Horton self-similarity of Kingman's coalescent

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(joint work with Ilya Zaliapin of U. Nevada)

Introduction.

When studying the tree graphs associated with random structures one often aims at discovering a particular symmetry or a consistent pattern such as self-similarity. There exist two important types of tree self-similarity related to the Horton-Strahler ordering and Tokunaga indexing schemes for tree branches.

The Horton-Strahler indexing assigns orders to the tree branches according to their relative importance in the hierarchy.

- Introduced in hydrology in the 1950s to describe the dendritic structure of river networks.

- Applications: ranking river tributaries, analysis of brain structure, designing optimal computer codes, etc.

Self-similar trees

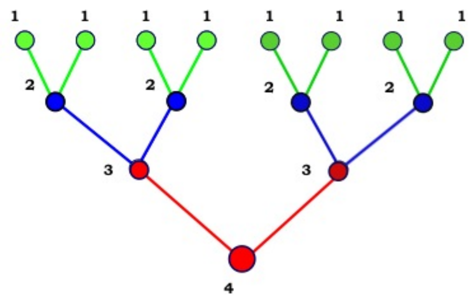
- A two-parametric class of *Tokunaga self-similar trees* closely approximates a surprising variety of trees in observed and modeled systems [Tokunaga, 1978; Peckham, 1995; Newman et al., 1997; Zanardo et al., 2013]

- Tokunaga self-similarity implies *Horton laws*, heavily used in hydrology since the 1950-s

- Horton laws can be interpreted as a power-law distribution of system element sizes, and hence are relevant to many hierarchical systems

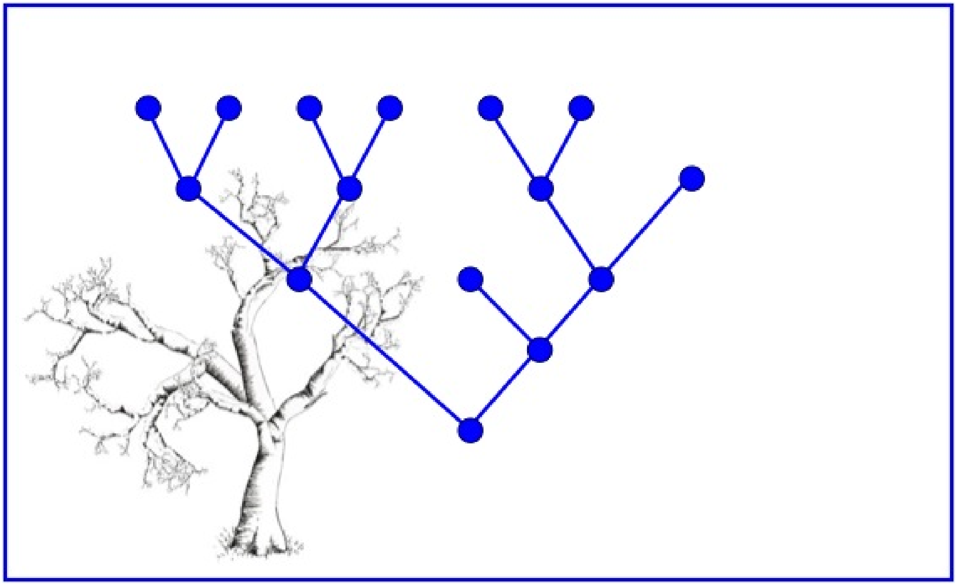
Horton-Strahler ordering.

- Horton and Tokunaga laws are based on *Horton-Strahler orders* that measure "importance" of tree branches within the hierarchy
- In a perfect binary tree (all leaves having the same depth) the orders are proportional to depth
- How to assign orders in a non-perfect tree?



Horton-Strahler ordering.

Rooted tree



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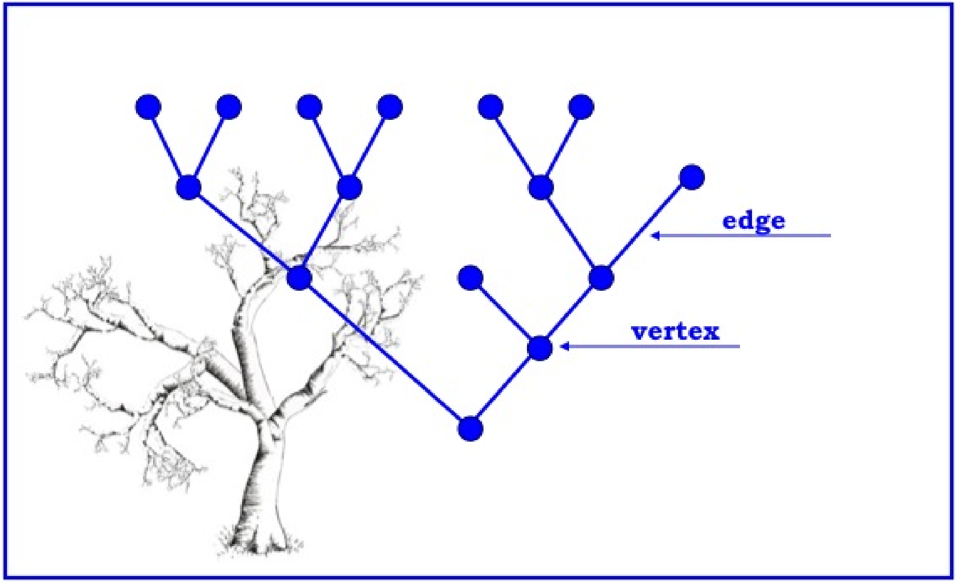

