Analysing degeneracies in networks spectra

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Abstract - Many real-world networks exhibit a high degeneracy at few eigenvalues. We show that a simple transformation of the network's adjacency matrix provides an understanding to the origins of the occurrence of high multiplicities in the networks spectra. We find that the eigenvectors associated with the degenerate eigenvalues shed light on the structures contributing to the degeneracy. Since these degeneracies are rarely observed in model graphs, we present results for various cancer networks. This approach gives the opportunity to search for structures contributing to degeneracy which might have an important role in a network.

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The paper written by Leonhard Euler on the Seven Bridges of Königsberg marks the beginning of the graph theory [1] by introducing a concept of graphs representing complex systems. The work was restricted to small system size. The revolution in computing power later provided the opportunity to analyse very large real-world systems in terms of networks. Further, the analysis of graph spectra has contributed significantly to our understanding of structural and dynamical properties of graphs [2,3]. Among other things, it has been noted that a symmetric spectrum about the origin is related to a bipartite graph [4]. Further, a bulk portion of eigenvalues has been shown to be modeled using the random matrix theory [5], whereas extremal eigenvalues have been shown to be modeled using the generalized eigenvalue statistics [6,7]. Recent investigations have revealed that real-world networks exhibit properties which are very different from those of the corresponding model graphs [8–10]. One of these properties is the occurrence of degeneracy at 0, −1 and −2 eigenvalues [2]. Few papers have related 0 and −1 eigenvalues to stars and cliques, respectively [11–13]. However, graphs in the absence of stars and cliques can still show a degeneracy at 0 and −1 eigenvalues, respectively. As a result, these reasons are not exhaustive and it turns out that the origins of degeneracy at these eigenvalues are more complex. For example, the 0 degeneracy has been shown to result from the complete and the partial duplications [14] of nodes which are particularly interesting for biological systems as they shed light on a fundamental process in the evolution related with gene duplication [15], hence an interest lies in investigating the origins of other degenerate eigenvalues. We will see in the following that two reasons emerge to explain the degeneracy of every eigenvalue. In particular cases, one of these reasons reveals the existence of characteristic structures in networks.

In this paper, we consider finite undirected graphs defined by $G = \{V, E\}$ with $V$ the node set, and $E$ the edge set such as $|V| = N$ and $|E| = m$. A graph is completely determined by its adjacency matrix for which its element $A_{ij}$ is 1 when there is an edge from vertex $i$ to vertex $j$, and 0 otherwise. In the following, the rows $i$ of every adjacency matrix will be denoted by $R_i$.

The eigenvalues are obtained by computing the roots of the characteristic polynomial of the adjacency matrix, $\chi_A(\lambda) = \det(A - \lambda I) = \prod_{i=1}^{N}(\lambda - \lambda_i)$ and denoted by $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$. Since the adjacency matrix of an undirected graph is symmetric with 0 and 1 entries, the eigenvalues are real. The associated eigenvectors $v_1, v_2, \ldots, v_N$ satisfy the eigen-equation $Av_i = \lambda_i v_i$ with $i = 1, 2, \ldots, N$.

A complete graph, denoted by $K_N$, is an undirected graph for which every pair of nodes is connected by a unique edge. This type of graphs is especially interesting since their spectra exhibit a very high multiplicity at the $-1$ eigenvalue. Specifically, a complete graph of $N$ nodes has $N - 1$ degeneracies for the $-1$ eigenvalue [2]. However, it is misleading to associate this special graph structure
with $-1$ degeneracy. Let us take as example the 5-nodes complete graph in which we have removed an edge. In the resulting graph, two $-1$ eigenvalues are retained, whereas the globally connected structure is destroyed, which indicates that the globally connected structure is not sufficient to explain the occurrence of the $-1$ degeneracy. We will see in the following that only one type of particular structure consisting of a complete graph and its variants contribute to the $-1$ eigenvalue.

