Lower bound for the cost of connecting tree with
given vertex degree sequence

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Abstract

The optimal connecting network problem generalizes many models of
structure optimization known from the literature, including communica-
tion and transport network topology design, graph cut and graph clus-
tering, structure identification from data, etc. For the case of connecting
trees with the given sequence of vertex degrees the cost of the optimal
tree is shown to be bounded from below by the solution of a semidefinite
optimization program with bilinear matrix constraints, which is reduced
to the solution of a series of convex programs with linear matrix inequality
constraints. The proposed lower bound estimate is used to construct
several heuristic algorithms and to evaluate their quality on a variety of
generated and real-life data sets. Optimal communication network, gen-
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1 Introduction

The shortcut network is used below for a simple connected undirected graph
with labeled vertices. So, networks with different labeling are considered dis-
tinct.

Let us consider the fixed set of terminals \( V = \{1, ..., n\} \) indexed from 1 to \( n \)
and denote a collection of networks over vertex set \( V \) with \( \Omega(V) \). Let us assume
we are given a symmetric non-negative flow matrix \( A = (\mu_{ij})_{i,j=1}^{n} \) (where \( \mu_{ij} \) is
an informational or material flow between the $i$-th and the $j$-th terminal, and set of admissible networks $\Omega \subseteq \Omega(V)$ (e.g., the set of all trees or of all bipartite graphs of order $n$, etc.).

The optimal connecting network (OCN) problem is that of finding an admissible network $G^* \in \Omega$ with the minimum weighted average distance between vertex pairs. In the other words, network $G^* \in \Omega$ is a solution of OCN problem if and only if $C_A(G^*) \leq C_A(G)$ for all $G \in \Omega$, where

$$C_A(G) := \sum_{\{i,j\} \subset V} \mu_{ij} d_G(i,j) = \frac{1}{2} \text{tr} D(G)A.$$  \hspace{1cm} (1)

Here $d_G(i,j)$ is distance between the $i$-th and the $j$-th vertices in graph $G$, and $D(G) = (d_G(i,j))_{i,j=1}^n$ is the distance matrix of graph $G \in \Omega$.

This framework, being simplistic at the first glance, however, has many classical problems of combinatorial optimization as special cases. Considering specific flow matrices, sets of admissible networks, and specifying a concrete notion of graph distance (the shortest-path distance, the resistance distance, or some weighted distance) one can obtain a quadratic assignment problem (QAP), a graph cut or clustering problem, or a sort of a problem of structure identification from data (see examples in Section 2).

In this article we study a special case of OCN problem, which encapsulates the essence of many difficulties that arise in OCN search. We consider the admissible set, which contains all trees with the given sequence of vertex degrees, and the (most popular) concept of the shortest-path graph distance.

If flow matrix $A$ has rank one, i.e., it can be represented as an outer product $A = \mu \mu^\top$, where $\mu$ is some non-negative sequence of vertex weights, cost function (1) reduces to the weighted Wiener index $W_I\mu(G) = \mu^\top D(G)\mu$ and OCN problem reduces to the recently solved problem of the Wiener index optimization over the set of trees with given vertex weight and degree sequences. In [17] the optimal tree is efficiently constructed with a modification of the famous Huffman algorithm for the optimal prefix code [24].

Below we approximate the general flow matrix $A$ by a rank-one matrix obtaining a lower-bound estimate for the optimal connecting tree cost. Calculation of the estimate reduces to the non-convex semidefinite program. We solve it iteratively through a series of constrained convex semidefinite programs effectively calculated with standard optimization tools (we used CVX package with SeDuMi solver). It takes reasonable time to calculate the estimate on a PC for trees with several hundreds of vertices.

The quality of the lower bound is evaluated on a number of generated flow matrices with dimension from 10 to 1000 and on the selected real-life origin-destination matrices with dimension varying from 12 to 300. High quality of the lower bound is verified in many practical cases, although in general the quality crucially depends on how accurately matrix $A$ can be approximated by a rank-one matrix.
2 Literature

2.1 Quadratic assignment problems

OCN problem is closely related to many structure optimization problems studied in the literature. If all networks in the set $Ω$ of admissible networks are isomorphic and differ only in the vertex labeling, the solution of OCN reduces to the assignment of terminals to network vertices, and we obtain a classical Koopmans-Beckmann’s quadratic assignment problem (QAP) \[28\]

$$\min_{\pi} \sum_{i,j=1}^{n} \mu_{ij} d_{\pi(i)\pi(j)}, \text{ where } \pi \text{ is a permutation of } 1, ..., n.$$ QAP is well-known as one of the most difficult problems of combinatorial optimization \[7, 30, 6\]. It has many unsolved instances of the dimension less than a hundred and does not have lower bounds of guaranteed quality.

2.2 Graph partitioning

If, in addition, the considered topology is a balanced tree of diameter 4 with $K + 1$ internal vertices and only flows between tree leaves are allowed, the model is equivalent to the optimal graph $K$-partitioning problem. If function $\pi(i)$ assigns a cluster number $1, ..., K$ to $i$-th terminal $i = 1, ..., n$, then the cost function reduces to

$$C_A(\cdot) = \sum_{k=1}^{K} \sum_{i: \pi(i) = k} \left[ 2 \sum_{j: \pi(j) \neq k} \mu_{ij} + \sum_{j: \pi(j) = k} \mu_{ij} \right] =$$

$$= \sum_{k=1}^{K} \sum_{i \in s_k} \sum_{j \notin s_k} \mu_{ij} + \text{const} = \text{Cut}(s_1, ..., s_K),$$

where $s_k := \{i : \pi(i) = k\}$. In a similar fashion, balanced graph cut problems \[23\] are obtained as a very special case of OCN.

Although the set of trees with the given sequence of vertex degrees includes the admissible sets of graph partitioning and balanced cut problems (and even of the QAP over the tree topology), the framework studied in this article is not completely equivalent to the above problems.

The wider set does not necessary results in the more complex problem (e.g., the complete graph is an obvious solution of the OCN over the set of all graphs of the fixed order). On the other hand, the problem studied in the present article can be seen as a variation of the balanced hierarchical clusterization problem, when not only terminals have to be optimally grouped into clusters, but clusters should also be rationally arranged into a hierarchy.

Business process decomposition and work breakdown structure (WBS) construction problems are among possible applications. In many classic notations
(IDEF, Aris, BPMN, UML Activity Diagrams, Event Process Chains, and others) a business process in an organization is represented as a directed graph where vertices are elementary operations (activities) and arcs are labeled with material or information flows between activities. In the same manner, vertices in a project schedule network are project operations (works), while arcs represent precedence relations between them.

A complex business process (or a project schedule) may have many thousands elementary activities. To simplify its representation and analysis, the activities are arranged in a hierarchy of diagrams so that only the limited number (typically, from 5 to 7) of activities along with their internal and external flows are combined in a single diagram (see Figure 1) hiding the complexity inside sub-diagrams.

![Hierarchical decomposition of the business process](image)

Figure 1: Hierarchical decomposition of the business process

During the business analysis most closely connected activities (those having the maximum number of connecting flows or the maximum flow volume between them) are located in a single diagram and are grouped together into a corresponding combined activity. Then combined activities are grouped again at a higher level of decomposition tree taking into account flows that connect them. It is commonly recognized that such “rational” decomposition reveals the information about internal structure of processes in an organization. In particular, business process partitioning is used to identify services in SOA (service-oriented architecture).

When a flow connects activities in different diagrams, it is depicted as an external flow both in the source and in the destination diagrams. This flow is also copied as external in all higher-level diagrams until the common parent diagram where it is depicted as an internal flow (see Figure 1).

Let the flow matrix $A$ be the adjacency matrix of the flow graph where the direction of arcs is ignored, and the tree-shaped network $G$ coincide with the process decomposition hierarchy. Then the total number of flows in all
diagrams (counting for flow copies in different diagrams) is given by expression (1), and rational business process decomposition reduces to OCN over the set of hierarchies (trees) with a limited maximum vertex degree (typically, it varies from 6 to 8).

