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Spectral reconstruction of complex networks[☆]

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ABSTRACT

In this paper we study the reconstruction of a network topology from the eigenvalues of its Laplacian matrix. We introduce a simple cost function and consider the tabu search combinatorial optimization method, while comparing its performance when reconstructing different categories of networks – random, regular, small-world, scale-free and clustered – from their eigenvalues. We show that this combinatorial optimization method, together with the information contained in the Laplacian spectrum, allows an exact reconstruction of small networks and leads to good approximations in the case of networks with larger orders. We also show that the method can be used to generate a quasi-optimal topology for a network associated to a dynamic process (like in the case of metabolic or protein–protein interaction networks of organisms).

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1. Introduction

In recent years there has been a growing interest in the study of complex networks, related to transportation and communication systems – WWW, Internet, power grid, etc. – including social and biological networks (like the metabolic or the protein–protein interaction networks of organisms). Many of these networks are large, with a number of nodes, very often in the thousands. To store the topological details of the network requires knowing the list of adjacencies and, although usually the networks are sparse, this means the use of a large amount of memory. In contrast, the spectrum of the network (eigenvalues of the associated adjacency or Laplacian matrix) contains important information with significantly less memory use. Also, the spectrum provides information on the behavior of dynamic processes supported by the network (see Ref. [1]). Therefore, it is of interest to reconstruct or generate a network from its spectrum.

In Ref. [2], Ipsen and Mikhailov use simulated annealing with an elaborated cost function based on the spectral density to perform such a reconstruction. The spectral density of a network has also been considered by different authors for classification purposes, see for example Refs. [3–5]. Here, we propose a simple cost function which, together with the information provided by the knowledge of the spectrum, drives the tabu search method towards a good network reconstruction. The method is probabilistic, i.e. it has a random component, and as a consequence we can not guarantee that the algorithm will find an optimal reconstruction, but we show that the final networks match the originals in their main topological properties.

We also show that the method can be used, without modifications, to generate a quasi-optimal topology for a network associated to a dynamic process. As an example, we have considered the Laplacian spectrum of the largest connected components from the metabolic network of *Saccharomyces cerevisiae* and the protein–protein interaction network of *Helicobacter pylori*, to generate new networks with a similar topology. This can be used to produce network models when the spectrum of a network is known or it can be inferred, even partially, from its dynamical properties.

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In the next section, we introduce the mathematical notation and concepts necessary for our study. Section 3 contains a description of tabu search, the combinatorial optimization algorithm considered, with details on its use with information provided by the spectrum. Our main results are presented in Section 4.

2. The Laplacian spectrum of a graph and its reconstruction

Let us consider the Laplacian of the graph $G = G(V, E)$, with vertex set V (order $n = |V|$) and edge set E , associated with a network. The Laplacian is a symmetric matrix with zero row-sums that accounts for the topology of the network, defined to be $L_{ij} = -1$ if nodes i and j are connected, $L_{ii} = \delta_i$ if node i has degree δ_i (i.e. is connected to δ_i other nodes), and $L_{ij} = 0$ otherwise. The Laplacian matrix can be related to the adjacency matrix A of G by $L = D - A$, where D is the diagonal matrix of vertex degrees of G .

The (Laplacian) spectrum of G consists of the n eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of the Laplacian matrix and they satisfy $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$. We have also considered the reconstruction of a network from the spectra of the sign-less Laplacian matrix, defined as $|L| = D + A$, and the normalized Laplacian matrix, defined to be $\bar{L}_{ij} = -1/\sqrt{\delta_i \delta_j}$ if nodes i and j are connected, $\bar{L}_{ii} = 1$ if node i has degree $\delta_i > 0$, and $\bar{L}_{ij} = 0$ otherwise. For this last matrix, the eigenvalues satisfy $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \leq 2$ and $1 < \lambda_2 \leq 2$. In this paper, when we refer to the Laplacian matrix we mean the first definition unless stated otherwise. The spectrum of a graph is important as it provides bounds on its diameter, maximum and minimum degrees, and gives information about possible partitions etc. It can also be used to count the number of paths of a given length in the network, number of triangles, total number of links, etc., see Refs. [6,7]. Dynamic properties of a network, like its synchronizability, can also be determined from the eigenvalues, see Refs. [8,1] We note that two isomorphic graphs have the same spectrum, independent of the labeling of the vertices, but there also exist non-isomorphic graphs (topologically different) with the same spectrum, known as cospectral graphs. For $n < 6$ there are no connected cospectral graphs with respect to the usual Laplacian matrix. For $n = 6$ there exist four pairs, there are 130 pairs for $n = 7$, 1767 pairs for $n = 8$, etc. The number of cospectral graphs increases rapidly with the order of the graph, but the fraction is very small (e.g. it is 0.09 for $n = 11$) and approaches zero as the order of the graph increases, see Refs. [9,10]. Hence, two graphs with the same spectrum would indeed be isomorphic with a high probability.

