Optimal transportation network with concave cost functions: loop analysis and algorithms*

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Transportation networks play a vital role in modern societies. Structural optimization of a transportation system under a given set of constraints is an issue of great practical importance. For a general transportation system whose total cost C is determined by $C = \sum_{i<j} C_{ij}(I_{ij})$, with $C_{ij}(I_{ij})$ being the cost of the flow I_{ij} between node i and node j, Banavar and co-authors [J. Banavar *et al.*, Phys. Rev. Lett. **84**, 4745-4748 (2000)] proved that the optimal network topology is a tree if $C_{ij} \propto |I_{ij}|^{\gamma}$ with $0 < \gamma < 1$. The same conclusion also holds in the more general case where all the flow costs are strict concave functions of the flow I_{ij}. To further understand the qualitative difference between systems with concave and convex cost functions, a loop analysis of transportation cost is performed in the present paper, and an alternative mathematical proof of the optimality of tree-formed networks is given. The simple intuitive picture of this proof then leads to an efficient global algorithm for the searching of optimal structures for a given transportation system with concave cost functions.

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I. INTRODUCTION

Structure, dynamics, and evolution are the three major themes of current researches on complex networks. The structure or topology of a network affects the robustness [1–3], efficiency [4, 5], and sensitivity [6] of dynamical processes on the network and, consequently, influence the performance of the network in fulfilling its intended functions. On the other hand, various feedback mechanisms exist in complex dynamical systems, which couple network dynamical processes with the evolution of the network's architecture. To understand the global topologies of many real-world complex networks from this viewpoint of function/dynamics-driven structural optimization is an on-going effort (see, e.g., Refs. [7–11]). This problem can be divided into two issues: i) For a given dynamical process, what are the corresponding optimal network structures? and ii) How does the network evolve to an optimal structure? The former issue, which concerns with the 'fixed points' of the network evolution dynamics, may serve as a first step in fully characterize the complex dynamics–structure coupling in a given networked systems.

Transportation networks are very interesting model systems to study complex network evolution and optimization [12–18]. Electricity power grids, river systems, global airline networks, the internet, urban road networks can all be regarded as transportation systems. Flows on the network, be they electronic currents or email messages, usually are associated with certain types of costs. The costs could be energy dissipation into heat, time delay between sending and receiving an email message, ect.. For a network containing N vertices, the total transportation cost C might be defined according to

$$C[\{I\}] = \sum_{i<j} C_{ij}(|I_{ij}|) \ , \tag{1}$$

where $\{I\} \equiv \{I_{ij} | 1 \leq i < j \leq N\}$ is a general flow pattern; I_{ij} is the flow between vertex i and vertex j of the network (if $I_{ij} > 0$ then the flow is from i to j; if $I_{ij} < 0$, it is from j to i; if $I_{ij} = 0$, then there is no flow between i and j); $C_{ij}(|I_{ij}|)$ is the cost of the flow I_{ij} between vertex i and j (without loss of generality, when $I_{ij} = 0$ we can assume $C_{ij} \equiv 0$). Notice that Eq. (1) contains only flow costs along the edges of the network. In some transportation systems

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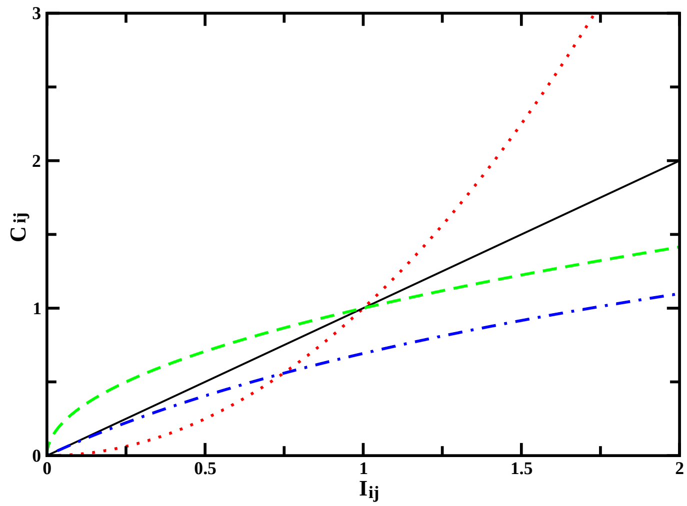