### 2.3 Wiener index

If $A$ is an all-ones matrix and $d_G(\cdot, \cdot)$ is the (edge) distance in graph $G$, then $C_A(G)$ in (1) reduces to the sum of distances in graph $G$, also known as the Wiener index, the one of the earliest and most popular topological graph invariants widely used in mathematical chemistry and network analysis as the measure of graph compactness. Compact connected graphs have the small value of the Wiener index while more scattered graphs have the larger index value. If $A = \mu \mu^T$, where $\mu = (\mu_1, \ldots, \mu_n)$ is a positive sequence of vertex weights, $C_A(\cdot)$ becomes a variant of the Wiener index for vertex-weighted graphs [27].

Mathematical properties of the Wiener index and its extensions are studied for decades by graph theorists (see the surveys in [11, 12, 1, 21, 20]). Also, they also employed by many applications including mathematical chemistry [22], analysis of social [16, 32] and communication [5, 25] networks.

Studies of extremal problems [33] is a valuable part the literature on the Wiener index. In particular, Fischermann et al. [15] have shown a sort of balanced trees (aka Volkmann trees) to minimize the Wiener index over the set of trees with the limited maximum vertex degree. The problem of Wiener index minimization over the set of trees with the given degree sequence was independently solved by [36, 35] and the optimal tree was characterized, being known as greedy tree in [35], and also as the breadth-first-search (BFS) tree in [36]. Later these results were extended to the Wiener index for vertex-weighted graphs. It has been shown in [17, 18] that the, so-called, generalized Huffman tree minimizes the Wiener index over the set of trees with given vertex weight and degree sequences. The present article is the further extension of these results. Although no efficient exact solution is proposed for the general flow matrix $A$, the cost of the generalized Huffman tree for the conveniently chosen vertex weights gives the lower bound of the cost of the optimal tree. Vertex weights corresponding to the best lower bound are calculated from a non-convex optimization problem. They are also used in the heuristic algorithm to efficiently construct a nearly optimal tree.

### 2.4 Structure learning

Another closely connected strand of the literature is learning the graph structure from data. In the basic setting some signals (time series) are collected at the vertices of an unknown graph and the problem is to elicit the edges (weighted, in general), of the graph using correlation of signals in its vertices as a clue. Typically, the lower the distance between signals is, the closer they should be located in a graph.
Let \( X = (x^{(1)}, ..., x^{(n)})^\top \) be an \( m \times n \) matrix, where \( x^{(i)} \) is an \( m \)-dimensional row representing the signal located in vertex \( i = 1, ..., n \) of an unknown graph \( G = (V, E) \) with edge weights \( w_{ij}, ij \in E \).

The search of the graph, in which \( i \)-th and \( j \)-th vertices are connected when the distance \( ||x^{(i)} - x^{(j)}|| \) between the corresponding signals is small, is often (see \[26, 14\] and the references therein) reduced to the minimization of the function

\[
\frac{1}{2} \sum_{i,j=1}^{n} w_{ij} ||x^{(i)} - x^{(j)}|| = \text{tr} X^\top L(G) X = \text{tr} L(G) A, \tag{2}
\]

where \( A := XX^\top \) is the covariance matrix\(^1\) and \( L(G) \) is the Laplacian matrix of graph \( G \):

\[
L_{ij} = \begin{cases} 
-w_{ij} & i \neq j, \\
\sum_k w_{ik} & i = j, \\
0 & \text{otherwise.}
\end{cases}
\]

The set of admissible graphs is additionally constrained to account for the \textit{a priori} information about the target graph (e.g., maximum vertex degree, connectedness, or edge density). Edge weights \( w_{ij} \) are sought in \[26\] while in \[13, 14\] the authors seek for the Laplacian matrix \( L \) further relaxing the admissible set to the set of all positive semidefinite matrices with zero row sums. Regularization terms are added to (2) in \[26, 14\] to obey local connectivity (every vertex must be connected to another vertex in a graph) and obtain the desired graph density.

In the present article a similar problem is solved for the distance matrix on the place of the graph Laplace matrix in (2). Although both criteria \[1, 2\] promote construction of the graph by connecting vertices with highly correlated signals, their mathematical properties are different. OCN is not directly reduced to the continuous (and even complex) optimization problem as in \[13, 26, 14\]. Instead we construct a lower bound estimate using the OCN with the rank-one flow matrix, for which an exact solution is known.

### 3 Weighted Wiener index

As noted in Section \[2, 1\] the general OCN is strongly NP-complete. At the same time, efficient algorithms are known for special cases. For example, as soon as the complete graph is admissible, it is an obvious solution of OCN problem.

The case of the flow matrix of rank one also appears computationally tractable. If \( A = \mu \mu^\top \), where \( \mu_i \geq 0 \) is a weight of terminal \( i = 1, ..., n \), then \( C_A(T) \) reduces to the vertex-weighted Wiener index \( WI_\mu(T) = \mu^\top D(T) \mu \), for which an optimal connecting tree for a given vertex degree sequence is effectively built by the generalized Huffman algorithm \[17\].

Below in this section we provide basic notation and definitions, and also introduce the generalized Huffman algorithm, which is extensively used below.

\(^1\)It plays the role of the flow matrix in these applications, so we use the same notation.
Let $d_G(v)$ be the degree of vertex $v \in V$ in network $G \in \Omega(V)$. Vertex degree sequence of network $G$ is a vector $d_G = (d_G(i))_{i=1}^n$. Vertex $v \in V$ is called pendent if $d_G(v) = 1$ and is called internal otherwise.

**Definition 1** Connected network $T \in \Omega(V)$ is called a tree if $\sum_{i=1}^n d_T(i) = 2(n - 1)$. The collection of trees over vertex set $V$ is denoted with $\mathcal{T}(V)$. 

**Definition 2** Natural sequence $d = (d_1, ..., d_n)$ is called generating if $\sum_{i=1}^n d_i = 2(n - 1)$. Let $\mathcal{T}(d) := \{T \in \mathcal{T}(V) : d_T = d\}$ denote the collection of trees with degree sequence $d$.

Let $K_{W,M}$ be the complete bipartite network over vertex subsets $W$ and $M$, i.e., $K_{W,M}$ has vertex set $W \cup M$ and edge set $W \times M$.

For a fixed weight sequence $\mu \in \mathbb{R}^n_{+}$ and generating degree sequence $d$ the generalized Huffman algorithm [18] builds a tree $H \in \mathcal{T}(d)$ as shown in Listing 1.

**Listing 1** Build a Huffman tree for weight sequence $\mu$ and degree sequence $d$

1: function HUFFMANTREE($\mu$, $d$) 
2: $V := \{1, ..., n\}$ \Comment{Vertex set: sequences $\mu$ and $d$ are assumed to have $n$ components} 
3: $W := \{i \in V : d_i = 1\}$ \Comment{Index set for vacant pendent vertices} 
4: $M := V \setminus W$ \Comment{Index set for vacant internal vertices} 
5: $H = \langle V, \emptyset \rangle$ \Comment{Start with empty network over vertex set $V$.} 
6: for $i = 1$ to $q - 1$ do 
7: Choose any $m \in \arg \min \{d_u | u \in \argin M \mu_u\}$ \Comment{$m$ has the least degree among vertices} 
8: \Comment{$m$ has the least weight in $M$.} 
9: for $j = 1$ to $d_m - 1$ do 
10: Choose any $w_j \in \arg \min \mu_w$ 
11: $W := W \setminus \{w_j\}$ 
12: $\mu_m := \mu_m + \mu_{w_j}$ 
13: end for \Comment{Pick the vertices $w_1, ..., w_{d_m-1}$ that have $d_m - 1$ least weights in $W$.} 
14: $H := H \cup \{w_1m\} \cup ... \cup \{w_{d_m-1}m\}$. \Comment{Add edges $\{w_1m\},...,\{w_{d_m-1}m\}$ to network $H$} 
15: $M := M \setminus \{m\}$, $W = W \cup \{m\}$ \Comment{Move $m$ to index set $W$ of vacant pendent vertices} 
16: end for 
17: $H = H \cup K_{W,M}$ \Comment{Finish the Huffman tree by adding the star $K_{W,M}$} 
18: return $H$ \Comment{By construction, at this moment $|M| = 1$, and $d_m = |W|$, where $\{m\} = M$} 
19: end function

**Note 1** Like the “classic” Huffman algorithm, this algorithm requires $\mathcal{O}(n \ln n)$ operations, and, so, is highly efficient.
Figure 2: Huffman tree (a) not isomorphic to the greedy tree (b)

**Note 2** Some freedom of choice is allowed at lines 7 and 10 of the algorithm, so, several distinct Huffman trees are possible, all sharing the same value of $WI_{\mu}(\cdot)$. Let $H(\mu, d)$ be the collection of Huffman trees for weight sequence $\mu$ and degree sequence $d$.

