RNA folding and tree growth models

François David [1], C. Hagendorf [2] & K. J. Wiese [2]

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Plan of the talk

1. RNA folding & the random RNA model
2. Greedy approximation
3. Arch deposition model
4. Tree growth model
5. Conclusion

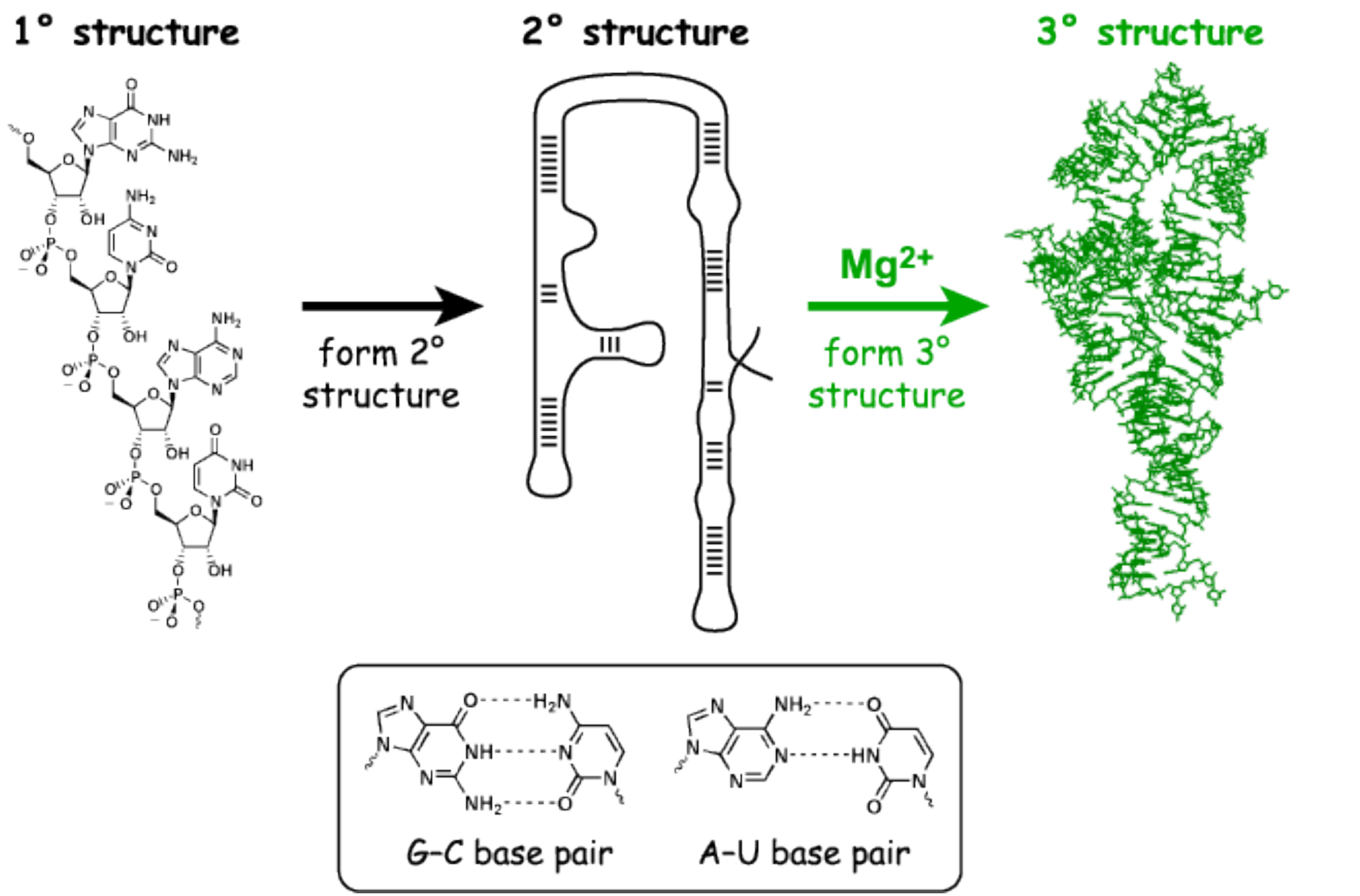
RNA folding

biological(ly inspired) physics: secondary structure of RNA strand

one-dimensional disordered system with long range interactions (pairing) & frustration (topology: planar or almost-planar structure)

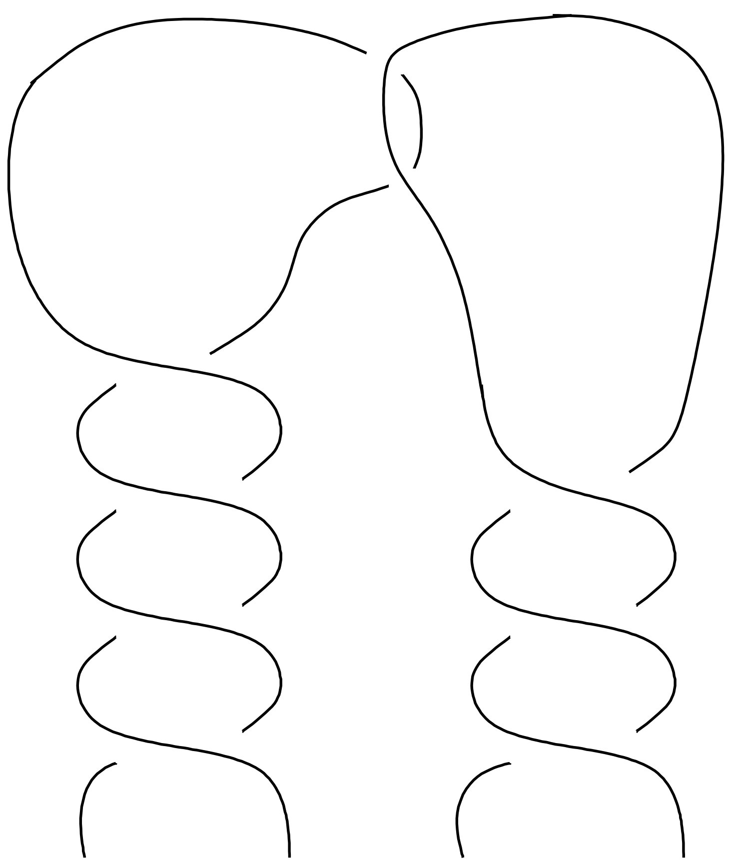
freezing transition, glass-like phase with non-trivial ground-state(s)

RNA primary, secondary and tertiary structure

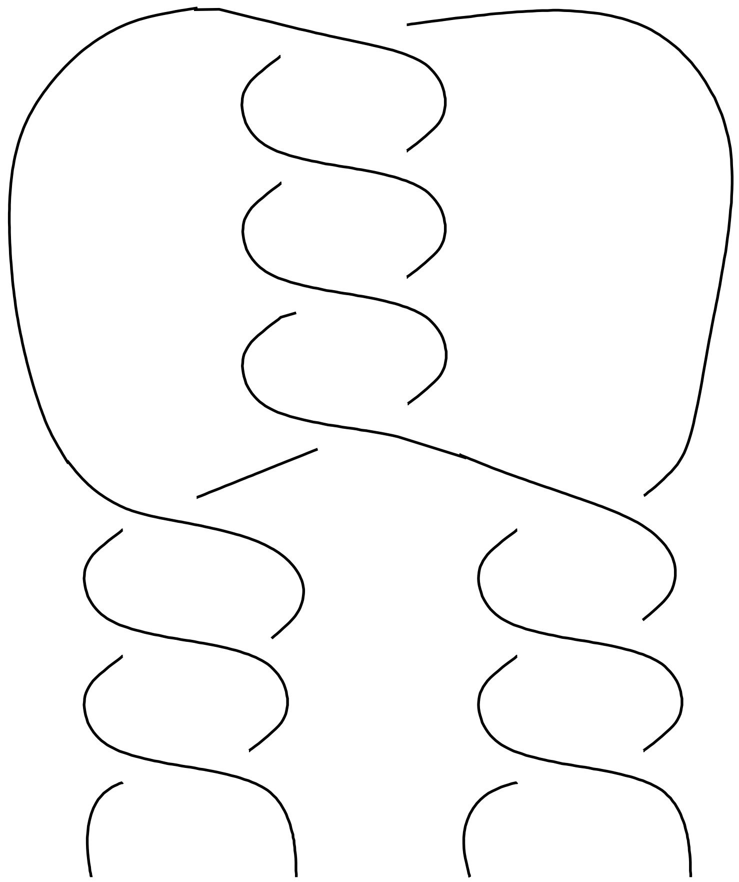


(borrowed from Scott K. Silverman scott@scs.uiuc.edu)

