Pareto Optimality in Multilayer Network Growth

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We model the formation of multilayer transportation networks as a multiobjective optimization process, where service providers compete for passengers, and the creation of routes is determined by a multiobjective cost function encoding a trade-off between efficiency and competition. The resulting model reproduces well real-world systems as diverse as airplane, train, and bus networks, thus suggesting that such systems are indeed compatible with the proposed local optimization mechanisms. In the specific case of airline transportation systems, we show that the networks of routes operated by each company are placed very close to the theoretical Pareto front in the efficiency-competition plane, and that most of the largest carriers of a continent belong to the corresponding Pareto front. Our results shed light on the fundamental role played by multiobjective optimization principles in shaping the structure of large-scale multilayer transportation systems, and provide novel insights to service providers on the strategies for the smart selection of novel routes.

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The interactions among the basic units of many natural and man-made systems, including living organisms, ecosystems, societies, cities, and transportation systems, are well described by complex networks [1–5]. Often these systems are subject to different types of concurrent, and sometimes competing, constraints and objectives, such as the availability of energy and resources, or the overall efficiency of the resulting structure. It is therefore reasonable to assume that the systems that we observe today are the result of a delicate balance between contrasting forces, which can be modeled by means of an underlying optimization process under a set of constraints [6–10]. For instance, the emergence of scale-free networks can be explained by simple optimization mechanisms [11–15], while it has been found that many of the properties of biological networks result from the simultaneous optimization of several concurrent cost functions [16–25]. However, multiobjective optimization has not yet been linked to the most recent advances in network science, based on multilayer network representations of real-world systems [26–29]. Recent studies have shown that the presence of many intertwined layers in a network is responsible for the emergence of novel physical phenomena including abrupt cascading failures [30–32], superdiffusion [33], explosive synchronization [34], and the appearance of new dynamical phases in opinion formation [35,36] and in epidemic processes [37,38]. Moreover, multiplexity can have an impact on practical problems such as air traffic management [39–41] and epidemic containment [42,43]. As a result, understanding how multilayer networks evolve [44–46] is becoming of central importance in various fields.

In this Letter we propose a model of multilayer network growth in which the formation of links at each layer is the result of a local multiobjective optimization (MOO), i.e., a process where two or more objective (cost) functions, often in conflict with each other, have to be simultaneously minimized or maximized. Within this framework, the concept of Pareto optimality naturally arises. By introducing the dominance strict partial order [47], the solution of a MOO problem consists of a set of *nondominated* or *Pareto-optimal* points in the solution space. Intuitively, these points represent those solutions for which no improvement can be achieved in one objective function without hindering the other objective functions. The collection of nondominated points constitutes the *Pareto surface* or *Pareto front* (PF) [48,49].

The multiplex multiobjective optimization (MMOO) model we propose is inspired by the observation that the formation of edges in many real-world transportation networks [50,51] is often subject to concurrent spatial and economical constraints [52–54]. On the one hand, there is the tendency to accumulate edges around nodes that are already well connected, in order to exploit the economy of scale associated with hubs. On the other hand, each service provider usually tends to minimize the competition with other existing service providers. We show that, by combining these two mechanisms, the MMOO model is able to reproduce quite accurately the structural features of three large-scale multiplex transportation systems, namely, the UK railway network, the UK coach network, and the six continental air transportation networks [55–58]. The MMOO model provides a reasonable explanation for the emergence of highly optimized heterogeneous multiplex networks.

Multiplex multiobjective optimization model.—Let us consider a multiplex transportation network with N nodes and M layers, where nodes represent locations and layers represent service providers, e.g., airline, train, or bus companies. Each layer is the graph of routes operated by one of the service providers. The network can be described by a set of adjacency matrices $\{A^{[1]}, A^{[2]}, \ldots, A^{[M]}\} \in \mathbb{R}^{N\times N\times M}$, where the entry $a_{ij}^{[\tau]}$ is equal to 1 if i and j are connected by a link at layer τ (meaning that provider τ, with $\tau = 1, 2, \ldots, M$ operates a route between location i and j), while $a_{ij}^{[\tau]} = 0$ otherwise. We denote by $k_i^{[\tau]} = \sum_j a_{ij}^{[\tau]}$ the degree of a node i at the layer τ, and by $K^{[\tau]} = \frac{1}{2}\sum_i k_i^{[\tau]}$ the total number of links of layer τ. An important multiplex property of a node i is the overlapping (or total) degree $o_i = \sum_\tau k_i^{[\tau]} = \sum_j o_{ij}$, namely, the total number of edges incident on node i at any of the layers of the multiplex [59], where $o_{ij} = \sum_\tau a_{ij}^{[\tau]}$ is the overlap of edge (i, j) [59,60], that is the number of layers at which i and j are connected by an edge.

