Counting Phylogenetic Networks with the Component Graph Method

(based on joint work with Y.-S. Chang, E.-Y. Huang, H. Liu, M. Wallner, G.-R. Yu, L. Zhang)

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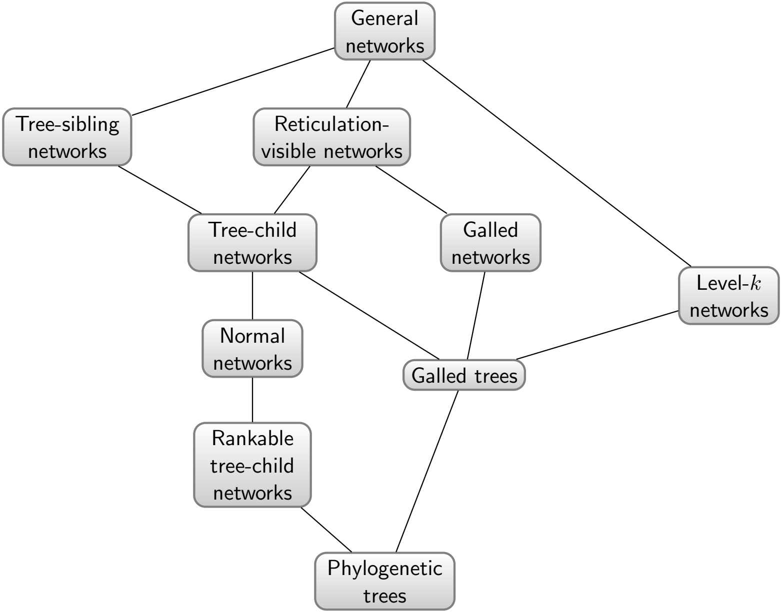
They are used to model reticulate evolution which contains reticulation events such as lateral gene transfer or hybridization.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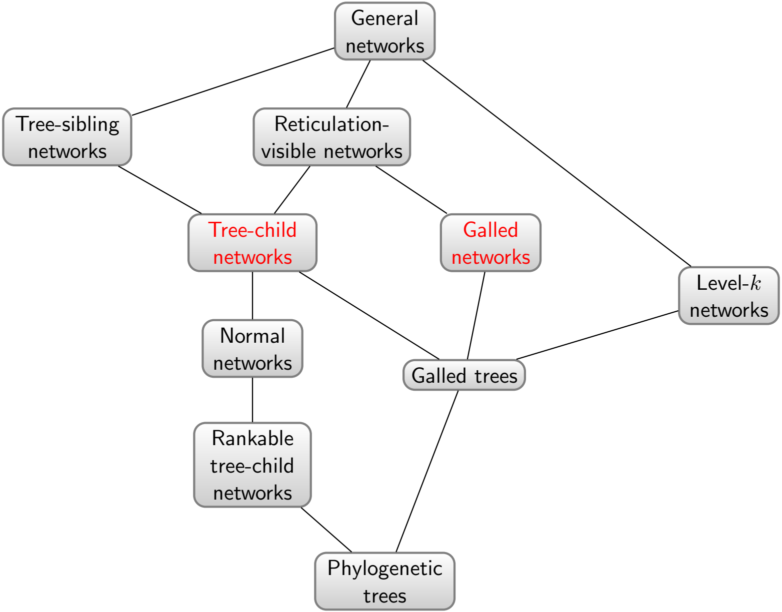
Phylogenetic trees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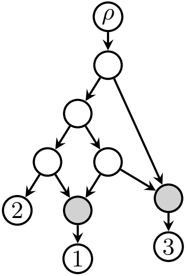

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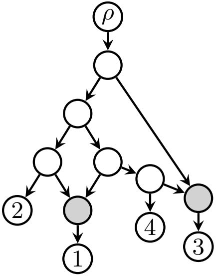

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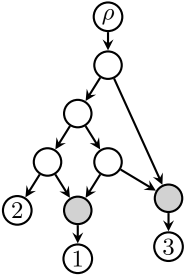

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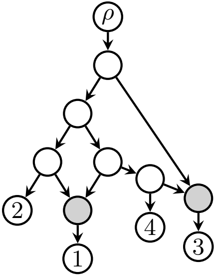

Figure: (a) is not a tc-network whereas (b) is a tc-network.

Method of Component Graphs

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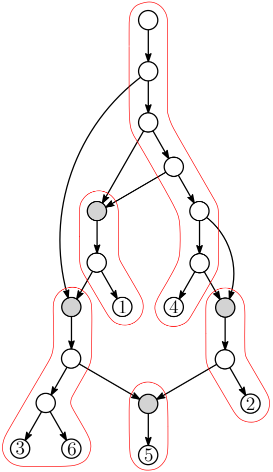

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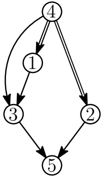

Counting TC-Networks

k_m ... # of component graphs with m nodes.

