

Data and text mining

Shuffle & untangle: novel untangle methods for solving the tanglegram layout problem

Nghia Van Nguyen¹, Kurdistan Chawshin¹, Carl Fredrik Berg ^{1,*} and Damiano Varagnolo^{2,3}

¹Department of Geoscience and Petroleum, NTNU, 7031 Trondheim, Norway, ²Department of Engineering Cybernetics, NTNU, 7034 Trondheim, Norway and ³Department of Information Engineering, University of Padova, 35122 Padova, Italy

*To whom correspondence should be addressed.

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Abstract

Motivation: A tanglegram is a plot of two-tree-like diagrams, one facing the other, and having their labels connected by inter-tree edges. These two trees, which could be both phylogenetic trees and dendrograms stemming from hierarchical clusterings, have thus identically labelled leaves but different topologies. As a result, the inter-tree edges of a tanglegram can be intricately tangled and difficult to be analysed and explained by human readers. To better visualize the tanglegram (and thus compare the two dendrograms) one may try to untangle it, i.e. search for that series of flippings of the various branches of the two trees that minimizes the number of crossings among the inter-tree edges. The untangling problem has received significant interest in the past decade, and several techniques have been proposed to address it. These techniques are computationally efficient but tend to fail at finding the global optimum configuration generating the least tangly tanglegram.

Results: We leverage the existing results to propose untangling methods that are characterized by an overall slower convergence method than the ones in the literature, but that produce tanglegrams with lower entanglements.

Availability and implementation: One of the algorithms is implemented in Python, and available from <https://github.com/schlegelp/tanglegram>.

Contact: carl.f.berg@ntnu.no

1 Introduction

A common strategy to visually compare two different dendrograms relative to the same sets of terminal vertices is by using tanglegrams, i.e. comparative drawings (embeddings) of a pair of dendrograms, side-by-side, with matching objects connected by straight-line segments called inter-tree edges (Andreas *et al.*, 2012). A crossing occurs in a tanglegram when two inter-tree edges intersect, while there is no crossing inside the individual trees. The number of crossings, in its turn, depends on the layout (also known as drawing) of the two dendrograms in the tanglegram. In practical terms, layouts, which lead to a high number of crossings are harder to interpret (Andreas *et al.*, 2012). This calls for finding a drawing of the tanglegram with as few crossings as possible. Finding a tanglegram layout (TL) of two trees that produces zero crossings, sometimes referred to as a drawable layout (Fertus *et al.*, 2010), is known as the planar embedding problem (Andreas *et al.*, 2012). It is known that every pair of trees of size smaller or equal to three has a drawable layout (Fertus *et al.*, 2010). However, only special cases allow for a layout with zero crossings. The problem of finding a graphical layout of

two trees that gives the minimum number of crossings is known as the TL problem (Ramsal *et al.*, 2009), or the two-tree crossing minimization (TTCM) problem (Fertus *et al.*, 2010). The TTCM problem is known to be NP-complete, meaning that there is no known algorithm to solve this problem in polynomial time with the tree size, but only in exponential time (Fertus *et al.*, 2010).

When one tree is fixed, the problem above is referred to as the one-tree crossing minimization (OTCM) (Fertus *et al.*, 2010). For arbitrary trees, the OTCM problem can be solved in $O(n \log n)$ time (with n the number of leaves) as in Venkatasubramanian *et al.* (2009) and Fertus *et al.* (2010). Ramsal *et al.* (2009), instead, presented an $O(n \log^2 n / \log \log n)$ algorithm for a generalized tanglegram.

A heuristics-based algorithm to tackle the TTCM problem was proposed in Dwyer and Schreiber (2004). Here, the authors repeatedly solve the OTCM problem for each tree, and eventually provide 2.5D graphical representations of the results. Another approximation algorithm for complete tanglegrams is provided in Buchin *et al.* (2009).

The TTCM for binary trees problem was shown in Fertus *et al.* (2010) to be fixed parameter tractable (FPT) with parameter k (the

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