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Drawing (Complete) Binary Tanglegrams:

Hardness, Approximation, Fixed-Parameter Tractability

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Abstract A *binary tanglegram* is a drawing of a pair of rooted binary trees whose leaf sets are in one-to-one correspondence; matching leaves are connected by inter-tree edges. For applications, for example, in phylogenetics, it is essential that both trees are drawn without edge crossings and that the inter-tree edges have as few crossings as possible. It is known that finding a tanglegram with the minimum number of crossings is NP-hard and that the problem is fixed-parameter tractable with respect to that number.

We prove that under the Unique Games Conjecture there is no constant-factor approximation for binary trees. We show that the problem is NP-hard even if both trees are complete binary trees. For this case we give an $O(n^3)$-time 2-approximation and a new, simple fixed-parameter algorithm. We show that the maximization version of the dual problem for binary trees can be reduced to a version of MaxCut for which the algorithm of Goemans and Williamson yields a 0.878-approximation.

Keywords Binary tanglegram · crossing minimization · NP-hardness · approximation algorithm · fixed-parameter tractability

1 Introduction

In this paper we are interested in drawing so-called *tanglegrams* [23], that is, comparative drawings of pairs of rooted trees whose leaf sets are in one-to-one correspondence. The need to visually compare pairs of

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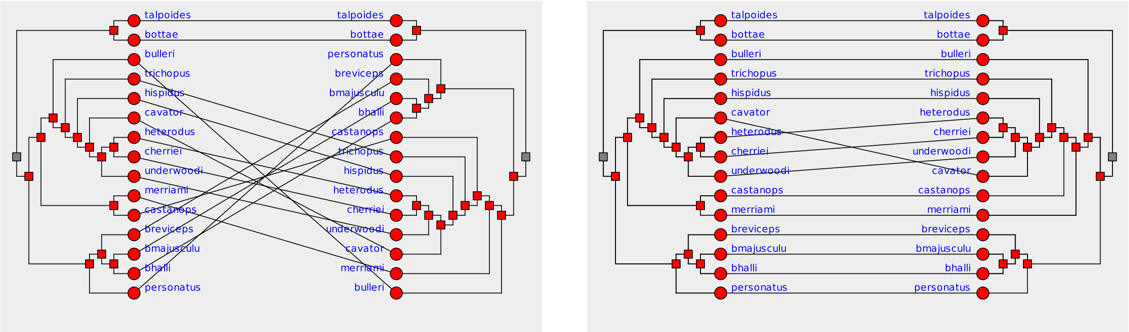


(a) arbitrary layout

(b) layout by our 2-approximation algorithm

Fig. 1: A binary tanglegram showing two evolutionary trees for lice of pocket gophers [16].

trees arises in applications such as the analysis of software projects, phylogenetics, or clustering. In the first application, trees may represent package-class-method hierarchies or the decomposition of a project into layers, units, and modules [17]. The aim is to analyze changes in hierarchy over time or to compare human-made decompositions with automatically generated ones. Whereas trees in software analysis can have nodes of arbitrary degree, trees from our second application, that is, (rooted) phylogenetic trees, are binary trees. This makes binary tanglegrams an interesting special case, see Fig. 1. Tanglegrams in phylogenetics are used, for example, to study cospeciation [23] or to compare evolutionary trees for the speciation of a single lineage but from different tree building methods. Hierarchical clusterings, our third application, are usually visualized by a binary tree-like structure called *dendrogram*, where elements are represented by the leaves and each internal node of the tree represents the cluster containing the leaves in its subtree. Pairs of dendrograms stemming from different clustering processes of the same data can be compared visually using tanglegrams. Note that we are interested in minimizing the number of crossings for visualization purposes. The minimum, as a number, is not primarily intended to be a tree-distance measure (since, for example, a crossing number of zero does not mean that two trees are equal). Examples of such measures are nearest-neighbor interchange and subtree transfer [8].

Let S and T be two rooted, unordered, n-leaf trees with node sets $V(S)$ and $V(T)$, edge sets $E(S)$ and $E(T)$, and leaf sets $L(S) \subseteq V(S)$ and $L(T) \subseteq V(T)$, respectively. In the remainder of the paper, unless explicitly stated otherwise, trees are considered to be rooted and unordered. We say that the pair of trees $\langle S,T\rangle$ is *uniquely leaf-labeled* if there are two bijective labeling functions $\lambda_S\colon L(S) \to \Lambda$ and $\lambda_T\colon L(T) \to \Lambda$, where $\Lambda = \{1,\dots,n\}$ is a set of labels. For a uniquely leaf-labeled pair of trees $\langle S,T\rangle$ we define the set $E(S,T) = \{uv \mid u \in L(S), v \in L(T), \lambda_S(u) = \lambda_T(v)\}$ of *inter-tree edges*, where each edge in $E(S,T)$ connects two leaves with the same label.

Tanglegram Layout Problem[1] **(TL)** Given a uniquely leaf-labeled pair of trees $\langle S,T\rangle$, find a *tanglegram* of $\langle S,T\rangle$, that is, a drawing of the graph $G = (V(S) \cup V(T), E(S) \cup E(T) \cup E(S,T))$ in the plane, with the following properties:

1. The subdrawing of S is a plane, *leftward* drawing of S with the leaves $L(S)$ on the line $x = 0$ and each parent node strictly to the left of all its children;
2. the subdrawing of T is a plane, *rightward* drawing of T with the leaves $L(T)$ on the line $x = 1$ and each parent node strictly to the right of all its children;
3. the inter-tree edges $E(S,T)$ are drawn as straight-line segments;
4. the number of crossings (between inter-tree edges) in the drawing is minimum.

In this paper we consider binary tanglegrams, that is, tanglegrams that consist of two rooted binary trees. We call the restriction of TL to binary trees the *binary TL problem*. We say that a rooted binary tree is *complete* (or *perfect*) if all its leaves have the same distance to the root. Accordingly, we call the restriction

[1] The name follows the common terminology in the biology literature [20, 23, 26]. Note that the problem has also been called the two-tree crossing minimization problem [12] or the stratified tree ordering problem [10].

of the binary TL problem to complete binary trees the *complete binary TL problem*. Figure 1 shows two binary tanglegrams for the same pair of trees, an arbitrary tanglegram and one with a minimum number of crossings.

The TL problem is purely combinatorial: Given a tree T, we say that a linear order of $L(T)$ is *compatible* with T if for each node v of T the nodes in the subtree of v form an interval in the order. For a binary tree T the linear orders of $L(T)$ that are compatible with T are exactly those orders that can be obtained from an initial plane leftward (or rightward) drawing of T by performing a sequence of subtree *swaps* that flip the order of the two child subtrees at an internal node. Given a permutation π of $\{1,\dots,n\}$, we call (i,j) an *inversion* in π if $i<j$ and $\pi(i)>\pi(j)$. For fixed orders σ of $L(S)$ and τ of $L(T)$ we define the permutation $\pi_{\tau,\sigma}$, which for a given position in τ returns the position in σ of the leaf having the same label. Now the TL problem consists in finding an order σ of $L(S)$ compatible with S and an order τ of $L(T)$ compatible with T such that the number of inversions in $\pi_{\tau,\sigma}$ is minimum.

Related problems. In graph drawing the so-called *two-sided crossing minimization problem* (2SCM) is an important problem that occurs when computing layered graph layouts. Such layouts were introduced by Sugiyama et al. [25] and are widely used for drawing hierarchical graphs. In 2SCM, vertices of a bipartite graph are to be placed on two parallel lines (called *layers*) such that vertices on one line are adjacent only to vertices on the other line. As in TL the objective is to minimize the number of edge crossings provided that edges are drawn as straight-line segments. In one-sided crossing minimization (1SCM) the order of the vertices on one of the layers is fixed. Even 1SCM is NP-hard [11]. In contrast to TL, a vertex in an instance of 1SCM or 2SCM can have several incident edges and the linear order of the vertices in the non-fixed layer is not required to be compatible with a tree. The following is known about 1SCM. The median heuristic of Eades and Wormald [11] yields a 3-approximation and a randomized algorithm of Nagamochi [21] yields an expected 1.4664-approximation. Dujmovič et al. [9] give an FPT algorithm that runs in $O^\star(1.4664^k)$ time, where k is the minimum number of crossings in any 2-layer drawing of the given graph that respects the vertex order of the fixed layer. The $O^\star(\cdot)$-notation ignores polynomial factors.

Previous work. Dwyer and Schreiber [10] draw series of related tanglegrams in 2.5 dimensions. Each tree is drawn on a plane, and the planes are stacked on top of each other. They consider a one-sided version of binary TL by fixing the layout of the first tree in the stack, and then, plane-by-plane, computing the leaf order of the next tree in $O(n^2 \log n)$ time each. Binary TL is also studied by Fernau et al. [12], although they refer to it as the *two-tree crossing minimization* problem. They show that binary TL is NP-hard and give a fixed-parameter algorithm that runs in $O^\star(c^k)$ time, where c is a constant estimated to be 1024 and k is the minimum number of crossings in any drawing of the given tanglegram. In addition, they show that the one-sided version of binary TL can be solved in $O(n \log^2 n)$ time. This improves on the result of Dwyer and Schreiber [10]. Fernau et al. also make the simple observation that the edges of the tanglegram can be directed from one root to the other. Thus the existence of a crossing-free tanglegram can be verified using a linear-time upward-planarity test for single-source directed acyclic graphs [3]. Later, apparently not being aware of the above mentioned results, Lozano et al. [20] give a quadratic-time algorithm for the same special case, to which they refer as *planar tanglegram layout*. Holten and van Wijk [17] present a visualization tool for general tanglegrams that heuristically reduces crossings (using the barycenter method for 1SCM on a per-level base) and draws inter-tree edges in bundles (using Bézier curves).

Our results. We first analyze the complexity of binary TL, see Section 2. We show that binary TL is essentially as hard as the MinUncut problem. If the (widely accepted) Unique Games Conjecture holds, it is NP-hard to approximate MinUncut—and thus binary TL—within any constant factor [19]. This motivates us to consider *complete* binary TL. It turns out that this special case has a rich structure. We start our investigation by giving a new reduction from Max2Sat that establishes the NP-hardness of complete binary TL.