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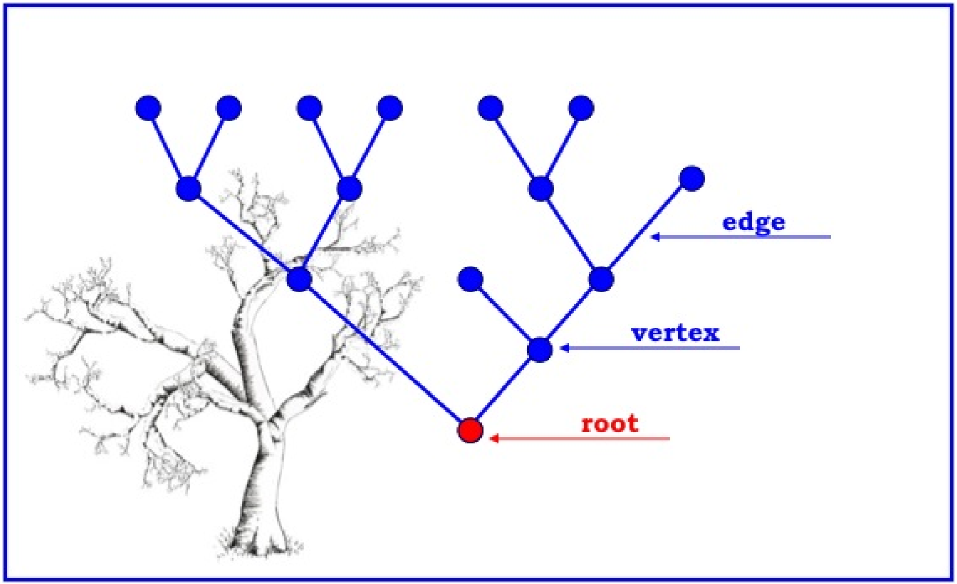

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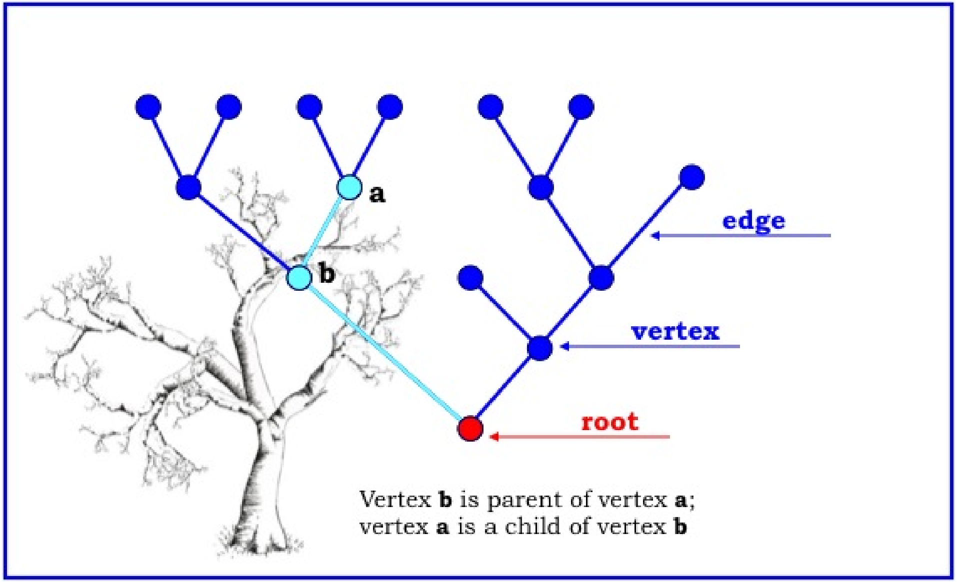

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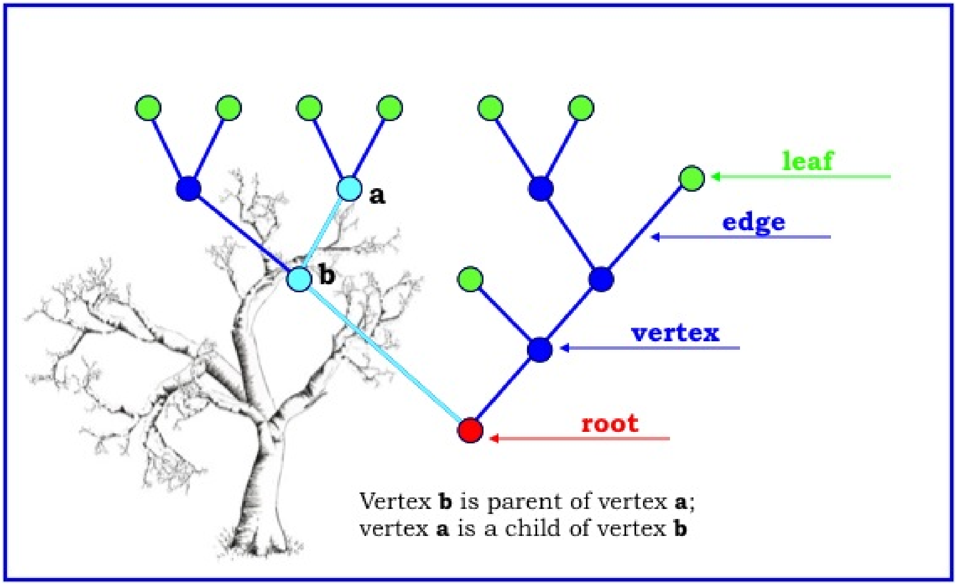


