p_2 = 0.5$, $p_3 = 0.1$ and $p_4 = 0.85$ and sample sizes (from top to bottom) 31, 51, 71, 101, and 131.
Table 2: The percentage of p-values bigger than a given level $\alpha$ over 1000 tests, with $\alpha = 0.05, 0.01, 0.1$

<table>
<thead>
<tr>
<th>$z = 0.36$</th>
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<th></th>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>31</td>
<td>51</td>
<td>71</td>
<td>101</td>
<td>131</td>
</tr>
<tr>
<td>0.01</td>
<td>4.5%</td>
<td>10.8%</td>
<td>32.5%</td>
<td>59.4%</td>
<td>81.9%</td>
</tr>
<tr>
<td>0.05</td>
<td>28.8%</td>
<td>36.3%</td>
<td>74.7%</td>
<td>88.7%</td>
<td>97.3%</td>
</tr>
<tr>
<td>0.1</td>
<td>43.8%</td>
<td>64.2%</td>
<td>85.7%</td>
<td>97.6%</td>
<td>99%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$z = 0.49$</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>31</td>
<td>51</td>
<td>71</td>
<td>101</td>
<td>131</td>
</tr>
<tr>
<td>0.01</td>
<td>3.5%</td>
<td>15.0%</td>
<td>25.9%</td>
<td>49.6%</td>
<td>69.9%</td>
</tr>
<tr>
<td>0.05</td>
<td>17.3%</td>
<td>47.7%</td>
<td>63.4%</td>
<td>86.1%</td>
<td>94.7%</td>
</tr>
<tr>
<td>0.1</td>
<td>34.8%</td>
<td>66.6%</td>
<td>81.1%</td>
<td>94.2%</td>
<td>98.6%</td>
</tr>
</tbody>
</table>

Figure 1 shows in two columns histograms of the test statistic values obtained in $N = M = 1000$ iterations. We have plotted the test statistic under null hypothesis on red and the one under the alternative on blue. The first column relates to the experiment made with $z = 0.36$ and the second column with $z = 0.49$. The rows show the changes in the histograms produced by the increase in the sample size, set as 31, 51, 71, 101, and 131. In Figure 2 we have plotted the p-values computed in $M = 1000$ iterations, each curve belonging to a different sample size. In Table 2 we evaluate the power of the test for three different values of the test level ($\alpha$, as 0.01, 0.05 and 0.1) as the percentage of p-values greater than the respective level $\alpha$. The change in the $z$ parameter from 0.36 to 0.49 increase a little the variance of the statistics, as seen in Figure 1, and reduce the power of the test, as observed in Table 2.

The second pair of parameters chosen $p_1 = 0.3$, $p_2 = 0.65$, $p_3 = 0.45$ and $p_4 = 0.5$ gives a different panorama, since the distributions of the populations are very close, and the corresponding distributions of the test under null hypothesis and alternative remain also close. Increasing the sample size reduces the variance and separates the means of the distributions but at a slow rate, increasing the computing cost of the statistic. We have studied the performance of the statistic with 10 different sample sizes, $n = [50, 100, 150, 200, 250, 300, 350, 400, 450, 500]$, fixing $z = 0.36$ and we have plotted the histograms for all sizes in Figure 3.

That Figure shows clearly the difficulty of the problem, the reader is invited to observe the first subplot, where the sample has 50 trees and the last subplot, (fifth row second plot) where the sample has 500 trees. The distributions are barely separated, even after increasing ten times the sample size.

Figure 4 shows two more plots, the left one shows 10 curves of 1000 p-values each, computed changing sample sizes, and the right one shows the percentage of rejection as a
Figure 2: p-values calculated 1000 times, with parameters $z = 0.36$, $p_1 = 0.45$, $p_2 = 0.5$, $p_3 = 0.1$, $p_4 = 0.85$ and sample size 31, 51, 71, 101, 131. Left plot: parameter $z = 0.36$. Right plot: parameter $z = 0.49$.

function of the sample size, each curve computed with a different $\alpha$ level. Besides sample fluctuations, the percentage of rejection increases with sample size, but at a quite slow rate.

6 Final Remarks

We have proposed a way to compute the statistic for the BFFS test to distinguish between populations of trees. We have applied the tests to Galton-Watson processes. The examples show that the test is powerful and that it can be applied to reasonably large trees. The aim now is to understand if it can be used with other types of trees, namely phylogenetic trees, suffix trees, probabilistic trees, search trees, tries and others, all of them with particularities related to the field of application from whom they have arisen. Particularly important are the applications in biology and computer science, although recently many other areas are using random trees. We are aware of a recent application in linguistic. In these examples the leaves of the tree may be more important than the root and its neighbors. In this case one might propose a different distance, or a different weight to the vertices when computing the distance. Our context works with quite general underlying distributions and distances, that allows –in principle– to include trees coming from different fields.