FIG. 1: Examples of convex and concave cost functions $C_{ij}(|I_{ij}|)$ associated with flow I_{ij} between two vertices i and j. The function $C_{ij}(|I_{ij}|) = |I_{ij}|^2$ (dotted line) is convex, while $C_{ij}(|I_{ij}|) = |I_{ij}|^{1/2}$ (dashed line) and $C_{ij}(|I_{ij}|) = \ln(1 + |I_{ij}|)$ (dot-dashed line) are concave. The thin solid line represents $C_{ij}(|I_{ij}|) = |I_{ij}|$.

there might be additional costs at the vertices (for example, in internet routing, congestion mainly takes place at different computer servers (nodes) of the internet), but in the present work we do not consider this complication. The network structure is defined by all those non-zero edge flows in the flow pattern $\{I\}$ and thus the searching of optimal structure could also be regard as searching of the optimal flow pattern. The optimal flow pattern problem, which is at the crossroads of network theory, complex systems, and economics, has been studied extensively in metabolic networks and other transportation networks (see, for example, Refs. [19–22]).

Naturally it is desirable to choose a network architecture which minimizes the total transportation cost. Empirically, it was observed that some transportation systems (such as electric power grids and urban road networks [23]) typically contains many loops, while other transportation systems (notably the global airline network and river networks [22, 24–26]) are tree-like, i.e., contain very few loops. To understand this qualitative distinction in network topologies, Banavar and co-authors [12] showed that, if in Eq. (1) all the edge costs C_{ij} increases sublinearly with the flow, i.e., $C_{ij}(|I_{ij}|) \propto |I_{ij}|^\gamma$ with $0 < \gamma < 1$ (see Fig. 1), then the optimal flow network will contain no loops; on the other hand, if C_{ij} increases with I_{ij} faster than linearly (Fig. 1), then the optimal flow network in general will be loop-rich. Reference [12] further mentioned that, the overall topology of a transportation network will be tree-like or loop-rich depending only on whether all the flow costs C_{ij} are strictly concave or strictly convex, respectively. This conclusion is intuitively easy to accept: if the flow cost on each edge increases with the flux faster than linearly (Fig 1), it might be preferable to distribute this flux through multiple pathways; on the other hand, if the cost increases with the flux slower than linearly (Fig 1), the accumulation of the flux on the optimal pathway might lower the total cost. The optimality of tree-shaped topologies has also been addressed in detail in Ref. [21], which also reviewed other developments. Transportation networks with concave cost functions initially arose in the optimal channel network problem [19, 20, 22]. In this context, it has been argued that the observed fractal forms in many real-world channel networks have a dynamical origin, i.e., are caused by evolution and optimization under certain constraints [22]. Furthermore, the observed allometric scaling of such systems can also be understood from the viewpoint of transportation optimization [27, 28].

In the present paper, we revisit the optimal transportation network problem and, based on a loop analysis technique, give an alternative proof of the general statement of Banavar and co-workers [12], namely that the optimal topology of a transportation network with all edge flow cost functions being strictly concave is a tree. Following the basic mathematical idea of this proof, we are able to design an efficient global algorithm to construct optimal tree-shaped transportation networks. We also demonstrate by working on some simple examples that, when all the edge cost functions are strictly convex, the resulting optimal transportation network may not necessarily contain loops; whether it is loop-rich or not also depends on the boundary conditions (i.e., input or output flux at every vertex).