In this paper, we study the reconstruction of graphs from their Laplacian spectra. Note that the number of different graphs of a given order n is large even for relatively small order. For example, for $n = 40$ there are roughly 10^{186} graphs. It makes no sense to check all of these graphs to find one matching spectrum, even in an approximate way. We are in the classical situation where combinatorial optimization algorithms are useful.

The generic process is as follows: we will reconstruct a given reference graph G_0 from its spectrum $\{\lambda_i^0, 0 \leq i \leq n\}$. In the reconstruction process, we generate an initial random graph G_{ini} using the information provided by the spectrum. The graph should have n vertices, $(\sum_{i=1}^n \lambda_i)/2$ edges and fulfill the following constraints on the degrees maximum and minimum: $\frac{4}{n\lambda_2} \leq \Delta \leq \frac{n-1}{n}\lambda_n$ and $\delta \geq \frac{n-1}{n}\lambda_2$, see [11]. Some bounds on the diameter provided by Mohar in Ref. [12] could also be considered: $\frac{4}{n\lambda_2} \leq D \leq 2\lceil \frac{\Delta+\lambda_2}{4\lambda_2} \ln(n-1) \rceil$.

Next we apply a process of change and selection. Change is done by random modifications of the pattern of connections, whereas the selection process is based on the spectral distance between two graphs, a concept which we discuss below.

A typical modification of a graph consists in reconnecting one edge, while keeping again the constraints deduced from the spectrum.

To decide if the changes should be accepted (that is, to perform *selection*), we need a measure (cost function) of the “distance” of a given graph G_t with eigenvalues $\{\lambda_i^t, 0 \leq i \leq n\}$ from the reference graph G_0 . This measure is given by a spectral distance ϵ . In this paper, we introduce a simple spectral distance based on the quadratic difference of the eigenvalues $\epsilon = \sum_{i=0}^n (\lambda_i^0 - \lambda_i^t)^2$. We have tested other spectral distances which give different weights to the eigenvalues, but they are more complex and their efficiency is similar. Also, our new distance is simpler than the distance considered in the related study by Ipsen and Mikhailov [2]. These authors use the distance function $\epsilon = \sqrt{\int_0^\infty [\rho(\omega) - \rho_0(\omega)]^2 d\omega}$, where $\rho(\omega)$ is the spectral density defined as $\rho(\omega) = K \sum_{k=1}^{n-1} \gamma / ((\omega - \omega_k)^2 + \gamma^2)$ with $\omega_k^2 = -\lambda_k$, K is a normalization constant and γ is the width of the Lorentz distribution. Note that the spectral distance, which has to be evaluated many times by the two algorithms, involves in both cases the computation of all the eigenvalues of the graph. After this, in our case, the distance is calculated with simple operations: the sum of the squares of the eigenvalue differences. The distance proposed in [2], on top of these last operations, requires an integration.

The main problem with the reconstruction of a graph is to relate the generated graph to the reference graph. The graphs can be isomorphic but with permuted vertices or non-isomorphic with topological similarity that might not be manifest. As in Ref. [2], we check the similarity between two graphs in terms of the singular value decomposition [13] of their adjacency matrices (the details of which are in Section 4). Recently, another method, which measures and visualizes the similarity between networks, has been published in Ref. [14]. It would be of interest to check if it can be also applied in this context.

3. Combinatorial optimization algorithms

When exact methods are not possible, sometimes it is sufficient to obtain an approximate solution with a fast easily

implemented method. These methods include simulated annealing, genetic algorithms, tabu search, ant colony based systems, and many other combinatorial optimization techniques.

To implement any of these optimization methods, we need a way to encode the problem which has to be solved, and a measure to quantify the “goodness” of a solution. In the case of a spectral reconstruction of a network, a possible solution is given by the adjacency list of the graph. As described in the previous section, the solution is changed by reconnecting one link for a random node, while maintaining the bounds derived from the original spectrum. The cost function simply measures the “distance” of the spectrum of the new graph with the target spectrum.