We consider the matrix $A + I$, where $I$ is the identity matrix, and we make a change of variables in the characteristic polynomial such as $\chi_{A+I}(\lambda) = \chi_A(\mu)$. By this way, $\mu$ is an eigenvalue of $A$ if and only if $\lambda$ is an eigenvalue of $A + I$. We can also prove that they have the same multiplicity. Hence, it is possible to reduce the computation of the $-1$ eigenvalue of $A$ to the $0$ eigenvalue of $A + I$. This is especially interesting since the origin and implications of the occurrence of the $0$ degeneracy in networks spectra are well characterized [14, 16]. The spectrum of a matrix of size $N$ and rank $r$ contains the $0$ eigenvalue with multiplicity $N - r$. Three conditions lead to the lowering of the rank of a matrix: i) the network has an isolated node ($R_i = 0 \cdots 0 \cdots 0$); ii) at least two rows are equal ($R_i = R_j$); iii) two or more rows together are equal to some other rows ($\sum a_i R_i = \sum b_j R_j$, where $a_i$ and $b_j$ take an integer value included $0$).

In the case of $A + I$, it is obvious that the condition i) is never met. We focus now on the condition ii). Let us consider a network of size $N$ for which two nodes labelled 1 and 2 verify $R_1 = R_2$ in the adjacency matrix added to the identity matrix,

$$ A + I = \begin{pmatrix} 1 & a_{1,2} & \cdots & a_{1,N} \\ a_{1,2} & 1 & \cdots & a_{1,2,N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1,N} & a_{2,N} & \cdots & 1 \end{pmatrix}. \tag{1} $$

The condition ii) is verified for any pair of rows, say 1st and 2nd, if and only if $a_{1,2} = 1$ and $a_{1,i} = a_{2,i}$ for $i = 3, 4, \ldots, N$.

So, the adjacency matrix $A$ takes the following form:

$$ A = \begin{pmatrix} 0 & 1 & \cdots & a_{1,N} \\ 1 & 0 & \cdots & a_{1,N} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1,N} & a_{1,N} & \cdots & 0 \end{pmatrix}. \tag{2} $$

The nodes 1 and 2 are interlinked and connected to the same set of other nodes. The rank of $A + I$ is $N - 1$, and hence we deduce that the spectrum associated to the $A$ matrix contains exactly one $-1$ eigenvalue. It is trivial to generalize this proof to the case $R_1 = R_2 = \ldots = R_n$. Hence, $n$ nodes forming a complete graph $K$ connected to the same set $S$ of other different nodes and denoted as $K * S$ (fig. 1) contribute to the $-1$ eigenvalue with multiplicity $n - 1$.

Next, we emphasize on the condition iii), which, for example, may correspond to $R_1 + R_2 = R_3 + R_4$ in the matrix $A + I$. For this particular case, the condition iii) is satisfied if and only if $a_{1,j} + a_{2,j} = a_{3,j} + a_{4,j}$ for $j = 1, 2, \ldots, N$. On this basis, we can clarify that the condition iii) implies for the node $j$ that $j = 5, 6, \ldots, N$. If the node $j$ is adjacent (respectively, non-adjacent) to both nodes labelled 1 and 2, it is also adjacent (respectively, non-adjacent) to both nodes 3 and 4. In the case in which the node $j$ is connected either to 1 or 2, the condition iii) imposes that $j$ is connected either to 3 or 4 (see table 1).

Let us now have a closer look at constraints which nodes 1, 2, 3 and 4 must obey. Since we have $a_{i,j} = 1$, $a_{i,j} = a_{j,i}$ and by considering the previous constraints,

$$ \begin{cases} 1 + a_{1,2} = a_{1,3} + a_{1,4}, \\ a_{1,2} + 1 = a_{2,3} + a_{2,4}, \\ a_{1,3} + a_{2,3} = 1 + a_{3,4}, \\ a_{1,4} + a_{2,4} = a_{3,4} + 1. \end{cases} \tag{3} $$

This set has more unknown variables than the number of equations. The system is underdetermined and has infinitely many solutions. As a result, it is difficult to define a typical structure which corresponds to the condition iii). Here we will limit ourselves to illustrate it with the graph in fig. 1(b) for which the adjacency matrix $A$ added to the identity matrix satisfies $R_1 + R_4 = R_2 + R_5$.

This relation is at the origin of the $-1$ eigenvalue observed in the spectrum of $A$. More generally, each linear combination of rows in $A + I$ leads to exactly one $-1$ eigenvalue. The power of this approach is that it can be extended to all the degenerate eigenvalues. In the case of a network which exhibits a high multiplicity at the $x$
eigenvalue, it is wise to reduce the computation of the \( \lambda \) eigenvalue to the study of the 0 eigenvalue of \( A - xI \) so that \( \chi_{A-xI}(\lambda) = \chi_A(\mu) \).

