Most probable paths in temporal weighted networks: 
An application to ocean transport

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(Dated: November 26, 2014)

PACS numbers: 89.75.Hc, 47.27.ed, 92.10.Lq

Many real-world systems can be studied by using the network paradigm [1 2]. Though in many of these situations the connections between network nodes are constant in time and it is sufficient to adopt a static network description, this approach may not be always suitable and a temporal network description is required [3]. Relevant examples are epidemic spreading, human communication or transportation networks, i.e. systems where the strong time variability plays a crucial role in determining connections and interactions [4–6]. Also, approaching continuous dynamical systems from a network perspective [7 8] requires a spatio-temporal discretization that, in the non-autonomous case, often determines a marked time-dependence of the resulting networks. This feature is clearly recognizable, in particular, in climate networks [9–12] and in networks describing connectivity by fluid flows [13 14].

Prominent connectivity patterns in networks can be revealed by introducing the concept of paths [1 2]. While its definition is simple and intuitive for static or aggregated networks, for the temporal case paths between nodes can suddenly appear and disappear in time [3 15–22]. Thus, there is recently a focus towards the definition and characterization of paths in temporal networks. The concept of shortest path in static network analysis has been generalized to include information on the time necessary to establish a space-time connection between nodes. This was the motivation behind the development of fastest path analysis, specially for unweighted and undirected networks [3 23]. Although it is relevant to study the time required to build a path among two nodes, it is equally crucial to understand how to quantify the importance and the distribution of such paths. This issue becomes essential when one tries to exploit this information in order to define and evaluate global network properties, for example betweenness centrality.

In this Letter we extend the concept of most probable path (MPP) [23 26] to the case of temporal, weighted and directed networks. We quantify the relative importance of the MPP with respect to the whole set of paths, and to the subset of highly probable paths which incorporate most of the connection probability. These concepts are used to provide alternative definitions of betweenness centrality. We apply our formalism to a transport network describing surface flow in the Mediterranean Sea. Despite the full transport dynamics is described by a very large number of paths we find that, for realistic time scales, only a very small subset of high probability paths (or even a single most probable one) is enough to characterize global connectivity properties of the network.

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In this Letter we extend the concept of most probable path (MPP) [23 26] to the case of temporal, weighted and directed networks. We quantify the relative importance of the MPP with respect to the whole set of paths, and to the subset of highly probable paths (HPPs) incorporating most of the connection probability. Using such sets of paths we are able to define a betweenness centrality measure for temporal weighted networks. The approach presented here is applied to a flow network describing ocean water transport by surface currents in the Mediterranean Sea. In this example we demonstrate that information contained in MPPs (or in small subsets of HPPs) suffices to describe all major transport properties, despite the number of such paths being just a very small fraction of the full set. The MPPs correspond to the main carriers of ocean mass transport (showing connectivity patterns) and MPP-betwenness to a measure for a clear identification of the main avenues of water transport in the Mediterranean Sea.

Definitions and notation. The analysis is restricted to a time interval \([t_0, t_M]\) in which \(M + 1\) snapshots are taken at times \(t_l = t_0 + l\tau\), \(l = 0, 1, ..., M\), with \(\tau\) the time between them. We consider a temporal, directed and weighted network of \(N\) nodes. Its time-dependent connectivity is described by a set of weighted adjacency matrices \(A^{(l)}\), \(l = 1...M\), in which the matrix element \(A^{(l)}_{ij} \geq 0\) specifies the strength of connectivity from \(i\) to \(J\) during the time interval \([t_{l-1}, t_l]\). A convenient way to analyze the system is using time-ordered graphs (TOGs) [19]. Formally, the TOG can be considered a static network of \(N \times (M + 1)\) nodes with directed and causal links. For each snapshot \(l\), a group \(V(t_l)\) of \(N\) nodes replicating the nodes of the original network can be defined. Links are then established only from nodes at successive times, i.e. from \(i_{l-1} \in V(t_{l-1})\) to \(j_l \in V(t_l)\) with the weights given by those in the original temporal network: \(A^{(l)}_{i_{l-1}, j_l}\).