For particular distributions (like Galton-Watson processes with Binomial offspring distribution) more simple tailor-made test can be developed. For instance, in this case we may take advantage that we know that at each node we have independent Binomial distributions, and perform a simpler test. On the contrary, our test tends to be universal for a quite general family of distributions over trees: the family of distributions that are determined by the mean distance.
Our simulations show that the BFFS test is able to distinguish between distributions determined by the vertex-marginal distributions, which is a reasonably large family of distributions for applications. This class includes tree laws with Markovian hypothesis, as shown in Proposition 3.2. Probably this can be extended to a larger class analogous to $k$ step Markov chains.

The study of the asymptotic behaviour of these Markovian processes over trees seems to be challenging.

The computational burden for our algorithm allow us to go to trees with up to $5^{10}$ nodes. If the database are sparse enough, it may also allow to handle trees with 20 generations and up to 20 offsprings.

The code is available from Jorge R. Busch (jbusch@fi.uba.ar) upon request.

A Mean distances and Markovian hypotheses

In this Appendix we show Lemma 3.1 and Proposition 3.2. We start with an elementary computation.

**Lemma A.1** Let $\nu$ be a distribution on $T$.

(a) If $T$ is a random tree with distribution $\nu$, then

$$ g_T(t) = \sum_{v \in V} \phi(v)(\mu_T(v) - t(v))^2 + \sum_{v \in \tilde{V}} \phi(v)\sigma_T^2(v), \quad (25) $$

$$ = \sum_{v \in V} \phi(v)\mu_T(v)(1 - 2t(v)) + \sum_{v \in \tilde{V}} \phi(v)t(v) \quad (26) $$

**Proof of Lemma 3.1** Notice first that from (26) it follows that

$$ g_T(t) - g_{T'}(t) = \sum_{v \in V} \phi(v)(\mu_T(v) - \mu_{T'}(v))(1 - 2t(v)). \quad (27) $$

which implies that if $\mu_T(v) = \mu_{T'}(v)$ for all $v \in \tilde{V}$, then $g_T(t) = g_{T'}(t)$. This proves sufficiency.

To prove necessity we proceed by induction. When $g_T(t) = g_{T'}(t)$ for all $t \in T$, from (27) we obtain

$$ 0 = \sum_{v \in \tilde{V}} \phi(v)(\mu_T(v) - \mu_{T'}(v))(1 - 2t(v)) $$

$$ = -\sum_{v \in t} \phi(v)(\mu_T(v) - \mu_{T'}(v)) + \sum_{v \not\in t} \phi(v)(\mu_T(v) - \mu_{T'}(v)) \quad (28) $$
for all $t \in \mathcal{T}$. Letting $t = \emptyset$, the empty tree, and $t = \{1\}$ in (28), we obtain

$$0 = \sum_{v \in \tilde{V}} \phi(v)(\mu_T(v) - \mu_{T'}(v))$$

(29)

$$0 = -\phi(1)(\mu_T(1) - \mu_{T'}(1)) + \sum_{v \neq 1} \phi(v)(\mu_T(v) - \mu_{T'}(v)).$$

(30)

Thus, $\mu_T(1) = \mu_{T'}(1)$.

**Inductive step** Let $t \in \mathcal{T}$, and $h \in \tilde{V} \setminus \{t\}$ such that $t_h := t \cup \{h\} \in \mathcal{T}$. We show that if $\mu_T(v) = \mu_{T'}(v)$ for all $v \in t$, then $\mu_T(h) = \mu_{T'}(h)$. First, we obtain from (28)

$$0 = \sum_{v \notin t} \phi(v)(\mu_T(v) - \mu_{T'}(v));$$

(31)

$$0 = -\phi(h)(\mu_T(h) - \mu_{T'}(h)) + \sum_{v \notin t_h} \phi(v)(\mu_T(v) - \mu_{T'}(v));$$

(32)

and it follows that $\mu_T(h) = \mu_{T'}(h)$. □

It is easy to prove the following lemma.

