A Mathematical Assessment of the Isolation Tree Method for Anomaly Detection in Big Data

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Abstract

We present the mathematical analysis of the Isolation Random Forest Method (IRF Method) for anomaly detection, introduced in [1] and [2]. We prove that the IRF space can be endowed with a probability induced by the Isolation Tree algorithm (iTree). In this setting, the convergence of the IRF method is proved, using the Law of Large Numbers. A couple of counterexamples are presented to show that the method is inconclusive and no certificate of quality can be given, when using it as a means to detect anomalies. Hence, a more robust version of the method is proposed whose mathematical foundation is fully justified. Finally, numerical experiments are presented to compare the performance of the classic method with the proposed one.

Keywords: Isolation Random Forest, Monte Carlo Methods, Anomaly Detection, Probabilistic Algorithms

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1. Introduction

Anomaly detection is an important field of research due to its applications; its presence may indicate disease of individuals, fraudulent transactions and network security breaches, among others. There is a remarkable number of methods for anomaly detection following different paradigms, some of these are distance-based (see [3, 4, 5]), classification-based (see [6, 7]), cluster-based (see [8]) and isolation-based presented first in [1] and later extended in [2]. In the present work we focus on the mathematical analysis of the latter method, from now on, referred as the IRF Method.

Despite the popularity of the IRF method, to the authors’ best knowledge, no mathematical analysis has been done to it. For instance, there is no rigorous proof that the method converges, there is no analysis about the number of iterations needed to assure confidence intervals for the computed values. Some scenarios where the methods performs poorly have been pointed out in [1] and [2], but there are no general recommendations/guidelines for a setting where the IRF Method runs successful. In the present work, all these aspects are addressed with mathematical rigor.

The paper is organized as follows, in the introductory section the notation and general setting are introduced; the IRF Method is reviewed for the sake of completeness and a prove is given that the iTree algorithm is well-defined. In the second section the method is analyzed for the 1D case, and proved to be a suitable tool for anomaly detection in this particular setting, this is done recalling a closely related algorithm, next, estimates for the values of the expected height and variance are given. Section 3 presents the analysis of the method in the general setting, the underlying probabilistic structure used by the method is revised, the convergence of the method is proven, the cardinality of the isolation random forest (IRF) is presented and finally two examples are
given to analytically prove the inconclusiveness of the IRF Method. Finally, section 4 proposes a more robust version of the method, together with numerical examples examining the performance of both algorithms.

1.1. Preliminaries

In this section the general setting and preliminaries of the problem are presented. We start introducing the mathematical notation. For any natural number \( N \in \mathbb{N} \), the symbol \([N] = \{1, 2, \ldots, N\}\) indicates the set/window of the first \( N \) natural numbers. For any set \( E \) we denote by \(#E\) its cardinal and \( p(E)\) its power set. A particularly important set is \( S_N \), where \( S_N \) denotes the set of all permutations in \([N]\), its elements will be usually denoted by \( \sigma, \tau \), etc. Random variables will be represented with upright capital letters, namely \( X, Y, Z, \ldots \) and its respective expectations with \( E(X), E(Y), E(Z), \ldots \). Vectors are indicated with bold letters, namely \( \mathbf{p}, \mathbf{q}, \mathbf{r} \ldots \) etc. The canonical basis in \( \mathbb{R}^d \) is written \( \{\mathbf{e}_1, \ldots, \mathbf{e}_d\} \), projections from \( \mathbb{R}^d \) onto the \( j\)-th coordinate are written as \( \pi_j(\mathbf{x}) = \mathbf{x} \cdot \mathbf{e}_j \), where \( \mathbf{x} \in \mathbb{R}^d \) for all \( j \in [d] \). Particularly important collections of objects will be written with calligraphic characters, e.g. \( A, D, E \) to add emphasis.

The isolation random tree algorithm (iT-Tree) for a set of points in \( \mathbb{R}^d \) is defined recursively as follows

**Definition 1 (The iT-Tree Algorithm).** Let \( S \stackrel{\text{def}}{=} \{x_0, x_1, \ldots, x_N\} \) be a set of points in \( \mathbb{R}^d \).

1. An isolation random tree \( T \) (iT-Tree), associated to this set is defined recursively as follows:
   
   a. Define the tree root as \( rt(T) \stackrel{\text{def}}{=} S \).

   b. Define the sets
      
      \[ \pi_j(S) \stackrel{\text{def}}{=} \{\mathbf{x} \cdot \mathbf{e}_j : \mathbf{x} \in S\}, \quad 1 \leq j \leq d, \quad \Omega_c \stackrel{\text{def}}{=} \{j \in [d] : \#\pi_j(\mathbf{S}) \geq 2\}. \]  
      
   c. If the set \( S \) has two or more points (equivalently, if \( \Omega_c \neq \emptyset \)), choose randomly \( j \) in \( \Omega_c \), then choose randomly \( p \in (\min \pi_j(S), \max \pi_j(S)) \) (the split value).

   d. Perform an isolation random tree on the left set of data \( S_l \stackrel{\text{def}}{=} \{\mathbf{x} \in S : \mathbf{x} \cdot \mathbf{e}_j < p\} \), denoted by \( T_l \).

   e. Perform an isolation random tree on the right set of data \( S_r \stackrel{\text{def}}{=} \{\mathbf{x} \in S : \mathbf{x} \cdot \mathbf{e}_j \geq p\} \), denoted by \( T_r \).

   f. Denote the set of all possible isolation random trees associated to the set \( S \) by \( \Omega_{\text{IRF}}(S) \), whenever the context is clear, we simply write \( \Omega_{\text{IRF}} \), and refer to it as the isolation random forest.

For the sake of completeness we present the iT-Tree Algorithm’s pseudocode in [1].

**Proposition 1.** Given an arbitrary set \( S \stackrel{\text{def}}{=} \{x_0, x_1, \ldots, x_N\} \) in \( \mathbb{R}^d \), the iT-Tree algorithm described in Definition 1 needs \( N \) instances to isolate every point in \( S \).

**Proof.** We proceed by induction on the number of data \( N \). For \( N = 1 \) the result is trivial. For \( N = 2 \) the result is direct given that two distinct points \( x_0 \) and \( x_1 \) must differ in at least one coordinate, namely \( j \in [d] \), moreover, the interval \((\min \{x_0 \cdot \mathbf{e}_j, x_1 \cdot \mathbf{e}_j\}, \max \{x_0 \cdot \mathbf{e}_j, x_1 \cdot \mathbf{e}_j\})\) is nonempty. Therefore, any hyperplane \( H \stackrel{\text{def}}{=} \{\mathbf{x} \in \mathbb{R}^d : \mathbf{x} \cdot \mathbf{e}_j = p\} \), with \( p \in (\min \{x_0 \cdot \mathbf{e}_j, x_1 \cdot \mathbf{e}_j\}, \max \{x_0 \cdot \mathbf{e}_j, x_1 \cdot \mathbf{e}_j\}) \) defines \( T_l = \{x_j : x_j = \min \{x_0 \cdot \mathbf{e}_j, x_1 \cdot \mathbf{e}_j\}\} \) and \( T_r = \{x_j : x_j = \max \{x_0 \cdot \mathbf{e}_j, x_1 \cdot \mathbf{e}_j\}\} \), which are both singleton trees. Hence, the algorithm stops after one instance.

Assume now that the result holds true for \( k \leq N - 1 \) and let \( S \stackrel{\text{def}}{=} \{x_0, x_1, \ldots, x_N\} \) be arbitrary in \( \mathbb{R}^d \). Since \( \#S \geq 2 \), the set \( \Omega_c \) (defined in [1]) must be nonempty. Choose randomly an index \( j \) in \( \Omega_c \) and choose randomly \( p \in (\min S_j, \max S_j) \). Thus, after one instance of the algorithm the left and right subsets are defined...
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Definition 3. related problem. We begin introducing some definitions.

2. The 1D Setting

by the iTree algorithm, will be postponed until Section 3, Theorem 11.

brevity, the proof showing that the isolation random forest can be endowed with a probability measure, defined

Observe that due to Proposition 1 the iTree Algorithm and consequently the IRF method are well-defined. For

and they satisfy \( \#S_l < N, \#S_r < N, \#S_l + \#S_r = N \). Then, applying the induction hypothesis on each the left and right subsets it follows that the total of needed instances is

\[
1 + (\#S_l - 1) + (\#S_r - 1) = \#S_l + \#S_r - 1 = N - 1,
\]

which completes the proof.

\[\Box\]

Definition 2 (The IRF Method). Input: data set \( S \stackrel{\text{def}}{=} \{x_1, \ldots, x_N\} \subseteq \mathbb{R}^d \), number of Bernoulli trials \( K \).

(i) For each Bernoulli trial \( k = 1, \ldots, K \), perform iTree on \( S \) (see Definition 1 and/or Algorithm 1) and store the heights \( \{h_k(x) : x \in S\} \) in a Log.

(ii) For each \( x \in S \), define \( H_{\text{IRF}}(x) \) as the average height of the collection of heights \( \{h_k(x) : k = 1, \ldots, K\} \).

