# ARN et arbres: problèmes de croissance et de repliement


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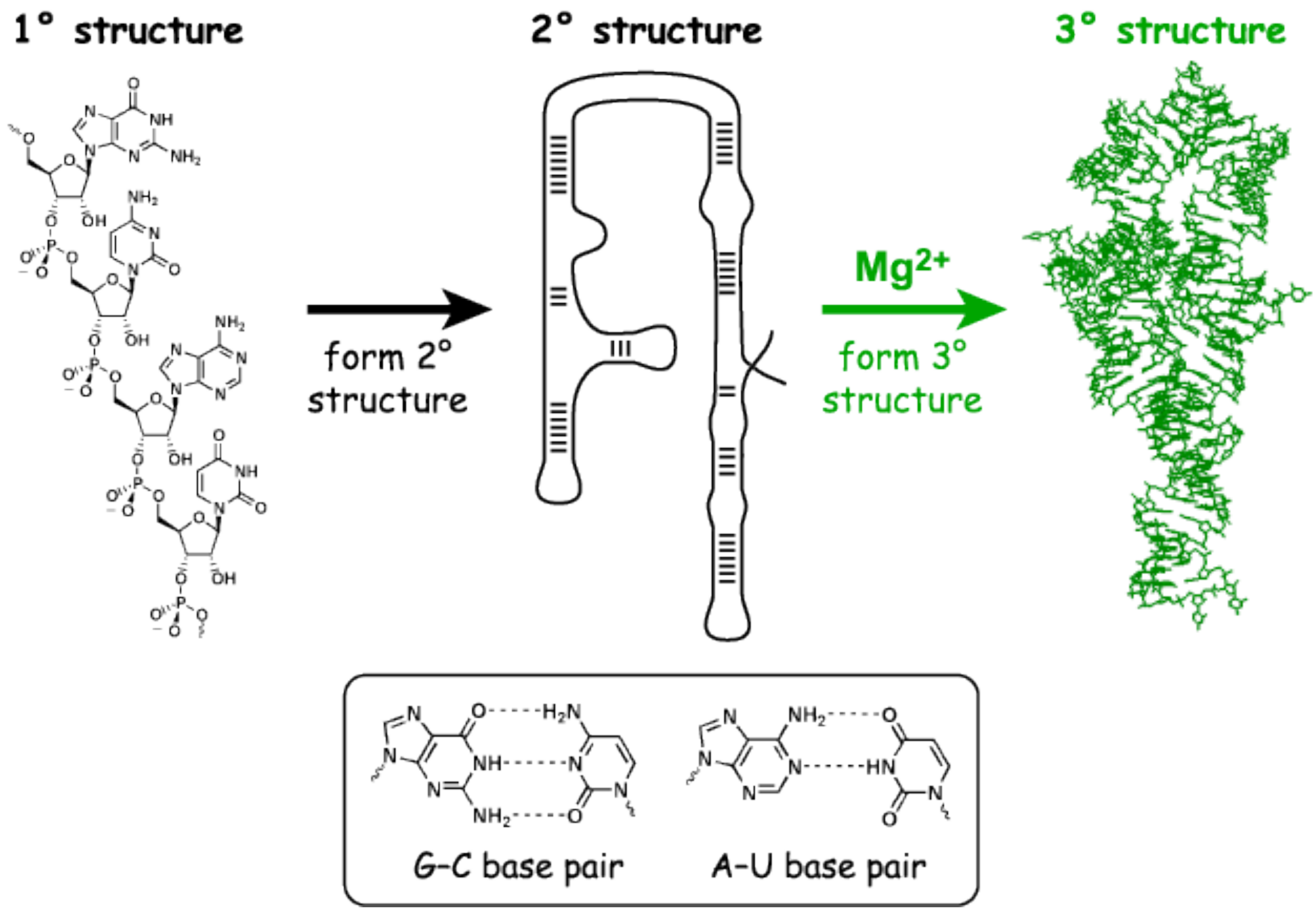
# Why trees?

- Population dynamics & genealogy
- Biology, Evolution
- Growth processes
- Branched polymers
- Statistical mechanics
- Spanning trees, random matrices
- Quantum gravity (2d & 3d)
- Combinatorics
- Computer science, data bases, XML, etc.
- Optimisation problems
- Social sciences, economics
- etc.

# First problem: RNA folding & random splitting trees

## RNA primary, secondary and tertiary structure




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

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

GCCUUAAUGCACAUGGGCAAGCCCACGUAGCUAGUCGCGACACCAGUCCCAAAUAAUGUUCACCCAACUCGCCUGACCGUCCCGCAGUA
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**

# Random bond RNA model (R. Bundshuh and T. Hwa)

Question: Which features are sequence dependent (biological functions) and which are generic?

Long chain with random sequence of bases

Allows numerical and analytical studies (in particular at IPhT...)

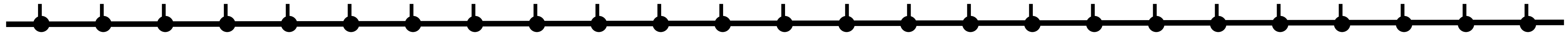
Exhibit a freezing transition at a finite temperature $T_g$

High temperature molten phase (many equivalent microstates - generic tree with fractal dimension 2)

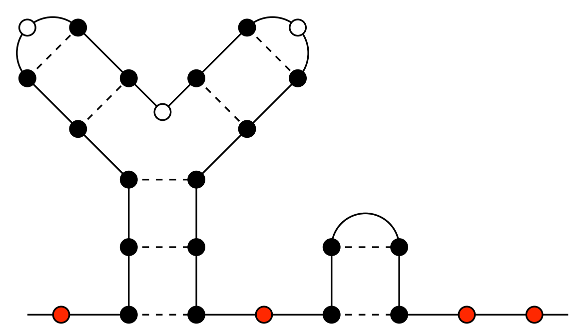
Low temperature frozen state (the system is frozen in one of the minimal energy configurations, like in a glass or a spin-glass)

# The (planar) random bond RNA folding model

1) Start from a strand made of L random bases $b_1 \; b_2 \; b_3 \; \cdots \; b_L$



2) Fold it in a planar way (neither knots nor pseudo-knots)



3) Assign to each configuration an energy
sum of an energy for each bond

$$\mathcal{E} = \sum_{\text{pairs } (ij)} e(i,j)$$

4) Take the bond energies to be independent
Gaussian quenched random variables

$$\overline{e(i,j)e_(k,l)} = \sigma\, \delta_{ik}\delta_{jl}$$

... instead of a function of the random bases $e(b_i, b_j)$

5) And find the lowest energy configuration (ground state at zero temperature)

......This is a difficult problem: infinite range forces & topological frustration

# Greedy algorithm

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A simple step-by-step strategy to find a (hopefully not too bad) approximation of the ground state

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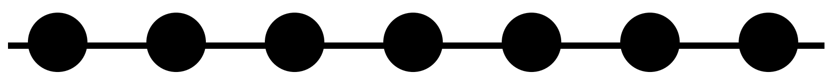
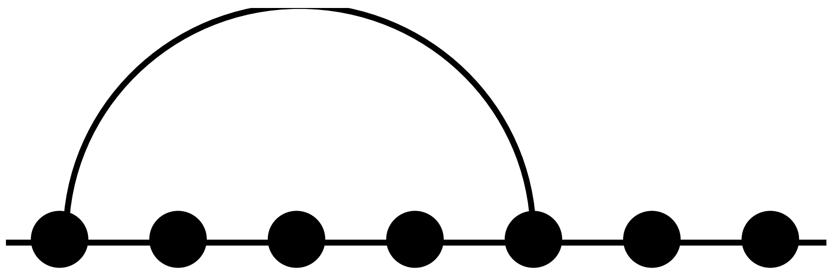
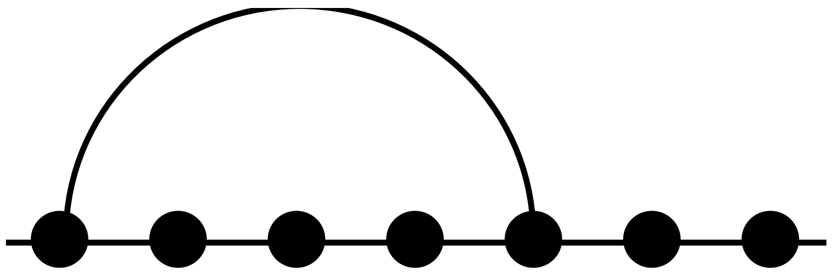
Iterate until we cannot add any pairing