The main result of this paper is a simple recursive factor-2 approximation algorithm for complete binary TL, see Section 3. It runs in $O(n^3)$ time and extends to d-ary trees. Our algorithm can also process non-complete binary tanglegrams—without guaranteeing any approximation ratio. It works well in practice and is quite fast when combined with branch-and-bound [22].

Next we consider a dual problem: maximize the number of edge pairs that do *not* cross. We show that this problem (for binary trees) can be reduced to a version of MAXCUT for which the algorithm of Goemans and Williamson [15] yields a 0.878-approximation.

Finally, we investigate the parameterized complexity of complete binary TL. Our parameter is the number k of crossings in an optimal drawing. We give a new FPT algorithm for complete binary TL that is much simpler and faster than the FPT algorithm for binary TL by Fernau et al. [12]. The running time of our algorithm is $O(4^k n^2)$, see Section 4. An interesting feature of the algorithm is that the parameter does *not* drop in each level of the recursion.

Subsequent work. Since the presentation of the preliminary version [5] of this work, the TL problem has received a lot of attention. We briefly summarize these recent developments. Böcker et al. [4] present a fixed-parameter algorithm for binary TL that runs in $O(2^k n^4)$ time. They further give a kernel-like bound for complete binary TL. Baumann et al. [2] study a generalized version of TL, in which the leaves no longer have to be in one-to-one correspondence; instead, the inter-tree edges may form any bipartite graph. They show how to formulate the problem as a quadratic linear-ordering problem with additional side constraints. Bansal et al. [1] study the same generalization, but restricted to binary TL. For the one-sided case (where the leaf order of one tree is fixed), they give a polynomial-time algorithm. On instances of (non-generalized) one-sided binary TL, their algorithm runs in $O(n \log^2 n / \log\log n)$ time, improving on the algorithm of Fernau et al. Finally, Venkatachalam et al. [26] give an $O(n \log n)$-time solution for the same problem.

2 Complexity

In this section we consider the complexity of binary TL, which Fernau et al. [12] have shown to be NP-complete. We strengthen their findings in two ways. First, we show that it is unlikely that an efficient constant-factor approximation for binary TL exists. Second, we show that TL remains hard even when restricted to *complete* binary tanglegrams.

We start by showing that binary TL is essentially as hard as MINUNCUT, the dual formulation of the classic MAXCUT problem [14]. This result relates the existence of a constant-factor approximation for binary TL to the Unique Games Conjecture (UGC). The UGC was introduced by Khot [18] in the context of interactive proofs. It concerns a scenario with two provers and a single round of answers to a question of the verifier. The word "unique" refers to the strategy of the verifier, who for any fixed answer of one of the provers will accept the proof only if the other prover gives the unique second part of the proof. The provers cannot communicate with each other. Still they want to maximize the probability of the proof being accepted given that questions of the verifier are drawn randomly from a given distribution. The UGC states that it is NP-hard to decide whether the optimal strategy of the provers gives them a high probability of success.

The UGC became famous when it was discovered that it implies optimal hardness-of-approximation results for problems such as MAXCUT and VERTEXCOVER, and forbids constant factor-approximation algorithms for problems such as MINUNCUT and SPARSESTCUT [19]. We reduce the MINUNCUT problem to the binary TL problem, which, by the result of Khot and Vishnoi [19], makes it unlikely that an efficient constant-factor approximation for binary TL exists.

The MINUNCUT problem is defined as follows. Given an undirected graph $G = (V,E)$, find a partition (V_1,V_2) of the vertex set V that minimizes the number of edges that are not cut by the partition, that is, $\min_{(V_1,V_2)} |\{uv \in E : \{u,v\} \subseteq V_1 \text{ or } \{u,v\} \subseteq V_2\}|$. Note that an optimal solution for MINUNCUT of a graph G is at the same time an optimal solution for MAXCUT of G. Nevertheless, the MINUNCUT problem is more difficult to approximate.

Theorem 2.1 *Under the Unique Games Conjecture it is NP-hard to approximate the TL problem for binary trees within any constant factor.*

Proof As mentioned above, we reduce from the MINUNCUT problem. Our reduction is similar to the reduction in the NP-hardness proof by Fernau et al. [12].

Consider an instance $G = (V,E)$ of the MINUNCUT problem. We construct a binary TL instance $\langle S,T \rangle$ as follows. The two trees S and T are isomorphic and there are three groups of edges connecting leaves

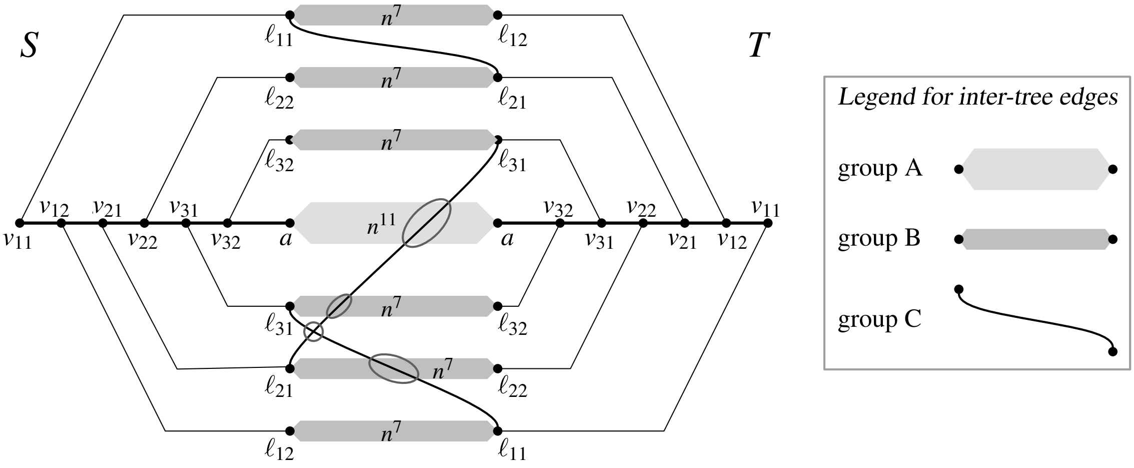


Fig. 2: Binary TL instance corresponding to the graph K_3 and the cut $(\{v_1\},\{v_2,v_3\})$. The crossings of the inter-tree edges are marked by gray ellipses.

of S to leaves of T. For simplicity of exposition, we permit multiple inter-tree edges between a pair of leaves and also an inter-tree connection of a leaf to many other leafs in the other tree. In the actual trees, we replace each such meta-leaf by a binary tree with the appropriate number of regular leaves.

Let $V = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of the graph G that constitutes our MINUNCUT instance. Then we construct both S and T as follows. We start with a *backbone* path $\langle v_{11}, v_{12}, v_{21}, v_{22}, \ldots, v_{n1}, v_{n2}, a\rangle$ from the root node v_{11} to a central leaf a. Additionally, for $i \in \{1,\ldots,n\}$ and $j \in \{1,2\}$, we attach each node v_{ij} to a leaf ℓ_{ij}. (The construction of S and T is illustrated, for the complete graph $K_3 = (\{v_1,v_2,v_3\},\{v_1v_2,v_2v_3,v_3v_1\})$, in Fig. 2.) In the remainder of this proof, where needed, we use a superscript to denote the tree to which a leaf belongs. The inter-tree edges between S and T form the following three groups.

- Group A contains n^{11} edges connecting the central leaves of the two trees.
- Group B contains, for each $v_i \in V$, n^7 edges connecting ℓ^S_{i1} with ℓ^T_{i2} and n^7 edges connecting ℓ^S_{i2} with ℓ^T_{i1}.
- Group C contains, for each $v_iv_j \in E$, a single edge from ℓ^S_{i1} to ℓ^T_{j1}.

Note that group C contains possibly more than one inter-tree edge attached to a single leaf in the described tree. The actual, final tree is then obtained by replacing each leaf of the tree described above by a tree with $O(n)$ new leaves such that no two inter-tree edges share a leaf. This replacement may cause new crossings, but no more than $O(n^2)$. Hence, these crossings can be neglected in the analysis, where only terms of order n^{11} will matter.

Next, we show how to transform any partition in G into a solution of the corresponding binary TL instance $\langle S,T\rangle$. For our reduction we will apply this transformation to the partition of an optimal solution to the given MINUNCUT instance. Let (V_1^*, V_2^*) be the given partition of G and suppose that k is the number of edges that are not cut. We now construct a drawing of $\langle S,T\rangle$ such that at most $k \cdot n^{11} + O(n^{10})$ pairs of edges cross. (In the example of Fig. 2 we consider the cut $(\{v_1\},\{v_2,v_3\})$ with the uncut edge v_2v_3.) We simply draw, for each vertex $v_i \in V_1^*$, the leaves ℓ^S_{i1} and ℓ^T_{i2} above the backbones, and the leaves ℓ^S_{i2} and ℓ^T_{i1} below the backbones. Symmetrically, for each vertex $v_i \in V_2^*$, we draw the leaves ℓ^S_{i1} and ℓ^T_{i2} below the backbones, and the leaves ℓ^S_{i2} and ℓ^T_{i1} above the backbones. Let us check the resulting number of crossings. There are $k \cdot n^{11}$ A–C crossings, no A–B crossings, at most $|E| \cdot n^8 \in O(n^{10})$ B–C crossings, and at most $|E|^2 \in O(n^4)$ C–C crossings. (In Fig. 2, we have $k = 1$, $|E| = 3$, and $n^{11} + 2n^7 + 1$ crossings in total.)