Observe that due to Proposition 1 the iTree Algorithm and consequently the IRF method are well-defined. For brevity, the proof showing that the isolation random forest can be endowed with a probability measure, defined by the iTree algorithm, will be postponed until Section 3, Theorem 11.

2. The 1D Setting

In order to study the problem for sets \( S = \{x_0, x_1, \ldots, x_N\} \) in \( \mathbb{R} \), it is strategic to start analyzing another related problem. We begin introducing some definitions.

Definition 3. A family \( \mathcal{P} = \{I_n : n \in [N]\} \) is said to be a monotone partition of an interval \([a, b]\) if there exists a monotone sequence \( a = x_0 < x_1 < \ldots < x_N = b \) such that the extremes of \( I_n \) are \( x_{n-1} \) and \( x_n \) for all \( n \in [N] \). (See Figure 1 (a) for an example with \( |\mathcal{P}| = 5 \).)

Definition 4. Let \( \mathcal{P} = \{I_n : n \in [N]\} \) be a monotone partition of the interval \( I = [a, b] \), with set of endpoints \( x_0 = a < x_1 < \ldots < x_N = b \), from now denoted by \( S(\mathcal{P}) \).
(i) A monotone random tree $T$, associated to this partition is defined recursively as follows (see Figures 1(a) and (b) for an example.):

a. If the partition is non-empty, choose $rt(T) = I_k \in \mathcal{P}$ randomly as the root of $T$, with probability
   \[ \frac{|I_k|}{|I|} = \frac{x_k - 1 - a}{b - a}. \]

b. Perform a monotone random tree on the **left partition** of intervals $\mathcal{P}_l \overset{\text{def}}{=} \{ I_n : n \in [N], n < k \}$, denoted by $T_l$. Next, include the arc $(rt(T), rt(T_l))$ in the edges of the tree $E(T)$; where $rt(T_l)$ indicates the root of $T_l$.

c. Perform a monotone random tree on the **right partition** of intervals $\mathcal{P}_r \overset{\text{def}}{=} \{ I_n : n \in [N], n > k \}$, denoted by $T_r$. Next, define the arc $(rt(T), rt(T_r))$ in the edges of the tree $E(T)$, where $rt(T_r)$ indicates the root of $T_r$.

(ii) We denote the set of all possible monotone random trees associated to the partition $\mathcal{P}$ by $\Omega_{\text{MRF}}(\mathcal{P})$, whenever the context is clear, we simply write $\Omega_{\text{MRF}}$, and we refer to it as the **monotone random forest**.

**Remark 1.** Labeling the edges of the monotone random tree is done to ease, later on, the connection between these trees and the iTrees for the 1D case.

**Proposition 2.** Let $T$ be in $\Omega_{\text{MRF}}$, then $T$ it is a binary tree.

**Proof.** We proceed by induction on the number of elements in the partition $\# \mathcal{P} = N$. For $\# \mathcal{P} = N = 1$, the result is trivial since there is only one possible tree. For $\# \mathcal{P} = N = 2$, the result also holds since there are only two possible trees. Assume now that the result holds whenever the monotone partition has cardinal less or equal than $N - 1$. Take $\mathcal{P} = \{ I_n : n \in [N] \}$ and $T \in \Omega_{\text{MRF}}$ with $rt(T), \mathcal{P}_l, \mathcal{P}_r$ its root, left and right partitions respectively. Given that $\# \mathcal{P}_l < N$ and $\# \mathcal{P}_r < N$, then $T_l$ and $T_r$ are both binary trees (one of them may be empty), with corresponding roots $rt(T_l)$ and $rt(T_r)$. Since the arcs $(rt(T_l), rt(T))$ and $(rt(T_r), rt(T))$ are included in the list of edges $E(T)$ by construction (whenever its respective tree is nonempty), it follows that $T$ is a binary tree.

Next we recall a classic definition, see [9]

**Definition 5.** Let $T$ be a binary tree, the **left** (resp. **right**) subtree of a vertex $v$ is the binary subtree spanning the left (resp. right)-child of $v$ and all of its descendants.
Theorem 3. Let \( P = \{ I_n : n \in [N] \} \) and \( \Omega_{MRF} \), be as in Definition \( \mathbb{E} \), then, the algorithm induces a probability measure in \( \Omega_{MRF} \).

Proof. We prove this theorem by induction on the cardinal of the monotone partition \#\( P \). For \#\( P = N = 1 \) the result is trivial because there is only one possible tree. For \#\( P = N = 2 \) the result also holds since there are only two possible trees. Assume now that the result is true for any monotone partition with cardinal less or equal than \( N - 1 \). Let \( P = \{ I_n : n \in [N] \} \) be a monotone partition and let \( T \in \Omega_{MRF} \) be arbitrary, with root rt\( (T) \), \( T_l, T_r \) left and right trees, \( P_l, P_r \) left and right partitions respectively. Therefore, the probability that the tree \( T \) occurs equals the probability of choosing \( rt(T) = I_k \) times the probability that \( T_\alpha \) occurs in \( P_\alpha \) when \( \alpha \in \{ l, r \} \), i.e.

\[
\mathbb{P}(T) \equiv \sum_{\{ I : l \in P \}} \mathbb{P}_l(T_l) \mathbb{P}_r(T_r).
\]

Here \( \mathbb{P}_\alpha(T_\alpha) \) indicates the probability that \( T_\alpha \) occurs in the space of monotone random trees \( \Omega_{MRF}(P_\alpha) \), defined on the partition \( P_\alpha \), for \( \alpha \in \{ l, r \} \). By the induction hypothesis, we know that \( \mathbb{P}_\alpha : \Omega_{MRF}(P_\alpha) \to [0, 1] \) is a well-defined probability, consequently \( \mathbb{P}(T) \) is nonnegative. Next we show that \( \sum \{ \mathbb{P}(T) : T \in \Omega_{MRF} \} = 1 \).

Consider the following identities

\[
\sum_{T \in \Omega_{MRF}} \mathbb{P}(T) = \sum_{k=1}^{N} \sum_{T \in \Omega_{MRF}(P_k) \cap \{ rt(T) = I_k \}} \mathbb{P}(T) = \sum_{k=1}^{N} \sum_{T \in \Omega_{MRF}(P_k) \cap \{ rt(T) = I_k \}} \frac{|rt(T)|}{\sum_{\{ I : l \in P \}} \mathbb{P}_l(T_l) \mathbb{P}_r(T_r)} \mathbb{P}_l(T_l) \mathbb{P}_r(T_r)
\]

The last sum can be written in the following way

\[
\sum_{T \in \Omega_{MRF}(P_k) \cap \{ rt(T) = I_k \}} \mathbb{P}(T) \mathbb{P}_r(T_r) = \sum_{T \in \Omega_{MRF}(P_k) \cap \{ rt(T) = I_k \}} \mathbb{P}_l(T_l) \mathbb{P}_r(T_r) = \sum_{T \in \Omega_{MRF}(P_k) \cap \{ rt(T) = I_k \}} \sum_{T \in \Omega_{MRF}(P_l)} \mathbb{P}_l(T_l) \mathbb{P}_r(T_r)
\]

Due to the induction hypothesis, each factor in the last term equals to one. Replacing this fact in the previous expression we get

\[
\sum_{T \in \Omega_{MRF}} \mathbb{P}(T) = \sum_{k=1}^{N} \sum_{\{ I : l \in P \}} \mathbb{P}_l(T_l) \mathbb{P}_r(T_r) = \sum_{\{ I : l \in P \}} \frac{1}{\sum_{\{ I : l \in P \}} \sum_{k=1}^{N} |I_k|} = 1.
\]

which completes the proof. \( \square \)

Remark 2. Observe that the space \( \Omega_{MRF}(P) \) with \#\( P = i \), is made of all possible binary trees on \( i \) vertices; to ease notation we write \( \Omega_{MRF}([i]) \). Denoting by \( b_i \) the number of all possible binary trees on \( i \) vertices, with the artificial convention that \( b_0 = 1 \), then \#\( \Omega_{MRF}([i]) = b_i \). Moreover, the set of all possible binary trees satisfies the Catalan recursion

\[
\# \Omega_{MRF}([N]) = b_N = \sum_{i=1}^{N-1} b_i b_{N-1-i} = \sum_{i=1}^{N-1} \# \Omega_{MRF}([i]) \# \Omega_{MRF}([N-1-i]). \tag{3}
\]

Therefore, the cardinal of the space is given by

\[
\# \Omega_{MRF}(P) \equiv \frac{1}{N+1} \binom{2N}{N}, \quad \#P = N. \tag{4}
\]
Let Lemma 4.

Notice that while \( H \)

Step 1. Suppose that the length of every interval in \( \mathcal{P} \).

Proof.

(i) It is direct to see that the depth of an interval equals the total number of its ancestors.

(ii) Consider the set \( S \) of all intervals with the uniform probability function, if and only if, all the intervals have the same length.

Definition 6. Let \( \mathcal{P} = \{ I_n : n \in [N] \} \), \( \Omega_{MRF} \) be as in Definition 4 and \( i \in [N] \) be fixed. Define

(i) \( H_i : \Omega_{MRF} \to \mathbb{N} \cup \{0\} \), \( H_i(T) = \) the depth of the interval \( I_n \) in the tree \( T \in \Omega_{MRF} \).

