Compression of flow can reveal overlapping modular organization in networks

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To better understand the overlapping modular organization of large networks with respect to flow, here we introduce the map equation for overlapping modules. In this information-theoretic framework, we use the correspondence between compression and regularity detection. The generalized map equation measures how well we can compress a description of flow in the network when we partition it into modules with possible overlaps. When we minimize the generalized map equation over overlapping network partitions, we detect modules that capture flow and determine which nodes at the boundaries between modules should be classified in multiple modules and to what degree.

With a novel greedy search algorithm, we find that some networks, for example, the neural network of C. Elegans, are best described by modules dominated by hard boundaries, but that others, for example, the sparse European road network, have a highly overlapping modular organization.

I. INTRODUCTION

To discern higher levels of organization in large social and biological networks [1,6], researchers have used hard clustering algorithms to aggregate highly interconnected nodes into non-overlapping modules [6,8] because they have assumed that each node only plays a single modular role in a network. Recently, because researchers have realized that nodes can play many roles in a network, they have detected overlapping modules in networks using three approaches: a hard clustering algorithm that is run multiple times [9,10]; a local clustering method that generates independent and intersecting modules [11,14]; and link clustering that assigns boundary nodes to multiple modules [15,17]. However, all these approaches have limitations. The first and second approaches require several steps or tunable parameters to infer overlapping modules and the third approach necessarily overlaps all neighboring modules. To find simultaneously the number of modules in a network, which nodes belong to which modules, and which nodes should belong to multiple modules and to what degree, we use an information-theoretic approach and the map equation [18].

We are interested in the dynamics on networks and what role nodes on the boundaries between modules play with respect to flow through the system. For example, in Fig. 1(a), Keflavik airport in Reykjavik connects Europe and North America in the global air traffic network. When we summarize the network in modules with long flow persistence times, should Reykjavik belong to Europe, North America, or both? In our framework, the answer depends on the traffic flow. That is, Reykjavik's role in the network depends on to what degree passengers visit Iceland as tourists versus to what degree they use Keflavik as a transit between North America and Europe. If we assign the boundary node to both modules, for returning flow we can increase the time the flow stays in the modules and decrease the transition rate between the modules, but for transit flow, the transition rate does not decrease and a single module assignment is preferable. By generalizing the information theoretic clustering method called the map equation [19] to overlapping structures, we can formalize this observation and use the level of compression of a modular description of the flow through the system to resolve the fuzzy boundaries between modules. With this approach, modules will overlap if they correspond to separate flow systems with shared nodes.

In the next section, we review the map equation framework, introduce the map equation for overlapping modules, and explain how it exploits returning flow near module boundaries. The mathematical framework works for both generalized and empirical flow, but here we illustrate the method by exploring the overlapping modular structure of several real-world networks built on the probability flow of a random walker. We also test the performance on synthetic networks and compare the results with other clustering algorithms. Finally, in the Materials and Methods section, we provide complete descriptions of the map equation for overlapping modules and the novel search algorithm.

II. RESULTS AND DISCUSSION

A. The map equation

The mathematics of the map equation are designed to take advantage of regularities in the flow that connects a system’s components and generates their interdependence. The flow can be, for example, passengers traveling between airports, money transferred between banks, gossip exchanged among friends, people surfing the web, or, what we use here as a proxy for real flow, a random walker on a network guided by the (weighted directed) links of the network. Specifically, the map equation measures how well different partitions of a network can be used to compress descriptions of flow on the network and utilizes the rationale of the minimum description length principle. Quoting Peter Grünwald [20]: “...[E]very regularity in the data can be used to compress the data, i.e., to...
describe it using fewer symbols than the number of symbols needed to describe the data literally.” That is, the
map equation gauges how successful different network partitions are at finding regularities in the flow on the
network.

We employ two regularities for compressing flow on a network. First, we use short code words for nodes visited
often and, by necessity, long code words for nodes visited rarely, such that the average code word length will be
as short as possible. Second, we use a two-level code for module movements and within-module movements,
such that we can reuse short node code words between modules with long persistence times.