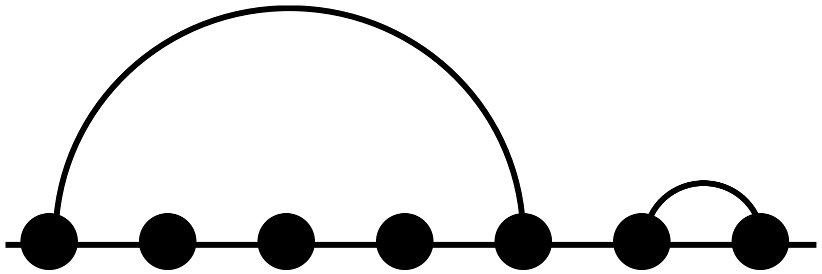
Since the pair energies are independent, this amounts to build an arch system by successive random deposition of arches







$$\frac{1}{21}$$



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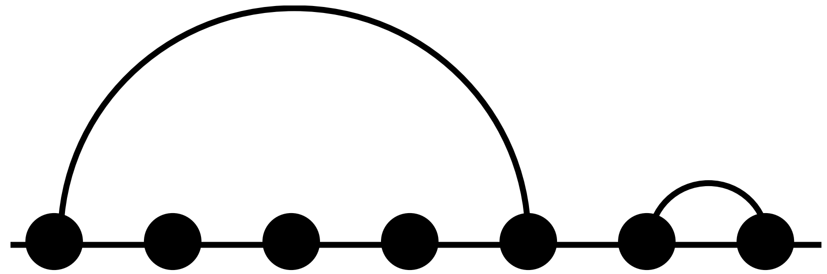
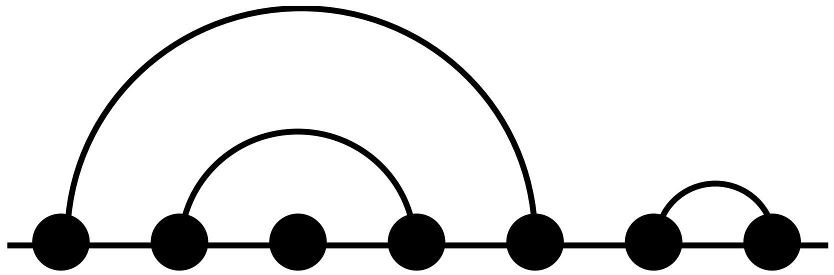


$$\frac{1}{21} \times \frac{1}{4}$$



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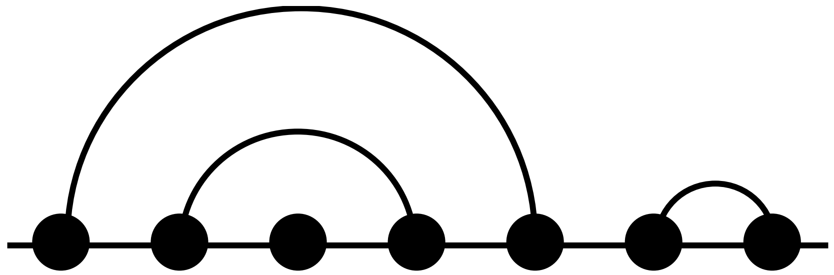

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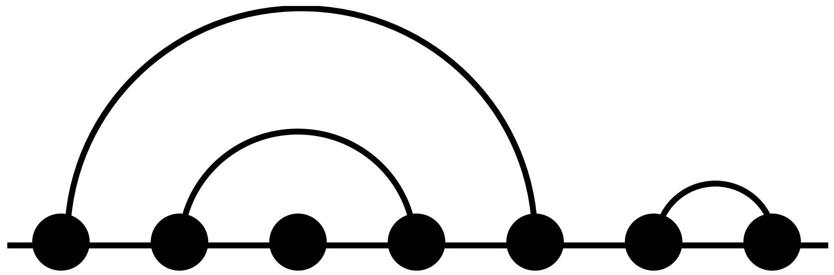

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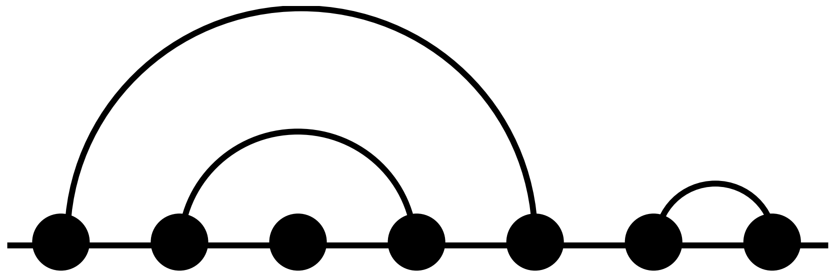
At each step, choose a new arch with uniform probability among all possible arches.
A final configuration is constructed via several deposition processes

Total probability



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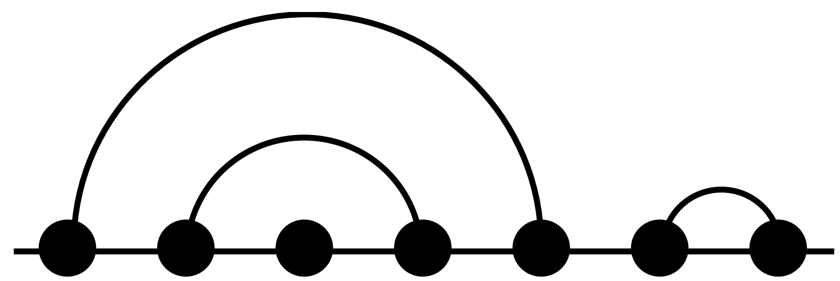
Total probability $\frac{1}{84}+\frac{1}{630}+\frac{1}{210}+\frac{1}{252}+2\,\frac{1}{126}=\frac{4}{105}$



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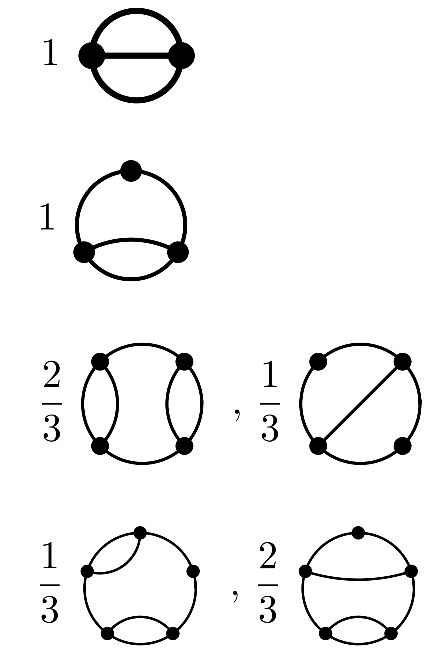
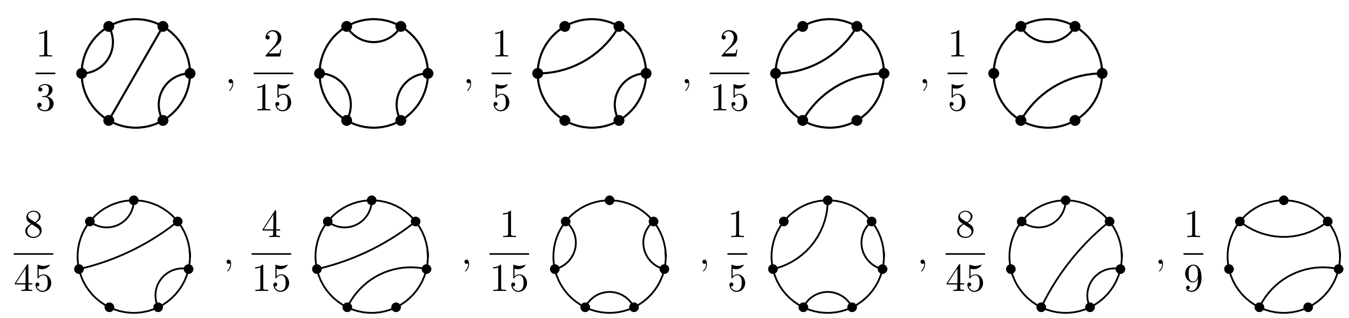
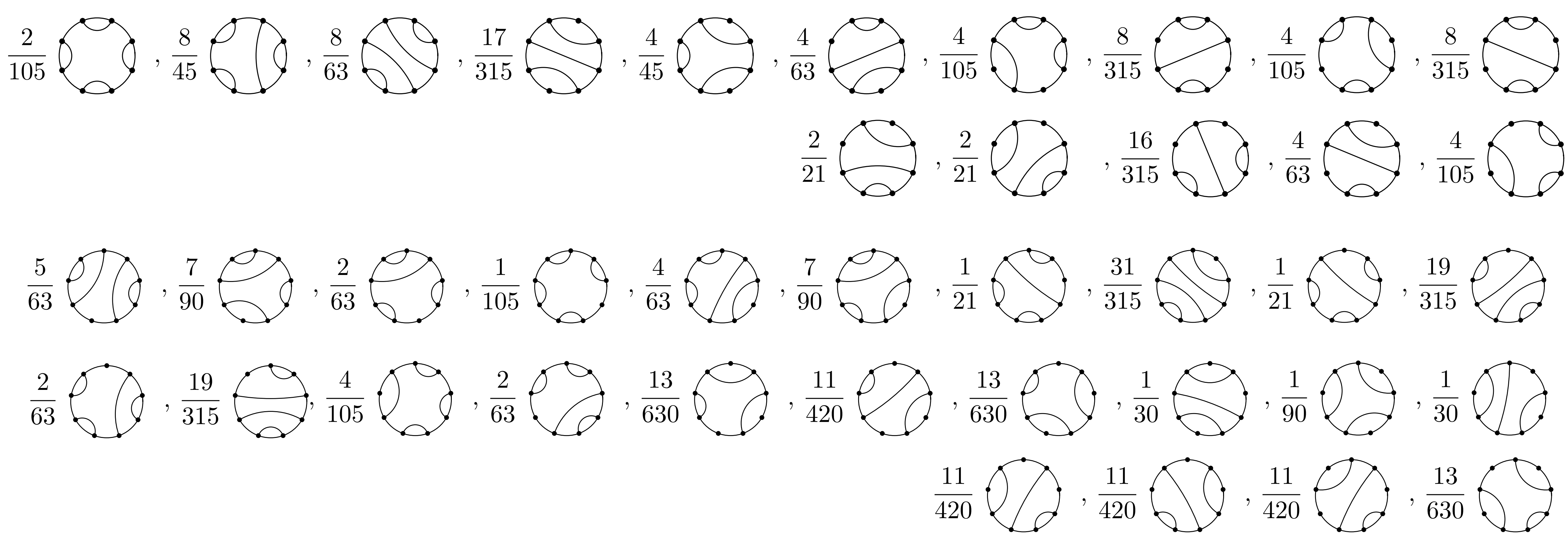
Relation to fragmentation models?