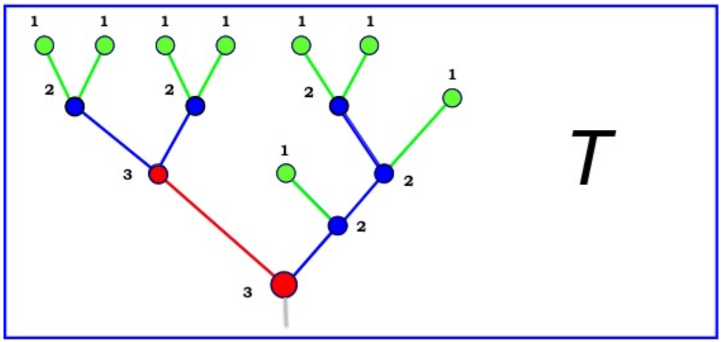
Horton-Strahler order (via pruning).

- *Pruning* $\mathcal{R}(T)$ of a finite tree T cuts the leaves and degree-2 chains connected to leaves.

- Nodes cut at k-th pruning, $\mathcal{R}^{k-1}(T) \setminus \mathcal{R}^{k}(T)$, have order k, $k \geq 1$.

- A chain of the same order vertices is called *branch*.

- N_k denotes the number of *branches* of order k in a finite tree T



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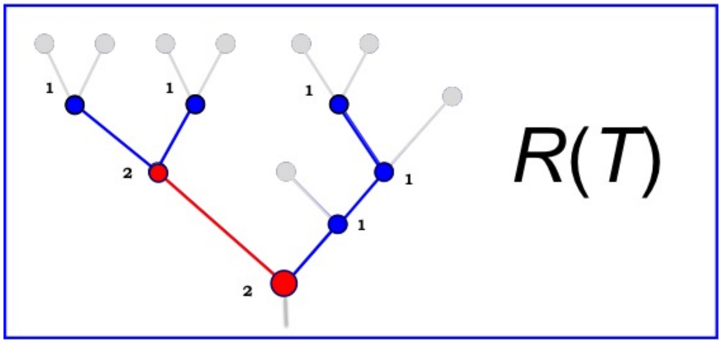

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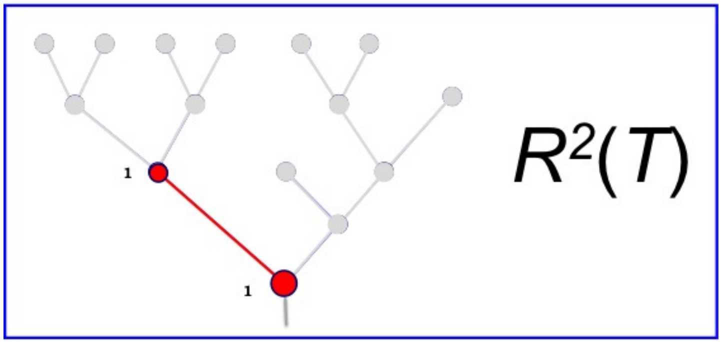

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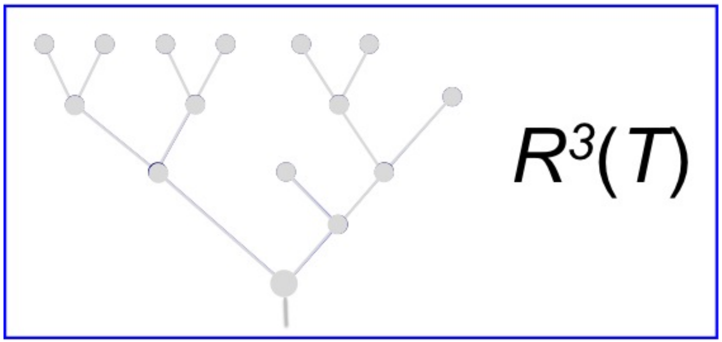

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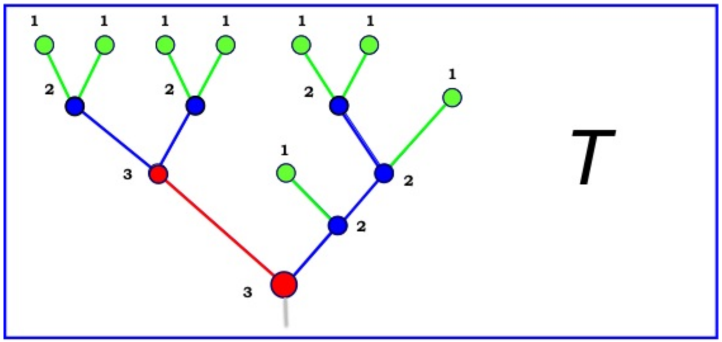
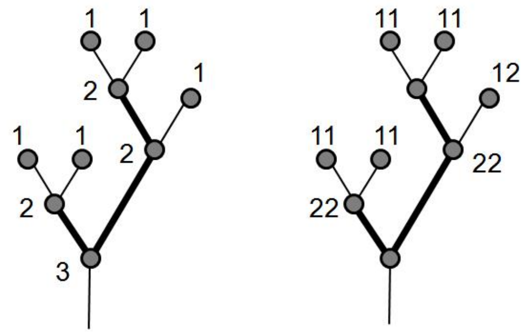


Horton-Strahler ordering and Tokunaga indexing.