In the model we assume that service providers join the system one after the other, each one with a predetermined number of routes that they can operate. This means that the multilayer network acquires a new layer at each (discrete) time step τ. When the layer joins the system, the new provider tries to place its routes in order to maximize its profit. To this end, a provider would prefer to have access to as many potential customers as possible (i.e., to connect locations with large population), while minimizing the competition with other providers (i.e., to avoid to operate a route if it is already operated by other providers). In order to mimic these two competing drives, we set the probability to create an edge between node i and node j at the new layer τ as

$$p_{ij}^{[\tau]} \propto \frac{o_i^{[\tau-1]} o_j^{[\tau-1]} + c_1}{o_{ij}^{[\tau-1]} + c_2} \qquad \tau = 2, \ldots, M, \tag{1}$$

where $o_i^{[\tau-1]}$ and $o_{ij}^{[\tau-1]}$ are, respectively, the overlapping degree of node i and the edge overlap of (i, j) at time $\tau - 1$. The non-negative constants c_1 and c_2 allow a nonzero probability to create a new edge to a node that is isolated at all the existing layers. The rationale behind Eq. (1) is that the overlapping degree o_i of node i can be used as a proxy of the population living at that location. Hence, in the same spirit of the "gravity model" [61,62], creating a link between node i and node j with a probability proportional to the product $o_i o_j$ will increase the chances for a provider to access a large set of customers. Similarly, by requiring that $p_{ij}^{[\tau]}$ is inversely proportional to the edge overlap $o_{ij}^{[\tau-1]}$ we discourage the creation of a new route between two locations if they are already served by a large number of other providers, thus modeling the tendency of providers to avoid competition. The two competing mechanisms we propose can be formalized as a MOO problem:

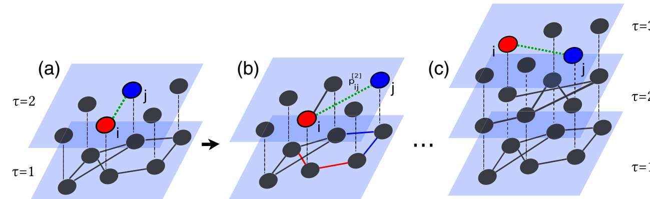

FIG. 1. Illustration of the airline growth model. (a) At time $\tau = 2$ a new layer arrives with $K^{[2]}$ links to be placed, and the first edge is placed uniformly at random among all possible pairs of nodes. (b) The remaining $K^{[2]} - 1$ links are placed according to the probability $p_{ij}^{[2]}$ in Eq. (1). (c) The same procedure is repeated for each layer τ until a multiplex with M layers is obtained.

$$\begin{cases} \max \mathbf{F} \\ \min \mathbf{G} \end{cases} = \begin{cases} F^{[\tau]} = \sum\limits_{i,j:a_{ij}^{[\tau]}=1} (o_i o_j + c_1) \\ G^{[\tau]} = \sum\limits_{i,j:a_{ij}^{[\tau]}=1} (o_{ij} + c_2) \end{cases} \tag{2}$$

where the efficiency function $F^{[\tau]}$ accounts for the number of potential customers, while $G^{[\tau]}$ measures the competition due to route overlaps.