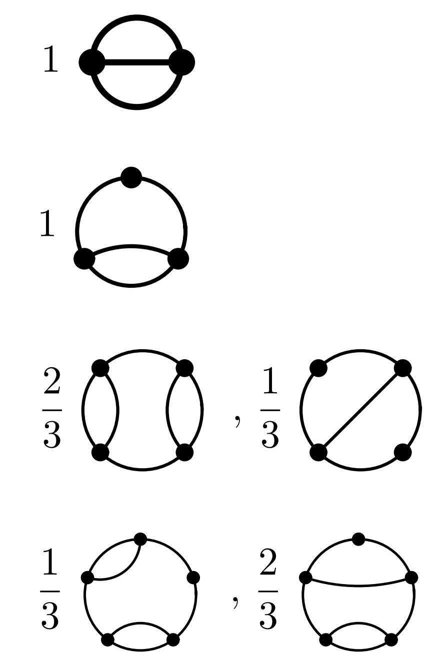
Not a model for real-time RNA folding

We generate an ensemble of configurations with non-trivial weights (different from those obtained by local processes, no combinatorics...)



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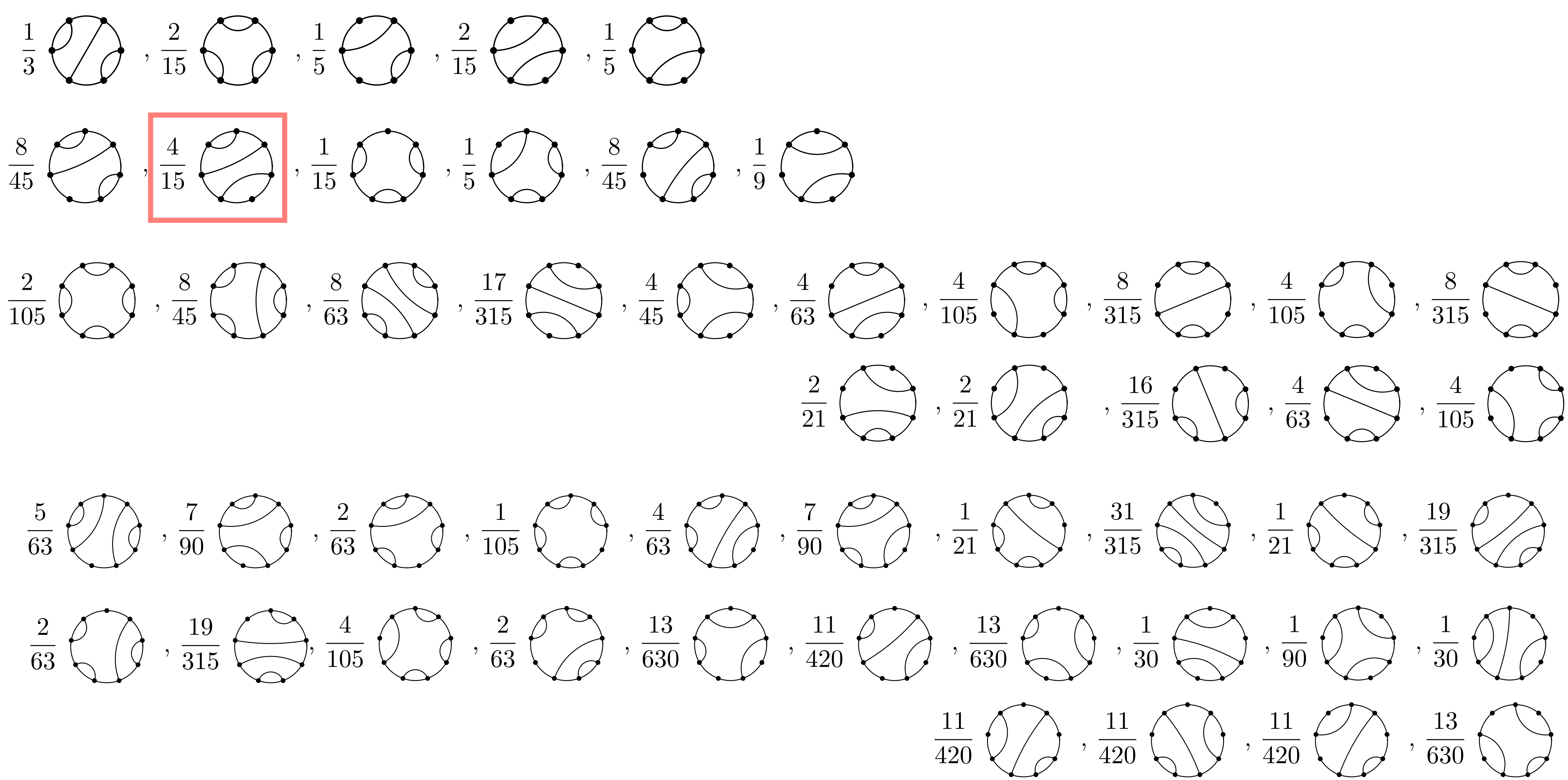
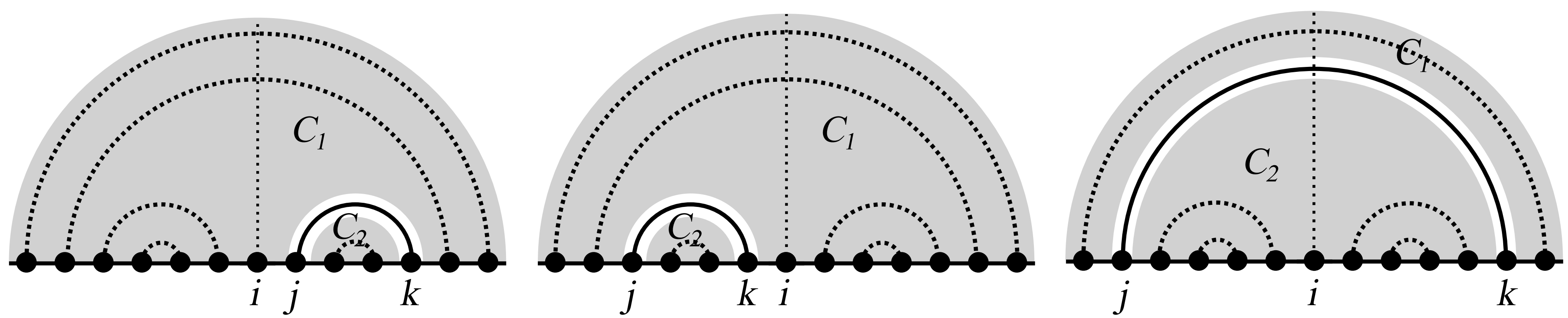


