Structure, Scaling, and Phase Transition in the Optimal Transport Network

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The structure and properties of optimal networks depend on the cost functional being minimized and on constraints to which the minimization is subject. We show here two different formulations that lead to identical results: minimizing the dissipation rate of an electrical network under a global constraint is equivalent to the minimization of a power-law cost function introduced by Banavar *et al.* [Phys. Rev. Lett. **84**, 4745 (2000)]. An explicit scaling relation between the currents and the corresponding conductances is derived, proving the potential flow nature of the latter. Varying a unique parameter, the topology of the optimized networks shows a transition from a tree topology to a very redundant structure with loops; the transition corresponds to a discontinuity in the slope of the power dissipation.

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The design of an optimal network for the distribution of valuables such as water, electricity, or telephone signals is a matter of great practical import in urban planning which has been studied since antiquity [1] and acquired renewed interest during "the war of the currents" between Westinghouse and Edison in the late 1800s [2]. An overview over hydraulic network design principles can be found in [3]. Recently, natural systems such as river networks and vascular systems have been fruitfully interpreted in this light [4–6]. A different family of transportation problems derives from the Monge-Kantorovich problem posed in 1781 [7]. Hence formal models of optimal transport networks have attracted attention over many years [8,9]. However, different studies use different definitions of network and optimize different functionals. For example, Durand [10,11] considers hydraulic networks whose currents derive from a potential, explicitly analogous to electrical networks; the networks are embedded in an ambient space, and he studies the optimal geometry and the relation between the local geometry and local topology. On the other side, Banavar *et al.* [6] propose a more abstract model where the graph is not assumed to be embedded in a target space, nor are the currents through the nodes explicitly constrained to derive from a potential. This allows them to furnish a strict proof that the topology of the optimized flow pattern [6] depends on the convexity of their cost function, but makes a direct physical interpretation of the model more elusive. In the following, we shall introduce a third model of an optimal transport network from whom both of these previous models can be derived, so all formulations are, in fact, equivalent.

Consider an electrical transport network on a graph composed of nodes k interconnected by links (k, l). There is a given current source i_k at each node and the total current input must add to zero: $\sum_k i_k = 0$. There are variable currents I_{kl} flowing through the links; the sum of all currents impinging on a given node k must equal the given current sources: $i_k = \sum_l I_{kl}$ (Kirchhoff's current law). We associate a resistor $R_{kl} \geq 0$ to each link (k, l) and decompose its value as $R_{kl} = (d_{kl}\kappa_{kl})^{-1}$, where $d_{kl} > 0$ is a given weight and the conductances κ_{kl} are variable; considering κ_{kl} as a conductivity per unit length, d_{kl} can be thought of as the length of the link. The dissipation rate J is then a function of the currents I_{kl} through the links and the conductances κ_{kl}:

$$J = \sum_{(k,l)} \frac{I_{kl}^2}{(d_{kl}\kappa_{kl})} \tag{1}$$

We shall minimize this dissipation rate J over the currents I_{kl} and the conductances κ_{kl} with the local constraint given by Kirchhoff's current law, and a supplementary global constraint that the sum over the conductances raised to a given power $\gamma > 0$ is kept constant:

$$K^\gamma = \sum_{(k,l)} \kappa_{kl}^\gamma.$$

One may interpret this constant as an amount of resources we have at our disposal to build the network [12].

Since we allow κ_{kl} and I_{kl} to vary independently, the currents are not explicitly constrained to derive from a potential at the nodes U_k and Kirchhoff's voltage law (the sum of the potential differences on a loop vanishes) need not apply.