Now, suppose there exists, for some constant α, an α-approximation algorithm for the binary TL problem. Applying this algorithm to the instance $\langle S,T\rangle$ defined above yields a drawing $D(S,T)$ with at most $\alpha \cdot k \cdot n^{11} + O(n^{10})$ crossings. Let us assume that n is much larger than α and than any of the constants hidden in the $O(\cdot)$-notation. We show that from such a drawing $D(S,T)$ we would be able to reconstruct a cut (V_1,V_2) in G with at most $\alpha \cdot k$ uncut edges. First, observe that nodes ℓ^S_{i1} and ℓ^T_{i2} must be drawn either both above or both below the backbones, otherwise there would be n^{18} A–B crossings. Similarly, ℓ^S_{i2} must be on the same side as ℓ^T_{i1}. Next, observe that nodes ℓ^S_{i1} and ℓ^S_{i2} must be drawn on different sides of the backbones, otherwise there would be $O(n^{14})$ B–B crossings. Finally, observe that if we interpret the set of vertices v_i for which ℓ^S_{i1} is drawn above the backbone as the set V_1 of a partition of G and its complement as the set V_2, then this partition leaves at most $\alpha \cdot k$ edges from E uncut.

Hence, an α-approximation for the binary TL problem would provide an α-approximation for the MinUncut problem, which would contradict the UGC. □

The above negative result for binary TL is our motivation to investigate the complexity of complete binary TL. It turns out that even this special case is hard. Unlike Fernau et al. [12], who showed hardness of binary TL by a reduction from MaxCut using extremely unbalanced trees, we use a quite different reduction from a variant of Max2Sat.

Theorem 2.2 *The TL problem is NP-complete even for complete binary trees.*

Proof Recall the Max2Sat problem which is defined as follows. Given a set $U = \{x_1, \ldots, x_n\}$ of Boolean variables, a set $C = \{c_1, \ldots, c_m\}$ of disjunctive clauses containing two literals each, and an integer K, the question is whether there is a truth assignment of the variables such that at least K clauses are satisfied. We consider a restricted version of Max2Sat, where each variable appears in at most three clauses. This version remains NP-complete [24].

Our reduction constructs two complete binary trees S and T, in which certain aligned subtrees serve as variable gadgets and others as clause gadgets. We further determine an integer K' such that the instance $\langle S, T \rangle$ has less than K' crossings if and only if the corresponding Max2Sat instance has a truth assignment that satisfies at least K clauses.

The high-level structure of the two trees is depicted in Fig. 3. From top to bottom, the four subtrees at level 2 on both sides are a clause subtree, a variable subtree, another clause subtree, and finally a dummy subtree. The subtrees are connected to each other by inter-tree edges such that in any optimal solution they must be aligned in the depicted (or mirrored) order. Each clause gadget appears twice, once in each clause subtree, and is connected to the variable gadgets belonging to its two literals. Pairs of corresponding gadgets in S and T are connected to each other. Finally, non-crossing dummy edges connect unused leaves in order to make S and T complete. In the following, we describe the gadgets in more detail.

Variable gadgets. The basic structure of a variable gadget consists of two complete binary trees with 32 leaves each as shown in Fig. 4. Each tree has three highlighted subtrees of size 2 labeled a, b, c and a', b', c',

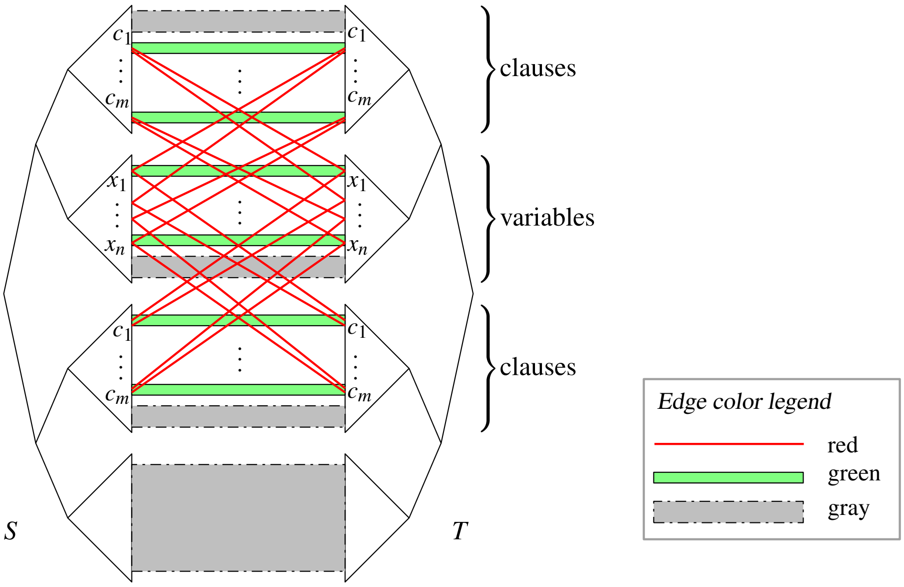
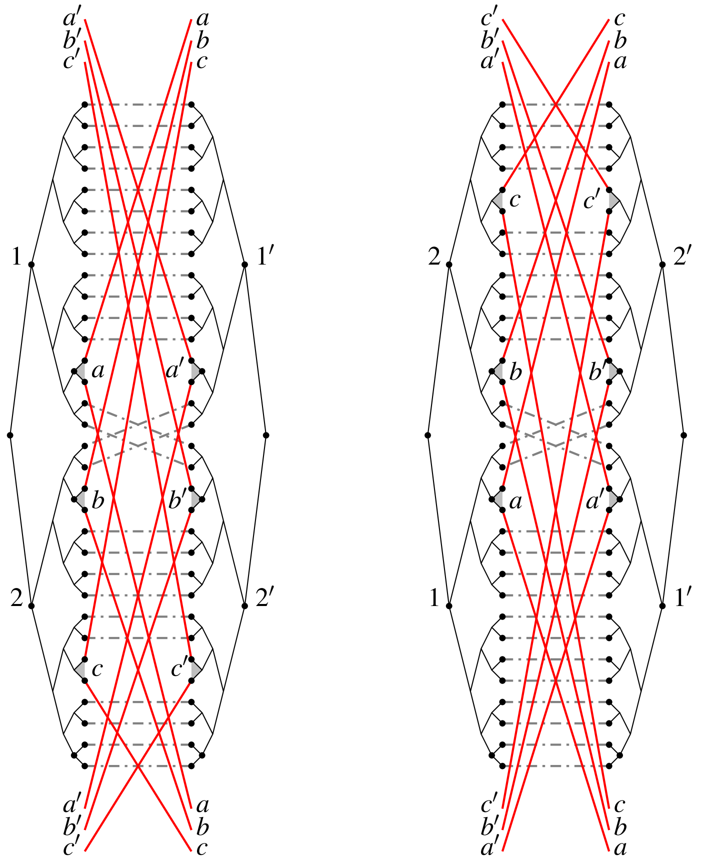


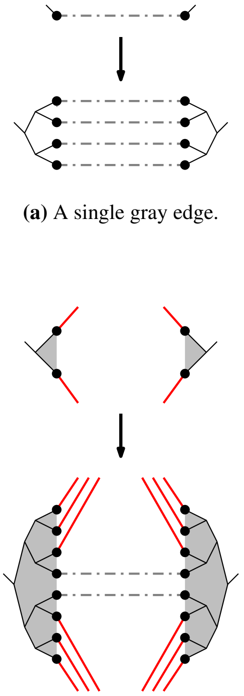
Fig. 3: High-level structure of the two trees S and T. Red edges connect clause and variable gadgets, green edges connect corresponding gadget halves, and gray edges are dummy edges to complete the trees.



(a) $x = \mathit{true}$

(b) $x = \mathit{false}$

Fig. 4: The variable gadget in its two optimal configurations with 184 crossings. Red edges are drawn solid, whereas dash-dot style is used for gray edges.



(a) A single gray edge.

(b) Two pairs of connector edges for a variable used in three clauses.

Fig. 5: Replacing each edge by four edges.

respectively. From each of these subtrees there is one red *connector* edge leaving the gadget at the top and one leaving it at the bottom. As long as two connector edges from the same tree do not cross each other, they transfer the vertical order of the labeled subtrees towards a clause gadget. We define the configuration in Fig. 4a as *true* and the configuration in Fig. 4b as *false*. If the configuration is in its *true* state, the induced vertical order of the connector edges is $a < b < c$, otherwise the order is inverse: $c < b < a$. It can easily be verified that both states have the same number of crossings. To see that it is optimal observe that each pair of connector edges from the same subtree (for example, subtree a) always crosses all 26 gray edges in the gadget. Furthermore, all 24 crossings of two connector edges in the figure are mandatory. Finally, the four crossings among the gray edges between subtrees 1 and $2'$ and subtrees 2 and $1'$ are also optimal. (Otherwise, if subtree 1 is aligned with subtree $2'$, there are 12 edges from the upper subtree on the left to the lower subtree on the right and 10 edges from the lower subtree on the left to the upper subtree on the right that yield in total at least 120 gray–gray crossings in addition to the 24 red–red crossings and the 156 red–gray crossings as opposed to a total of 184 crossings in either configuration of Fig. 4.) Note that some internal swaps within the subtrees 1, 2, $1'$, $2'$ are possible that do not affect the number of crossings; none of them, however, changes the order of the connector edges since in any optimal solution the subtrees of the four crossing gray edges must always stay in the center of the gadget.

Note that so far the gadget in the figure is designed for a single appearance of the variable since the four connector-edge triplets are required for a single clause. For the MAX2SAT reduction, however, each variable can appear up to three times in different clauses. By appending a complete binary tree with four leaves as in Fig. 5 to each leaf of the gadget in Fig. 4 and copying each edge accordingly the above arguments still hold for the enlarged trees with 128 leaves each. Unused connector edges in opposite subtrees are linked to each other (a to a', b to b', c to c') as in Fig. 4b such that the number of crossings in the gadget remains balanced for both states.

Clause gadgets. For each clause $c_i = l_{i1} \vee l_{i2}$, where l_{i1} and l_{i2} denote the two literals, we create two clause gadgets: one in the upper clause subtrees and one in the lower clause subtrees (recall Fig. 3). Each gadget itself consists of two parts: one part that uses the connectors from the first variable in the left tree and those from the second variable in the right tree and vice versa. Figure 6 shows one such part of the gadget in the lower clause subtrees, where the connector edges lead upwards. The gadget in the upper clause subtree is simply a mirrored version.