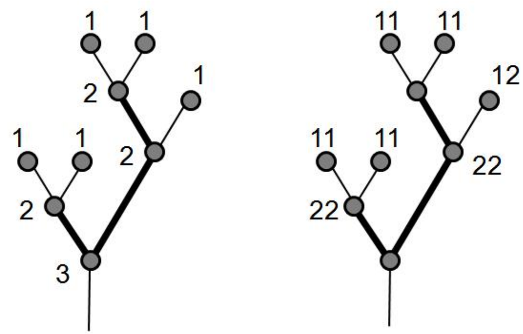
(a) Horton-Strahler orders (b)Tokunaga indices

Example: (a) Horton-Strahler ordering

(b) Tokunaga indexing.

Two order-2 branches are depicted by heavy lines in both panels. The Horton-Strahler orders refer, interchangeably, to the tree nodes or to their parent links. The Tokunaga indices refer to entire branches, and not to individual vertices.

Horton-Strahler ordering.



(a) Horton-Strahler orders (b)Tokunaga indices

The **Horton-Strahler ordering** of the vertices of a finite rooted labeled binary tree is performed in a hierarchical fashion, from leaves to the root:

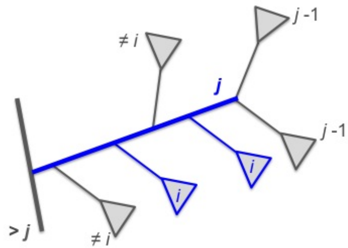
(i) each leaf has order $r(\text{leaf}) = 1$;

(ii) when both children, c_1, c_2, of a parent vertex p have the same order r, the vertex p is assigned order $r(p) = r + 1$;

(iii) when two children of vertex p have different orders, the vertex p is assigned the higher order of the two.

Tokunaga indexing.

- Let $\tau_{ij}^{(k)}$, $1 \le k \le N_j$, $1 \le i < j \le \Omega$, denote the number of branches of order i that join the non-terminal vertices of the k-th branch of order j



- Let N_{ij} be the total number of instances when an order-i branch merges an order-j branch

$$N_{ij} = \sum_k \tau_{ij}^{(k)}, i < j$$

- The Tokunaga index T_{ij} is the average number of order-i branches that join an order-j branch:

$$T_{ij} = \frac{N_{ij}}{N_j}$$

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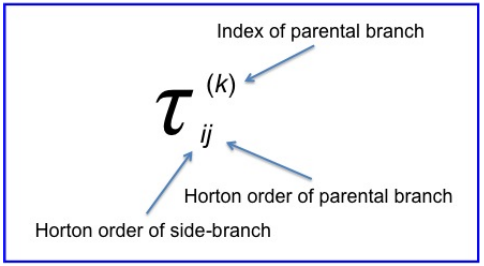

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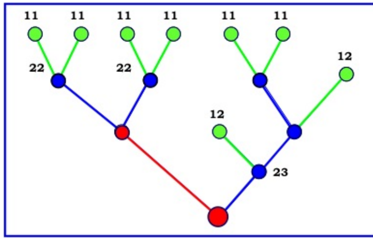

i \ j	1	2	3	N_i
1	6	2	0	8
2		2	1	2

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Tree self-similarity

Definition 1 (Self-similarity)**.** A random tree T of order Ω is self-similar if

$$\mathsf{E}\left[\tau^{(j)}_{i(i+k)}\right] =: T_k$$

for $1 \le j \le N_{i+k}$, $2 \le i+k \le \Omega$.

Definition 2 (Tokunaga self-similarity)**.** A random self-similar tree is *Tokunaga self-similar* if

$$T_{k+1}/T_k = c \quad \Leftrightarrow \quad T_k = a\,c^{k-1} \quad a, c > 0,\ 1 \le k \le \Omega{-}1.$$

Tree self-similarity

The matrix of Tokunaga indices

$$\mathbb{T} = \begin{bmatrix} T_{12} & T_{13} & T_{14} & \dots & T_{1\Omega} \\ 0 & T_{23} & T_{24} & \dots & T_{2\Omega} \\ 0 & 0 & T_{34} & \dots & T_{3\Omega} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & T_{\Omega-1\Omega} \end{bmatrix}$$

becomes a Toeplitz matrix for a self-similar tree:

$$\mathbb{T}_{\mathsf{SS}} = \begin{bmatrix} T_1 & T_2 & T_3 & \dots & T_{\Omega-1} \\ 0 & T_1 & T_2 & \dots & T_{\Omega-2} \\ 0 & 0 & T_1 & \dots & T_{\Omega-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & T_1 \end{bmatrix}; \quad \mathbb{T}_{\mathsf{TSS}} = \begin{bmatrix} a & ac & ac^2 & \dots & ac^{\Omega-2} \\ 0 & a & ac & \dots & ac^{\Omega-3} \\ 0 & 0 & a & \dots & ac^{\Omega-4} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & a \end{bmatrix}$$

Horton self-similarity.