# Tools: recursion relations for probabilities and height

heights = number of arches above a point (Dyck & Motzkin paths)




Many explicit results

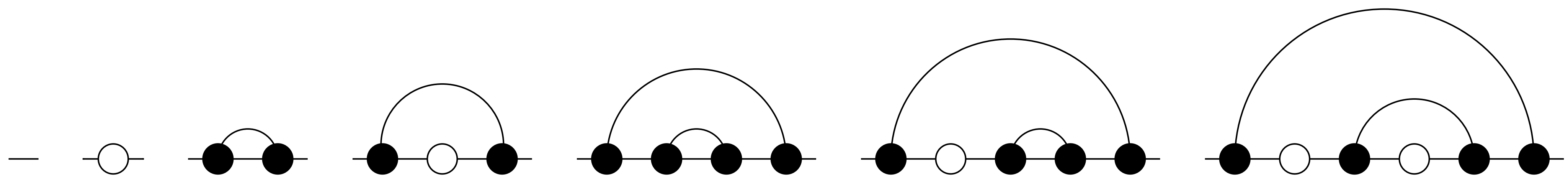
Hausdorff dimension

$$\zeta^2 + 3\zeta = 2\,, \quad \zeta = \frac{\sqrt{17}-3}{2} = 0.561\ldots\,, \quad \mathrm{d_F} = \frac{1}{\zeta} = 1.78\ldots < 2$$

Scaling functions in term of hypergeometric functions

# This model is equivalent to a tree growth model !

Random deposition point model: successive deposition of points on intervals & create an arch whenever it is possible



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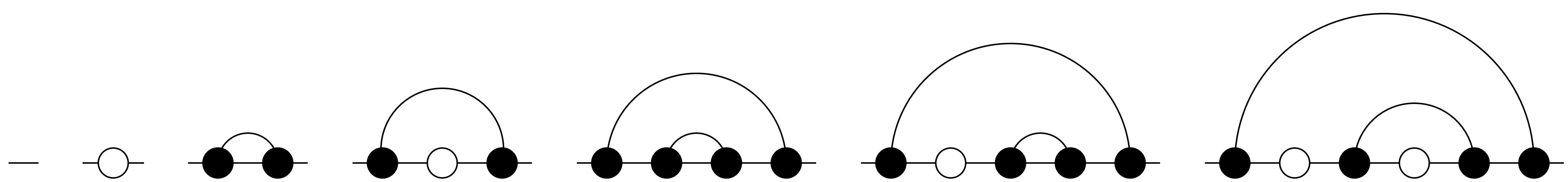
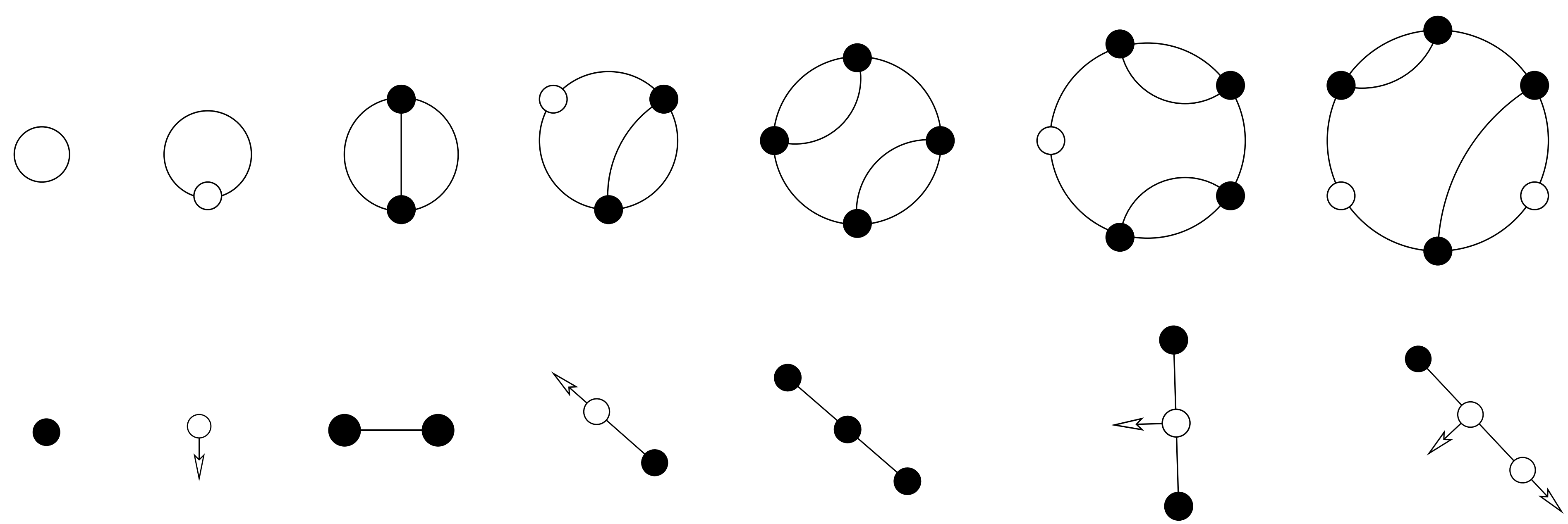


Closing + duality gives a decorated tree growth model



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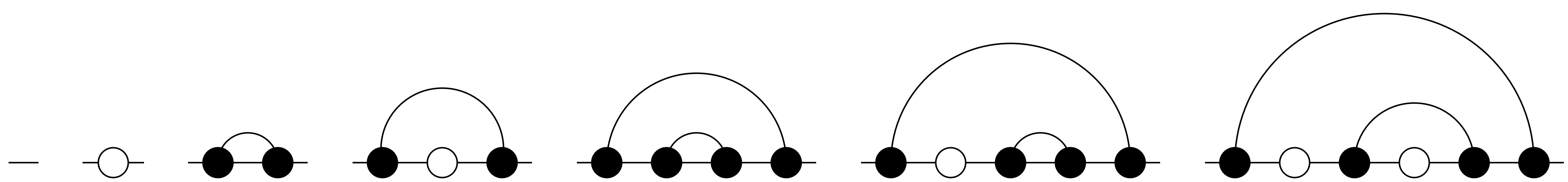

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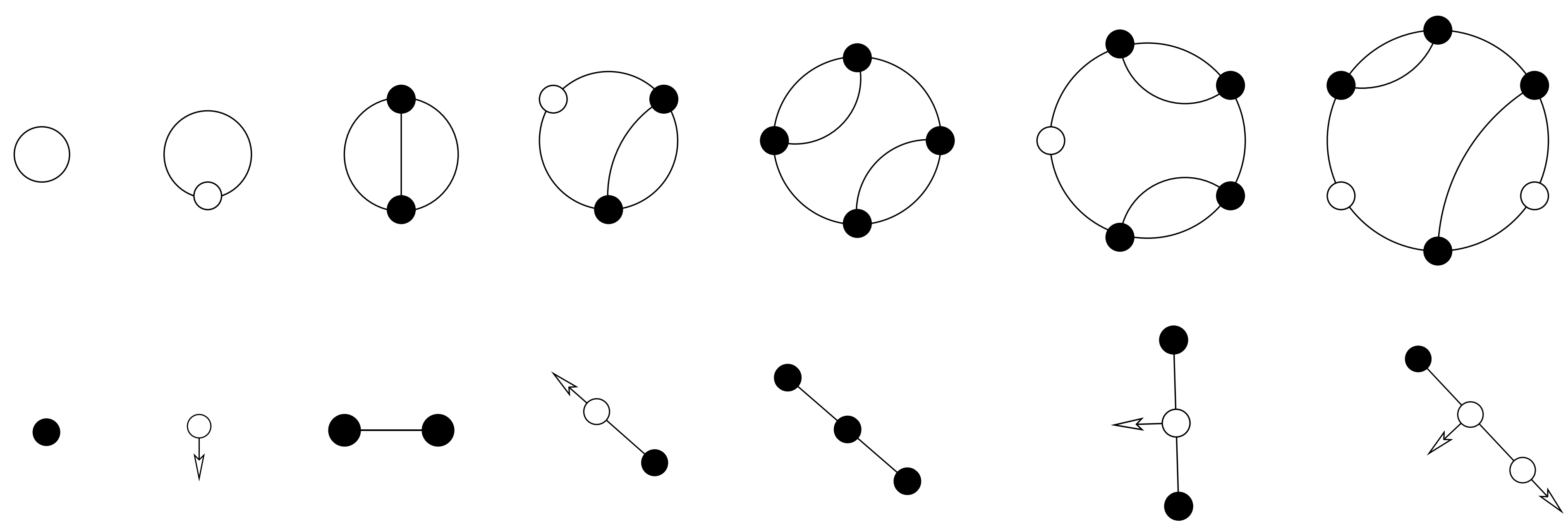
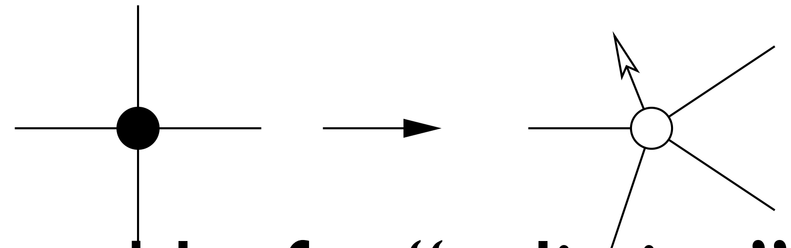