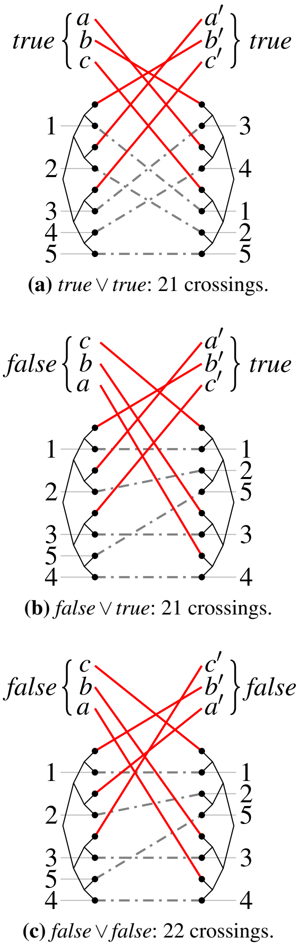
The basic structure consists of two aligned subtrees with eight leaves as depicted in Fig. 6. Three of the leaves on each side serve as the missing endpoints for the triplets of connector edges from the corresponding variables. Recall that for a positive literal with value *true* the order of the connector edges is $a < b < c$, and for a positive literal with value *false* it is $c < b < a$. (For negative literals the meaning of the orders is inverted.) The two connector leaves for the edges labeled a and b are in the same four-leaf subtree, the connector leaf for c is in the other subtree. Three cases need to be distinguished. If (1) both literals are *true*, then the configuration in Fig. 6a is optimal with 21 crossings. If (2) only one literal is *true*, then Fig. 6b shows again an optimal configuration with 21 crossings. Here the tree on the right side swapped the subtrees of the root node. Finally, if (3) both literals are *false*, there are at least 22 crossings in the gadget as shown in Fig. 6c. Since this substructure is repeated four times for each clause we have 84 induced crossings for satisfied clauses and 88 induced crossings for unsatisfied clauses.

Reduction. We construct the gadgets for all variables and clauses and link them together as two trees S and T, which are filled up with dummy leaves and edges such that they become complete binary trees. The general layout is as depicted in Fig. 3, where each dummy leaf in S is connected to the opposite dummy leaf in T such that there are no crossings among dummy edges. In each of the four main subtrees all dummy edges are consecutive. Thus of all dummy edges only those in the variable subtree have crossings with exactly half the connector edges.

It remains to compute the minimum number M of crossings that are always necessary, even if all clauses are satisfied. Then the MAX2SAT instance has a solution with at least K satisfied clauses if and only if the constructed TL instance has a solution with at most $K' = M + 4(|C| - K)$ crossings. We get the corresponding variable assignment directly from the layout of the variable gadgets.

The first step for computing M is to fix an (arbitrary) order for the variable gadgets in the variable subtree. Let this order be $x_1 < x_2 < \ldots < x_n$. We want to achieve that any other order would increase the number of crossings by a number that is too large for it to be part of an optimum solution. We first establish neighbor links between adjacent variable gadgets. For these neighbor links we need eight of the 128 leaves in each half of each variable gadget as shown in Fig. 7. Since both subtrees below the root of x_i in S and both subtrees below the root of x_{i+1} in T are connected to each other, the minimum number of crossings of those edges is independent of the truth state of each gadget. The next step is to enlarge the variable gadgets even further by repeatedly doubling all leaves until each variable gadget has at least cm^2 gray edges for some constant c. (Note that in subtrees containing red connector edges, we do not duplicate any red edges but rather create new gray edges, similarly to Fig. 4b.) Now changing the variable order causes at least $8cm^2$ additional crossings since at least eight neighbor links would cross at least one variable gadget. We explain how to choose c later.

Once the order of the variables is fixed, we sort all clauses lexicographically (a clause with variables $x_i < x_j$ is smaller than a clause with variables $x_k < x_l$ if $x_i < x_k$ or if $x_i = x_k$ and $x_j < x_l$) and place smaller clauses towards the top of the clause subtrees. Consider two clause gadgets in the same clause subtree. Then, in the given clause order, there are crossings between their connector-edge triplets if and only if the intervals between their respective variables intersect in the variable order. Since these crossings are unavoidable for the given variable order, the number of connector-triplet crossings in the lexicographic order of the clauses is optimal. There are at most 36 crossings between the connector-edge triples of any pair of clause gadgets in each of the two clause subtrees. So for all clause pairs in both clause subtrees we get at most $\gamma = 2 \cdot 36 \cdot m(m-1)/2$ crossings. If we choose the constant c so that $8cm^2 > \gamma$, it never pays off



(a) *true* ∨ *true*: 21 crossings.

(b) *false* ∨ *true*: 21 crossings.

(c) *false* ∨ *false*: 22 crossings.

Fig. 6: Gadget for the clause $c_i = l_{i1} \vee l_{i2}$.

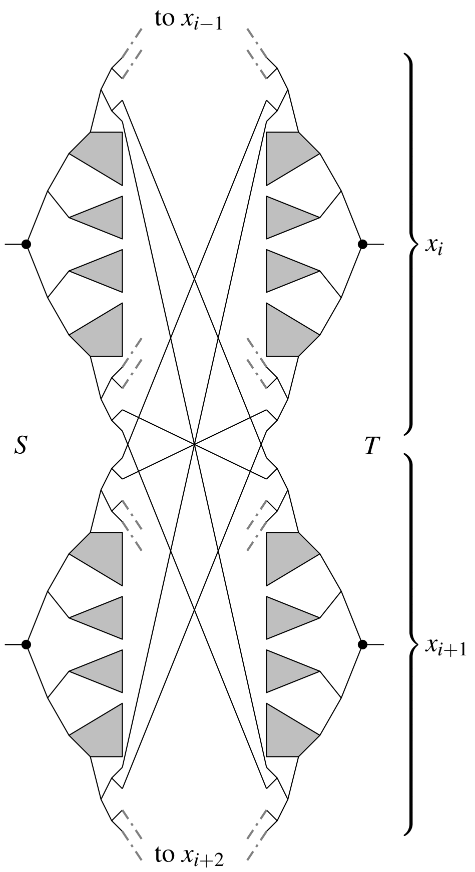


Fig. 7: Linking adjacent variable gadgets for x_i and x_{i+1}.

to change the given variable order. So we can finally compute all necessary crossings between connector edges, dummy edges and intra-gadget edges which yields the number M.

Since each gadget has polynomial size, the two trees and the number M can be computed in polynomial time. It is obvious that the complete binary TL problem is in $\mathscr{NP}$. □

3 Approximation Algorithm

We start with a basic observation about binary tanglegrams. As we have noted in the introduction, TL is a purely combinatorial problem, that is, it suffices to determine two leaf orders σ and τ that are compatible with the input trees S and T, respectively. These orders are completely determined by fixing an order of the two subtrees of each inner node $v \in S^\circ \cup T^\circ$, where S° and T° denote the set of inner nodes of S and T. The algorithm will recursively split the two trees S and T at their roots into two equally sized subinstances and determine leaf orders of S and T by choosing a locally optimal order of the subtrees below the left and right root of the current subinstance.

Let $\langle S_0, T_0 \rangle$ be an input instance for complete binary TL. We assume that an initial layout of S_0 and T_0 is given, that is, the subtrees of each $v \in S_0^\circ \cup T_0^\circ$ are ordered (otherwise choose an arbitrary initial layout). The root of a tree T is denoted as v_T. For a binary tree T with the two ordered subtrees T_1 and T_2 of v_T, we use the notation $T = (T_1, T_2)$. For each subinstance $\langle S, T \rangle$ with $S = (S_1, S_2)$ and $T = (T_1, T_2)$, we need to consider the four configurations $(S_1, S_2) \times (T_1, T_2)$ (initial layout), $(S_2, S_1) \times (T_1, T_2)$ (swap at v_S), $(S_1, S_2) \times (T_2, T_1)$

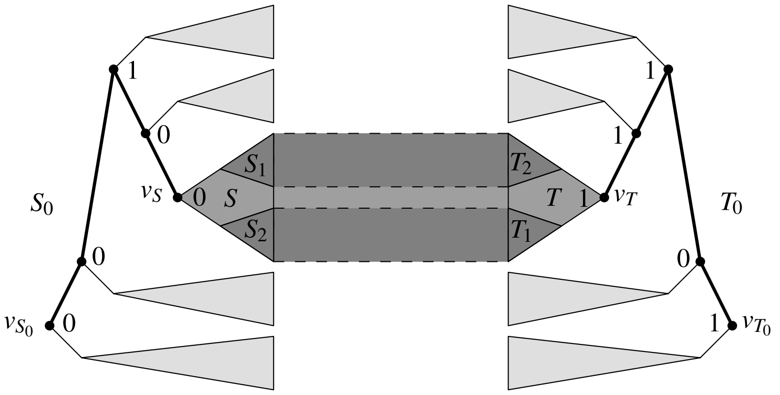


Fig. 8: The context of an instance $\langle S,T \rangle$ that is split into the subinstances $\langle S_1,T_2 \rangle$ and $\langle S_2,T_1 \rangle$ since T_1 and T_2 are swapped at v_T. The swap history is indicated by binary swap variables along the paths to the roots v_{S_0} and v_{T_0}.

(swap at v_T), and $(S_2,S_1) \times (T_2,T_1)$ (swap at v_S and v_T). For each configuration, we recursively solve two subinstances and then choose the configuration with the minimum number of crossings.

We always split the instance $\langle S,T \rangle$ into an upper and a lower half, that is, the subinstances depend on the swap decision. If we swap both v_S and v_T or none, the two subinstances are $\langle S_1,T_1 \rangle$ and $\langle S_2,T_2 \rangle$; if only one side is swapped, the subinstances are $\langle S_1,T_2 \rangle$ and $\langle S_2,T_1 \rangle$. We solve both subinstances independently. In order to achieve the desired approximation ratio, however, we cannot ignore the swap history of the predecessor nodes of v_T and v_S. This history can be regarded as two bit strings h_S and h_T that represent the *swap* and *no-swap* decisions made at the previous steps of the recursion. Figure 8 shows an instance $\langle S,T \rangle$ and its swap history.

