Phylogenetic Diversity on Split Systems

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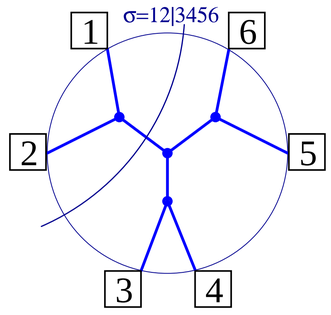
Phylogenetic Diversity on Trees

Biodiversity: is the variability among living organisms from all sources, including, 'inter alia', terrestrial, marine, and other aquatic ecosystems, and the ecological complexes of which they are part: this includes diversity within species, between species and of ecosystems [UN Earth Summit, 1992].

Phylogenetic Diversity: a measure of the content of feature diversity of a taxon subset $W \subseteq \mathcal{X}$ relative to the entire variation of the phylogenetic tree (sensu Faith, 1992).

Task: Assume that you can only support k taxa. Which subset of k taxa has the highest phylogenetic diversity?

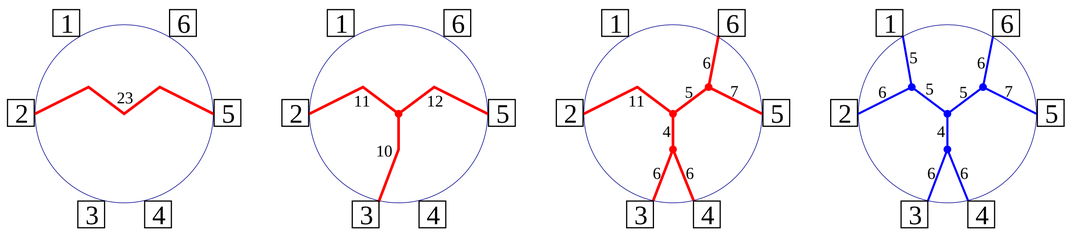


Let $\mathcal{T} = (\mathcal{V}, \mathcal{E})$ denote the tree describing the relationship of the taxon set $\mathcal{X}$ with respect to a certain feature (morphological, gene-level). The nonnegative number $\lambda(e)$ is the length of edge $e \in \mathcal{E}$. The tree $\mathcal{T}_W$ for a taxon subset W contains all connecting edges from $\mathcal{T}$ and the interior nodes whose degree remains larger than two. If an interior node vanishes and its incident edges merge, the length $\lambda_W(.)$ of the new edge is the sum of the length of the merged edges. The diversity of the taxon subset W is the sum of the length of the edges in $\mathcal{E}_W$, i.e.

$$\mathrm{PD}(W) = \sum_{e \in \mathcal{E}_W} \lambda_W(e).$$

Greedy works on Trees

For all taxon sets $W \in \mathrm{PD}_j$ exists a taxon $w \in \mathcal{X} - W$ such that $W \cup \{w\} \in \mathrm{PD}_{j+1}$.



Optimality of greedy algorithm on trees proven independently by Steel (2005) and Pardi and Goldman (2005); fast implementation by Minh *et al.* (2006).

Phylogenetic Diversity on Circular Networks

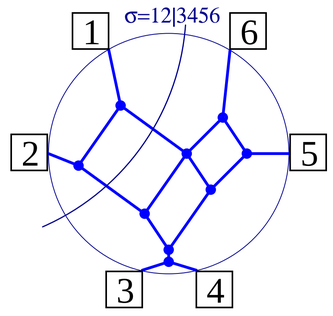
Assume we wish to put our decision not on one but on multiple features. Each feature suggests a tree, and these trees are not necessarily compatible. Which structure can simultaneously regard conflicting information?

Split: Decomposition $A|B$ of taxon set $\mathcal{X}$, i.e. $A \cap B = \emptyset,\ A \cup B = \mathcal{X}$.

Trees: Each edge in a tree uniquely identifies a split. Collecting all splits from the feature trees gives us a split system that might not identify a tree.

Split Networks: This visualization is introduced in Bandelt and Dress (1992). Splits are now illustrated by parallel or single edges in the graph.

Circular: A split system has a circular representation if all taxa can be placed on an circle and each split can be illustrated by a line intersecting the circle exactly twice.

