Random trees

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Nordita & Alba Nova, Stockholm

Outline

- Introduction - Motivation: Physics, Mathematics, Biology, ...
- Principal questions
- Models
- Methods
- Results

Random Walks

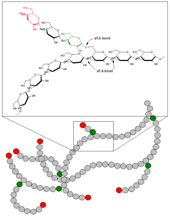
- Universal theoretical tool: diffusion, functional integrals, ...
- No intrinsic structure: properties come from imbedding into an ambient space, e.g. $\mathbb{R}^d$
- Strong universality results - central limit theorem
- Rigorous continuum theory, Wiener integral, potential theory

Random geometry

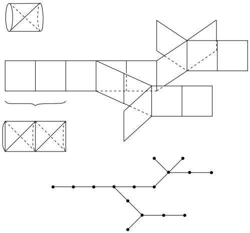
- Intrinsic and extrinsic degrees of freedom
- Trees
- Surfaces: Phase boundaries, membranes, string theory, 2-dimensional quantum gravity, ...
- Higher dimensional manifolds: gravity in dimensions ≥ 3, mainly numerical results
- General graphs, networks

Random trees

- Physical tree-like objects: branched polymers

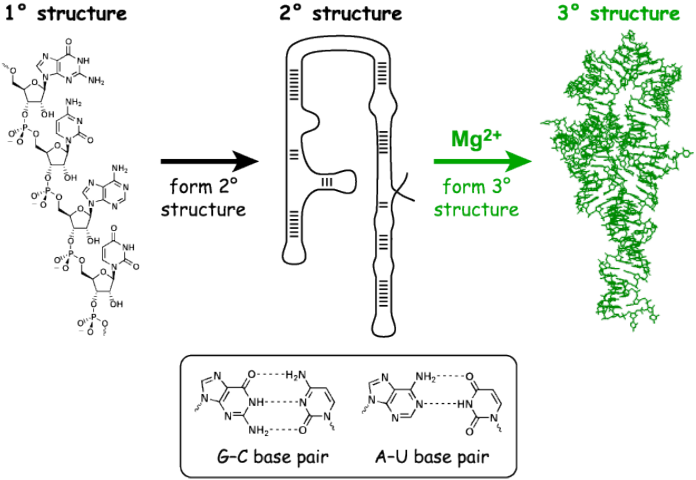


- Surfaces and higher dimensional manifolds can have a phase where they degenerate into trees



Random trees

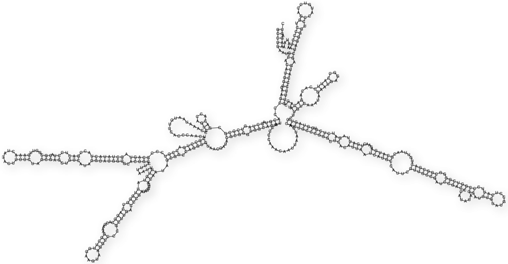
- Secondary structure of macromolecules, e.g. RNA



(borrowed from Scott K. Silverman scott@scs.uiuc.edu)

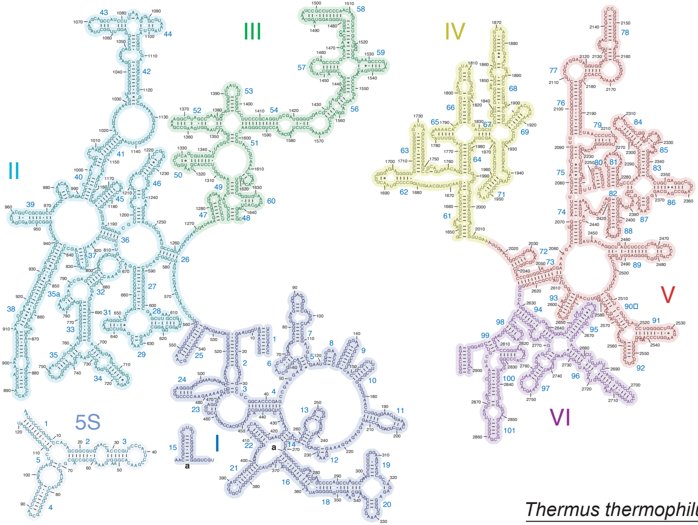
Problem: find the secondary (and the tertiary) structure from the base sequence

GCCUUAAUGCACAUGGGCAAGCCCACGUAGCUAGUCGCGCGACACCAGUCCCAAAUAAUGUUCACCCAACUCGCCUGACCGUCCCGCAGUA
GCUAUACUACCGACUCCUACGCGGUUGAAACUAGACUUUUCUAGCGAGCUGUCAUAGGUAUGGUGCACUGUCUUUAAUUUUGUAUUGGGCC
AGGCACGAAAGGCUUGGAAGUAAGGCCCCGCUUGACCCGAGAGGUGACAAUAGCGGCCAGGUGUAACGAUACGCGGGUGGCACGUACCCCA
AACAAUUAAUCACACUGCCCGGGCUCACAUUAAUCAUGCCAUUCGUUGCCGAUCCGACCCAUAUAGGAUGUGUAUGCCUCAUUCCCGGUCG
GGGCGGCGACUGUUAACGCAUGAGAACUGAUUAGAUCUCGUGGUAGUGCUUGUCAAAUAGAAUGAGGCCAUUCCACAGACAUAGCGUUUCC
CAUGAGCUAGGGGUCCCAUGUCCAGGUCCCCUAAAUAAAAGAGUC