**Definition 3** Weights $\mu$ are **monotone** in degrees $d$ if for all $i, j \in V$ from $1 < d_i < d_j$ it follows that $\mu_i \leq \mu_j$.

**Theorem 1** [17, 18] If weights $\mu$ are monotone in degrees $d$ and tree $T$ minimizes $WI_{\mu}(T)$ over $T(d)$, then $T \in H(\mu, d)$ (i.e., $T$ is a Huffman tree).

**Note 3** Huffman tree can be built for any weight sequence $\mu$ but Theorem 1 may fail if weights are not monotone in degrees.

**Note 4** Only weights of internal vertices must be monotone in degrees in Theorem 1. Assume that, in addition, weights of pendent vertices are required to not exceed those of internal vertices in $\mu$. Then, as shown in [17], all optimal trees for the degree sequence $d$ are isomorphic to the greedy tree (see Section 2.3 for details). But, in general, Huffman trees may have diverse topology. For example, Huffman tree for weight sequence $(1, 1, 2, 4, 8, 16, 32, 0, 0, 0, 0, 0)$ and degree sequence $(1, 1, 1, 1, 1, 1, 3, 3, 3, 3, 3)$ shown in Figure 2(a) is not isomorphic to the corresponding greedy tree shown in Figure 2(b).

## 4 Lower bound of optimal connecting tree cost

In this article we study the following optimal connecting tree problem:

$$\min_{T \in T(d)} C_A(T) = \min_{T \in T(d)} \text{tr } D(T)A$$

for given non-negative symmetric flow matrix $A$ and generating sequence $d = (d_1, ..., d_n)$ of vertex degrees, and in this section a closed-form expression is

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2We omit here the technical assumption $\mu_i > 0 \iff d_i = 1$ imposed in [18] to simplify the proofs.
derived for the lower bound estimate of the optimal tree cost. The main idea is to approximate flow matrix $A$ by the sum of some non-negative rank-one matrix and a diagonal matrix. The latter plays a role similar to that of the diagonal perturbation in [34] and improves the quality of approximation.

Let us denote $n \times n$ all-ones matrix with $J$ and define matrix $P(T) := \frac{n-1}{2} J - D(T)$. It is shown in [2] that $P(T)$ is positive semidefinite for any tree $T$ of order $n$.

Theorem 2 If real vector $\alpha \in \mathbb{R}^n$ and non-negative vector $\mu \in \mathbb{R}^n_+$ are chosen such that weights $\mu$ are monotone in degrees $d$ and matrix $\text{diag}(\alpha) + \mu \mu^\top - A$ is positive semidefinite, then for any tree $T \in T(d)$

$$C_A(T) \geq LB(\alpha, \mu) := \frac{n-1}{2} \sum_{i,j=1}^n \mu_{ij} - \left( \frac{n-1}{2} \sum_{i=1}^n \alpha_i + \frac{n}{2} \mu^\top P(H(\mu)) \mu \right), \quad (4)$$

where $H(\mu) \in \mathcal{H}(\mu, d)$ is a Huffman tree for weight sequence $\mu$. In other words, $LB(\alpha, \mu)$ is the lower bound estimate for the problem (3).

Proof Since matrices $P(T)$ and $\text{diag}(\alpha) + \mu \mu^\top - A$ are positive semidefinite and diagonal elements of $P(T)$ are equal to $\frac{n-1}{2}$,

$$C_A(T) = \text{tr} D(T) A = \frac{n-1}{2} \sum_{i,j=1}^n \mu_{ij} - \text{tr} P(T) A \geq \frac{n-1}{2} \sum_{i,j=1}^n \mu_{ij} - \frac{n-1}{2} \sum_{i=1}^n \alpha_i - \mu^\top P(T) \mu =$$

$$= \frac{n-1}{2} \sum_{i,j=1}^n (\mu_{ij} - \mu_i \mu_j) - \frac{n-1}{2} \sum_{i=1}^n \alpha_i + 2W_I \mu(T). \quad (5)$$

From Theorem [1] we know that $W_I \mu(T) \geq W_I \mu(H(\mu))$. Hence,

$$C_A(T) \geq \frac{n-1}{2} \sum_{i,j=1}^n (\mu_{ij} - \mu_i \mu_j) - \frac{n-1}{2} \sum_{i=1}^n \alpha_i + 2W_I \mu(H(\mu)) =$$

$$= \frac{n-1}{2} \sum_{i,j=1}^n \mu_{ij} - \left( \frac{n-1}{2} \sum_{i=1}^n \alpha_i + \mu^\top P(H(\mu)) \mu \right). \quad (6)$$

This completes the proof.

5 Calculation of Lower bound

Inequality (4) is valid for any combination of vectors $\alpha$ and $\mu$ that satisfy conditions of Theorem [2]. Generally, we are interested in the best (i.e., the largest)
lower bound, which can be found by maximizing $LB(\alpha, \mu)$ over all admissible combinations of $\alpha$ and $\mu$. In this section we characterize the corresponding optimization problem, discuss its algorithmic aspects and propose the optimization algorithm.

Taking into account Expression (4), this problem is equivalent to the minimization of the function

$$\mu^\top P(H(\mu))\mu + \frac{n-1}{2} \sum_{i=1}^{n} \alpha_i.$$  \hspace{1cm} (7)

Since $\mu^\top P(G)\mu = \text{const} - 2WI_\mu(G)$ for fixed $\mu$ and any $G \in \Omega(V)$, from Theorem 1 we know that

$$\mu^\top P(H(\mu))\mu = \max_{T \in T(d)} \mu^\top P(T)\mu,$$  \hspace{1cm} (8)

and, so, function (7) is convex as an upper boundary of a family of convex functions.

Finally, the best lower bound can be calculated from the minimization of a linear function

$$\min_{\alpha, \mu, \varphi} [\varphi + \frac{n-1}{2} \sum_{i=1}^{n} \alpha_i]$$  \hspace{1cm} (9)

under the bilinear matrix inequality (BMI) constraint\footnote{Notation $B \succeq 0$ means that matrix $B$ is positive semidefinite.}

$$\text{diag}(\alpha) + \mu\mu^\top - A \succeq 0$$  \hspace{1cm} (10)

and convex constraints

$$\mu_i \geq 0, \ i = 1, ..., n,$$  \hspace{1cm} (11)

$$\varphi \geq \mu^\top P(H)\mu \text{ for all } H \in \mathcal{H},$$  \hspace{1cm} (12)

$$\mu_j \geq \mu_i \text{ for all } i, j : d_j - d_i = 1, d_i > 1,$$  \hspace{1cm} (13)

where $\mathcal{H} = \bigcup_d \mathcal{H}(\mu, d)$ is the collection of Huffman trees for vertex degree sequence $d$ and all monotone weight sequences.

The number of trees in $\mathcal{H}$ is finite but large enough for the problem to become intractable. At the same time, only the small number of inequalities in (12) are active (i.e., make an equality at the optimal point), which makes constraint generation a promising idea.

Constraint generation is an approach to optimization problems with a large number of constraints \footnote{In our case it involves two steps that run in a cycle. At the first step of iteration $t$ a relaxed problem (9) containing only a subset $\mathcal{H}_t \subset \mathcal{H}$ of the constraints in (12) is solved. Then, at the second step, a special separation procedure adds inequalities that are violated by the relaxed solution $\alpha(t), \mu(t), \varphi(t)$ forming the set of constraints $\mathcal{H}_{t+1}$ for the next iteration. The process is iterated until no violated inequality is found (and, thus, $\mathcal{H}_t = \mathcal{H}_{t+1}$).}. In our case it involves two steps that run in a cycle. At the first step of iteration $t$ a relaxed problem (9) containing only a subset $\mathcal{H}_t \subset \mathcal{H}$ of the constraints in (12) is solved. Then, at the second step, a special separation procedure adds inequalities that are violated by the relaxed solution $\alpha(t), \mu(t), \varphi(t)$ forming the set of constraints $\mathcal{H}_{t+1}$ for the next iteration. The process is iterated until no violated inequality is found (and, thus, $\mathcal{H}_t = \mathcal{H}_{t+1}$).
It is clear that if $\alpha(t), \mu(t), \varphi(t)$ is an optimal solution of the relaxed problem \((9)\) for some constraint subset $H_t \subset H$, and Huffman tree $H(\mu(t))$ for weight sequence $\mu(t)$ belongs to the set $H_t$, then $\varphi(t) \geq \mu(t)^\top H\mu(t)$ for any $H \in H_t$, i.e., the relaxed solution is also the optimal solution of problem \((9)\) with the complete constraint set $H$. On the contrary, if $H(\mu(t)) \notin H_t$, the relaxed solution cannot be the optimal solution for the complete constraint set. Therefore, in our case the separation procedure just adds the tree $H(\mu(t))$ to the constraint set $H_t$.