We say that a sequence of probability laws $\{\mathcal{P}_N\}_{N\in\mathbb{N}}$ has **well-defined asymptotic Horton-Strahler orders** if for each $k \in \mathbb{N}$, random variables

$$\frac{N_k^{(\mathcal{P}_N)}}{N} \longrightarrow \mathcal{N}_k \quad \text{in probability as} \quad N \to \infty,$$

where quantity $\mathcal{N}_k$ is called the **asymptotic ratio** of the branches of order k.

The notion of Horton self-similarity characterizes the cases when the sequence $\mathcal{N}_k$ decreases in a regular geometric fashion with k going to infinity. Informally,

$$\mathcal{N}_k \asymp N_0 \cdot R^{-k}$$

Horton self-similarity.

The notion of Horton self-similarity characterizes the cases when the sequence $\mathcal{N}_k$ decreases in a regular geometric fashion with k going to infinity. Informally, $\mathcal{N}_k \asymp N_0 \cdot R^{-k}$. Formally, we define three types of Horton self-similarity.

A sequence $\{\mathcal{P}_N\}_{N\in\mathbb{N}}$ of probability laws over binary trees with well-defined asymptotic Horton-Strahler orders is said to obey a Horton self-similarity law if and only if at least one of the following limits exists and is finite and positive:

$$\text{(a) root law :} \quad \lim_{k\to\infty} \left(\mathcal{N}_k\right)^{-\frac{1}{k}} = R > 0,$$

$$\text{(b) ratio law :} \quad \lim_{k\to\infty} \frac{\mathcal{N}_k}{\mathcal{N}_{k+1}} = R > 0,$$

$$\text{(c) geometric law :} \quad \lim_{k\to\infty} \mathcal{N}_k \cdot R^k = N_0 > 0.$$

The constant R is called the Horton exponent.

Background.

• A classical model that exhibits Horton and Tokunaga self-similarity is critical binary Galton-Watson tree (Burd, Waymire, and Winn, 2000). This model has $R = 4$ and $(a, c) = (1, 2)$.

Theorem [Shreve, 1969; Burd et al., 2000]. A critical binary Galton-Watson tree is Tokunaga self-similar with

$$(a, c) = (1, 2),$$

that is

$$T_k = 2^{k-1} \quad \text{and} \quad R = 4.$$

Theorem [Burd et al., 2000].

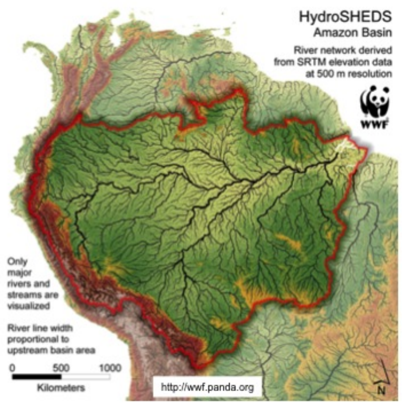
1. Let $P_{\mathsf{GW}}(p_k)$ denote the Galton-Watson distribution on the space of finite trees with branching probabilities p_k, $k = 0, 1, \ldots$. A tree $T \sim P_{\mathsf{GW}}(p_k)$ is self-similar if and only if $\{p_k\}$ is the critical binary distribution $p_0 = p_2 = 1/2$.

2. Any critical Galton-Watson tree T, $\sum k\, p_k = 1$, converges to the binary critical tree under the operation of pruning, $\mathcal{R}^n(T)$, $n \to \infty$.

Background.

• Peckham'95 : high-precision extraction of river channels for Kentucky River, Kentucky and Powder River, Wyoming.

Reported Horton exponents and Tokunaga parameters: $R \approx 4.6$ and $(a, c) \approx (1.2, 2.5)$.



River networks: Shreve 1966, 1969; Tokunaga, 1978; Peckham, 1995; Burd et al., 2000; Z et al., 2009; Zanardo et al., 2013

Background.

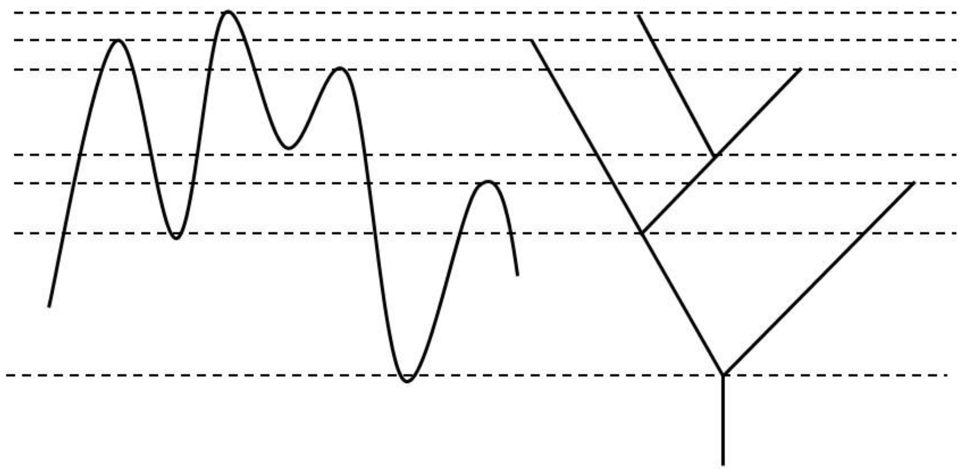
• Beyond river networks: botanical leaves, diffusion limited aggregation, two dimensional site percolation, nearest-neighbor clustering in Euclidean spaces, a general hierarchical coagulation model of Gabrielov introduced in the framework of self-organized criticality, etc.