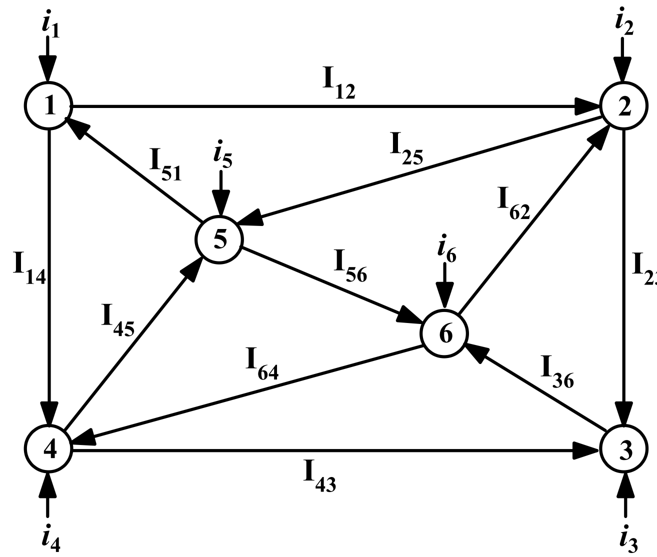

FIG. 2: A simple transportation system. The system is consisted of $N = 6$ vertices, each of them receiving an external flux i_j ($j = 1, 2, \ldots, N$). (If the external flux on vertex j is an input flow, then i_j is positive; if it is an output flow, then i_j is negative.) The external input fluxes are then distributed in the transportation network by internal flows I_{ij} and finally transported out of the system. In this figure, the arrow head of an internal edge denotes the direction of the flow on this edge. The internal flows satisfy the Kirchhoff condition Eq. (3) at each vertex.

II. LOOP ANALYSIS ON TRANSPORTATION FLOWS

A. The model system

Consider a transportation system with N vertices (in the example shown in Fig. 2, $N = 6$ and only those edges with non-zero fluxes are drawn). Each vertex j of the system receives an external flux i_j, which can either be positive (flux in) or be negative (flux out). Since there is no net accumulation of flux within the system, we have the following global condition that

$$\sum_{j=1}^{N} i_j \equiv 0 \ , \tag{2}$$

which means that the total amount of input flux to the system is exactly balanced by the total amount of output flux. The external input flux is transported through the network by internal flows I_{ij} along the edges (i, j) of the system. Since there is no net accumulation of flux at each vertex of the network, the internal flows must satisfy the following Kirchhoff condition for each vertex:

$$i_j \equiv \sum_{k \neq j} I_{jk}, \qquad \text{for } \ i = 1, 2, \ldots, N \ . \tag{3}$$

In Eq. (3) the internal flux satisfies $I_{jk} = -I_{kj}$.

For a transportation system with specified input and output fluxes $\{i_j : j = 1, 2, \ldots, N\}$, an optimal network structure corresponds to a flow pattern $\{I\} \equiv \{I_{ij} : 1 \leq i < j \leq N\}$ of minimal total cost $C[\{I\}]$ as defined by Eq. (1), with the constraint Eq. (3) being observed at all the vertices. In the next subsection we will investigate the case where all the cost functions C_{ij} in Eq. (1) are strictly concave, namely that

$$C_{ij}\big(\lambda |I_{ij}^{(1)}| + (1-\lambda)|I_{ij}^{(2)}|\big) \ > \ \lambda C_{ij}\big(|I_{ij}^{(1)}|\big) + (1-\lambda) C_{ij}\big(|I_{ij}^{(2)}|\big) \ , \tag{4}$$

for any $0 < \lambda < 1$.