For the first iteration we take the constraint set $H_1 = \{H\}$ containing only Huffman tree $H \in H(1, d)$ for all-ones weight sequence $1$ (aka BFS-tree \[36]\) aka greedy tree \[35]\). Greedy tree is a good starting point because in Section \[7\] it is shown that for large random flow matrices it is almost always optimal. Numeric experiments also show that typically just a few constraint generation iterations are enough to converge.

Unfortunately, even for the limited constraint set problem \((9)\) is not trivial, because BMI constraint \((10)\) bounds a non-convex region due to the bilinear term $\mu\mu^\top$ (mathematical properties of this region are summarized in Appendix). At the same time, this BMI can be linearized with respect to $\mu$ in the neighborhood of any point $\nu$ as follows. Inequality \((10)\) is equivalent to

$$\text{diag}(\alpha) + \mu\nu^\top + \nu\mu^\top - \nu\nu^\top - A \succeq 0.$$

Suppressing the last term (which is an always non-negative and positive semidefinite matrix) naturally gives the following linear matrix inequality (LMI) in $\alpha$ and $\mu$:

$$\text{diag}(\alpha) + \mu\nu^\top + \nu\mu^\top - \nu\nu^\top - A \succeq 0, \quad (14)$$

which always bounds a convex region being a subset of the region bounded by BMI \((10)\).

Linearized problem \((9)\) with BMI \((10)\) replaced with LMI \((14)\) is a convex SDP (semidefinite program), which can be conveniently coded using the disciplined programming notation of CVX package for Matlab \[19]\) and efficiently solved by any available SDP solver like SDPT4, SeDuMi, or Gurobi (we use SDPT4, the default solver for CVX shell).

To obtain the solution of the initial problem \((9)\) we combine the majorization-minimization (MM) approach \[29]\) with the alternating directions (AD) method \[4]\) solving in a cycle the linearized problem and adjusting $\mu$ from the solution of the non-linearized problem under fixed $\alpha$, the step, which is explained below.

Let us define symmetric matrix $A_{\alpha} := A - \text{diag}(\alpha)$, and denote its eigenvalues $\lambda_i(A_{\alpha})$ listed in the descending order, and the corresponding eigenvectors $u^{(i)}(A_{\alpha})$, $i = 1, \ldots, n$.

For fixed $\alpha$ BMI \((10)\) is inconsistent whenever $\lambda_2(A_{\alpha}) > 0$ (see Lemma \[4]\) and is satisfied for any $\mu$ whenever $\lambda_1(A_{\alpha}) \leq 0$ (see Lemma \[2]\). Otherwise (see Lemma \[5]\), the region bounded by BMI is an interior of two convex sheets of a two-sheet hyperboloid defined by the inequality

$$\frac{(\mu^\top u^{(1)}(A_{\alpha}))^2}{\lambda_1(A_{\alpha})} \geq 1 - \sum_{i=2}^n \frac{(\mu^\top u^{(i)}(A_{\alpha}))^2}{\lambda_i(A_{\alpha})}. \quad (15)$$
Alternatively the points satisfying (15) are characterized by the following pair (for “+” and for “−”) of inequalities:

\[ \pm \frac{\mu^\top u^{(1)}(A_{\alpha})}{\sqrt{\lambda_1(A_{\alpha})}} \geq \sqrt{1 + \sum_{i=2}^{n} \frac{(\mu^\top u^{(i)}(A_{\alpha}))^2}{|\lambda_i(A_{\alpha})|}}. \]  

(16)

Absolute eigenvalues are used in (16) to emphasize that \( \lambda_i(A_{\alpha}) \leq 0 \) for all \( i = 2, \ldots, n \). With notation

\[ z := \left( 1, \frac{\mu^\top u^{(2)}(A_{\alpha})}{\sqrt{|A_2(A_{\alpha})|}}, \ldots, \frac{\mu^\top u^{(n)}(A_{\alpha})}{\sqrt{|A_n(A_{\alpha})|}} \right)^\top \]  

(17)

conic inequalities (16) can be written in the canonic form

\[ \pm \frac{\mu^\top u^{(1)}(A_{\alpha})}{\sqrt{\lambda_1(A_{\alpha})}} \geq \|z\|_2. \]  

(18)

Therefore, for fixed \( \alpha \), \( \mu \)-adjustment step reduces to the minimization of \( \phi \) with respect to \( \mu \) and \( \phi \) under constraints (11), (12), (13), and (18) (for “+” and for “−”). This pair of conic programs is efficiently coded with CVX and solved using almost any available convex programming tool (CPLEX, SDPT4, SeDuMi, Gurobi, etc.) Finally, the adjusted \( \mu \) is used as a new linearization point at the next iteration of the algorithm.

**Note 5** If \( \lambda_i(A_{\alpha}) = 0 \) for some \( i = 1, \ldots, n \), the corresponding term in conic inequalities (16) is omitted, and the new condition \( \mu^\top u^{(i)}(A_{\alpha}) = 0 \) is added instead.

We need a feasible starting point to begin iterations. Lemma 19 says that for the feasible set to be not empty, \( \alpha \) must be chosen such that \( \lambda_2(A_{\alpha}) \leq 0 \). Therefore, let us choose \( \alpha(0) = \lambda_2(A)1 \), so that \( \lambda_i(A_{\alpha(1)}) = \lambda_i(A) - \lambda_2(A) \). Eigenvectors of matrix \( A_{\alpha(1)} \) coincide with those of matrix \( A \), so, according to Lemma 3, let us choose feasible \( \mu(1) \) := \( \sqrt{\lambda_1(A) - \lambda_2(A)} u^{(1)}(A_{\alpha}) \), which can be used as the first linearization point in (14).

Function MAXIMIZELB that solves problem (9) under constraints (10)-(13) is presented in Listing 2. Combination of MM and AD steps highly improves convergence compared to MM and AD applied separately.

**Note 6** Since the linearized solution is always feasible, \( \mu^* \) and \( \phi^* \) from SOLVE-LINEARIZED can be a starting point in ADJUSTMU for algorithms that require an internal starting point.

**Note 7** Two conic problems are solved in ADJUSTMU, one for “+” sign and the other for “−” sign in (18). However, for instance, cplexqcp utility of CPLEX package solves both in a single run taking inequality (19) as an input.

4Due to nonnegativity and monotonicity constraints (11) and (13) one of these programs is typically inconsistent, which does not make a problem.
Listing 2 Calculate the best parameters for the lower bound $LB(\alpha, \mu)$

1: function MaximizeLB
2: \[ \mathcal{H}_1 := \{ \text{HuffmanTree}(1, d) \} \] ▷ Start from a single constraint in \((12)\)
3: \[ t := 0 \]
4: repeat
5: \[ t := t + 1 \]
6: \[ (\alpha(t), \mu(t), \varphi(t)) := \text{SolveRelaxed}(\mathcal{H}_t) \]
7: \[ H := \text{HuffmanTree}(\mu(t), d) \] ▷ $H$ is a Huffman tree for weight sequence $\mu(t)$
8: \[ \mathcal{H}_{t+1} = \mathcal{H}_t \cup \{ H \} \] ▷ Extend the set of constraints
9: until \[ (\varphi(t) \geq \mu(t)^\top P(H) \mu(t)) \]
10: return \((\alpha(t), \mu(t))\)
11: end function