Not so poor approximation

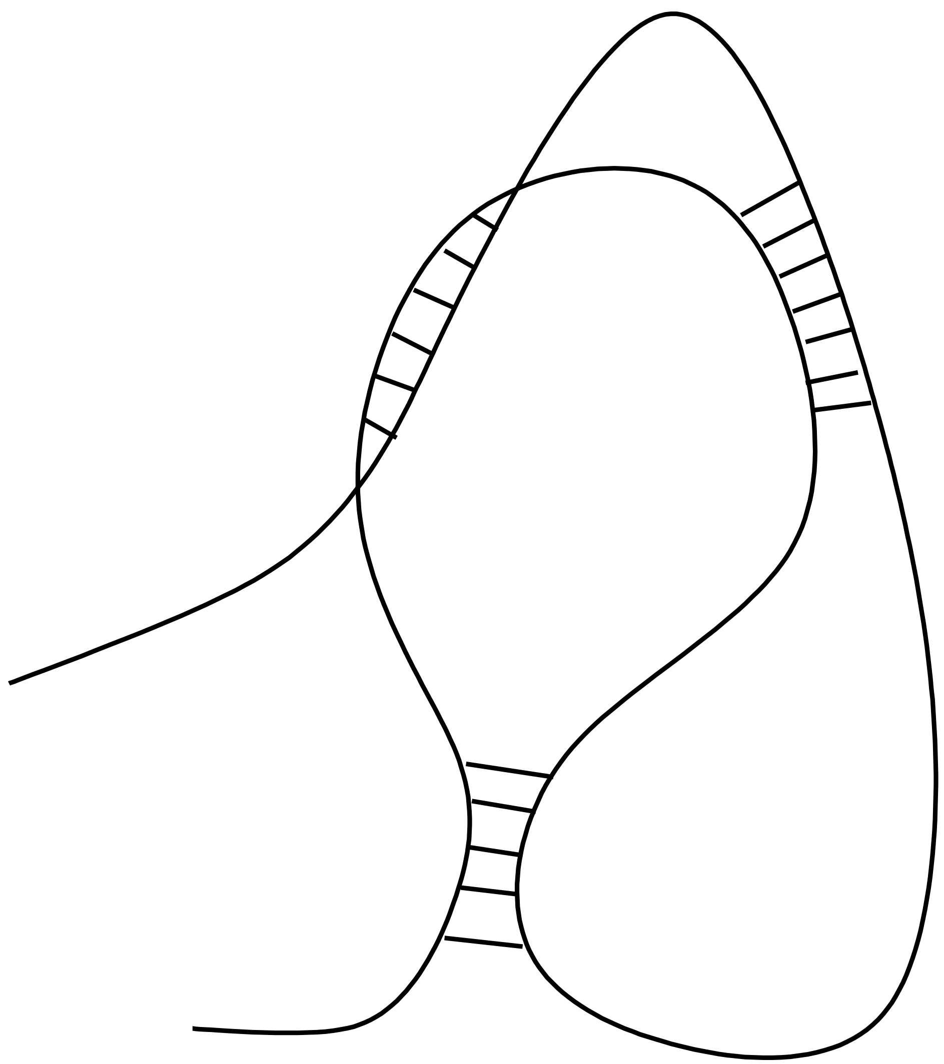


no pseudo-knot

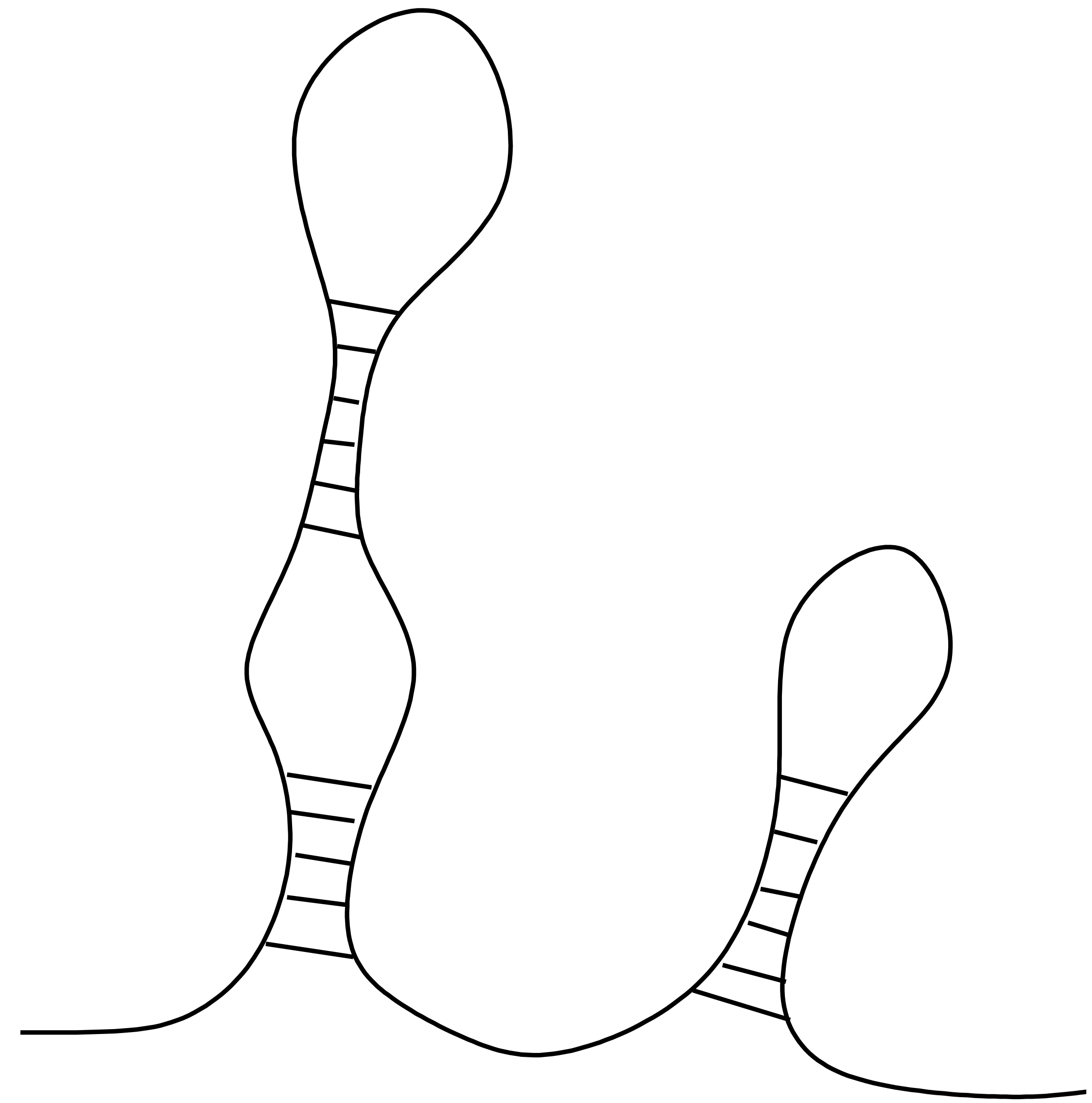


no knot

only planar configurations



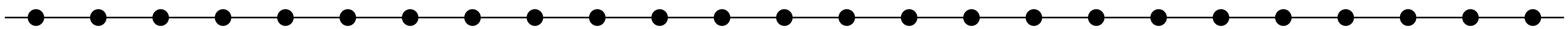
~~non-planar~~



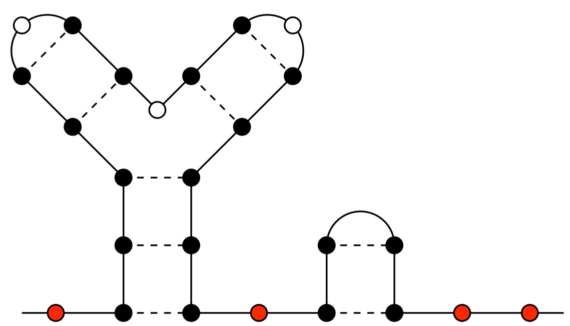
planar = tree

The random bond RNA folding model

1) Start from a strand made of L monomers



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



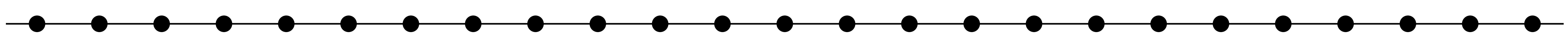
3) Assign to each configuration an energy sum of an energy for each bond

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

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

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

Pairings = Trees = Arch systems = Dyck-like paths



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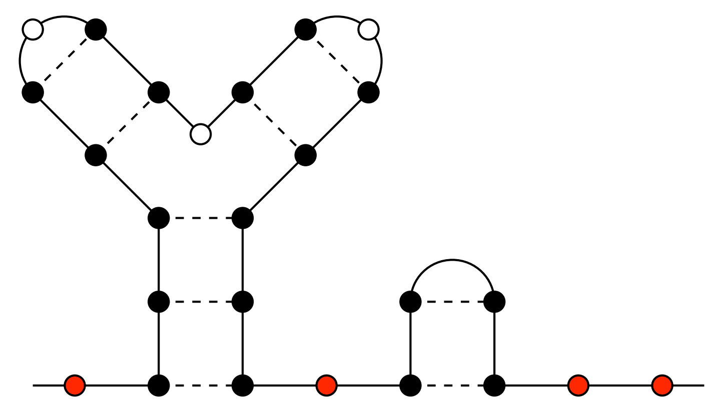

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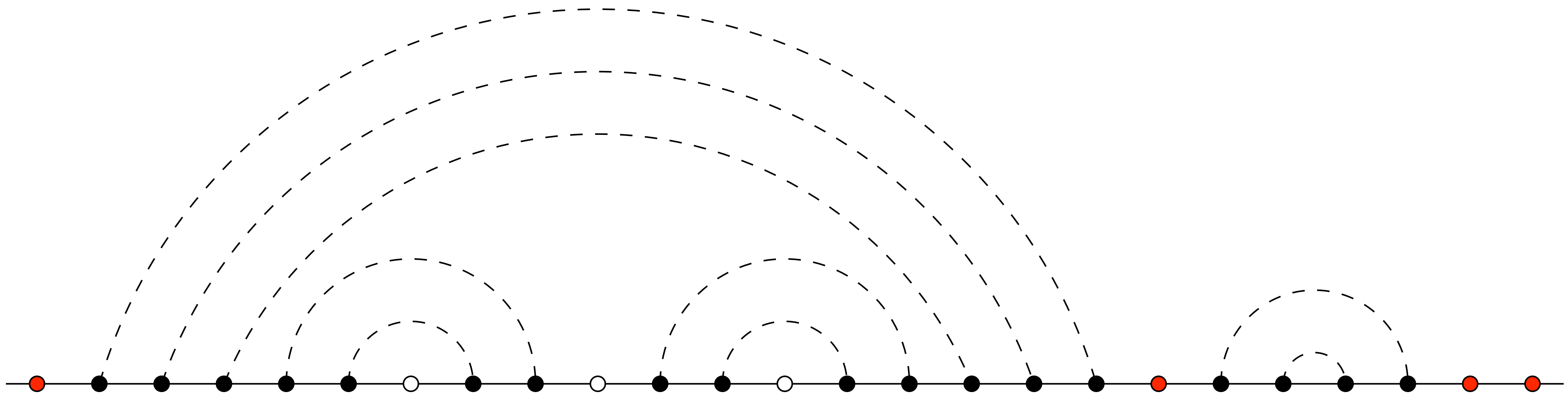

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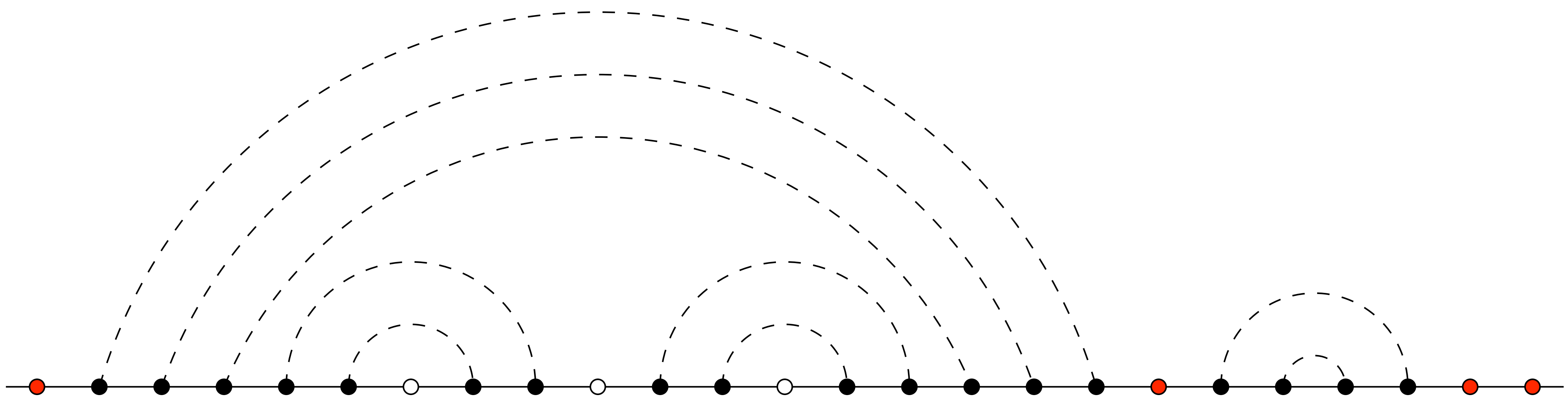

pairing probabilities $\Phi(i, j) \propto |i - j|^{-\rho}$

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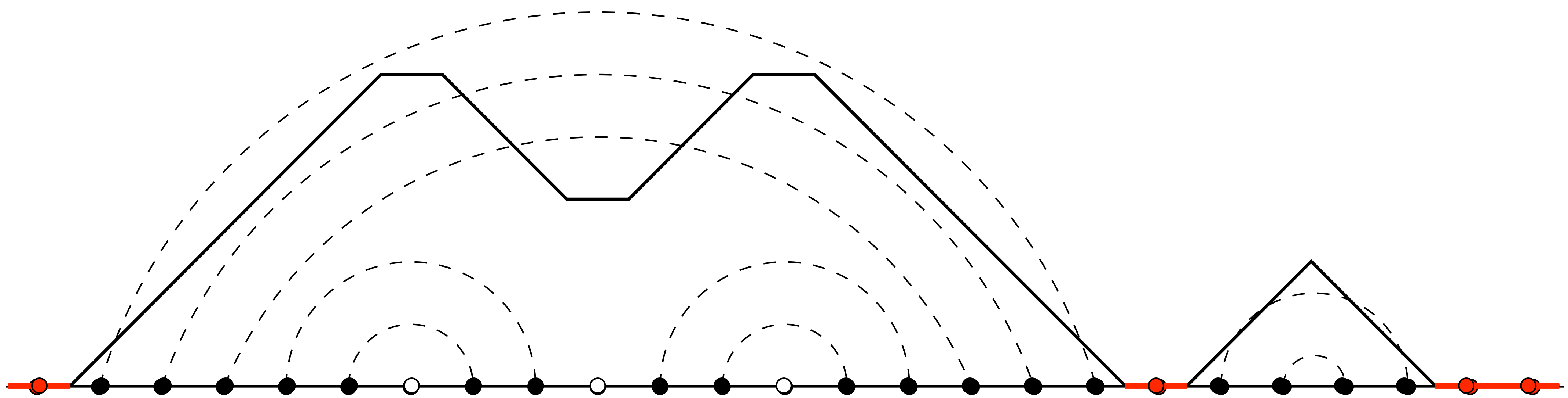

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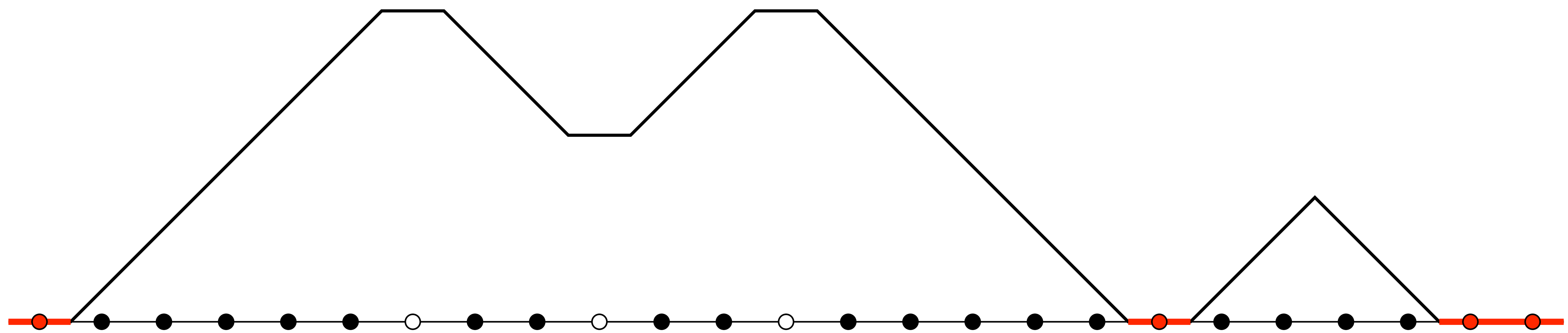