(ii) Given \( k \in [N] - \{i\} \), define \( X_{i,k} : \Omega_{MRF} \to \{0, 1\} \) as \( X_{i,k}(T) = 1 \) if \( l_k \) is ancestor of \( i \) in \( T \) and \( X_{i,k}(T) = 0 \) otherwise.

(iii) For \( k \neq i \) define the quantity

\[
  w_{i,k} \overset{\text{def}}{=} \sum_{\ell = \min\{i,k\}}^{\max\{i,k\}} |l_{\ell}|.
\]

Notice that while \( H_i \), \( X_{i,k} \) are random variables, depending on the tree, the quantities \( w_{i,k} \) are not, moreover \( w_{i,k} = w_{k,i} \).

Lemma 4. Let \( \mathcal{P} = \{ I_n : n \in [N] \} \) and \( \Omega_{MRF} \) be as in Definition 4. Then

(i) The height of the interval \( I_i \) satisfies \( H_i = \sum_{k \neq i} X_{i,k} \).

(ii) \( \mathbb{E}(X_{i,k}) = \frac{|l_k|}{w_{i,k}} \), with \( w_{i,k} \) as defined in (5).

Proof. (i) It is direct to see that the depth of an interval equals the total number of its ancestors.

(ii) Consider the set \( S \) of all intervals with the uniform probability function, if and only if, all the intervals have the same length. Therefore, \( k \) is the ancestor of \( i \) if and only if \( l_k \) is the first interval chosen in the family \( S \). The probability of this event is given by \( \frac{|l_k|}{w_{i,k}} \) and since \( X_{i,k} \) states whether or not the event took place, its expectation is equal to the probability of the event, which gives the result.

Theorem 5. Let \( \mathcal{P} = \{ I_n : n \in [N] \} \), and \( \Omega_{MRF} \) be as in Definition 4. Then the expected depth of the interval \( I_i \) satisfies

\[
\mathbb{E}(H_i) = \mathcal{O}\left( \log \left( \frac{\sum \{ |l| : l \in \mathcal{P} \}}{|I_i|} \right) \right)
\]

Proof. Step 1. Suppose that the length of every interval in \( \mathcal{P} \) is an integer i.e., \( |l_n| \in \mathbb{N} \) for all \( n \in [N] \). Due to the first and the second part of Lemma 4, we know that

\[
\mathbb{E}(H_i) = \sum_{k \neq i} \mathbb{E}(X_{i,k}) = \sum_{k \neq i} \frac{|l_k|}{w_{i,k}}
\]

Observe that since \( |l_k| \) and \( w_{i,k} \) are positive integers with \( |l_k| < w_{i,k} \), then

\[
\frac{|l_k|}{w_{i,k}} \leq \frac{1}{w_{i,k}} + \frac{1}{w_{i,k} - 1} + \frac{1}{w_{i,k} - 2} + \ldots + \frac{1}{w_{i,k} - |l_k| + 1} = \sum_{\ell = w_{i,k} - |l_k| + 1}^{w_{i,k}} \frac{1}{\ell}
\]
Also observe that $w_{i,k+1} - |l_{k+1}| + 1 = w_{i,k} + 1$ for any $k < N$. Then,

$$\sum_{k > i} |l_k| \leq \sum_{k > i} \ell = \sum_{\ell = |l_i|+1}^{|l_k|} \frac{1}{\ell} = \sum_{\ell = |l_i|+1}^{w_{i,n}} \frac{1}{\ell},$$

$$\sum_{k < i} |l_k| \leq \sum_{k < i} \ell = \sum_{\ell = |l_i|+1}^{w_{i,n}} \frac{1}{\ell} = \sum_{\ell = |l_i|+1}^{w_{i,n}} \frac{1}{\ell},$$

because the index $\ell$ becomes consecutive from one sum to the next. As for the limits of the sum, in the first row the minimum value that $\ell$ would take is $|l_i| + 1$, when $k = i + 1$ and its maximum value is $w_{i,n}$, when $k = N$ since $k > i$. In the second row, given that $k < i$, the maximum possible value that $\ell$ takes is $w_{i,1}$, when $k = 1$ and the minimum possible value is again $|l_i| + 1$, when $k = i - 1$. Using these bounds in (7) we get

$$\mathbb{E}(H_i) = \sum_{k > i} \frac{|l_k|}{w_{i,k}} + \sum_{k < i} \frac{|l_k|}{w_{i,k}} \leq \sum_{\ell = |l_i|+1}^{w_{i,n}} \frac{1}{\ell} + \sum_{\ell = |l_i|+1}^{w_{i,1}} \frac{1}{\ell} \leq \log \left( \frac{w_{i,n}}{|l_i|} \right) + \log \left( \frac{w_{i,1}}{|l_i|} \right) \leq 2 \log \left( \frac{w_{i,n}}{|l_i|} \right).$$

The last line holds because $w_{n,1} = \max \{w_{i,k} : i, k \in [N], i \neq k \}$. Hence, the first step is complete.

**Step 2.** Suppose that the length of every interval in $\mathcal{P}$ is rational i.e., $|l_n| \in \mathbb{Q}$ for all $n \in [N]$. Since $\mathcal{P}$ is a monotone partition, clearly $a_i = \min \{x : x \in \bigcup_{n \in [N]} I_n \}$. Let $q \in \mathbb{N}$ be such that $q|l_n| \in \mathbb{N}$ for all $n \in [N]$ and consider the monotone partition $\mathcal{P}_0$ def $\{J_n : n \in [N]\}$ with $J_n = q(l_n - a_1) = \{q(x - a_1) : x \in I_n \}$. The number of intervals in both partitions is equal and all the ratios between the intervals are preserved. Then, there exists a bijection $\varphi : \Omega_{\text{MRF}}(\mathcal{P}) \rightarrow \Omega_{\text{MRF}}(\mathcal{P}_0)$ such that $\mathbb{P}(T) = \mathbb{P}_0(\varphi(T))$ for all $T \in \Omega_{\text{MRF}}(\mathcal{P})$; where $\mathbb{P}$, $\mathbb{P}_0$ are the probabilities in the spaces $\Omega_{\text{MRF}}(\mathcal{P})$ and $\Omega_{\text{MRF}}(\mathcal{P}_0)$ respectively. Denoting by $H_{i,j}$ the heights of the intervals $I_i$ and $J_j$ respectively, and recalling the first step we have

$$\mathbb{E}(H_{i,j}) = \mathbb{E}(H_{i,j}) \leq O\left( \sum_{\{J : j \in \mathcal{P}_0\}} \frac{1}{|l_i|} \right) = O\left( \sum_{\mathcal{P}} \frac{\{J : j \in \mathcal{P}\}}{|l_i|} \right).$$

**Step 3.** Suppose that there are no restriction on the length of the intervals i.e., $|l_n| > 0$ for all $n \in [N]$. The proof is done building a sequence of partitions whose intervals have rational lengths, approximating the expected height. To see this, take a vector $\mathbf{q} \in \mathbb{Q}^N$ with rational coordinates such that

$$q_i > |l_i|,$$

$$q_k < |l_k|, \quad \sum_{\ell = \min\{i,k\}}^{\max\{i,k\}} q_\ell < w_{i,k}, \quad \text{for all } k \in [N] - \{i\}. \quad (8)$$

Due to the density of the rationals in the reals, such choice can be made. Then, for every $k \in [N] - \{i\}$ the following inequalities hold

$$\frac{|l_i|}{w_{i,k}} \leq \frac{|l_i|}{|l_i| + (w_{i,k} - |l_i|)} < \frac{q_i}{q_i + (w_{i,k} - |l_i|)} = \frac{q_i}{q_i + \left( \sum_{\ell = \min\{i,k\}}^{\max\{i,k\}} q_\ell - q_i \right)} = \frac{q_i}{\sum_{\ell = \min\{i,k\}}^{\max\{i,k\}} q_\ell}.$$
In order to analyze the independence of the random variables involved in the expression above we proceed by

Recall that

**Proof.**

\[ V \left( X_{i,k} \right) = \frac{\left| I_i \right|}{w_{i,k}} \leq \frac{\left| J_n^q \right|}{w_{i,k}} = E(X_{i,k}^q), \]

for every \( k \in [N] - \{i\} \). Denote by \( H_i^q \), the random variable indicating the depth of the interval \( J_i \) in \( T \in \Omega_{\text{MRF}}(\mathcal{P}^q) \) and recall that \( H_i^q = \sum_k X_{i,k}^q \) (see Lemma 4 (i)). Next, computing expectations we get

\[ E(H_i) = \sum_{k \neq i} E(X_{i,k}) \leq \sum_{k \neq i} E(X_{i,k}^q) = E(H_i^q) \leq 2 \log \left( \frac{\sum \left\{ \left| J_n^q : n \in [N] \right| \right\}}{\left| J_n^q \right|} \right), \]

where the last estimate holds due to part (ii). Observe that due to the density of the rationals in the real line, it is possible to choose a sequence \( \{\eta_\ell : \ell \in \mathbb{N}\} \subseteq \mathbb{Q}^N \) satisfying the conditions \( [8] \) and such that \( \left\| \eta_\ell - I_i \right\| \to 0 \) for all \( i \in [N] \). Since the estimate \( [9] \) holds for every rational satisfying the conditions, in particular it holds for every \( \eta_\ell \) then, letting \( \ell \to \infty \) the result follows.

\[ \square \]

2.1. Variance and Confidence Intervals of the Monotone Random Forest \( \Omega_{\text{MRF}} \)

In the present section we estimate the variance of the heights through the monotone random forest and use this information to give a number of Bernoulli trials (random sampling) in order to guarantee a confidence interval with a confidence level for the computed value of the expected height.