12: function SolveRelaxed($\mathcal{H}$)
13: \[ t := 0 \]
14: \[ \mu(0) := \sqrt{\lambda_1(A) - \lambda_2(A)\mu(t)}(A) \]
15: \[ t := 0 \]
16: repeat
17: \[ t := t + 1 \]
18: \[ \alpha(t) := \text{SolveLinearized}(\mathcal{H}, \mu(t - 1)) \]
19: \[ (\mu(t), \varphi(t)) := \text{AdjustMu}(\mathcal{H}, \alpha(t)) \]
20: until \[ |\varphi(t - 1) - \varphi(t) + \frac{n-1}{2} \sum_{i=1}^{n} [\alpha_i(t) - \alpha_i(t)]| < \delta \] ▷ Improvement below tolerance
21: return \((\alpha(t), \mu(t), \varphi(t))\)
22: end function

23: function SolveLinearized($\mathcal{H}, \nu$)
24: Find \((\alpha^*, \mu^*, \varphi^*) \in \text{Arg min}_{\alpha, \mu, \varphi} [\varphi + \frac{n-1}{2} \sum_{i=1}^{n} \alpha_i] \) under constraints \([11]-[14]\) ▷ Convex SDP
25: return $\alpha^*$
26: end function

27: function AdjustMu($\mathcal{H}, \alpha$)
28: Find \((\mu^*, \varphi^*) \in \text{Arg min}_{\mu, \varphi} \varphi \) under constraints \([11]-[13], [18]\) ▷ Pair of conic programs
29: return \((\mu^*, \varphi^*)\)
30: end function

Note 8 The algorithm in SolveRelaxed converges, since objective function \([4]\) is bounded, and every iteration improves the solution. Numeric tests in Section 7 show fast convergence in average (less than in a dozen iteration), however, in general, no fast convergence can be guaranteed.

Note 9 To find the best values of the parameters of the lower bound the algorithm solves the non-convex optimization problem. For such problems there is no universal criterion of convergence to the global optimum. At the same time, global optimality is not critical for lower bound evaluation since any admissible
solution of problem (9) with constraints (10)-(13) gives a lower bound.

6 Heuristics

One of applications of the lower bound estimate introduced in Section 4 is performance evaluation of heuristic algorithms that build nearly optimal trees for the given degree sequence. Since any heuristic algorithm gives an upper bound to the optimal tree cost, the gap between the upper and the lower bounds measures the possible performance loss, justifies the price of algorithm improvement, and motivates future research.

Heuristic algorithms may base on different ideas. In this section we describe two algorithms that employ rank-one approximation of the flow matrix and the optimality of Huffman trees.

Approximation of flow matrix $A$ with some matrix $\mu\mu^T$ of rank one results in assigning non-negative weights $\mu_i$, $i = 1,\ldots,n$, to the terminals. It is known that the first principal component of a non-negative symmetric matrix $A$ is its Perron vector $u^{(1)}(A)$. This means that $u^{(1)}(A) = \arg\min_{\mu} \|A - \mu\mu^T\|_2$, so, the Perron vector is the best approximation (in $L_2$ norm) of matrix $A$ by a rank-one matrix. This justifies the choice of weight sequence $u^{(1)}(A)$. By Perron-Frobenius theorem, the Perron vector is positive, so, $u^{(1)}(A)$ is a valid weight sequence, to which the Huffman algorithm can be applied. Although $u^{(1)}(A)$ has not be monotone with respect to degree sequence $d$ and, so, Theorem 1 may not hold, the topology of the Huffman tree is still a good choice for a connecting tree with weight sequence $\mu$. Hence we introduce

$$\text{Heuristics1} := \text{HuffmanTree}(u^{(1)}(A), d).$$

Another low-rank approximation of the flow matrix goes from the lower bound calculation (see the previous section). For $(\cdot, \mu^{[2]}) = \text{MAXIMIZELB}$ let us define

$$\text{Heuristics2} := \text{HuffmanTree}$$

The advantage of Heuristics2 is that weight sequence $\mu^{[2]}$ is always, by construction, monotone with respect to $d$ and, therefore, the Huffman tree is an optimal connecting tree for the approximated flow matrix. We postpone comparative performance analysis of both heuristics to the next section.

7 Numeric simulations

Several numeric tests on generated and real-world data were run to evaluate the quality of the lower bound estimate proposed in Section 4 compared to the quality of two heuristic algorithms introduced in Section 6. The performance is also estimated of the algorithm (see Section 5) for calculation of the best parameter values of the lower bound.
7.1 Random rank-one flow matrices

First we check that the lower bound is tight when flow matrix $A$ has rank one. 100 degree sequences were generated for trees of order from 50 to 250 with degrees of internal vertices uniformly distributed from 2 to 5. For every degree sequence $d$ a monotone random vertex weight sequence $\nu$ was generated such that $\nu_i = \text{rnd}^\beta$, where rnd is a random number uniformly distributed on $[0,1]$, and $\beta \geq 0$ is a diversity factor (for $\beta = 0$ all weights are equal to unity, for $\beta = 1$ we have the uniform distribution of weights, while for large $\beta$ most weights, except some outliers, are close to zero).

The flow matrix $A$ was set to $\nu^\top - \text{diag}(\nu_1^2, \ldots, \nu_n^2)$ (diagonal entries of flow matrix are equal to zero). For all cases MAXIMIZELB was called to find the best parameters of the lower bound. Two upper bounds and the corresponding nearly optimal trees $H_1 := \text{HEURISTICS}1$ and $H_2 := \text{HEURISTICS}2$ were obtained along with the breadth-first-search tree $BFS := \text{HUFFMAN TREE}(1, d)$. The “best found tree” was selected as $H^* = \text{Arg min}_{H \in \{H_1, H_2, BFS\}} C_A(H)$. Finally, we calculated the average cost $C_{\text{avg}}$ of 100 random trees from $T(d)$.

In all cases less than four iterations inside a single run of \textsc{SolveRelaxed} function were enough to find the best parameters of the lower bound. Two upper bounds and the corresponding nearly optimal trees $H_1 := \text{HEURISTICS}1$ and $H_2 := \text{HEURISTICS}2$ were obtained along with the breadth-first-search tree $BFS := \text{HUFFMAN TREE}(1, d)$. The “best found tree” was selected as $H^* = \text{Arg min}_{H \in \{H_1, H_2, BFS\}} C_A(H)$. Finally, we calculated the average cost $C_{\text{avg}}$ of 100 random trees from $T(d)$.

$BFS$ tree is a “perfectly balanced tree” that can be calculated once for degree sequence $d$ and used as a “universal solution” being more or less good for all monotone vertex weight sequences. The relative gap $\Delta_{\text{BFS}} = \frac{C_A(BFS) - C_A(T^*)}{C_A(T^*)}$ between the cost of $BFS$ and the cost of the best found solution $H^*$ shows the price of knowing flow matrix $A$. The relative gap $\Delta_{\text{avg}} = \frac{C_{\text{avg}} - C_A(T^*)}{C_A(T^*)}$ shows the price of solving OCN problem in comparison with picking a random tree as a solution.

From [8] it is known that for QAP the relative gap between the best and the worst solution tends to zero when the dimension of the problem increases. For OCN problem, however, the gap depends on the weight distribution parameter $\beta$. In Figure 3(a) three typical relations are shown between the $BFS$ gap and the weight distribution parameter $\beta$ for different problem dimension $n$. For $\beta$ being close to zero most weights are close to unity, and $BFS$ tree is optimal. However, for larger $\beta$ $BFS$ tree is almost always suboptimal irrespective of the problem dimension. Therefore, even for random flow matrices the solution of OCN problem can be non-trivial.

The curves in Figure 3(b) show how much we lose in average from choosing a random tree instead of seeking for a “good” tree for $\beta \in [0,2]$. Three typical curves for different problem dimension $n$ show the significant gap, which increases when the problem dimension grows.
Then the lower bound was tested against a collection of random flow matrices. Again, 100 degree sequences were generated for trees of order from 50 to 250 with degrees of internal vertices uniformly distributed from 2 to 5. For every degree sequence \( d \) of dimension \( n \) a random flow matrix \( A = (\mu_{ij})_{i,j=1}^{n} \) was generated such that \( \mu_{ij} = \mu_{ji} = \text{rnd}^2 \), where \( \text{rnd} \) is a random number uniformly distributed on \([0,1]\), and \( \beta > 0 \) is a diversity factor. Then each matrix was loosed to the desired density degree \( \sigma \). The lower bound for the best parameter values, two heuristics, and BFS tree were calculated. As before, the “best found solution” was defined as \( H^* = \text{Arg min}_{H \in \{H_1, H_2, \text{BFS}\}} C_A(H) \), and the gap of the lower bound was evaluated as \( \Delta_{LB} = C_{A(H^*)} - LB_A(d) \).

