

Towards Optimal Transport Networks

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ABSTRACT

Our ultimate goal is to design transportation networks whose dynamic performance metrics (e.g. passenger throughput, passenger delay, and insensitivity to weather disturbances) are optimized. Here the focus is on optimizing static features of the network that are known to directly affect the network dynamics. First, we present simulation results which support a connection between maximizing the first non-trivial eigenvalue of a network's Laplacian and superior airport network performance. Then, we explore the effectiveness of a tabu search heuristic for optimizing this metric by comparing experimental results to theoretical upper bounds. We also consider generating upper bounds on a network's algebraic connectivity via the solution of semidefinite programming (SDP) relaxations. A modification of an existing subgraph extraction algorithm is implemented to explore the underlying regional structures in the U.S. airport network, with the hope that the resulting localized structures can be optimized independently and reconnected via a "backbone" network to achieve superior network performance.

1. INTRODUCTION

The current hub-and-spoke topology of the U.S. air transport network is ill-equipped to handle the three-fold demand increase projected for the coming decade [13]. We are interested in developing rigorous methods for improving the transportation network topology. With this in mind, our goal is twofold: (1) to establish relationships between global network metrics and airport network performance measures, and (2) develop algorithms that exploit these relationships as part of a larger optimization framework. Computing global network metrics first requires that we define what is meant by a "network" in our current context. For our purposes, a network is a simple (connected) graph $G = (N, E)$, where N is the set of n nodes

and E is the set of undirected edges between nodes. Of course air flights are directed, but here we assume that if a flight exists from one airport to another, the reverse flight also exists. Thus feasible flight direction need not be encoded in the static network definition. Such networks are typically given by an $n \times n$ adjacency matrix A , where $a_{ij} = 1$ if there is an edge $(i, j) \in E$ connecting nodes i and j and $a_{ij} = 0$ otherwise. In our application, $a_{ij} = 1$ is equivalent to the existence of a direct flight between airports i and j . Given this network definition, we wish to uncover functional dependencies of dynamic performance of the airport network on explicit topological variables and implicit topological functions that would allow us to optimize network performance in terms of topological variables. Section 3 describes our use of simulation to gain insight into these functional dependencies.

2. METRICS OF INTEREST

The network performance measures with which we are currently concerned are average time in air, average holding time, average number of hops, average distance traveled (averages taken over all flights) and the average number of planes in queue over all airports in the network. Here a "hop" refers to a direct flight between two airports in the network. So, the number of hops required for a flight is equivalent to the number of edges that must be traversed in the network representation to travel from origin airport to destination airport. These measures are subject to a particular dynamic instance of the static network G , i.e., a schedule of flights through the network. Initially, we sought to determine how two popular network metrics correlated with these performance measures.

The first metric is the algebraic connectivity of the network, λ_2 , which is the first non-trivial eigenvalue of the network's Laplacian. The Laplacian L is defined by

$$L = D - A \quad (1)$$

where D is the diagonal matrix of node degrees. The degree of a node i is the number of edges in G inci-

dent to i . As before, A is the adjacency matrix of G . The λ_2 metric can be interpreted as a measure of the network's connectivity, and is a metric relevant to the system's propensity to "synchronize", i.e., behave in a regular or predictable manner while maintaining stability. (see, e.g., [4],[14]). A λ_2 of zero means that the network is disconnected. Second eigenvalues near zero suggest a nearly disconnected network, while a large λ_2 is consistent with high connectivity. (see, e.g., [2]).

The second metric of interest is $s(G)$. Given an undirected graph G with edge set E define

$$s(G) = \sum_{(i,j) \in E} d_i d_j. \quad (2)$$

Here d_i is the degree of the i^{th} node in the network. The $s(G)$ metric is strongly related to assortativity, the extent to which high degree nodes are adjacent to other high degree nodes. Graphs with large $s(G)$ typically display a more hub-like topology, much akin to the current U.S. air transport network. (see, e.g., [10]). The following section summarizes our early experimental results regarding the connection between airport network performance measures and the two metrics as defined above.