Flows in networks and most probable paths. We now consider a flow or transport process by releasing inde-
dependent random walkers in each node of the network. Their motion is assumed to be Markovian and is defined by single-step transition probabilities proportional to the entries in the adjacency matrices. Specifically the probability of reaching node \( k_l \) at time \( t_l \) under the condition of being at \( k_{l-1} \) at time \( t_{l-1} \) is \( T_{k_{l-1},k_l}^{(l)} \). Here \( A_{k_{l-1},k_l}^{(l)} \) is the out-degree of node \( k_l \) during time step \( l \), so that \( \sum_j T_{k_j}^{(l)} = 1 \). A generic \( M \)-step path \( \mu \) between two nodes \( I \) and \( J \) is defined as a \((M + 1)\)-uplet \( \mu \equiv \{ I, k_1, ..., k_{M-1}, J \} \) providing a sequence of nodes crossed to reach \( J \) at time \( t_M \) from \( I \) at time \( t_0 \). Under the Markovian assumption the probability for a random walker to take the path \( \mu \) is:

\[
(p_{IJ}^M)_{\mu} = T_{k_1}^{(1)} T_{k_{l-1},k_l}^{(l)} T_{k_{M-1},J}^{(M)}
\]

The most probable path (MPP) \( n_{IJ}^M \) is the path that maximizes Eq. (1) with respect to the intermediate nodes \( k_2, ..., k_{M-1} \). Its probability is denoted by \( P_{IJ}^M = \max_{\mu} (p_{IJ}^M)_{\mu} \). The exact maximization of Eq. (1) can be obtained iteratively by noting that in the first step the maximum probability to reach a given node \( k_1 \) is simply \( P_{IK}^1 = T_{k_1}^{(1)} \), and then using the recurrence

\[
P_{IK}^{l+1} = \max_{k_l} (P_{IK}^l T_{k_{l+1}}^{(l+1)})
\]

for \( l = 1, 2, ..., M - 1 \) until reaching \( k_M = J \). This type of iterative optimization is similar (taking logarithms of the probabilities involved) to the one used to find optimal configurations of directed polymers in random media [27] and can be considered as an adaptation of the classical Dijkstra algorithm [28] to the layered and directed structure of the TOG. The computational cost of the maximization is strongly reduced by calculating first accessibility matrices [21] and restricting the maximization search to the set of nodes that are accessible from \( I \) and for which \( J \) results accessible as well.

The number of paths connecting two nodes increases with \( M \), therefore one could argue whether the most probable path alone is a good representation of the transport dynamics. A proper quantity to assess this is \( \lambda_{IJ}^M = P_{IJ}^M / \sum_{\mu} (p_{IJ}^M)_{\mu} \), determining the fraction of probability carried by the MPP between \( I \) and \( J \) with respect to the sum of the probabilities of all paths connecting these nodes after \( M \) steps. Note that the sum in the denominator can be efficiently computed as the entry \((I,J)\) in the matrix product \( \prod_{l=1}^M T^{(l)} \). Depending on the network under investigation, the MPP can actually carry a significant fraction of the total connection probability. When this is not the case we can relax the definition of MPP and define a subset of HPPs which carry most of the probability. In particular we want to identify paths characterized by individually carrying a probability larger than a fraction \( \epsilon \) of the MPP probability, i.e. larger than \( \epsilon P_{IJ}^M \), with \( 0 \leq \epsilon \leq 1 \). Exhaustively searching for all such paths becomes computationally prohibitive except for the smallest \( N \) and \( M \) values. Here we compute the set \( Q_{IJ}^M \) of all paths of \( M \) steps between \( I \) and \( J \) that are constructed by joining the MPP from \( I \) to an intermediate \( k_l \) and the MPP from \( k_l \) to \( J \). In principle there would be \((M - 2) \times N\) such paths, one for every choice of the intermediate \( k_l \), but this number is in fact much smaller when considering that \( k_l \) should be accessible from \( I \) [21], that \( J \) should be accessible from \( k_l \) itself, and that many of the resulting paths turn out to be repeated. Out of these we consider the subset \( K_{IJ}^M (\epsilon) = \{ \mu \in Q_{IJ}^M | (p_{IJ}^M)_{\mu} > \epsilon P_{IJ}^M \} \). This set contains the MPP, and although it may miss some of the paths with probability larger than \( \epsilon P_{IJ}^M \), we expect it to contain a sufficiently representative sample of them. This can be checked by calculating \( \lambda_{IJ}^M (\epsilon) = \sum_{\mu \in K_{IJ}^M (\epsilon)} (p_{IJ}^M)_{\mu} / \sum_{\mu} (p_{IJ}^M)_{\mu} \), the fraction of probability carried by this set of HPPs.