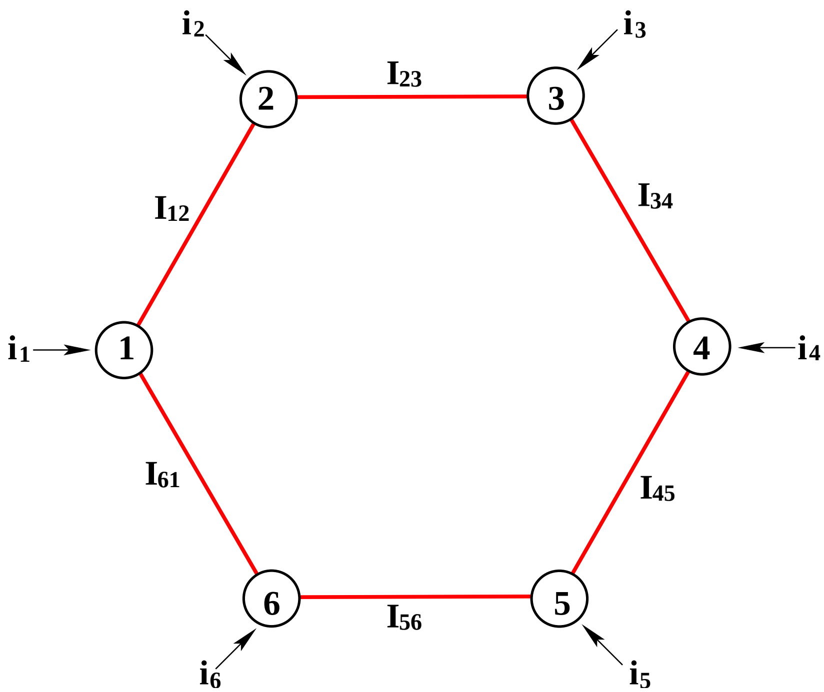

FIG. 3: A transportation loop of $n = 6$ vertices. As there is no net accumulation of currents in the loop, the sum of the external fluxes to the loop satisfies Eq. (2).

B. Optimality of tree-shaped topologies

Let us first consider a transportation network of size n which is in the shape of a single loop (see Fig. 3). Let us fix the flow current $I_{n,1}$ between vertex n and vertex 1 of the loop system. Then all the other edge fluxes along the loop are related to $I_{n,1}$ through

$$I_{i,i+1} = I_{n,1} - f_{i,i+1} \ , \tag{5}$$

where $f_{i,i+1}$ is determined by

$$f_{i,i+1} = -f_{n,1} - \sum_{j=1}^{i} i_j \ , \qquad \text{for} \ \ i = 1, 2, \ldots, n-1 \tag{6}$$

with $f_{n,1} \equiv 0$. The total flow cost of the loop as defined by Eq. (1) is therefore a function of $I_{n,1}$, and hereafter we denote this cost as $C(I_{n,1})$. The n values of $f_{i,j}$ in Eq. (6) depend on the external environment (the $\{i_j\}$ values); some of them may take identical values. For the convenience of later discussions, we denote the $m \leq n$ different values of the $f_{i,j}$ parameters as $\phi_1, \phi_2, \ldots, \phi_m$, with $\phi_1 < \phi_2 < \ldots < \phi_m$.

When the flow current $I_{n,1}$ is restricted to the range of $I_{n,1} \geq \phi_m$, the flow cost on each edge of the loop satisfies $C_{i,i+1}(|I_{i,i+1}|) \equiv C_{i,i+1}(|I_{n,1} - f_{i,i+1}|) \geq C_{i,i+1}(\phi_m - f_{i,i+1})$, due to the fact that the flow cost is an increasing function of the flux. It is obvious to see that the total flow cost $C(I_{n,1})$ will attain its minimal value at $I_{n,1} = \phi_m$ when $I_{n,1}$ is restricted to $I_{n,1} \geq \phi_m$. Similarly it is easy to prove that if $I_{n,1}$ is restricted to $I_{n,1} \leq \phi_1$, $C(I_{n,1})$ will attain its minimal value at $I_{n,1} = \phi_1$. Therefore, to discuss the minimality of the total flux $C(I_{n,1})$ we need only to consider the parameter range of $\phi_1 \leq I_{n,1} \leq \phi_m$.

