Inversion method for content-based networks

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In this paper, we generalize a recently introduced Expectation Maximization (EM) method for graphs and apply it to content-based networks. The EM method provides a classification of the nodes of a graph, and allows to infer relations between the different classes. Content-based networks are ideal models for graphs displaying any kind of community or/multipartite structure. We show both numerically and analytically that the generalized EM method is able to recover the process that led to the generation of such networks. We also investigate the conditions under which our generalized EM method can recover the underlying contents-based structure in the presence of randomness in the connections. Two entropies, $S_q$ and $S_c$, are defined to measure the quality of the node classification and to what extent the connectivity of a given network is content-based. $S_q$ and $S_c$ are also useful in determining the number of classes for which the classification is optimal.

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I. INTRODUCTION

Classifying items with respect to their properties is a fundamental and very old problem. If the properties are inherent to the objects, the difficulty is deciding first how many groups are required and then establishing the discrimination thresholds for each. The matter becomes more complicated when instead of the inherent properties, one tries to classify elements based on mutual interactions. Of course, such classifications would be very useful for a better understanding of the mechanisms underlying the behavior of systems encountered in scientific disciplines as diverse as Sociology, Biology or Physics [1, 2, 3, 4]. As an example, consider social systems which are often modeled as networks. The vertices represent individuals and the edges interactions between them. These interactions can be of many types: friendship, belonging to the same club or school, working together, etc. In these graphs, it is important to be able to group the nodes into what is commonly known as communities. That is, groups of vertices that share a higher number of connections among themselves than with the rest of the network [5, 6, 7, 8] (see also [9] for a recent review). This partition bears information on which persons have a stronger interdependence and may allow to predict the actors that drive the dynamics of the group as a whole. In Biology, on the other hand, network methods have been used to understand gene regulatory patterns [10]. Here each vertex corresponds to a gene and an edge contains information on how the associated protein regulates the synthesis of the protein associated to the second gene. Since regulation of gene activity plays a fundamental role in the functioning of the cell [11], the community structure points towards the different functional subunits (see [12] and references therein). Given the relevance of communities, the last years have seen an increase in the number of techniques proposed to detect them. To name a few: some of them are based on the concept of betweenness (number of paths passing through a link) and modularity [8, 9, 14], others on synchronization of oscillators [15, 16] or on other dynamical systems running on the network [17, 18, 19], detection of overlapping cliques [20] or the diffusion of random walkers [21, 22, 23].

Nevertheless, communities are not the only relevant information that can be extracted from networks. It is also possible to search for vertices with similar connection patterns (not necessarily having connections among themselves, as in the case of communities) that are expected to play equivalent functional roles. In the social networks literature such nodes are referred to as structurally equivalent [24] and have lead to an analysis of social networks based on Block Modeling [1, 25]. In many types of networks, like those formed by webpages or social actors, the connection between nodes is often due to some intrinsic properties of the nodes, which we will refer to henceforth as their "contents". Thus it is possible to consider an alternative point of view in which a network structure arises as a result of node contents, leading one to the notion of contents-based networks [26, 27, 28, 29].

In many cases, network analysis approaches based on communities and those based on some form of node similarity are aimed towards the understanding of very different questions. When viewed within the framework of contents based networks, however, these differences disappear as will be argued below. We will also show that
an extension of Newman and Leicht’s Expectation Maximization (EM) method [30] is well-suited for uncovering content-based structure underlying a network, inverting in practice the process that lead to its formation.

The organization of the paper is as follows: in Section II, content-based networks are formally introduced. Next, we describe in Section III our generalization of the EM method to directed graphs. In Section IV, we show how the EM method can be used to solve the inverse problem, namely to recover the underlying contents-based structure from a given network. We present in Section V analytical results regarding the application of the EM method to contents-based networks and the recovery of the contents-based structure. These results will be complemented with a numerical study in Sections VI and VII. In Section VII, we consider a more realistic situation and ask to what extent an underlying contents-based structure can be recovered in the presence of disorder in the connections. Finally, we summarize our results and present the conclusions in Section VIII.

II. CONTENT BASED NETWORKS

Let us define first content-based networks. Consider a set of nodes \( i = 1, 2, \ldots, N \) each of which has a content \( x_i \) assigned with \( x_i \in \mathcal{X} = \{1, 2, \ldots, N_c\} \), and where \( 1, 2, \ldots \) are labels for the possible contents. The structure of the connectivity pattern of the associated content-based network is determined by the function \( c(x_i, x_j) \in \{0, 1\} \), which is defined for all ordered pairs of contents \( (x_i, x_j) \in \mathcal{X} \). The adjacency matrix of the graph is then given by

\[
A_{ij} = c(x_i, x_j).
\]

We see immediately that nodes having the same contents \( x \) also have the same connection patterns, and thus are structurally equivalent [24]. As explained before, this can imply a functional equivalence in the process that generated the network. The point of view that we will take in this article is to regard contents-based networks as ideal networks, from which the ”real” networks are obtained through alteration or removal of some of the connections. Note that the range of topologies that can be generated via contents-based network is very broad: if the connectivity function \( c(x, y) \) shows a close to diagonal configuration, the network will be formed by a set of almost insulated cliques. The ideal configuration would be a family of independent communities without interconnections. Another configuration that can be easily reprinted with content-based networks are bipartite graphs. In its most simplest from, it is enough to allow the nodes to take one of two possible contents and letting the connectivity function \( c \) to be non-zero only for the off-diagonal elements. Much more complicated connectivity patterns can be actually achieved by introducing finer contents distinctions and more intricate connectivity functions. Thus a content-based graph can in general include all sorts of combinations between community-like and/or multipartite graphs, as can be seen in the example plotted in Figure 1.