3. NUMERICAL RESULTS

To explore the connection between $s(G)$, λ_2 and airport network performance, we developed the Airport Network Simulation Program (ANSP), a tool which allows the user to simulate the dynamic aspects of a customized airport network. Alterable input parameters include (but are not limited to) a network adjacency matrix, airport capacities, origin-destination pairs for flights, and three-dimensional flight paths. All networks must be simple and connected. A module also exists which keeps track of pairwise airplane separation throughout the simulation, so that Required Navigation Performance (RNP) constraints can be enforced. The simulation is written in C, and a Fortran driver code allows for batch runs and more flexible control of ANSP in a Linux/Unix environment.

As an early experiment to gauge the relationship between our two network metrics of interest and network performance, we generated a collection of counterparts to the 336 node 1990 U.S. airport network — each heuristically rewired using tabu search (see [12]) to achieve target levels (i.e., minimization and maximization) of the global network metrics λ_2 and $s(G)$.

Tabu search is a metaheuristic — i.e., a heuristic that can be embedded as a subroutine within other heuristics — that controls the search trajectory of a

traditional local search so that many locally optimal solutions can be uncovered. Here "trajectory" refers to the sequence by which feasible solutions are visited by the algorithm from one iteration to the next. Of particular importance here is the set of moves that are allowed to be made. Given a particular graph G , we define the set of neighboring solutions to consist of all graphs obtainable from G by "swapping" any pair of edges as long as the original network's degree distribution is preserved and the graph is connected. A swap is performed by first identifying a set of four nodes, consisting of two pairs of adjacent nodes. Then, the two edges corresponding to these adjacencies are removed from the graph, and two edges are added such that each node is newly adjacent to a node in the set of four with which it was not originally paired. Special care must be taken so that a swap does not disconnect the graph. At each iteration of the tabu search procedure we chose to implement the first improving swap encountered — i.e., the first swap leading to an improved network metric — while generating the neighborhood of allowable moves. At this juncture only the most basic features of tabu search (aspiration criterion and tabu list) have been employed.

Early experiments (see Figure 1) demonstrate that the 1990 U.S. airport network topology with heuristically maximized λ_2 exhibits the "best" overall performance when the performance metrics are: time average number of customers in queue over all airports, average number of hops for each flight, average time in air for each flight, average distance traveled by each flight, average holding time for each flight.

4. REGIONAL SUBSTRUCTURES

The tabu search routines described above optimize over the entire network structure and do not isolate regional substructures during the optimization process. In reality, however, airport networks can be partitioned geographically by regional carriers. A superior rewiring algorithm might take advantage of this partitioning by optimizing each disjoint component independently, and then reconnecting the components with a secondary objective in mind. Chung and Lu [8] provide a local subgraph extraction algorithm, which we modified to allow for arc distances of any real length (as opposed to arcs of unit length). The algorithm requires four inputs, $k \in \mathbb{Z}^+$, $l \in \mathbb{Z}^+$, $l' \in \mathbb{R}^+$, and a simple graph G . By "simple" we mean a connected, undirected graph with no self loops or multiples edges. The algorithm systematically removes arcs from G in order to expose the underlying substructure. First, all arcs of length larger than l' are removed. We then create an arbitrary ordering of the remaining arcs, as the resulting extraction is independent of the initial ordering. Each arc is considered in turn. For the current arc e , the number of arc-