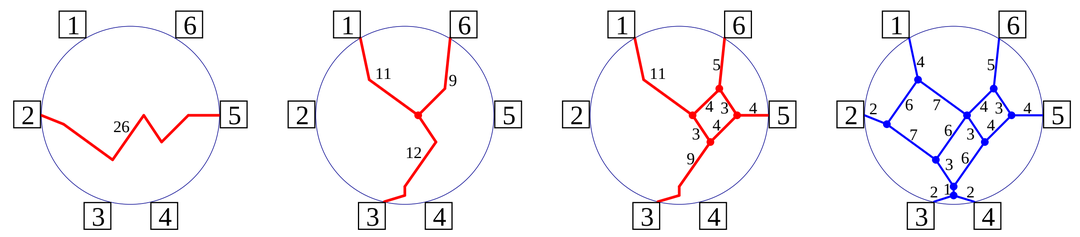


Let Σ denote a split system for taxon set $\mathcal{X}$. For each split $\sigma \in \Sigma$ the symbol $\lambda(\sigma)$ may denote its weight. For a taxon subset W the split subsystem Σ_W is given by $\{A|B \in \Sigma :, \exists a, b \in W : a \in A, b \in B\}$. The phylogenetic diversity of W is then

$$\mathrm{PD}(W) = \sum_{\sigma \in \Sigma_W} \lambda(\sigma).$$

Greedy does not work on Split Systems

Greedy never gives up what it already has acquired. As the example below shows, this is not always a good strategy, especially if the two elements from the optimal 2-set are not in the optimal 3-set.



Therefore, an alternative approach to acquire optimal subsets is needed. And we have a suggestion.

Circular Tours and Phylogenetic Diversity

Define the distance between two taxa u and v as the sum of the weights of splits separating u from v, i.e.

$$d_{uv} = \sum_{\substack{A|B \in \Sigma \\ u \in A, B \in v}} \lambda(A|B).$$

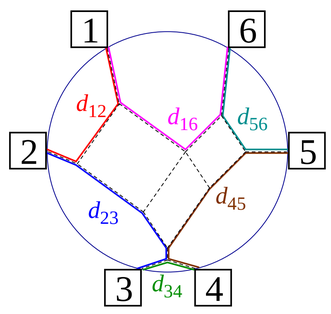
A circular split network always comes with a circular order of the taxa. From results from the traveling salesman problem (e.g., Korostensky and Gonnet, 2000) we learn that for a circular network with circular order $(u_1, u_2, \ldots, u_n)$ of taxa the shortest tour visiting all taxa and returning to the starting taxa is exactly the sum of the distance of consecutive taxa, i.e.

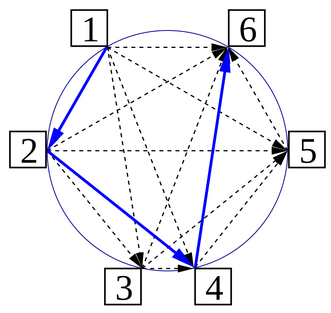
$$\Lambda_{[1,n]} = d_{u_1 u_n} + \sum_{j=1}^{n-1} d_{u_j u_{j+1}},$$

which is also twice the length of the network. Circular order and pairwise distances are retained in subsystems. Therefore, for taxon subset W of size k with inherited taxon order $w_1, \ldots, w_k$ the phylogenetic diversity is calculated by

$$\mathrm{PD}(W) = \frac{1}{2}\left(d_{w_1 w_k} + \sum_{j=1}^{k-1} d_{w_j w_{j+1}}\right).$$

With this the structure on which to optimize can be depicted as an acyclic graph with taxon set $\mathcal{X}$ where each pair (u, v) of taxa is connected by a directed edge with length d_{uv}.





A Dynamic Programming Algorithm

Input: Circular order of taxa $(1, 2, \ldots, n)$, split-distance matrix (d_{uv}), set size k.

Initialization: Length of longest ordered 2-path between taxa $u < v$: $L^2_{uv} = d_{uv}$.

Iteration: In each step i compute for all pairs of taxa $u < v$ the *longest ordered i-path* by

$$L^i_{uv} = \max_{u<w<v} \{L^{i-1}_{uw} + d_{wv}\}.$$

and store L^i_{uv} and $\alpha^i_{uv} = \mathrm{argmax}\, L^i_{uv}$.