Background.

• Zaliapin and K., 2012: established Horton and Tokunaga self-similarity for the level-set tree representation of a homogeneous discrete Markov chain and infinite-tree representation of a regular Brownian motion in continuous time.

This expands the class of Horton and Tokunaga self-similar processes beyond the critical binary Galton-Watson branching, since the tree representation of Markov chains in general is not equivalent to the Galton-Watson process.

Level-set tree of a function.



(a) Function X_t (b) Tree LEVEL(X)

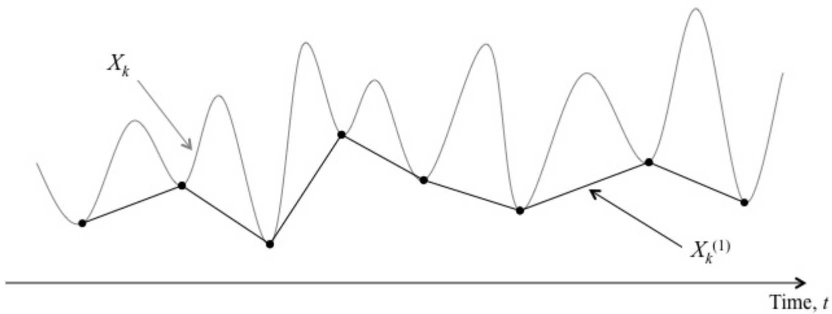
Function X_t (panel a) with a finite number of local extrema and its level-set tree level(X) (panel b).

Pruning of time series

Proposition [Zaliapin and K., 2012]: The transition from a time series X_k to the time series $X_k^{(1)}$ of its local minima corresponds to the pruning of the level-set tree level(X). Formally,

$$\text{level}\left(X^{(m)}\right) = \mathcal{R}^m\left(\text{level}(X)\right), \forall m \geq 1,$$

where $X^{(m)}$ is obtained from X by iteratively taking local minima m times (i.e., local minima of local minima and so on.)



Horton and Tokunaga self-similarity for Markov chains

Let X_k, $k = 1, \ldots, N$ be a symmetric homogeneous Markov chain and $T = \text{shape}(\text{level}(X))$ be the combinatorial level set tree of X_k.

Theorem [Zaliapin and K., 2012].

1. Tree T is Tokunaga self-similar with parameters $(a, c) = (1, 2)$:

$$\mathsf{E}\left[\tau^{(j)}_{i(i+k)}\right] =: T_k = 2^{k-1},$$

   and geometric-Horton self-similar, asymptotically in N, with $R = 4$.

2. Accordingly, a combinatorial level-set tree for regular Brownian motion is Tokunaga and Horton self-similar, with $(a, c) = (1, 2)$, and $R = 4$.

Horton and Tokunaga self-similarity for fractional Brownian motions

Conjecture [Zaliapin and K., 2012]. The tree tree $\left(B^H\right)$ of a fractional Brownian motion B_t^H, $t \in [0,1]$ with the Hurst index $0 < H < 1$ is Tokunaga self-similar with $T_{i(i+k)} = T_k = c^{k-1}$, $c = 2H + 1$, $i, k \geq 1$.

Background.

• K. and Zaliapin, 2015: established the *root-Horton law* for the Kingman's coalescent. Showed that the tree that describes a Kingman's coalescent is combinatorially equivalent to the level-set tree of a white noise.

Perform numerical experiments that suggest that the Kingman's coalescent, and hence the level-set tree of a white noise, are Horton self-similar in a regular stronger sense as well as asymptotically Tokunaga self-similar.

Finite coalescent process via a collision kernel.

[Markus, 1968; Lushnikov, 1978; Aldous, 1999; Pitman, 2006]

- The process starts at $t = 0$ with N particles (clusters) of mass one.

- The cluster formation is governed by a collision rate kernel

$$K(i,j) = K(j,i) > 0,$$

  $1 \leq i,j \leq N-1$. Specificallyly, a pair of clusters with masses i and j coalesces at the rate $K(i,j)/N$, independently of the other pairs, to form a new cluster of mass $i+j$.

- The process continues until there is a single cluster of mass N.

Kingman's N-coalescent process.

The best studied coalescent processes (as $N \to \infty$) are:

- Kingman's coalescent: $K(x, y) \equiv 1$
- Additive coalescent: $K(x, y) = x + y$
- Multiplicative coalescent: $K(x, y) = xy$

See [Aldous, *Bernoulli* **5**(1), 1999, 3–48] for review.

Coalescent tree.

A merger history of Kingman's N-coalescent process can be naturally described by a time-oriented binary tree $T_{\mathsf{K}}^{(N)}$ constructed as follows.