Another point to note is that originally these networks were proposed in a context where the relation between contents was an order relation [21, 31, 32]. This implies that the relation between nodes is not symmetric and the network is therefore more naturally represented by a directed graph. In this case, the connectivity function \( c \) is non-symmetric in its arguments. Apart from directionality, realistic graphs may present, as well, a certain degree of disorder in their connection patterns. This effect can be incorporated into the mathematical description by regarding the values of \( c(x, y) \) as probabilities of having a link from a node of content \( x \) to a node of content \( y \). This view transforms the content-based network into a hidden variable graph [33, 34, 35]. As we will see later, the EM method is still able to extract information from networks produced in this way but the failure rate increases the further \( c(x, y) \) deviates from a binary-valued function.

Contents based networks have proven to be very useful in the description of phenomena that include an underlying relation of hierarchy or ordering. The simplest way of achieving such a relation is to associate with each node a string of letters and letting the relation between any two nodes be based on string inclusion: namely that one string is contained as an uninterrupted subsequence in the other. Networks generated from random strings in this manner have been successfully used to model receptor-ligand interactions in the immune system [31, 32], and the transcription factor based gene regulatory network in yeast [24, 27, 28, 29].

In this article, our goal is to address the inverse problem: Given a network of which we know nothing in advance, is it possible to decide whether there is an underlying contents-based structure and, if so, can we deduce the class membership of its nodes and the class connectivity function? Moreover, can this be achieved in the presence of noisy connections? Seen in this way, the problem at hand becomes one of statistical inference, very well-suited to EM methods [36, 37].

![An example of content based network](image-url)
III. THE EM METHOD FOR NETWORKS AND ITS GENERALIZATION

Given a graph $\mathcal{G}$ of $N$ nodes and an adjacency matrix $A_{ij}$, the Expectation Maximization (EM) algorithm searches for a partition of the nodes into $N_c$ groups such that a certain log-likelihood function for the graph is maximized. Henceforth we will refer to the groups into which the EM method divides the nodes, as classes. Note that $N_c$ must not be confused with the number of contents $N_x$, described in the previous section. Ideally, the optimal number of classes would be $N_x$, but a criterion independent from the EM algorithm is required to determine its value since we assume that in general $N_x$ will not be known in advance. The variables of the algorithm are the probabilities $\pi_r$ that a randomly selected node is assigned to class $r$, with $r = 1, 2, \ldots, N_c$, and the set of probabilities $\theta_{rj}$ of having a connection from a node belonging to class $r$ to a certain node $j$. Assuming that the functions $\theta$ and $\pi$ are given, the probability $\Pr(A, g|\pi, \theta)$ of realizing the given graph under a node classification $g$, such that $g_i$ is the class that node $i$ has been assigned to, can be written as

$$\Pr(A, g|\pi, \theta) = \prod_i \pi_{g_i} \left[ \prod_j A_{ij} \theta_{g_i j} \right], \quad (2)$$

$\Pr(A, g|\pi, \theta)$ is the likelihood to be maximized, but it turns out to be more convenient to consider its logarithm instead

$$\mathcal{L}(\pi, \theta) = \sum_i \ln \pi_{g_i} + \sum_j A_{ij} \ln \theta_{g_i j}. \quad (3)$$

Treating the a priori unknown class assignment $g_i$ of the nodes as statistical "unknown data", one introduces next the auxiliary probabilities $q_{ir} = \Pr(g_i = r|A, \pi, \theta)$ that a node $i$ is assigned to class $r$, and considers the averaged log-likelihood constructed as

$$\bar{\mathcal{L}}(\pi, \theta) = \sum_{ir} q_{ir} \left[ \ln \pi_r + \sum_j A_{ij} \ln \theta_{rj} \right]. \quad (4)$$

The maximization of $\bar{\mathcal{L}}$ must be performed taking into account the following normalization conditions for the probabilities $\pi$ and $\theta$

$$\sum_{r=1}^{N_c} \pi_r = 1 \quad (5)$$
$$\sum_{j=1}^{N} \theta_{rj} = 1. \quad (6)$$

The final results are

$$\pi_r = \frac{1}{N} \sum_i q_{ir} \quad (7)$$
$$\theta_{rj} = \frac{\sum_i A_{ij} q_{ir}}{\sum_i k_i q_{ir}} \quad (8)$$

where $k_i$ is the total degree of node $i$. The still unknown probabilities $q_{ir}$ are then determined a posteriori by noting that

$$q_{ir} = \Pr(g_i = r|A, \pi, \theta) = \frac{\Pr(A, g_i = r|\pi, \theta)}{\Pr(A|\pi, \theta)}, \quad (9)$$

from which one obtains

$$q_{ir} = \frac{\pi_r \prod_j \theta_{rj}^{A_{ij}}}{\sum_s \pi_s \prod_j \theta_{rj}^{A_{ij}}}. \quad (10)$$

Eqs. (7), (8) and (10) form a set of self consistent equations for $q_{ir}, \theta_{rj}$ and $\pi_r$ that any extremum of the expected log-likelihood must satisfy.

Thus, given a graph $\mathcal{G}$, the EM algorithm consists of picking a number of classes $N_c$ into which the nodes are to be classified and searching for solutions of Eqs. (7), (8) and (10). These equations were derived by Newman and Leicht. They also showed that when applied to diverse type of networks the resulting $q_{ir}$ and $\theta_{rj}$ yield useful information about the internal structure of the network. Note that only a minimal amount of a priori information is supplied: the number of classes $N_c$ and the network.