**Theorem 6.** Let \( \mathcal{P} = \{I_n : n \in [N]\} \), and \( \Omega_{\text{MRF}} \) be as in Definition [4]. Then

\[ \var(H_i) = \sum_{k \neq i} E(X_{i,k}) + \sum_{k \neq i} E(X_{i,k}) \sum_{\ell \neq i} E(X_{i,\ell}) - E^2(H_i), \]

\[ \var(H_i) \leq E(H_i), \]

for all \( i = 0, \ldots, N \).

**Proof.** Recall that \( \var(H_i) = E(H_i^q) - E^2(H_i) \) and that \( H_i = \sum_k X_{i,k} \), then

\[ \var(H_i) = E(H_i^q) - E^2(H_i) = \sum_{k \neq i} E(X_{i,k}) + \sum_{k \neq i} \sum_{\ell \neq i} E(X_{i,k}X_{i,\ell}) - E^2(H_i). \]

In order to analyze the independence of the random variables involved in the expression above we proceed by cases

\[ k < i < \ell \text{ or } \ell < i < k : \]

\[ \mathbb{P}(X_{i,k}X_{i,\ell} = 1) = \mathbb{P}(X_{i,k} = 1)\mathbb{P}(X_{i,\ell} = 1). \]
\[ k < \ell < i \text{ or } i < \ell < k : \]
\[ \mathbb{E}(X_{i,k}X_{i,\ell}) = \mathbb{P}(X_{i,k}X_{i,\ell} = 1) = \mathbb{P}(X_{i,k} = 1)\mathbb{P}(X_{i,\ell} = 1|X_{i,k} = 1) = \mathbb{E}(X_{i,k})\mathbb{E}(X_{i,\ell}). \]

\[ \ell < k < i \text{ or } i < k < \ell : \]
\[ \mathbb{E}(X_{i,k}X_{i,\ell}) = \mathbb{P}(X_{i,k}X_{i,\ell} = 1) = \mathbb{P}(X_{i,k} = 1)\mathbb{P}(X_{i,\ell} = 1|X_{i,k} = 1) = \mathbb{E}(X_{i,k})\mathbb{E}(X_{i,\ell}). \]

Using the latter, to bound the second summand of the former expression we get,
\[ \sum_{k \neq i} \sum_{\ell \neq i} \mathbb{E}(X_{i,k}X_{i,\ell}) = \sum_{k \neq i} \sum_{\ell \neq i} \mathbb{E}(X_{i,k})\mathbb{E}(X_{i,\ell}) \]
\[ = \sum_{k \neq i} \mathbb{E}(X_{i,k}) \sum_{\ell \neq i} \mathbb{E}(X_{i,\ell}) \]
\[ \leq \sum_{k \neq i} \mathbb{E}(X_{i,k}) \sum_{\ell \neq i} \mathbb{E}(X_{i,\ell}) = \mathbb{E}^2(H_i). \]

Combining the equality of the second line above with (11), Equation (10a) follows. Finally, combining the inequality of the third line in the expression above with (11), the estimate (10b) follows.

Getting an estimate of the variance is useful to determine the number of Bernoulli trials (sampling) that has to be done in order to assure a confidence level of our numerical results. For instance, if the confidence interval is to furnish, respectively a 90% and 95% confidence, the number of trials is given by (see [10])
\[ K_0 \overset{\text{def}}{=} (\frac{1.645}{0.1})^2 \text{Var}(H_i), \quad K_0 \overset{\text{def}}{=} (\frac{1.96}{0.05})^2 \text{Var}(H_i). \quad (13) \]

Therefore, we would like the value of \( \max_{j=1}^{N} \text{Var}(H_j) \). However, it is not possible to give a closed formula, hence we aim for an estimate. For a fixed number of \( N \) points distributed inside a fixed interval, namely \( (0,1) \), it is well-known that the variance of the heights will be maximum when the points are equidistant i.e., the chances for an interval to be chosen attain its maximum level of uncertainty. Consequently, we adopt the maximum possible variance of a monotone partition \( \mathcal{P} \) whose endpoints are \( x_i, i = 0, 1, \ldots, N \). We use the equality (11) to compute numerically such maxima, the table 1 displays certain important values.

Consequently, we compute the corresponding value \( \delta_N^2 \) for the problem at hand or simply adopt it from a tables such as [1] or a regression model such as Equation (15), to plug in Equation (13) and compute the number of necessary Bernoulli trials \( K \) according to the desired confidence level
\[ K \overset{\text{def}}{=} (\frac{1.645}{0.1})^2 \delta_N^2, \quad K \overset{\text{def}}{=} (\frac{1.96}{0.05})^2 \delta_N^2. \quad (14) \]

An elementary linear regression adjustment gives
\[ \text{Var}(\lambda^3) = 1.99j - 2.38, \quad \kappa = 0.9967, \quad \sigma = 0.076. \]

Here \( \kappa \) is the correlation coefficient and \( \sigma \) is the standard error. A quick change of variable gives
\[ \text{Var}(n) = \frac{1.99}{\log 3} \log n - 2.38, \quad \kappa = 0.9967, \quad \sigma = 0.076, \quad (15) \]

where \( n \) is the number of intervals in the monotone partition \( \mathcal{P} \).

**Theorem 7** (Computational Cost of the Methods). \( (i) \) The DIRF method computational cost is \( \mathcal{O}(n \log n) \), as suggested in [4] [3].
Table 1: Maximum Variance Table

| Exponent | Intervals | Maximum Variance |
|----------|-----------|------------------|
| 1        | 3         | 0.25             |
| 2        | 9         | 1.32             |
| 3        | 27        | 3.22             |
| 4        | 81        | 5.32             |
| 5        | 243       | 7.48             |
| 6        | 729       | 9.67             |
| 7        | 2187      | 11.86            |

(ii) Under the hypothesis that DIRF and IRF have variance of the same order, the IRF method computational cost $O(n \log n)$. (As suggested in [1, 2].)

Proof. (i) Combining (14) and (15) with Proposition 1 the result follows.

(ii) The hypothesis on the IRF variance implies that (14) and (15) are valid. Therefore, the previous reasoning applies and the proof is complete.

\[ \text{\hspace{1cm} } \]

2.2. The Relationship Between Monotone Random Trees and iTrees

In the present section, we illustrate the link between the monotone random tree algorithm introduced in Definition 4 and the iTree introduced in Definition 1 for the 1D setting. To that end we first recall a definition and a proposition from basic graph theory (see [9]).

Definition 7. The line graph $L(G)$ of a graph $G$ has a vertex for each edge of $G$, and two vertices in $L(G)$ are adjacent if and only if the corresponding edges in $G$ have a vertex in common.

Proposition 8. The line graph of a tree is also a tree. Moreover, $h(L(T)) = h(T) - 1$, where $h(\cdot)$ denotes the height of the graph.

Proof. See [9].

In order to illustrate the relationship between monotone random trees and iTrees consider the tree $T$ of Figure 1 and transform it into the one displayed in Figure 2 (a), denoted by $E(T)$. The set of data $S$ is given by the extremes of the intervals in $P$, each node hosting an interval has two children and the edges were relabeled, using corresponding left and right subsets generated when the interval is chosen. Abstract vertices were added: whenever the label had a singleton, one as the root of $E(T)$ together with an edge connecting $rt(E(T))$ with $rt(T)$, labeled by the full set $S$. Once the $E(T)$ tree is constructed, it is direct to see that its line graph $L(E(T))$ is an isolation tree (iTree) of the data $S$.

Remark 3. Although it is possible to furnish a mathematically rigorous algorithm that would give a probability-preserving bijection between the spaces $\Omega_{MRF}$ and $\Omega_{IRF}$ in 1D. This would deliver relationships between expected heights and topological properties, as well as properties of the variance for the 1D $\Omega_{IRF}$. However, such construction is highly technical and contributes little to our topic of interest, therefore we omit it here. On the other hand we present Theorem 9 as simpler theoretical proof relating expected heights and topological properties.

