Combinatorics of Phylogenetic Networks

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Evolutionary Biology

Charles Darwin
(1809-1882)

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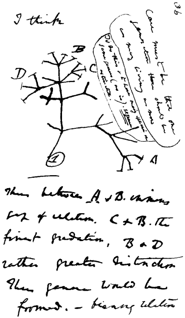
First notebook on Transmutation of Species (1837)



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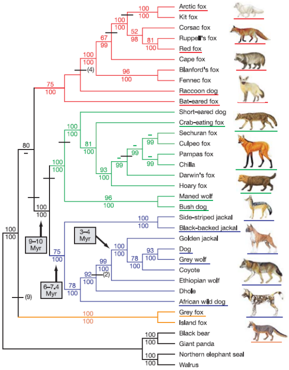

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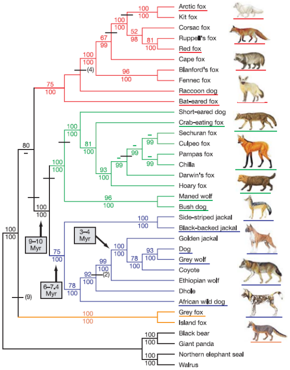

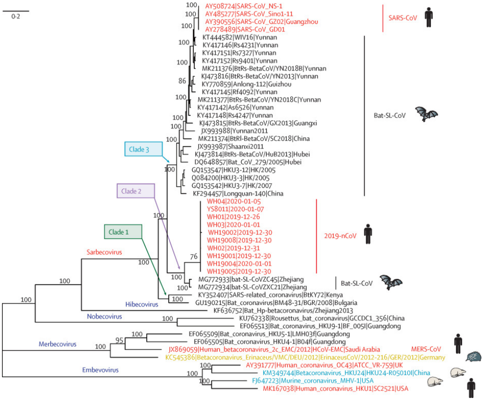

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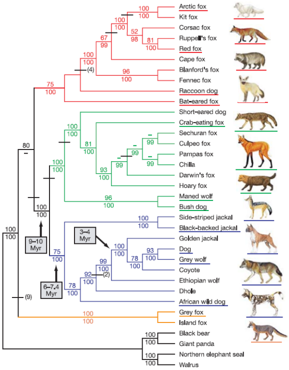

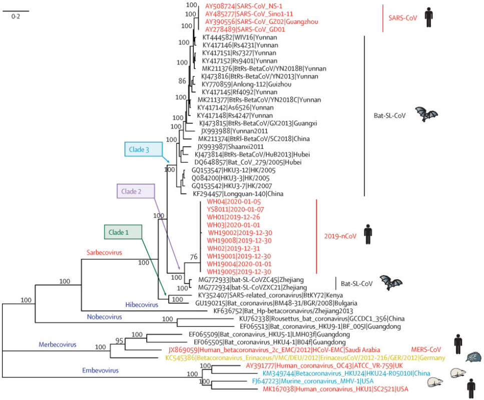

A phylogenetic tree is a rooted, non-plane, binary tree with leaves labeled by X.

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Thus,

$$\mathrm{T}_n = (2n-3)\mathrm{T}_{n-1}$$

and by iteration

$$\mathrm{T}_n = (2n-3)!!.$$

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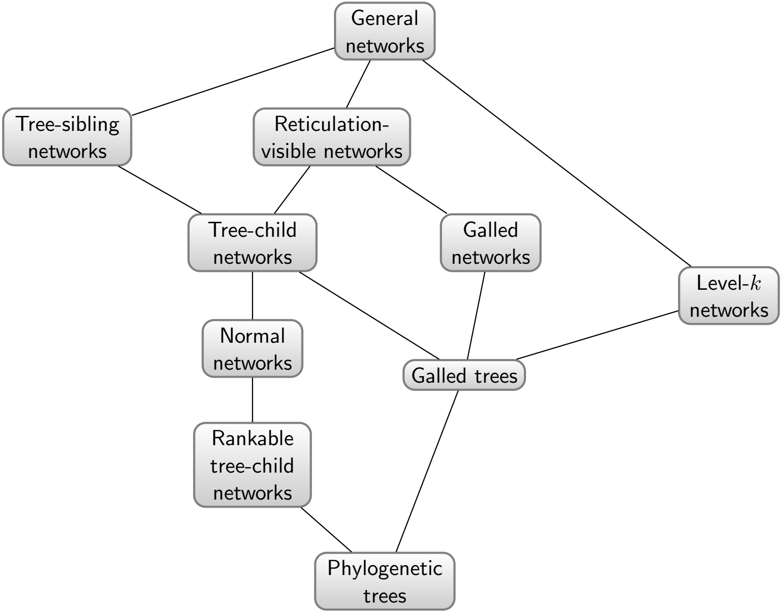
Phylogenetic networks have become increasingly popular in recent decades.