The history is used to compute the number of *current-level crossings* of $\langle S,T \rangle$, that is, the number of crossings that are caused by the swap decisions made for the current subinstance. The number of current-level crossings and the recursively computed numbers of crossings of the subinstances determine which of the four configurations of the current instance is the best one. Let $\operatorname{lca}(a,b)$ be the lowest common ancestor of two nodes a and b of the same tree. An important observation that is necessary to compute the number of current-level crossings is the following.

Observation *For each pair of inter-tree edges ab and cd, $a,c \in L(S)$ and $b,d \in L(T)$, the swap decisions at the lowest common ancestors $\operatorname{lca}(a,c)$ and $\operatorname{lca}(b,d)$ completely determine whether ab and cd cross or not. Given the order of the subtrees of $\operatorname{lca}(a,c)$, swapping or not swapping the subtrees of $\operatorname{lca}(b,d)$ (and vice versa) causes or removes the crossing of ab and cd.*

When considering the current-level crossings of a subinstance $\langle S,T \rangle$ we know from the swap history which of the nodes on the paths P_S and P_T from v_S and v_T to the roots v_{S_0} and v_{T_0} of the full trees, respectively, have swapped their subtrees. Hence, for v_S we can compute the current-level crossings of all pairs of edges ab and cd with $a \in L(S_1)$, $c \in L(S_2)$, and $\operatorname{lca}(b,d) \in P_T$; analogously, we can compute the crossings of all pairs of edges ab and cd with $b \in L(T_1)$, $d \in L(T_2)$, and $\operatorname{lca}(a,c) \in P_S$. Note that if $\operatorname{lca}(b,d)$ or $\operatorname{lca}(a,c)$ is not one of the predecessor nodes of v_T or v_S, but it is a node in the subtree T or S, then the crossing of the edges ab and cd will be considered in a subsequent step. Otherwise, our algorithm cannot account for the crossing and we may underestimate the number of crossings. Yet, we are able to bound this error later in Theorem 3.2.

Algorithm 1 defines the recursive routine `RecSplit` that computes our tanglegram layout. It is initially called with the parameters `RecSplit` $(S_0,T_0,\varepsilon,\varepsilon)$, where ε is the empty string.

In order to quickly calculate the number of current-level crossings we use a preprocessing step. To that end, we compute two tables $C^=$ and $C^\times$ of size $O(n^2)$. For each pair (v,w) of inner nodes in $S^\circ \times T^\circ$, the entry $C^=[v,w]$ stores the number of crossings of edge pairs ab and cd with $\operatorname{lca}(a,c) = v$ and $\operatorname{lca}(b,d) = w$ if either both or none of v and w swap their subtrees. An entry $C^\times[v,w]$ stores the analogous number of crossings if only one of v and w swap their subtrees.

Lemma 3.1 *The tables $C^=$ and $C^\times$ can be computed in $O(n^2)$ time.*

```
Algorithm 1: RecSplit $(S,T,h_S,h_T)$
  Input:  $n$-leaf trees $S=(S_1,S_2)$ and $T=(T_1,T_2)$, swap histories $h_S$ and $h_T$
  Output: lower bound $\mathrm{cr}_{ST}$ on the number of crossings created by the algorithm;
          orders $\sigma$ and $\tau$ for the leaves of $S$ and $T$, respectively
  if $n=1$ then
      return $(\mathrm{cr}_{ST},\sigma,\tau)=(0,v_S,v_T)$
  else
      $\mathrm{cr}_{ST}=\infty$
      foreach $(\mathrm{swp}_S,\mathrm{swp}_T)\in\{0,1\}^2$ do
          loop through all four cases to swap subtrees of S and T
          $\mathrm{cl}\leftarrow$ current level crossings induced by $(\mathrm{swp}_S,\mathrm{swp}_T)$
          $(\mathrm{cr}_1,\sigma_{1+\mathrm{swp}_S},\tau_{1+\mathrm{swp}_T})\leftarrow \texttt{RecSplit}(S_{1+\mathrm{swp}_S},T_{1+\mathrm{swp}_T},(h_S,\mathrm{swp}_S),(h_T,\mathrm{swp}_T))$
          $(\mathrm{cr}_2,\sigma_{2-\mathrm{swp}_S},\tau_{2-\mathrm{swp}_T})\leftarrow \texttt{RecSplit}(S_{2-\mathrm{swp}_S},T_{2-\mathrm{swp}_T},(h_S,\mathrm{swp}_S),(h_T,\mathrm{swp}_T))$
          if $\mathrm{cl}+\mathrm{cr}_1+\mathrm{cr}_2<\mathrm{cr}_{ST}$ then
              $\mathrm{cr}_{ST}\leftarrow\mathrm{cl}+\mathrm{cr}_1+\mathrm{cr}_2$
              if $\mathrm{swp}_S=0$ then
                  $\sigma\leftarrow(\sigma_1,\sigma_2)$
              else $\sigma\leftarrow(\sigma_2,\sigma_1)$
              if $\mathrm{swp}_T=0$ then
                  $\tau\leftarrow(\tau_1,\tau_2)$
              else $\tau\leftarrow(\tau_2,\tau_1)$
      return $(\mathrm{cr}_{ST},\sigma,\tau)$
```

Proof We initialize all entries as 0 and preprocess S_0 and T_0 in linear time to support lowest-common-ancestor queries in $O(1)$ time [13]. Then we determine for each pair of inter-tree edges their lowest common ancestors in S_0 and T_0 and increment the corresponding table entry depending on which two configurations yield the crossing. This takes $O(n^2)$ time for all edge pairs. □

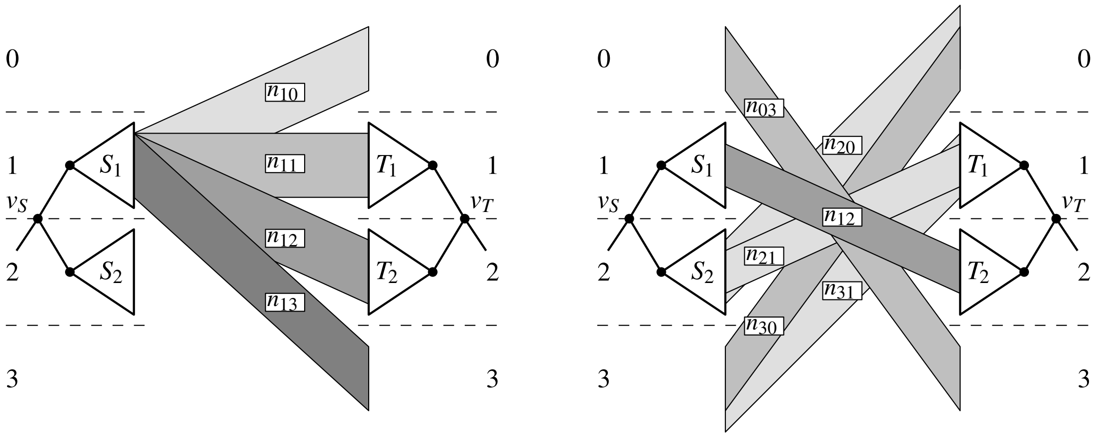
Once we have computed $C^=$ and $C^\times$, we can determine the number of current-level crossings for any subinstance $\langle S,T\rangle$ in $O(\log n)$ time by summing up the appropriate table entries depending on the swap history along the paths P_T and P_S, which are of length $O(\log n)$.

The running time Algorithm 1 satisfies the recurrence $T(n)\leq 8T(n/2)+O(\log n)$, which solves to $T(n)=O(n^3)$ by the master method [7]. We now prove that the algorithm yields a 2-approximation.

Theorem 3.2 *Given a complete binary TL instance $\langle S_0,T_0\rangle$ with n leaves in each tree, Algorithm 1 computes in $O(n^3)$ time a drawing of $\langle S_0,T_0\rangle$ that has at most twice as many crossings as an optimal drawing.*

Proof Fix any drawing δ of $\langle S_0,T_0\rangle$. Algorithm 1 tries, for each subinstance $\langle S,T\rangle$ of $\langle S_0,T_0\rangle$, all four possible configurations of $S=(S_1,S_2)$ and $T=(T_1,T_2)$—among them the configuration in δ. Assume that the configuration in δ is $\langle(S_1,S_2),(T_1,T_2)\rangle$. We determine an upper bound on the number of crossings that the algorithm fails to count for the drawing δ. In each of the trees S_0 and T_0 we distinguish four different areas for the endpoints of the edges: above S_1, in S_1, in S_2, below S_2 and similarly above T_1, in T_1, in T_2, below T_2. We number these regions from 0 to 3, see Fig. 9. This allows us to classify the edges into 16 groups (two of which, 0–0 and 3–3, are not relevant). We denote the number of *i–j edges*, that is, edges from area i to area j, by $n_{ij}(S,T)$ (for $i,j\in\{0,1,2,3\}$). Figure 9a shows the four groups of *i–j* edges for $i=1$.

The only crossings that the algorithm does not take into account are crossings between edges whose lowest common ancestors lie in parts of S_0 and T_0 that are split apart into different branches of the recursion. For the subinstance $\langle S,T\rangle$, which is split into $\langle S_1,T_1\rangle$ and $\langle S_2,T_2\rangle$, this means that for all $n_{12}(S,T)$ edges that run between S_1 and T_2, we fail to consider all crossings between pairs of two such edges. Similarly, we do not consider any pair of the $n_{21}(S,T)$ edges between S_2 and T_1.



(a) Edges incident to $L(S_1)$ are separated into four groups by the area of their second endpoint.

(b) All edge groups that cross the n_{12} 1–2 edges between $L(S_1)$ and $L(T_2)$.

Fig. 9: Areas of the endpoints and types of edges incident to $L(S)$ and $L(T)$. Cardinalities $n_{ij}(S,T)$ are abbreviated as n_{ij}.