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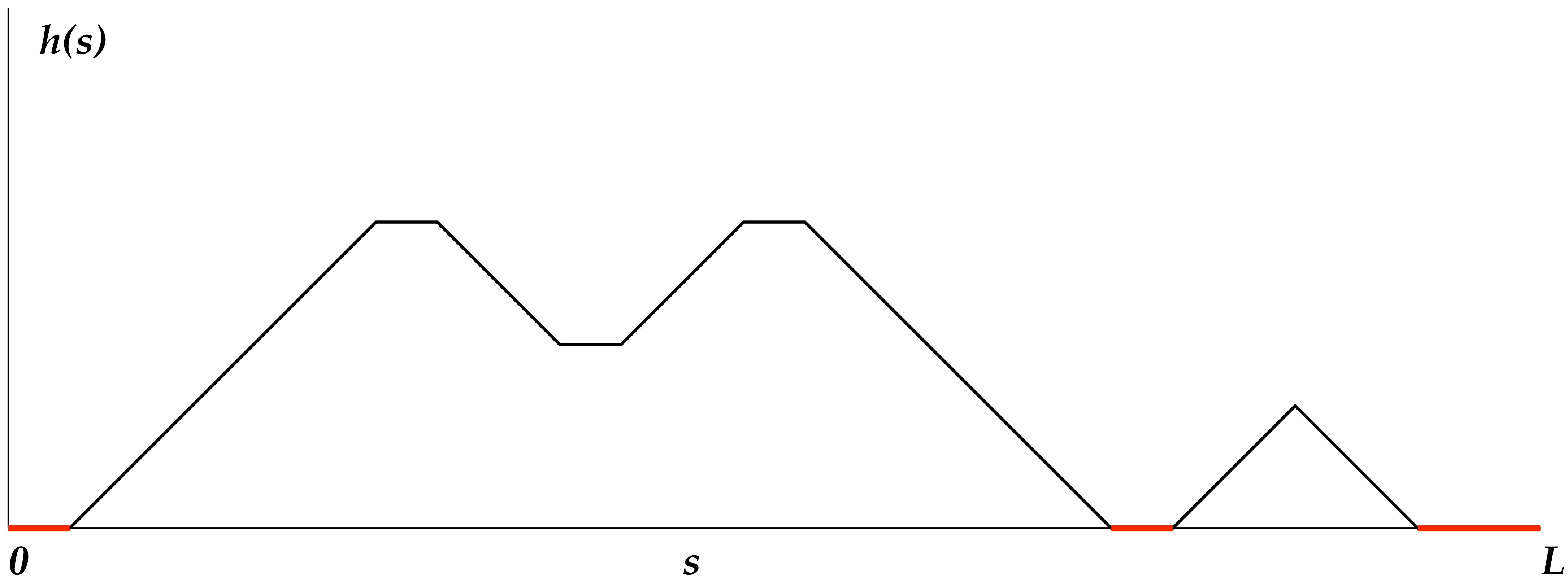

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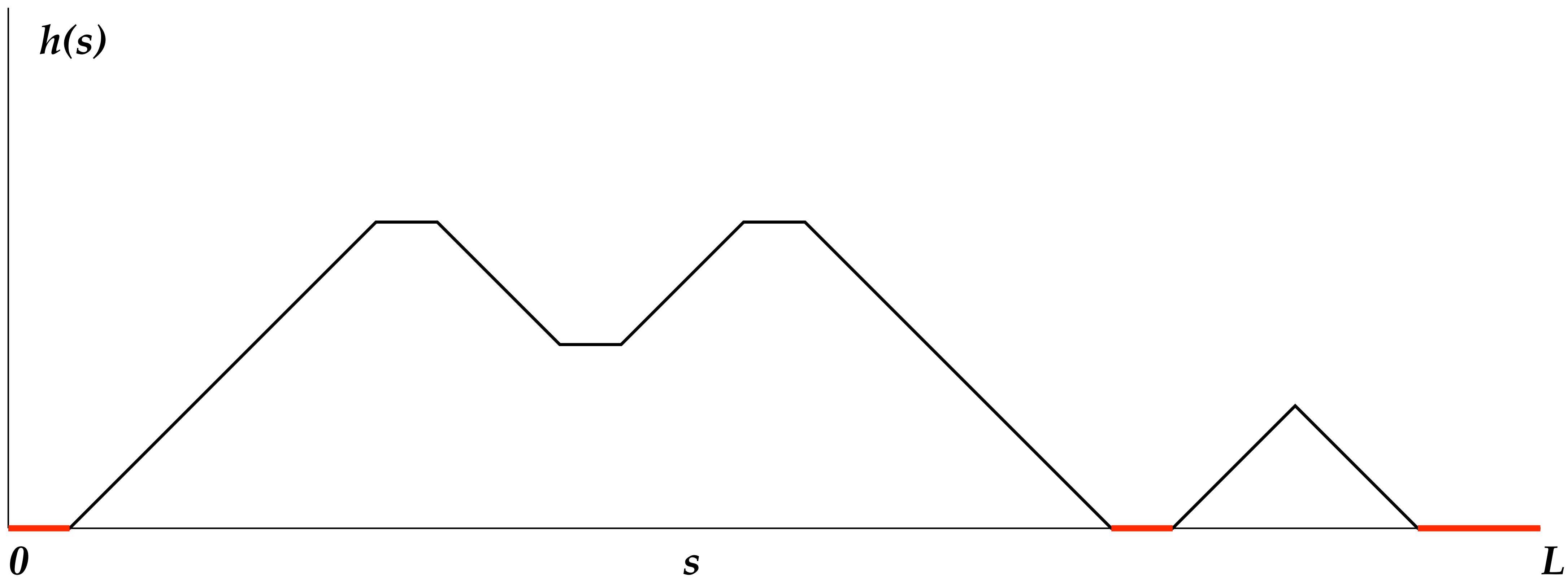

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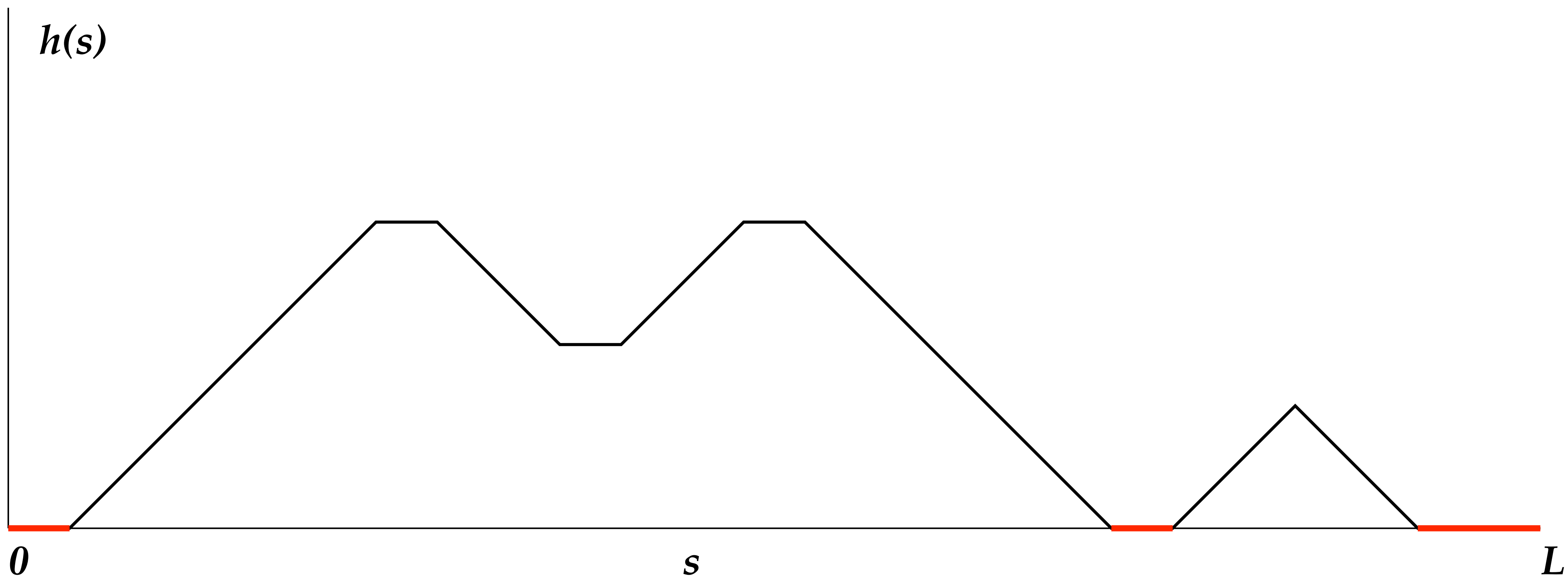

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fractal dimension of the tree $d_f = \dfrac{1}{\zeta}$

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* already considered in Markus Müller's thesis (2002)

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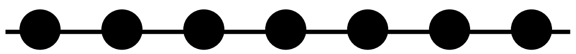

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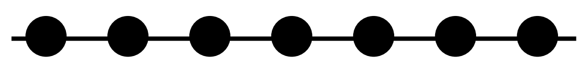

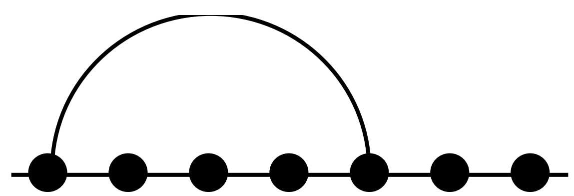

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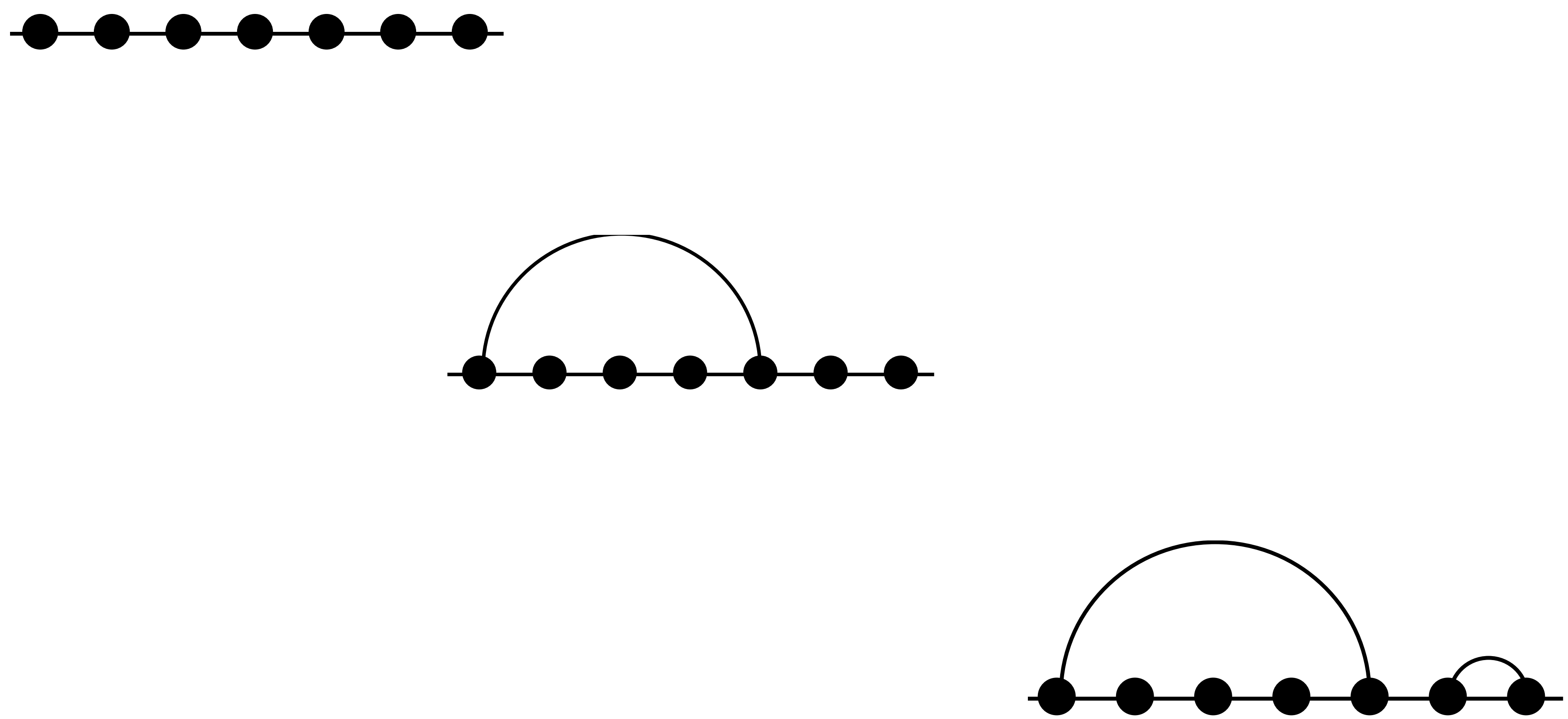