They are used to model reticulate evolution which contains reticulation events such as lateral gene transfer or hybridization.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Reticulation-visible networks
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Galled networks
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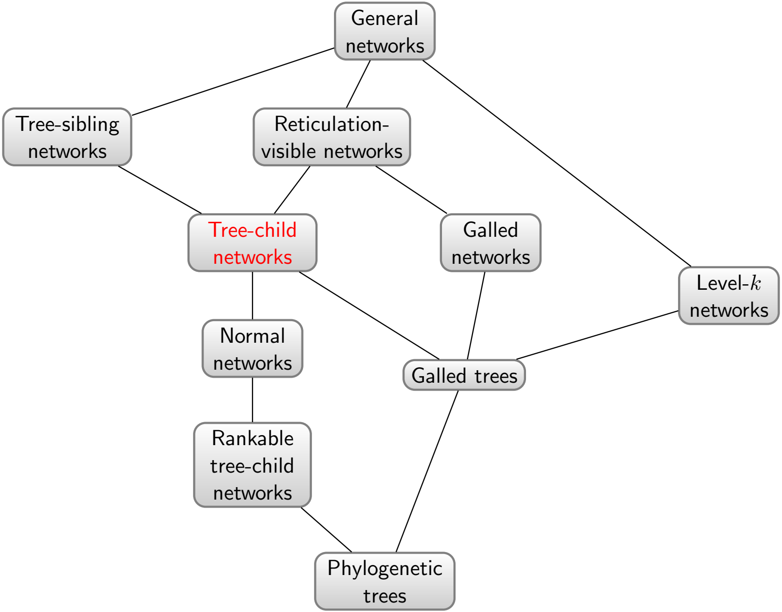
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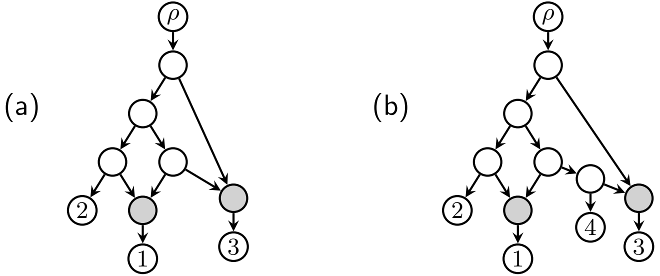

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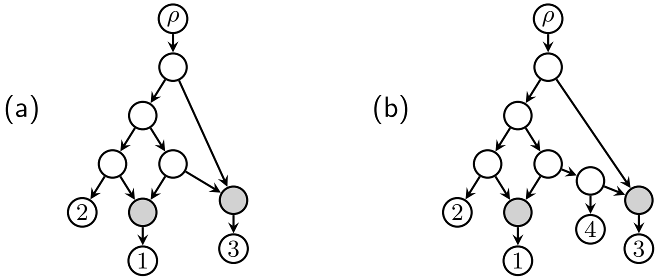

Figure: (a) is not a tc-network whereas (b) is a tc-network.

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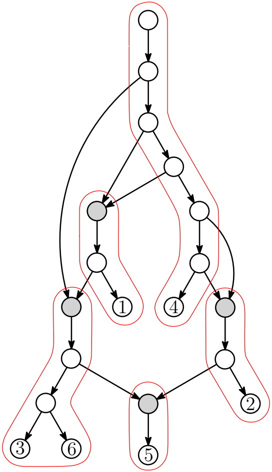

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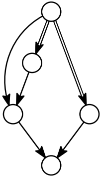

Counting TC-Networks

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

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

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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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Computation becomes more and more cumbersome because the number of component graphs increases rapidly!