The results are presented in Figure 4. For \( \beta = 0 \) we have \( A = J - I \), and OCN problem reduces to the Wiener index minimization whose solution is BFS tree \([35, 36]\). The algorithm easily finds optimal weights (being equal to unity), and the lower-bound gap is equal to zero (see curves for \( \beta = 0 \) in Figures 4(a) and 4(b)).

Figure 4(a) shows that the relative gap \( \Delta_{LB} \) decreases (and, hence, the lower bound quality increases) with problem dimension. This effect is probably due to the random nature of the underlying flow matrices: in a large matrix the effect of an individual flow is easier to conceal. Again, the average tree gap \( \Delta_{avg} \) in Figure 4(c) increases with problem dimension, so the potential gain from solving...
Figure 4: Results of numeric tests for random flow matrices.
OCN problem increases for large-scale problems. At the same time, Figure 4(d) shows that BFS tree, the “universal” solution that does not depend on the flow matrix, can be very attractive (at least, when compared to the existing heuristics).

In general, the more diverse are the flows, the lower is the quality of the lower bound. For example, the sparser matrix enjoys the larger weight diversity, and the relative gap $\Delta_{LB}$ decreases in matrix density (see Figure 4(b)). From Figure 4(d) we see that the quality of BFS tree also decreases in weights’ diversity $\beta$, and the gain from accounting for the specific flows’ pattern increases.

It is important to note that the average number of calls of $\text{SOLVERELAXED}$ function does not increase in problem dimension (see Figure 4(e)), so even for large-scale problems we need not consider bulky constraint sets in (12). At the same time, several large-scale convex problems are solved inside $\text{SOLVERELAXED}$, which requires more calculus when the problem dimension grows. The computation time increases rapidly in problem dimension $n$ (see Figure 4(f)). However, problems with several hundreds terminals are still solved in reasonable time (see details in Figure 4(f)) on a laptop (we used Lenovo™ Thinkpad© with Intel™ Core i5 2.3GHz).

7.3 Real-world datasets

Different free data sources from transportation industry (public transport and airline statistics reports) and demography (migration reports) were used to build several real-world flow matrices with various size and flows’ pattern. Below we briefly characterize all sources. Information about all elicited datasets is consolidated in Table 1. In all cases, we symmetrize obtained origin-destination (OD) matrices to obtain a symmetric flow matrix. The flow matrices can be downloaded from [http://www.mtas.ru/upload/ODmatrices.zip](http://www.mtas.ru/upload/ODmatrices.zip).

1. London Tube and Rail Transport (LTRT)
   It is possible to travel on Tube, DLR, London Overground, TfL Rail and most National Rail services using contactless or Oyster card to pay. Two data sets located at [https://tfl.gov.uk/maps/track/dlr](https://tfl.gov.uk/maps/track/dlr) provide information about the traffic between London Tube and Rail Stations based upon the card touch-in/touch-out information.

2. Queensland Government Data – TransLink OD trips (TransLink)
   Several datasets were derived from the Queensland State’s Government, Australia, [https://data.qld.gov.au/dataset/go-card-transaction-data/resource/8a99a319-6b70-4945-b87e-e58b178deae3](https://data.qld.gov.au/dataset/go-card-transaction-data/resource/8a99a319-6b70-4945-b87e-e58b178deae3) storing data about trip count for many transportation modes and carriers.

3. Greater Cambridge ANPR Data: OD Reports (ANPR)
   These origin-to-destination reports are derived from the Automatic Number Plate Recognition (ANPR) camera traffic survey undertaken in 2017.
across the Cambridge area from June 10 to 17. The reports provide information on the first and the last cameras triggered on vehicle journeys across the city. We summarize the data into an OD matrix.

4. **The Air Carrier Statistics database – T-100 Segment (T100)**
   The source located at [https://www.transtats.bts.gov/Fields.asp?Table_ID=293](https://www.transtats.bts.gov/Fields.asp?Table_ID=293) contains domestic and international T-100 segment data reported by U.S. and foreign air carriers and non-stop segment data by aircraft type and service class for transported passengers, freight and mail, available capacity, scheduled departures, departures performed, aircraft hours, and load factor. Flights with both origin and destination in a foreign country are not included. OD matrix is built using the fields “OriginAirportID”, “DestAirportID”, “Passengers”, and “UniqueCarrier”.

5. **Airline Origin and Destination Survey (US Air)**
   The Airline Origin and Destination Survey ([https://data.world/us-dot-gov/02210b59-4330-440d-acf4-d4fb276f1d74](https://data.world/us-dot-gov/02210b59-4330-440d-acf4-d4fb276f1d74)) is a 10% sample of airline tickets from reporting carriers collected by the U.S. Office of Airline Information of the Bureau of Transportation Statistics in the first quarter of 1993. Data includes origin, destination and other itinerary details of passengers transported. This database is used to determine air traffic patterns, air carrier market shares and passenger flows. We analyze only fields “OriginAirportID”, “DestAirportID”, “Coupons”. If it were several airports in an itinerary, we take the first airport as origin an the last as destination. If the first airport coincide with the last, we split the itinerary on two itineraries: from the first airport to the penultimate and from the penultimate to the last one.

6. **Canada Aircraft Movement Statistics (Canadian)**
   The survey located at [http://www23.statcan.gc.ca/imdb/p2SV.pl?Function=getSurvey&SDDS=2715](http://www23.statcan.gc.ca/imdb/p2SV.pl?Function=getSurvey&SDDS=2715) provides estimates of aircraft movements in Canada. The source table contains the hyphen-separated pair of cities and the passenger flow between these cities.

7. **EU Country to Country Migration (EU Migration)**
   [https://www.imi.ox.ac.uk/data/demig-data/demig-c2c-data](https://www.imi.ox.ac.uk/data/demig-data/demig-c2c-data)
   The DEMIG C2C (country-to-country) database contains bilateral migration flow data for 34 reporting countries and from up to 236 countries over the 1946–2011 period. It includes data for inflows, outflows and net flows, respectively for citizens, foreigners and/or citizens and foreigners combined, depending on the reporting countries. We take “Reporting country”, “Countries”, and “Value” columns for both genders.

8. **U.S. Census Bureau Migration Reports (US Migration)**
   The U.S. Census Bureau has been releasing county-to-county and county/minor civil division (MCD)-to-county/MCD migration flow estimates based on the American Community Survey (ACS) since 2012. We
Table 1: Data sets used to build real-world flow matrices

| Source     | Dataset                                                                 | Abbrev. | Dimension |
|------------|-------------------------------------------------------------------------|---------|-----------|
| LTRT       | The London Underground Limited operator                                  | LUL     | 266       |
| LTRT       | The Docklands Light Railway light metro system                           | DLR     | 61        |
| TransLink  | All carriers in June 2017                                               | TL      | 723       |
| TransLink  | One week of June 2017 for the carrier “BCC Ferries”                     | BCC     | 20        |
| TransLink  | One week of June 2017 for the carrier “Sunbus”                          | Sunbus  | 846       |
| TransLink  | Carrier “Park Ridge Transit” in June 2017                               | PRT     | 498       |
| TransLink  | Carrier “Mt Gravatt Bus Service” in June 2017                           | MGBS    | 364       |
| TransLink  | Carrier “Queensland Rail” in June 2017                                 | QR      | 154       |
| ANPR       | Summary data for June 10, 2017                                          | ANPR    | 91        |
| T100       | Carrier “Hawaiian Airlines Inc” in January 2017                         | HA      | 29        |
| T100       | Carrier “Compass Airlines” in January 2017                              | CA      | 55        |
| US Air     | Carrier “America West Airlines Inc.” (IATA code HP)                     | HP      | 105       |
| US Air     | Carrier “Trans World Airways LLC” (IATA code TW)                        | TW      | 176       |
| US Air     | Carrier “US Airways Inc.” (IATA code US)                                | US      | 269       |
| US Air     | Carrier “Midwest Express Airlines” (IATA code YX)                       | YX      | 59        |
| Canadian   | The annual report for 2005                                              | Canadian | 72       |
| EU Migration | EU to EU migration in 2007 by country                          | EU    | 13        |
| US Migration | Migration between counties of Alabama in 2014                    | Alabama | 67        |

Several typical flow patterns are presented in Figure 5. Transportation and migration datasets were used because of their availability, although we clearly understand that minimizing the number-of-edges graph distance over the set of trees is not of much practical interest for them.