Theorem 9. Let $S \equiv \{x_0, x_1, \ldots, x_N\}$ be an arbitrary set of points on the line such that $x_0 < x_1 < \ldots < x_N$. Let $H_i : \Omega_{IRF} \to \mathbb{N}$ be the random variable with $H_i(T)$ defined as the depth of the data $x_i$ in the isolation random tree $T$. Then

\[
E(H_i) = O\left( \log \left( \frac{x_N - x_0}{\text{dist}(x_i, S - \{x_i\})} \right) \right),
\]

(16)
Proof. Define the intervals \( I_n \defeq x_n - x_{n-1} \) for every \( n \in [N] \) and the partition \( P \defeq \{ I_n : n \in \mathbb{N} \} \). Denote by \( H_i \) the random variable indicating the depth in \( \Omega_{\text{IRF}} \) of the interval \( I_i \), then the following relations are direct
\[
H_i = 1 + \max\{ H_i, H_{i-1} \} \quad i \in \{1, \ldots, N\},
\]
\[
H_0 = 1 + H_0, \quad H_N = 1 + H_N.
\]
Since \( H_j \geq 0 \) for all \( j \in [N] \), then \( H_i \leq 1 + \tilde{H}_i + \tilde{H}_{i-1} \), for all \( i \in [N] \); hence
\[
\mathbb{E}(H_i) \leq 1 + \mathbb{E}(\tilde{H}_i) + \mathbb{E}(\tilde{H}_{i-1})
\]
\[
\leq 1 + O\left( \log\left( \frac{\sum\{ |I_i| : n \in [N] \}}{|I_i|} \right) \right) + O\left( \log\left( \frac{\sum\{ |I_i| : n \in [N] \}}{\min\{ |I_{i-1}|, |I_i| \}} \right) \right)
\]
\[
\leq O\left( \log\left( \frac{\sum\{ |I_i| : n \in [N] \}}{\min\{ |I_{i-1}|, |I_i| \}} \right) \right).
\]
Since \( x_N - x_0 = \sum\{ |I_i| : n \in [N] \} \) and \( \text{dist}(x_i, S - \{ x_i \}) = \min\{ |I_{i-1}|, |I_i| \} \) the proof is complete. \( \square \)

2.3. The Quality of the Bound \( b(H) \)

In this section we discuss the quality of the bound \( b \) first for a monotone partition \( P = \{ I_i : 1 \leq i \leq N \} \) we introduce the quantity
\[
b(H_i) \defeq \log \frac{\sum\{ |I_i| : l \in P \}}{|I_i|}, \quad i = 1, \ldots, N.
\]

**Theorem 10.** Consider a monotone partition \( P = \{ I_n : n \in [N] \} \) defined by the sequence of points
\[
S \defeq \{ 0, d, x_2, \ldots, x_{N-1}, 1 \}, \quad 0 < d < x_2 < \ldots < x_{N-1} < 1.
\]
Then,
\[
\frac{\mathbb{E}(H_i)}{b(H_i)} \xrightarrow{d 	o 0} 0, \quad \frac{\mathbb{E}(H_i)}{b(H_i)} \xrightarrow{d 	o 1} 1.
\]
(Notice that there are no conditions for \(x_k\) with \(k = 2, \ldots, N - 1\), other than the monotonicity and the boundedness detailed above.)

Proof. Recall that the height of the interval \(I_1\) is given by \(H_1 = \sum_{k=2}^{N} X_{1,k}\). From Lemma 4 we have \(E(X_{1,k}) = \frac{x_k - x_{k-1}}{x_k}\). Hence,

\[
E(H_1) = \sum_{k=2}^{N} \frac{x_k - x_{k-1}}{x_k} \leq \sum_{k=2}^{N} \frac{x_k - x_{k-1}}{d} = \frac{1 - d}{d},
\]

next

\[
E(H_1) = \sum_{k=2}^{N} \frac{x_k - x_{k-1}}{x_k} \geq \sum_{k=2}^{N} \frac{x_k - x_{k-1}}{1} = 1 - d.
\]

On the other hand,

\[
b(H_1^{(j)}) = \log \frac{1}{d} = -\log d.
\]

Combining the above, the ratio has the following bounds

\[
0 \leq \frac{d - 1}{d \log d} \leq \frac{E(H_1)}{b(H_1)} \leq \frac{d - 1}{d \log d}.
\]

Letting \(d \to 0\), the upper bound above delivers the first limit in (18); while letting \(d \to 1\), the lower bound in the expression above yields the second limit in (18).

Remark 4. The theorem above states that the quality of the bound \(b(H_1)\) improves as the point becomes more of an outlier and it deteriorates as the point gets closer to the cluster of points. Hence, \(E(H_1)\) contains reliable topological information for outliers, though its quality of information is poor for cluster points.

3. The General Setting

The present section presents the features of the isolation random forest that can be proved in general, these are the its probability structure, its cardinality and the fact that the IRF method converges and it is well-defined. For the analysis of general case first we need to introduce a hypothesis

**Hypothesis 1.** Given a set of data \(S = \{x_0, \ldots, x_N\} \subseteq \mathbb{R}^d\), from now on it will be assumed that no coordinates are repeated i.e.

\[
\#\pi_j(S) = N + 1, \quad \text{for all } j = 0, 1, \ldots, N.
\]

Here \(\pi_j(S)\) is the \(j\)-th projection of the set \(S\) as defined in Equation (1).

**Definition 8.** Let \(S = \{x_0, \ldots, x_N\} \subseteq \mathbb{R}^d\) be a data set satisfying Hypothesis 1 for each \(j \in [d]\).

(i) Denote by \(P^{(j)} \overset{\text{def}}{=} \{I_{n}^{(j)} : n \in [N]\}\) the family of intervals defined by sorting points of the set \(\pi_j(S) = \{x_n \cdot \hat{e}_j : n = 0, \ldots, N\}\).

(ii) Define the grid of the set by \(G \overset{\text{def}}{=} \prod_{j=1}^{d} \pi_j(S)\).

(See Figure 3(a) for an illustration when \(S \subseteq \mathbb{R}^2\).)
Remark 5. (i) Observe that Hypothesis 1 is mild because, it will be satisfied with probability one for any given configuration/set.

(ii) Notice that, for any data set \( S \subseteq \mathbb{R}^d \) the partitions \( \{ P(j) : j \in [d] \} \) are a monotone partition the interval \( (\min \pi_j(S), \max \pi_j(S)) \) for all \( j \in [d] \).

Next we prove that given a data set, its isolation random forest is a probability space.

**Theorem 11.** Let \( S \overset{\text{def}}{=} \{ x_0, x_1, \ldots, x_N \} \subseteq \mathbb{R}^d \) and let \( \Omega_{\text{IRF}} \) be as in Definition 2. Then, the algorithm induces a probability measure in \( \Omega_{\text{IRF}} \).

**Proof.** We prove this theorem by induction on the cardinal of the set \#\( S \). For \#\( S = N = 1 \) the only possible tree is the trivial one. For \#\( S = N = 2 \) the result also holds. Due to Theorem 1 only one instance is needed to form the only possible isolation tree. Given that the isolation tree is unique, it has probability one.

Assume now that the result is true for any data set satisfying Hypothesis 1 with cardinal less or equal than \( N - 1 \). Let \( S = \{ x_0, \ldots, x_N \} \) be a set and let \( T \in \Omega_{\text{IRF}} \) be arbitrary, such that \( j \in [d] \) was the first direction of separation, with corresponding split value \( p^T \in (\min \pi_j(S), \max \pi_j(S)) \). \( T_l, T_r \) left & right subtrees and \( S_l, S_r \) left & right sets (as in Definition 1). Suppose that \( p^T \) belongs to the interval \( l_{\alpha}^{(j)} \) then, the probability that \( T \) occurs, equals the probability of choosing the direction \( j \in [d] \), times the probability of choosing \( l_{\alpha}^{(j)} \) among \( P(j) \), times the probability that \( T_\alpha \) occurs in \( S_\alpha \) when \( \alpha \in \{l, r\} \), i.e.

\[
\mathbb{P}(T) = \frac{1}{d} \sum_{\{l\} : l \in \mathcal{P}(j)} |l_{\alpha}^{(j)}| \mathbb{P}_l(T_l) \mathbb{P}_r(T_r).
\]
Here \( \mathbb{P}_\alpha(T_\alpha) \) indicates the probability that \( T_\alpha \) occurs in the space of isolation random trees defined on the sets \( S_\alpha \), for \( \alpha \in \{I, R\} \); which is well-defined since \( \#S_\alpha \leq N - 1 \). Denoting by \( \Omega_{\text{IRF}}(\mathbb{P}_\alpha) \) the space of isolation random trees defined on the set \( S_\alpha \), by the induction hypothesis we know that \( \mathbb{P}_\alpha : \Omega_{\text{IRF}}(\mathbb{P}_\alpha) \to [0, 1] \) is a well-defined probability, consequently \( \mathbb{P}(T) \) is nonnegative. Next we show that \( \sum (\mathbb{P}(T) : T \in \Omega_{\text{IRF}}) = 1 \). Consider the following identities:

\[
\sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T) = \sum_{j=1}^{d} \sum_{T \in \Omega_{\text{IRF}}} \frac{1}{d} \sum_{l \in I_l^{(j)}} \mathbb{P}(T) = \sum_{j=1}^{d} \sum_{l \in I_l^{(j)}} \frac{1}{d} \sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T) = \sum_{j=1}^{d} \sum_{l \in I_l^{(j)}} \frac{1}{d} \sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T)
\]

The sum nested in the third level can be written in the following way:

\[
\sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T) = \sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T) = \sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T) = \sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T) = 1
\]

Due to the induction hypothesis, each factor in the last term equals to one. Replacing this fact in the former expression we get:

\[
\sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T) = \sum_{j=1}^{d} \sum_{n=1}^{N} \frac{1}{d} \sum_{T \in \Omega_{\text{IRF}}} \mathbb{P}(T)
\]

which completes the proof.

\[\square\]

**Corollary 12.** Let \( S \) be as in Definition 1. Given a sequence of random \( \text{iTree} \) algorithm experiments (or Bernoulli trials), denoted by \( (T_n)_{n \in \mathbb{N}} \), denote by \( (H_\alpha(T_n))_{n \in \mathbb{N}} \) the sequence of corresponding depths for the point \( x \in S \). Then,

\[
\frac{H_\alpha(T_1) + H_\alpha(T_2) + \ldots + H_\alpha(T_n)}{n} \to \mathbb{E}(H_\alpha).
\]

In particular, the IRF method converges and it is well-defined.