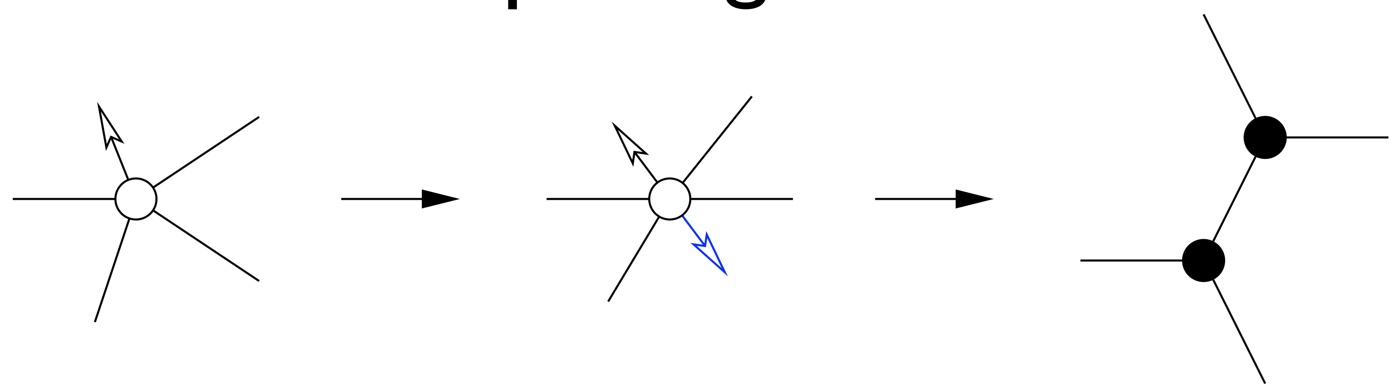
arch/tree growth at time $t$ = arch deposition for size $n=t$ !

2 steps growth process:

- add a leaf to a vertex: 1 black → 1 white



- add a second leaf = "splitting" 1 white → 2 black

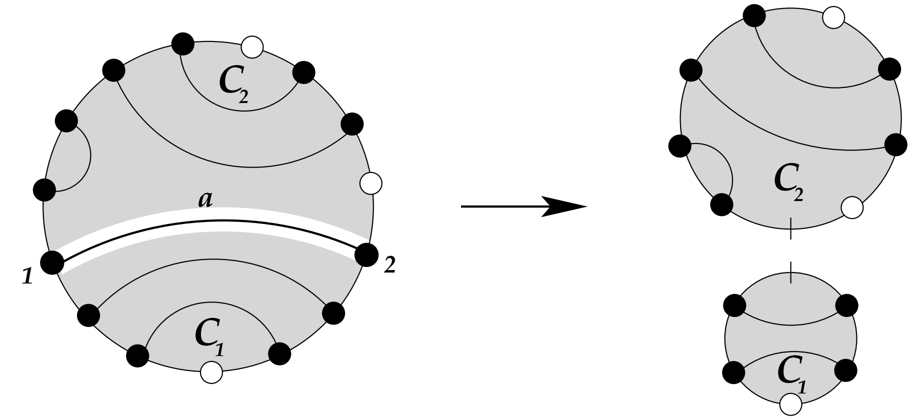


$$k \, \textit{white} \; \to (k_1, k_2) \; \text{black} \qquad k_1 + k_2 = k + 2$$

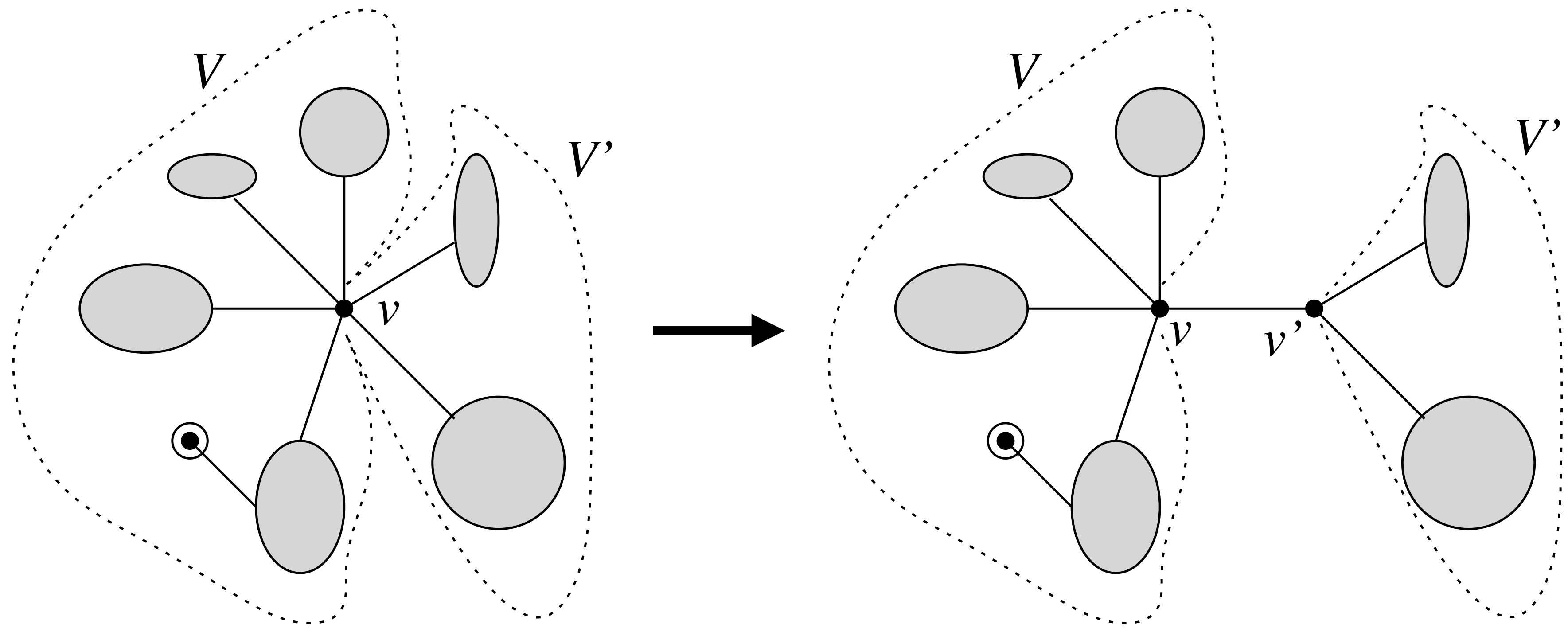
NB: attachment is just a special case

$$k_1 = 1 \,, \;\; k_2 = k + 1$$

Proof of the equivalence
deposition = growth by splitting
Use the recursion relation for
probabilities for both models



# Simpler but more general model: growth of planar trees by splitting




$$k \to (k_1, k_2) \quad , \qquad k_1 + k_2 = k + 2$$

Relative probability for specific splitting of a vertex

$$w_{k_1,k_2}$$

Relative probability for splitting of a vertex

$$w_k = \frac{k}{2} \sum_{k_1+k_2=k+2} w_{k_1,k_2}$$

# This includes attachement processes

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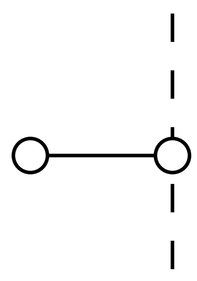