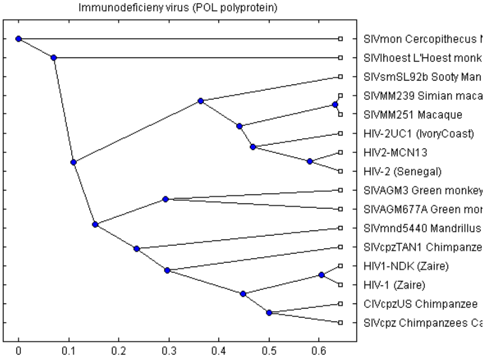
1. “kissing hairpins” & interlaced strands are rare (unfavored by kinematics & topology)

2. RNA can (to some extent) be considered as a **planar tree**

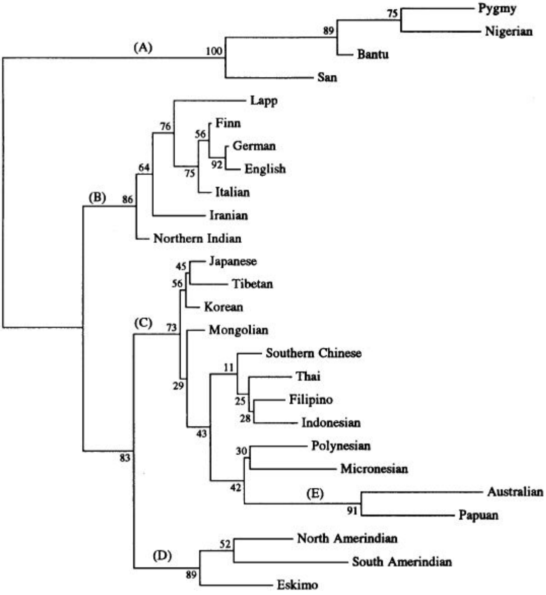


Thermus thermophilus
large subunit ribosomal RNA

- Family trees
- Phylogenetic trees

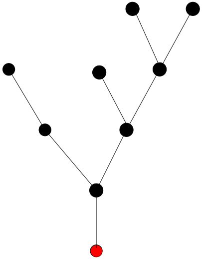


- Fragmentation and coagulation models, river networks, blood vessels, search algorithms, citation networks, random surfaces, etc. etc.


Pygmy
Nigerian
Bantu
San
Lapp
Finn
German
English
Italian
Iranian
Northern Indian
Japanese
Tibetan
Korean
Mongolian
Southern Chinese
Thai
Filipino
Indonesian
Polynesian
Micronesian
Australian
Papuan
North Amerindian
South Amerindian
Eskimo
(A)
(B)
(C)
(D)
(E)
100
89
75
86
64
76
56
92
75
83
73
56
45
29
43
11
25
28
42
30
91
89
52

Random trees

- Extensive mathematics literature: branching processes etc.
- Theory of continuous trees (Aldous et al.)
- Has been used to construct a theory of continuous random surfaces (Le Gall et al.)
- Today we will consider trees which are discrete
- Rooted planar tree graphs



Two main approaches

1. Equilibrium statistical mechanics

   $\mathcal{T}$= Set of graphs, μ a probability measure on $\mathcal{T}$

   $$\mu(T) = Z^{-1}e^{-\beta E(T)}$$

2. Growing trees $T_n \mapsto T_{n+1}$, time discrete

   Growth rules induce a probability measure on $\mathcal{T}_t$, the trees that can arise in t steps

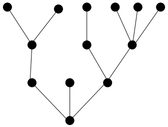
- Sometimes (1) is more natural
- Sometimes (2) is more natural
- Sometimes (1) and (2) are known to be equivalent

Problems to study

- What are the prinicipal characteristics of the trees under consideration?
- Universality classes
- Distribution of vertex degrees
- Correlations
- Fractal dimensions: Hausdorff, spectral, ...
- The "shape" of trees

Galton-Watson trees

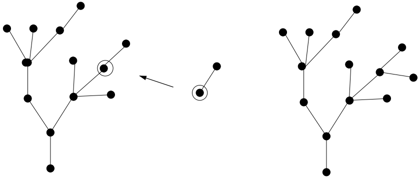
- p_n = probability of having n descendents, $\sum_n p_n = 1$, $m = \sum_n np_n$



- $m < 1$ subcritical, $m > 1$ supercritical, $m = 1$ critical
- n generations at time $t = n - 1$ if no extinction
- Well understood

Preferential attachment trees

- In each timestep one new edge is attached to a preexisting tree



- Probability of attaching to a vertex v of order k

$$P_v = \frac{w_k}{\sum_k n_k w_w}, \quad w_k \geq 0.$$

- Growth rule induces a probability measure on $\mathcal{T}_t$.