Proposition

k_m satisfies $k_m = \sum_{s=1}^{m-1} k_{m,s}$ where $k_{1,1} = 1$ and

$$k_{m,s} = \sum_{1\le t\le m-1-s} \binom{m}{s} \sum_{0\le \ell\le t} (-1)^{\ell} \binom{t}{\ell} \binom{m-s-\ell+1}{2}^{s} k_{m-s,t}.$$

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$\mathrm{TC}_{n,k}$ ... # of tc-networks with n leaves and k reticulation nodes.

Theorem (Cardona & Zhang; 2020)

$$\mathrm{TC}_{n,k} = \frac{1}{2^{n-1-k}} \sum_{\{B_j\}_{j=1}^{k+1}} \sum_{G \in \mathcal{K}_{k+1}} \prod_{j=1}^{k+1} \frac{(2b_j + g_j - 2)!}{(b_j - 1)! \prod_{\ell=1}^{k+1} (g_{j,\ell})!}.$$

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Cardona & Zhang:

$k \setminus n$	2	3	4	5	6	7
1	2	21	228	2805	39330	623385
2		42	1272	30300	696600	16418430
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Computation becomes more and more cumbersome because the number of component graphs increases rapidly!

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Chang & Liu & F. & Wallner & Yu (2023+) recently also found the following recursive formula:

$$\mathrm{TC}_{n,k} = \frac{n!}{2^{n-1-k}} w_{n-1,k},$$

where

$$\omega_{n,k} = \sum_{m \geq 1} b_{n,k,m}$$

with $b_{n,km}$ given recursively by:

$$b_{n,k,m} = \sum_{j=1}^{m} b_{n-1,k,j} + (n+m+k-2) \sum_{j=1}^{m} b_{n-1,k-1,j}.$$

Formulas for small k

Theorem (Cardona & Zhang; 2020)

We have,

$$\mathrm{TC}_{n,1} = \frac{n!(2n)!}{2^n n!} - 2^{n-1} n!.$$

and

$$\begin{aligned}\mathrm{TC}_{n,2} &= \frac{n!}{2^n} \sum_{j=1}^{n-2} \binom{2j}{j} \binom{2n-2j}{n-j} \frac{j(2j+1)(2n-j-1)}{2n-2j-1} \\ &\quad + n(n-1)n!2^{n-3} - \frac{(2n-1)!n}{3 \cdot 2^{n-1}(n-2)!} \\ &= n! \left(\frac{n(n+1)(n-1)(3n+2)}{6(2n+1)2^n} \binom{2n+2}{n+1} - n(n-1)2^n \right).\end{aligned}$$

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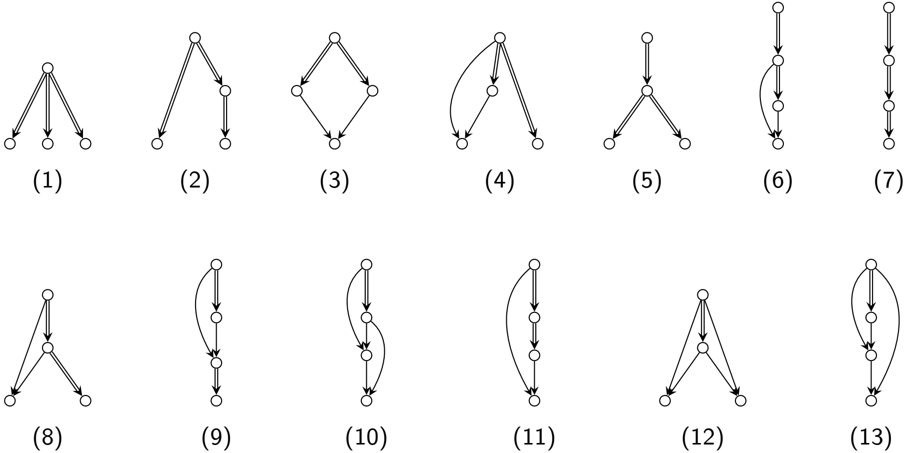
En-Yu Huang (master student; 2022) derived a formula for $k = 3$.