Let's return to the drawing δ and consider the set $\mathscr{I}$ of subinstances that correspond to δ, that is, all pairs of opposing subtrees in δ. For each subinstance $\langle S,T\rangle \in \mathscr{I}$ we do not account for crossings of pairs of 1–2 edges and pairs of 2–1 edges since these edges run between two subinstances that are solved independently. In the worst case all these edge pairs cross and the algorithm misses $\binom{n_{12}(S,T)}{2} + \binom{n_{21}(S,T)}{2}$ crossings. Let c_δ be the number of crossings of δ counted by the algorithm, and let $|\delta|$ be the actual number of crossings of δ. Clearly, we have $c_\delta \leq |\delta|$. We can bound $|\delta|$ from above by

$$|\delta| \leq c_\delta + \sum_{\langle S,T\rangle \in \mathscr{I}} \left[\binom{n_{12}(S,T)}{2} + \binom{n_{21}(S,T)}{2} \right] \leq c_\delta + \sum_{\langle S,T\rangle \in \mathscr{I}} \frac{n_{12}^2(S,T) + n_{21}^2(S,T)}{2}. \tag{1}$$

We now show that $\sum_{\langle S,T\rangle \in \mathscr{I}} (n_{12}^2(S,T) + n_{21}^2(S,T)) \leq 2c_\delta$. For the sake of convenience, we abbreviate $n_{ij}(S,T)$ by n_{ij} in the following. We will bound n_{12}^2 by the number of crossings of the 1–2 edges in δ that are counted by the algorithm. This number is at least

$$c_{12} = n_{12} \cdot (n_{03} + n_{20} + n_{21} + n_{30} + n_{31}) \tag{2}$$

as can be seen in Fig. 9b. All these crossings are current-level crossings at this or some earlier point in the algorithm. Since our (sub)trees are complete and thus S_1 and T_1 have the same number of leaves, we obtain

$$n_{10} + n_{12} + n_{13} = n_{01} + n_{21} + n_{31}. \tag{3}$$

Furthermore, we have the following equality for the edges from areas 0 on both sides

$$n_{01} + n_{02} + n_{03} = n_{10} + n_{20} + n_{30}. \tag{4}$$

From (3) we obtain $n_{12} \leq n_{01} - n_{10} + n_{21} + n_{31}$ and from (4) we obtain $n_{01} - n_{10} \leq n_{20} + n_{30}$. Hence, we have $n_{12} \leq n_{20} + n_{30} + n_{21} + n_{31}$. With (2) this yields

$$n_{12}^2 \leq n_{12} \cdot (n_{20} + n_{30} + n_{21} + n_{31}) \leq c_{12}, \tag{5}$$

that is, n_{12}^2 is bounded by the number of crossings that involve a 1–2 edge in δ and that are counted by the algorithm. Analogously, we obtain

$$n_{21}^2 \leq n_{21} \cdot (n_{02} + n_{03} + n_{12} + n_{13}) \leq c_{21}, \tag{6}$$

that is, n_{21}^2 is bounded by the number of crossings counted by the algorithm that involve a 2–1 edge in δ.

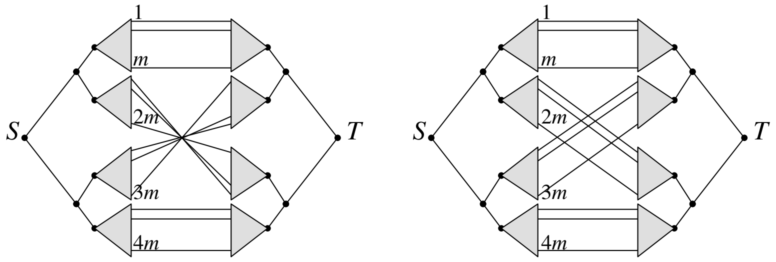


Fig. 10: Example of a tanglegram for which our algorithm may output a drawing (left) that has roughly twice as many crossings as the optimal drawing (right).

So from (5) and (6) we have $n_{12}^2 \le c_{12}$ and $n_{21}^2 \le c_{21}$. Applying this argument to all subinstances $\langle S,T\rangle \in \mathscr{I}$ we get

$$\sum_{\langle S,T\rangle\in\mathscr{I}} (n_{12}^2(S,T)+n_{21}^2(S,T)) \le \sum_{\langle S,T\rangle\in\mathscr{I}} c_{12}(S,T) + \sum_{\langle S,T\rangle\in\mathscr{I}} c_{21}(S,T) \le 2\cdot c_\delta. \tag{7}$$

The fact that $\sum_{\langle S,T\rangle\in\mathscr{I}} c_{12}(S,T) \le c_\delta$ holds is due to each edge crossing δ appearing in at most one term $c_{12}(S,T)$. This can be seen as follows. Let ab be a 1–2 edge in the subinstance $\langle S,T\rangle$. Then in all parent instances of the recursion, ab was still a 1–1 edge or a 2–2 edge; such edges do not appear in any previous c_{12}-term. In a subsequent instance $\langle S',T'\rangle$ below $\langle S,T\rangle$ in the recursion the edge ab might in fact reappear, for example as a 0–3 edge. At that point, however, it is considered as an edge that crosses one of the 1–2 edges of $\langle S',T'\rangle$, say cd. But then cd was considered as a 1–1 or 2–2 edge in all previous instances. Hence, the crossing between ab and cd does not appear in any other c_{12}-term. Analogous reasoning yields $\sum_{\langle S,T\rangle\in\mathscr{I}} c_{21}(S,T) \le c_\delta$

Plugging (7) into (1) yields $|\delta| \le 2c_\delta$. Now let $A^\star$ be the solution computed by Algorithm 1 and let $S^\star$ be an optimal solution. We denote their actual numbers of crossings by $|A^\star|$ and $|S^\star|$, respectively. By $c_{A^\star}$ and $c_{S^\star}$ we denote the number of crossings counted by our algorithm for the drawings $A^\star$ and $S^\star$, respectively. Since $|\delta| \le 2c_\delta$ for any drawing δ we get

$$|A^\star| \le 2c_{A^\star} \le 2c_{S^\star} \le 2|S^\star|,$$

that is, the algorithm is indeed a factor-2 approximation. □

We note that the approximation factor of 2 is tight: let $n = 4m$, let S have leaves ordered $1,\dots,4m$, and let T have leaves ordered $1,\dots,m,3m,\dots,2m+1,\ m+1,\dots,2m,3m+1,\dots,4m$ (see Fig. 10). Then our algorithm may construct a drawing with $m^2 + 2\binom{m}{2} = 2m^2 - m$ crossings, while the optimal drawing has only m^2 crossings.

Non-complete binary trees. Algorithm 1 can also be applied to non-complete tanglegrams with minor modifications. The only essential difference is that during the algorithm we can encounter the situation that a single leaf v of one tree is paired with a larger subtree T' of the other tree. In that case we continue the recursion for those subtrees of T' that contain an edge to v in order to find their locally optimal swap decisions. For non-complete tanglegrams, however, the approximation factor does not hold any more. Nöllenburg et al. [22] have evaluated several heuristics for binary TL, among them the modified version of Algorithm 1.

Generalization to d-ary trees. The algorithm can be generalized to complete d-ary trees. The recurrence relation of the running time changes to $T(n) \le d\cdot(d!)^2\cdot T(n/d) + O(\log n)$ since we need to consider all $d!$ subtree orderings of both trees, each triggering d subinstances of size n/d. This resolves to $T(n) = O(n^{1+2\log_d(d!)})$. For $d \ge 3$ the running time is upper-bounded by $O(n^{2d-1.7})$. At the same time the approximation factor increases to $1+\binom{d}{2}$. This is because for any pair (i,j) with $1 \le i < j \le d$ the algorithm fails to account for potential crossings between the trees S_i and T_j as well as between S_j and T_i. This number can be bounded for each of the $\binom{d}{2}$ pairs by the number of crossings in the optimal solution using our arguments for binary trees.

Maximization version. Instead of the original TL problem, which minimizes the number of pairs of edges that cross each other, we now consider the dual problem TL* of maximizing the number of pairs of edges that do not cross. The sets of optimal solutions for the two problems are the same, but from the perspective of approximation the problems differ a lot, at least in the binary case: in contrast to binary TL, which is hard to approximate as we have shown in Theorem 2.1, binary TL* has a constant-factor approximation algorithm. We show this by reducing binary TL* to a constrained version of the MAXCUT problem, which can be solved approximately with the semidefinite programming (SDP) rounding algorithm of Goemans and Williamson [15]. Their algorithm runs in polynomial time; solving the underlying SDP relaxation of the problem is the most time-consuming step. Still, SDP relaxations of MAXCUT instances of up to 7000 variables can be solved in practice [6].

Theorem 3.3 *There exists a polynomial-time algorithm with approximation factor* 0.878 *for binary TL**.

Proof Let $\langle S,T\rangle$ be an instance of binary TL*. Fix any initial drawing of $\langle S,T\rangle$. As before, we associate a decision variable with each inner node of the two trees. The variable decides whether we do or do not swap the children at the corresponding node. We model this situation by a weighted graph $G=(V,E)$; a swap decision corresponds to deciding to which side of a cut the corresponding vertex is assigned. More precisely, for each inner node u of $\langle S,T\rangle$, the graph G contains two vertices u and u'. We will also impose a constraint that u and u' must be separated by a cut we are looking for. As we will indicate later, we can use the algorithm of Goemans and Williamson [15] to find large cuts among those separating all pairs of type (u,u').

For each pair ab and cd of inter-tree edges with $a,c\in L(S)$ and $b,d\in L(T)$, the graph G contains a weighted edge that we construct as follows. Let $v=\mathrm{lca}(a,c)$ and $w=\mathrm{lca}(b,d)$ be the lowest common ancestors of the edge pair. If ab and cd cross in the initial drawing, we add the edge vw with weight 1 to G. If the edge is already present, we increase its weight by one. If the two edges do not cross in the initial drawing, then we analogously add the edge vw' to G or increase its weight by one.