**Lemma A.2** If $T$ is a random tree satisfying the Markov hypotheses with tree-shift $f$ then,

1. Given $T(v) = 1$, the variables $T(w) : w \in f^{-1}(v)$ are independent.

2. If $v = f(w)$,

$$\mathbb{P}(T(w) = 1|T(v) = 1) = \frac{\mu_T(w)}{\mu_T(v)}$$

(33)

**Proof of Proposition 3.2** First, notice that

$$\nu(\emptyset) = 1 - \mu_T(1)$$

(34)

From Lemma A.2,

$$\nu(\{1\}) = \mu_T(1) \prod_{h \in f^{-1}(1)} \left(1 - \frac{\mu_T(h)}{\mu_T(1)}\right)$$

(35)

Let $t$ be a not empty finite tree, $t \neq \tilde{V}$ and $h$ be a node such that $h \notin t$ and $v = f(h) \in t$. We shall show that

$$\nu(t \cup \{h\}) = \nu(t) \frac{\mu_T(h)}{\mu_T(v) - \mu_T(h)}$$

(36)
First, we have
\[
\nu(t \cup \{h\}) = \mathbb{P}(T_t = 1, T(h) = 1, T_{(t\cup\{h\})^c} = 0)
= \mathbb{P}(T(h) = 1 | T_t = 1, T_{(t\cup\{h\})^c} = 0) \mathbb{P}(T_t = 1, T_{(t\cup\{h\})^c} = 0)
= \mathbb{P}(T(h) = 1 | T(v) = 1) \mathbb{P}(T_t = 1, T_{(t\cup\{h\})^c} = 0) \tag{37}
\]

On the other hand,
\[
\nu(t) = \mathbb{P}(T_t = 1, T(h) = 0, T_{(t\cup\{h\})^c} = 0)
= \mathbb{P}(T(h) = 0 | T(v) = 1) \mathbb{P}(T_t = 1, T_{(t\cup\{h\})^c} = 0)
= (1 - \mathbb{P}(T(h) = 1 | T(v) = 1)) \mathbb{P}(T_t = 1, T_{(t\cup\{h\})^c} = 0) \tag{38}
\]

From (37) and (38) it follows that
\[
\nu(t \cup \{h\}) = \nu(t) \frac{\mathbb{P}(T(h) = 1 | T(f(h)) = 1)}{1 - \mathbb{P}(T(h) = 1 | T(f(h)) = 1)} \tag{39}
\]

This shows (36). Our main statement follows now by induction from (35) and (36), noticing that any finite tree may be constructed from \{1\} in this way. \qed

### B Redefining the variational problem

In this Appendix we prove Proposition 4.1 for the variational problem (16). The case (15) is analogous.

Let \(T = (T_1, \ldots, T_n)\) be a random sample with law \(\nu\). A computation analogous to Lemma A.1 shows that
\[
g_T(t) = \sum_{v \in V} \phi(v)(T(v) - t(v))^2 + k(T), \tag{40}
\]
\[
= \sum_{v \in V} \phi(v) T(v)(1 - 2t(v)) + \sum_{v \in V} \phi(v) t(v) \tag{41}
\]
where \(k(T) = \sum_{v \in V} \phi(v) T(v)(1 - T(v))\) does not depend on \(t\).

**Lemma B.1** The set (16) is contained in the union of the sets
\[
\arg \min_{t \in T} \sum_{v \in V} \phi(v)(T(v) - \mu_T(v))(1 - 2t(v)), \tag{42}
\]
\[
\arg \min_{t \in T} \sum_{v \in V} \phi(v)(\mu_T(v) - T(v))(1 - 2t(v)). \tag{43}
\]
Proof. From (26) and (41),
\[ g_T(t) - g_T(t) = \sum_{v \in V} \phi(v)(T(v) - \mu_T(v))(1 - 2t(v)) \]  
\[ = -\sum_{v \in V} \phi(v)(\mu_T(v) - \overline{T}(v))(1 - 2t(v)) \]  
(44)  
(45)

Since to maximize \(|A(t)|\) is sufficient to minimize \(A(t)\) and \(-A(t)\), the result follows. \(\square\)

Notice that
\[ \sum_{v \in V} \phi(v)(\mu_T(v) - \overline{T}(v))(1 - 2t(v)) = K(T, \mu_T) + 2\mathcal{L}(t) \]  
(46)

where \(K(T, \mu_T) = \sum_{v \in V} \phi(v)(\mu_T(v) - \overline{T}(v))\) does not depend on \(t\) and
\[ \mathcal{L}(t) = \sum_{v \in V} \phi(v)(\overline{T}(v) - \mu_T(v))t(v). \]  
(47)

The maximization problem is then reduced to find trees that minimize \(\pm \mathcal{L}(t)\). In order to handle both minimizing problems simultaneously, we consider the general problem of minimizing
\[ \mathcal{L}(t) = \sum_{v \in V} \phi(v)\Delta(v)t(v). \]  
(48)

when \(|\Delta(v)| \leq 1\) for all \(v\).