For each flow matrix the degree sequence was generated with degrees of internal vertices uniformly distributed from 2 to 5. The lower bound, two upper bounds, BFS tree, and the average tree cost $C_{avg}$ were calculated. The results are presented in Table 2 and in Figure 6.

Table 2 shows that, distinct to random flows (see Figure 4(d)), BFS tree can have unacceptable quality for real datasets. Also, in most cases, Heuristics2 gives the best tree. Therefore, in spite of the complexity of MAXIMIZE LB procedure, it provides the highly valuable information for heuristic algorithm construction.

From Figure 6 we see that the quality of the lower bound (the value of the relative gap $\Delta_{LB}$) may vary in a wide range: from the modest gap $\Delta_{LB} = 22\%$ for “HA” dataset to the huge gap $\Delta_{LB} = 363\%$ for “MGBS” dataset. In the latter case the lower bound becomes almost uninformative (although it is still twice as big as a trivial lower bound, the sum of all flows). At the same time, we do not see the quality of the lower bound to decrease with the problem dimension. So, good quality of the lower bound can be expected for
Figure 5: Typical OD matrices before symmetrization (flow intensity grows from blue to red)
Table 2: Results for real-world datasets. The cost of the best found tree is marked with bold.

| Dataset  | Dimension | $\Delta_{LB}$ | $\Delta_{BFS}$ | $\Delta_{avg}$ | LB Heur. 1 | Heur. 2 | BFS tree | $C_{avg}$ |
|----------|-----------|---------------|----------------|---------------|-----------|---------|----------|-----------|
| EU       | 13        | 52% 24% 47%   | 0.339 0.517    | 0.515         | 0.639     | 0.756   |
| BCC      | 20        | 89% 15% 20%   | 0.331 0.626    | 0.660         | 0.717     | 0.754   |
| HA       | 29        | 22% 42% 53%   | 0.462 0.568    | 0.565         | 0.802     | 0.865   |
| CA       | 55        | 100% 37% 57%  | 0.331 0.687    | 0.662         | 0.905     | 1.041   |
| YX       | 59        | 39% 44% 103%  | 0.346 0.998    | 0.660         | 0.951     | 1.340   |
| DLR      | 61        | 168% 20% 54%  | 0.229 0.613    | 0.789         | 0.736     | 0.946   |
| Alabama  | 67        | 147% 18% 52%  | 0.245 0.605    | 0.652         | 0.712     | 0.919   |
| Canadian | 72        | 101% 54% 93%  | 0.307 0.714    | 0.619         | 0.951     | 1.192   |
| ANPR     | 91        | 171% 0% 26%   | 0.294 1.044    | 0.821         | 0.799     | 1.009   |
| HP       | 105       | 54% 45% 97%   | 0.408 0.845    | 0.629         | 0.915     | 1.243   |
| QR       | 154       | 94% 21% 85%   | 0.384 1.025    | 0.745         | 0.903     | 1.380   |
| TW       | 176       | 57% 61% 121%  | 0.394 1.284    | 0.620         | 0.959     | 1.370   |
| LUL      | 266       | 53% 2% 35%    | 0.833 1.405    | 1.272         | 1.293     | 1.721   |
| US       | 269       | 71% 41% 106%  | 0.377 1.171    | 0.646         | 0.911     | 1.329   |
| MGBS     | 364       | 363% 0% 54%   | 0.176 0.942    | 0.853         | 0.815     | 1.259   |
| PRT      | 498       |                |                |               | Stopped after several hours of computation |
| TL       | 723       |                |                |               | Stopped after several hours of computation |
| Sunbus   | 846       |                |                |               | Stopped after several hours of computation |

Figure 6: Results for real datasets (normalized to the sizing factor $n^2 \ln n$). The lower bound is depicted with the height of a dotted rectangle, “+” shows the cost of HEURISTICS1 tree, while “×” stands for HEURISTICS2 tree. Circle “o” shows the cost of BFS tree, and the horizontal bar points out the cost of the average tree.
bigger samples, at least for some application areas. Potentially, after the careful optimization of the algorithm, the best parameters of the lower bound can be calculated for OCN problems with thousand terminals or more.

8 Conclusion

An optimal connecting network (OCN) has the minimum possible weighted sum of distances between pairs of its vertices among all admissible networks. Weights of vertex pairs are given by a flow matrix $A$. In general, finding OCN is a complex problem of combinatorial optimization.

In this article a lower bound estimate is constructed for the cost of an optimal connecting tree with the given degree sequence. The lower bound is parameterized by two vectors, $\alpha \in \mathbb{R}^n$ and $\mu \in \mathbb{R}^n_+$. The problem of finding the best combination of parameter values reduces to the non-convex semidefinite problem, for which an algorithm is proposed. The algorithm solves the non-convex problem through a series of its convex relaxations.

Although the optimization problem involves a (rather demanding) semidefinite constraint and several quadratic constraints with dense matrices, numeric tests show that the lower bound can be calculated in reasonable time (minutes on a PC) for trees with several hundreds vertices. However, calculation of the lower bound for huge trees with thousands vertices is still an open problem, which can be the subject of future research. At the same time, if we do not insist on the best parameter values and are satisfied with any admissible $\alpha$ and $\mu$, calculation time can be considerably decreased by increasing tolerance parameter $\delta$ in Listing 2.

The quality of the lower bound depends on how accurately flow matrix $A$ can be approximated by the sum of the diagonal matrix $\text{diag}(\alpha)$ and the non-negative rank-one matrix $\mu\mu^\top$. It is shown in Section 7 that for $A$ having rank one we have the perfect approximation, and the lower bound is equal to the optimal tree cost. In this case every terminal can be endowed with non-negative weight $\mu_i$, $i = 1, \ldots, n$, and the flow between the terminals $i$ and $j$ is written as $\mu_{ij} = \mu_i\mu_j$. Weights of terminals are explained by the following simplistic model. Let us assume that the $i$-th terminal is active at a given period of time with probability proportional to its weight $\mu_i$. If active, a terminal sends a unique piece of information to all terminals being active at this moment. If all terminals are independent, then the average volume of information circulating between terminals $i$ and $j$ is proportional to $\mu_i\mu_j$.

Many real-world flow patterns, however, are far from this model, and the lower bound may sometimes have poor quality. It is an open question, which flow matrix is the least convenient for approximation by a rank-one matrix, and, hence, for which flow matrix the lower bound has the least quality. These results may be used when developing the new lower bounds with the better guaranteed quality.

The strategic direction of research, however, is connected with generalizing the approach to the general networks with loops.
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A Properties of bilinear matrix inequality $xx^\top - A \succeq 0$

In this appendix properties are studied of the set

$$X_A := \{ x \in \mathbb{R}^n : xx^\top - A \succeq 0 \}$$

where $A$ is a symmetric real $n \times n$ matrix.

Recall that with $\lambda_i(A), i = 1, ..., n$ we denote (real) eigenvalues of real symmetric matrix $A$ listed in the descending order while $u^{(i)}(A)$ standing for the corresponding eigenvectors. Let $\mathbb{S}^{n-1} := \{ x \in \mathbb{R}^n : x^\top x = 1 \}$ denote the unit sphere in $\mathbb{R}^n$.