Because we are not interested in the actual code words, but only in the theoretical limit of compression, we use
Shannon’s source coding theorem \[21\], which establishes the Shannon entropy \( H(p) \) as the lower limit of the aver-
age number of bits per code word necessary to encode a message, given the probability distribution \( p \) of the code
words,

\[
H(p) = - \sum_i p_i \log_2 p_i .
\]

For example, if there is a message “ABABBAAB...” for which the symbols “A” and “B” occur randomly with the
same frequency, that is, “A” and “B” are independent and identically distributed, the source coding theorem
states that no binary language can describe the message with less than \( \frac{1}{2} \log_2 \frac{1}{2} - \frac{1}{2} \log_2 \frac{1}{2} = 1 \) bit per symbol.
However, if “A” occurs twice as often as “B”, the regularity

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use and which nodes should be in which modules to best capture the dynamics on the network. See [http://www.mapequation.org](http://www.mapequation.org) for a dynamic visualization of the mechanics of the map equation. Because the map equation only depends on the rates of node visits and module transitions, it is universal to all flow for which the rates of node visits and module transitions can be measured or calculated. The code structure of the map equation can also be generalized to make use of higher-order structures. In ref. [22], we show how a multilevel code structure can reveal hierarchical organization in networks, and in the next section, we show that we can capitalize on overlapping structures by releasing the constraint that a node can only belong to one module codebook.

### B. The map equation for overlapping modules

The code structure of the map equation framework is flexible and can be modified to uncover different structures of a network as long as flow on the network can be unambiguously coded and decoded. As we will show here, by releasing the constraint that a node can only belong to one module codebook and allowing nodes to be *information free ports*, we can reveal overlapping modular organization in networks. To see how, let us again study the air traffic between North America and Europe in Fig. 1(a). Suppose that cities in North America and Europe belong to two different modules, for simplicity identical in size and composition, and we are to assign membership to Reykjavik between North America and Europe. For a hard partition, we would assign Reykjavik to the module that most passengers travel to and from, and if the traffic flow were the same, we could choose either module. But if the flow to and from Reykjavik were dominated by American and European tourists visiting Iceland for sightseeing before returning to their home continent, both Americans and Europeans would consider Iceland as part of their territory. We can accommodate for this view if we allow nodes to belong to multiple module codebooks; depending on the origin of the flow, we use different code words for the same node.

With the map equation for overlapping modules, we can measure the description length of flow on the network with nodes assigned to multiple modules. By minimizing the map equation for overlapping modules, we can not only resolve into how many modules a network is organized and which nodes belong to which modules, but also which nodes belong to multiple modules and to what degree.

The pattern of flow, returning tourists to Iceland or intransit businessmen on intercontinental trips, determines whether we should assign Reykjavik to North America, Europe, or both. Or, conversely, when we decide whether Reykjavik should be assigned to North America, Europe, or both, we reveal the pattern of boundary flow between modules, as Fig. 1 illustrates. In this hypothetical example, assigning cities to two non-overlapping modules is always better than assigning all cities to one module. But for a sufficiently high proportion of returning flow, the overlapping modular solution with Reykjavik in both modules as a free port provides the most efficient partition to describe flow on the network.

The map equation for overlapping modules can take advantage of regularities in the boundary flow between modules. To measure the length of an overlapping modular description of flow on a network, we must decide how the flow switches modules to calculate the node-visit rates from different modules of multiply assigned nodes. In the Materials and Methods section, we provide a detailed description of how a random walker moves in an overlapping modular structure, but the rule is simple: when a random walker arrives at a node assigned to multiple modules, the walker remains in the same module if possible. Otherwise, the random walker switches, with equal probability, to one of the modules to which the node is assigned.

Figure 2 illustrates the code structure of a hard and a fuzzy partition of an example network with the dynamics derived from a random walker. For this network, the figure shows that an overlapping modular description allows us to describe the path of a random walker with fewer bits than we could do with a hard network partition. With overlapping modules, we halve the use of the index codebook, since the rate of module switching halves. Because we consequently use the exit codes in the new identical module codebooks less often, the description of movements within modules also becomes shorter, even if the average code word length increases. Turning the reasoning around again, given the overlapping modular organization, we have learned that returning flow characterizes the boundary flow between the modules.