Tabu search

We have considered *tabu search*, a method described in its current form by Glover in 1986 [15,16]. In our preliminary tests [17], tabu search outperformed other combinatorial optimization methods (simulated annealing and a multiagent optimization algorithm) and we recommend it for its simplicity. The overall approach is to avoid cycles in the solution space by forbidding or penalizing moves that would take the current solution to others previously visited. This ensures that new regions of the solution space will be investigated.

The tabu search starts by finding a local minimum. To avoid retracing the steps used, the method records recent moves in a list (tabu list). The tabu lists form the tabu search memory. The role of the memory can change as the algorithm proceeds. At initialization the goal is to make a coarse examination of the solution space, known as “diversification”, but as candidate locations are identified the search becomes more focused to produce locally optimal solutions in a process known as “intensification”.

- (1) Generate an initial random graph. Tabu list empty.
- (2) Repeat until stop criterion
 - (a) Select vertex at random and modify edge not in tabu list. Compute cost.
 - (b) If better, accept new graph.
 - (c) If worse, undo modification.
 - (d) Add edge to tabu list. Delete old items from list.

Cost function

We have considered different cost functions to measure the quality of the solutions. All of them are based on the quadratic difference between the eigenvalues of the Laplacian of the tested and the reference graphs, $\sum_{i=0}^n (\lambda_i^0 - \lambda_i^t)^2$, and in some cases they include rank ponderation. The cost functions tested are:

$$\left(\sum_{i=0}^n (\lambda_i^0 - \lambda_i^t)^2 \right)^{1/2}, \quad \left(\sum_{i=0}^n |\lambda_i^0 - \lambda_i^t|^3 \right)^{1/2}, \quad \left(\sum_{i=0}^n (i+1)(\lambda_i^0 - \lambda_i^t)^2 \right)^{1/2},$$

$$\left(\sum_{i=0}^n (n-i)(\lambda_i^0 - \lambda_i^t)^2 \right)^{1/2}, \quad \text{and} \quad \left(\sum_{i=0}^n |\lambda_i^0 - \lambda_i^t|(n-1)^{1.5} \right)^{1/2}.$$

The experiments with these cost functions to reconstruct random, regular, small-world, scale-free, and clustered graphs, show that the quality of the reconstructions is comparable for all of the cost functions and graphs with a variation of at most ten percent in the worst case. The tests were performed considering one hundred instances of each category of graph. The best results were obtained with the first simpler cost function, which was then used in the main set of experiments. We have also tested sets of eigenvalues coming from the standard Laplacian, the normalized Laplacian, and the sign-less Laplacian and the coefficients of the characteristic polynomial. Again, there are no important differences in the results obtained. Therefore, the final experiments were performed using the cost function $\sqrt{\sum_{i=0}^n (\lambda_i^0 - \lambda_i^t)^2}$ where the eigenvalues are those of the Laplacian matrix of the graph.

4. Results

The algorithm was implemented in C++ using DEV-C++ and executed on a PC (Pentium IV CPU at 2.41 GHz) under Windows XP. Each reconstruction test was limited to 300 s, which for this computer roughly corresponds to 30,000 iterations of the algorithm, each one involving the computation of all the eigenvalues of the graph. We note that the cost of the algorithm depends essentially on this computation which was done using the CLAPACK package (a C version of LAPACK) [18]. The algorithms in this package are $O(n^3)$ for dense graphs, where n is the number of vertices, but the complexity is $O(n^2)$ for most graphs and $O(n)$ if the graph is sparse, see Refs. [19,20]. We note that graphs associated to complex systems (like those considered in this paper) are in most cases sparse. Other factors which affect the performance of the algorithm are the precision required for the computed eigenvalues, and the size of the tabu list.

We tested the tabu search method and the cost functions on graphs of small orders (up to 14 vertices) and in all cases we were able to reconstruct exactly the graph. We also performed experiments to check the behavior of the algorithm in the case of cospectral graphs. In particular, we ran 1000 reconstructions from the spectrum $\{0, 3 - \sqrt{5}, 2, 3, 3, 3 + \sqrt{5}\}$ of the

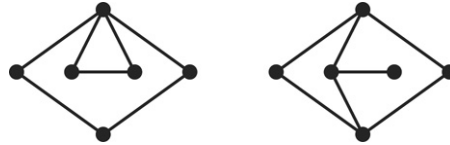


Fig. 1. Two distinct Laplacian cospectral graphs of order six.