**Proof.** It is a direct consequence of the Law of the Large Numbers, see [11].

Next we present the cardinal of the space \( \Omega_{\text{IRF}} \).
Theorem 13 (Cardinal of the Isolation Random Forest). Let $S \overset{\text{def}}{=} \{x_0, x_1, \ldots, x_N\} \subseteq \mathbb{R}^d$ and $\Omega_{\text{IRF}}$ be as in Hypothesis 11, then

$$\# \Omega_{\text{IRF}}(N) \equiv \frac{1}{N} \binom{2(N-1)}{N-1} d^{N-1} = C_{N-1} d^{N-1}, \quad \forall N \geq 1. \quad (22)$$

Here $C_{N-1}$ denotes the $N-1$ Catalan number.

Proof. Let $t_i$ be the number of all possible isolation trees on $i$ data, with the artificial convention $t_0 = 0$. From the proof of Theorem 11 it also follows that $t_1 = 1$. Then, the following recursion is satisfied

$$t_{N+1} = \sum_{T \in \Omega_{\text{IRF}}(N+1)} \prod_{j=1}^d \sum_{n=1}^{N_n} 1 = \sum_{n=1}^N \sum_{j=1}^d t_n t_{N+1-n} = d \sum_{n=0}^{N+1} t_n t_{N+1-n}, \quad \forall N \in \mathbb{N}. \quad (23)$$

Notice that if $\rho^T \in I^{(n)}_n$ then $\# S_l = n$ and $\# S_r = N + 1 - n$. Therefore, the sum $\sum \{1 : T \in \Omega_{\text{IRF}}, \rho^T \in I^{(n)}_n\}$ counts all the possible combinations of trees on $S_l$ times the trees on $S_r$, whose cardinals are $t_n$ and $t_{N+1-n}$ respectively. Replacing the latter in the expression above, we have

$$t_{N+1} = \sum_{j=1}^d \sum_{n=1}^N t_n t_{N+1-n} = d \sum_{n=0}^{N+1} t_n t_{N+1-n}. \quad \forall N \in \mathbb{N}. \quad (23)$$

Let $g(x) \overset{\text{def}}{=} \sum_{i \geq 1} t_i x^i$ be the generating function of the sequence $(t_i)_{i \geq 1}$, then the relation $dg^2(x) + x = g(x)$ holds which, solving for $g(x)$ and recalling that $g(0) = t_0 = 0$ gives

$$g(x) = \frac{1 - \sqrt{1 - 4dx}}{2d}. \quad (24)$$

The generalized binomial theorem states

$$g(x) = \frac{1}{2d} \left(1 - \sum_{k \geq 0} \binom{1/2}{k} (-4dx)^k\right) = \frac{1}{d} \sum_{k \geq 1} \binom{1/2}{k} (-1)^{k+1} 2^{2k-1} d^k x^k. \quad (25)$$

Recalling that

$$\binom{1/2}{k} = \frac{(-1)^{k-1}}{2^k} \frac{1 \cdot 3 \ldots \cdot (2k - 3)}{1 \cdot 2 \ldots \cdot k},$$

we conclude

$$t_k = \frac{1}{k} \left(\frac{2(k-1)}{k-1}\right) d^{k-1}. \quad (26)$$

The above concludes the proof. \qed

3.1. The Inconclusiveness of the Expected Height.

In the present section, it will be seen that the expectation of the depth, depending on the configuration of the points, has different topological meaning, when working in multiple dimensions. This is illustrated with two particular examples in 2D. Before presenting them some context needs to be introduced.

Hypothesis 2. The data set $S \subseteq \mathbb{R}^2$ satisfies

(i) All the data are contained in the first quadrant of the plane.

(ii) The set $S$ contains the origin 0.
(iii) The set $S$ verifies the hypothesis 1 of Section 3.

From now on we concentrate on analyzing the depth of origin $0$ in the $\Omega_{\text{IRF}}$. Notice that in this case the potential ancestors of $0$ have the structure $A = S \cap R$ where $R \subseteq \mathbb{R}^2$ is a rectangle whose edges are parallel to the coordinate axes, see Figure 3(a). Given that infinitely many rectangles satisfy this conditions we consider $R_A \overset{\text{def}}{=} \{ R : A = R \cap S \}$, and $R$ is a rectangle. Now, $R_A$ can be identified with its upper right corner, moreover, given a set $S$ with associated grid $G_S = \{0, p_1, \ldots, p_N\} \times \{0, q_1, \ldots, q_N\}$, we denote a potential ancestor by $[p_i, q_j] \overset{\text{def}}{=} \{ x \in S : x \cdot \hat{e}_1 \leq p_i, x \cdot \hat{e}_2 \leq q_j \}$, see Figure 3. Notice that, depending on the configuration of $S$, not every element of $G_S$ defines a potential ancestor, also observe that the different configurations/sets may have an ancestor identified by the same pair, as it is the case of $[p_i, q_j]$ in see Figure 3(b). Finally, we introduce the indicator function analogously to the one given in Definition 4.

Recalling Lemma 4 it is direct to see $H_0 = \sum_{i \in [N]} X_{[p_i, q_j]} : [p_i, q_j]$ is a potential ancestor of $0$).

**Lemma 14** (Inconclusiveness in 2D). Given a set $S = \{x_0, x_1, \ldots, x_N\}$ in $\subseteq \mathbb{R}^2$, the topological meaning of the expected height, found by the IRF method is inconclusive and no general quality certificate can be established for the method.

**Proof.** Consider the following two sets.

Set 1. (A monotone configuration.) Let $S_1 = \{x_0, x_1, \ldots, x_N\} \subseteq \mathbb{R}^2$ satisfy Hypothesis 2. Let $G_S = \{0, p_1, \ldots, p_N\} \times \{0, q_1, \ldots, q_N\}$ be its associated grid and suppose that $x_i = p_i \hat{e}_1 + q_i \hat{e}_2$ for $i \in [N]$. In this particular case, the ancestors are identified with the points $x_i \in S$, moreover they are the upper right corner of the associated rectangle.

$$H_0 = \sum_{i \in [N]} X_{[p_i, q_j]}.$$ Adopting the convention that $p_0 = q_0 = 0$ we have

$$\mathbb{E}(X_{[p_i, q_j]}) = \begin{cases} \frac{1}{2} \frac{p_{i+1}-p_i}{p_{i+1}}, & 1 \leq i \leq N-1, \\ \frac{1}{2} \frac{q_{i+1}-q_i}{q_{i+1}}, & i = N, \\ 1, & \end{cases}$$

Thus, the expectation is given by

$$\mathbb{E}(H_0) = 1 + \sum_{i=1}^{N-1} \frac{1}{2} \frac{q_{i+1}-q_i}{q_{i+1}} + \frac{1}{2} \frac{p_{i+1}-p_i}{p_{i+1}},$$

and the distance from the origin to the rest of the set is given by

$$d_i \overset{\text{def}}{=} \text{dist } (x_0, S - \{x_0\}) = \sqrt{p_i^2 + q_i^2}.$$ (24a)

Set 2. (A strategic transposition.) Let $S_2 = \{y_0, y_1, \ldots, y_N\} \subseteq \mathbb{R}^2$ satisfy Hypothesis 2. Let $G_S = \{0, p_1, \ldots, p_N\} \times \{0, q_1, \ldots, q_N\}$ be its associated grid and suppose that

$$y_1 = \begin{pmatrix} p_1 \\ q_2 \end{pmatrix}, \quad y_2 = \begin{pmatrix} p_2 \\ q_1 \end{pmatrix}, \quad y_i = \begin{pmatrix} p_i \\ q_i \end{pmatrix}, \quad \text{for all } i = 3, \ldots, N.$$ (24b)
In this particular case, all the points \( y_i \in S \) define each one a potential ancestor, but there is an additional one, the potential ancestor \([p_2, q_2]\). Then

\[
H_0 = X_{[p_2, q_2]} + X_{[p_1, q_2]} + \sum_{i=1}^{N} X_{[p_i, q_i]} \\
= X_{[p_1, q_2]} + X_{[p_2, q_1]} + \sum_{i=2}^{N} X_{[p_i, q_i]}.
\]