With the mathematical foundation in place, we need an algorithm that can discover the best partition of the network. In particular, which nodes should belong to multiple modules and to what degree? For this optimization problem, we have developed a greedy search algorithm that we call Fuzzy infomap and detail in the Materials and Methods section. Here we give a short summary of Fuzzy infomap designed to provide good approximate solutions for large networks. We start from Infomap’s hard clustering of the network and then execute the two-step algorithm. In the first step, we measure the change in the description length when we assign boundary nodes, one by one, to multiple modules. This calculation is fast, but aggregating the changes in the second step is expensive and often requires recalculating all node-visit rates. Therefore, we rank the individual multiple module assignments and, in a greedy fashion, aggregate the individual best ones to minimize the description length.
the European roads network, which is a sparse network for overlaps. We find the highest compression gain from highest to lowest compression gain when allowing for overlaps. The networks are sorted by compression of flow on the network.

Boundaries between research groups lead to optimal compression of flow, as the size of the modules and the fraction of returning flow on the network. The map equation can capitalize on regularities, information they can subsequently share with other researchers and induce a flow of information on the network. The map equation can capitalize on regularities, and Fig. 3 highlights one area of the co-authorship network, Leskovec is strongly associated with Dasgupta, Mahoney, Lang, and Backstrom, but also with groups at Cornell University, Carnegie Mellon University, Stanford University, and Yahoo Research. The underlying co-authorship network is derived from the reference lists in the three review articles [11, 16, 23]. In this weighted undirected network, we connect two researchers with a weighted link if they have co-authored one or more research papers. For every co-authored paper, we add to the total weight of the link a weight inversely proportional to the number of authors on the paper. Our premise is that two persons who have co-authored a paper have exchanged information, information they can subsequently share with other researchers and induce a flow of information on the network. The map equation can capitalize on regularities in this flow, and Fig. 3 highlights one area of the co-authorship network with several overlapping research groups. For example, assigning Jure Leskovec to four research groups contributes to maximal compression of a description of a random walker on the network. Based on this co-authorship network, Leskovec is strongly associated with Dasgupta, Mahoney, Lang, and Backstrom, but also with groups at Cornell University, Carnegie Mellon University, Stanford University, and Yahoo Research. The size of the modules and the fraction of returning flow at the boundary nodes determine whether hard or fuzzy boundaries between research groups lead to optimal compression of flow on the network.

Table I shows the level of compression and overlap of a number of real-world networks. The networks are sorted from highest to lowest compression gain when allowing for overlaps. We find the highest compression gain in the European roads network, which is a sparse network with intersections as nodes and roads as links. Many intersections at boundaries between modules are classified in multiple modules, because intersections only connect a few roads and the return rate of the random flow is relatively high.

By contrast, compressing random flow in overlapping modules only gives a marginal gain over hard clustering in the highly interconnected and directed network of C. elegans, where less than three percent of the neurons are classified in multiple modules. Even if there is evidence that the neural network is modular, we most likely underestimate the degree of overlap with a random walk model of flow.

In the middle of the table, the world air routes network shows a relatively low compression gain, given the many cities classified in multiple modules. For this network, the compression gain would be much higher if, instead of random flow on the links, we were to describe real passenger flow with a higher return rate.