However, the EM method in the form presented so far does not yet serve our purposes for the following reason: as remarked before, content-based networks are usually represented as directed graphs. The probability $\theta_{rj}$ was defined as the probability that a node $j$ receives a directed connection from a node belonging to class $r$. Together with the normalization condition for $\theta_{rj}$, Eq. (6), this implies that the classification must be such that each

![FIG. 2: A simple scenario in which the EM method for directed networks, as defined in (30), has problems to classify the nodes of the network in two classes. The configurations a) and b) are possible outputs of the original EM method since both satisfy the normalization condition of Eq. (6). The solution a) comes together with values for $q_{ir} = 1/2$ for all the nodes and classes, while the solution b), which has a lower likelihood, produces $q_{ir} \approx 0.99$ for all the nodes in one class and a very small probability for the other. The plot on the right, solution c), is the output offered by the generalization of EM with values of $q_{ir}$ virtually one and/or zero.](image-url)
class $r$ has at least one member with non-zero out-degree. This constraint forces the EM algorithm to classify a simple bi-partite graph in the manner depicted in Figures 2a or 2b. From a content-based point of view, on the other hand, the classification that would be more natural is the one displayed in Figure 2c which is forbidden by the condition of Eq. (6). This difficulty is not resolved by re-defining $\theta_{rj}$ instead as the probability that a node $j$ makes a directed connection to a node belonging to class $r$, since now the classification must be such that each class $r$ has at least one member with non-zero in-degree.

We therefore have to generalize the EM approach in such a way that the node directionality does not restrict the possible classification of the nodes. This can be achieved by introducing the probabilities

- $\theta_{ri}$ of having a uni-directional link from a vertex of class $r$ to a node $i$,
- $\bar{\theta}_{ri}$ of having a uni-directional link from node $i$ to a node in class $r$, and
- $\tilde{\theta}_{ri}$ of having a bidirectional link between $i$ and a node in class $r$.

With these new definitions Eq. (2) becomes

$$L = \sum_i q_{ir} \left( \ln \pi_r + \sum_j \left[ (A_{ji} (1 - A_{ij})) \ln \theta_{r,j} + (A_{ij} (1 - A_{ji})) \ln \theta_{r,j} \right] \right),$$

which has to be maximized under the following constraint on the probabilities $\theta_{rj}$,

$$\sum_i (\theta_{r,i} + \bar{\theta}_{r,i} + \tilde{\theta}_{r,i}) = 1, \quad (13)$$

implying that there is no isolated node. The probability $\pi_r$, that a randomly selected node belongs to class $r$, is again given by Eq. (7).

Introducing the Lagrange multipliers $\beta$ and $\lambda_r$, to incorporate the constraints, Eqs. (15) and (13), the expression to be extremized becomes

$$\hat{L} = \hat{L} + \beta \left( 1 - \sum_r \pi_r \right) - \sum_r \lambda_r \left( 1 - \sum_i (\theta_{r,i} + \bar{\theta}_{r,i} + \tilde{\theta}_{r,i}) \right). \quad (14)$$

As before, the extremal condition on $\hat{L}$ with respect to $\pi$ gives us

$$\frac{\partial \hat{L}}{\partial \pi_r} = 0 \iff \pi_r = \frac{1}{N} \sum_i q_{ir} \quad \text{and} \quad \beta = N, \quad (15)$$

where $N$ is the total number of nodes. Differentiating $\hat{L}$ with respect to the $\theta$ variables, we get

$$\frac{\partial \hat{L}}{\partial \theta_{rj}} = 0 \iff \sum_i q_{ir} A_{ji} (1 - A_{ij}) - \bar{\theta}_{rj} \lambda_r = 0 \quad \text{and} \quad \frac{\partial \hat{L}}{\partial \bar{\theta}_{rj}} = 0 \iff \sum_i q_{ir} A_{ij} (1 - A_{ji}) - \bar{\theta}_{rj} \lambda_r = 0,$$

Putting together the three previous expressions and summing over the index of the nodes $j$, we obtain the following result for the Lagrange multipliers

$$\lambda_r = \sum_i q_{ir} (\bar{k}_i^j + \bar{k}_i^o - \bar{k}_i^b), \quad (17)$$

where $\bar{k}_i^j$, $\bar{k}_i^o$ and $\bar{k}_i^b$ are the in-degree, out-degree and bi-degree of node $i$, respectively. Inserting this relation into the previous set of equations, we extract the new extremal conditions for the $\theta$'s

$$\bar{\theta}_{rj} = \frac{\sum_i q_{ir} A_{ji} (1 - A_{ij})}{\sum_i q_{ir} (k_i^j + k_i^o - k_i^b)},$$

$$\bar{\theta}_{rj} = \frac{\sum_i q_{ir} A_{ij} (1 - A_{ji})}{\sum_i q_{ir} (k_i^j + k_i^o - k_i^b)}.$$

These expressions have to be again supplemented with the self-consistent equation for $q_{ir}$ which now reads

$$q_{ir} = \frac{\pi_r \prod_j \bar{\theta}_{rj}^{A_{ji}} (1 - A_{ij})}{\sum_s \pi_s \prod_j \bar{\theta}_{sj}^{A_{sj}} (1 - A_{sj})} \prod_j \bar{\theta}_{sj}^{A_{sj}} (1 - A_{sj}) \prod_j \bar{\theta}_{rj}^{A_{rj}}, \quad (19)$$

Note that when we have only bi-directional links so that $A_{ij} = A_{ji}$, it follows from Eq. (18) that $\bar{\theta}_{rj} = \bar{\theta}_{rj} = 0$. Thus we recover the original EM equations under the identification $\theta_{rj} = \bar{\theta}_{rj}$.