In this manner, we are able to understand the origin of every degenerate eigenvalue, thus enabling to focus on their implications. We note that the condition ii) is never met for \( \lambda < -1 \) and \( 0 < \lambda \) since the entries of the adjacency matrix are equal to 0 or 1.

We have seen that the \(-1\) degeneracy in networks spectra is related to some typical structures. However, the study of eigenvalues and their multiplicities is not sufficient to determine the number and size of these structures in networks. For example, the graphs of fig. 2 lead to the same number of the \(-1\) degeneracy but have different structures. The question we ask now is: how can we identify nodes which contribute to degenerate eigenvalues? In order to address this, we consider eigenvectors associated to the degenerate eigenvalues of \( A \). First we focus on the \(-1\) degeneracy and note that eigenvectors of the \(-1\) eigenvalue, such as \( Av = \lambda_1v \), are the same as the eigenvectors corresponding to the 0 eigenvalues of \( A + I \) which verify \((A + I)v = \lambda_0v\).

We find that most of the entries of such eigenvectors (corresponding to the 0 eigenvalue) are equal to zero. It turns out that non-null entries reveal nodes which contribute to decreasing the rank of a matrix. Moreover, nodes belonging to the same structure, say \( K \ast S \), are linked by the following relation (derivation is in the Supplementary Material Supplementary material.pdf (SM)\(^1\)):

\[
\{ \sum_{i \in K_v} v_i = 0 \quad \text{with} \quad v_i \neq 0 \quad \text{and} \quad p = 1, 2, \ldots, n_{K \ast S}, \quad v_j \in \{K_1 \cup K_2 \cup \ldots \cup K_{n_{K \ast S}}\} = 0, \}
\]

where \( n_{K \ast S} \) is the number of \( K \ast S \) structures in the network. This relation, arising directly from \( R_i = R_j \), enables us to distinguish each structure contributing to the \(-1\) degeneracy through condition ii). The same reason holds for condition iii). Indeed, nodes belonging to the same linear combination verify

\[
\sum_{i \in (LC)_p} v_i = 0 \quad \text{with} \quad v_i \neq 0 \quad \text{and} \quad p = 1, 2, \ldots, n_{LC},
\]

\[
v_j \in (LC)_1 \cup (LC)_2 \cup \ldots \cup (LC)_n_{LC} = 0,
\]

where \( n_{LC} \) is the number of linear combinations of rows in the network. The derivation of eq. (5) follows the same reasoning as that of eq. (4) seeing that \( R_k = R_i \) is a particular case of \( \sum_i a_i R_k = \sum_j b_j R_j \). It is also interesting to note that eqs. (4) and (5) can be proved using row equivalent forms of adjacency matrices (see footnote \(^1\)). Since the assumptions are only based on the conditions ii) and iii), the proofs provided in the SM show that eqs. (4) and (5) are valid for any arbitrary network. These properties give the opportunity to find in every network the nodes which contribute to the \(-1\) degeneracy. We can go further by distinguishing the nodes which satisfy the condition ii) and those which satisfy the condition iii). In order to do it, we can have a rather easy computation of the rows of \( A + I \) such as \( R_i = R_j \). Then, by considering one of the eigenvectors associated to the \(-1\) eigenvalue, we can find all the non-zero entries. Among these non-zero entries, those which do not correspond to the nodes computed previously, satisfy the condition iii). Besides being able to find the nodes leading to the \(-1\) degeneracy, we can associate them to ii) or iii). As we did in the previous section, we extend this approach to all the degenerate eigenvalues. Indeed, eigenvectors of \( x \) of the \( A \) matrix which satisfy \((A - xI)v = \lambda_0v\) are the same as the eigenvectors corresponding to 0 eigenvalues of \( A - xI \) so that \( Av = \lambda_xv \).

So, we can find precisely the origin of every degenerate eigenvalue, namely the condition ii) or the condition iii). In addition, we are able to identify the nodes which contribute to high multiplicity of eigenvalues. In brief, this approach provides a quantitative measure of degeneracy in networks spectra.