Adopting the convention that \( p_0 = q_0 = 0 \) we have

\[
E(X_{[p_i, q_i]}) = \begin{cases} 
\frac{1}{2} \frac{p_2 - p_1}{p_2}, & i = 2, j = 1, \\
\frac{1}{2} \frac{q_2 - q_1}{q_2}, & i = 1, j = 2, \\
\frac{1}{2} \frac{p_2 - p_{i-1}}{p_i} + \frac{1}{2} \frac{q_2 - q_{i-1}}{q_i}, & 2 \leq i = j \leq N - 1, \\
1, & i = j = N.
\end{cases}
\]

Computing the expectation we get

\[
E(H_0) = \frac{1}{2} \frac{q_2 - q_1}{q_2} + \frac{1}{2} \frac{p_2 - p_1}{p_2} + \sum_{i=2}^{N-1} \frac{1}{2} \frac{q_i - q_{i-1}}{q_i} + 1 + \frac{1}{2} \frac{p_i - p_{i-1}}{p_i}
\]

\[
= 1 + \sum_{i=1}^{N-1} \frac{1}{2} \frac{q_i - q_{i-1}}{q_i} + \frac{1}{2} \frac{p_i - p_{i-1}}{p_i}.
\]

Hence, the expected height is given by

\[
E(H_0) = 1 + \sum_{i=1}^{N-1} \frac{1}{2} \frac{q_i - q_{i-1}}{q_i} + \frac{1}{2} \frac{p_i - p_{i-1}}{p_i}, \quad (25a)
\]

and the distance from the origin to the rest of the set is given by

\[
d_2 \overset{\text{def}}{=} \text{dist}\left(\{x_0\}, S - \{x_0\}\right) = \min\left\{\sqrt{p_1^2 + q_1^2}, \sqrt{p_2^2 + q_2^2}\right\}. \quad (25b)
\]

Notice that if for both sets \( S^1 \) and \( S^2 \) the expected height has identical value, as Equations \( 24a \) and \( 25a \) show. However, the topological distance from \( \emptyset \) to the set \( S \) is different as Equations \( 24b \) and \( 25b \) show. Moreover, for simplicity assume that \( p_1 = q_1, p_2 = q_2 \) and let \( p_1 \to 0 \). Then, the distances behave as follows

\[
d_1 \overset{p_1 \to 0}{\longrightarrow} 0, \quad d_2 \overset{p_1 \to 0}{\longrightarrow} p_2.
\]

Since \( p_2 \) can take any value in \( \mathbb{R} \), the difference between distances can be arbitrarily large while their expected heights remain equal. In other words, in the first case the point is close to the set while in the second one \( p_2 \in \mathbb{R} \) can be chosen so that \( \emptyset \) becomes an anomaly, but the expected heights are identical and can not be used to distinguish between cases.

From the discussion above, it follows that although the IRF method is well-defined and it converges to \( E(H_x) \) for every \( x \in S \) (see Corollary \( 12 \)), the topological-metric meaning of such expected value may change according to the combinatorial configuration of the data. More specifically the value \( E(H_x) \) is inconclusive from the topological-metric point of view and therefore, its reliability to assess whether or not a point is an anomaly is uncertain. Moreover, the limits' analysis of the previous part shows that no general quality certificate about the method can be given.
Remark 6. A third example can be constructed similarly to the sets 1 and 2 above. Let \( S = \{z_0, z_1, \ldots, z_N\} \subseteq \mathbb{R}^2 \) be given by

\[
z_1 = \left( \frac{p_1}{q_N} \right), \quad z_i = \left( \frac{p_i}{q_{i-1}} \right), \text{ for all } i = 2, \ldots, N.
\]

Then, in this third configuration \( E(H_0) \) satisfies the the identity (25a), while the distance from the origin to the rest of the set is given by

\[
d_3 \overset{\text{def}}{=} \text{dist} (x_0, S - \{x_0\}) = \min \left\{ \sqrt{p_1^2 + q_N^2}, \sqrt{p_2^2 + q_1^2} \right\}.
\]

This third example ads even more inconclusiveness to the IRF method in multiple dimensions, in addition to that detected by the analysis presented in Lemma 14.

Theorem 15 (Inconclusiveness of the IRF Method). Given a set \( S = \{x_0, x_1, \ldots, x_N\} \subseteq \mathbb{R}^d \), the topological meaning of the expected height, found by the IRF method is inconclusive and no general quality certificate can be established for the method.

Proof. We proceed as in the proof of Lemma 14. In particular the result has been already shown for \( d = 2 \), then, from now on we assume that \( d \geq 3 \).

Consider a sequence of numbers \( 0 = r_0 < r_1 < \ldots < r_n \), recall the sets \( S_1, S_2 \) introduce in the proof of Lemma 14 and for \( k = 1, 2 \), define the sets

\[
\tilde{S}_k \overset{\text{def}}{=} \{ \tilde{x}_0, \tilde{x}_1, \ldots, \tilde{x}_N \}, \quad \tilde{x}_i \cdot \hat{e}_1 + \tilde{x}_i \cdot \hat{e}_j = x_i \in S_k, \quad \forall j \in \{3, 4, \ldots, N\}, \forall i \in [N].
\]

Since \( \tilde{S}_1, \tilde{S}_2 \) are embeddings of the sets \( S_1, S_2 \) in higher dimensions, it is direct to see that they have similar properties to the sets \( S_1, S_2 \), in particular the number and description of their potential ancestors. Therefore, the values of the expected height for the point \( 0 \) will agree but the distances from it to the nearest point can arbritrally disagree as already shown in Lemma 14.

3.2. A Modification of the IRF Method

In the current section we present a more robust version of the IRF Method. The Directional Isolation Random Forest Method (DIRF Method) works as follows

Definition 9 (The DIRF Method). Input: data set \( S \overset{\text{def}}{=} \{x_0, x_1, \ldots, x_N\} \subseteq \mathbb{R}^d \), number of Bernoulli trials \( K \).

(i) Find the principal directions of the set \( S \).

(ii) Project the data on each direction, i.e., generate \( \pi_j(S) \overset{\text{def}}{=} \{x \cdot \hat{e}_j : x \in S\} \), for \( j = 1, \ldots, d \).

(iii) For each Bernoulli trial, select at random one direction, namely \( \hat{e}_j \in [d] \). Perform iTree (see Definition 1 and/or Algorithm 1) on \( \pi_j(S) \) and store the heights \( \{h(x) : x \in S\} \) in a Log.

(iv) For each \( x \in S \), define \( H_{\text{DIRF}}(x) \) as the average height of the collection of heights \( \{h_k(x) : k = 1, \ldots, K\} \).

Here, it is understood that the number of Bernoulli trials \( K \) (see Section 2.1), is chosen to assure a confidence level for the computed value of the expected heights. Notice that

\[
H_{\text{DIRF}}(x) \overset{\text{def}}{=} \lim_{K \to \infty} \frac{1}{d} \sum_{i=1}^{d} H_i(x), \quad \text{for all } x \in S.
\]
Here $\mathbf{H}_i(\mathbf{x})$ indicates the expected height of the data $\mathbf{x} \cdot \hat{e}$, within the IRF of the set $S_i$, for all $i \in [d]$. The statement (26) can be easily seen as follows: define $A_i \overset{\text{def}}{=} \{ k \in [K] : \text{trial } k \text{ chose direction } i \}$, then

$$
\mathbf{H}_{\text{DIRF}}(\mathbf{x}) = \frac{1}{K} \sum_{k=1}^{K} h_k(\mathbf{x}) = \frac{1}{K} \sum_{i=1}^{d} \frac{|A_i|}{|A_i|} \sum_{k \in A_i} h_k(\mathbf{x}).
$$

(27)

Due to the Law of Large Numbers (see [11]) it is clear that for all $i \in [d]$, it holds that $\frac{|A_i|}{K} \rightarrow 1$ and due to Corollary 12 it is clear that for all $i \in [d]$, it holds that $\frac{1}{|A_i|} \sum_{k \in A_i} h_k(\mathbf{x}) \rightarrow H_i(\mathbf{x})$

4. Numerical Experiments.

The present section is devoted to the design and execution of numerical experiments in order to compare the performance of both algorithms; the following aspects are important in the execution and design of experiments

(i) The codes are implemented in python, some of the used libraries are pandas, scipy, numpy and matplotlib.

(ii) Although the experiments use benchmarks already labeled, we also use a distance-based definition of outlier, introduced in [3]

Definition 10. Let $r > 0$ and $0 \leq p \leq 1$ be two fixed parameters and $S \subseteq \mathbb{R}^d$ be a set. A point $\mathbf{x} \in S$ is said to be an outlier with respect to the parameters $r$ and $p$ if

$$
\frac{|B(\mathbf{x},r) \cap S|}{|S|} \leq p.
$$

(28)

Here $B(\mathbf{x},r) \overset{\text{def}}{=} \{ \mathbf{z} \in \mathbb{R}^d : \| \mathbf{x} - \mathbf{z} \| \leq r \}$, with $\| \cdot \|$ the Euclidean norm.

(iii) The number of Bernoulli trials $K$ is computed combining (14) and (15).