Component Graphs for $k = 3$



Asymptotics of TC-Networks with fixed k

Proposition

Let $S_{n,k}$ be the number of tc-networks arising from the star-component graph. Then,

$$S_{n,k} \sim \frac{2^{k-1}\sqrt{2}}{k!}\left(\frac{2}{e}\right)^{n} n^{n+2k-1}.$$

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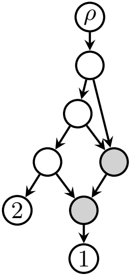

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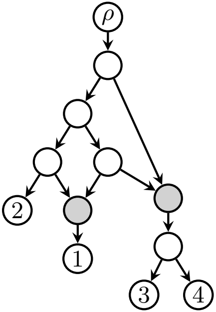

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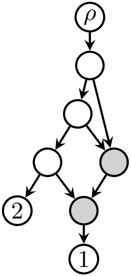

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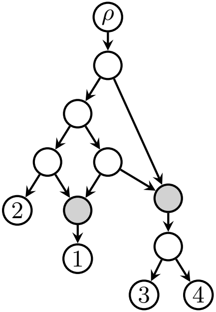

Figure: (a) is not a galled network whereas (b) is a galled network.

Component Graphs for Galled Networks

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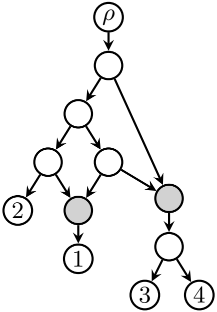

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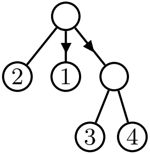

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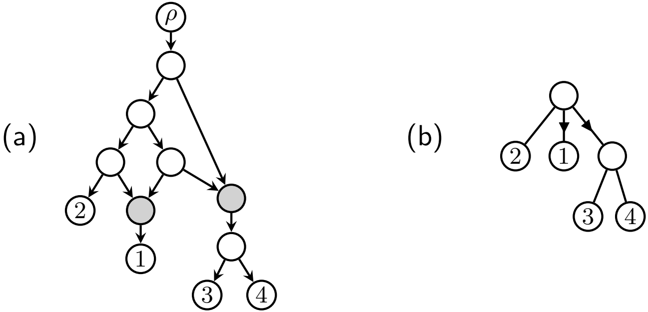

Theorem (Gunawan & Rathin & Zhang; 2022)

$$\mathrm{GN}_n = \sum_{\mathcal{T}} \prod_{v \in \mathcal{I}(\mathcal{T})} \sum_{j=c_{\mathrm{nlf}}(v)}^{c(v)} \binom{c_{\mathrm{lf}}(v)}{j - c_{\mathrm{nlf}}(v)} N_{c(v)+1}^{(j)}.$$

Asymptotics of Galled Networks (i)

We have,

$$\mathrm{OGN}_{n,k} = \binom{n}{k} N_{n+1}^{(k)},$$

where

$$N_n^{(k)} = (n+k-3)N_n^{(k-1)} + (k-1)N_n^{(k-2)} + \frac{1}{2}\sum_{1\le d\le k-1}\binom{k-1}{d}(2d-1)!!\left(N_{n-d}^{(k-1-d)} - N_{n-d+1}^{(k-1-d)}\right).$$

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Theorem (F. & Yu & Zhang; 2022)

As $n \to \infty$,

$$\mathrm{OGN}_n \sim \frac{\sqrt{2e\sqrt{e}}}{4} n^{-1}\left(\frac{8}{e^2}\right)^n n^{2n}.$$

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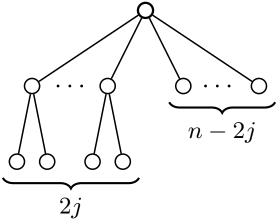

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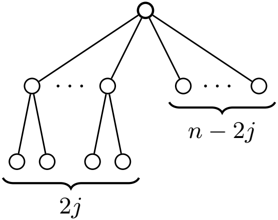

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where for $j \geq 0$ *and* $k \geq -j$,

$$\mathbb{P}(X = j, Y = k) = \frac{e^{-7/8}}{16^j j!}[z^{j-k}]e^{1/(2z)}\left(1 + 2z + 3z^2\right)^j.$$

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E.g., as a consequence,

$$\mathbb{E}(Y_n) = n - \frac{3}{8} + o(1) \qquad \text{and} \qquad \mathrm{Var}(Y_n) = \frac{3}{4} + o(1).$$

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- What is the asymptotics of the number of reticulation-visible networks with n leaves? Does it contain a stretched example?

Some References

1. G. Cardona and L. Zhang (2020). Counting and enumerating tree-child networks and their subclasses, *J. Comput. System Sci.*, **114**, 84–104.

2. Y.-S. Chang, M. Fuchs, H. Liu, M. Wallner, G.-R. Yu. Enumerative and distributional results for d-combining tree-child networks, 48 pages, submitted.

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