Local trees

- Weight factor of a tree T

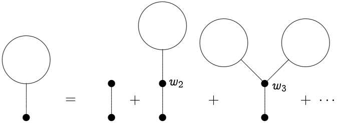
$$W(T) = \prod_{i \in T} w_{\sigma(i)}$$

$\sigma(i)$ = order of the vertex i

- Partition functions

$$Z_N = \sum_{T:|T|=N} W(T), \quad Z = \sum_N \zeta^N Z_N, \quad |\zeta| < \zeta_0$$

- Generating function $g(z) = \sum_n w_n z^{n-1}$, radius of convergence ρ
- Main equation



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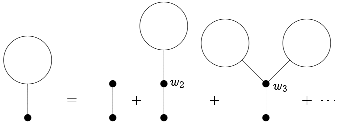
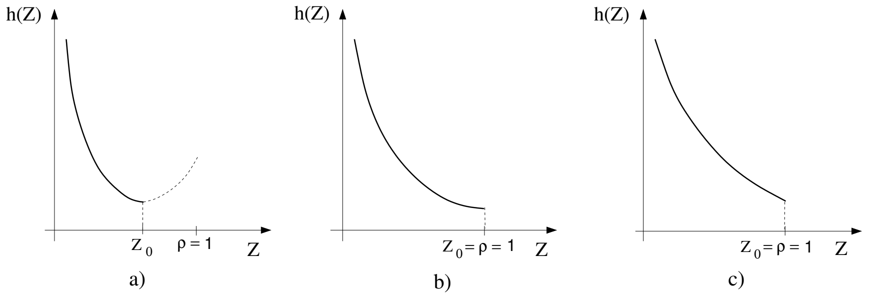


- Algebraically

$$Z(\zeta) = \zeta g(Z(\zeta)) = \zeta \sum_{i=0}^{\infty} w_{i+1} Z^i(\zeta)$$

- Define $Z_0 = \lim_{\zeta \to \zeta_0} Z(\zeta)$
- If $Z_0 < \rho$ then we say that the trees are *generic*.
- $Z(\zeta) - Z_0 \sim \sqrt{\zeta_0 - \zeta}$



Here we have defined

$$h(Z) = \frac{g(Z)}{Z}$$

and the weights have been scaled so that $\rho = 1$

- Define

$$\mu(T) = Z_0^{-1} \zeta_0^{|T|} \prod_{i \in T} w_{\sigma(i)}$$

Probability measure

- This measure is the same as the one obtained from a Galton-Watson process with

$$p_n = \zeta_0 w_{n+1} Z_0^{n-1}$$

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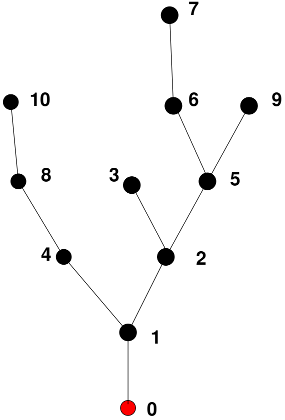
Another equivalence

- Preferential attachment trees $\approx$ Causal trees
- Weight proportional to the number of *causal labelings*



- More branchings, more ways to grow

Some results about generic trees

Work with B. Durhuus and J. Wheater

- Let $V_T(R)$=volume of a ball of radius R centered on the root

$$\langle V_T(R)\rangle \sim R^{d_H}, \quad R\to\infty \quad \text{defines } d_H$$

- Let $p_T(t)$ = probability that a random walker is back at the root after t steps on T

$$\langle p_T(t)\rangle \sim t^{-d_s/2}, \quad t\to\infty \quad \text{defines } d_s$$

cf.

$$K_t(x,y) = (2\pi t)^{-d/2} e^{-(x-y)^2/2t}$$

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- Averages taken w.r.t. a measure on infinite trees

$$\nu_N = Z_N^{-1} \prod_{i \in T} w_{\sigma(i)}$$

$$\nu_N \to \nu_\infty \ \text{ as } \ N \to \infty$$

- **Theorem.**
  (i) $d_H = 2$
  (ii) $d_s = 4/3$
  (iii) There is a unique infinite simple path whose outgrowths are critical GW-trees
  (iv) Vertex degrees are uncorrelated

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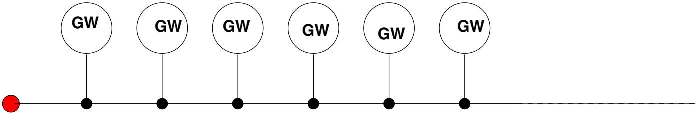

- One spine due to entropy
- The number of rooted planar trees with ℓ edges is

$$N(\ell) \sim \ell^{-3/2} C^{\ell}$$

$$\max\{N(\ell_1)N(\ell_2) : \ell_1 + \ell_2 = \ell\} \approx N(\ell)$$

- Main tool for analysing the spectral dimension is the generating function

$$Q_T(x) = \sum_{t=0}^{\infty} p_T(t)(1-x)^{t/2}$$

and its ensemble average

$$Q(x) = \langle Q_T(x) \rangle$$

$$Q(x) \sim x^{-1/3} \Longrightarrow d_s = 4/3$$

Non-generic trees

- Critical exponents change
- There can arise a vertex of infinite order in the thermodynamic limit (Bialas, Burda, Johnston) - numerical work
- Proven in a special case (S. Stefansson)