Using a Lagrange multiplier λ, we define the function $\Xi(\{\kappa_{kl}\}, \{I_{kl}\})$ as

$$\Xi(\{\kappa_{kl}\}, \{I_{kl}\}) = \sum_{(k,l)} \frac{I_{kl}^2}{(d_{kl}\kappa_{kl})} - \lambda \sum_{(k,l)} \kappa_{kl}^\gamma. \tag{2}$$

The necessary conditions for a minima of J with constant K are then

$$\frac{\partial \Xi}{\partial I_{kl}} = 0, \qquad \frac{\partial \Xi}{\partial \kappa_{kl}} = 0. \tag{3}$$

Let us first consider the derivatives with respect to I_{kl}. Let

$\{\tilde{I}_{kl}\}$, $\{\tilde{\kappa}_{kl}\}$ minimize J. Adding a circular current X_α on a loop α to the currents (Fig. 1) does not violate the constraints. We (re)define the directions of the currents $\tilde{I}_{kl}$ on the loop to be parallel to the loop current X_α. Then

$$0 = \frac{\partial \Xi}{\partial X_\alpha}\bigg|_{X_\alpha=0} = \sum_{\text{loop}\alpha} \tilde{R}_{kl}\tilde{I}_{kl}. \tag{4}$$

Thus Kirchhoff's voltage law holds at the minimum of J, so the currents though the links derive from potential differences between the nodes: $\tilde{I}_{kl} = \tilde{R}_{kl}(U_l - U_k)$. Note that this is not the case for every arbitrary current distribution. For instance, if all currents on the loop in Fig. 1 are positive $\tilde{I}_{kl} > 0$, then there exists no set of $\tilde{R}_{kl} \geq 0$ to fulfill this relation. Let us now consider the derivatives of Ξ with respect to κ_{kl} [Eq. (3)]. With the constraint of a constant K, we obtain an explicit scaling relation between the currents and the conductivity in the minimal configuration:

$$\kappa_{kl} = \frac{(I_{kl}^2/d_{kl})^{1/1+\gamma}}{\left(\sum_{(m,n)}(I_{mn}^2/d_{mn})^{\gamma/1+\gamma}\right)^{1/\gamma}} K. \tag{5}$$

We can now write the total dissipation [Eq. (1)] in terms of the currents alone as

$$J(\{I_{kl}\}) = \frac{1}{K}\left(\sum_{(k,l)}(I_{kl}^2/d_{kl})^{\gamma/1+\gamma}\right)^{1+(1/\gamma)}. \tag{6}$$

Since for $\gamma > 0$, the function $x^{1+(1/\gamma)}$ is monotonically increasing, the original minimization problem is reduced to the minimization of

$$C(\{I_{kl}\}) = \sum_{(k,l)}(I_{kl}^2/d_{kl})^{\gamma/1+\gamma}. \tag{7}$$

By setting

$$\Gamma = \frac{2\gamma}{\gamma+1} \tag{8}$$

and rescaling the weights as $w_{kl} = d_{kl}^{-(\gamma/1+\gamma)}$, the quantity to be minimized is now

$$C(\{I_{kl}\}) = \sum_{(k,l)} w_{kl} I_{kl}^{\Gamma} \tag{9}$$

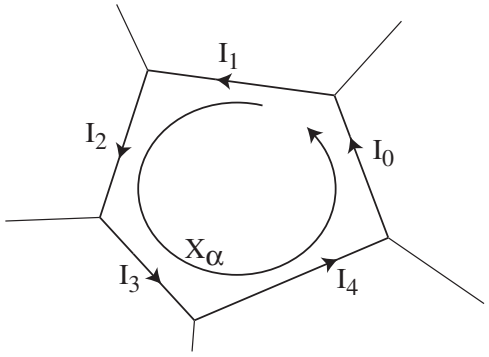

FIG. 1. Sketch of a loop α indicating the direction of the currents. Every perturbation of the I_{kl} satisfying the constraints can be written as a weighted sum of such loops.

which is exactly the model used by Banavar *et al.* [6]. They give a strict proof that for $\Gamma < 1$, the resulting structure may not have any loop, and each spanning tree is a local minimum. For $\Gamma > 1$, there are in general loops and a unique minimum. Because of the correspondence between γ and Γ, this result must apply also to our original model where $\gamma < 1$ ($\gamma > 1$) corresponds to a $\Gamma < 1$ ($\Gamma > 1$).