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

$$\mathrm{TC}_{n,2} = \frac{n!}{2^n} \sum_{j=1}^{n-2} \binom{2j}{j} \binom{2n-2j}{n-j} \frac{j(2j+1)(2n-j-1)}{2n-2j-1} + n(n-1)n!2^{n-3} - \frac{(2n-1)!n}{3 \cdot 2^{n-1}(n-2)!}$$

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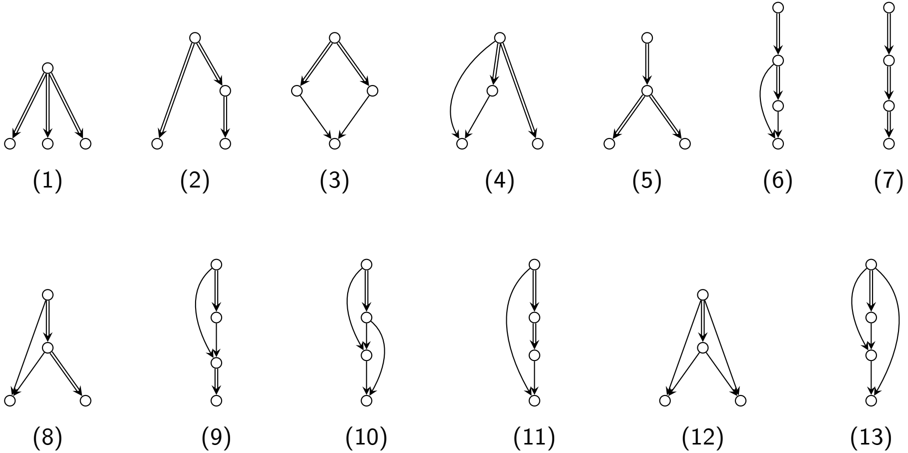
En-Yu Huang (2022) derived a formula for $k = 3$.

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,

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Theorem (McDiarmid, Semple, Welsh; 2015)

(a) *$\#$ of reticulation nodes $\sim n$ for almost all tc-networks;*

(b) *The number of cherries is $o(n)$ for almost all tc-networks.*

General TC-Networks (ii)

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A213863 was submitted on June 23rd, 2012 by Alois P. Heinz who gave its first 17 terms and a (brute-force) Maple program to compute them; tc-networks are not mentioned in his entry.

A Counting Sequence of Words

Definition (OEIS; A213863)

Denote by a_n the number of words on letters $\{\omega_1, \dots, \omega_n\}$ so that

(i) *each letter occurs exactly 3 times;*

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$$\frac{\mathrm{TC}_{n,n-1}}{n!} = a_{n-1}.$$

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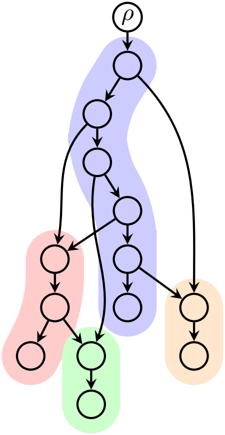

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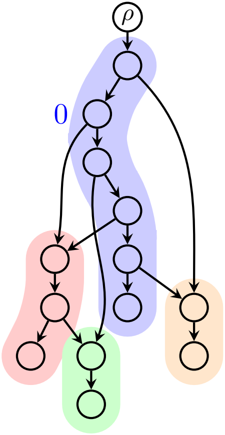

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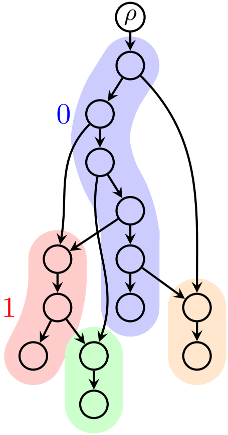

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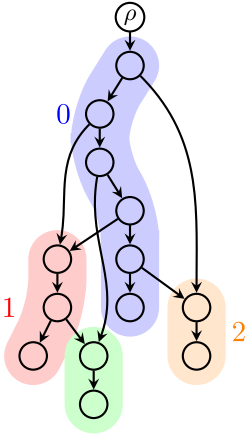