It is easily shown that the solutions of the EM equations, Eqs. (16), (18) and (19), are such that if two nodes $i$ and $j$ are structurally equivalent, i.e. $A_{ik} = A_{jk}$ as well as $A_{ki} = A_{kj}$, for all $k$ then they will be classified in the same manner: $q_{ir} = q_{ij}$, and $\theta_{ri} = \theta_{rj}$, $\bar{\theta}_{ri} = \bar{\theta}_{rj}$ and $\tilde{\theta}_{ri} = \tilde{\theta}_{rj}$ for all $r$. This property of the solutions obtained from the EM methods renders it very well-suited for detecting any underlying contents-based structure.
IV. THE INVERSION METHOD

One important shortcoming of the EM method is that $\mathcal{N}_c$ has to be provided as an external parameter. The algorithm lacks a means to evaluate how good a classification is, and consequently one cannot decide which number of classes furnishes an optimal classification of the nodes of a graph. To overcome this problem, we propose to define a measure of the quality of a classification as follows:

$$S_q = \frac{1}{N} \sum_{i,r} q_{ir} \ln(q_{ir}),$$

(20)

where the sum runs over all the nodes $i$ and classes $r$. $S_q$ is the average entropy of the classification and as such measures the certainty with which the nodes are assigned to their respective classes. One can easily see that $0 \leq S_q \leq \ln N_c$. For a sharp classification $S_q = 0$, while the worst-case scenario occurs when $q_{ir} = 1/N_c$. We will later argue that $S_q$ is a useful statistic to infer $N_c$.

Once an optimal classification has been found, it is possible to determine the connectivity structure among the classes. Given an EM classification, we will define $c(r,s)$ as the probability that a node in class $r$ has a connection to one in class $s$. This probability can be estimated as

$$c(r,s) = \frac{\sum_{i,j} q_{ir} A_{ij} q_{js}}{\sum_i q_{ir} \sum_j q_{js} \left( 1 + \frac{\delta_{rs}}{\sum_i q_{ir} - 1} \right),}$$

(21)

by noting that

$$p(i|r) = \frac{q_{ir}}{\sum_j q_{jr}}$$

(22)

is the posterior probability that given that a node has been assigned to class $r$, the node is $i$. The second term on the right hand side of Eq. (21) must be included as a correction for the absence of self-connections, since by convention, we assume that $A_{ii} = 0$ for all $i$.

$c(r,s)$, as defined above, is the probability of regarding a connection between two nodes in the graph as being one between nodes of type $r$ and $s$. As we will show in the following section, if the underlying graph is a contents-based network, a successful application of the EM algorithm should result in sharp assignments of nodes into classes and $c(r,s)$ should thus be binary valued (and moreover be equal to the connectivity function $c(x,y)$). It is possible to also define a measure of how close the connectivity function resembles one that corresponds to a content-based network by considering the entropy for $c$,

$$S_c = -\frac{2}{N_c^2 \ln 2} \sum_{r,s} c(r,s) \ln c(r,s).$$

(23)

We have that $0 \leq S_c \leq 1$. The maximum of $S_c$ occurs when $c(r,s) = 1/2$, i.e. when none of the classes have any preferred connection pattern to any class.

The generalization of the EM method, the entropies $S_q, S_c$ and the estimation of $c(r,s)$ are in general applicable to any kind of graph. However, for the purpose of this article we will focus only on their applications to content-based networks. We will address the general case in a subsequent work [39], where we will also show that contents-based networks play a special role for the classifications of the EM method.

V. ANALYTICAL RESULTS FOR CONTENTS-BASED NETWORKS

Assume that we are given a contents-based graph $G$ that has been constructed from a set of nodes of unknown contents, and an unknown connectivity function $c(x,y)$. In this setting, we suppose that the optimal number of classes $\mathcal{N}_c$ has already been found and that it is equal to the number of contents $\mathcal{N}_c$. We would like to know under which conditions the EM algorithm can infer the class membership of the nodes as well as the connectivity function. In other words, given the adjacency matrix $A_{ij}$, we are looking for a solution of the generalized EM equations, Eqs. (15) and (19), with

$$q_{ir} = \delta_{r,x_i}$$

(24)

along with the unknown class-connectivity function $c(r,s)$ that ideally should coincide with the original $c(x,y)$. Note that the Ansatz Eq. (24) implies that for such a solution $S_q = 0$.

Substituting the above Ansatz into Eq. (18), we find

$$\bar{\theta}_{rj} = \frac{c(x_j,r) [1 - c(r,x_j)]}{k^o_r + k^o_r - k^b_r}$$

(25)

$$\bar{\theta}_{rj} = \frac{c(r,x_j) [1 - c(x_j,r)]}{k^o_r + k^o_r - k^b_r}$$

$$\bar{\theta}_{rj} = \frac{c(r,x_j) c(x_j,r)}{k^o_r + k^o_r - k^b_r},$$

where $\bar{k}^o_r$ and $\bar{k}^b_r$ are the average in-degree, out-degree and bi-directional degree of nodes belonging to class $r$,

$$\sum_{i} \delta_{x_i,r} \left( \bar{k}^o_r + \bar{k}^o_r - \bar{k}^b_r \right) = n_r \left( \bar{k}^o_r + \bar{k}^o_r - \bar{k}^b_r \right)$$

(26)

so that $\bar{k}_r$ is the total degree of each of the $n_r$ nodes belonging to class $r$. Note that in Eq. (25), the node index $j$ enters only through its content $x_j$, so that $\theta_{rj}$ is the same for all the nodes that have the same content as $j$. The same turns out to be true for the $q_{ir}$. We thus have $q_{ir} = q_{ir}$ for all nodes $i$ such that $x_i = x$, and from Eq. (19) we obtain

$$q_{ir} = \frac{\gamma t \pi_r}{k^b_r} \prod_s \left\{ \frac{[c(r,s) (1 - c(s,r))]^{c(t,s) (1 - c(t,s))}}{[c(s,r) (1 - c(r,s))]^{c(s,t) (1 - c(t,s))}} \times [c(r,s) c(s,r)]^{c(s,t) c(t,s)} \right\},$$

(27)
where \( \gamma_i \) is the normalization constant for \( q_{tr} \).