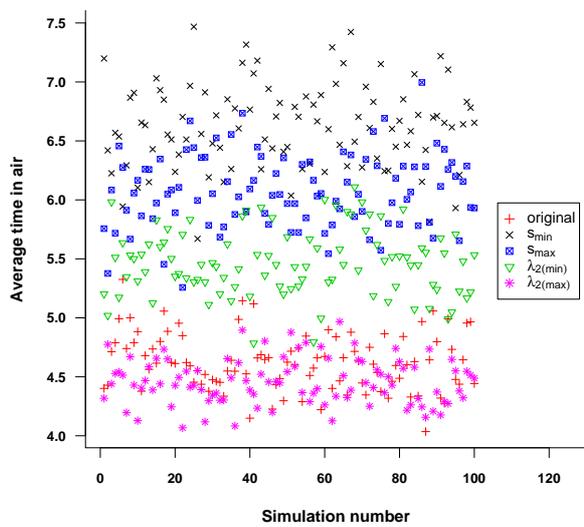
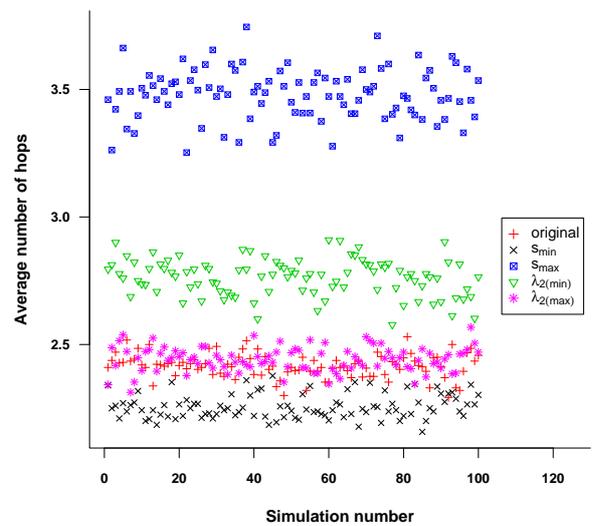
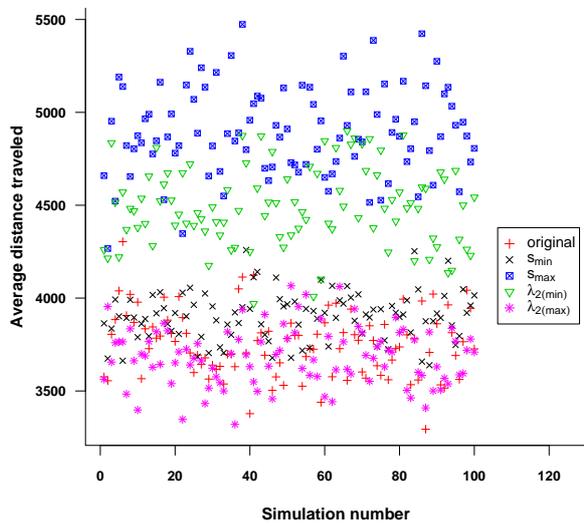
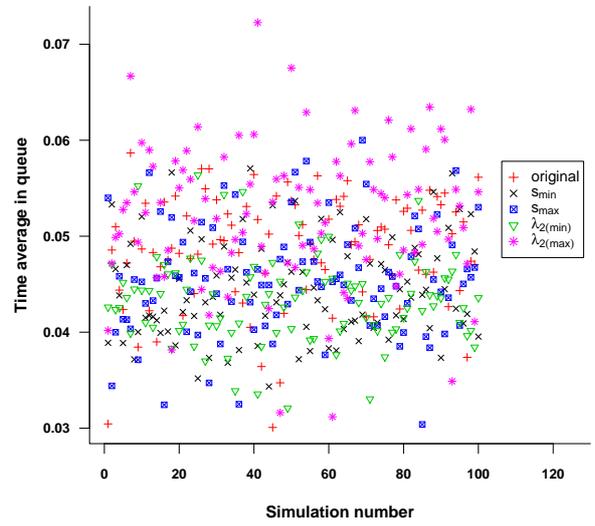
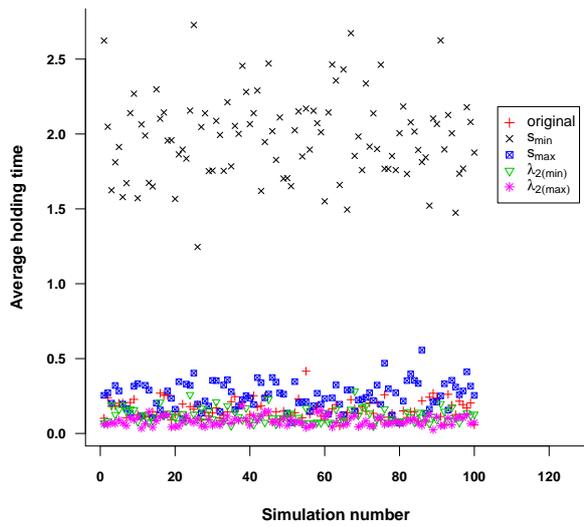


Figure 1: A graphical performance comparison between the 1990 U.S. airport network and its rewired counterparts

disjoint paths with at most l arcs passing through e is counted. If this number exceeds k , then the arc is deleted from the network. Otherwise, it is retained and the next arc in the ordering is considered. Once the algorithm cycles through all remaining arcs in the list, without executing the removal procedure, the algorithm is terminated. This modified algorithm was tested on the 1990 U.S. airport network (see Figure 2). For the majority of k, l, l' parameters tested, the algorithm extracted subgraphs corresponding to the western U.S., the northeast, and the southeast. The subgraphs correspond to geographic areas where regional carriers are likely to operate.