Preferential attachment trees

Results obtained with F. David, P. di Francesco and E. Guitter

- In general many infinite simple paths
- $d_H = \infty$ in many cases (all cases?)
- Broad distribution of sizes of subtrees
- Lesson: The vertex degree distribution alone does not characterize a random tree

The vertex splitting model

Work with F. David, M. Dukes and S. Stefansson

- A model of randomly growing rooted, planar trees
- Degree of vertices is bounded by an integer d
- The parameters of the model are

$$\begin{bmatrix} 0 & w_{1,2} & w_{1,3} & \cdots & w_{1,d-1} & w_{1,d} \\ w_{2,1} & w_{2,2} & w_{2,3} & \cdots & w_{2,d-1} & w_{2,d} \\ w_{3,1} & w_{3,2} & w_{3,3} & \cdots & w_{3,d-1} & 0 \\ w_{4,1} & w_{4,2} & w_{4,3} & & 0 & 0 \\ \vdots & \vdots & \vdots & \iddots & \vdots & \vdots \\ w_{d,1} & w_{d,2} & 0 & \cdots & 0 & 0 \end{bmatrix}$$

a symmetric matrix of non–negative *partitioning weights*.

- The *splitting weights* $w_1, w_2, \ldots, w_d$ are defined by

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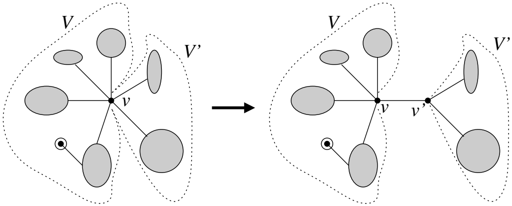
Vertex splitting rules

Given a fixed initial tree

(i) Choose a vertex v of degree i with relative probability w_i.

(ii) Partition the edges incident with v into two disjoint sets, V containing $k-1$ adjacent edges and V' containing the rest, with relative probability $w_{k,i+2-k}$.

(iii) Move all edges in V' from v to a new vertex v' and create an edge joining v to v'.



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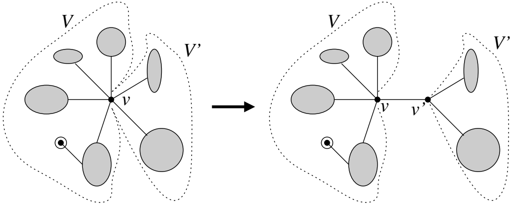

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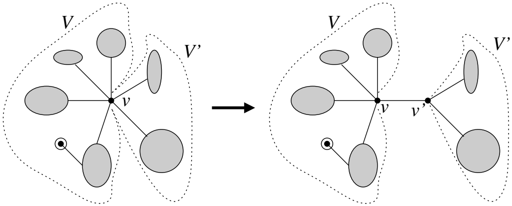
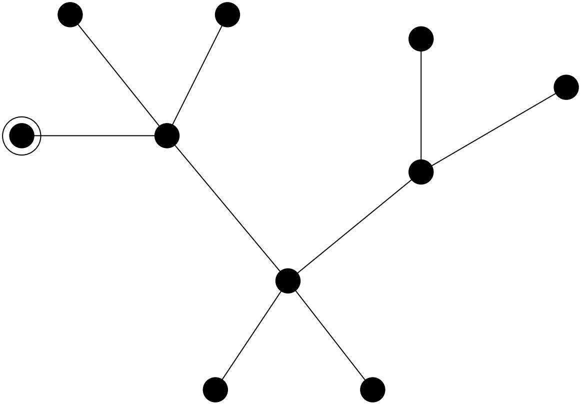


A tree



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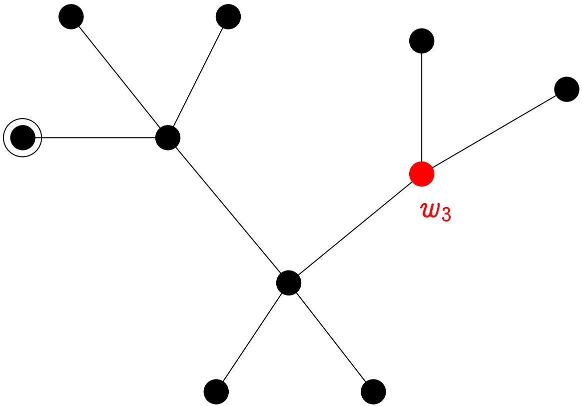