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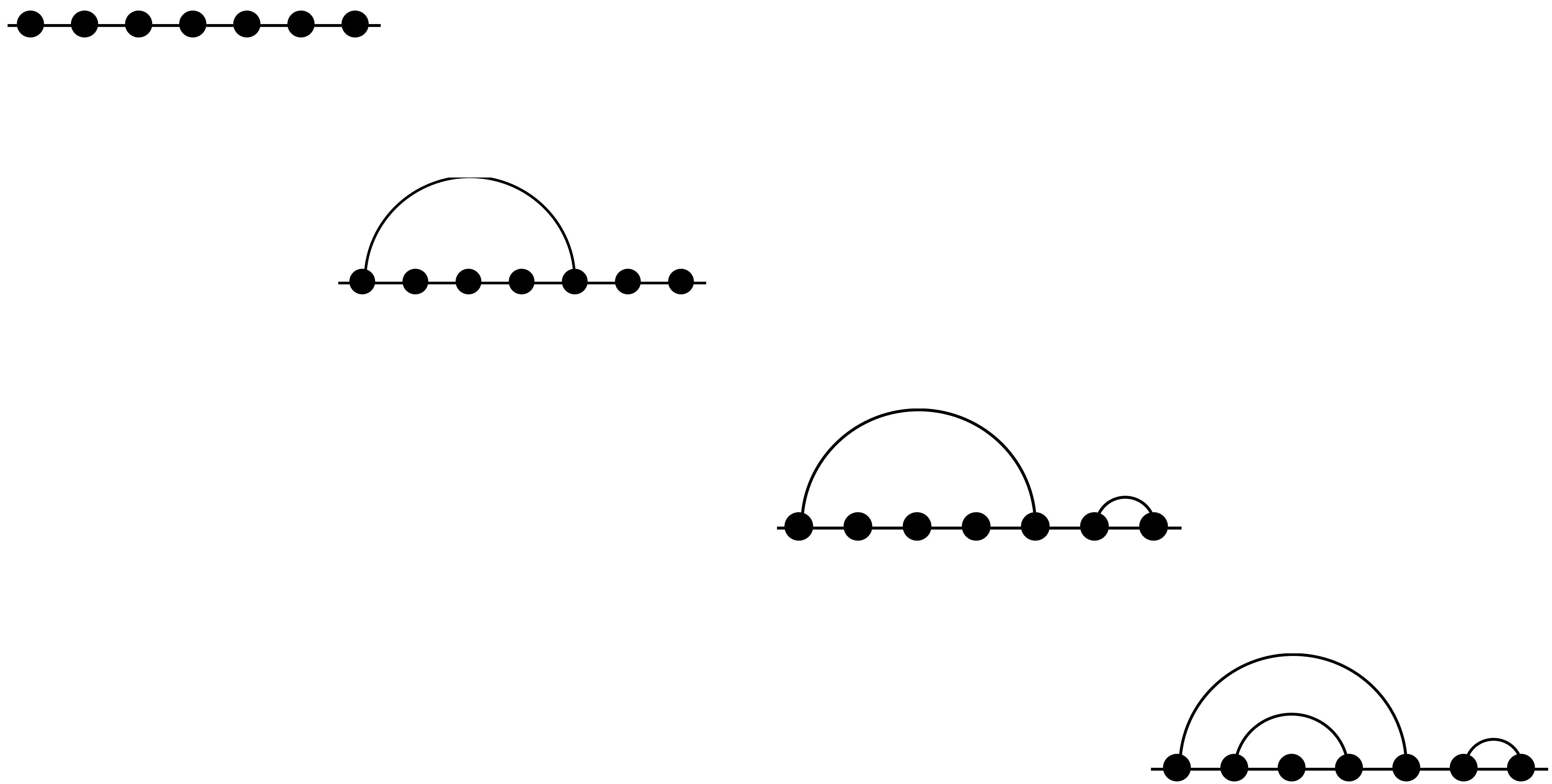

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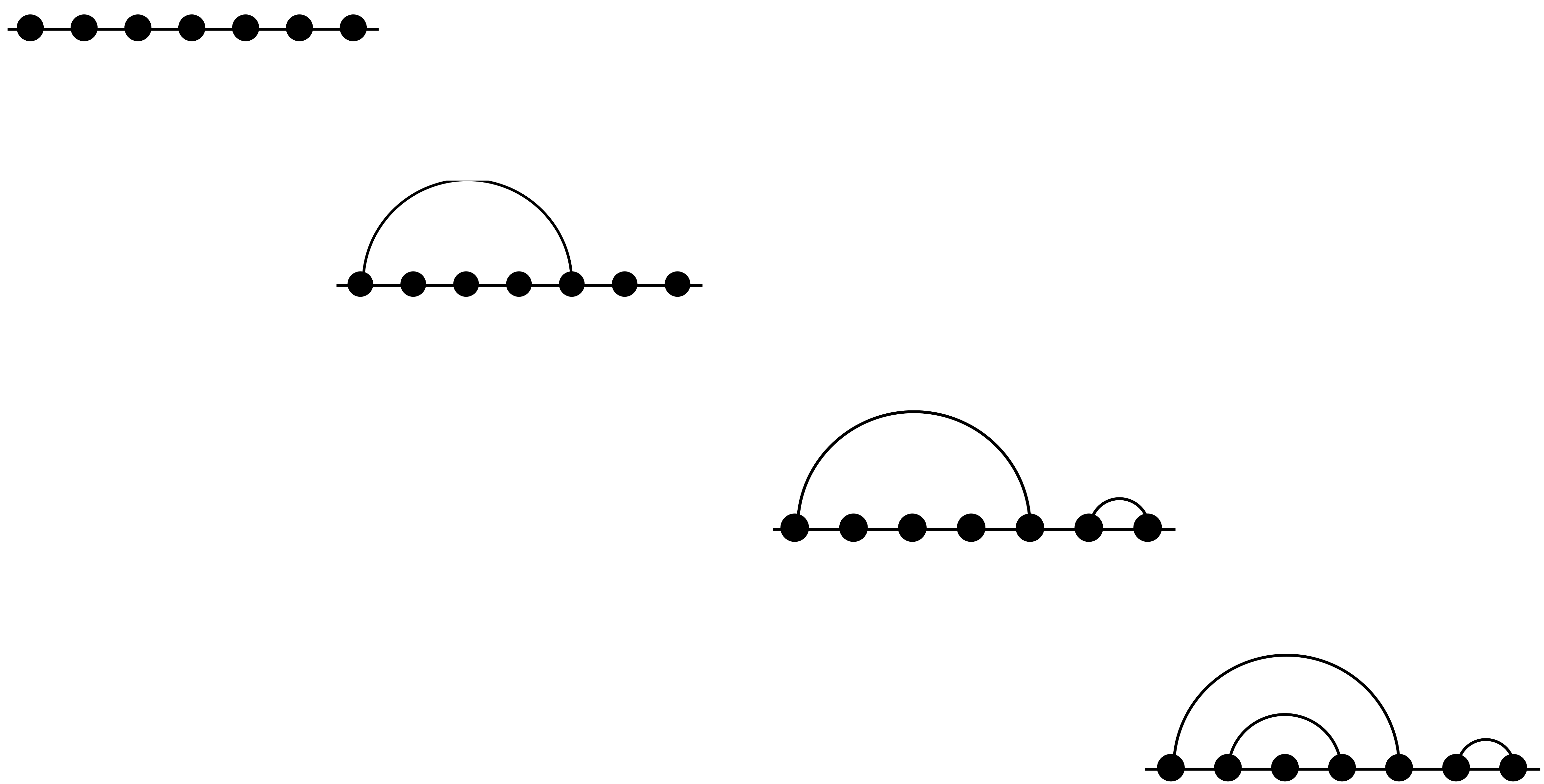

Relation to fragmentation models?

Recursion relations

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for configuration probabilities of arch structures

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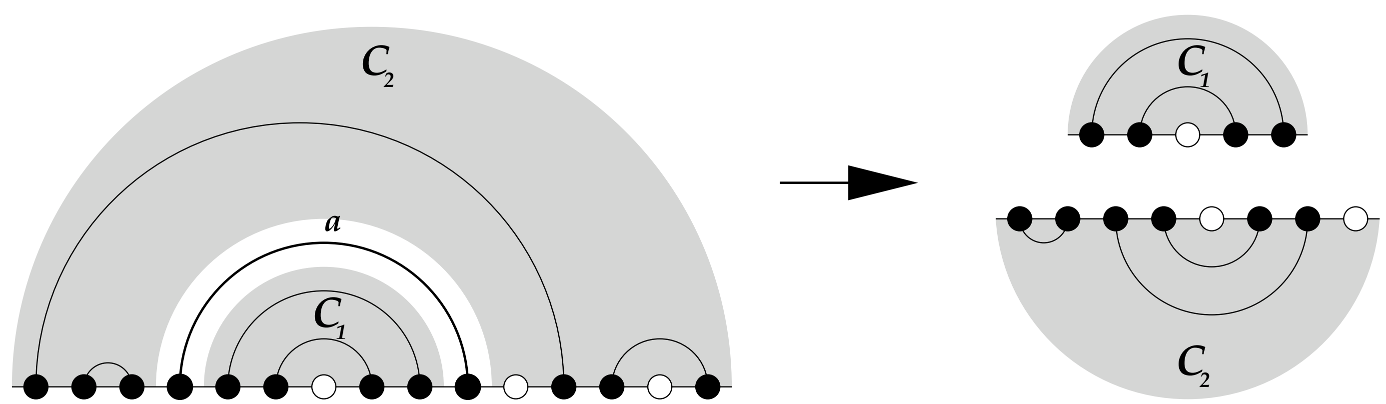
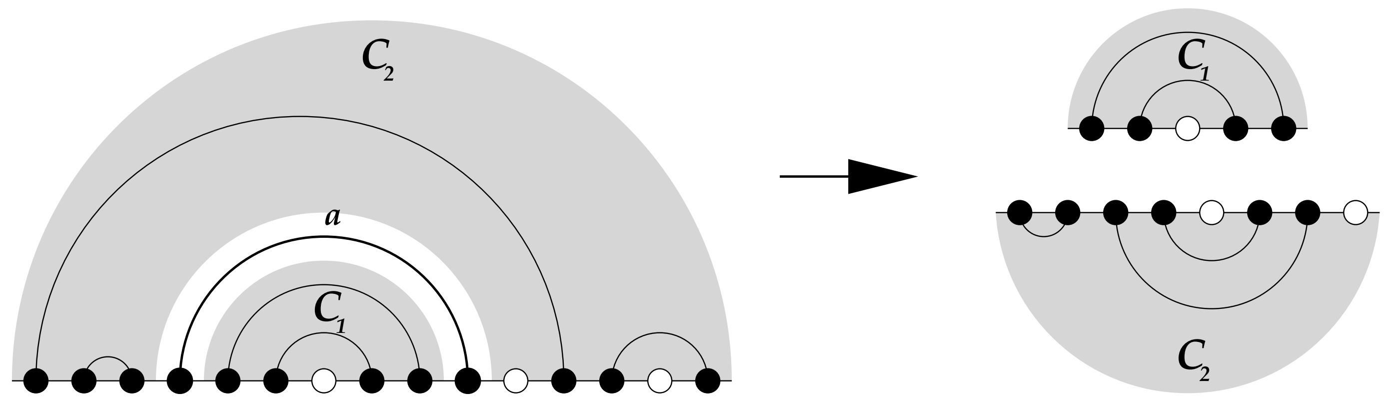


$$P(\mathcal{C}) = \sum_{\substack{\text{first arch}\\ a\in\mathcal{C}}} \sum_{\substack{\text{substructures}\\ \mathcal{C}_1\,\&\,\mathcal{C}_2}} \frac{2}{n(n-1)}\, P(\mathcal{C}_1)\, P(\mathcal{C}_2)$$

Recursion relations

for configuration probabilities of arch structures



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for heights = number of arches above a point

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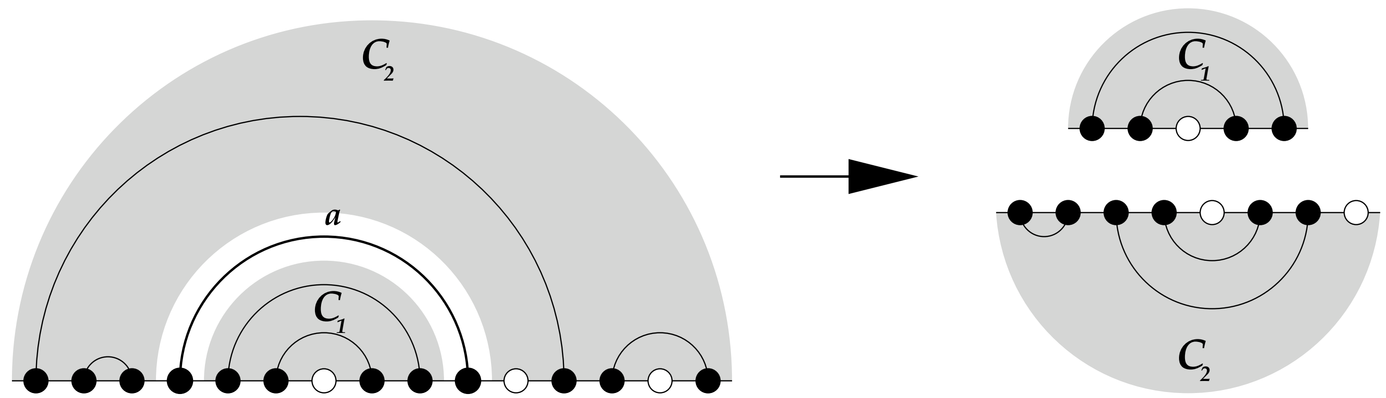

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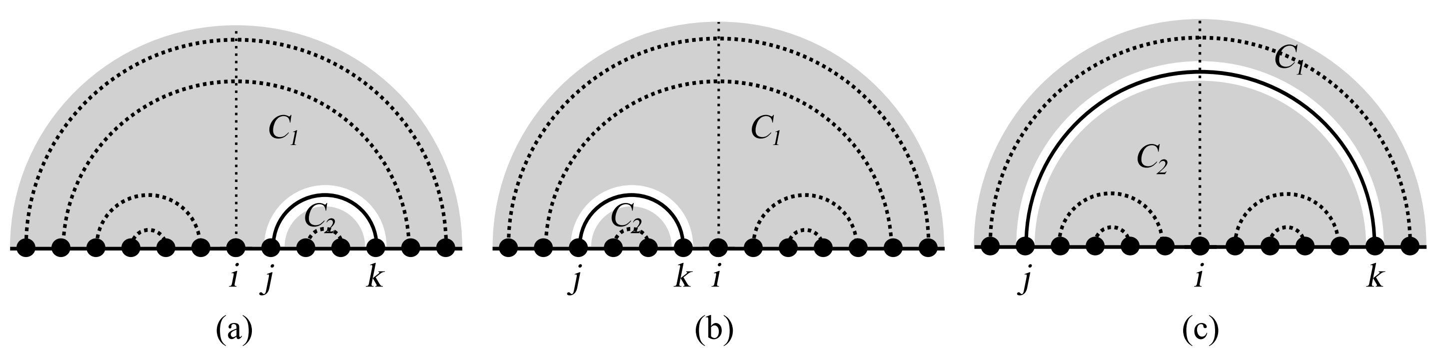

$$\begin{aligned}\frac{n(n-1)}{2} h(i,n) &= \sum_{i<j<k<n} h(i, n-k+j-1) + \sum_{0<j<k\leq i} h(i-k+j-1, n-k+j-1) \\ &+ \sum_{0<j\leq i<k<n} [h(j-1, n-k+j-1) + h(i-j, k-j-1) + 1]\end{aligned}$$