Let us assume that $\phi_k \leq I_{n,1} \leq \phi_{k+1}$. For the flow cost $C_{i,i+1}(|I_{n,1} - f_{i,i+1}|)$, we know from the concavity condition Eq. (4) that

$$C_{i,i+1}(|I_{n,1} - f_{i,i+1}|) \ \geq \ \frac{\phi_{k+1} C_{i,i+1}(|\phi_k - f_{i,i+1}|) - \phi_k C_{i,i+1}(|\phi_{k+1} - f_{i,i+1}|)}{\phi_{k+1} - \phi_k}$$

$$+I_{n,1}\frac{C_{i,i+1}(|\phi_{k+1}-f_{i,i+1}|)-C_{i,i+1}(|\phi_k-f_{i,i+1}|)}{\phi_{k+1}-\phi_k}\ , \tag{7}$$

where the equality holds *only* when $I_{n,1} = \phi_k$ or $I_{n,1} = \phi_{k+1}$. Applying this inequality to each edge of the transportation loop of Fig. (3), for $\phi_k \le I_{n,1} \le \phi_{k+1}$, we finally obtain the following inequality concerning the total transportation cost

$$C(I_{n,1}) \ge c_1 + c_2 I_{n,1}\ , \tag{8}$$

where c_1 and c_2 are independent of $I_{n,1}$. The equality of Eq. (8) holds *only* when $I_{n,1} = \phi_k$ or $I_{n,1} = \phi_{k+1}$. From Eq. (8) we can conclude that: (a) if $c_2 > 0$, then $C(I_{n,1})$ reaches its local minimum at $I_{n,1} = \phi_k$ in the interval of $\phi_k \le I_{n,1} \le \phi_{k+1}$; (b) if $c_2 < 0$, then $C(I_{n,1})$ reaches its local minimal at $I_{n,1} = \phi_{k+1}$; and (c) if $c_2 = 0$, there are two equal local minima of $C(I_{n,1})$ at $I_{n,1} = \phi_k$ and $I_{n,1} = \phi_{k+1}$.

The above analysis demonstrates that, the local minima of the function $C(I_{n,1})$ can only locate at some or all of the m points of $I_{n,1} = \phi_k$. Consequently the global minimal of $C(I_{n,1})$ can also only locate at some or all of these ϕ_k values. (This fact was demonstrated earlier in Fig. 20 and Fig. 22 of Ref. [21].) Let us assume $I_{n,1} = \phi_k$ is a global minimum of $C(I_{n,1})$, then from Eq. (5) we know that one of the edge fluxes, say $I_{i,i+1}$ must vanish, i.e., $I_{i,i+1} \equiv 0$.

We are now ready to prove the general statement of Ref. [12] that, the structure of an optimal transportation network with strictly concave flow cost functions is a tree. Let us assume that this state is not true and there exist at least one loop of non-zero edge fluxes in the optimal transportation network. We can then take this loop as a new transportation system and regard the fluxes in and out of this loop as external conditions (the i_j value of Fig. 3 now are understood as the sum of the fluxes between the loop and the remaining part of the whole transportation system, plus the external input or output flow at vertex j). Then from the above-mentioned analysis we know that the flux on one edge of this loop must be identically zero to minimize cost. This contradict our original assumption. Therefore, in the optimal transportation network there must not be any loops. The proof finishes.

If the edge flow cost functions are concave but not strictly concave (e.g., $C_{ij}(|I_{ij}|) = |I_{ij}|$), then the equality in Eq. (7) might also hold at intermediate values of $\phi_k < I_{n,1} < \phi_{k+1}$. As a result, some loop-containing transportation structures might be equally optimal as loop-free structures when the total transportation cost is concerned.