C. Overlapping modular organization in real-world networks

To illustrate our flow-based approach, we have clustered a number of real-world networks. Figure 3 shows researchers organized in overlapping research groups in network science. The underlying co-authorship network is derived from the reference lists in the three review articles [11, 16, 23]. In this weighted undirected network, we connect two researchers with a weighted link if they have co-authored one or more research papers. For every co-authored paper, we add to the total weight of the link a weight inversely proportional to the number of authors on the paper. Our premise is that two persons who have co-authored a paper have exchanged information, information they can subsequently share with other researchers and induce a flow of information on the network. The map equation can capitalize on regularities in this flow, and Fig. 3 highlights one area of the co-authorship network with several overlapping research groups. For example, assigning Jure Leskovec to four research groups contributes to maximal compression of a description of a random walker on the network. Based on this co-authorship network, Leskovec is strongly associated with Dasgupta, Mahoney, Lang, and Backstrom, but also with groups at Cornell University, Carnegie Mellon University, Stanford University, and Yahoo Research. The size of the modules and the fraction of returning flow at the boundary nodes determine whether hard or fuzzy boundaries between research groups lead to optimal compression of flow on the network.

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D. Comparing the map equation for overlapping modules with other methods

Depending on the system being studied and the research question at hand, researchers develop clustering algorithms for overlapping modules based on different principles. For example, while some researchers take a statistical approach and see modules as non-random features of a network, other researcher use a local definition and identify independent and intersecting modules, or take a link perspective and assign all boundary nodes to multiple modules. Consequently, the final partitions are quite different, and it is interesting to contrast our information theoretic and flow-based approach, implemented in fuzzy infomap with these approaches, here represented by OSLOM [13], Clique Percolation [31], and Link Communities [16].

OSLOM defines a module as the set of nodes that maximizes a local statistical significance metric. In other words, OSLOM identifies possibly overlapping modules that are unlikely to be found in a random network. Clique percolation identifies clusters by sliding fully connected k-cliques to adjacent k-cliques that share k-1 vertices with each other. A module is defined as the maximal set of nodes that can be visited in chained iterations of this operation, and the overlaps consist of the shared nodes between modules that do not support the slide operation across the boundary. Finally, the Link Communities approach creates highly overlapping modules by aggregating nodes that are part of a link community. The link communities themselves are built using a similarity measure between links, the primal actors of the method.

To compare the methods at different degrees of overlap, we used a set of synthetic networks presented in ref. [32]. In Table I we included six statistics for the four methods applied to synthetic networks with 1000 nodes and three different degrees of overlap (see table...
FIG. 3. Network scientists organized in overlapping research groups. The colors of the nodes represent overlapping research groups identified by the map equation and the pie charts represent the fractional association with the different research groups.
and $-2$ for the node degree distribution

Table II shows that Fuzzy infomap and OSLOM generated with three different degrees of overlap [32]: Low overlap corresponds to 100, medium overlap corresponds to 300, and high overlap corresponds to 500 nodes in multiple modules. As a result, with the overlapping partitions generated by Fuzzy infomap, random flow can be described with fewer bits. But the difference is small and shows up only in the second decimal place when up to half of all the nodes are assigned to multiple modules.

Clique percolation generates partitions with more modules but fewer assignments than both Fuzzy infomap and OSLOM. From a flow perspective, smaller modules with less overlap give more module switches that cannot be compensated for by a shorter module codeliness. The strength of the Clique percolation method is the simple definition that allows for easy interpretation of the results.

Designed with links as the primal actors used to identify pervasive overlap in networks, the results of Link Communities are quite different. For example, independent of the degree of overlap of the synthetic networks, each node belongs to on average ten modules. From the perspective of a random flow model, the persistence time is short in the many small modules, and the information necessary to encode the many transitions is much larger than for the other methods. This result is expected, as Link Communities is tailored to identify pervasive overlap in social networks in which people belong to several modules. And information flow is far from random.

Often the performance is an important aspect to consider when choosing a clustering method. Therefore, we measured the time it took to cluster the synthetic networks with the different clustering algorithms. We stress that we used presumably non-optimized research code made available online by its developers and that the performance, of course, depends on the network. Per 1000 node synthetic network used in our comparison, Fuzzy infomap used on average 1.7 seconds for a single iteration of module growth and 240 seconds for multiple iterations (caption for details).

The first group of partition numbers describe the number of detected modules, the number of nodes that are assigned to multiple modules, and the total number of assignments. To interpret the results from a flow perspective, we included the index, module, and total codeliness for describing a random walker on the network given the network partition.