Introduce the space of configurations
\[ \Sigma := \{0, 1\}^V. \]

Remark B.2 In the larger space \(\Sigma\) minimizing configurations satisfy: \(t \in \arg \min_{y \in \Sigma} \mathcal{L}(y)\) if and only if
\[ t(v) = \begin{cases} 0 & \text{if } \Delta(v) > 0, \\ 1 & \text{if } \Delta(v) < 0. \end{cases} \]  
(49)

Configurations given by (49) are not necessarily trees.

Let \(l_-\) and \(l_+\) the values of the minimum and maximum of \(\mathcal{L}(t)\) over \(\Sigma:\)
\[ l_- = \sum_{v \in \tilde{V}^-} \phi(v)\Delta(v), \quad l_+ = \sum_{v \in \tilde{V}^+} \phi(v)\Delta(v), \]  
(50)

where \(\tilde{V}^-\) is the set of all nodes where \(\Delta(v) < 0\) and \(\tilde{V}^+\) is the set of all nodes where \(\Delta(v) > 0\). Notice that
\[ l_+ - l_- = \sum_{v \in V} \phi(v)|\Delta(v)| \leq \sum_{v \in V} \phi(v) \]  
(51)
Penalization  We penalize the configurations of $\Sigma$ that are not trees with the number of orphan vertices:

$$\mathcal{P}(t) = \sum_{\text{gen}(v) < M} \sum_{a \in A} t(va)(1 - t(v)).$$

(52)

It is clear that $\mathcal{P}(t) \geq 0$ and $\mathcal{P}(t) = 0$ if and only if $t \in \mathcal{T}$.

Hamiltonian function  Consider Hamiltonian functions of the form

$$\mathcal{H}_\beta(t) = \beta \mathcal{P}(t) + \mathcal{L}(t)$$

(53)

where $\beta$ is a positive constant.

Trees minimizing $\mathcal{L}$ will also minimize $\mathcal{H}_\beta$ for all positive $\beta$: If $t \in \mathcal{T} \cap \arg \min_{y \in \Sigma} \mathcal{L}(y)$, then $t \in \arg \min_{y \in \Sigma} \mathcal{H}_\beta(y)$ for all $\beta > 0$. On the other hand, if $\beta$ is big enough we expect the configurations minimizing $\mathcal{H}_\beta(t)$ to be trees. Since on the set of trees the form $\mathcal{P}(t)$ vanishes, the minimizing trees should also minimize $\mathcal{L}(t)$. This is proven in the following Lemma.

Lemma B.3  If $\beta > \sum_{v \in \widetilde{V}} \phi(v)$, then

$$\arg \min_{t \in \Sigma} \mathcal{H}_\beta(t) = \arg \min_{t \in \mathcal{T}} \mathcal{L}(t).$$

(54)

Proof.  For all $t \in \Sigma$ it holds

$$\mathcal{H}_\beta(t) \geq l_- + \beta \sum_{v \in \widetilde{V}} \sum_{a \in A} t(va).$$

(55)

If $t$ is not a tree, there exists $v \in \widetilde{V}$ and $a \in A$ such that $t(v) = 0$ and $t(va) = 1$, hence

$$\mathcal{H}_\beta(t) \geq l_- + \beta > l_- + \sum_{v \in \widetilde{V}} \phi(v) \geq l_+.$$  

(56)

by (51). On the other hand, $\mathcal{H}_\beta(t) = \mathcal{L}(t) \leq l_+$ for any tree $t$. Hence, for these values of $\beta$, if $t$ is not a tree, then $\mathcal{H}_\beta(t) > \max_{y \in \mathcal{T}} \mathcal{H}_\beta(y)$, and the result follows.  