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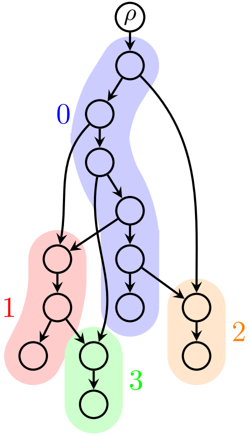

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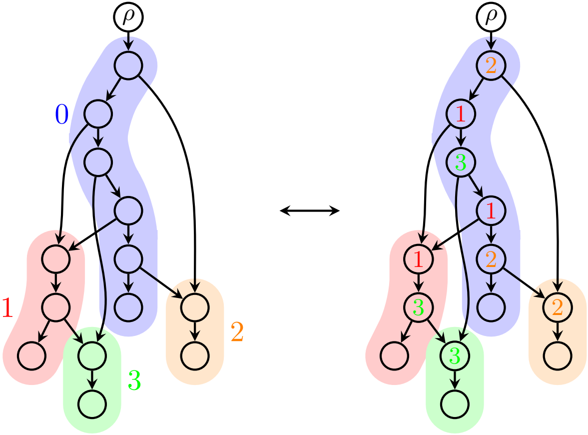

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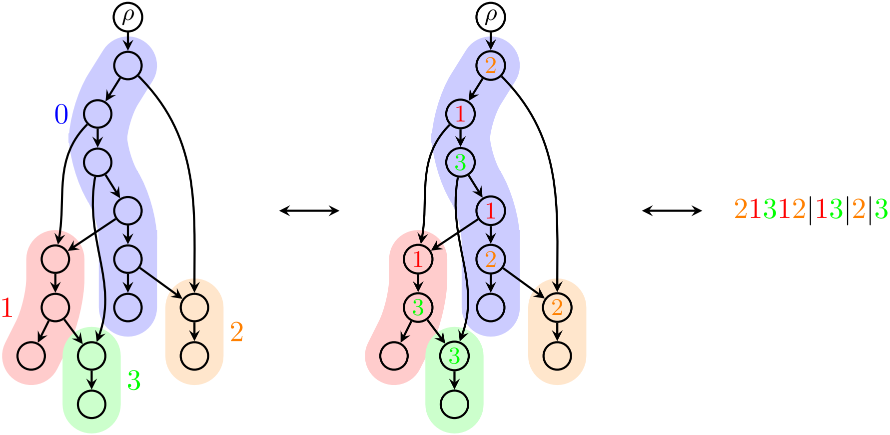

Asymptotics of General TC-Networks

Define

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

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Exact Enumeration of General TC-Networks

Definition

Denote by $w_{n,k}$ the number of words on letters $\{\omega_1, \ldots, \omega_n\}$ so that

(i) *k letters occur 3 times; $n-k$ letters occur 2 times, where the 0-th, 1-st, 2-nd occurrence counts as the 1-st, 2-nd, 3-rd.*

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Define,

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$$\mathbb{E}(\#\ \textit{of cherries}) = \mathcal{O}(1).$$

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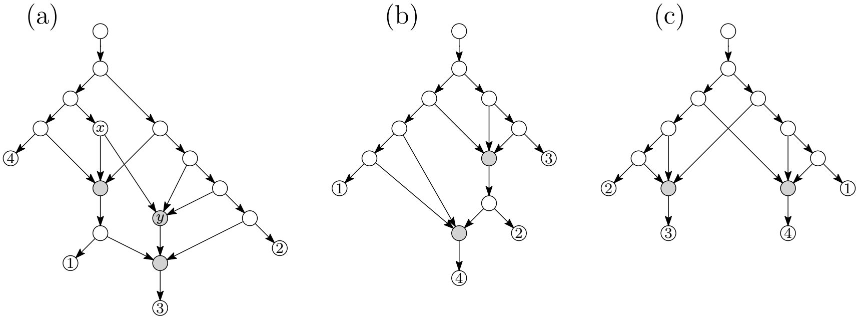

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We have,

$$\mathrm{TC}_n^{[d]} = \Theta\left((n!)^d\,\gamma(d)^n\,e^{3a_1\beta(d)n^{1/3}}n^{\alpha(d)}\right),$$

where a_1 is the largest root of the Airy function of the first kind and

$$\alpha(d) = -\frac{d(3d-1)}{2(d+1)}, \qquad \beta(d) = \left(\frac{d-1}{d+1}\right)^{2/3}, \qquad \gamma(d) = 4\frac{(d+1)^{d-1}}{(d-1)!}.$$

