10th International Congress on Industrial and Applied Mathematics, Poster Presentation at Waseda University, Tokyo, Japan. August 24, 2023

Constructing a Phylogenetic X-cactus from a Distance Matrix

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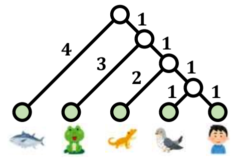
Background

Trees have been studied due to their usefulness in describing the evolutionary processes of organisms. However, when considering factors such as hybridization between different species, phylogenetic networks become necessary.

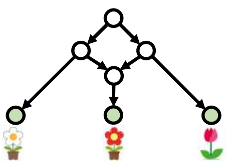
A distance matrix D on X for representing dissimilarities

	0	2	4	6	8
	2	0	4	6	8
	4	4	0	6	8
	6	6	6	0	8
	8	8	8	8	0

A realization of (X, D) $(d_G(x,y) = d(x,y))$



A phylogenetic network



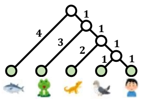
1965	1974	1987	2004
Uniqueness of phylogenetic tree [Hakimi & Yau]	Characterization of tree metric [Buneman]	Algorithm of constructing tree [Saitou & Nei]	Algorithm of constructing Network [Bryant & Moulton]

Tree metric

	0	2	4	6	8
	2	0	4	6	8
	4	4	0	6	8
	6	6	6	0	8
	8	8	8	8	0

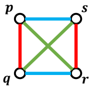
1 to 1

Tree

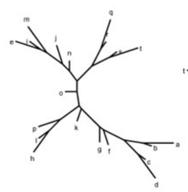


A distance d on X is tree metric $\Leftrightarrow$ d satisfies **"four-point condition"** such that $\forall p, q, r, s \in X$,

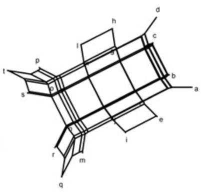
$$d(p,q) + d(r,s) \le \max\begin{cases} d(p,r) + d(q,s) \\ d(p,s) + d(q,r) \end{cases}$$



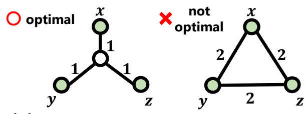
Neighbor-Joining algorithm



Neighbor-Net algorithm



We consider "optimal" realizations which are realizations of least total weight.



Saitou & Nei solved the following problem.

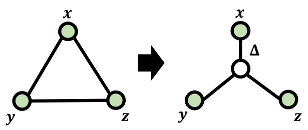
Problem 1

Propose an algorithm that satisfies the following conditions.

Input: A tree metric d on X

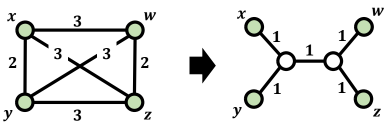
Output: The optimal realization of (X, d)

Define the operation "tightening".

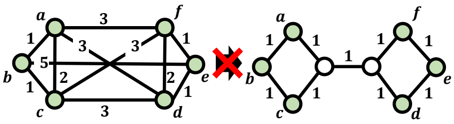


Determine how much each vertex "extends" from the set of other vertices using tightening.

$$\Delta := \min_{y,z \in X \setminus \{x\}} \left\{ \frac{1}{2}\left(d(x,y) + d(x,z) - d(y,z)\right) \right\}$$



If an input is a tree metric, the optimal realization can be obtained through tightening.



However, in cases where it is not a tree metric, the optimal realization might not be obtained.

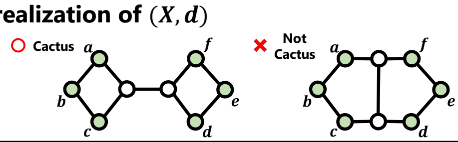
Problem 2

Propose an algorithm that satisfies the following conditions.