MPP-betweenness. Equipped with the above definitions we can now characterize network properties that are dependent on optimal paths in different ways. One of these is the concept of betweenness centrality, which is generally defined as the proportion of shortest paths passing through a node. We introduce here a definition based on the number of most probable paths crossing a node. Specifically we define the betweenness of node \( K \) after \( M \) steps as \( B_K^M = \sum_{I,J,K} g_{IJ,K}^M / N_M \), where the sum is over all pairs of initial nodes \( I \) and final accessible nodes \( J \), \( N_M \) is the total number of connected pairs of nodes at time step \( M \) (computable from accessibility matrices [21]), and \( g_{IJ,K}^M \) is the number of times the node \( K \) appears in the most probable path connecting \( I \) and \( J \). Fixing the time interval \( M \) corresponds to considering paths with the same temporal duration. In this way we ignore connections that are occurring at shorter or longer times [19] and that can be significantly more probable. It is possible to overcome this limitation by performing a multistep analysis: we can look at all MPP’s with \( M \) in a given interval \([M_{\min}, M_{\max}]\) and choose the MPP, \( g_{IJ}^{[M_{\min}, M_{\max}]} \), with the highest probability. The multistep analysis leads to an alternative definition of betweenness, i.e a multistep MPP-betweenness \( B_K^{[M_{\min}, M_{\max}]} \) which is calculated considering the multistep MPPs instead of the fixed-\( M \) one.

Mediterranean flow network. We apply the previous concepts to a specific network describing surface water transport in the Mediterranean Sea [13, 14]. Fluid transport is typically studied from a Lagrangian perspective, by following trajectories of particles released in the flow. Recent works have approached the problem from a discretized point of view [13, 14, 29, 31]. Most of these studies are focused on the analysis and identification of coherent structures like vortices, barriers, or regions where trajectories of fluid parcels tend to be confined. Less
insight is available on the pathways followed by fluid masses during transport and in the resulting connectivity patterns. In this regard, our approach complements the standard Lagrangian toolbox as will be illustrated with this oceanic flow example.

Velocity data have been collected from the Mediterranean Forecasting System Model, Physics Reanalysis component [82]. We use the horizontal surface velocity daily field of the whole Mediterranean basin at a resolution of 1/16 degrees during 10 years of simulation (2002-2011). For the first months of each year a temporal flow network has been constructed by partitioning the surface of the Mediterranean sea in \( N = 3270 \) two-dimensional square-boxes (approximate lateral size of 28 km), each of which is identified with a network node. Link's weights are assigned from the effective mass transport driven by ocean currents between two boxes during a given time interval [13][14]. To build the adjacency matrices at each time \( t_l \) \((l=1,...M)\) we homogeneously initialize \( n = 500 \) ideal fluid particles in each node and integrate the surface velocity for a given time \( \tau \). The matrix element \( A^{(l)}_{IJ} \) is the number of particles starting from node \( I \) at time \( t_{l-1} \) and arriving to node \( J \) at \( t_l \). The normalized matrices \( T^{(l)} \) define a flow network. In fact, since \( s_{\text{out}}^{(l)}(i) \approx s_{\text{in}}^{(l-1)}(i) \) is approximately valid for every \( i,l \), our MPPs coincide with maximum flow pathways [33], i.e. paths that maximize the exported fraction of water from the source node to the destination node.