Table II shows that Fuzzy infomap and OSLOM generate similar partitions for low and medium degrees of overlap, but the trend when going to higher degrees of overlap indicates fundamental differences. By assigning boundary nodes to more modules than OSLOM prefers, Fuzzy infomap identifies modules with longer persistence times. The shorter index codeliness resulting from the fewer transitions compensates for the longer module codeliness from the larger modules. As a result, with the overlapping partitions generated by Fuzzy infomap, random flow can be described with fewer bits. But the difference is small and shows up only in the second decimal place when up to half of all the nodes are assigned to multiple modules.

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The table below shows the comparison of four different overlapping clustering methods. We run Fuzzy infomap, OSLOM, and Link communities with their default settings and use clique size four for the Clique percolation method. All values are averaged over ten instantiations of random undirected and unweighted networks with 1000 nodes and predefined community structure, generated with three different degrees of overlap [32]: Low overlap corresponds to 100, medium overlap corresponds to 300, and high overlap corresponds to 500 nodes in multiple modules. All other parameters were held constant: The number of nodes that multiply-assigned nodes are assigned to was set to two; each cluster consisted of on average 20 nodes with a minimum of 10 and a maximum of 50 nodes; and the power law exponent was set to $-2$ for the node degree distribution and $-1$ for the module size distribution. Finally, the mixing parameter that controls the proportion of links within and between modules was set to 0.1.

| Network                  | n    | l    | C    | $\Delta C_{\text{fuzzy}}$ | $N_{\text{fuzzy}}/N$ |
|--------------------------|------|------|------|---------------------------|----------------------|
| European roads network   | 1018 | 1274 | 46.2%| 10.4%                     | 35.5%                |
| Western states power grid| 4941 | 6994 | 53.4%| 8.8%                      | 27.5%                |
| Human diseases network   | 516  | 1188 | 46.4%| 2.87%                     | 15.3%                |
| Coauthorship network     | 552  | 1317 | 48.9%| 2.47%                     | 14.6%                |
| World air routes         | 3618 | 14142| 31.1%| 1.24%                     | 13.9%                |
| U.S. political blogs     | 1222 | 16714| 4.13%| 0.35%                     | 5.81%                |
| Swedish political blogs  | 855  | 10315| 0.50%| 0.18%                     | 4.79%                |
| Neural net. of C. Elegans| 297  | 2345 | 1.16%| 0.13%                     | 2.69%                |

| Partition numbers | Codeless (bits) |
|-------------------|-----------------|
|                   | modules | overlaps | assignments | index | module | total | n | l |
| Low overlap       | Fuzzy Infomap  | 44     | 105      | 1228   | 1.7   | 5.9   | 7.6  |
|                   | OSLOM    | 44     | 89       | 1089   | 1.8   | 5.8   | 7.6  |
|                   | Clique Percolation | 43     | 104      | 1108   | 1.7   | 6.0   | 7.7  |
|                   | Link Communities | 3415   | 1000     | 9215   | 8.1   | 3.5   | 12   |
| Medium overlap    | Fuzzy Infomap  | 53     | 303      | 1830   | 2.2   | 6.0   | 8.2  |
|                   | OSLOM    | 54     | 276      | 1277   | 2.3   | 5.9   | 8.2  |
|                   | Clique Percolation | 55     | 268      | 1283   | 2.3   | 6.1   | 8.3  |
|                   | Link Communities | 4457   | 1000     | 11628  | 8.7   | 3.5   | 14   |
| High overlap      | Fuzzy Infomap  | 56     | 398      | 1676   | 2.6   | 6.1   | 8.8  |
|                   | OSLOM    | 61     | 462      | 1465   | 2.8   | 6.0   | 8.8  |
|                   | Clique Percolation | 73     | 388      | 1429   | 2.9   | 6.1   | 9.0  |
|                   | Link Communities | 4298   | 1000     | 11063  | 10    | 3.7   | 11   |
III. MATERIALS AND METHODS

Here we detail the map equation for overlapping modules and describe our greedy search algorithm.