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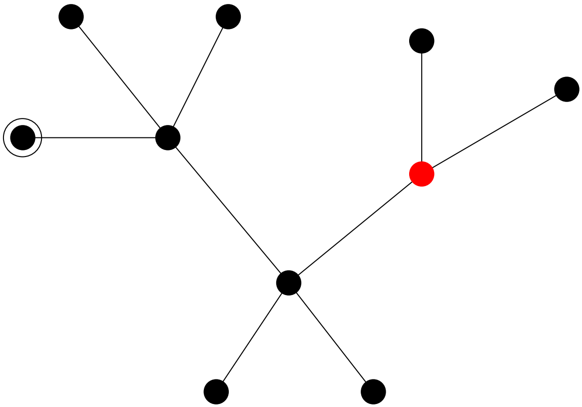

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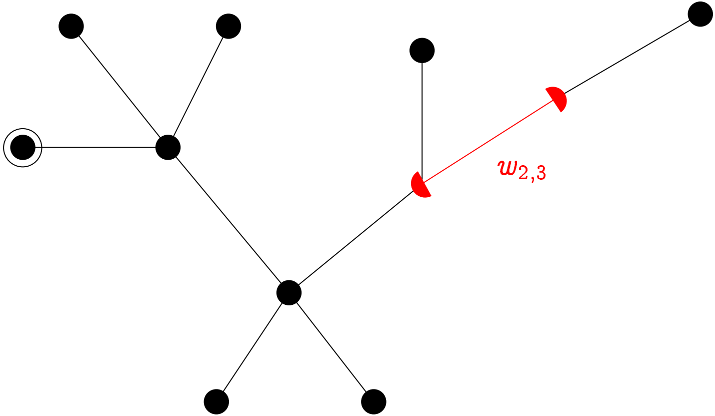

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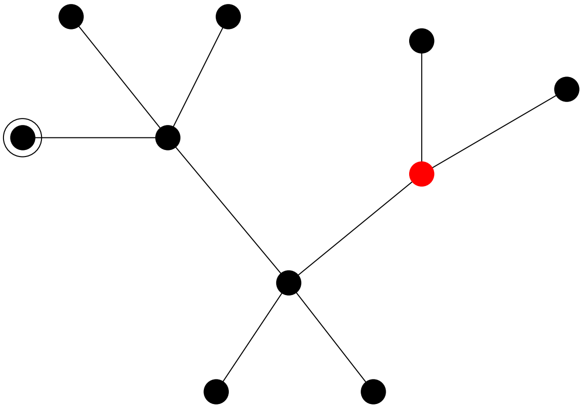

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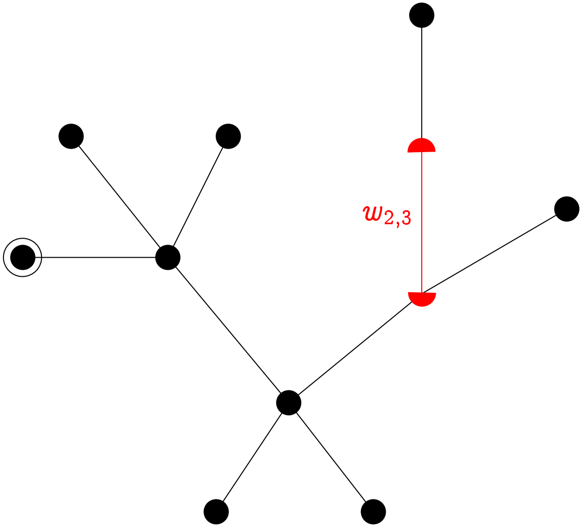

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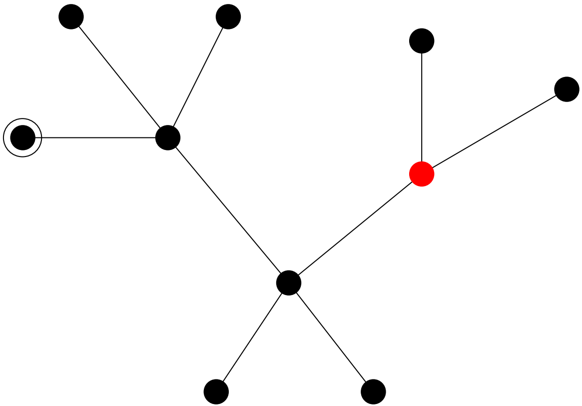

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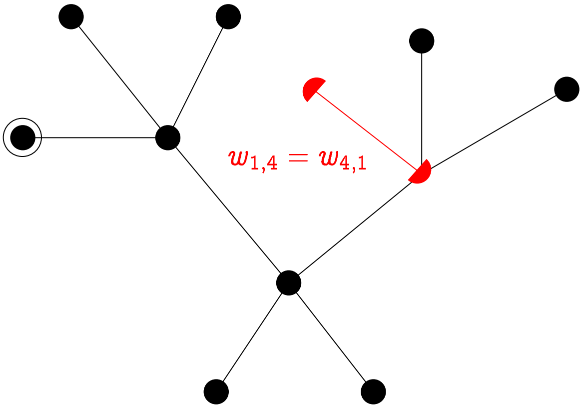