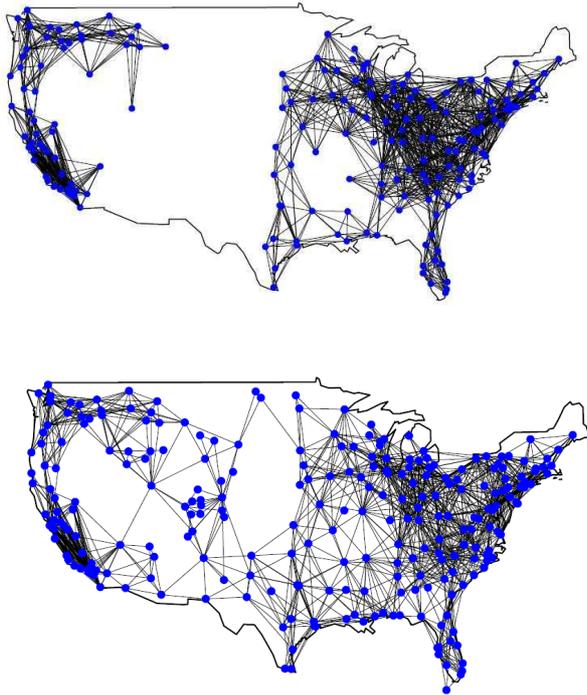


Figure 2: Two applications of the subgraph extraction algorithm to the 1990 U.S. airport network; top, $k = 3, l = 4, l' = 600.0$ (kilometers); bottom, $k = 2, l = 2, l' = 500.0$

5. UPPER BOUNDS FOR λ_2

It is worth considering the extent to which our tabu search heuristic succeeds in maximizing the λ_2 metric. An upper bound on λ_2 is given for general graphs in [19]. Let G be a graph and let s and t be any two non-adjacent nodes in G . It follows that

$$\lambda_2(G) \leq \frac{1}{2}(d_s + d_t), \quad (3)$$

where d_i denotes the degree of node i in G . Thus if a graph G contains two non-adjacent nodes of degree

one, then we must have $\lambda_2(G) \leq 1$. This result holds for the 336 node 1990 U.S. airport network. It has also been shown that for a graph G with node set N

$$\lambda_2(G) \leq \frac{n}{n-1} \min_{i \in N} \{d_i\}. \quad (4)$$

Thus, if at least one node has degree one then the bound is $n/(n-1)$ which is nearly 1 for large n . During our tabu search experiments, a maximum λ_2 of 0.97 was realized. It is interesting to note that this value of λ_2 was not achieved while explicitly maximizing λ_2 , but rather while minimizing $s(G)$. This pattern has remained consistent through repeated applications of our tabu search heuristic to many types of randomly generated graphs (e.g., geometric, Erdős-Rényi [11]). In fact, this relationship is not a coincidence.

Apparently unknown to the authors of [15], $s(G)$ is equivalent to a well known metric in computational chemistry. For a (chemical) network, the general Randić index $R_\alpha(G)$ is defined as the sum of products $(d_i \times d_j)^\alpha$ over all edges (i, j) of G . That is,

$$R_\alpha(G) = \sum_{(i,j) \in E} (d_i \times d_j)^\alpha. \quad (5)$$

Thus, when $\alpha = 1$, $s(G)$ and $R_1(G)$ are equivalent. In 1975, the chemist Milan Randić [20] proposed the topological index $R_\alpha(G)$ for $\alpha = -1$ or $-1/2$ under the name *branching index*. He explained the utility of R in measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Bollobás and Erdős [5] generalized this index by allowing α to take on any real number. An up to date summary of results for the Randić index can be found in [17]. A result of particular interest in [18] relating λ_2 , λ_n and $R_\alpha(G)$ is the following theorem.