The Number of Reticulation Nodes

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Theorem (Chang & F. & Liu & Wallner & Yu; 2023+)

Let $d \geq 3$. The limit law of the number of reticulation nodes is degenerate. More precisely,

$$n - 1 - \text{\# of reticulation nodes} \xrightarrow{L_1} 0.$$

Fixed Number of Reticulation Nodes

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Theorem (Chang & F. & Liu & Wallner & Yu; 2023+)

We have,

$$\mathrm{TC}_{n,1}^{[3]} = \frac{n(2n+1)}{3}(2n-1)!! - n^2(2n-2)!!;$$

$$\mathrm{TC}_{n,2}^{[3]} = n(n-1)\left(\frac{70n^2+244n+177}{315}(2n+1)!! - \frac{16n+13}{48}(2n+2)!!\right).$$

In addition, as $n \to \infty$*,*

$$\mathrm{TC}_{n,k} \sim \frac{2^{dk-1}\sqrt{2}}{(d!)^k k!}\left(\frac{2}{e}\right)^n n^{n+dk-1}$$

for any fixed k*.*

Open Problems

- Can one obtain the first-order asymptotics? E.g., for $d = 2$, is there a constant c such that

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- How about results for height and Sackin index?

Some References

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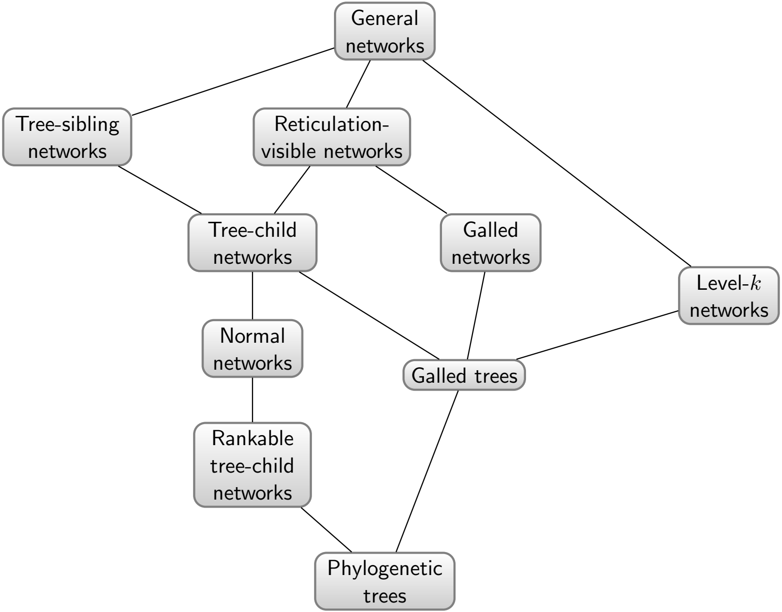
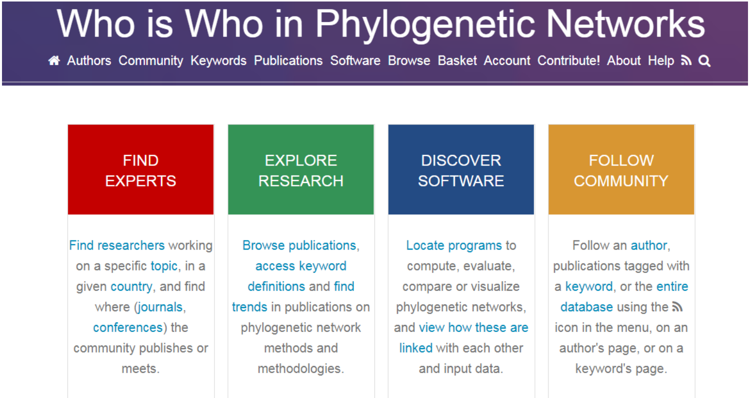

General networks
Tree-sibling networks
Reticulation-visible networks
Tree-child networks
Galled networks
Level-k networks
Normal networks
Galled trees
Rankable tree-child networks
Phylogenetic trees

There are more classes of phylogenetic networks:

http://phylnet.univ-mlv.fr/



Thanks for your attention!