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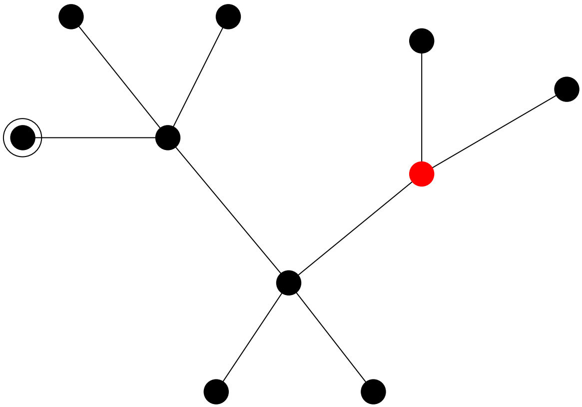

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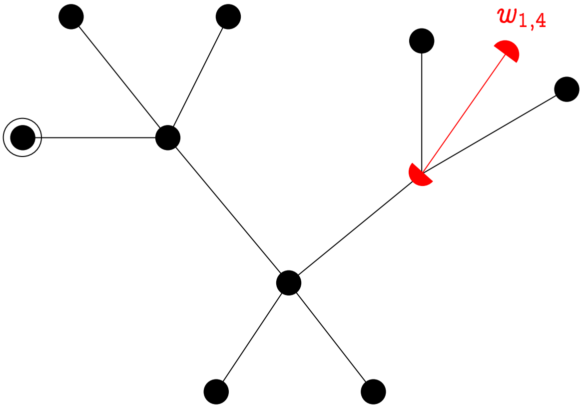

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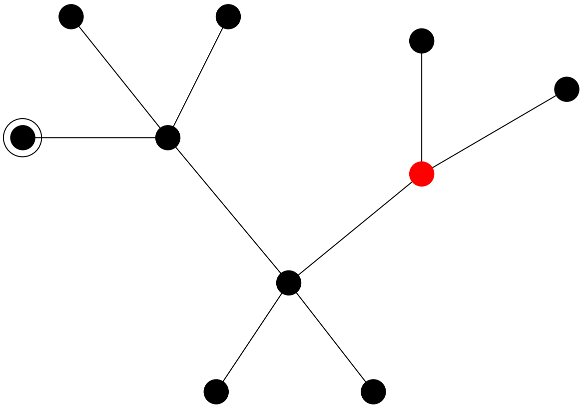

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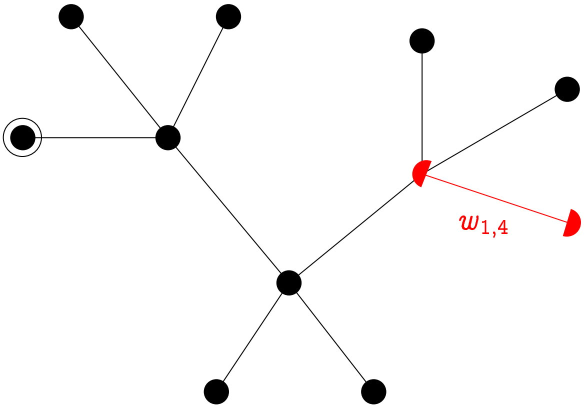

Relation to other models

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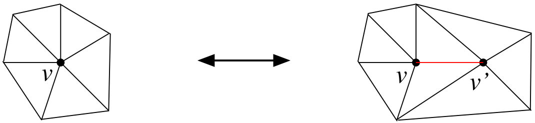

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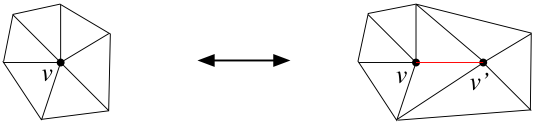

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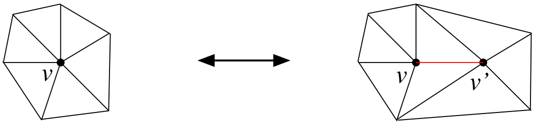

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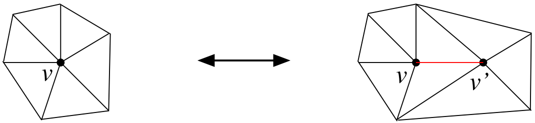

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Main problems

- Distribution of vertex degrees
- Correlations between vertex degrees of neighbouring vertices
- Shape of trees - Hausdorff dimension

If we consider linear splitting weights

$$w_i = ai + b.$$

the analysis simplifies due to the Euler relation for trees

$$\sum_{i=1}^{d} n_i(T) = |T|, \quad \sum_{i=1}^{d} i n_i(T) = 2(|T| - 1)$$

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Vertex degree distribution

For an infinite tree that has evolved in this way, let ρ_i be the proportion of vertices of degree i.