PDE for generating functions

$$G(u,v;z) = \sum_{n=0}^{\infty} \sum_{i=0}^{n} \left\langle e^{z\, h_{\mathcal{C}}(i,n)} \right\rangle u^i v^{n-i}$$

$$\left[\frac{1}{2} \left(u^2 \frac{\partial^2}{\partial u^2} + v^2 \frac{\partial^2}{\partial v^2} \right) + uv \frac{\partial^2}{\partial u \partial v} \right] G(u,v;z)$$

$$= \left[\frac{u^2}{(1-u)} \left(u \frac{\partial}{\partial u} + 1 \right) + \frac{v^2}{(1-v)} \left(v \frac{\partial}{\partial v} + 1 \right) \right] G(u,v;z) + uv\, e^z\, G(u,v;z)^2$$

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for the average mean height

$$K(t) = \left. \frac{\partial}{\partial z} G(t,t,z) \right|_{z=0} = \sum_n t^n \sum_{i=0}^{n} \langle h(i,n) \rangle$$

$$(1-t)^2 K''(t) - 2t(1-t)K'(t) - 4(2-t)K(t) = \frac{2}{(1-t)^2}$$

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$$(1-t)^2K''(t)-2t(1-t)K'(t)-4(2-t)K(t)=\frac{2}{(1-t)^2}$$

Scaling

$$K(t)\underset{t\to 1}{\propto}(1-t)^{-2-\zeta}\quad\Longrightarrow\quad\zeta^2+3\zeta=2\quad\Longrightarrow\quad\zeta=\frac{\sqrt{17}-3}{2}=0.561\ldots$$

NB: value for ζ obtained in M. Müller's PhD thesis (2002), assuming scaling

Scaling function for average height

$$\langle h(i,n)\rangle \underset{n\to\infty}{=} n^{\zeta}\,\mathcal{H}(x)\ ,\qquad x = i/n$$

$$\mathcal{H}(x) = \mathbf{E}\,x^{\zeta}(1-x)^{\zeta}\ ,\qquad \zeta = \frac{\sqrt{17}-3}{2}\ ,\qquad \mathbf{E} = 0.888309\ldots$$

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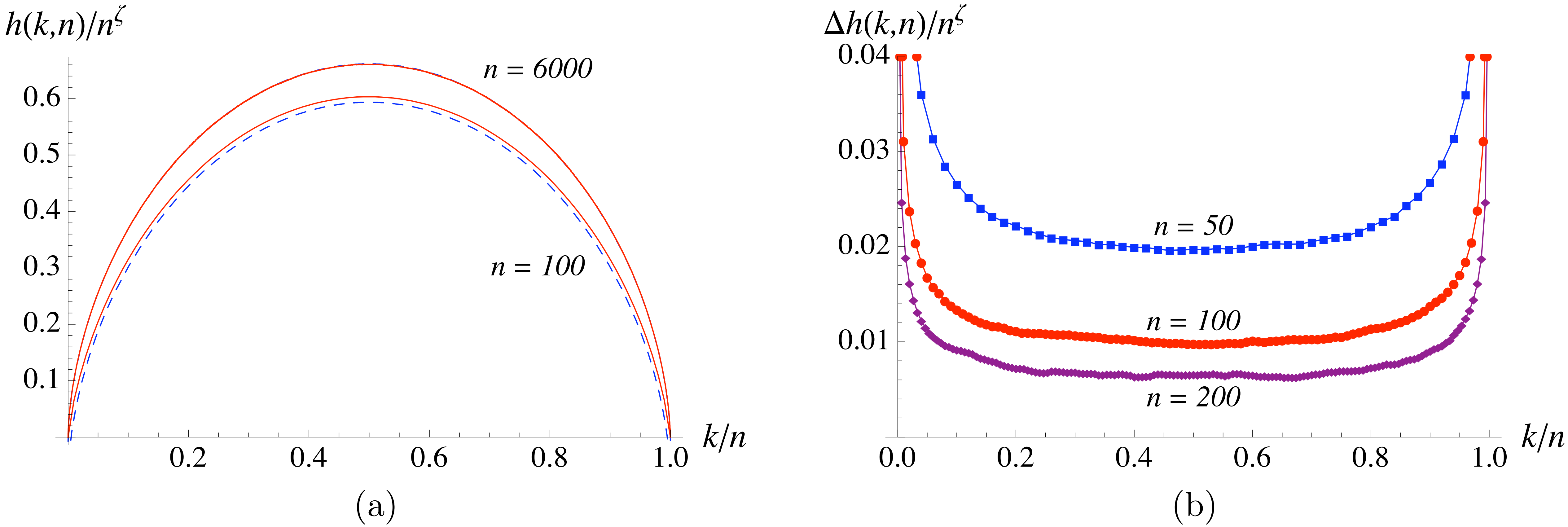
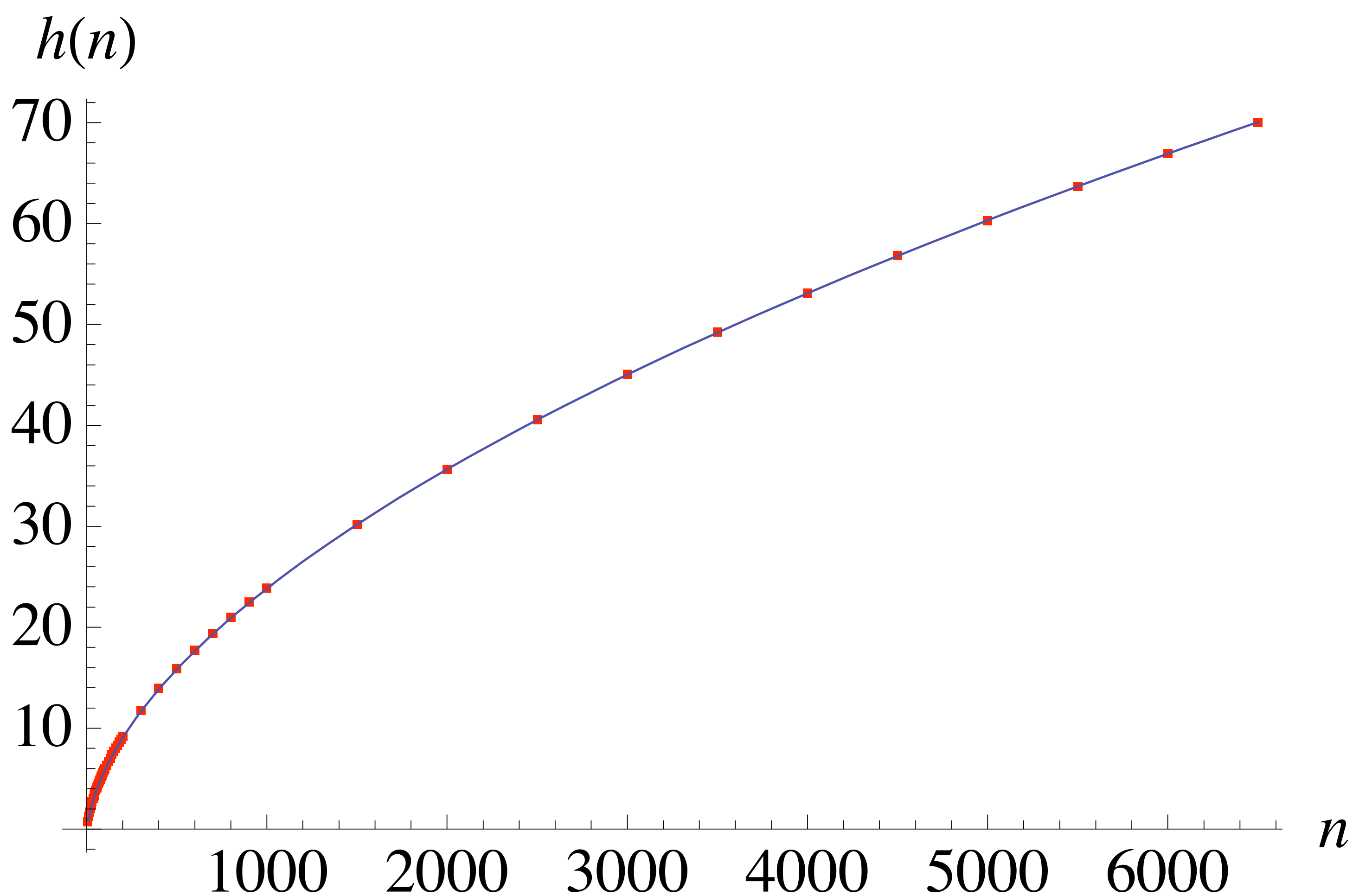
Numerical checks



Hypergeometric equations for many observables
example: mean height

$$K(v) = \frac{\mathbf{C}_+}{(1-v)^{\zeta+2}}\, M(-\zeta, -2-2\zeta; 2-2v) - \frac{1}{(1-v)^2} + \frac{\mathbf{C}_-}{(1-v)^{-1-\zeta}} M(\zeta+3, 2\zeta+4; 2-2v)$$

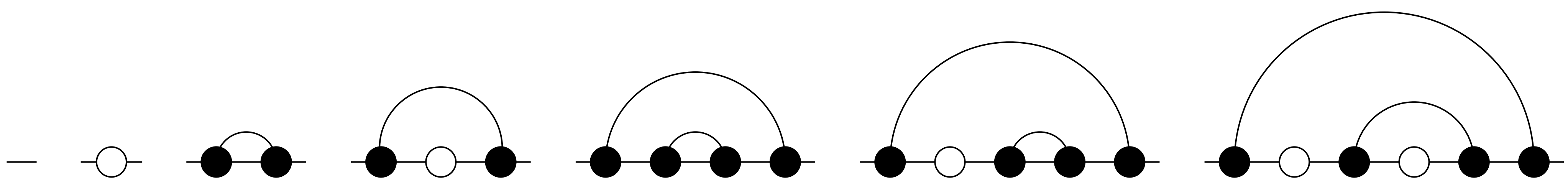
$\mathbf{C}_+ = 0.713263\ldots$ $\quad \mathbf{C}_- = 0.519299\ldots$ $\quad M$ confluent hypergeometric function (Kummer)



Allows to estimate finite size effects

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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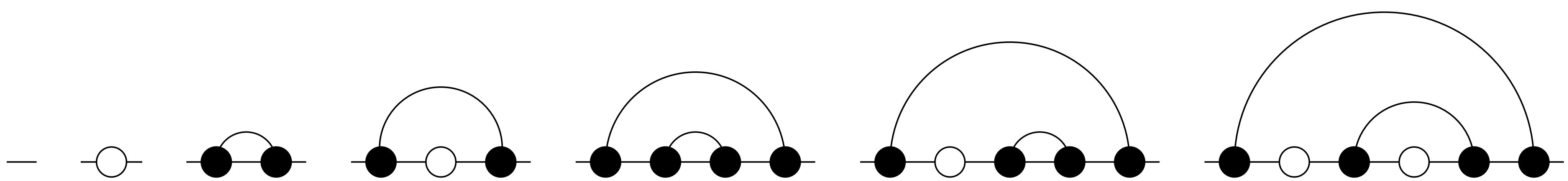
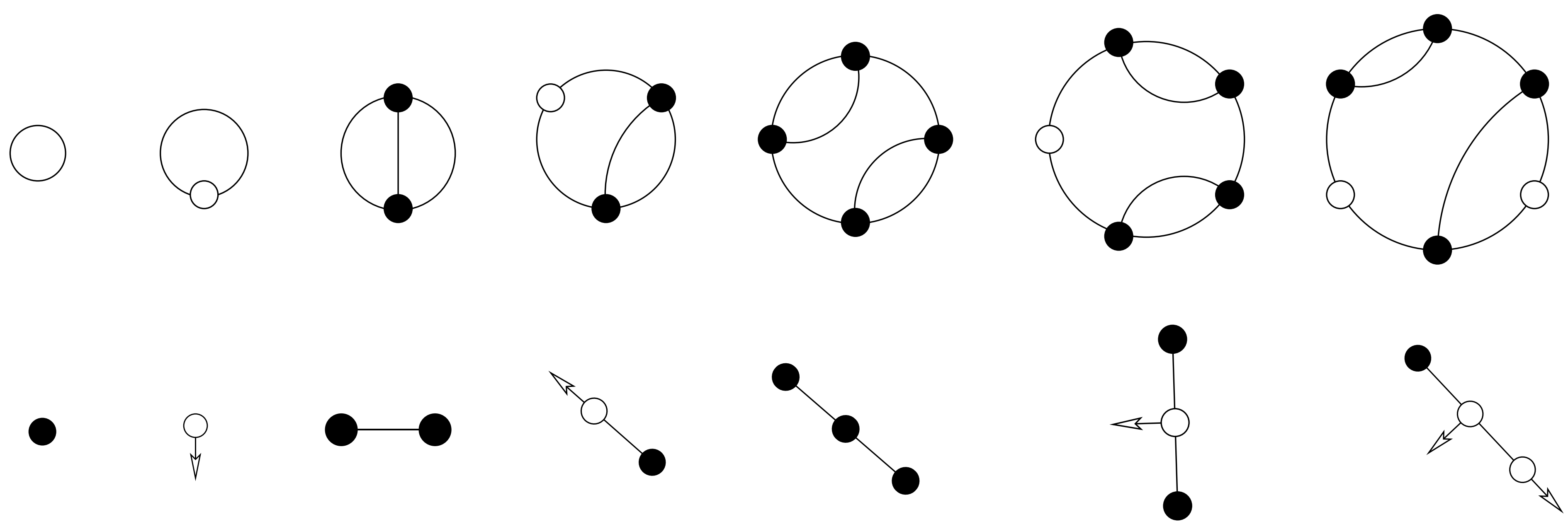