We perform the calculations using a time step of \( \tau = 10 \) days, and considering \( M \) from 6 to 9 steps (i.e. in between 2 and 3 months, a time interval during which the horizontal-flow assumption remains a good approximation). We build therefore 10 temporal networks, each one having \( t_0 \) as January 1st of each of the years available in the simulation database (2002 – 2011).

In Fig. [left panel] we show on map the set of all the MPPs of \( M = 9 \) time steps starting from a given node in one of our temporal networks (the one corresponding to 2011), and we notice how many different connections are possible from a single starting node. The \( P^{M}_{IJ} \) values span several orders of magnitude and this behavior is typical for the distribution of probability across MPPs. We stress here that MPPs do not coincide in general with fastest paths: the faster connection among two nodes is not always the most probable one for its value of \( M \). This underlines further the importance of our weighted description of the network.

To assess how representative of the whole dynamics are MPPs such as the ones shown in Fig. [left panel] we show in Fig. [middle panel] the distribution of \( \lambda^M_{IJ} \) and \( \lambda^M_{IJ}(\epsilon) \) for two values of \( M \). The distributions are collected from the \( \lambda \)-values of the whole set of accessible pairs \((I,J)\) in our ten temporal networks. For small \( M \) most of the MPP have significant \( \lambda \)-values, but as \( M \) increases the peak in the distribution of \( \lambda^M_{IJ} \) shifts towards zero meaning that the single MPP becomes increasingly unimportant, as a consequence of the dramatic increase with \( M \) of the number of available paths between two nodes. Then, it becomes important to consider larger sets of paths such as \( K^M_{IJ}(\epsilon) \). For the cases plotted, i.e. \( M = 5,6 \) and \( \epsilon = 0.1 \), the mean values of \( \lambda^M_{IJ}(\epsilon) \) are around 0.5. This means that, despite \( K^M_{IJ}(\epsilon) \) may not contain the full set of paths which individually carry a probability larger than \( \epsilon P^M_{IJ} \), it is large enough so that, for most of the \((I,J)\) pairs, it contains globally over 50% of the connection probability. This result further gains meaning if we consider that the number of paths in \( K^M_{IJ}(\epsilon) \) is on average well below 1% of the total number of paths of \( M = 5 \) and 6 steps. Hence, despite the strong particle dispersion characterizing our flow networks it is true that only a small subset of paths contribute significantly to the main transport features. This conclusion will also show up when studying global network properties, such as the betweenness centrality measure.

In Fig. [right panel] we show the multistep MPP-betweenness \( B^M_P \), averaged over our ten networks. Spatial patterns determined by the transport dynamics of the flow are clearly evident in the figure where high betweenness areas are organized in one dimensional-like structures corresponding to the main corridors of transport, i.e. narrow pathways that connect different regions of the ocean. Main paths of the Mediterranean sea are observed like Cyprus and Rhodes Gyres, surrounding the Ionian basin, the Algerian current and those along the Sicily strait, etc. Note that because of the ten-years average, individual short lived mesoscale features (eddies and fronts) are averaged out. We checked that the result is robust under different choices of the duration of a single time step. This means that very similar results are obtained when considering different \( M \) and \( \tau \) values but the same total duration \( M \tau \).