For linear splitting weights and certain not so restrictive conditions, the limiting densities

$$\rho_1, \ldots, \rho_d$$

exist and are the unique positive solution to the linear equations

$$\rho_k = -\frac{w_k}{w_2}\rho_k + \sum_{i=k-1}^{d} i\frac{w_{k,i+2-k}}{w_2}\rho_i.$$

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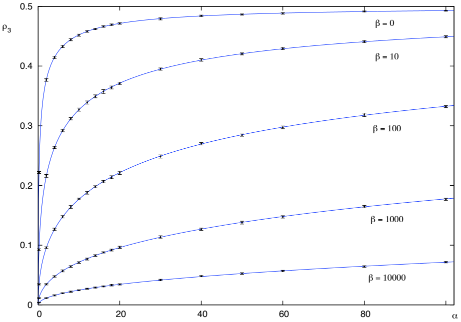

FIGURE 4. The value of ρ_3 as given in (2.45) compared to results from simulations. Each point is calculated from 20 trees on 10000 vertices.

A comparison of the theoretical prediction with simulations in the case d=3 and uniform partitioning weights.

$$\alpha = \frac{w_2}{w_1}, \quad \beta = \frac{w_3}{w_1}$$

Unbounded vertex degrees

- Can solve the equation for ρ_i with $d = \infty$ and linear splitting weights
- Perron Frobenius does not work here so a proof of convergence is missing
- ρ_i falls off factorially with i
- $\rho_i(w_j = 1) = \frac{1}{e(k-1)!}$

Correlations

In a typical infinite tree, what is the proportion of edges whose endpoints have degrees j and k ?

Let $n_{j,k}$ = number of such edges in a finite tree of size t, where the vertex of degree j is closer to the root

Let $\rho_{j,k} = \lim_{t\to\infty} \frac{n_{j,k}}{n}$. Then

$$\rho_{jk} = -\frac{w_j + w_k}{w_2}\rho_{jk} + (j-1)\frac{w_{j,k}}{w_2}\rho_{j+k-2} + (j-1)\sum_{i=j-1}^{d}\frac{w_{j,i+2-j}}{w_2}\rho_{ik} + (k-1)\sum_{i=k-1}^{d}\frac{w_{k,i+2-k}}{w_2}\rho_{ji}.$$

This result is obtained by assuming the existence of the limit and it agrees with simulations.
Can solve in simple cases and find nontrivial correlations

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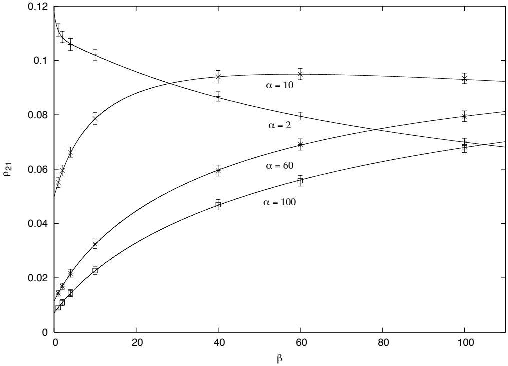

$$\alpha = \frac{w_2}{w_1}, \quad \beta = \frac{w_3}{w_1}, \quad d = 3$$

Correlations

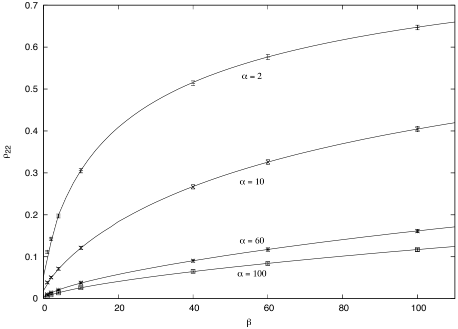

FIGURE 17. The solution (5.5) for the density ρ_{22} plotted as a function of β for a few values of α. Each datapoint is calculated from simulations of 100 trees on 10000 vertices.

$$
\begin{aligned}
\rho_{22} \quad = \quad & \frac{16}{3}\Big(284\,\alpha^2\beta^4\gamma - 177\,\alpha^5\beta\gamma + 3564\,\alpha^3 + 18\,\alpha^6\gamma + 161\alpha\,\beta^5\gamma - 873\,\gamma + 11979\,\alpha^2\beta^3 \\
& -2259\,\alpha^5 - 39\,\alpha^6\beta - 207\,\alpha^5\gamma + 6516\,\alpha^2\beta^4 - 5205\,\alpha^5\beta - 1419\,\alpha^4\beta\gamma + 996\,\alpha\beta^5 \\
& -5994\,\alpha^4 - 892\,\alpha^4\beta^2\gamma + 1543\,\alpha^2\beta^5 - 18\,\alpha^7 - 668\,\alpha^3\beta^4 + 324\,\alpha^2\gamma + 909\,\alpha\beta^3\gamma \\
& -2600\,\alpha^5\beta^2 - 975\,\alpha^3\beta^3 + 222\,\alpha\beta^6 - 1533\,\alpha^3\beta^2\gamma + 10206\,\alpha^2\beta^2 - 11799\,\alpha^4\beta \\
& -5300\,\alpha^4\beta^3 - 1521\,\alpha^3\beta\gamma + 1899\,\alpha^2\beta^2\gamma + 1059\alpha^2\,\beta^3\gamma + 1269\,\alpha^3\beta^2 + 3240\alpha^2\,\beta \\
& +756\,\alpha\beta^3 + 4860\,\alpha^3\beta + 6\,\beta^6\gamma - 11703\,\alpha^4\beta^2 + 1728\alpha^2\,\beta\gamma - 162\,\alpha^3\gamma + 486\alpha\,\beta^2\gamma \\
& +18\,\beta^4\gamma + 1530\,\alpha\beta^4 + 624\alpha\,\beta^4\gamma - 772\,\alpha^3\beta^3\gamma - 9\,\alpha^6 + 24\,\beta^5\gamma\Big)\Big/\Big((3\,\alpha + 2\,\beta + \gamma + 6) \\
& \times \left(11\,\alpha^2 + 25\,\alpha\beta + 5\,\alpha\gamma + 3\,\beta\gamma + 12\,\alpha + 4\,\beta^2\right)(-\alpha + \gamma)\,(1 - 2\,\alpha + \beta)\,(7\,\alpha + 2\,\beta + \gamma)^2\Big)
\end{aligned}
$$