Start with N leaves that represent the initial N particles and have time mark $t = 0$. When two clusters coalesce (a transition occurs), merge the corresponding vertices to form an internal vertex with a time mark of the coalescent.

The final coalescence forms the tree root.

The resulting time-oriented tree represents the history of the process. It is readily seen that there is one-to-one map from the trajectories of an N-coalescence process onto the time-oriented trees with N leaves.

Coalescent tree.

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Results.

In Zaliapin and K. 2015, we consider the asymptotic proportion

$$\mathcal{N}_k = \lim_{N\to\infty} N_k/N$$

of the number N_k of branches of Horton-Strahler order k in Kingman's N-coalescent process with constant collision kernel.

We have a construction that allows one to interpret $\mathcal{N}_k$ also as the proportion of branches of order k in the infinite tree that corresponds to the Kingman's coalescent.

We show that

$$\mathcal{N}_k = \frac{1}{2}\int_0^\infty g_k^2(x)\,dx,$$

where the sequence $g_k(x)$ solves:

$$g'_{k+1}(x) - \frac{g_k^2(x)}{2} + g_k(x)g_{k+1}(x) = 0, \quad x \geq 0$$

with $g_1(x) = 2/(x+2)$, $g_k(0) = 0$ for $k \geq 2$.

Results.

Equivalent relation:

$$\mathcal{N}_k = \int_0^1 [1-(1-x)\,h_{k-1}(x)]^2\,dx,$$

where

$$h'_{k+1}(x) + h_k^2(x) - 2h_k(x)h_{k+1}(x) = 0, \qquad x \in [0,1]$$

with $h_0 \equiv 0$, $h_1 \equiv 1$, and $h_k(0) = 1$ for $k \geq 1$.

Theorem. The asymptotic Horton ratios $\mathcal{N}_k$ exist and finite and satisfy the convergence $\lim\limits_{k\to\infty} (\mathcal{N}_k)^{-\frac{1}{k}} = R$ with $2 \leq R \leq 4$.

Conjecture. The tree associated with Kingman's coalescent process is Horton self-similar with

$$\lim_{k\to\infty} \frac{\mathcal{N}_k}{\mathcal{N}_{k+1}} = \lim_{k\to\infty} (\mathcal{N}_k)^{-\frac{1}{k}} = R \quad \text{and} \quad \lim_{k\to\infty} (\mathcal{N}_k R^k) = const.,$$

where $R = 3.043827\ldots$ and Tokunaga self-similar, asymptotically in k:

$$\lim_{i\to\infty} T_{i,i+k} =: T_k \quad \text{and} \quad \lim_{k\to\infty} \frac{T_k}{c^{k-1}} = a$$

for some positive a and c.

Results.

Theorem. The asymptotic Horton ratios $\mathcal{N}_k$ exist and finite and satisfy the convergence $\lim_{k\to\infty} (\mathcal{N}_k)^{-\frac{1}{k}} = R$ with $2 \le R \le 4$.

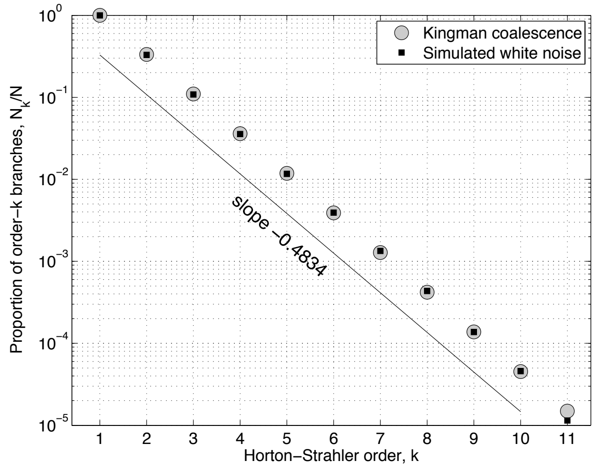
Consider now a time series X with N local maxima separated by $N-1$ internal local minima such that the latter form a discrete white noise; we call X an *extended discrete white noise*.

Theorem. The combinatorial level set tree of an extended discrete white noise X with N local maxima has the same distribution on $\mathcal{T}_N$ as the combinatorial tree generated by Kingman's N-coalescent.

The equivalence leads to the Horton self-similarity for discrete white noise.

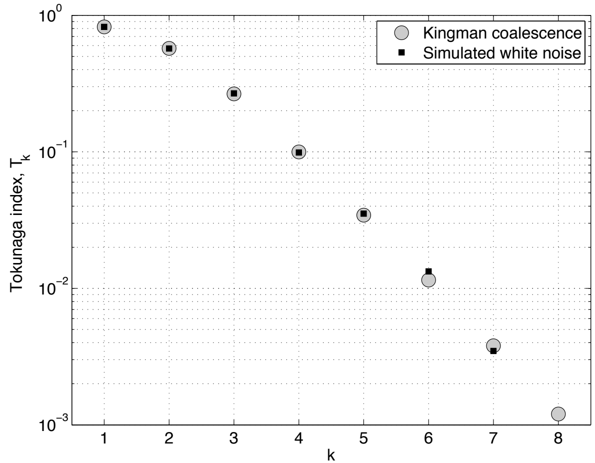
Corollary. The combinatorial level set tree of a discrete white noise is root-Horton self similar with the same Horton exponent R as for Kingman's coalescent.