Closing + duality gives a decorated tree growth model



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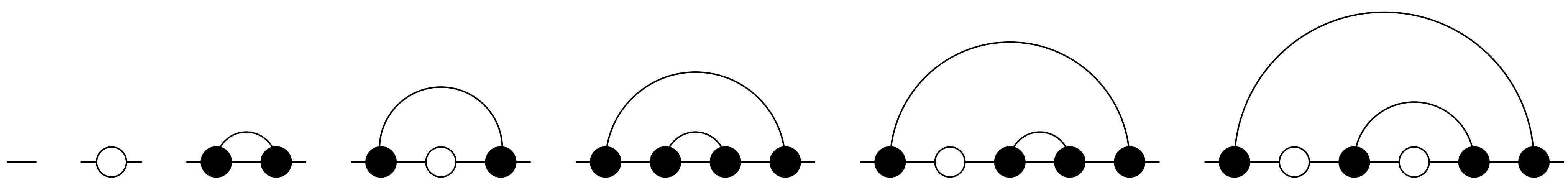

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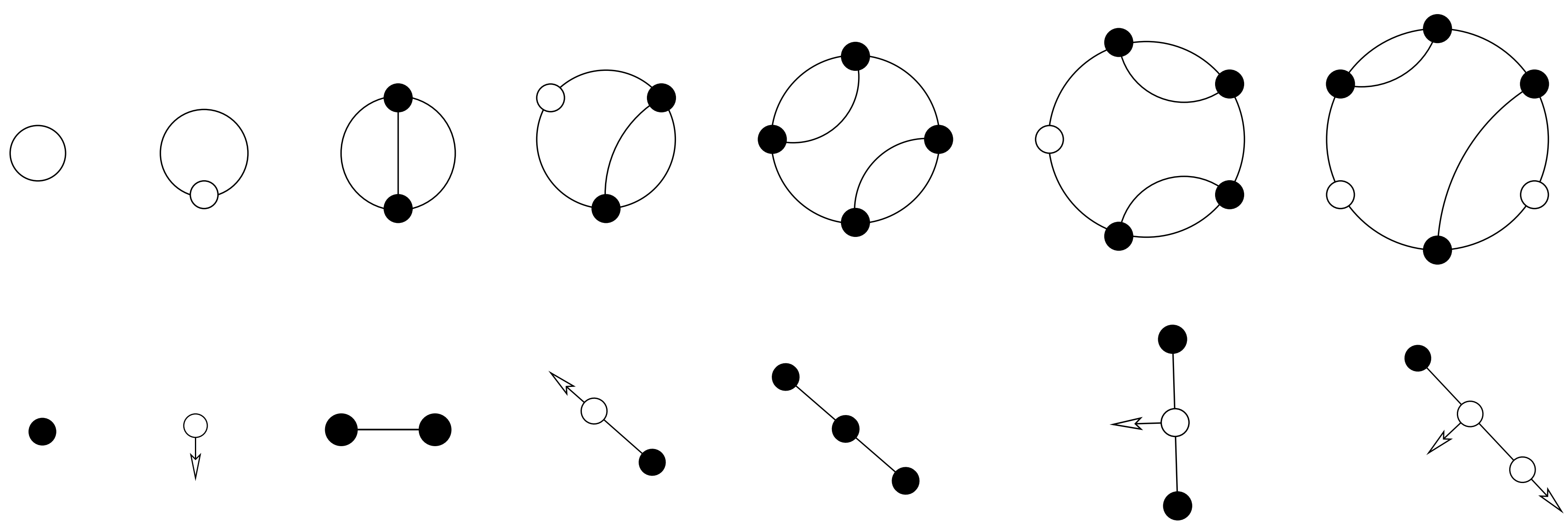
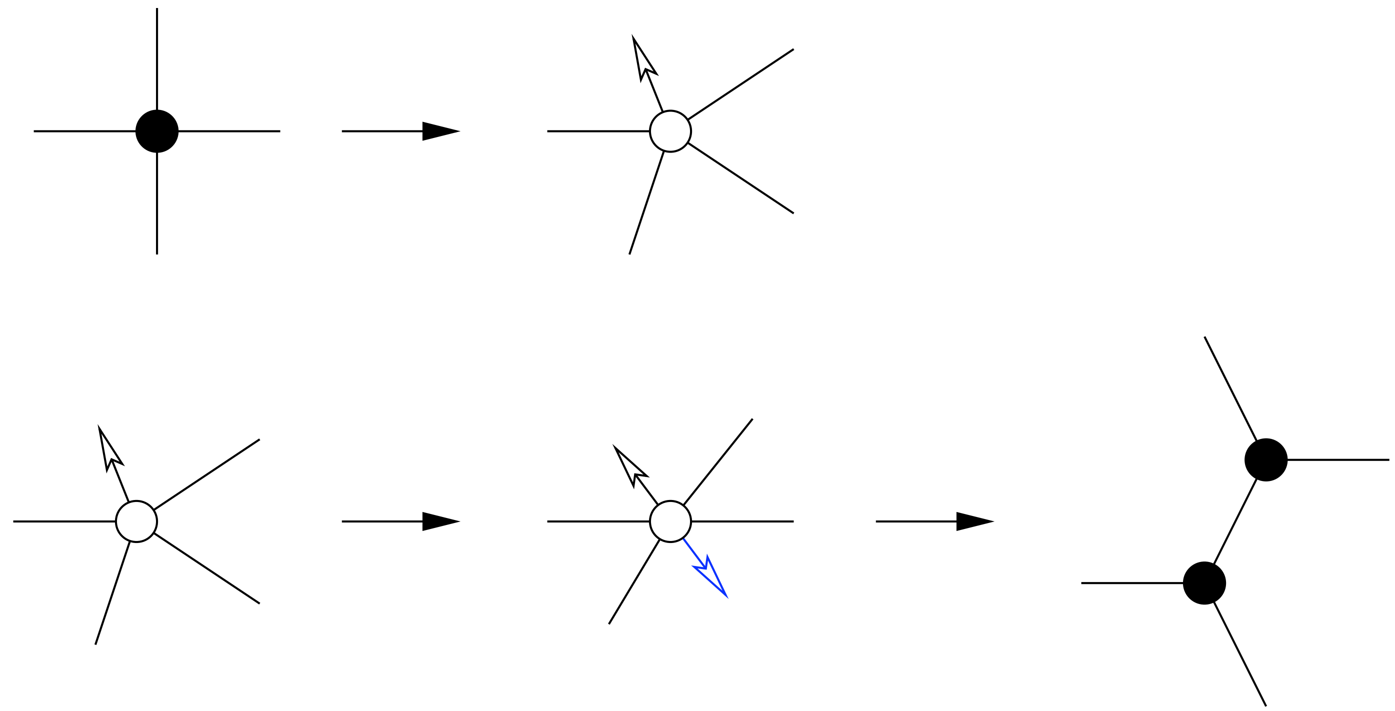


arch/tree growth at time t = arch deposition for size $n=t$!

2 steps growth process:

- add a leaf to a vertex
- add a second leaf = “budding” i.e. 1 vertex $\longrightarrow$ 2 vertices



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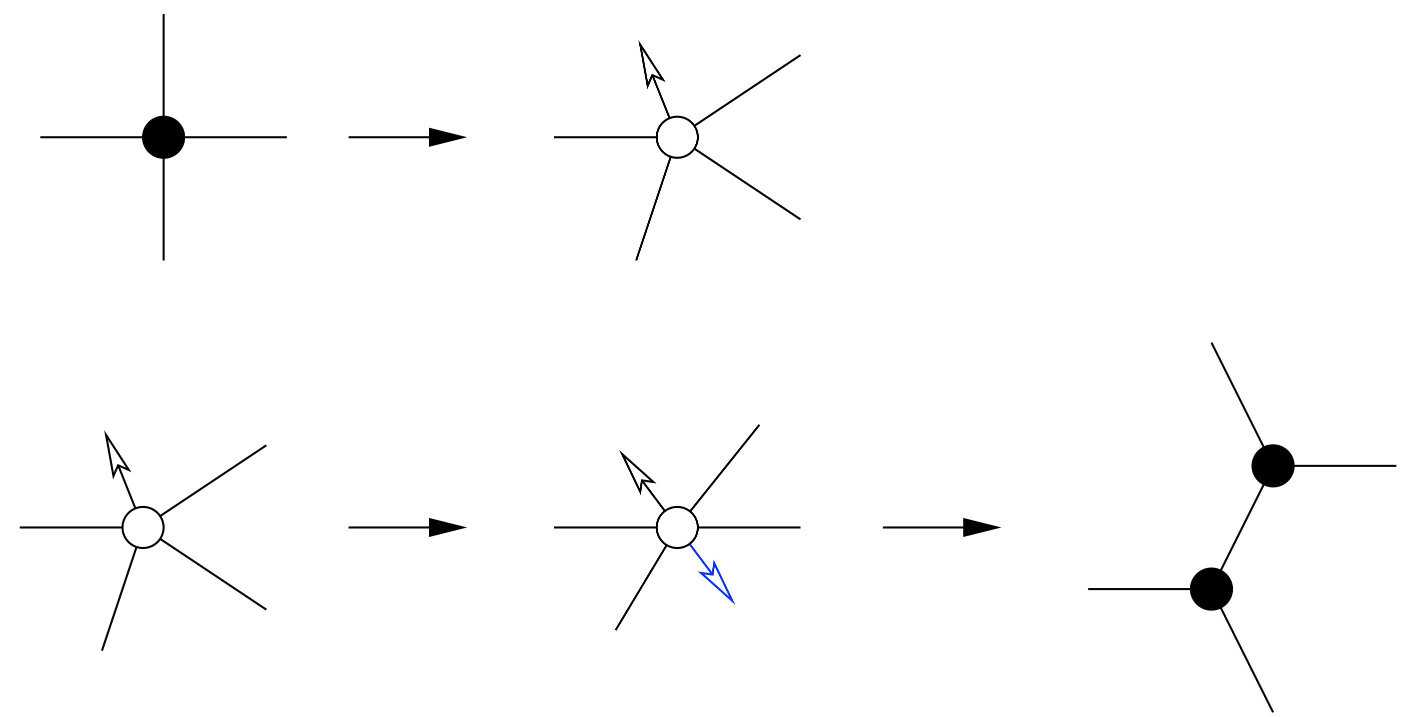

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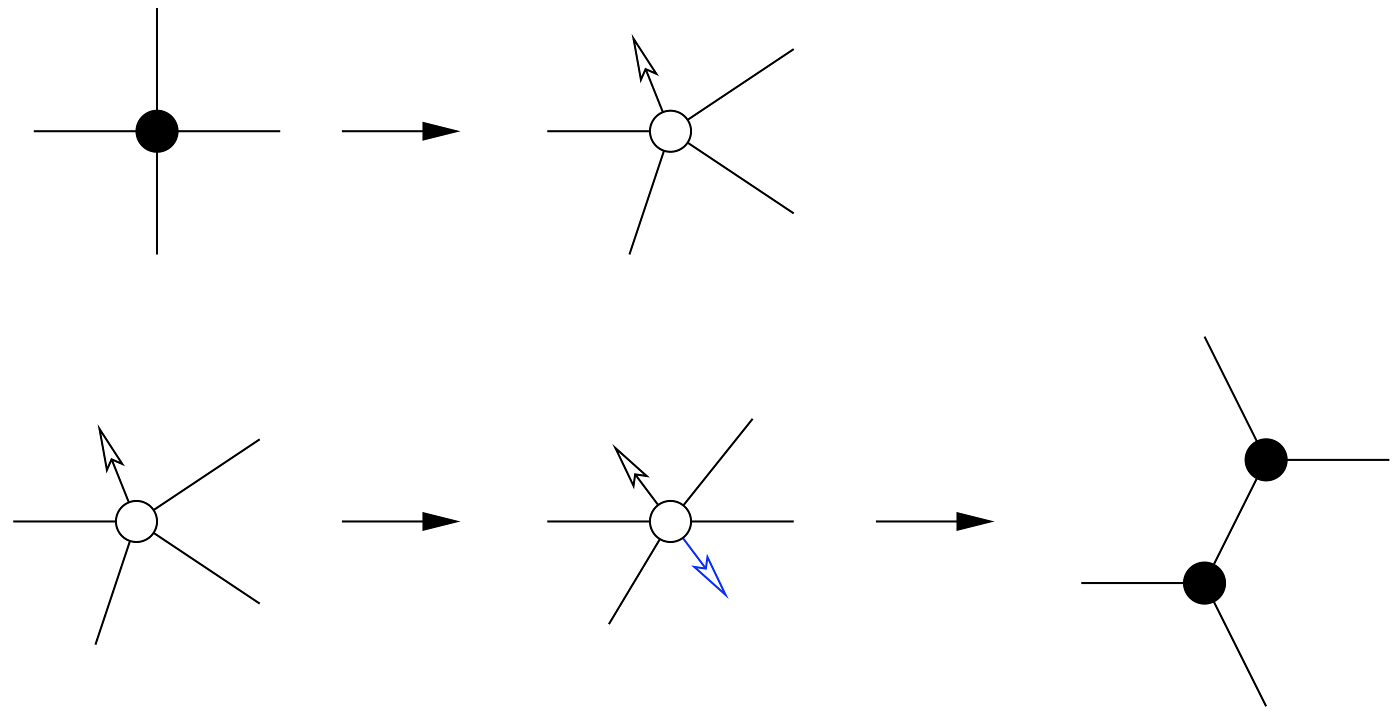