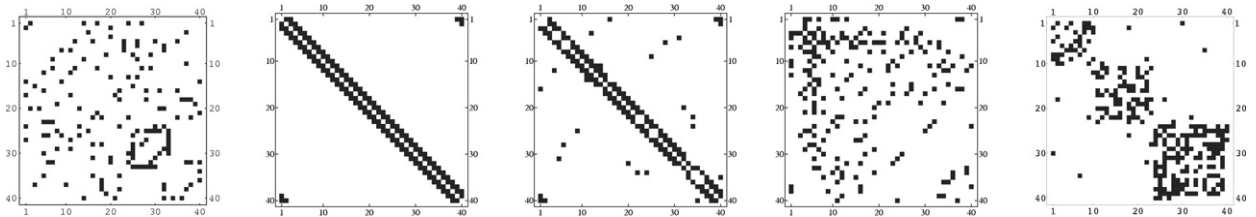


Fig. 2. Adjacency matrices of the reference graphs: random, regular (circulant), Watts-Strogatz small-world, scale-free and clustered. All graphs have order 40.

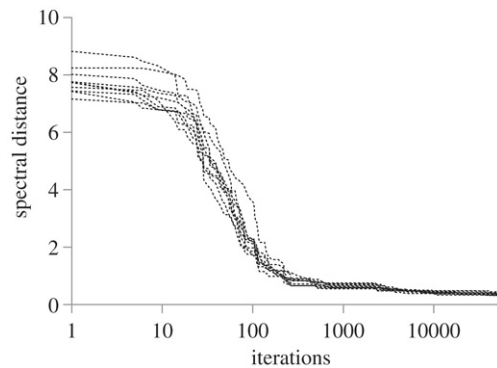


Fig. 3. Spectral distance evolution for ten distinct executions of the tabu search algorithm for the scale-free reference graph. Spectrum size: 40. Eigenvalue tolerance: 0.0001. Tabu list: 400. Tabu iterations after a change: 20.

two cospectral graphs of order six of Fig. 1, using the tabu search method and we obtained the graph on the left 554 times and the graph on the right 446 times.

There is no known polynomial time algorithm to decide if two graphs are isomorphic, although the problem has not been proved to be NP-complete [21,22]. We recall that a problem is NP-complete if it is NP, i.e. when a solution is given it can be verified in non-deterministic polynomial time, and at the same time an algorithm for solving it can be translated into one that solves any other NP problem.

Schmidt and Druffel [23] propose the method which we have implemented in our study. Their algorithm is not guaranteed to run in polynomial time, but has been shown to perform efficiently for a large class of graphs. Two isomorphic graphs should have the same exact degree distribution. After checking this property, the Schmidt and Druffel algorithm uses information from the distance matrices of the graphs to establish an initial vertex partition. Then, the distance matrix information is applied in a backtracking procedure to reduce the search for possible mappings between the vertices of the two graphs. The algorithm returns this mapping if the original and reconstructed graphs are indeed isomorphic.

As stated in Section 2, a problem occurs in the reconstruction process when we want to compare two networks which are different but similar in some context (in our case their spectra are close). In this case, we consider the singular values decomposition method for their adjacency matrices and use the spectral distance defined there.

The combinatorial optimization algorithm and cost functions considered in our study were tested systematically as follows:

We generate one sample graph of order 40 for each of the categories considered: random, regular (circulant), Watts-Strogatz small-world [24], scale-free [25], and clustered. Fig. 2 shows a graphic representation of the adjacency matrices of these graphs.