When the system's edge flow cost functions are all strictly convex, in general the optimal transportation network will contain loops. However, external conditions are also important now. Just as a simplist example, for a small transport system consisted of only three vertices and the cost functions defined as $C_{ij}(|I_{ij}|) = R_{ij} I_{ij}^2$, we find that if the external inputs of the system satisfies $i_1/i_2 = R_{23}/R_{13}$, the optimal transportation network will be a V-like tree with $I_{12} = 0$.

III. FROM THE LOOP ANALYSIS TO AN EFFICIENT GLOBAL ALGORITHM

The preceding section proved that the optimal transportation network with strictly concave edge flow cost functions should be in a tree topology. Inspired by the loop analysis of Sec. II B, here we introduce a global heuristic algorithm, called the Transient Loop Relaxation (TLR) algorithm, to actually construct such an optimal tree structure.

The TLR algorithm works as follows:

(i) Construct a random initial tree network connecting all the N vertices of a transportation system. Calculate the fluxes on each edge of the tree.

(ii) In each time interval $\Delta t = 1/N$, randomly select a pair of non-neighboring vertices, say vertex i and vertex j, and link an edge between these two vertices. This will lead to the formation of a loop. Then remove one edge of this loop and recalculate the fluxes on all the remaining edges of this loop, while keeping all the input and output fluxes to the loop unchanged. The removed edge is chosen to be one of the edges which make the total flow cost of the loop attain its global minimum.

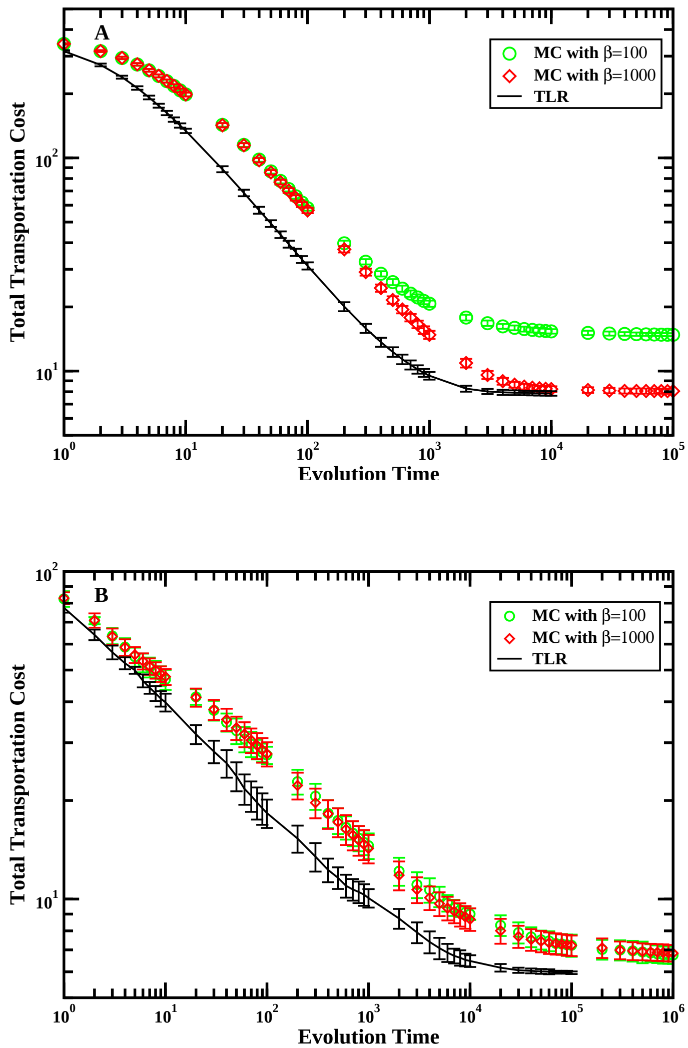

FIG. 4: Comparison of the performances of the two optimization algorithms described in the main text, the Monte Carlo importance sampling algorithm and the TLR (transient loop relaxation) algorithm. (A) Simulation on an artificial system A of the main text. This system contains $N = 1,000$ vertices. (B) Simulation on an artificial system B of the main text. The system has $N = 100$ vertices. In both (A) and (B) each data point is the average over 100 different network structural evolution trajectories. One evolution time step in both figures corresponds to N elementary updates of the algorithm.