We now have to consider the conditions on \( c(r, s), c(s, r), c(t, s), \) and \( c(s, t) \) such that given the classes \( r \) and \( t \), the terms in the product on the right hand side of Eq. (27) are non-zero for all \( s \), when \( r = t \), and zero for at least one \( s \) when \( r \neq t \). This is a statement about the kind of connections that the nodes of type \( r \) and \( t \) make to or receive from nodes of all possible classes \( s \). An inspection of the \( c^{e} \) type terms in the product shows that their contribution to \( q_{tr} \) is non-zero if and only if the following two conditions are satisfied for all \( s \):

- If there is a connection between \( t \) and \( s \), there must be also a connection between \( r \) and \( s \) of the same kind, namely either in, out, or bi-directional.
- Whenever there is no connection between \( t \) and \( s \), there can be any kind of connection between \( r \) and \( s \), as well as none at all.

The satisfaction of both conditions can be regarded as constituting a cover type of relation between \( r \) and \( t \), i.e. nodes belonging to class \( r \) connect in the same way with all the classes that nodes belonging to class \( t \) connect, but they have also some extra connections. We will denote this relation by \( r \triangleright t \) and say that \( r \) covers \( t \). From its definition it is clear that the cover relation is transitive, \( r \triangleright t, t \triangleright s \implies r \triangleright s \). When \( r \triangleright t \), we also define \( E(r; t) \) as the set of extra classes that \( r \) connects to (or receives connections from) relative to those of \( t \).

With the above definition, it can be readily seen that when \( r \triangleright t \)

\[
\tilde{k}_t = \tilde{k}_t + \sum_{v \in E(r; t)} n_v,
\]

where the index \( v \) runs over the extra classes to which \( r \) is connected. This implies that

\[
\frac{\tilde{k}_r}{k_t} = \frac{\tilde{k}_r}{k_t} \left( 1 + \frac{\sum_{v \in E(r; t)} n_v}{k_t} \right) \tilde{k}_t.
\]

Thus we find that

\[
q_{tr} = \begin{cases} 
\frac{n_r}{k_t} \left( 1 + \frac{\sum_{v \in E(r; t)} n_v}{k_t} \right)^{-\tilde{k}_t} & r = t, \\
0 & r \triangleright t, \end{cases}
\]

(30)

(with \( E(t; t) \equiv \emptyset \)). Thus, when \( r \triangleright t \) and for large \( \tilde{k}_t \), \( q_{tr} \) deviates from our Ansatz, Eq. (24), by an exponentially small amount.

Treating the deviations caused by the presence of cover relations among the classes, as a small perturbation to our Ansatz, Eq. (24), we can obtain the leading order expression for \( q_{tr} \) as

\[
q_{tr} = \begin{cases} 
1 - \sum_{r \triangleright t} \frac{n_t}{\pi_t} \left( 1 + \frac{\sum_{v \in E(r; t)} n_v}{k_t} \right)^{-\tilde{k}_t} & r = t, \\
\frac{\pi_r}{\pi_t} \left( 1 + \frac{\sum_{v \in E(r; t)} n_v}{k_t} \right)^{-\tilde{k}_t} & r \triangleright t, \end{cases}
\]

(31)

Thus, when \( r \triangleright t \), there is a non-zero probability for a node \( t \) to be also classified as belonging to class \( r \). We will refer to this as a leakage in the class assignment. However as can be seen from Eq. (31), the leakage probabilities vanish exponentially with the size of the classes. A detailed account of the solution structure for contents-based networks as well as more general types of networks will be given elsewhere [39].

When the contents-based network is cover-free, the generalized EM equations have a leak-free solution and thus the entropy of the class assignments \( S_q \) vanishes. On the other hand, in the presence of cover relations, the EM method will produce assignments with some nodes in multiple classes, i.e. leaks. We have already found above the leading order behavior for the leakage. It is not too hard to show that, in that case, \( S_q \) is given by

\[
S_q = \sum_r \sum_{t \text{ has a cover } r \triangleright t} n_t \alpha(r; t) \left( 1 + \frac{\alpha(r; t)}{k_t} \right)^{-\tilde{k}_t},
\]

(34)

where \( \alpha(r; t) = \sum_{v \in E(r; t)} n_v \) is the number of nodes to which nodes in class \( r \) are connected in addition to those
that nodes in class \( t \) connect. In many practical situations, the number of contents is fixed. This implies that if the probability of being in class \( r \) is given by \( p_r \), the actual number of nodes in the \( r \) class will grow on average as \( n_r = N p_r \) with the system size. Therefore, the factor \( \alpha(r;t) \) of Eq. (34) can also be written as
\[
\alpha(r;t) = N \tilde{\alpha}(r;t), \tag{35}
\]
where \( \tilde{\alpha}(r;t) \) is a constant depending on the connectivity function that generated the network. Under these assumptions, the entropy \( S_r \) will decrease exponentially with the network size, meaning that even for moderately sized networks the leakages will be in general too small to cause significant misclassification.

As shown in Section IV, the solution of the EM equations provides us with an estimate for the class connectivity, \( \tilde{c}(r,s) \), given by Eq. (21). For contents-based networks in the absence of any cover relation among classes, we have, cf. Eq. (22), \( p(r) = \delta_{x,r}/n_r \), and from Eq. (21) we immediately find that \( \tilde{c}(r,s) = c(r,s) \) with \( S_r = 0 \). In the presence of cover relations among the classes, there will be corrections that vanish exponentially with the number of nodes in the relevant classes. These results demonstrate that the EM algorithm is capable of inferring the hidden class connectivity function that generated the network.