(iv) It is not our intention to debate the definition of an anomaly classifying threshold here. Therefore, our analysis runs through several quantiles acting as thresholds, which we adopt empirically based on observations of each case/example.

(v) Our study will analyze, not only anomalies correctly detected but also the performance of the method against false positives. In practice, both methods IRF and DIRF need a threshold under which all the values are declared anomalies by the method. This will include a number of false positives which we also quantify in our examples.

Example 1. The first example uses the benchmark “Breast Cancer Wisconsin (Diagnosis) Data Set”, downloaded from https://www.kaggle.com/uciml/breast-cancer-wisconsin-data. Although the original data base contains 569 individuals, 213 patients (37.2%) were diagnosed with cancer. It is clear that the patients diagnosed with cancer can not be considered anomalies if the full data base is used for the analysis. Therefore the original data set was modified: the subset of healthy patients was left intact and 20 randomly chosen patients with cancer (3.5%) were chosen to complete the set.

Two labels were used, the diagnosis label coming from the original data set itself and a distance-based label computed according to Definition 10 with parameters $r = 350$, $p = 0.05$. The number of Bernoulli trials is given by $K = 2250$. The original dataset contains 32 columns, therefore we combine our technique with the PCA method (Principal Components Analysis), see [12]. In this particular example the number of components was chosen according to the eigenvalues’ order magnitude; hence, we analyze the problem with its 1, 2, 4, 5, 7, 8 and 11 first components. Moreover, our experiments show that both methods severely decay their
Figure 4: Anomaly detection percentages for Example 1, Breast Cancer Diagnosis. All the graphics have the number of principal components in the $x$-axis and multiple curves for the quantiles to be used as a threshold. Figure (a) and (c) depict anomalies detected by both methods with the original labeling, while figures (b) and (d) display false positives introduced by both methods with the original labeling.

Table 2: Table of differences IRF – DIRF, Breast Cancer Diagnosis, Example 1. All the values are difference of percentages. The columns “A” and “F” stand for anomalies and false positives respectively.

| quantile [%] | 0.5 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|--------------|-----|---|---|---|---|---|---|---|
| components   | A   | F | A | F | A | F | A | F |
| 1            | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 2            | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | -5.0 | 8.3 |
| 4            | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 5.0 | -5.0 | -8.3 |
| 5            | 0.0 | 0.0 | 0.0 | -5.0 | 12.5 | 0.0 | 0.0 | 5.0 |
| 7            | 0.0 | 0.0 | 0.0 | 0.0 | -5.0 | 12.5 | 10.0 | 16.7 |
| 8            | 0.0 | 0.0 | 0.0 | -5.0 | 12.5 | -5.0 | 8.3 | -10.0 |
| 11           | 0.0 | 0.0 | 0.0 | -5.0 | 12.5 | -10.0 | 16.7 | -5.0 |

quality from 11 components on (due to the noise introduced by the lower order components). In particular both perform really poorly with the 32 components to be considered a viable option. Finally, the quantiles are 0.5, 1, 2, 3, 4, 5, 6 and 7; chosen from observing the behavior of this particular case.

The table reports the difference of achievements attained by both methods when subtracting the DIRF to
IRF. The predominance of negative and positive values in the columns “A” and “F” of the table respectively. This shows that the DIRF method performs better than the IRF method. Specially in the detection of false positives where DIRF performs significantly better than IRF: the former method presents convex curves, while the latter method shows concave (or pseudo-convex) curves (see Figure (b) and (d)).

Observe that the use of the quantiles is “dual” in the following sense. It is clear that all the curves tend to shift upwards when the quantile is amplified. This is good from the anomaly detection point of view but bad from the false positives inclusion point of view and it is hardly surprising: the larger the threshold, the more likely we are to detect more anomalies, but also the higher the price of including false positives. For our particular example using a quantile of 4% seems to be the “balanced choice”.

It must be observed that the quality of DIRF deteriorates with respect to IRF as we move along the diagonal of the table in particular DIRF performs poorly with respect to IRF from 7 PCA components and from the 6% quantile on.

The same experiments were performed but using the artificial distance-based labeling introduced in Definition 10. It can be observed that both methods perform better for the anomaly detection, which is not unexpected because the DIRF method is strongly related to a distance function for anomalies, as shown in Theorem 10. However, both methods perform worse from the false positives inclusion point of view. Finally, the DIRF method performs better than the IRF method, although its superiority in the false positives inclusion is not as remarkable as in the first case.

Example 2. The second example uses a benchmark of lymphoma diagnosis, downloaded from www.kaggle.com. The dataset consists of 148 patients, with only 6 of them diagnosed with cancer, i.e. 4%.

Two labels were used, the diagnosis label coming from the original data set itself and a distance-based label computed according to Definition 10 with parameters \( r = 300, p = 0.05 \). The number of Bernoulli trials is given by \( K = 1800 \). The original dataset contains 18 columns, consequently we apply the PCA method as in the previous example. In contrast with Example 1, in this case the order of magnitude of the eigenvalues does not change as abruptly, hence we work with the 1, 3, 6, 9 and 13 first components. Our experiments show that none of the methods has a good performance for any number of components and its quality decays even more from 6 components on (due to the noise introduced by the lower order components). Finally, the quantiles are 0.5, 1, 2, 3, 4, 5, 6 and 7; chosen from observing the behavior of this particular case.

Table 3: Table of differences IRF – DIRF Lymphoma Diagnosis, Example 2. All the values are difference of percentages. The columns “A” and “F” stand for anomalies and false positives respectively.

| quantile [%] | components | A  | F  | A  | F  | A  | F  | A  | F  | A  | F  | A  | F  | A  | F  | A  | F  |
|-------------|------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 1.0         | 0.0        | 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0|
| 3.0         | 0.0        | 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 16.7| -20.0| 16.7| -16.7| 16.7| -12.5| 16.7| -11.1| 16.7| -9.1|
| 6.0         | 16.7| -100.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0|
| 9.0         | 0.0        | 0.0| 0.0| 0.0| 16.7| -33.3| 16.7| -20.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0|
| 13.0        | -16.7| 100.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0| 0.0|

The table reports the difference of achievements attained by both methods when subtracting the DIRF to IRF. Contrary to the previous example, there is a predominance of positive and negative values in the columns “A” and “F” of the table respectively, showing that the IRF method performs better than the DIRF method with some few exceptions, as Figure displays.

As in the previous example, the 4% quantile seems to be the “balanced choice”. In particular DIRF and IRF perform identically from 9 PCA components and from the 6% quantile on.

The same experiments were performed but using the artificial distance-based labeling introduced in Definition 10. In this case, both methods perform almost identically worse than in the case of the original labeling.
Figure 5: Anomaly detection percentages for Example 2, Lymphoma Diagnosis. All the graphics have the number of principal components in the x-axis and multiple curves for the quantiles to be used as a threshold. Figure (a) and (c) depict anomalies detected by both methods with the original labeling, while figures (b) and (d) display false positives introduced by both methods with the original labeling.

5. Conclusions and Final Discussion.

The present work yields several conclusions listed below.

(i) The IRF anomaly detection method introduced in [1, 2] has been mathematically analyzed. The well-posedness (Proposition 1) and the convergence of the method (Corollary 12) have been established as well as the cardinality (size) of the probabilistic space (Theorem 13).

(ii) Under mild assumptions, it has been proved (see Theorem 7) that the IRF method has a computational cost of the order $O(n \log n)$, as claimed in [1, 2].

(iii) It has been shown that although the IRF method is well-defined and convergent, its target values $\{E(H_x) : x \in S\}$ are inconclusive when used as parameters for anomaly detection (see Lemma 14 and Theorem 15). Moreover, the IRF method can be analyzed deeply in the 1D case (Theorem 9) and it has been shown from the theoretical point of view that the its relationship with a notion of topological distance is not certain (see Theorem 10 and Remark 4).
Taking advantage of the **tractability** of IRF for the 1D case, we have given theoretical estimates of the variance (Equation (15)) and a number of Bernoulli trials (Equation (14)) to guarantee confidence intervals for the empirical values of the expected heights. We have suggested a **modification** of the method in Section 3.2 named DIRF method (Directional Isolation Random Forest).

From the numerical examples in Section 4

It is **unclear** whether or not the IRF or the DIRF method are **recommendable** for the outlier detection task. As pointed out in Theorem 10 the relationship of the method with a notion of distance is not certain. Moreover, the examples above indicate there is definitely **correlation** between the heights computed by the methods (IRF and DIRF), but it could be strong as in Example 1 or weak as in Example 2.

Both numerical examples may suggest that the adequate number of PCA components to introduce in the IRF and DIRF methods is **one third** of its total number of dimensions. However, two experiments do not furnish enough numerical evidence to support such a conjecture.

Finally,

Although we have proved that the IRF method is inconclusive as a means to classify anomalies, experience shows that it can provide satisfactory results in practice, it follows that the method is **correlated** with anomalies. There are two possible approaches for enhancement of the method:

a. Find sufficient conditions for the data combinatorial configuration, to assure a quality certificate of IRF.

b. Look for additional statistical parameters for anomaly detection (with computational cost no bigger than $O(n \log n)$) to complement/contrast the information furnished by IRF.

Both research lines will be explored in future work.

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