Hausdorff dimension

- Let T be a tree with ℓ edges and v a vertex of T.
- Denote the graph distance between v and the root by $d_T(v)$.
- We define the radius of T as

$$R_T = \frac{1}{2|T|} \sum_{v \in T} d_T(v)\, \sigma(v),$$

- The definition of the Hausdorff dimension of the tree, d_H, by the scaling law for large trees ($\ell = |T|$)

$$\langle R_T \rangle \;\sim\; \ell^{1/d_H} \qquad \ell \to \infty$$

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Structure functions

- Define $q_{ki}(\ell_1, \ell_2) =$ probability that a vertex of order k in a tree of seize ℓ has i right subtrees of total volume ℓ_2 and the the remaining $k-i$ subtrees have a total volume ℓ_1
- These functions satisfy a linear system of equations
- They can be related to the Hausdorff dimension

$$\langle R \rangle_\ell = \frac{\ell+1}{2\ell} \sum_{\ell_2=0}^{\infty} (2\ell_2+1) \sum_{k=1}^{d} q_{k,k-1}(\ell-\ell_2, \ell_2)$$

- Using scaling assumptions about the q functions

$$q_{ki}(\ell_1, \ell-\ell_1) = \ell^{-\rho} \omega_{ki}(\ell_1/\ell) + O(\ell^{\rho+1})$$

we reduced the problem of calculating d_H to finding an eigenvalue of a $\binom{d}{2} \times \binom{d}{2}$ matrix

Hausdorff dimension

Linear weights and $d = 3$

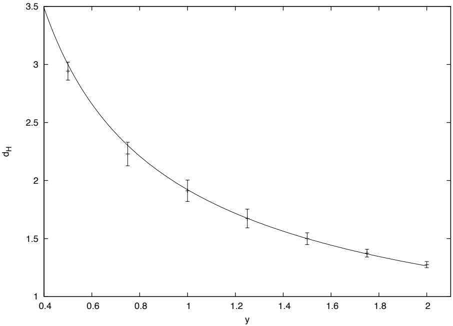

FIGURE 13. Equation (4.25) compared to simulations. The Hausdorff dimension, d_H, is plotted against $y = w_3/w_2$. The leftmost datapoint is calculated from 50 trees on 50000 vertices and the others are calculated from 50 trees on 10000 vertices.

Hausdorff dimension

General solution for $d = 3$

$$d_H = \frac{(w_{2,2} - 2w_{3,1}) + \sqrt{(w_{2,2} - 2w_{3,1})^2 + 8w_{3,1}(w_{2,1} + 3w_{3,2})}}{(w_{2,2} - 2w_{3,1}) + \sqrt{(w_{2,2} - 2w_{3,1})^2 + 16w_{3,1}w_{3,2}}}.$$

$w_{3,2} = w_3/3$

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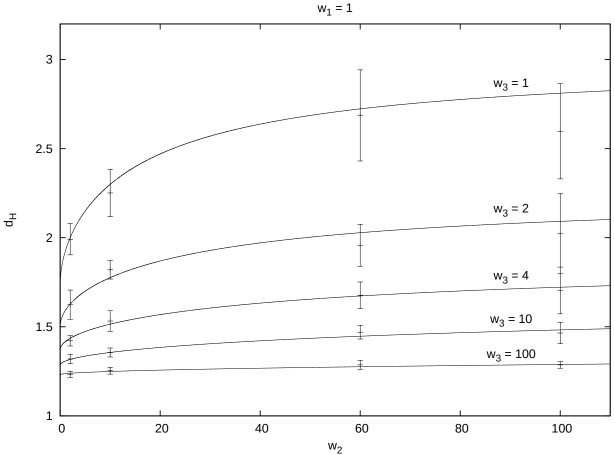

Conclusions and problems

- Random trees are a universal mathematical tool in science
- It remains to understand what types of behaviour can occur - what constitutes a universality class?
- What classes of continuum trees exist?
- Explore relations to SLE and 2d conformal field theory
- Many concrete problems: nongeneric local trees, equilibrium description of splitting vertex trees, spectral properties, etc. etc.
- Knowing the properties of the trees which arise in a physical system (or in some other context) may shed light on the mechanisms that produce the trees
- Export techniques and results from trees to graphs with loops

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