On the other hand, the correspondence between the different models allows an important conclusion about the model of Banavar *et al.* Since in both formulations, the minimum is obtained by the same set of currents, and since in our model these currents must derive from potential differences between the nodes, this must be true for the minimum of the Banavar *et al.* model, too (see also [13]). We can furthermore write down directly the values of the corresponding resistors as

$$R_{kl} = (d_{kl}\kappa_{kl})^{-1} = A w_{kl} |I_{kl}|^{\Gamma-2} \tag{10}$$

with an arbitrary positive constant A. R_{kl} thus scales explicitly with the local currents for $\Gamma \neq 2$.

Since positive γ corresponds to $0 < \Gamma < 2$, the equivalence of the two models is restricted to this parameter range. $\Gamma > 2$ corresponds to values $\gamma < -1$, for which our model collapses into infinitely many degenerate minima. The relations (3) correspond instead to a saddle node of J: a minimum with respect to the I_{kl} and a maximum with respect to the κ_{kl}. Nevertheless direct inspection shows that the current flow in the Banavar *et al.* model is potential with the set of resistors given by Eq. (10) even for $\Gamma > 2$ [14].

To get a deeper insight into the transition at $\gamma = 1$, we search numerically for the minimal dissipation configuration of an example network, a triangular network of conductivities with a hexagonal border, with equal weights $d_{kl} \equiv 1$. The total number of nodes N_{nodes} scales roughly as the square of the linear dimension of the network, given by the diameter of the graph N_{dia}. Except for those on the border, each node is linked by conductivities to six neighboring nodes.

We place a current source at a corner of the hexagon (i_0), the remaining $(N_{\text{nodes}} - 1)$ nodes present homogeneous distributed sinks; each node absorbs $i_k = -i_0/(N_{\text{nodes}} - 1)$. As an order parameter, we will consider the normalized dissipation rate $J_{\text{min}}/J_{\text{homo}}$, where J_{homo} is the total dissipation with a constant conductivity distribution $\kappa_{kl} \equiv$ const, and J_{min} is the dissipation for the optimized distribution of the conductivities. Note that J_{homo} corresponds also to $\gamma \to \infty$.

The previous discussion allows us to simplify the minimization problem enormously: using the scaling relation between κ_{kl} and I_{kl}, one can restrict the search of the minimum to the space of the currents or the space of conductivities. Furthermore, we can use the fact that the optimized current distribution derives from a potential U_k to construct a simple relaxation algorithm. Starting with a random distribution of κ_{kl}, we calculate first the values of

the potential at the nodes by solving the system of linear equations $i_k = \sum_l R_{kl}(U_k - U_l)$, then the currents through the links I_{kl} are determined. We use these currents to determine a first approximation of the optimal conductivities on the basis of the scaling relation. Then, the currents are recalculated with this set of conductivities, and the scaling relation is reused for the next approximation. These steps are repeated until the values have converged. We check by perturbing the solution that it actually is a minimum of the dissipation, which was always the case.

For all $\gamma > 1$, independently of the initial conditions, the same conductivity distribution is obtained, which conforms to the analytical result of [6]: there exists a unique minimum which is therefore global.

Furthermore, the distribution of κ_{kl} is "smooth," varying only on a "macroscopic scale," as show in Fig. 2(a). No formation of any particular structure occurs. However, the conductivity distribution is not isotropic. We can interpret the conductivity distribution as a discrete approximation of a continuous, macroscopic conductivity tensor (see also [10]). The smooth aspect of the distribution is conserved while approaching $\gamma \to 1$ while the local anisotropy increases, while the values of all κ_{kl} remain finite, even if they get very small. For $\gamma = 1.5$ and $N_{\text{dia}} = 15$, the conductivity distribution spreads already over eight decades and becomes still broader as $\gamma \to 1^+$, in which limit the number of iteration steps diverges as the minima becomes less and less steep.

$\gamma = 1$ presents a marginal case. The results of the simulation suggest that the minimum is highly degenerate; i.e., there are a large number of conductivity distributions yielding the same minimal dissipation.