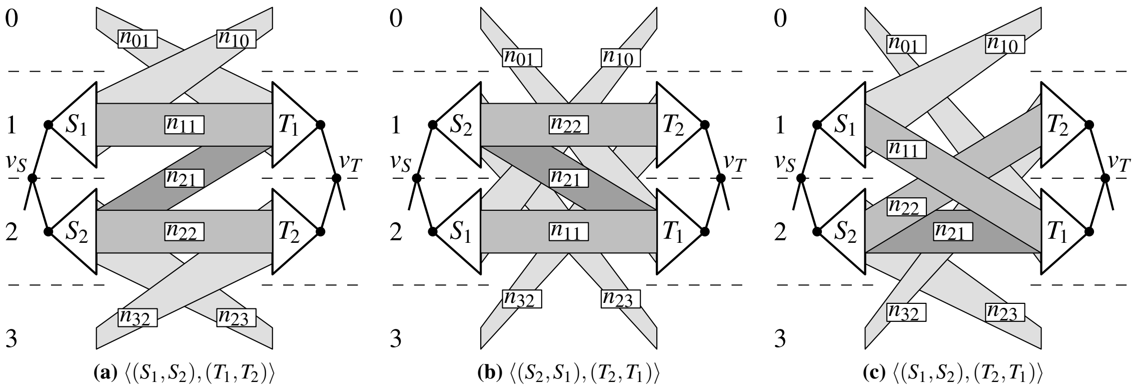
Consider a cut in G that for each inner node u of $\langle S,T\rangle$ separates u and u'. We claim that any such cut encodes a drawing of $\langle S,T\rangle$. To see this, let $(F,N=(V\setminus F))$ be such a cut. Starting from the initial drawing we construct a new drawing as follows. Let u be an inner node of $\langle S,T\rangle$. If $u\in F$ and $u'\in N$, we swap the children of the inner node u of the current drawing. If $u\in N$ and $u'\in F$, we do nothing. (Note that exchanging the roles of the sets F and N yields the mirrored drawing with the same number of crossings.)

For a moment, think of G as of a multigraph that is obtained by replacing each edge of weight k by k edges of weight one. Let us argue that the above described procedure to decode drawings from cuts has the property that in the resulting drawing of $\langle S,T\rangle$, pairs of inter-tree edges that do not cross correspond one-to-one to edges in G that are cut by (F,N). Consider first the cut corresponding to the initial drawing, namely the cut with $u\in N$ for each inner node u of $\langle S,T\rangle$ and observe that the claim holds for this cut. Now consider a single swap operation at an inner node u of $\langle S,T\rangle$ and the corresponding change in the cut. Note that it changes the "cut status" of exactly those pairs of edges that have u as the lowest common ancestor of two of their endpoints; at the same time it also changes the cut status of exactly the edges in G corresponding to these pairs of edges in the drawing. Since any cut in G may be reached by a finite sequence of such swap operations from the initial one, the property holds for any cut. Therefore, the number of pairs of non-crossing inter-tree edges in the obtained drawing equals the total weight of the cut (in the original, weighted version of G).

The resulting optimization problem is the MAXRESCUT problem, that is, MAXCUT with additional constraints forcing certain pairs of vertices to be separated by the cut. Goemans and Williamson [15], when describing their famous algorithm for the MAXCUT problem, observed that adding constraints to separate certain pairs of vertices does not make the problem harder to approximate. It is sufficient to encode these constraints as additional linear constraints in the SDP relaxation and to observe that random hyperplanes used to separate vertices always separate such constrained pairs.

We use their SDP rounding algorithm for MAXRESCUT to compute a 0.878-approximation of the largest cut in G. This cut determines which of the subtrees in the initial drawing must be swapped to obtain a drawing that is a 0.878-approximation to binary TL*. □

Note that our proof also works in a slightly more general case, namely for pairs of (not necessarily binary) trees where for each inner node the only choice for arranging the children is between a given permutation and the reverse permutation obtained by swapping the whole block of children.



(a) $\langle(S_1,S_2),(T_1,T_2)\rangle$ **(b)** $\langle(S_2,S_1),(T_2,T_1)\rangle$ **(c)** $\langle(S_1,S_2),(T_2,T_1)\rangle$

Fig. 11: Edge types and crossings of the instance $\langle S,T\rangle$. Only non-empty classes of edge types are shown.

4 Fixed-Parameter Tractability

We consider the following parameterized variant of the complete binary TL problem. Given a complete binary TL instance $\langle S,T\rangle$ and a non-negative integer k, decide whether there exists a layout of S and T with at most k induced inter-tree edge crossings. Our algorithm makes use of the same technique to count current-level crossings as the 2-approximation algorithm. Hence, we precompute the crossing tables $C^=$ and $C^\times$ in $O(n^2)$ time as before, see Lemma 3.1. The algorithm traverses the inner nodes of S in breadth-first order. It starts at the root of S and its corresponding node in T (in this case the root of T), branches into all four possible subtree configurations (at the root it actually suffices to consider two of them), and subtracts from k the number of current-level crossings in each branch. Then we proceed recursively with the next node v in S, its corresponding opposite node w in T, and the reduced parameter k' of allowed crossings. In each node of the search tree we count the current-level crossings for each of the subtree orders of v and w by summing up in linear time the appropriate entries in $C^=$ and $C^\times$ for v (or w) and all of the $O(n)$ subtree orders that are already fixed in T (or S). Once we reach a leaf of the search tree we know the exact number of crossings since each pair of edges ab and cd is counted as soon as the subtree orders of both $\mathrm{lca}(a,c)$ and $\mathrm{lca}(b,d)$ are fixed. Obviously, we stop following a branch of the search tree when the parameter value drops below 0.

For the search tree to have bounded height, we need to ensure that whenever we move to the next subinstance, the parameter value decreases at least by one. At first sight this seems problematic: if a subinstance does not incur any current-level crossings, the parameter will not drop. The following key lemma—which does not hold for non-complete binary trees—shows that there is a way out. It says that if there is an order of the subtrees in a subinstance that does not incur any current-level crossings, then we can ignore the other three subtree orders and do not have to branch.

Lemma 4.1 *Let $\langle S,T\rangle$ be a complete binary TL instance, and let v_S be a node of S and v_T a node of T such that v_S and v_T have the same distance to their respective root. Further, let (S_1,S_2) be the subtrees incident to v_S and let (T_1,T_2) be the subtrees incident to v_T. If the subinstance $\langle(S_1,S_2),(T_1,T_2)\rangle$ does not incur any current-level crossings, then each of the subinstances $\langle(S_1,S_2),(T_2,T_1)\rangle$, $\langle(S_2,S_1),(T_1,T_2)\rangle$, and $\langle(S_2,S_1),(T_2,T_1)\rangle$ has at least as many crossings as $\langle(S_1,S_2),(T_1,T_2)\rangle$, for any fixed ordering of the leaves of S_1, S_2, T_1 and T_2.*

Proof If the subinstance $\langle(S_1,S_2),(T_1,T_2)\rangle$ does not incur any current-level crossings, this excludes certain types of edges. We categorize the inter-tree edges originating from the four subtrees according to their destinations as before, and use the notation n_{ij} for the number of edges between area i on the left and area j on the right—see Fig. 11a. First of all, there are no edges between S_1 and T_2 or between S_2 and T_1. We consider only the first case, that is, $n_{12}=0$; the second case $n_{21}=0$ is symmetric. In both cases, we have $n_{13}=n_{31}=n_{20}=n_{02}=0$. Since we consider complete binary trees, we obtain the three equalities $n_{10}=n_{01}+n_{21}$, $n_{32}=n_{23}+n_{21}$, and $n_{01}+n_{11}=n_{23}+n_{22}$.

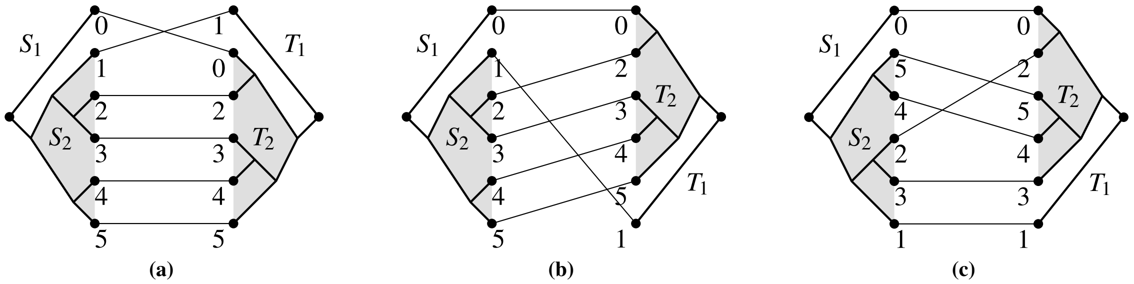


Fig. 12: Example of a binary TL instance with an optimal layout that has one crossing (a). The same order of the leaves in the subtrees S_2 and T_2 yields four crossings for a configuration without current-level crossings (b). The best layout that avoids the current-level crossing still has two crossings (c).

We fix an ordering σ of the leaves of the four subtrees S_1, S_2, T_1, and T_2. We first compare the number of crossings in the subinstance $\langle (S_1,S_2),(T_1,T_2)\rangle$ with the number of crossings in the subinstance $\langle (S_2,S_1),(T_2,T_1)\rangle$, see Figures 11a and 11b. The subinstance $\langle (S_1,S_2),(T_1,T_2)\rangle$ can have at most $n_{21}(n_{11}+n_{22})$ crossings that do not occur in $\langle (S_2,S_1),(T_2,T_1)\rangle$. However, $\langle (S_2,S_1),(T_2,T_1)\rangle$ has at least $n_{10}(n_{23}+n_{21}+n_{22})+n_{23}n_{11}+n_{32}(n_{01}+n_{21}+n_{11})+n_{01}n_{22}$ crossings that do not appear in $\langle (S_1,S_2),(T_1,T_2)\rangle$. Plugging in the above equalities for n_{10} and n_{32}, we get $(n_{01}+n_{21})(n_{23}+n_{21}+n_{22})+n_{23}n_{11}+(n_{23}+n_{21})(n_{01}+n_{21}+n_{11})+n_{01}n_{22} \geq n_{21}(n_{11}+n_{22})$. Thus, the subinstance $\langle (S_2,S_1),(T_2,T_1)\rangle$ has at least as many crossings with respect to the fixed leaf order σ as $\langle (S_1,S_2),(T_1,T_2)\rangle$ has.