Termination: Determine the *longest circular k-tour* by

$$\ell^k = \max_{u,v} \{L^k_{uv} + d_{uv}\}.$$

and the taxa of the k-tour by backtracking through (α^i_{uv}), $i = 2, \ldots, k$.

Optimal Substructure: If $(s_1, s_2, \ldots, s_j)$ is the longest ordered j-path from s_1 to s_j then $(s_1, s_2, \ldots, s_{j-1})$ is the longest ordered $j-1$-path from s_1 to s_{j-1}.

Complexity: $O(kn^3)$ time complexity and $O(kn)$ memory complexity.

Budget considerations

Just fixing the size of the taxon subset is not a very justifiable criterion. Moulton *et al.* (2006) suggest a variety of constraints which will influence the actual selection and give the set of k taxa more biological relevance. Weitzman (1998) proposed an economical side condition, namely that the taxon selection is not fixed by size but by a budget B for supporting the conservation efforts. To this end, each taxon $u \in \mathcal{X}$ is assigned the nonnegative preservation cost $c(u)$. The preservation cost $c(W)$ of a taxon subset W is the sum of preservation costs of its taxa.

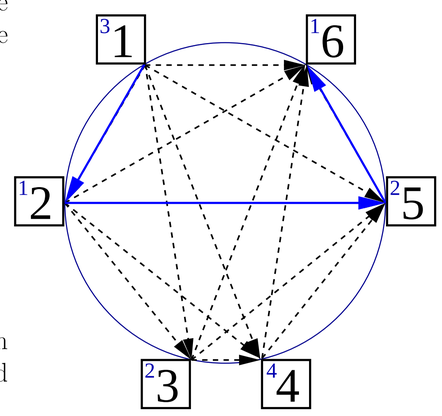
Task: Find the most diverse set W whose preservation cost $c(W)$ does not exceed a given budget B.

Replace in the algorithm the counters from k to B, i.e. regard the symbols L^b_{uv} and α^b_{uv} for $b = 0, 1, \ldots, B$. This replacements retains all properties of the algorithm.

An Example

Reconsider the network introduced in the above panel and assume an overall budget of $B = 7$. The example network introduces the following distance matrix and DAG.

$$(d_{uv}) = \begin{pmatrix} - & 12 & 23 & 23 & 22 & 20 \\ 12 & - & 15 & 15 & 26 & 24 \\ 23 & 15 & - & 4 & 17 & 21 \\ 23 & 15 & 4 & - & 17 & 21 \\ 22 & 26 & 17 & 17 & - & 12 \\ 20 & 24 & 21 & 21 & 12 & - \end{pmatrix}$$



The below table summarizes the optimization process. As we can see, the longest 7-tour has length 70 and starts in taxon 1 and returns to 1 from 6. The associated taxon subset is $\{1, 2, 5, 6\}$.

L^b_{uv}	v	0	1	2	3	4	5	6	7	$L^7_{uv} + d_{uv}$
L^b_{1v}	2	-	-	-	12	12	12	12	12	24
	3	-	-	-	-	-	23	27 (2)	27 (2)	50
	4	-	-	-	-	-	-	-	23	46
	5	-	-	-	-	-	22	38 (2)	40 (3)	62
	6	-	-	-	-	20	36 (2)	44 (3)	**50** (5)	**70**
L^b_{2v}	3	-	-	-	15	15	15	15	15	30
	4	-	-	-	-	-	15	15	19 (3)	34
	5	-	-	-	26	26	32 (3)	32 (3)	32 (4)	58
	6	-	-	21	21	38 (5)	38 (5)	44 (5)	44 (5)	68
L^b_{3v}	4	-	-	-	-	-	-	4	4	8
	5	-	-	-	-	17	17	17	17	34
	6	-	-	-	21	21	29 (5)	29 (5)	29 (5)	50
L^b_{4v}	5	-	-	-	-	-	-	17	17	34
	6	-	-	-	-	-	21	21	29 (5)	50
L^b_{5v}	6	-	-	-	12	12	12	12	12	24

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