A. The map equation for overlapping modules

Below we explain in detail how we derive the transition rates of a random walker between overlapping modules. We also derive the conditional probabilities for nodes assigned to multiple modules. We then express the map equation (Eq. 1) in terms of these rates, which allows for fast updates in the search algorithm.

1. Movements between nodes assigned to multiple modules

To calculate the map equation for overlapping modules, we need the visit rates \( p_{\alpha i} \) for all modules \( i \in M_\alpha \) a node \( \alpha \) is assigned to and the inflow \( q_{i\rightarrow} \) and the outflow \( q_{\rightarrow i} \) of all modules. We derive these quantities from the weighted and directed links \( W_{\alpha \beta} \), which we normalize such that \( w_{\alpha \beta} \) correspond to the probability of the random walker moving to node \( \beta \) once at node \( \alpha \):

\[
w_{\alpha \beta} = \begin{cases} 0, & \text{if there is no link from } \alpha \text{ to } \beta \\ \frac{W_{\alpha \beta}}{\sum_\beta W_{\alpha \beta}}, & \text{otherwise} \end{cases} \tag{2}
\]

When necessary, we use random teleportation to guarantee a unique steady state distribution. That is, for directed networks, at rate \( \tau \), or whenever the random walker arrives at a node with no out-links, the random walker teleports to a random node in the network. To simplify the notation, we set \( w_{\alpha \beta} = 1/n \) for all nodes \( \alpha \) with no out-links to all \( n \) nodes \( \beta \) in the network.

The movements between multiply assigned nodes and overlapping modules are straightforward. Whenever the random walker arrives at a node that is assigned to multiple modules, she remains in the same module if possible or switches to a random module if not possible. For example, assuming that the random walker is in module \( i \), she remains in module \( i \) when moving to node \( \beta \) if node \( \beta \) is assigned to module \( i \). But if node \( \beta \) is not assigned to module \( i \), she switches with equal probability to any of the modules node \( \beta \) is assigned to.

\[
\delta_{\alpha,i,j} = \begin{cases} 1, & \text{if } i = j \\ \frac{1}{|M_\beta|}, & \text{if } i \neq j \text{ and } i \notin M_\beta \\ 0, & \text{if } i \neq j \text{ and } i \in M_\beta \end{cases} \tag{3}
\]

we can now define the visit rates by the equation system

\[
p_{\alpha i} = \sum_{\beta} \sum_{j \in M_\beta} p_{\beta j} \delta_{\alpha, i j} \left[ (1 - \tau) w_{\beta \alpha} + \tau \frac{1}{n} \right] \tag{4}
\]

We solve for the unknown visit rates with the fast iterative algorithm BiCGStab. Since every node in module \( i \) guides a fraction \( (1 - \tau) \sum_{\beta \neq i} w_{\beta \alpha} \) and teleports a fraction \( \tau \frac{n_{\neq i}}{n} \) of its conditional probability \( p_{\alpha i} \) to nodes outside of module \( i \), the exit probability of module \( i \) is

\[
q_{i\rightarrow} = \sum_{\alpha} p_{\alpha i} \left[ (1 - \tau) \sum_{\beta \neq i} w_{\alpha \beta} + \tau \frac{n_{\neq i}}{n} \right] \tag{5}
\]

where \( n_i \) is the number of nodes assigned to module \( i \).

2. The expanded map equation for overlapping modules

To make explicit which terms must be updated in a given step of a search algorithm, here we expand the entropies of the map equation (Eq. 1) in terms of the visit and transition rates \( p_{\alpha i} \) and \( q_{i\rightarrow} \). When teleportation is included in the description length as above, the outflow of modules balances the inflow, but here we derive for the general case when \( q_{i\rightarrow} \neq q_{i\rightarrow} \).