To support our interpretation of most probable paths as main carriers of connectivity we considered also betweenness using subsets of paths, so that \( g^M_{I,J,K} \) is now the number of times node \( K \) appears in the set \( K^M_{IJ}(\epsilon) \) of HPPs between \( I \) and \( J \), with \( \epsilon = 0.1 \), without noticing any qualitative or quantitative difference in the results. Indeed the Pearson correlation coefficient between the two betweenness is larger than 0.9. Hence, despite the MPPs represent a small portion of the paths in the \( K^M_{IJ}(\epsilon) \) subsets (between 3 – 10% for \( \epsilon = 0.1 \), depending on the value of \( M \)), which is itself a very small fraction of the full set of paths in the network, they seem to be representative of the main spatio-temporal structures describing the global dynamics. Indeed, center and right panels of Fig. [right panel] show that most of the relevant paths remain spatially close to the MPP. This observation is confirmed by calculations of the spatial dispersion between paths in \( K^M_{IJ}(\epsilon) \), whose average turns out to be of the order of the size of the boxes defining the nodes.
FIG. 1: Paths of \( M = 9 \) steps (three months) in the Mediterranean flow network with starting date January 1st 2011, represented as straight segments joining the path nodes. Left: MPPs originating from a single node (black star) and ending in all accessible nodes. Color gives the \( P_{I,J}^{M} \) value of the paths in a normalized log-scale between the minimum value (\( 10^{-15} \), deep blue) and the maximum (\( 10^{-5} \), dark red). Center and right: all the paths in the \( K_{I,J}^{M}(\epsilon) \) set with \( \epsilon = 0.1 \), initial point marked by a cross and final point marked by a triangle. The center panel shows the 18 HPPs, out of a total of 54276 paths between the two sites. The MPP, with \( P_{I,J}^{M} = 3 \times 10^{-9} \), is displayed in dark red, whereas the other paths are colored with a normalized logarithmic scale according to their \( (p_{I,J}^{M})_{\epsilon} \) values in \( [\epsilon P_{I,J}^{M}, P_{I,J}^{M}] \). Right panel shows the 39 HPPs, out of a total of \( 61 \times 10^6 \), in a similar logarithmic scale normalized in \( [\epsilon P_{I,J}^{M}, P_{I,J}^{M}] \) with \( P_{I,J}^{M} = 1.4 \times 10^{-6} \).

FIG. 2: Normalized histogram \( f(\lambda) \) of coefficients \( \lambda_{I,J}^{M} \) for \( M = 5 \) (black curve) and \( M = 6 \) (green curve), and \( \lambda_{I,J}^{M}(\epsilon) \), with \( \epsilon = 0.1 \) for \( M = 5 \) (blue curve) and \( M = 6 \) (red curve). The statistics is compiled from all connected pairs of nodes \((I, J)\) and the ten temporal flow networks corresponding to the first months of the ten years of velocity data. The mean values are: \( \langle \lambda_{I,J}^{5} \rangle = 0.24 \); \( \langle \lambda_{I,J}^{6} \rangle = 0.16 \); \( \langle \lambda_{I,J}^{5}(0.1) \rangle = 0.52 \); \( \langle \lambda_{I,J}^{6}(0.1) \rangle = 0.42 \).

FIG. 3: Multistep MPP-betweenness \( B_{K}^{6,9} \) at each geographical node \( K \), computed for each of our ten (2002-2011) temporal networks and then averaged over them.

To conclude, in this paper we introduced tools to compute highly probable paths in weighted temporal networks and to evaluate their relative importance. Betweenness centrality measures based on them have also been introduced. We applied this approach to characterize connectivity in the Mediterranean Sea from a network-theory perspective. Here, MPPs correspond also to the set of paths that maximize the fraction of transported mass, giving therefore a clear physical interpretation of connection probabilities. Despite MPPs represent only a small fraction of the whole set of paths, we found that they suffice to highlight the main transport pathways across our oceanic network, since most of the HPPs remain geographically close to them. We believe that the study of fluid transport as a network will provide new tools and insights complementing standard Lagrangian methods. In particular, estimation of most probable paths may improve the forecasting of oil spill trajectories in strongly diffusive situations and help in search and rescue operations. Beyond the fluid dynamics context, MPPs and the MPP-betweenness measure here introduced could be easily transferred to other kinds of weighted temporal networks. This could be relevant, for instance, in defining vulnerability metrics in disease spreading processes, or in detecting bottlenecks of reaction chains in metabolic networks.

Acknowledgments. We acknowledge financial support from FEDER and MINECO (Spain) through the ESCOLA (CTM2012- 39025-C02-01) and INTENSE@COSYP (FIS2012-30634) projects, and from European Commission Marie-Curie ITN program (FP7-320 PEOPLE-2011-ITN) through the LINC project (no. 289447). We acknowledge helpful discussions with P. Fleurquin and V. Rossi.
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