Theorem Let G be a simple connected graph of order n . Then

$$\frac{1}{2} \sum_{i=1}^n d_i^{2\alpha+1} - \frac{k}{2} \lambda_n \leq R_\alpha(G) \leq \frac{1}{2} \sum_{i=1}^n d_i^{2\alpha+1} - \frac{k}{2} \lambda_2 \quad (6)$$

where

$$k = \sum_{i=1}^n d_i^{2\alpha} - \frac{(\sum_{i=1}^n d_i^\alpha)^2}{n}$$

is a graph invariant. As we have previously noted $s(G) = R_1(G)$. In addition, if we restrict our attention to simple connected graphs with a fixed degree sequence, we see that the all the terms in the upper and lower bounds are fixed except for the eigenvalues of the Laplacian, λ_2 and λ_n . It is worth noting that

these two eigenvalues are precisely the ones linked to network synchronization in the literature.

Recall that our simulation experiment found those networks optimized by tabu search to maximize λ_2 directly to perform best — better than the networks which actually exhibited the largest λ_2 values, i.e, the networks for which tabu search explicitly minimized $s(G)$. This does not mean that the maximization of λ_2 as a valid optimization criterion should be abandoned. The plots in Figure 1 demonstrate that the minimized $s(G)$ graphs suffer, largely due to excessive holding times, which our oversimplified system likely fails to model with sufficient accuracy.

When considering transportation networks in which all nodes have relatively large degrees, the λ_2 bounds presented above may not be sufficiently tight. For this reason other means of bounding the algebraic connectivity of simple graphs are needed. Boyd and Gosh ([6],[7]) formulate a semidefinite program (SDP) relaxation for this problem. Note that L_{ij} is the element in the i^{th} row and j^{th} column of the Laplacian matrix L .

$$\begin{aligned}
 & \text{maximize} && s \\
 & \text{subject to} && s(I - \mathbf{1}\mathbf{1}^T/n) \preceq L \\
 & && L^T = L \\
 & && L\mathbf{1} = \mathbf{0} \\
 & && \mathbf{0} \leq L_{ij} \leq \mathbf{1}, \quad i \neq j. \quad (7)
 \end{aligned}$$

Note that $s = \lambda_2$, where λ_2 is the second eigenvalue of L . The degree distribution $\mathbf{d} = (d_1, d_2, \dots, d_n)$ associated with the SDP can be fixed by enforcing the following set of constraints.

$$L_{ii} = d_i \quad i = 1, 2, \dots, n. \quad (8)$$

Because this SDP formulation is a relaxation, the L_{ij} are unlikely to satisfy the binary requirements of the discrete optimization problem. Thus, one shortcoming of the the SDP approach is that no feasible Laplacian for the discrete problem is generated as part of the solution. However, the SDP problem has the potential to be used as a subroutine in a branch and bound algorithm to solve the discrete problem exactly. A naive approach would be to branch by fixing one element of the Laplacian returned by the SDP relaxation to 0 or 1, and resolving. Due to the computational effort required to solve the SDP for networks with $n > 50$, a more viable alternative might be to develop an approximation algorithm based on the SDP problem.

6. CONCLUDING REMARKS

First, it is worth considering how good the bounds are on the Randić index in (6) for the $\alpha = 1$ case. Does this mean that optimizing $s(G)$, which appears to be easier, will automatically optimize λ_2 and λ_n ?

In addition to improving the performance of tabu search and providing better bounds on λ_2 it is possible to formulate optimization models whose goal is to design a network with maximum λ_2 . In [6] a binary optimization problem is formulated that begins with an initial *base* graph and a collection of additional edges E that may be added. The optimization model adds k edges from E so that λ_2 is maximized. An SDP results by considering a linear relaxation of the binary constraints. The authors of [6] provide a heuristic that yields feasible solutions to the binary optimization model. One application of this model for transport network design is to assist in decisions regarding the selection of new routes to add to an existing network. That is, select k routes from a larger set of proposed routes so that λ_2 is maximized. A second application is to use as a base graph the results from the subgraph extraction algorithm. The set of edges E from which we select k edges would re-connect the subgraphs in a way that maximizes λ_2 .

In addition to directly optimizing a particular static graph metric in the hope of affecting the system dynamics it is possible to link network topology with a given model of the network dynamics. For example, in [9] a particular diffusive system dynamics model led to Ramanujan (expander) graphs as best. Ramanujan graphs are regular graphs with large algebraic connectivity. Clearly, the complete U.S. air transport network does not have this structure as the airports (nodes) are not identical. However, if a slightly different coupling function is used [9] a dramatically different network topology emerges as *best*. For this system an optimal topology emerges whose degree distribution is shown to decay faster than an exponential (power law). To our knowledge, there is currently no dynamical system model for the U.S. air transport network.

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