The MMOO model is illustrated in Fig. 1. The first layer is a connected random graph with $K^{[1]}$ edges. At each step τ, with $\tau = 2, \ldots, M$, a new layer is created. The first of the $K^{[\tau]}$ edges of the new layer is placed uniformly at random among the $\binom{N}{2}$ possible edges. In order to obtain a connected network, the remaining $K^{[\tau]} - 1$ links are created according to the probability in Eq. (1), yet ensuring that one of the two endpoints of the selected edge belongs to the connected component at that layer. The total number of links at each of the M layers are external parameters of the model. Although considering the routes of each company as fixed over time may look like an unrealistic oversimplification, in all the systems we have considered, providers update their network of routes normally at a very slow rate, which justifies our assumption to consider the routes on each layer as quasi-static. In fact, rearranging a set of train services or flights entails substantial logistic and economic investments, since railway licenses and airport slots are normally allocated over time scales of several years.

Results.—We have used the MMOO model to reproduce the structure of three different multiplex transportation systems. The first data set includes six multiplex air

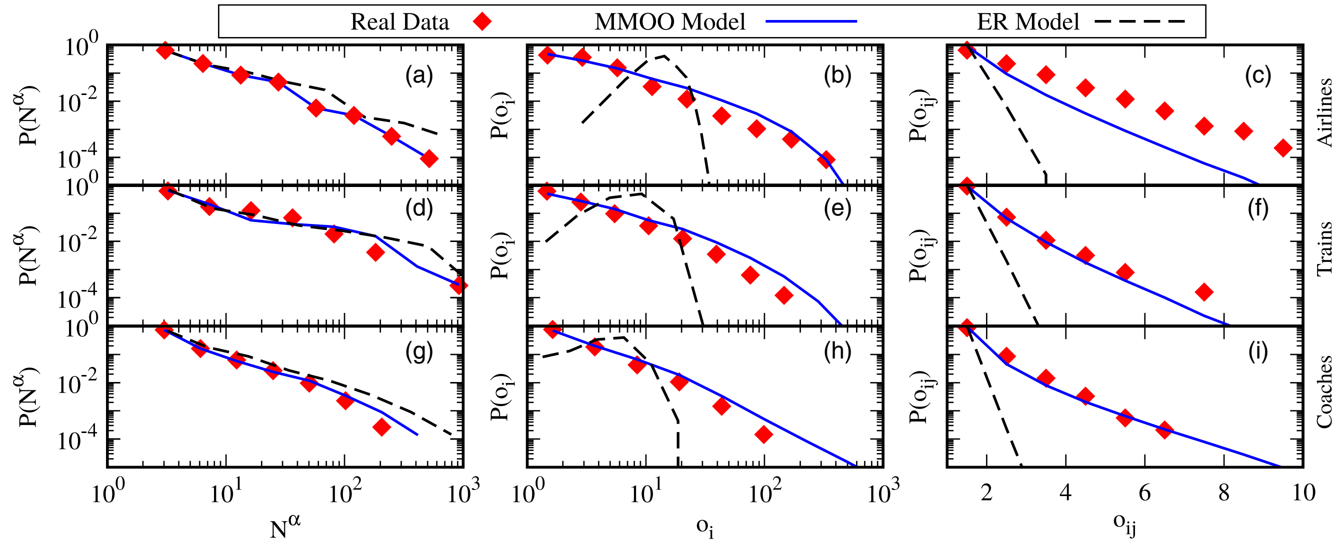

FIG. 2. Distributions of layer activity $N^{[\alpha]}$ (left column), node total degree o_i (middle column), and edge overlap o_{ij} (right column). The multiplex networks (red diamonds) of North America airlines (top row), UK train services (middle row), and UK coach services are compared to the corresponding multiplex networks generated by the MMOO model (solid blue lines) and to multiplex networks whose layers are Erdös-Rényi graphs [67] (dashed lines). The results shown are averaged over 10^3 realizations (standard deviations are indistinguishable from the symbols).