### A. An Example

In order to further illustrate the theoretical results above, we turn next to an example. Consider a network generated from six kinds of contents to be denoted by \( A, B, C, D, E \) and \( F \), and with the connectivity function as shown in Figure 3. The following cover relations are present: \( B \succ A \succ F \); that is, \( B \succ A \), \( B \succ F \), and \( A \succ F \). In fact, we have chosen this particular example to elucidate the effect of having nested covers and to show that the cover relation is transitive. For each of the cover relations, the sets of connections to additional classes are

\[ \mathcal{E}(B;A) = \{D\}, \mathcal{E}(B;F) = \{D,C\} \text{ and } \mathcal{E}(A;F) = \{C\}. \]

When inserted into Eq. (31), these relations yield
\[
q_{AA} = 1 - \frac{n_B}{n_A} \left( 1 + \frac{n_D}{n_E + n_C} \right)^{-n_E - n_C},
\]
\[
q_{AB} = \frac{n_B}{n_A} \left( 1 + \frac{n_D}{n_E + n_C} \right)^{-n_E - n_C},
\]
\[
q_{FF} = 1 - \frac{n_A}{n_F} \left( 1 + \frac{n_C}{n_E} \right)^{-n_E} - \frac{n_B}{n_F} \left( 1 + \frac{n_C + n_D}{n_E} \right)^{-n_E},
\]
\[
q_{FA} = \frac{n_A}{n_F} \left( 1 + \frac{n_C}{n_E} \right)^{-n_E},
\]
\[
q_{FB} = \frac{n_B}{n_F} \left( 1 + \frac{n_C + n_D}{n_E} \right)^{-n_E},
\]
with \( q_{BB} = q_{CC} = q_{DD} = q_{EE} = 1 \) and all the other values of \( q_{rt} = 0 \). These results are in agreement with what one would expect intuitively. For example, since \( B \succ A \) and \( B \succ F \), there is a non-zero probability of mistaking nodes of type \( A \) or \( F \) by nodes of \( B \), i.e. \( q_{AB}, q_{FB} \), and \( q_{FA} \) are all non-zero. However this probability vanishes exponentially with the number of nodes in the classes \( E \) and \( C \). In the large network size limit, the leakage on \( q_{rt} \), and how far \( S_r \) deviates from zero, are determined by the pair of classes \( (r,t) \) such that \( r \) is the "tightest" cover of \( t \), these are the pairs \( r \succ t \) for which \( \alpha(r;t) \) is smallest, \( A \succ F \) and \( B \succ A \), in our example.

![FIG. 5: An example of classification, the original network is on the top and on the bottom the probability \( q_{ir} \) is represented graphically. The color of the symbols correspond to the contents of the nodes (green \( A \), red \( B \), magenta \( C \), blue \( D \) and cyan \( E \)). On the bottom, the spheres radius is proportional to the probability \( q_{ir} \). On the left, the network is generated using the connectivity function \( c_A \) of Figure 4 with no cover relation among the classes, while on the right we have used \( c_B \), which incorporates a single cover relation between \( A \) and \( B \) such that \( A \succ B \).](Image 318x284 to 429x360)
VI. SIMULATION RESULTS, EM APPLIED TO CONTENT-BASED NETWORKS

In the following, we study numerically the ideas introduced in the previous sections. The generalized version of EM will be applied to directed content-based networks generated randomly from the connectivity functions shown in Figure 4. The nodes of these networks have a content assigned that is selected at random out of $N_c = 5$ five possible contents, denoted by $A$, $B$, $C$, $D$, and $E$. Since the presence of coverage relations can change the quality of an EM classification, we have considered two connectivity functions $c(x, y)$ (see Fig. 4); one without class coverage, $c_A$, and another, $c_B$, with a single cover relation between contents $A$ and $B$, such that $A \succ B$. In order to improve our numerical estimation of the classification with maximum likelihood, we implemented a simulated-annealing type of procedure for the optimization of $\mathcal{L}$.

In the previous section, we have shown that our generalized EM method is able to infer the underlying content-based structure that generated the network. These calculations were carried out assuming that the number of contents $N_x$ coincides with the number of classes $N_c$. Let us therefore start by setting $N_x = N_c = 5$. In Figure 5, we show graphically the classifications obtained from the generalized EM method as applied to an ensemble of networks of size $N = 50$ generated with the connectivity functions of Figure 4. The color coding is based on the contents of the nodes and will be such that it matches in all the subsequent figures of the paper ($A$ green, $B$ red, $C$ blue, $D$ magenta and $E$ cyan). The size of the spheres in the bottom plots are proportional to the probabilities $q_{ir}$.

For these examples the classification is rather good even in the case when a cover relation is present, as can be readily seen from the bottom diagrams where no major color is misplaced. In other words, there are not misclassifications, although for the $B$ case a small amount of leakage can be noticed.

To try to quantify the quality of these results, we can, as a first measure, count the number of network realizations in our ensemble for which at least two nodes with different contents have been assigned to the same class, with the understanding that a node $i$ is assigned to a class $r$ whenever $q_{ir} > 1/2$. This is a strict criterion, since it may well be that we are considering as erroneous a classification with only a single node misclassified. The result can also slightly depend on the method applied to optimize the likelihood. Still, this definition is a way to play on safe ground and avoid to complicate too much the detection of mistakes in the classification. Let us call this then the error rate of the classification $\epsilon$. For each of the two connectivity functions of Fig. 4, we have studied over 2000 realizations of networks of size $N = 50$. In none of them the generalized EM method misclassified a single node. This result is in agreement with our earlier observation that the EM method classifies structurally equivalent nodes in the same way.