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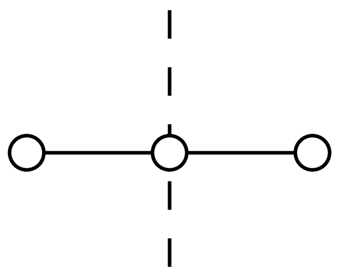

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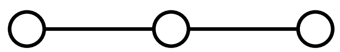

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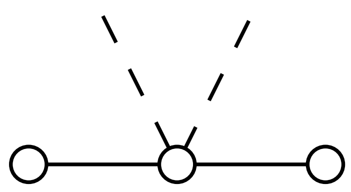

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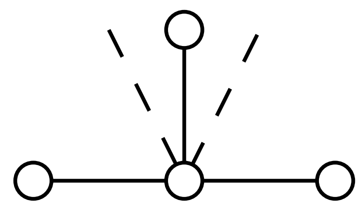

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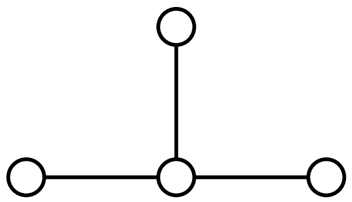

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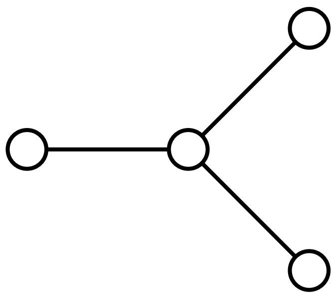

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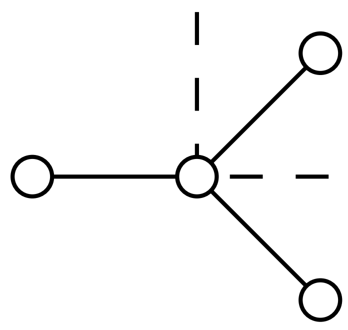

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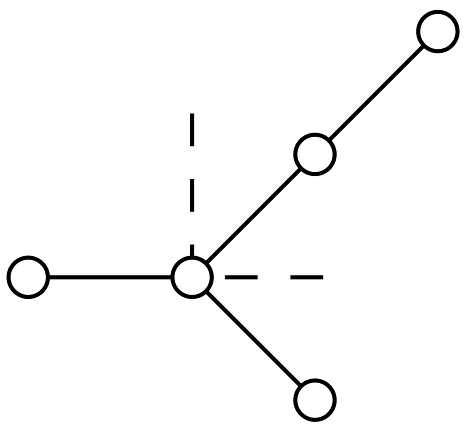

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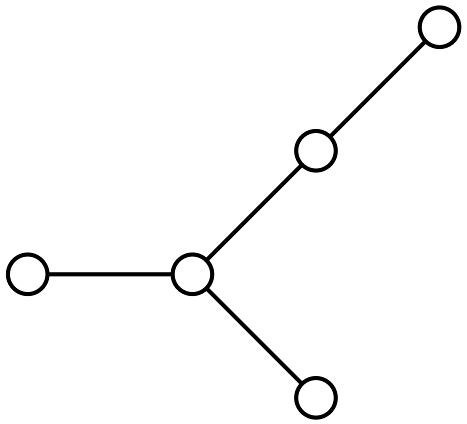

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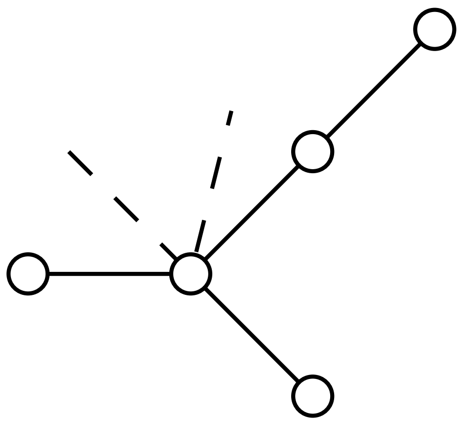

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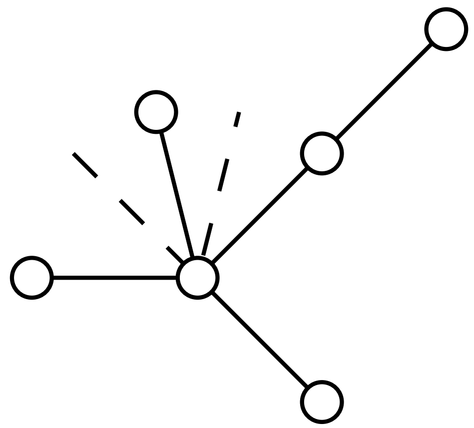

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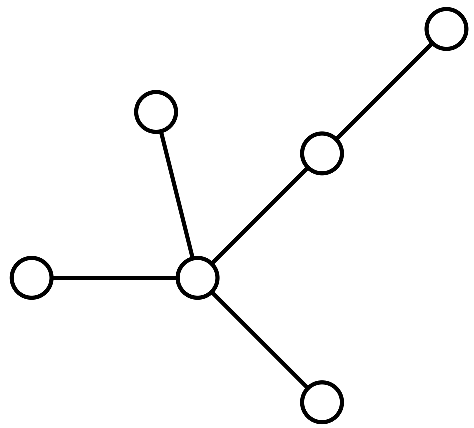

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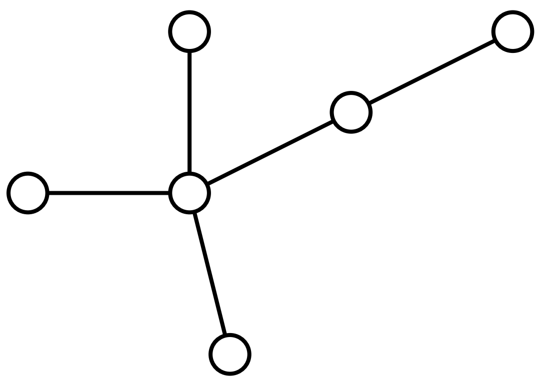

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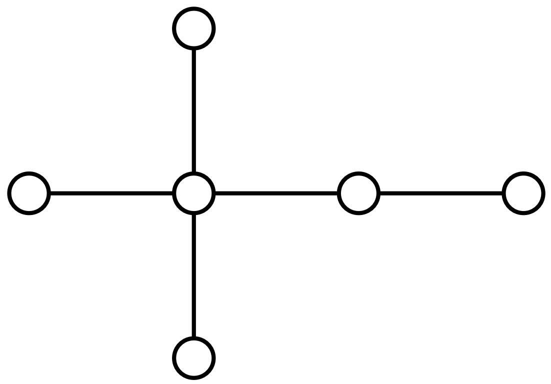

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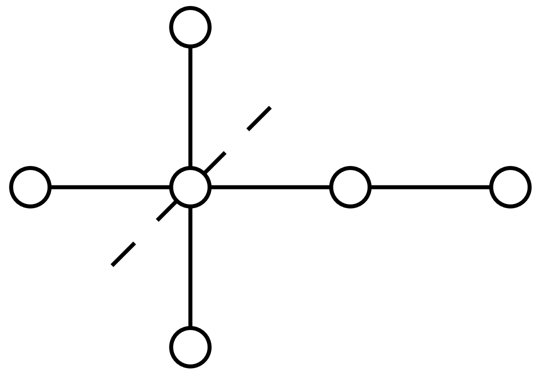

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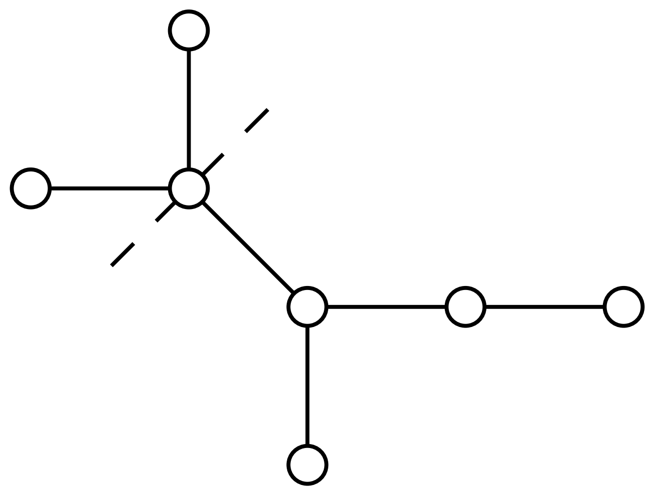