transportation networks, each representing the airline routes operated in a continent. Each network has between 200 and 1000 nodes (airports) and between 35 and 200 layers (carriers) [57]. We have constructed the other two data sets, respectively, from the UK national railway timetable (41 companies operating over about 1600 stations) and from the UK national coach timetable (1207 companies and over 12 000 coach stations). See Ref. [58] for details. For each network, we generated 10^3 independent permutations of the sequence $\{K^{[1]}, K^{[2]}, \ldots, K^{[M]}\}$ of the total number of links at each layer in the data set. Then, for each permutation, we ran 50 independent realizations of the model. In our simulations we used a Metropolis-Hastings algorithm [63] to sample form the distribution in Eq. (1). In Fig. 2 we report the distributions of layer activity $N^{[\alpha]}$ (number of nonisolated nodes at each layer), total node degree o_i, and edge overlap o_{ij} of the multiplex networks obtained with the MMOO model, where we set $c_1 = c_2 = 1$. The two-sample Cramer–von Mises statistical test [64] provides convincing evidence that the synthetic distributions are compatible with the original ones [p value < 0.01, except for panel (c), where $p < 0.2$]. It is worth noticing that the MMOO model naturally reproduces the heterogeneous distribution of node total degree and the decreasing exponential behavior of the edge overlap o_{ij}, which respectively mirror the heavy-tailed distribution of city size [65,66] and the tendency of service providers to reduce the competition on single routes [56]. It is also possible to fine-tune the values of c_1 and c_2 in Eq. (1) in order to accurately reproduce also other structural properties of the three transportation networks, such as the distributions of node activity B_i (number of layers at which node i is not

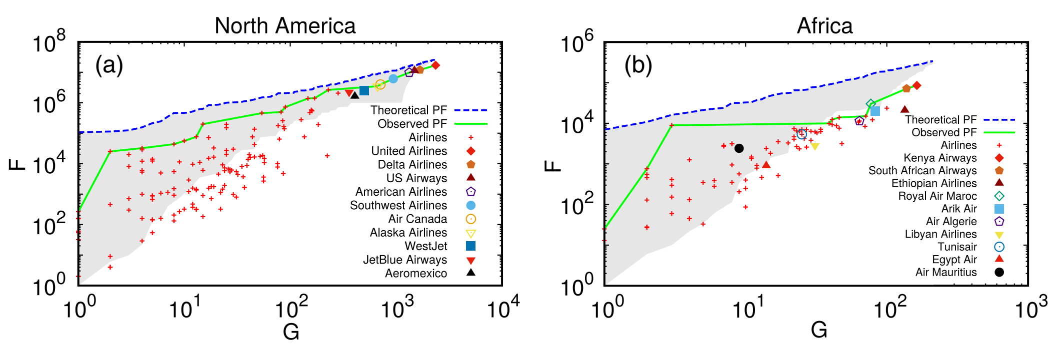

FIG. 3. Observed (solid green line) and theoretical (dashed blue line) Pareto fronts for the continental airline networks of (a) North America and (b) Africa. The top ten airlines by number of passengers in 2013 are highlighted. For each system, the theoretical Pareto front was obtained as the nondominated points of 10^5 realizations of the MMOO model (the range of variability of the simulations is indicated by the shaded grey region).

TABLE I. The potential improvement attainable by a system in the $F - G$ plane is measured by the normalised relative hypervolume Δ_H, where smaller values of Δ_H correspond to more optimized networks. The ranking of continents by Δ_H is reported in the table together with the economical performance of each continent, as measured by the average GPD per capita.

Continent	Δ_H	GDP (US \$)
North America	6.82×10^{-5}	17 892
Asia	7.79×10^{-5}	14 070
Europe	1.07×10^{-4}	36 784
South America	5.50×10^{-4}	9359
Oceania	5.81×10^{-4}	13 064
Africa	8.82×10^{-4}	2843

isolated) and the pattern of pairwise interlayer correlations. See Ref. [58] for more details.

Pareto fronts and system efficiency.—By considering the multiobjective optimization framework formally defined in Eq. (2), it is possible to compare providers by looking at their position in the efficiency-competition plane defined by the two functions F and G and shown in Fig. 3. We focused on the air transportation networks and extracted from the empirical data the *observed Pareto front* of each continental network, i.e., the set of all the nondominated points in the F-G plane. Surprisingly, we found that most of the Pareto-optimal points correspond to the most important companies in the continent (e.g., flagship, mainline, and large low-cost carriers), and in particular with those carrying the largest number of passengers.