For each reference graph, we compute the spectrum and use it to reconstruct the graph with the tabu search method. We fix the reconstruction time for each graph to be 300 s, which, as it has been said before, corresponds to 30,000 algorithm iterations. This should allow the process to converge as it is shown in Fig. 3. Next, we compute the main topological parameters (diameter, average distance, degree distribution, clustering) for the best graph obtained and we check the similarity of its adjacency matrix with the original graph. Each test is repeated 100 times and the results are averaged. The final

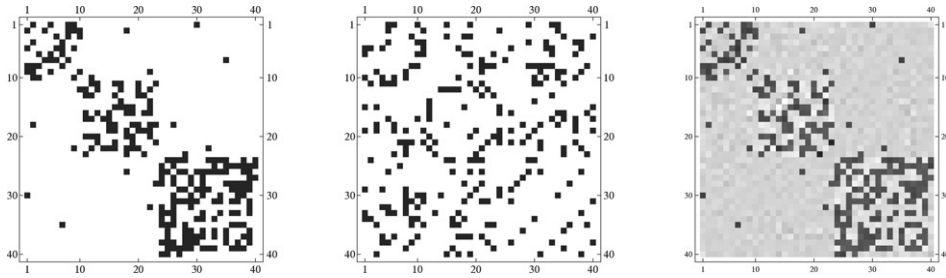


Fig. 4. Reconstruction of a clustered graph using tabu search. Left: The adjacency matrix of the original graph. Center: The adjacency matrix of the reconstructed graph. Right: Matrix F of the reconstructed graph.

Table 1

Tabu search

		Random		Circulant		Small-world		Scale-free		Clustered	
		Orig.	Rec.	Orig.	Rec.	Orig.	Rec.	Orig.	Rec.	Orig.	Rec.
Diameter	Min.		6		6		7		4		4
	Avg.	6	6.4	12	9.7	9	7.9	4	4.1	5	5
	Max.		7		18		9		5		6
Average distance	Min.		2.822		1.032		3.451		2.256		2.174
	Avg.	2.894	2.9	6.185	4.222	3.973	3.721	2.315	2.320	2.646	2.226
	Max.		2.964		7.441		3.956		2.379		2.277
Degree	Min.	1	1	4	1	2	1	1	1	2	1
	Avg.	3.8	3.8	4	4	3.9	3.9	4.95	4.95	6.3	6.3
	Max.	8	8	4	5	6	6	17	17	13	13
Clustering	Min.		0.163		0.604		0.461		0.138		0.189
	Avg.	0.199	0.217	0.7	0.727	0.529	0.489	0.225	0.191	0.372	0.216
	Max.		0.284		0.798		0.504		0.260		0.254
δ	Min.		0.011		0.035		0.022		0.012		0.064
	Avg.		0.017		0.079		0.042		0.019		0.076
	Max.		0.050		0.145		0.064		0.034		0.088

Results for the average of 100 reconstructions for each reference graph. Spectrum size: 40. Eigenvalue tolerance: 0.0001. Tabu list: 400. Tabu iterations after a change: 20.

graph could be isomorphic to the reference graph but with permuted vertices or non-isomorphic with some topological similarity that might not be manifest. We use the singular value decomposition technique [13], as described in Ref. [2], to quantify this similarity. We recall that a matrix A can be decomposed into two matrices U and V and a diagonal singular value matrix Σ which satisfy $A = U\Sigma V^T$ and $\Sigma = U^T A V$. For any two graphs G_1 and G_2 with adjacency matrices A_1 and A_2 , consider the function $F = F(A_1, A_2) = U_1 \Sigma_2 V_1^T = U_1 U_2^T A_2 V_2 V_1^T$ which is constructed from the singular vectors of G_1 and G_2 . If the two graphs are isomorphic and their adjacency matrices only differ because of a different ordering of the vertices, it will happen that $A_1 = F(A_1, A_2)$. However, if the two graphs are not isomorphic, F will have real values not far from the values of A_1 . Therefore, it is possible to define $\Delta = A_1 - F$ and use the norm $\delta = \sqrt{\sum_{i,j} \Delta_{ij}^2 / n}$ to measure similarity between the graphs.

Fig. 4 shows a typical reconstruction: the left matrix corresponds to the adjacency matrix of the original graph (a clustered graph), the central matrix is the adjacency matrix of the reconstructed graph and the right matrix is the F matrix obtained from this adjacency matrix after performing the singular value transformation. We see, in a visual way, the quality of the reconstruction (which can also be described more precisely by the parameters in Table 1). In this figure, the matrix elements are represented by using gray-scale color maps whose limits are determined by their minimum and maximum values. Even though the matrix F does not coincide with the adjacency matrix of the reference graph, it is very close to it. Its distance (norm) to the reference graph matrix is $\delta = 0.07$. In Table 1, we present a set of results for the tabu search method. More details for the whole set of experiments (other spectral distances and methods) are available from the authors and are included in Ref. [17].