Let $\gamma(v)$ count the number of parents minus the number of children of node $v$:

$$\gamma(v) := \begin{cases} 
-m & \text{if } v \text{ is root} \\
-m + 1 & \text{if } \text{gen}(v) \leq M - 1 \\
1 & \text{if } \text{gen}(v) = M 
\end{cases}$$

and let

$$\varphi(v) := \beta \gamma(v) + 2\varphi(v)\Delta(v)$$

(57)

(58)

The notation $v' \sim v$ means that $v'$ is a child of $v$. 
Lemma B.4

\[ 2\mathcal{H}_\beta(t) = \sum_{v \in V} |\varphi(v)| \mathbf{1}\{t(v) \neq t_{\varphi}(v)\} \]

\[ + \beta \sum_{\text{gen}(v) < M} \sum_{v' \sim v} \mathbf{1}\{t(v) \neq t(v')\} + \sum_{v \in V} \varphi(v)^- \]  

(59)

(where \( \varphi(v)^- = \min(\varphi(v), 0)\)).

Proof. We have

\[ \mathcal{P}(t) = \sum_{\text{gen}(v) < M} a \sum_{v} t(va) - \sum_{\text{gen}(v) < M} a \sum_{v} t(va)t(v) \]

\[ = \sum_{\text{gen}(v) < M} a \sum_{v} (1 - t(v)) - \sum_{\text{gen}(v) < M} a \sum_{v} (1 - t(va))(1 - t(v)) \]

Adding these expressions,

\[ 2\mathcal{P}(t) = \sum_{\text{gen}(v) < M} a \sum_{v} \left[t(va) + (1 - t(v))\right] - \sum_{\text{gen}(v) < M} a \sum_{v} \mathbf{1}\{t(va) = t(v)\} \]

\[ = \sum_{\text{gen}(v) < M} a \sum_{v} t(va) - \sum_{\text{gen}(v) < M} a \sum_{v} \mathbf{1}\{t(va) \neq t(v)\} \]

\[ = \sum_{v \in V} \gamma(v)t(v) + \sum_{\text{gen}(v) < M} a \sum_{v} \mathbf{1}\{t(va) \neq t(v)\} \]  

(60)

Hence

\[ 2\beta\mathcal{P}(t) + 2\mathcal{L}(t) = \sum_{v \in V} \left[\beta \gamma(v) + 2\varphi(v)\Delta(v)\right] t(v) + \beta \sum_{\text{gen}(v) < M} a \sum_{v} \mathbf{1}\{t(va) \neq t(v)\} \]

\[ = \sum_{v \in V} \varphi(v)t(v) + \beta \sum_{\text{gen}(v) < M} a \sum_{v' \sim v} \mathbf{1}\{t(v') \neq t(v)\} \]  

(61)

To conclude, write

\[ \sum_{v \in V} \varphi(v)t(v) = \frac{1}{2} \sum_{v \in V} \varphi(v) \left[2t(v) - 1\right] + \frac{1}{2} \sum_{v \in V} \varphi(v) \]

\[ = \sum_{v \in V} |\varphi(v)| \mathbf{1}\{t(v) \neq t_{\varphi}(v)\} + \sum_{v \in V} \varphi(v)^- \]  

(62)

to get (59).
Proof of Proposition 4.1 We prove the Proposition for the case (16). The case (15) is analogous. By Lemma B.1, the set (16) is contained in the union of (42) and (43). By (46) and (47) this is the same as to find trees minimizing $L(t)$ for $\Delta(t) = T(t) - \mu_T(t)$ and for $-\Delta(t)$. Fix $\Delta$ and take $\beta > \sum_{v \in V} \phi(v)$. By Lemma B.3, to minimize $L(t)$ in the space of trees is the same as to minimize $H_\beta$ in the space of configurations $\Sigma$. When $\varphi$ is given by (58),

$$2H_\beta = H_{\beta, \varphi} + K_1$$

where $K_1 = \sum_{v \in V} \varphi(v)$—does not depend on $t$. Hence, to minimize $H_\beta$ is the same as to minimize $H_{\beta, \varphi}$. Switching $\Delta$ to $-\Delta$ we get the proposition. \qed

References


Figure 3: Histogram of the test statistic under null hypothesis (red line) and alternative (blue line), with parameters $z = 0.36$, $p_1 = 0.3$, $p_2 = 0.65$, $p_3 = 0.45$ and $p_4 = 0.5$, each subplot related to a different sample size 50, 100, 150, 200, 250, 300, 350, 400, 450, 500.
Figure 4: Left plot: p-values computed 1000 times, with parameters $p_1 = 0.3$, $p_2 = 0.65$, $p_3 = 0.45$ and $p_4 = 0.5$, each curve related to a different sample size 50, 100, 150, 200, 250, 300, 350, 400, 450, 500. Right plot: percentage of rejection as a function of the sample size, each curve computed with a different $\alpha$ level, 0.01 in blue, 0.05 in green and 0.1 in red.