In order to quantify the potential improvement attainable by a system in the F-G plane, we used a multiobjective optimization algorithm [68] to generate 10^5 synthetic multiplex networks for each continent. We then computed the so-called *theoretical Pareto front*, consisting of the Pareto-optimal points resulting from all the simulations, reported in Fig. 3 as a dashed blue line. The closer the observed PF is to the theoretical PF, the better the system approaches the best possible solution in the F-G plane. Interestingly, the observed PF of the North American airline network is relatively closer to its theoretical PF, while for the African airlines we observe a larger gap between the two curves. This means that, on average, the African airlines may obtain a greater improvement in the F-G plane than North American companies. A quantitative way to associate a number to a Pareto Front $\mathcal{P}$ is by means of the hypervolume indicator $I_H(\mathcal{P})$, that is the Lebesgue measure of the union of the rectangles defined by each point in the front $\mathcal{P}$ and a reference point [58,69,70]. The distance between an observed PF, $\mathcal{P}^{\mathrm{obs}}$, and the corresponding theoretical PF, $\mathcal{P}^{\mathrm{th}}$, can be quantified through the relative normalized hypervolume $\Delta_H = |I_{H_{\mathcal{P}\mathrm{obs}}} - I_{H_{\mathcal{P}\mathrm{th}}}|/(I_{H_{\mathcal{P}\mathrm{th}}} K)$. By dividing the relative hypervolume difference by the total number of routes K, it is possible to compare the level of

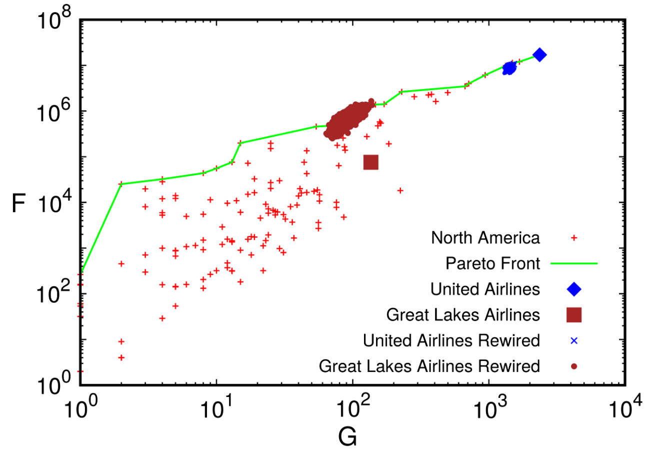

FIG. 4. Reshaping the routes of two North American airlines in the F-G plane. United Airlines, a Pareto-optimal company (blue diamonds), cannot be improved any further by our model, while Great Lakes Airlines (brown squares) can potentially get much closer to the Pareto front.

potential improvement of two multiplex networks with respect to their corresponding theoretical PF. We argue that the value of Δ_H can be used as a proxy of the technological advancement of a transportation system, with smaller values of Δ_H indicating more optimized configurations. Table I reports the ranking of the continents induced by Δ_H, where North America and Asia lead the pack, while Africa is lagging behind. Interestingly, that ranking is positively correlated with the ranking induced by continental GDP per capita [71] (Kendall's $\tau_b = 0.6$, $p \approx 9 \times 10^{-2}$).

Finally, we show that our model can in principle be used by new companies entering the market, as a guide to place their routes in the most effective way. We run simulations of a slightly different version of the model, where all the layers are fixed and identical to the observed ones except for one of them, which represents a new service provider. The last layer is constructed according to Eq. (1). As shown in Fig. 4, we found that in general the companies lying on the observed Pareto front cannot substantially improve their position in the F-G plane, meaning that their routes have evolved over time according to an effective optimization process. Conversely, our model is able to improve the position in the F-G plane of suboptimal and nonoptimal airlines.

Conclusions.—The introduction of multiobjective optimization principles in the modeling of multilayer systems allows us to obtain simple, effective explanations for the evolution of real-world transportation networks. In particular, the systematic exploration of the possible local improvements in the efficiency-competition plane at the level of single carriers, that we have used here to characterize the technological advancement of a continent and the effectiveness of the network of single carriers, can be employed in practice to inform the placement of new routes, and to compare alternative expansion strategies. The proposed methodology can be readily applied to any system whose multilayer structure is the result of the interactions between two or more conflicting objective functions, paving the way to a more accurate characterization of many different natural and man-made complex systems.

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