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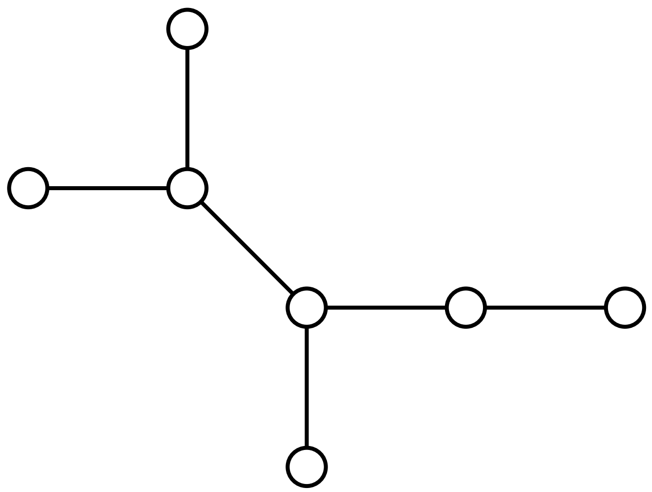

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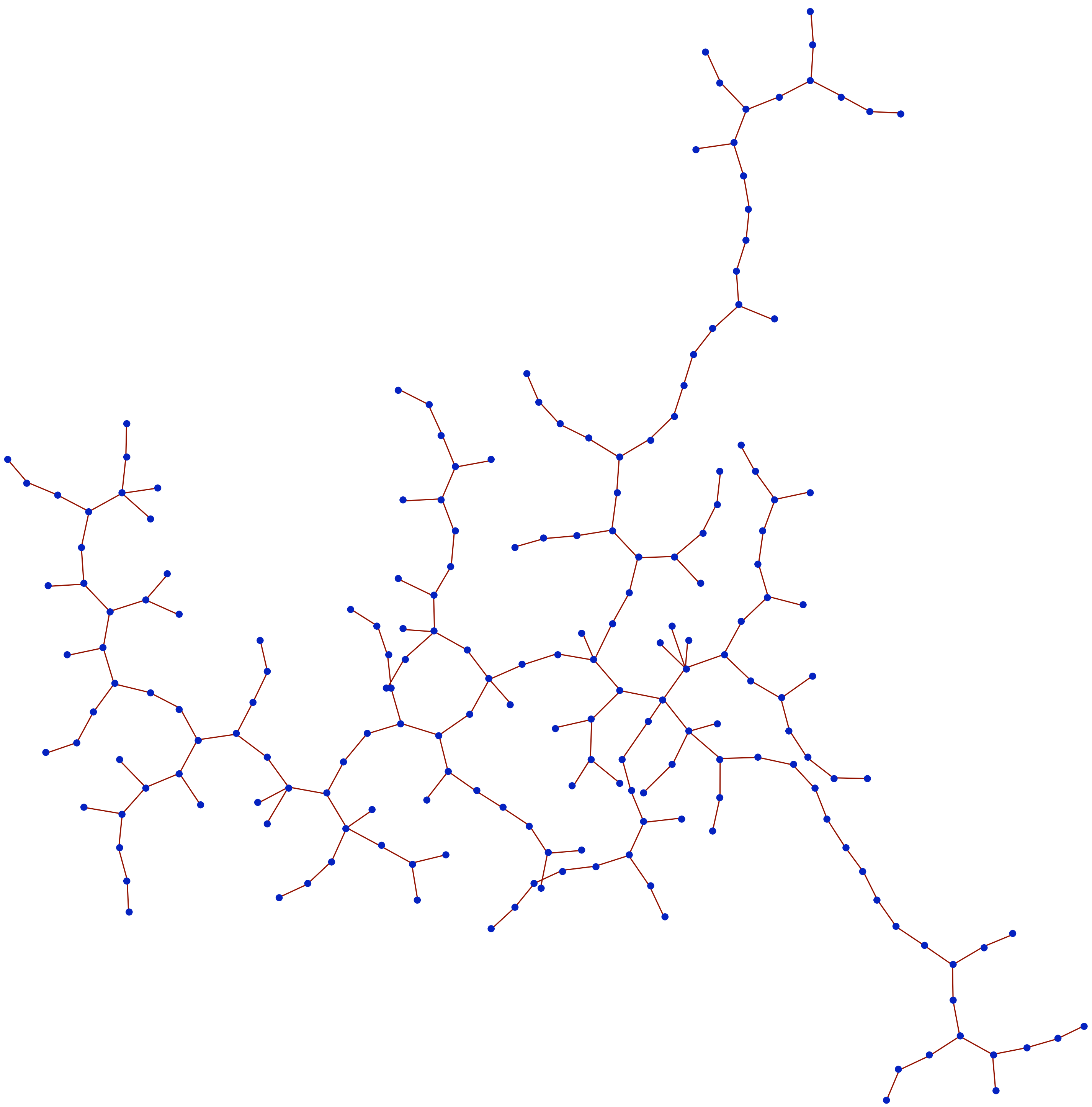

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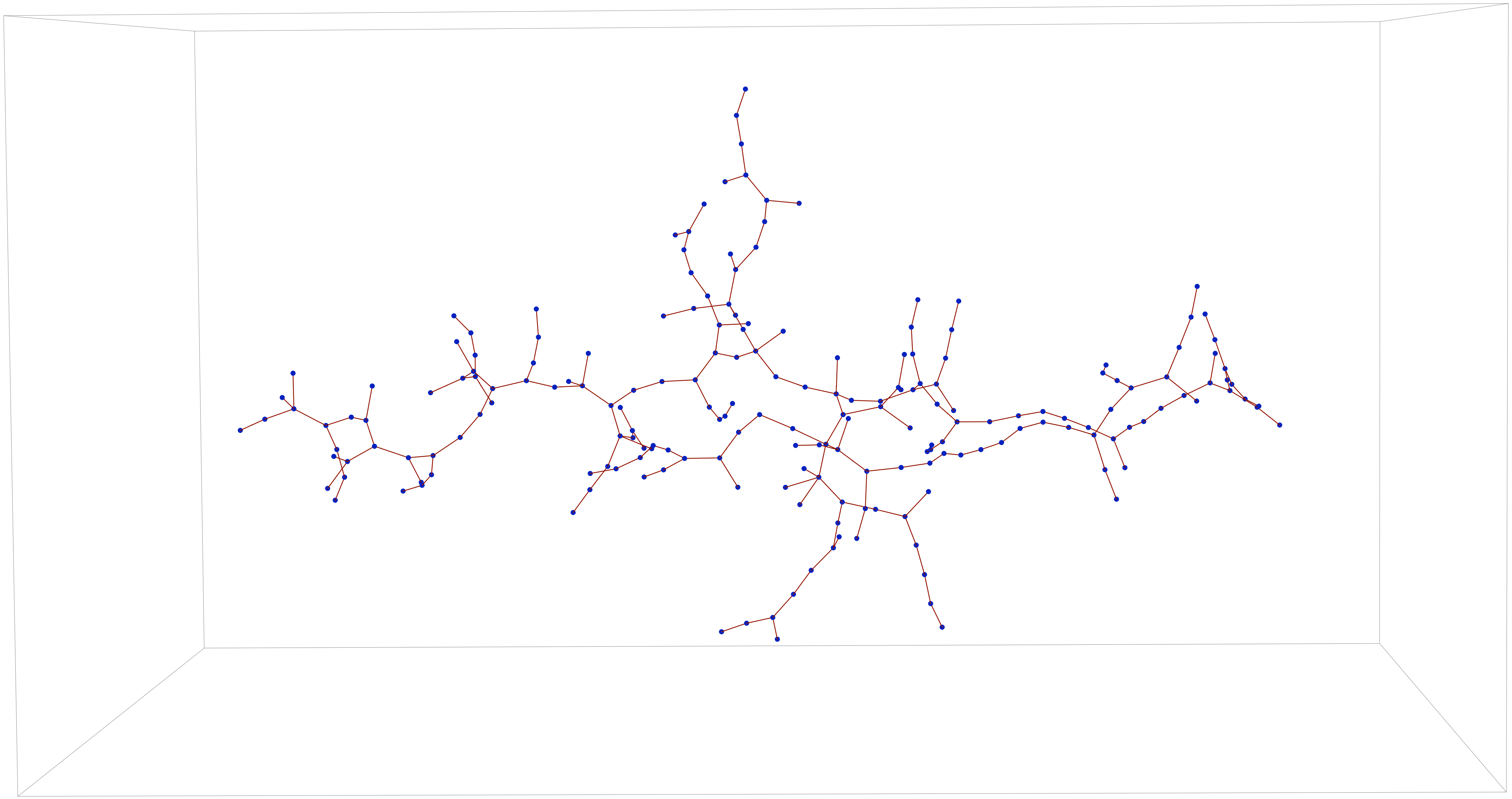


- What kind of trees do we get?