The next question is then: how can the optimal $N_c$ be determined? If the networks studied are content-based, there are several possible answers to this. Here we will outline two of them and will discuss at the end of this section a third one in the context of inferring the class connectivity function. In Section IV, we have introduced a measure $S_q$ for the quality of an EM classification of the
network. We have also shown that when $N_c = N_x$, $S_q$ is either zero or exponentially small for large content-based networks. Therefore, a signal on $S_q$ can be expected for $N_c = N_x$, if the EM algorithm is faced with the challenge of classifying a content-based network with a series of values $N_c$. This effect happens because the normalization conditions of Eqs. (5) and (13) impose that no class can be left totally unassigned, $\pi_r > 0$ for all $r$. The more redundant classes the method has to assign nodes to, the higher $S_q$ becomes. In other words, we are providing the EM algorithm with a larger degree of freedom than required to properly classify the nodes. The extra freedom leads to structural leakage. The evolution of $S_q$ with $N_c$ is displayed in Figure 6 for the two networks of Fig. 5. These are, of course, particular examples but some general features can be deduced. First, the value of $S_q$ is rather small or even zero for $N_c < N_x$. This may be a generic property of content-based networks. As noted before, the structural equivalence of nodes with the same content prevents the EM algorithm from putting such nodes into different classes. This means that once the contents are classified by the classes the leakage comes from cover relations between classes and can become very small for big networks. On the other hand, when $N_c > N_x$, the availability of excess classes that cannot be left totally unassigned causes $S_q$ to be non-zero and to increase steadily with $N_c$. The boundary between these two types of behaviors is precisely the unknown $N_c = N_x$.

Another peculiarity of the EM method applied to contents-based networks is that when $N_c < N_x$, the landscape of the likelihood seems to have a very clear and unique maximum. The solution at the point of maximum $\mathcal{L}(\pi, \theta)$ has also a well determined value of $S_q$. However, if $N_c > N_x$, the landscape of the likelihood becomes rough, with a large number of local maxima. The search for the global maximum under such conditions is therefore much harder. And even, in the cases where it can be numerically found, say when $N_c = N_x$, it is formed by a set of degenerate extrema with the same value of $\mathcal{L}$ but very different values of $S_q$. Indeed, the values of the entropy shown in Fig. 6 for $N_c > N_x$ are averages over the best likelihood solutions found in different realizations of the optimization methods along with their standard deviations $\sigma_S$. The dispersion $\sigma_S$ of $S_q$ around its average, can be used in practice as another estimator for the optimal number of classes (see Fig. 6).

Once $N_x$ is known, it is possible to recover $c(r, s)$ as explained in Section IV. In the top panels of Figure 7, the recovered $c(r, s)$ is displayed for the content based networks of Figure 5. After the classes of $c(r, s)$ have been properly reordered, it is impossible to distinguish the top panels of Fig. 7 from the connectivity functions given in Fig. 4. Also, in the lower panels of Figure 7, we have included the evolution of the entropy $S_c$, as a function of $N_c$. $S_c$ also shows a clear change of behavior at $N_c = N_x$, suggesting that the best content-based partition of the network happens when the number of classes equals the number of contents. Consequently, $S_c$, apart from being an estimator of how much a network deviates from a purely content-based graph, is also a useful quantity for deciding when $N_c$ is optimal.

VII. EM AND NOISY CONNECTIONS IN CONTENT-BASED NETWORKS

It is unlikely that in real-world networks the generating processes is error-free. Even if the underlying structure is expected to be a content-based network, errors in the connecting pattern could naturally arise. We try to mimic the unexpected connections as well as the absence of expected connections, by introducing the corresponding error probabilities to the process of network generation from its contents. As before, each node $i$ has a content $x_i$ assigned at random from the set of possible contents (in the case of our example networks the same five possibilities: $A, B, C, D$ and $E$). Once the contents are established, the structure of the content-based network should be determined completely by the connectivity function $c(x_i, x_j)$: If $c(x_i, x_j) = 1$, there ought to be a link from node $i$ to $j$, and none if $c(x_i, x_j) = 0$. As a way of gradually losing the content-based structure of the connections, we introduce now the probabilities $P_\alpha$, and $P_\beta$, of not having a link, when $c(x_i, x_j) = 1$ and having a link although $c(x_i, x_j) = 0$, respectively. The networks constructed in this way can be regarded as hidden variable graphs \cite{33, 34, 35} for which the probability of connection between any nodes $i$ and $j$ is expressed as

$$r(x_i, x_j) = c(x_i, x_j) (1 - P_\alpha) + [1 - c(x_i, x_j)] P_\alpha. \quad (37)$$

In other words, where in the absence of noise the probability of having a connection was one, it now is $1 - P_\alpha$, and likewise, where it was zero, it now is $P_\alpha$. The extreme limit of this model occurs when $P_\alpha = P_\beta = 1/2$, so that the probability of connecting to a node of other class is maximally random and independent of the connectivity function. We are more interested here in the limit when both $P_\alpha$ and $P_\beta$ are much smaller than $1/2$, and the resulting graphs can be seen as a slight modification of a content-based network. For the sake of simplicity, all of the results shown below are for $P_\alpha = P_\beta$.

Let us begin by looking at how the networks change with increasing assignment error. In the top panels of Figure 8, we display a series of networks generated with the connectivity function $c_A$, for different values $P_\beta = P_\alpha$. It is readily seen that the connection patterns associated with the different kinds of content become more and more diffuse. On the bottom panels of the same figure, we show the corresponding class assignment probabilities $q_{ir}$. While these are just examples, there are some features that are worth pointing out. The problems in the classification seem to appear somewhere between $P_\alpha = P_\beta = 1\%$ and $P_\alpha = P_\beta = 10\%$. Even at $10\%$ of error the number of nodes misclassified in these networks is not very high. A closer inspection of the solution found shows that actually only two of the node contents-classes
are mingled up, while all the remaining node classes are perfectly assigned. With the aim of quantifying these observations, the behavior of $\epsilon$ is plotted in Figure 9 versus the disorder probability. This plot is, of course, susceptible to slight changes depending on the method used to search for the maximum likelihood and depends on how many realizations of the content-based graphs were considered (in this case 1000). Nevertheless, in our simulations the threshold for a sharp classification of all the nodes of the network is around $P_\alpha = P_\mu \approx 5\%$ for graphs without coverage, connectivity function $c_A$, and much the order of magnitude of the threshold beyond which the content-based structure cannot be recovered anymore.