**Lemma 1** $X_A \neq \emptyset$ if and only if $\lambda_2(A) \leq 0$.

**Proof** Vector $x$ belongs to $X_A$ if and only if for any vector $z \in \mathbb{S}^{n-1}$ inequality $z^\top (xx^\top - A) z \succeq 0$ holds. Consequently, $X_A = \emptyset$ if and only if for any $x \in \mathbb{R}^n$
there exists such \( z \in \mathbb{S}^{n-1} \) that \( z^\top (A - xx^\top) z > 0 \). In the other words, \( X_A = \emptyset \) when
\[
\inf_{a \geq 0} \min_{x \in \mathbb{S}^{n-1}} \max_{z \in \mathbb{S}^{n-1}} z^\top (A - axx^\top) z > 0. \tag{19}
\]

It is clear that the left-hand side of inequality (19) will not increase if we narrow the maximization area, and, therefore,
\[
\inf_{a \geq 0} \min_{x \in \mathbb{S}^{n-1}} \max_{z \in \mathbb{S}^{n-1}, z \perp x} z^\top (A - axx^\top) z = \inf_{a \geq 0} \min_{x \in \mathbb{S}^{n-1}} \max_{z \in \mathbb{S}^{n-1}, z \perp x} z^\top Az = \lambda_2(A). \tag{20}
\]
The last equality follows from the Courant-Fischer theorem, which says that
\[
\lambda_2(A) = \min_{z \in \mathbb{S}^{n-1}, z \perp x} \max_{x \in \mathbb{S}^{n-1}} z^\top Az.
\]

On the other hand, the left-hand side of inequality (19) will not decrease if minimization over \( x \in \mathbb{S}^{n-1} \) if replaced with the concrete \( x = u^{(1)}(A) \):
\[
\inf_{a \geq 0} \min_{x \in \mathbb{S}^{n-1}} \max_{z \in \mathbb{S}^{n-1}, z \perp x} z^\top (A - a \cdot xx^\top) z \leq \inf_{a \geq 0} \max_{z \in \mathbb{S}^{n-1}} z^\top (A - au^{(1)}(A))u^{(1)}(A)^\top z = \inf_{a \geq 0} \lambda_1(A - au^{(1)}(A))u^{(1)}(A)^\top \tag{21}
\]
The last equality also follows from Courant-Fischer theorem.

The spectrum of matrix \( A - a \cdot u^{(1)}(A))u^{(1)}(A)^\top \) differs from that of matrix \( A \) only in one component: the eigenvalue \( \lambda_1(A) \) is replaced with \( \lambda_1(A) - a \), and so,
\[
\inf_{a \geq 0} \lambda_1(A - au^{(1)}(A))u^{(1)}(A)^\top \leq \inf_{a \geq 0} \min_{\lambda_1(A) - a, \lambda_2(A)} = \lambda_2(A). \tag{22}
\]

From inequalities (20) and (22) it follows that the left-hand side of inequality (19) is equal to \( \lambda_2(A) \), and the inequality \( \lambda_2(A) > 0 \) is necessary and sufficient for inequality (19) to be valid, which, in turn, implies that \( X_A \) is empty. 

\textbf{Lemma 2} If matrix \( A \) is negative definite, then \( X_A = \mathbb{R}^n \).

\textbf{Proof} The proof follows immediately from positive semidefiniteness of matrix \( xx^\top \) for arbitrary \( x \in \mathbb{R}^n \).

\textbf{Lemma 3} if \( X_A \) is not empty, then \( x := \sqrt{\lambda_1(A)}u^{(1)}(A) \in X_A \).
The spectrum of matrix $A - xx^\top$ is equal to the spectrum of matrix $A$ up to replacing $\lambda_1(A)$ with zero. Since $X_A$ is not empty, from Lemma 1 if follows that all other eigenvalues are non-positive, and so, matrix $A - xx^\top$ is negative semidefinite.

**Lemma 4** If $x \in X_A$, then $ax \in X_A$ for all $a > 1$.

**Proof** The proof is straightforward.

**Lemma 5** If $X_A \neq \emptyset$ and $X_A \neq \mathbb{R}^n$, then

$$X_A = \left\{ x \in \mathbb{R}^n : \sum_{i=1}^{n} \frac{(x^\top u^{(i)}(A))^2}{\lambda_i(A)} \geq 1 \right\}. \quad (23)$$

**Proof** Let us denote with $I$ the identity $n \times n$ matrix. By definition of $X_A$, from $x \in X_A$ it follows that the characteristic equation $\det(A - xx^\top - \rho I) = 0$ has no positive roots. Since eigenvalues are continuous with respect to matrix elements, identity $\lambda_1(A - xx^\top) = 0$ holds on the boundary of $X_A$. Therefore, if vector $x$ belongs to the boundary of $X_A$, then $\rho = 0$ is a root of the characteristic equation, i.e,

$$\det(A - xx^\top) = 0. \quad (24)$$

To solve equation (24), let us consider the spectral decomposition $U \text{diag} (\lambda) U^\top$ of matrix $A$, where $\lambda = (\lambda_i(A))_{i=1}^n$, $U = (u^{(1)}(A), \ldots, u^{(n)}(A))$.

The characteristic equation and its roots are insensitive to orthogonal transformations. Hence, $\det(A - xx^\top) = \det(\text{diag}(\lambda) - y y^\top)$, where $y := U^\top x$.

Therefore, equation (24) can be written as

$$\det\begin{pmatrix}
\lambda_1(A) - y_1^2 & -y_1 y_2 & \cdots & -y_1 y_n \\
-y_2 y_1 & \lambda_2(A) - y_2^2 & \cdots & -y_2 y_n \\
\vdots & -y_3 y_2 & \ddots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
-y_n y_1 & -y_n y_2 & \cdots & \lambda_n(A) - y_n^2
\end{pmatrix} = 0.$$

Let us transform the matrix to the triangular form with elementary row operations not affecting the roots of the equation.

First we assume that $y_i \neq 0$, $i = 1, \ldots, n$. Let us divide $i$-th row by $y_i$, $i = 1, \ldots, n$, and subtract the first row from all other rows obtaining the equation

$$\det\begin{pmatrix}
\frac{\lambda_1(A)}{y_1} - y_1 & -\frac{y_1}{y_2} & \cdots & -\frac{y_1}{y_n} \\
-\frac{\lambda_1(A)}{y_1} & \frac{\lambda_2(A)}{y_2} & 0 & \cdots & 0 \\
\vdots & 0 & \ddots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
-\frac{\lambda_1(A)}{y_1} & 0 & \cdots & \frac{\lambda_n(A)}{y_n}
\end{pmatrix} = 0.$$
Let us multiply $i$-th row, $i = 1, \ldots, n$, by $\frac{y_i}{\lambda_i(A)}$ and add to the first row all other rows, multiplying them by $y_i$. Finally we obtain the desired lower triangular form:

$$
\begin{vmatrix}
\frac{\lambda_1(A)}{y_1} - y_1 - \sum_{i=2}^{n} \frac{y_i^2 \lambda_1(A)}{y_i \lambda_i(A)} & 0 & \cdots & 0 \\
- \frac{y_2 \lambda_1(A)}{y_1 \lambda_2(A)} & 1 & 0 & \cdots \\
\vdots & 0 & \ddots & \vdots \\
\vdots & \vdots & \ddots & \vdots \\
- \frac{y_n \lambda_1(A)}{y_1 \lambda_n(A)} & 0 & \cdots & 1
\end{vmatrix} = 0. \quad (25)
$$

The determinant of a triangular matrix is equal to the product of its diagonal element, so, equation (25) can be written as

$$
\frac{\lambda_1(A)}{y_1} - y_1 - \sum_{i=2}^{n} \frac{y_i^2 \lambda_1(A)}{y_i \lambda_i(A)} = 0.
$$

Multiplying both sides of the equation by $\frac{y_i}{\lambda_i(A)}$, we finally obtain

$$
\sum_{i=1}^{n} \frac{y_i^2}{\lambda_i(A)} = 1. \quad (26)
$$

If $y_i = 0$ for some $i$, $i$-th row is already diagonal, no transformation needed, so the case when some $y_i$ are equal to zero is considered in a similar manner.

Since $X_A$ is not empty and $X_A \neq \mathbb{R}^n$, it follows from Lemmas 1 and 2 that $\lambda_1(A) > 0$, $\lambda_2(A) \leq 0$. Therefore, equation (26) defines the two-sheet hyperboloid in the $n$-dimensional space:

$$
\frac{y_1^2}{\lambda_1(A)} - \sum_{i=2}^{n} \frac{y_i^2}{|\lambda_i(A)|} = 1. \quad (27)
$$

The boundary of the set $X_A$ belongs to this hyperboloid. Using Lemmas 3 and 4 one can easily check that both sheets defined by the inequality

$$
\frac{y_1^2}{\lambda_1(A)} - \sum_{i=2}^{n} \frac{y_i^2}{|\lambda_i(A)|} \geq 1 \quad (28)
$$

have points from $X_A$ and, hence, belong to $X_A$. The space between these sheets does not belong to $X_A$, since point $x = u_2(A)$ is obviously does not belong to $X_A$.

Taking into account that $y = U^T x$, we obtain the desired inequality. ■