- Like scale-free networks? (vertex with large coordination, infinite Hausdorff dimension)

- Or like generic trees (finite coordination, finite Hausdorff dimension)

- Universal properties?

- Do the Hausdorff dimension depend on the details of the transition rates matrix

Simple example:

Maximal coordination 3

Uniform transition rates

$$w_{1,2} = w_{2,1} = \frac{w_1}{2}$$
$$w_{1,3} = w_{2,2} = w_{3,1} = \frac{w_2}{3}$$
$$w_{3,2} = w_{2,3} = \frac{w_3}{2}$$

Linear k-dependence

$$w_k = ak + b$$

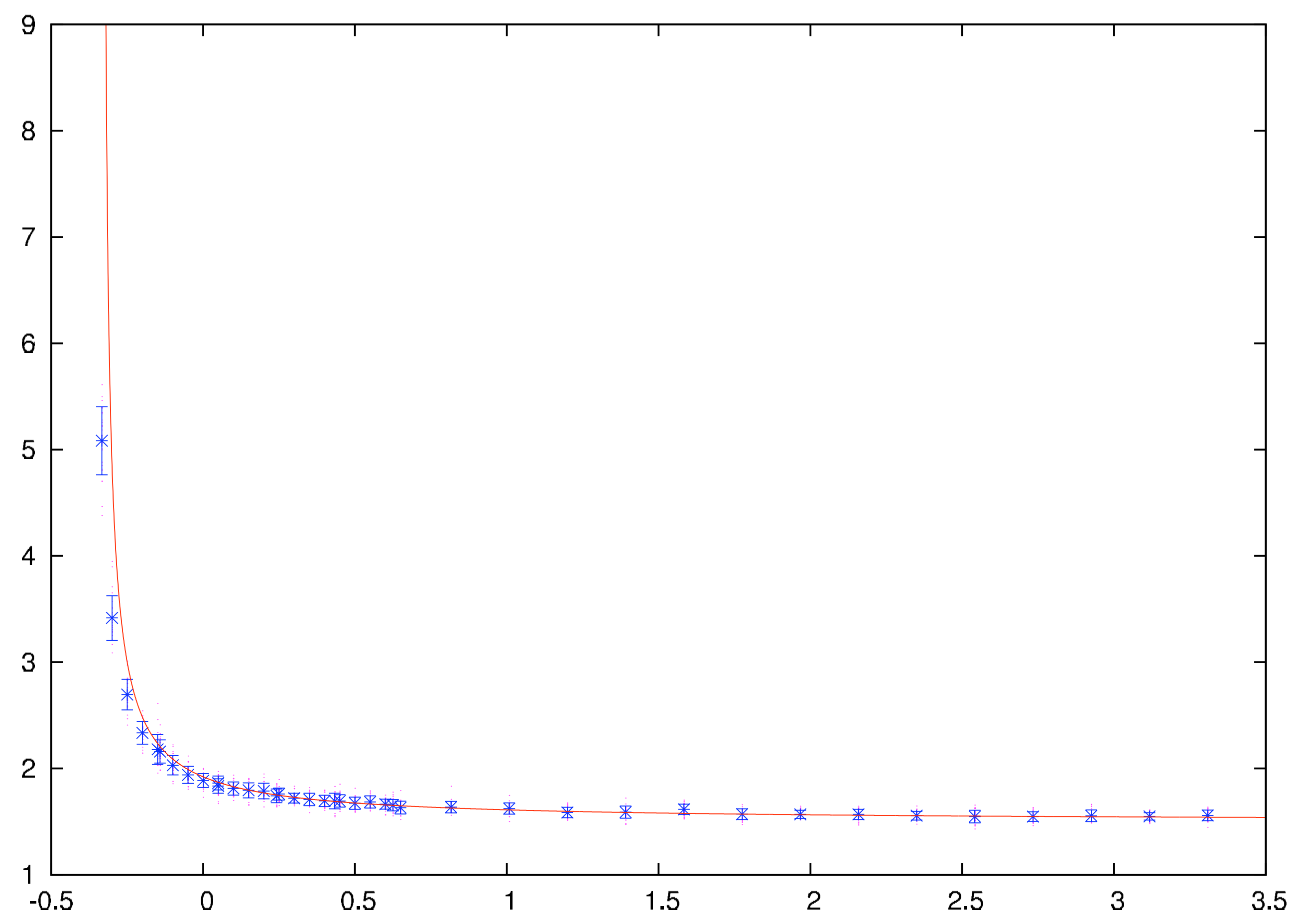
General approach: recursions for correlations

$$x = a/b$$

$$d_H = \frac{3(\sqrt{100x^2 + 84x + 17} + 2x + 1)}{8(3x + 1)}$$

# Hausdorff dimension varies continuously

$$1 < d_H < \infty$$



# Conclusion: the world as a tree?

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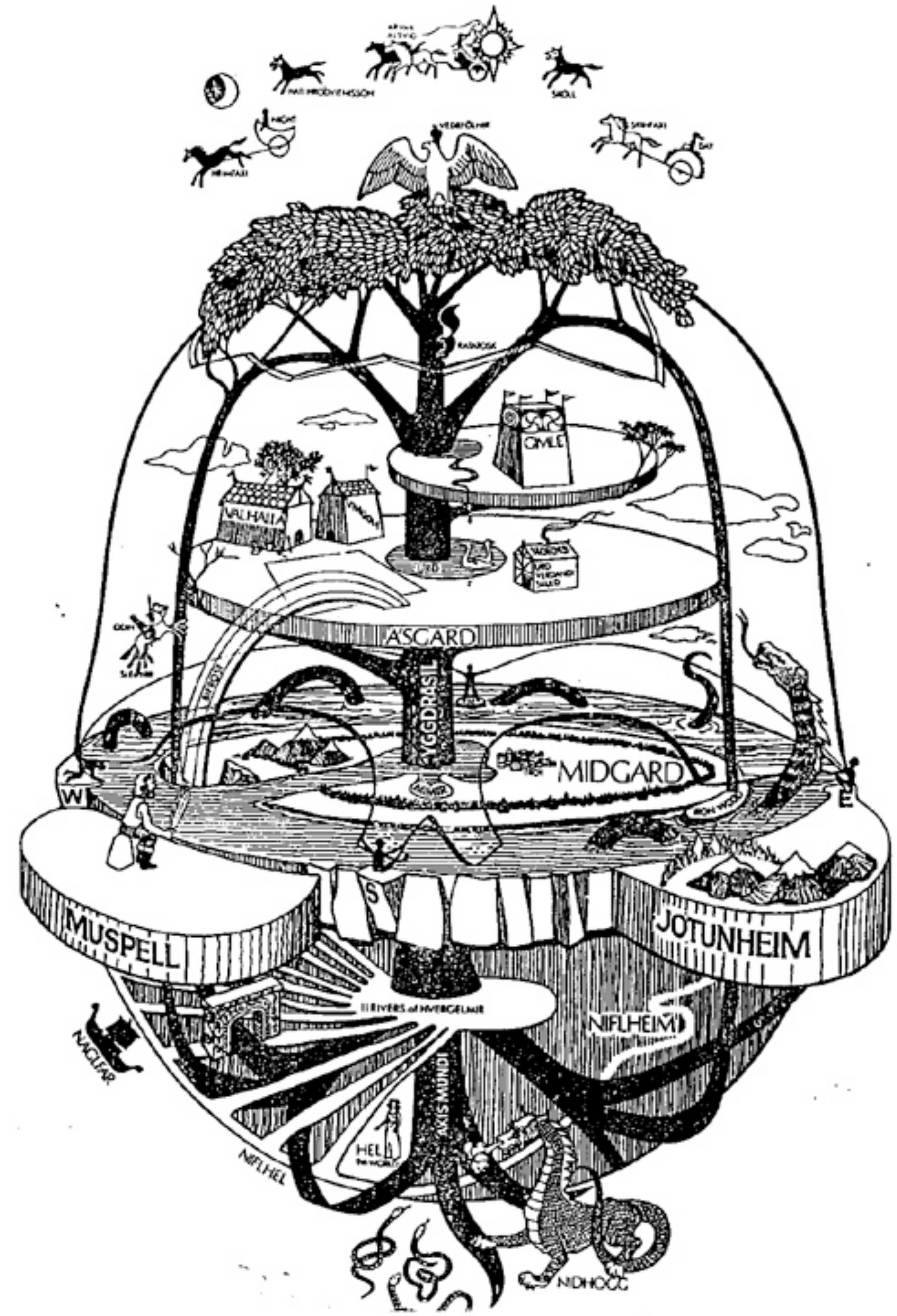

# Thanks to the organizers!