For $\gamma < 1$, the output of the relaxation algorithm is qualitatively different [Fig. 2(b)]. A large number of conductivities converge to zero so that no loop remains. The highly redundant network is transformed to a spanning tree topology and the currents are canalized in a hierarchical manner. This, too, is predicted by the analytical results [6]. In contrast to $\gamma > 1$, the conductivity distribution cannot be interpreted as a discrete approximation of a conductivity tensor: for $N_{\text{dia}} \to \infty$, the structure becomes fractal.

For different initial conditions, the relaxation algorithm yields trees with different topologies: each local minima in the high-dimensional and continuous space of conductivities $\{\kappa_{kl}\}$ corresponds to a different tree topology. To find the global minima with $\gamma < 1$, we search consequently in the (exponentially large) space of tree topologies using a Monte Carlo algorithm. (We start with some initial tree and then switch links without creating loops and without disconnecting a part of the network.) Note that for a tree topology, the currents do not depend on the values κ_{kl} and, using the scaling relation, one may directly write down the dissipation rate for a given tree; the iterative relaxation is not necessary here. This regime has been widely explored in the context of river networks [4,5,13,15], mainly for a set of parameters that corresponds, in our case, to $\gamma = 0.5$. An example of a resulting minimal dissipation tree structure is given in Fig. 2(c). Note also, that the scaling relations can be seen as some kind of erosion model: the more currents flows through a link, the better the link conducts [4].

The qualitative transition is reflected also quantitatively in the value of the minimal dissipation [Fig. 3(a)]. The points for $\gamma > 1$ were obtained with the relaxation algorithm, the points $\gamma < 1$ by optimizing the tree topologies with a Monte Carlo algorithm. For $\gamma \to \infty$, $J_{\text{min}}/J_{\text{homo}} \to 1$ by definition; for $\gamma \to 0$, $J_{\text{min}}/J_{\text{homo}} \to 0$, because the vanishing κ_{kl} allow the remaining $\kappa_{kl} \to \infty$.

Figure 3(b) shows the behavior of minimal dissipation rate close to $\gamma = 1$. For γ smaller than 1, the relaxation method only furnishes a local minimum, the Monte Carlo algorithm searching for the optimal tree topologies gives lower dissipation values. The different values corresponding to different realization indicate that the employed Monte Carlo method does not find the exact global minima. For $\gamma > 1$, the optimal tree obtained by the Monte Carlo algorithm is not the optimal solution since the absolute and only minima has loops. The dissipation rate which results from the relaxation algorithm is then, of course, lower than the dissipation of any tree. While the curve is continuous, the crossover at $\gamma = 1$ shows a clear change in the slope of $J_{\text{min}}(\gamma)$. One could interpret this behavior as a second order phase transition. (The change in

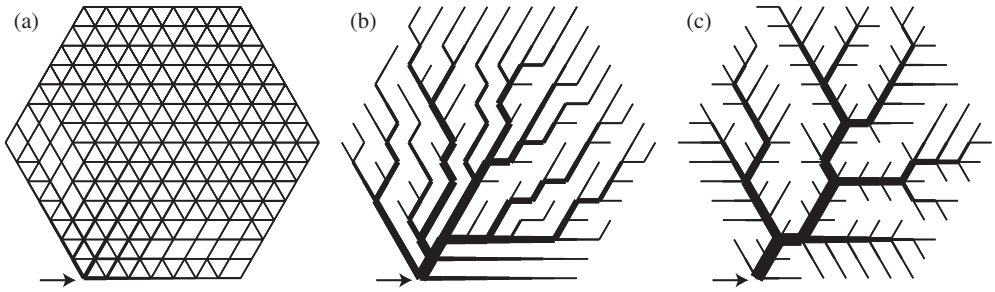

FIG. 2. Examples of the optimized conductivity distributions obtained by the relaxation method for (a) $\gamma = 2.0$ and (b) $\gamma = 0.5$. For $\gamma < 1$, the relaxation leads in general only to a local minimum. The global minimum can be approached by searching in the space of tree topologies. The result for $\gamma = 0.5$ is shown in (c). The arrows indicate the localized inlet.