We note that the values for δ are in the same range than those in Ref. [2] where a simulated annealing algorithm with an elaborated cost function involving an integration was used. Tests with a standard greedy algorithm provide values that are around ten times worse for the same graphs.

We have also used data from the metabolic network of *S. cerevisiae* and the protein–protein interaction network of *H. pylori* [26], to generate new networks with a topology similar to the original network. We considered for each of these

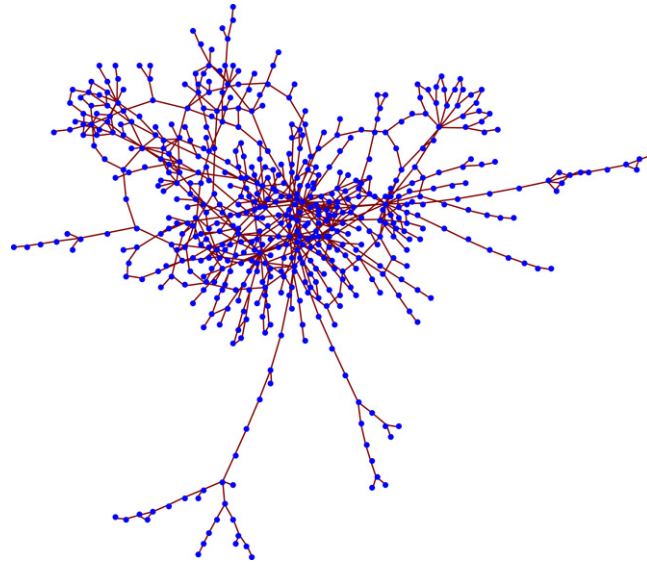


Fig. 5. Largest connected component of the metabolic network of *Saccharomyces cerevisiae* which has 570 vertices and 776 edges.

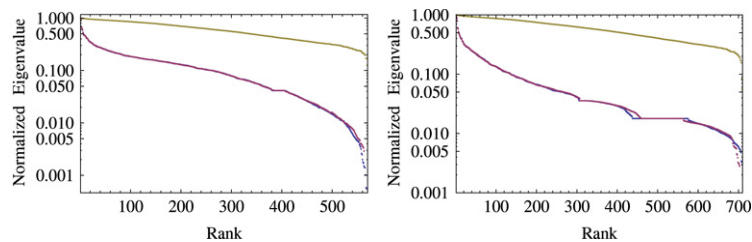


Fig. 6. Spectra of original and reconstructed networks of the largest connected components of the *Saccharomyces cerevisiae* metabolic network (left) and the *Helicobacter pylori* protein–protein interaction network (right.) Upper points correspond to the spectra values of the initial networks considered in the reconstruction process.

Table 2

Reconstruction of the largest component of the *Helicobacter pylori* metabolic and *Saccharomyces cerevisiae* protein–protein interaction networks

	Order		Size		Max. deg.		Min. deg.		Diameter		Avg. dist		Clust.	
	Orig.	Rec.	Orig.	Rec.	Orig.	Rec.	Orig.	Rec.	Orig.	Rec.	Orig.	Rec.	Orig.	Rec.
<i>H. pylori</i>	710	710	1396	1396	55	55	1	1	9	9	4.15	3.88	0.02	0.02
<i>S. cerevisiae</i>	570	570	776	776	23	23	1	1	27	25	8.22	7.75	0.07	0.06

networks their largest connected component (Fig. 5). After running the algorithm (10 h for the *S. cerevisiae* network and 20 h for the *H. pylori* network, with the computer resources mentioned above), the spectra of the reconstructed networks matches well the original spectra as we can visualize in Fig. 6. In this figure, upper points correspond to the spectra of the initial randomly generated networks in the reconstruction process. In Table 2 we present some relevant topological parameters for the original and the reconstructed networks. Thus, our algorithm can be useful as a tool to generate models for real life complex networks.

5. Conclusion

The results show that tabu search, with a simple cost function – the quadratic difference of eigenvalue –, reconstructs small graphs exactly from their spectra and obtains topologically good approximations for larger graphs. We have tested graphs with up to 2000 nodes and 20,000 edges. Because of the simplicity of the cost function, the method is easy to implement, and results in a fast algorithm. The algorithm provides a new tool for the study and modeling of complex real life networks and can be used, without modifications, to generate quasi-optimal topologies for networks associated with dynamic processes.

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