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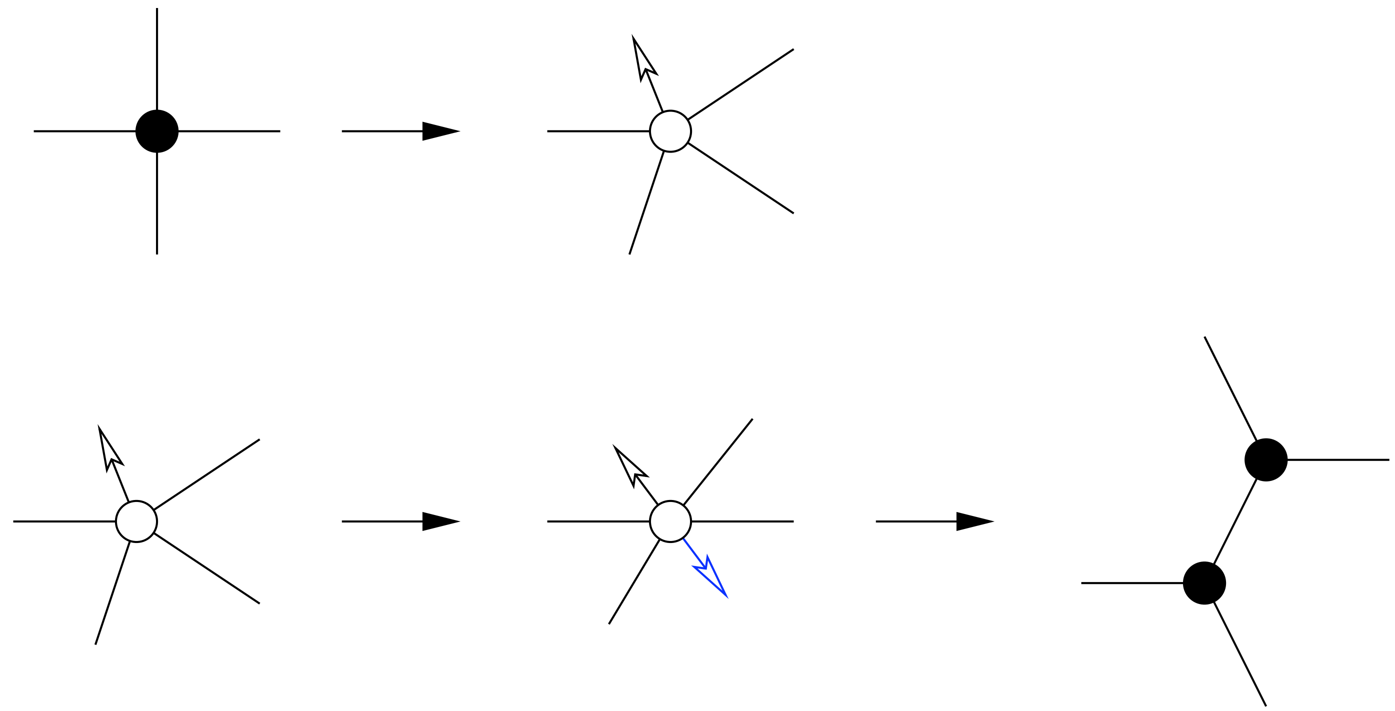

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$$\beta_k = \frac{1}{e^2}\frac{2^k}{(k+1)!} \quad , \qquad \omega_k = \frac{1}{e^2}\frac{k\ 2^k}{(k+2)!}$$

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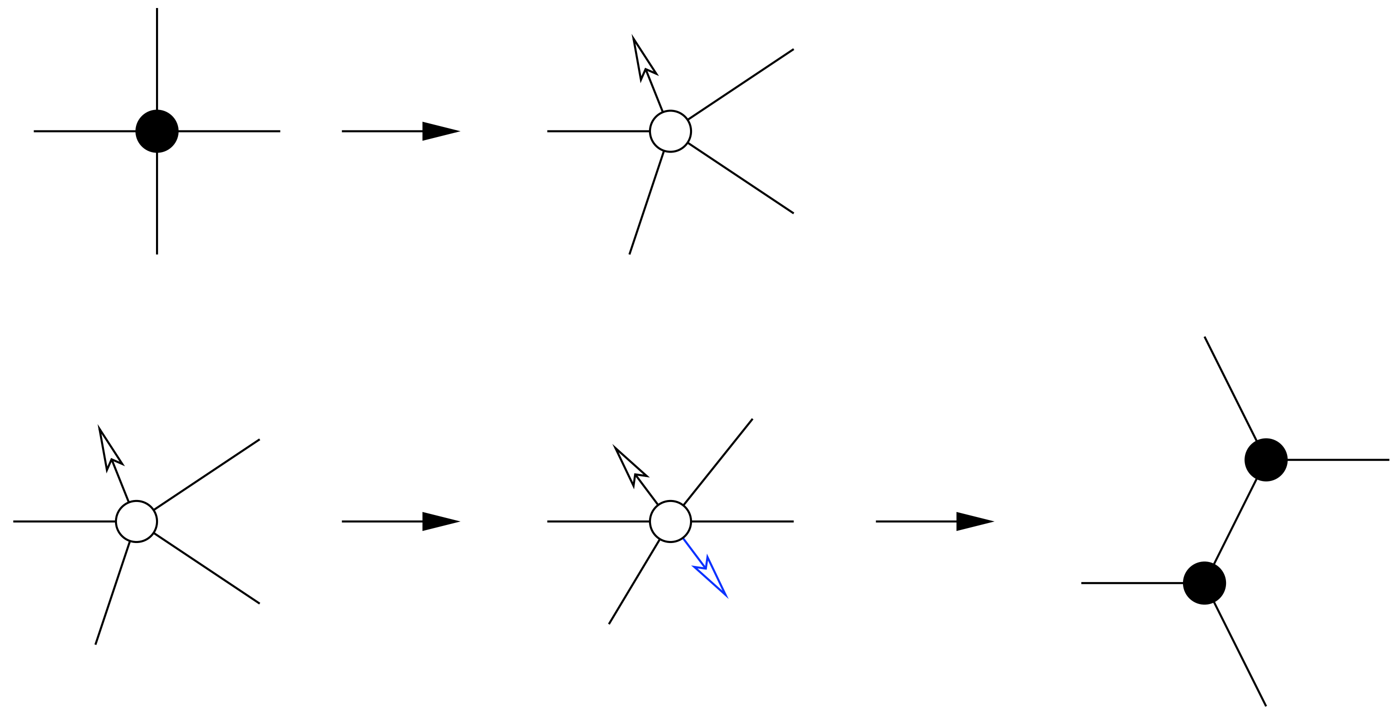

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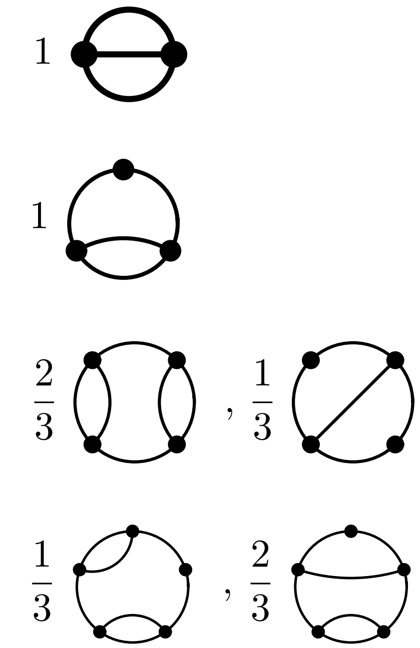
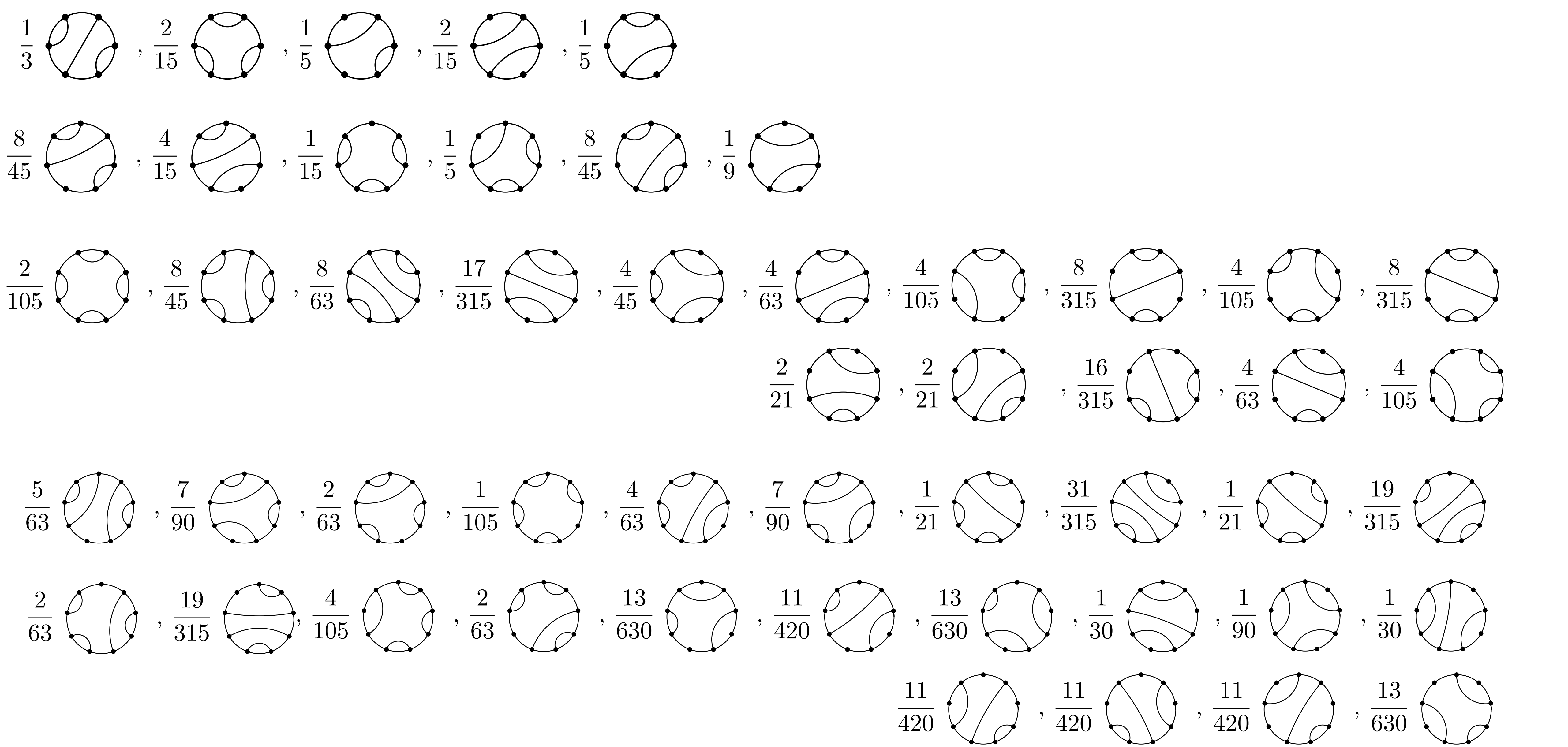
and for what more ? ....