A next aspect to consider is how the entropies $S_q$ and $S_c$ are affected by the intensity of the disorder, and whether they are still valid estimators to determine the magnitude of the threshold beyond which the content-based structure cannot be recovered anymore.

FIG. 10: The average entropies over different realizations for content-based networks generated with the connectivity functions of Figure 4. In the top panels, $S_c$ is represented as a function of the number of classes $N_c$ for two different levels of disorder: the circles are $P_\alpha = P_\mu = 1\%$, while the triangles for $P_\alpha = P_\mu = 10\%$. On the bottom panels, $S_q$ and $\sigma_S$ versus $N_c$ for the disorder probabilities $P_\alpha = P_\mu = 1\%$, circles ($S_q$) and squares ($\sigma_S$), and $P_\alpha = P_\mu = 10\%$, triangles ($S_q$) and stars ($\sigma_S$).
optimal number of classes. To answer this question, we fix the probabilities $P_\alpha = P_\mu = 1\%$, which seems to be a value where one might plausibly expect to obtain good classifications for both type of networks. In Figure 10, we display $S_q$, $\sigma_S$ and $S_c$, as function of the number of classes $N_c$ with the results averaged over different content-based realizations. Indeed, at this level of disorder the entropies can still be used to estimate $N_c$. The noise in the connections introduces a small constant background for $N_c$, which we will denote by $S^*_c$, and which can be determined in both examples from the behavior at high values of $N_c$. We can estimate the value of $S^*_c$ by noting that when $N_c = N_c$ any non-zero entropy should essentially be due to the background from the random connections. Substituting the expression for $r(x, y)$, Eq. (37), into the definition of $S_c$, Eq. (28), should therefore give us an estimate for $S^*_c$,

$$S^*_c \approx -\frac{2}{N_c^2} \ln 2 \sum_{x, y} r(x, y) \ln r(x, y)$$  \hspace{1cm} (38)

For $P_\alpha = P_\mu = 1\%$, this yields $S^*_c \sim 0.112$, close to the value observed in the Figure 10 for $N_c \geq 5$. To check how well our estimate for $S^*_c$ agrees with the values obtained from simulations, we plot in Figure 11 $S_c$ vs. the disorder probability at $N_c = 5$. When the disorder becomes very strong, on the other hand, it might not be possible to find an optimal $N_c$. Moreover, the presence of very different connection patterns for nodes with the same content renders the existence of such optimal number dubious. Therefore, apart from the obvious classification $N_c = N$, there may be not any other sharp classification. The effects of high disorder can be seen in Figure 10, where the entropies $S_c$ and $S_q$ are represented as a function of $N_c$ for $P_\alpha = P_\mu = 10\%$. The results depend on the connectivity function, $c_A$ seems a little more robust to the disorder as was confirmed by Fig. 9, but the signal in $S_q$ or $\sigma_S$ is clearly lost or has moved to higher values of $N_c$. Also $S_c$ has lost its capacity to predict $N_c$ and smoothly falls for higher and higher values of $N_c$. It is worthy also noting that in spite of the lack of a method to find $N_c$, if $N_c = 5$ the EM method retrieves the appropriate hidden variable theory connectivity function $r(x, y)$ as can be inferred from the good fit produced by Eq. (38) to $S_c$ shown in Figure 11.

The numerical findings of this section show that the classifications of the EM method are robust to the introduction of noise in the connection patterns up to a certain point. The certainty of the classification will suffer, the stronger the disorder becomes. In fact this is one of the major merits of the EM method: it is able to extract the underlying content-based structure even in the presence of a certain level of noisy connections.

VIII. CONCLUSIONS

In summary, we have shown how the EM method for the classification of nodes of a network can be applied to content-based networks in order to extract the underlying content-based structure even in the presence of a certain level of disorder in the connections. The application of the EM method to content-based networks is a natural concept that follows from the observation that the EM method classifies structurally equivalent nodes in an identical manner. In this sense, the EM method can be related to the Block Modeling techniques proposed in Social Sciences. Content based networks, on the other hand, are of great relevance, since they can be regarded as idealized paradigms of networks with communities or multipartite structures, including mixtures of both. Since in many realistic graphs the vertices carry additional attributes which might influence or even determine their connections to other vertices, being able to extract any content-based pattern can provide information about how the networks emerged.

Our approach in this paper has been to start out with pure content-based graphs, and to show analytically as well as numerically that the EM method can infer the content-based connectivity pattern. We have shown also that the existence of cover-relations between contents leads to non-zero probabilities of mistaking nodes belonging to different classes. However, these probabilities vanish exponentially with the increasing number of nodes, i.e., the more discriminating information provided to the method. By regarding more realistic networks as perturbations of content-based networks under the addition or removal of connections, we then asked under which circumstances the EM method is still able to perform satisfactorily. There is a certain level of disorder beyond which the inference of the content-based structure, specially the number of contents, becomes rather hard if not impossible.

In order to estimate the quality of the classification and how far the structure of the network is from a content-based structure, we have introduced two entropies, $S_q$ and $S_c$, which actually can be useful for the classification of any kind of graphs, including real-world networks. We have also shown that these entropies are applicable to deduce the optimal number of classes needed by the EM method to obtain a sharp classification of the nodes of

![FIG. 11: The average entropy $S_c$ as a function of the disorder probability $P_\alpha = P_\mu$ for content-based networks generated with the connectivity functions $c_A$ and $c_B$ depicted in Figure 4. The red curves correspond to the value of $S^*_c$.](image-url)
the network.

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