Next, we compare the number of crossings in the subinstance $\langle (S_1,S_2),(T_1,T_2)\rangle$ with the number of crossings in the subinstance $\langle (S_1,S_2),(T_2,T_1)\rangle$, see Figures 11a and 11c. Now the number of additional crossings of $\langle (S_1,S_2),(T_1,T_2)\rangle$ is at most $n_{21}n_{22}$, and the subinstance $\langle (S_1,S_2),(T_2,T_1)\rangle$ introduces at least $(n_{01}+n_{11})(n_{32}+n_{22})+n_{32}n_{21}$ additional crossings. With the equality $n_{01}+n_{11}=n_{23}+n_{22}$ and the inequality $n_{32}+n_{22}\geq n_{21}$ we get $(n_{01}+n_{11})(n_{32}+n_{22})+n_{32}n_{21}\geq (n_{23}+n_{22}+n_{32})n_{21}\geq n_{22}n_{21}$. Thus, the subinstance $\langle (S_1,S_2),(T_2,T_1)\rangle$ has at least as many crossings with respect to σ as $\langle (S_1,S_2),(T_1,T_2)\rangle$ has.

By symmetry, the same holds for the last case $\langle (S_2,S_1),(T_1,T_2)\rangle$, which incurs at least as many crossings as $n_{11}n_{21}$, the number of crossings that can be present in $\langle (S_1,S_2),(T_1,T_2)\rangle$ but not in $\langle (S_2,S_1),(T_1,T_2)\rangle$.

□

Counting the current-level crossings takes $O(n)$ time for each node that fixes its subtree order. If an order does not incur any current-level crossings we might need to fix in total up to $O(n)$ subtree orders and count the incurred crossings until we reach a new node of the search tree. Thus we spend $O(n^2)$ time for each of the $O(4^k)$ search-tree nodes. Including the preprocessing this yields a total running time of $O(n^2+4^k n^2)$. If the algorithm reaches a leaf of the search tree it has fixed all subtree orders in S and T and thus found a layout of the input instance that has at most k inter-tree edge crossings. If the search stops without reaching a leaf there is no layout of $\langle S,T\rangle$ with at most k inter-tree edge crossings.

Theorem 4.2 *Given a complete binary TL instance $\langle S,T\rangle$ with n leaves in each tree and an integer k, in $O(4^k n^2)$ time we can either determine a layout of $\langle S,T\rangle$ with at most k inter-tree edge crossings or report that no such layout exists.*

Finally, the fact that Lemma 4.1 relies on the completeness of the two trees is illustrated in Fig. 12. Here we have an example of an instance whose optimal layout requires a current-level crossing (Fig. 12a). At the same time, the configuration $\langle (S_1,S_2),(T_2,T_1)\rangle$ has no current-level crossing. According to Lemma 4.1 the leaf order of the optimal layout copied into the layout without current-level crossings would produce at most as many crossings as in the other layout. Figure 12b shows that this is not true in our example. The best solution of the configuration $\langle (S_1,S_2),(T_2,T_1)\rangle$ still has two crossings and is not optimal (Fig. 12c). Hence, we do have to consider *all* subtree orders even if one of them incurs no current-level crossings. This means that we cannot bound the size of the search tree in terms of the parameter k as we have done for complete binary trees.

5 Open Problems

We have shown that one cannot expect to find a constant-factor approximation for binary TL. Would it help if *one* of the two given trees was complete? We have given a factor-2 approximation for complete binary TL. It is natural to ask whether we can do better.

An alternative optimization goal is to remove a minimum number of inter-tree edges in order to obtain a planar tanglegram.

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References

1. M. S. Bansal, W.-C. Chang, O. Eulenstein, and D. Fernández-Baca. Generalized binary tanglegrams: Algorithms and applications. In S. Rajasekaran, editor, *Proc. 1st Internat. Conf. Bioinformatics Comput. Biol. (BICoB'09)*, volume 5462 of *Lecture Notes Comput. Sci.*, pages 114–125. Springer-Verlag, 2009.
2. F. Baumann, C. Buchheim, and F. Liers. Exact bipartite crossing minimization under tree constraints. In P. Festa, editor, *Proc. 9th Internat. Sympos. Experimental Algorithms (SEA'10)*, volume 6049, pages 118–128. Springer-Verlag, 2010.
3. P. Bertolazzi, G. Di Battista, C. Mannino, and R. Tamassia. Optimal upward planarity testing of single-source digraphs. *SIAM J. Comput.*, 27(1):132–169, 1998.
4. S. Böcker, F. Hüffner, A. Truss, and M. Wahlström. A faster fixed-parameter approach to drawing binary tanglegrams. In J. Chen and F. Fomin, editors, *Proc. 4th Internat. Workshop Parameterized and Exact Comput. (IWPEC'09)*, volume 5917 of *Lecture Notes Comput. Sci.*, pages 38–49. Springer-Verlag, 2009.
5. K. Buchin, M. Buchin, J. Byrka, M. Nöllenburg, Y. Okamoto, R. I. Silveira, and A. Wolff. Drawing (complete) binary tanglegrams: Hardness, approximation, fixed-parameter tractability. In I. G. Tollis and M. Patrignani, editors, *Proc. 16th Internat. Symp. Graph Drawing (GD'08)*, volume 5417 of *Lecture Notes Comput. Sci.*, pages 324–335. Springer-Verlag, 2009.
6. S. Burer and R. D. Monteiro. A projected gradient algorithm for solving the Maxcut SDP relaxation. *Optimization Methods and Software*, 15:175–200, 2001.
7. T. H. Cormen, C. E. Leiserson, R. L. Rivest, and C. Stein. *Introduction to Algorithms*. MIT Press, 2nd edition, 2001.
8. B. DasGupta, X. He, T. Jiang, M. Li, J. Tromp, and L. Zhang. On distances between phylogenetic trees. In *Proc. 18th Annu. ACM-SIAM Sympos. Discrete Algorithms (SODA'97)*, pages 427–436, 1997.
9. V. Dujmović, H. Fernau, and M. Kaufmann. Fixed parameter algorithms for one-sided crossing minimization revisited. *J. Discrete Algorithms*, 6(2):313–323, 2008.
10. T. Dwyer and F. Schreiber. Optimal leaf ordering for two and a half dimensional phylogenetic tree visualization. In N. Churcher and C. Churcher, editors, *Proc. Australasian Sympos. Inform. Visual. (InVis.au'04)*, volume 35 of *CRPIT*, pages 109–115. Australian Comput. Soc., 2004.
11. P. Eades and N. Wormald. Edge crossings in drawings of bipartite graphs. *Algorithmica*, 10:379–403, 1994.
12. H. Fernau, M. Kaufmann, and M. Poths. Comparing trees via crossing minimization. In R. Ramanujam and S. Sen, editors, *Proc. 25th Intern. Conf. Found. Softw. Techn. Theoret. Comput. Sci. (FSTTCS'05)*, volume 3821 of *Lecture Notes Comput. Sci.*, pages 457–469. Springer-Verlag, 2005.
13. H. N. Gabow and R. E. Tarjan. A linear-time algorithm for a special case of disjoint set union. In *Proc. 15th Annu. ACM Symp. Theory Comput. (STOC'83)*, pages 246–251, 1983.
14. M. R. Garey and D. S. Johnson. *Computers and Intractability*. W. H. Freeman, 1979.
15. M. X. Goemans and D. P. Williamson. Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming. *J. ACM*, 42(6):1115–1145, 1995.
16. M. S. Hafner, P. D. Sudman, F. X. Villablanca, T. A. Spradling, J. W. Demastes, and S. A. Nadler. Disparate rates of molecular evolution in cospeciating hosts and parasites. *Science*, 265:1087–1090, 1994.
17. D. Holten and J. J. van Wijk. Visual comparison of hierarchically organized data. In *Proc. 10th Eurographics/IEEE-VGTC Sympos. Visualization (EuroVis'08)*, pages 759–766, 2008.
18. S. Khot. On the power of unique 2-prover 1-round games. In *Proc. 34th Annu. ACM Sympos. Theory Comput. (STOC'02)*, pages 767–775, 2002.
19. S. Khot and N. K. Vishnoi. The unique games conjecture, integrality gap for cut problems and embeddability of negative type metrics into l_1. In *Proc. 46th Annu. IEEE Sympos. Foundat. Comput. Sci. (FOCS'05)*, pages 53–62, 2005.
20. A. Lozano, R. Y. Pinter, O. Rokhlenko, G. Valiente, and M. Ziv-Ukelson. Seeded tree alignment and planar tanglegram layout. In R. Giancarlo and S. Hannenhalli, editors, *Proc. 7th Internat. Workshop Algorithms Bioinformatics (WABI'07)*, volume 4645 of *Lecture Notes Comput. Sci.*, pages 98–110. Springer-Verlag, 2007.

21. H. Nagamochi. An improved bound on the one-sided minimum crossing number in two-layered drawings. *Discrete Comput. Geom.*, 33(4):565–591, 2005.
22. M. Nöllenburg, M. Völker, A. Wolff, and D. Holten. Drawing binary tanglegrams: An experimental evaluation. In *Proc. 11th Workshop Algorithm Engineering and Experiments (ALENEX'09)*, pages 106–119. SIAM, 2009.
23. R. D. M. Page, editor. *Tangled Trees: Phylogeny, Cospeciation, and Coevolution*. University of Chicago Press, 2002.
24. V. Raman, B. Ravikumar, and S. S. Rao. A simplified NP-complete MAXSAT problem. *Inform. Process. Lett.*, 65:1–6, 1998.
25. K. Sugiyama, S. Tagawa, and M. Toda. Methods for visual understanding of hierarchical system structures. *IEEE Trans. Syst. Man Cybern.*, 11(2):109–125, 1981.
26. B. Venkatachalam, J. Apple, K. St. John, and D. Gusfield. Untangling tanglegrams: Comparing trees by their drawings. *IEEE/ACM Trans. Comput. Biol. Bioinf.*, PrePrints, 2010. (doi: 10.1109/TCBB.2010.57)