Horton self-similarity.



Filled circles: The asymptotic ratio $\mathcal{N}_k$ of the number N_k of branches of order k to N in Kingman's coalescent, as $N \to \infty$. Black squares: The empirical ratio N_k/N_1 in a level-set tree for a single trajectory of a white noise of length $N = 2^{18}$.

Asymptotic Tokunaga self-similarity.



Filled circles: The asymptotic Tokunaga indices T_{i9} in Kingman's coalescent, as $N \to \infty$. Black squares: The empirical Tokunaga indices averaged over 100 level-set trees for white noises of length $N = 2^{17}$.

Smoluchowski-Horton ODEs.

Let $K(i,j) \equiv 1/N$ in Kingman's N-coalescent process, and let $\eta_{(N)}(t) := |\Pi_t^{(N)}|/N$ be the total number of clusters relative to the system size N.

Then $\eta_{(N)}(0) = N/N = 1$ and $\eta_{(N)}(t)$ decreases by $1/N$ with each coalescence of clusters at the rate of

$$\frac{1}{N}\binom{N\,\eta_{(N)}(t)}{2} = \frac{\eta_{(N)}^2(t)}{2} \cdot N + o(N), \quad \text{as } N \to \infty$$

The limit relative number of clusters $\eta(t) = \lim\limits_{N\to\infty} \eta_{(N)}(t)$ satisfies the following ODE:

$$\frac{d}{dt}\eta(t) = -\frac{\eta^2(t)}{2}.$$

Smoluchowski-Horton ODEs.

For any $j \in \mathbb{N}$ we define $\eta_{j,N}(t)$ to be the number of clusters of Horton-Strahler order j at time t relative to the system size N.

Initially,

$$\eta_{j,N}(0) = \delta_1(j).$$

At any time t, $\eta_{j,N}(t)$ increases by $1/N$ with each coalescence of clusters of Horton-Strahler order $j-1$ with rate

$$\frac{1}{N}\binom{N\,\eta_{(j-1),N}(t)}{2} = \frac{\eta^2_{(j-1),N}(t)}{2} \cdot N + o(N).$$

Thus $\frac{\eta^2_{(j-1),N}(t)}{2} + o(1)$ is the instantaneous rate of increase of $\eta_{j,N}(t)$.

Smoluchowski-Horton ODEs.

For any $j \in \mathbb{N}$ we define $\eta_{j,N}(t)$ to be the number of clusters of Horton-Strahler order j at time t relative to the system size N.

Similarly, $\eta_{j,N}(t)$ decreases by $1/N$ when a cluster of order j coalesces with a cluster of order strictly higher than j with rate

$$\eta_{j,N}(t)\ \left(\eta_{(N)}(t) - \sum_{k=1}^{j} \eta_{k,N}(t)\right) \cdot N,$$

and it decreases by $2/N$ when a cluster of order j coalesces with another cluster of order j with rate

$$\frac{1}{N}\binom{N\,\eta_{j,N}(t)}{2} = \frac{\eta_{j,N}^2(t)}{2} \cdot N + o(N).$$

Thus the instantaneous rate of change of $\eta_{j,N}(t)$ is

$$\eta_{j,N}(t)\ \left(\eta_{(N)}(t) - \sum_{k=1}^{j} \eta_{k,N}(t)\right) + \eta_{j,N}^2(t) + o(1).$$

Smoluchowski-Horton ODEs.

Informally write the limit rates-in and the rates-out via the following *Smoluchowski-Horton system* of ODEs:

$$\frac{d}{dt}\eta_j(t) = \frac{\eta_{j-1}(t)}{2} - \eta_j(t)\left(\eta(t) - \sum_{k=1}^{j-1}\eta_k(t)\right)$$

with $\eta_j(0) = \delta_1(j)$.

Formally, we prove **hydrodynamic limit**.

We show $\eta_k(t) = \lim_{N\to\infty} \eta_{k,N}(t)$ exists, and let $\eta_0 \equiv 0$.

Since $\eta_j(t)$ has the instantaneous rate of increase $\frac{\eta^2_{j-1}(t)}{2}$, the relative total number of clusters of Horton-Strahler order j is given by

$$\mathcal{N}_j = \delta_1(j) + \int_0^\infty \frac{\eta^2_{j-1}(t)}{2} dt.$$

Smoluchowski-Horton ODEs.

Lemma. The Horton ratios N_k/N converge in probability to a finite constant $\mathcal{N}_k = \delta_1(k) + \int_0^\infty \frac{\eta_{k-1}^2(t)}{2} dt$ as $N \to \infty$.

$$\mathcal{N}_1 = 1, \quad \mathcal{N}_2 = \frac{1}{3}$$

and

$$\mathcal{N}_3 = \frac{e^4}{128} - \frac{e^2}{8} + \frac{233}{384} = 0.109686868100941\ldots$$

Hence, we have $\mathcal{N}_1/\mathcal{N}_2 = 3$ and $\mathcal{N}_2/\mathcal{N}_3 = 3.038953879388\ldots$

Our numerical results yield, moreover,

$$\lim_{k\to\infty} \left(\mathcal{N}_k\right)^{-\frac{1}{k}} = \lim_{k\to\infty} \frac{\mathcal{N}_k}{\mathcal{N}_{k+1}} = 3.0438279\ldots$$