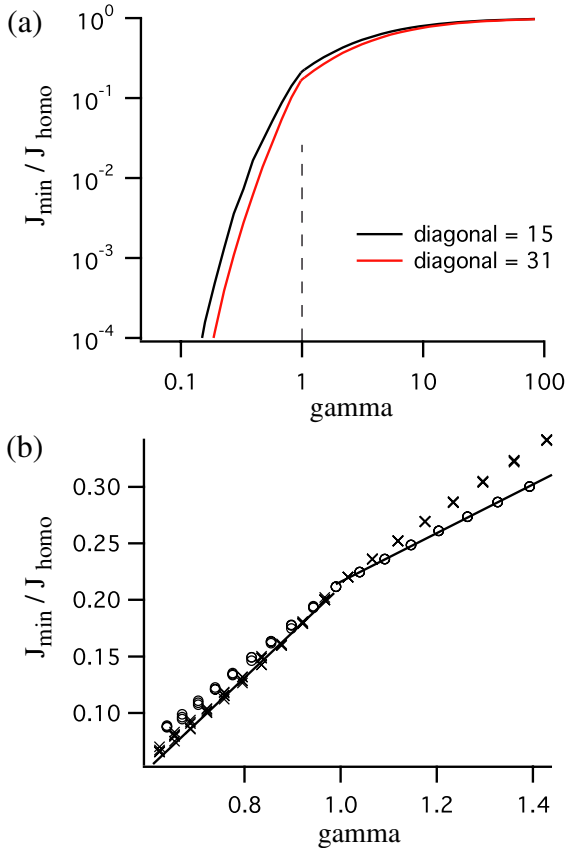

FIG. 3 (color online). (a) The normalized minimum dissipation rate $J_{\min}/J_{\text{homo}}$ as a function of γ for a network with $N_{\text{dia}} = 15$ (462 links) and a network with $N_{\text{dia}} = 31$ (2070 links, in red or in gray). Note the discontinuity of the slopes at $\gamma = 1$. (b) A detailed view of the crossover at $\gamma = 1$ for $N_{\text{dia}} = 15$. Cross symbols show data points obtained by optimizing a tree topology, circles show the output of the relaxation algorithm. The continuous lines indicate the actual minimum.

slope is, of course, preserved in the function $C(I_{kl})$ used by [6].)

As an intriguing practical application of these models, one may, for instance, cite the venation of plant leaves. The leaf venation pattern forms a hierarchical and shows an enormous redundancy of loops [16,17]. Secondary veins branch from a central primary vein and connect on the other end to other secondary veins; third order veins are connected at both ends to either first or second order veins, and only at the very small scale (veins of the order of nine or ten), the veins do not close loops but form small trees. It has been argued that this particular structure optimizes the water distribution in the leaf [18,19]. From experimental evidence [20] it is known that this water transport through the veins derives from a pressure gradient; our model should therefore a rather good description of this biological network. However, we showed that optimization either leads to a tree topology, or to no structure at all. The hierarchical loop structure of the venation network can thus not be explained by the optimization of a steady state water transport, even if Murray's law seems to hold at the nodes of the network [21].

[1] While most Roman water piping was suboptimally laid out as individual parallel pipes from homes to the *castella* (water towers), the water grid at Antioch was arranged hierarchically along the street grid; see A. Trevor Hodge, *Roman Aqueducts and Water Supply* (Duckworth Publishing, London, 2002), 2nd ed., pp. 320–321.
[2] T. A. Edison, U.S. Patent No. 602, 1880, p. 4, lines 20–24, states "from main conductors on principal streets subsidiary main conductors are laid through side streets; from the street conductors, wherever desired, derived circuits are led into the houses. . .."
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[14] Given a field $\mathbf{v}$ with a curl, a scalar field ϕ such that $\nabla \wedge \phi\mathbf{v} = \mathbf{0}$ is called an integrating factor; integrating factors always exist in two dimensions, or, in their discrete versions, for planar graphs as in here. But while there could be in principle a set of resistors that would make arbitrary currents in a planar model derive from a potential, such resistors would neither be guaranteed to be positive nor to depend only locally on the currents, as our result shows.
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