We use the per-step probabilities of entering the modules \( q_{i\rightarrow} \) to calculate the average code word length of the
index code words weighted by their rates of use, which is given by the entropy for the index codebook

$$H(Q) = - \sum_{i=1}^{m} \frac{q_{i\bowtie}}{\sum_{j=1}^{m} q_{j\bowtie}} \log_2 \left( \frac{q_{i\bowtie}}{\sum_{j=1}^{m} q_{j\bowtie}} \right), \quad (6)$$

where the sum runs over the $m$ modules of the modular partition. The contribution to the average description length from the index codebook is the entropy $H(Q)$ weighted by its rate of use $q_{\bowtie}$,

$$q_{\bowtie} = \sum_{j=1}^{m} q_{j\bowtie}. \quad (7)$$

Substituting Eq. 7 into Eq. 6 we can express the contribution to the per-step average description length from the index codebook as

$$q_{\bowtie} H(Q) = -\sum_{i=1}^{m} q_{i\bowtie} \left[ \sum_{i=1}^{m} \frac{q_{i\bowtie}}{q_{\bowtie}} \log_2 \frac{q_{i\bowtie}}{q_{\bowtie}} \right] = -\sum_{i=1}^{m} q_{i\bowtie} \left[ \log_2 q_{i\bowtie} - \log_2 q_{\bowtie} \right] = q_{\bowtie} \log_2 q_{\bowtie} - \sum_{i=1}^{m} q_{i\bowtie} \log_2 q_{i\bowtie}. \quad (8)$$

We use the per-step probabilities of exiting the modules $q_{i\bowtie}$, and the visit rates $p_{\alpha_{i}}$ to calculate the entropy of each module codebook:

$$H(P_{i}) = -\frac{q_{i\bowtie}}{q_{i\bowtie} + \sum_{\beta \in \bar{i}} p_{\beta_{i}}} \log_2 \frac{q_{i\bowtie}}{q_{i\bowtie} + \sum_{\beta \in \bar{i}} p_{\beta_{i}}} - \sum_{\alpha \in \bar{i}} \frac{p_{\alpha_{i}}}{q_{i\bowtie} + \sum_{\beta \in \bar{i}} p_{\beta_{i}}} \log_2 \frac{p_{\alpha_{i}}}{q_{i\bowtie} + \sum_{\beta \in \bar{i}} p_{\beta_{i}}} = -\frac{1}{p_{\bar{i}_{\bowtie}}} \left[ q_{i\bowtie} \log_2 q_{i\bowtie} + \sum_{\alpha \in \bar{i}} p_{\alpha_{i}} \log_2 p_{\alpha_{i}} - p_{\bar{i}_{\bowtie}} \log_2 p_{\bar{i}_{\bowtie}} \right]. \quad (9)$$

with $p_{\bar{i}_{\bowtie}}$ for the rate of use of the $i$-th module codebook,

$$p_{\bar{i}_{\bowtie}} = q_{i\bowtie} + \sum_{\beta \in \bar{i}} p_{\beta_{i}}. \quad (10)$$

Finally, summing over all module codebooks, the description length given by the overlapping module partition $M$ is

$$L(M) = q_{\bowtie} \log_2 q_{\bowtie} - \sum_{i=1}^{m} q_{i\bowtie} \log_2 q_{i\bowtie} - \sum_{i=1}^{m} q_{i\bowtie} \log_2 q_{i\bowtie} \quad (11)$$

$$- \sum_{i=1}^{m} \sum_{\alpha \in \bar{i}} p_{\alpha_{i}} \log_2 p_{\alpha_{i}} + \sum_{i=1}^{m} p_{\bar{i}_{\bowtie}} \log_2 p_{\bar{i}_{\bowtie}}. \quad (11)$$

The only visible difference between this expression and the map equation for non-overlapping modules is the sum over conditional probabilities for nodes assigned to multiple modules, which is no longer independent of the overlapping module partition $M$. But since the transition rates depend on the conditional probabilities (see Eq. 5), all terms depend on the overlapping configuration.

B. The greedy search algorithm for overlapping modules

To detect the overlapping modular organization of a network, ultimately we want to find the global minimum of the map equation over all possible overlapping modular configurations of the network, but only with an exhaustive enumeration of all possible solutions can we guarantee the optimal solution. This procedure is, of course, impractical for all but the smallest networks. However, we can construct an algorithm that finds a good approximation. Figure 5 explains the concept of our algorithm, which builds on an iterative two-step procedure.