Input: A cactus metric d on X

Output: The optimal realization of (X, d)

Cactus:
Each edge belongs to at most one cycle

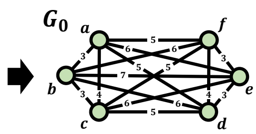


The Idea of proposed method

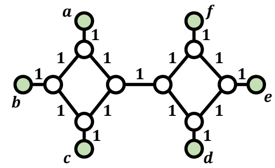
We demonstrate the proposal method with a small example.

Preliminary Step: Input distance matrix

	a	b	c	d	e	f
a	0	3	4	5	6	5
b	3	0	3	6	7	6
c	4	3	0	5	6	5
d	5	6	5	0	3	4
e	6	7	6	3	0	3
f	5	6	5	4	3	0



Optimal realization



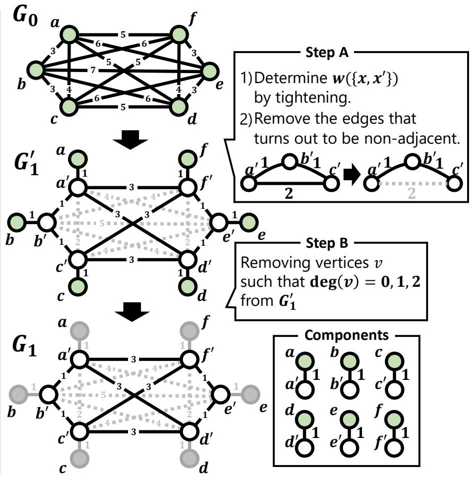
Main Step: Construct G^*

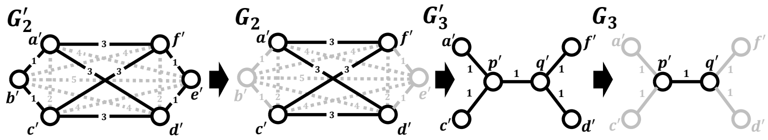
Repeat this "Main Step" until the number of vertices is 2 or fewer.

Step A: Construct G_1' from G_0
Determine how much each vertex "extends" from the set of other vertices using tightening.
Investigating adjacency relationships, including newly added vertices, for each vertex where $d(x,y) = d(x,t) + d(t,y)$ and x and y are not adjacent.

Step B: Remove vertices with $\deg(v) = 0, 1, 2$ and hold the removed elements as determined components of G^*.

Repeat this operation on G_1, and create G_2', G_2, G_3', G_3.
G_3 has 2 vertices, so the algorithm ends.

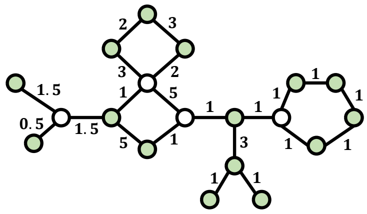




Examples

Illustrating successful examples using a Python program. This program runs on a laptop.

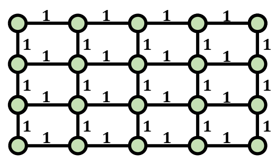
Example 1: A Cactus Metric



We were able to obtain the optimal realization fast using a cactus metric as the input.

Time: 0.2776 s

Example 2: A Grid (not cactus)



We were able to obtain the optimal realization fast not only a cactus metric.
The Neighbor-Net algorithm failed this example.

Time: 0.3961 s

Execution Environment

CPU: 11th Gen Intel(R) Core(TM) i7-1195G7 @ 2.90GHz 2.92 GHz
Python version: Python 3.11.4, Memory: 16.0GB, Operating System: Windows 11 22H2

Future works

Determining the metric spaces in which this method operates correctly. Furthermore, expanding to other metric spaces.

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GitHub (Programs)

References

[1] M. Hayamizu, K. T. Huber, V. Moulton, and Y. Murakami, "Recognizing and realizing cactus metrics," Information Processing Letters, vol. 157, p. 105916, 2020.
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