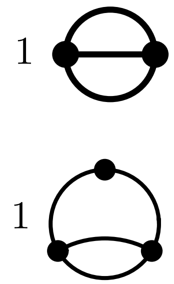

1
1
2/3 , 1/3
1/3 , 2/3
1/3 , 2/15 , 1/5 , 2/15 , 1/5
8/45 , 4/15 , 1/15 , 1/5 , 8/45 , 1/9
2/105 , 8/45 , 8/63 , 17/315 , 4/45 , 4/63 , 4/105 , 8/315 , 4/105 , 8/315
2/21 , 2/21 , 16/315 , 4/63 , 4/105
5/63 , 7/90 , 2/63 , 1/105 , 4/63 , 7/90 , 1/21 , 31/315 , 1/21 , 19/315
2/63 , 19/315 , 4/105 , 2/63 , 13/630 , 11/420 , 13/630 , 1/30 , 1/90 , 1/30
11/420 , 11/420 , 11/420 , 13/630

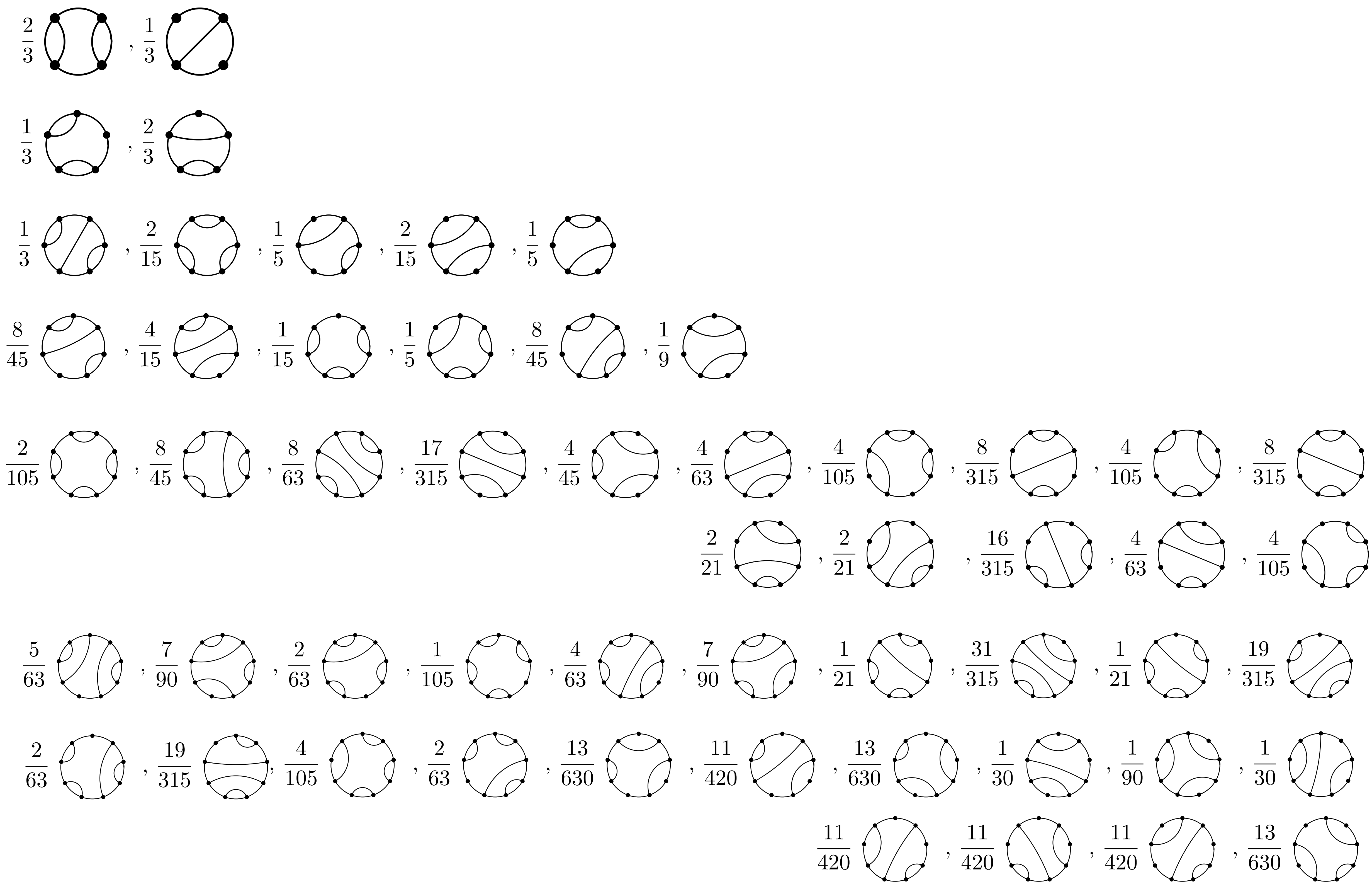
Interesting arch/tree statistics from growth process

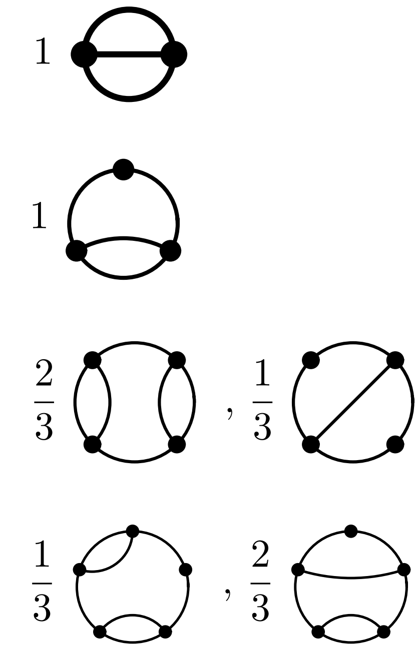




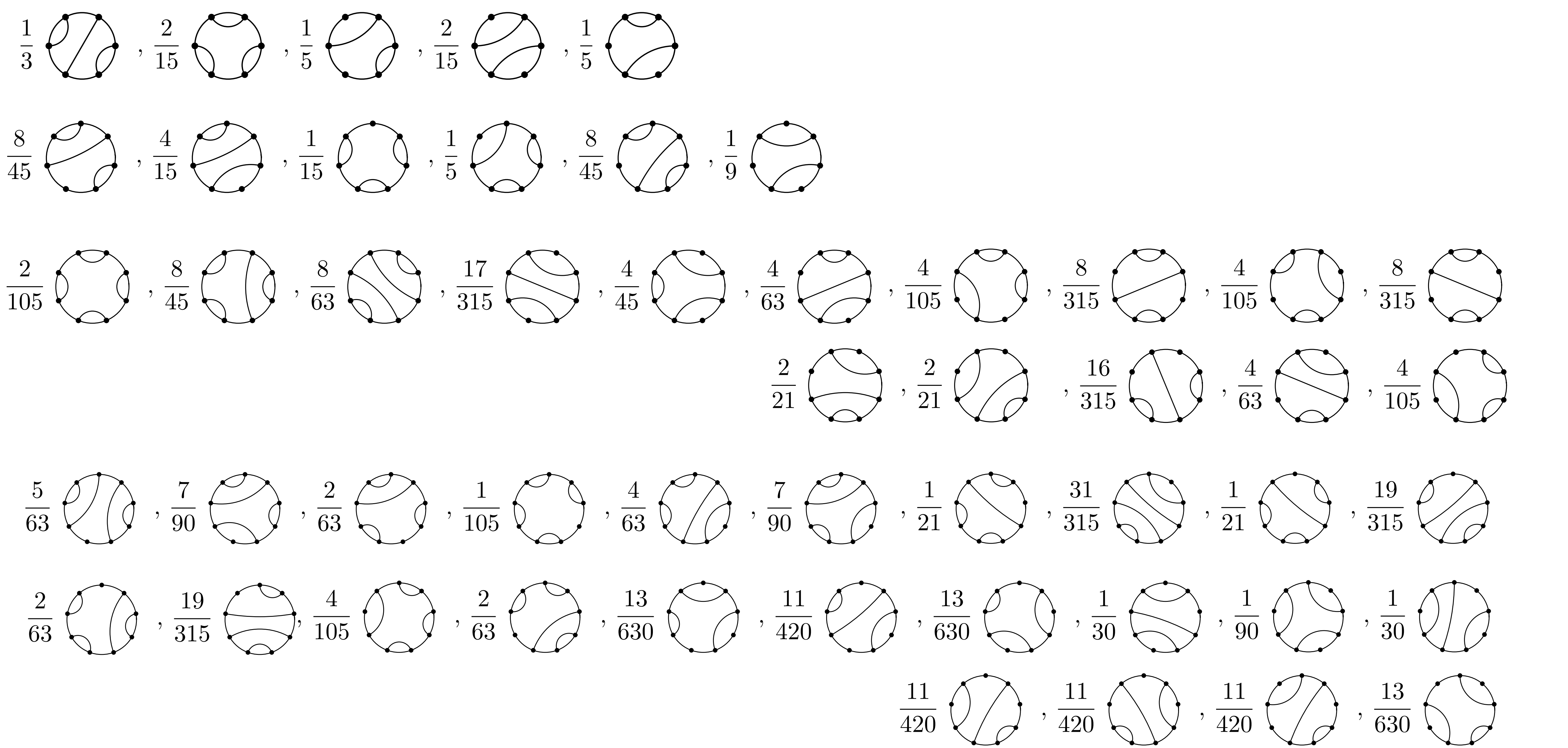
Interesting arch/tree statistics from growth process quite different from generic or causal trees

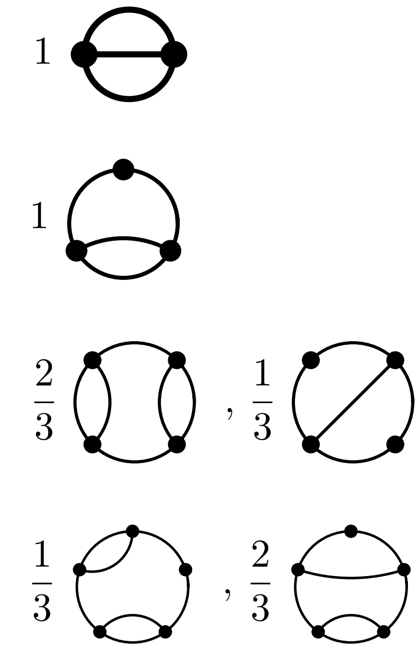




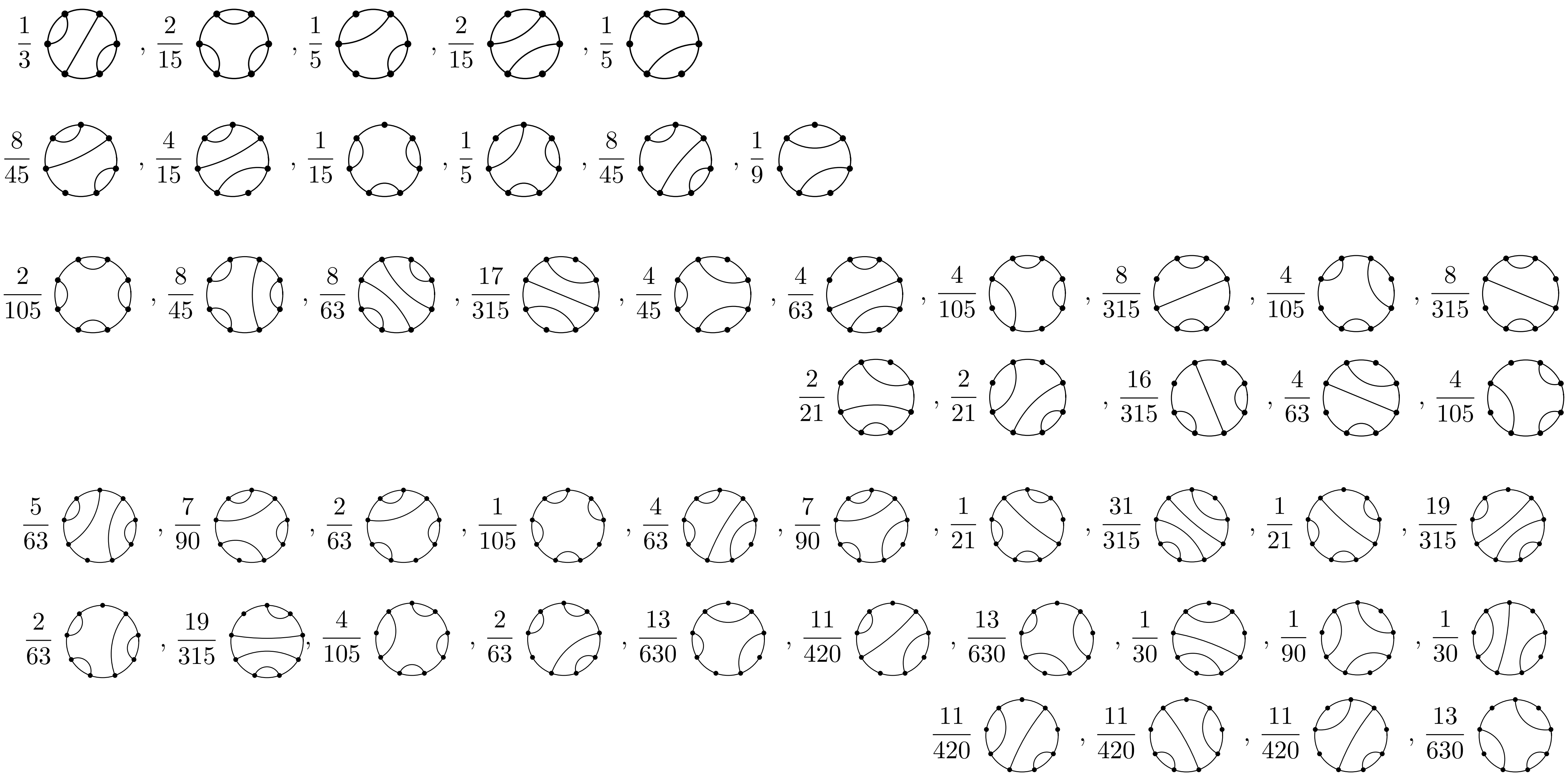


Interesting arch/tree statistics from growth process quite different from generic or causal trees and from growth by attachement trees





Interesting arch/tree statistics from growth process quite different from generic or causal trees and from growth by attachement trees
Is it new? is it universal?



Interesting arch/tree statistics from growth process
quite different from generic or causal trees
and from growth by attachement trees
Is it new? is it universal?
good for something?