(iii) Repeat step (ii) for a number of times until the total flow cost never decreases.

(iv) Output the final tree connection pattern.

An alternative way of searching for an optimal transportation network structure is by Monte Carlo (MC) importance sampling (similar ideas were also used in earlier studies of the Dial model of traffic research [29, 30] and the single-link-flip dynamics in searching of optimal channel network [21, 22] which is equivalent to the zero-temperature limit of the MC sampling method). In this MC algorithm, starting from a randomly constructed tree, at each interval $\Delta t = 1/N$ the following updating is proposed: cutting a randomly chosen branch of the tree and grafting it to another randomly chosen part of the remaining tree. This proposal is accepted if it leads to a decrease in the total transportation cost; if, on the other hand, the transportation cost increases with an amount ΔC, the proposal is accepted with probability $\exp(-\beta \Delta C)$. Here β is an adjustable parameter of the algorithm.

We have compared the performance of the TLR algorithm and the MC algorithm using two simple artificial systems. Both systems, A and B, are composed of N vertices. In system A, $N - 1$ of these N vertices have the same external input flow $i_j \equiv 1$, while in system B, the external flow on vertex j ($j = 1, 2, \ldots, N-1$) is a quenched random integer uniformly distributed in the the interval $[-m, m]$ (we set $m = 10$ in our numerical experiment). In both system A and system B, the edge flow cost function between a pair of vertices is set to be

$$C_{ij}(|I_{ij}|) = \ln(1 + r_{ij}|I_{ij}|) \ , \tag{9}$$

where r_{ij} is a quenched random variable uniformly distributed in the real interval $(0, 1)$.

Our simulation results are shown in Fig. 4A for an artificial system A and in Fig. 4B for an artificial system B. Both figures demonstrate that, the TLR algorithm is much faster than the MC algorithm (either measured by the total number of elementary optimization updates or measured by the absolute searching time), and it also finds network connection patterns with lower total transportation costs than those of the network structures reported by the MC algorithm. Figure 4B also suggests that, when the optimization task becomes more harder, the gap between the performance of the TLR algorithm and that of the MC algorithm becomes more large.

IV. CONCLUSION AND DISCUSSION

In summary, in this paper we have given a proof of the general statement of Ref. [12] that, the optimal structure of a transportation network with strictly concave edge flow cost functions should contain no loops. The proof is based on the mathematical idea of loop analysis, which appears to be more easier to understand compared with the analysis presented in Ref. [12]. Based on the same loop analysis idea, we have constructed a global heuristic algorithm TLR (transient loop relaxation) to search for an optimal loop-free structure for a given transportation system. This TLR algorithm was tested on two artificial transportation systems and was found to be superior to the importance-sampling-based Monte Carlo algorithm.

An unsolved algorithm issue is: does there exist an exact algorithm of polynomial complexity to find a global optimal tree-shaped structure for a given transportation system? It is relatively easy to construct a tree-shaped transportation network which is stable with respect to any single-loop perturbations (i.e., with the addition of an edge between any two non-neighboring vertices). Will such an locally optimal structure always be a structure with the *global* minimal total transportation cost? At the moment, we are unable to give a concrete answer to this important question.

The transient-loop-relaxation algorithm may also be helpful in the searching of optimal network structures for a transportation systems in which all the edge cost functions are convex. In this case, if we assume that the first derivative of each edge cost functions is also continuous, then the cost function $C(I_{n,1})$ of any loop (as defined in Sec. II B) has only one minimal point, and this minimal point is located between two consecutive ϕ values, i.e., $\phi_i \leq I_{n,1} \leq \phi_{i+1}$. The determination of the optimal flow $I_{n,1}$ for this loop is thus made simpler.

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