In the first step, we individually assess which nodes are most likely to be assigned to multiple modules. Starting from a hard partition generated by Infomap [18] in the first iteration, we go through all nodes at the boundary between modules and assign each boundary node to adjacent modules. That is, one node and one adjacent module at a time, we assign the node to the extra module, measure the map equation change, and then return to the previous configuration (see Fig. 3(c)). Because the multiply assigned nodes only connect to singly assigned nodes in the first iteration, the conditional probabilities and the change in the map equation can be updated quickly without a full recalculation of the visit rates. This first step produces 3-tuples of local changes of the form (node, extra-module, map-equation-change).

In the second step, we combine a fraction of all local changes generated in the first step into a global solution. Every time two or more multiply assigned nodes are connected, we need to solve a linear system to calculate the conditional probabilities. When a majority of nodes are assigned to multiple modules, this can take as long as calculating the steady-state distribution of random walkers in the first place. For good performance, we therefore try to test as few combinations of local changes as possible. After testing several different approaches, we have opted for a heuristic method in which we first sort the tuples from best to worst in terms of map equation change and then determine the number of best tuples that minimizes the map equation. The method works well, because good local changes often are good globally.

As a side remark, the map equation for link community [17] allows for straightforward and fast calculation of all conditional probabilities and transition rates, since each link belongs to only one module. But this constraint enforces module switches between boundary nodes that belong to the same module, because all boundary nodes
FIG. 5. General scheme of the two-step greedy search algorithm for overlapping modules. (a) Pseudocode with first step (c) and second step (d) of the algorithm that can be iterated as shown in (b). Starting from a hard partition generated by Infomap [18], each iteration successively increases the overlap between modules to minimize the map equation for overlapping modules. In the first step (c), one by one, each boundary node is assigned to adjacent modules. In the second step (d), we first sort the local changes from best to worst and then iteratively apply quadratic fitting to find the number of best local changes that minimizes the map equation.

belong to multiple modules in the link community approach.

Figure 5(d) shows the value of the map equation as a function of the number of aggregated tuples ordered from best to worst. Combinations of tuples that individually generate longer description lengths can generate a shorter description length if they are applied together. This fact, together with the greedy order in which we aggregate the tuples, generates noise in the curve. To quickly approach the global minimum, we must overcome bad local minima caused by the noise and evaluate as few aggregations as possible. Therefore, we iteratively fit a quadratic polynomial to the curve by selecting new points at the minimum of the polynomial. A quadratic polynomial only requires three points to be fully specified, but in order to deal with the noise, we use a moving local least squares fit. In practice, we evaluate around ten points for each quadratic fit and repeat this procedure a few times to obtain a good solution.

Step 1 and step 2 can now be repeated, each time starting from the obtained solution with overlapping modules from the previous iteration. Figure 5(b) illustrates that by repeating the two steps, we sometimes can extend the overlap between modules, but this comes at a cost. After the first iteration of the algorithm, step 1 also can involve solving a linear system to calculate the conditional probabilities. Thus, the first step is no longer guaranteed to be as fast as in the first iteration. Still, for medium-sized networks, multiple iterations are feasible. For example, for the networks presented in Table 1, the first iteration took a few seconds and multiple iterations until the point of no further improvements took less than two minutes on a normal laptop. We have made the code available here: https://sites.google.com/site/alcidesve82/

IV. CONCLUSIONS

In this paper, we have introduced the map equation for overlapping modules. When we allow nodes to belong to multiple module codebooks and minimize the map equation over possibly overlapping network partitions, we can determine which nodes belong to multiple modules and to what degree. Compared to hard partitions detected by the map equation, we have further compressed descriptions of a random walker on all tested real-world networks, and therefore revealed more regularities in the flow on the networks. We find the highest overlapping modular organization in sparse infrastructure networks, but this result depends on our random-walk model of flow. Since the mathematical framework is not limited to random flow, it would be interesting to compare our results with results derived from empirical flow.
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