What we have done so far is finding subgraphs behind the occurrence of degeneracy. The question we ask now is: do they play a significant role in real-world networks? In order to answer this, we are going to assess whether randomness enables to observe this kind of structures using various model graphs. The 0 degeneracy being the subject of a previous discussion [14], we focus in the following on degeneracy at the \(-1\) eigenvalue. First, we consider Erdös-Rényi model (ER) [17] in which each edge has a probability \( p \) of existing. Since the edges are placed randomly, most of the nodes have a degree close to the average degree \((k)\) of the graph [17]. So, the probability \( p \) equals \( \frac{k}{N} \).

We note that such networks are almost surely disconnected if \( p < \frac{\ln(N)}{N} \) [17]. In other words, if the previous equation is verified, there are at least two nodes such that no path has them as endpoints. We construct ER networks with different average degrees \((k)\) and sizes \( N \). As depicted by fig. 3, ER networks exhibit a low degeneracy for small average degrees. We can explain this by referring to \( n \)-complete graphs percolation [18]. Indeed, it has been shown that in such graphs, complete subgraphs occur beyond a certain probability \( p \). The threshold of this percolation is defined as \( p_c(n) = [(n-1)N]^{-\frac{1}{n-1}} \) [18].

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\(^1\)The SM contains the derivation of the relation linking nodes to the \( K \ast S \) structure.
The higher \( n \), the greater the increase in the threshold of percolation. Put another way, the more \( n \) augments, the more the probability to have \( n \)-complete graphs in the ER graphs gets diminished. Because \( p = \frac{k}{N} \) and by referring to \( p_c \), it is very easy to show that \( n \)-complete subgraphs appear in a network if the average degree is more than \( \langle k \rangle_c \approx N \frac{n}{n-1} \) [19]. For example, \( \langle k \rangle_c \approx 31.62 \) for \( n = 3 \) and \( N = 1000 \). In the case in which \( \langle k \rangle \) is smaller than \( \langle k \rangle_c \), we do not observe \( n \)-complete subgraphs in ER networks. So, the structure \( K \ast S \) being not obtained, the condition ii) is not met. If \( \langle k \rangle \) is smaller than \( \langle k \rangle \), it is possible to find cliques in the networks. However, randomness which characterizes the ER model may not give the opportunity to organized structures such as \( K \ast S \) to emerge. Nevertheless, the previous explanations are not exhaustive since the condition iii) can contribute to the \(-1\) degeneracy. For the condition not corresponding to a defined structure, it is more difficult to predict its contribution. Finally, the alert reader may inquire why we observe degeneracies for \( \langle k \rangle = 2 \). As it is specified earlier, in the case in which \( p < \frac{\ln(N)}{N} \) is verified, the network is most probably disconnected. More particularly, for a given \( N \), the lower the value of \( p \) (and hence \( \langle k \rangle \)), the higher the number of isolated nodes and two connected nodes [17]. Two connected nodes constitute a \( K \ast S \) structure where \( K \) contains two nodes and \( S \) contains no node. That is why the \(-1\) degeneracy exists for the low average degree.

We focus now on scale-free (SF) networks [20]. This model is particularly interesting since its degree distribution follows a power law as was also observed for many real-world networks [17]. We generate the SF networks by using a preferential attachment process. Each new node is attached to the existing nodes with a probability which is proportional to their degrees. As a result of the power law, SF networks contain a few high-degree nodes and a large number of low-degree nodes and the \(-1\) degeneracy is not observed in most of the cases (fig. 3). As explained in [14], any two nodes having a low degree are more susceptible to connect to the high-degree nodes, leading to two nodes having the same neighbors. However, the preferential attachment makes it less probable for these nodes to be interlinked. So, it is unlikely to find the \( K \ast S \) structure in SF networks. In the case of \( \langle k \rangle = 2 \), we find the \(-1\) degeneracy. Thanks to the eigenvectors analysis, we observe that only the condition iii) contributes to high multiplicity in this particular case. As we have already said, there is no typical structure corresponding to this condition. Therefore, it is difficult to provide an explanation to this observation.

As we have just seen, the \(-1\) degeneracy is not observed in ER and SF networks, leading us to believe that randomness is not conducive to degeneracy in networks spectra. In order to convince us, we study small-world (SW) networks constructed with the Watts-Strogatz mechanism [21]. This graph model is interesting since it illustrates small-world phenomenon according to which the distance between nodes increases as the logarithm of the number of nodes in the network [22]. The generating mechanism consists of a regular ring lattice where each node is connected to \( k \) neighbors and for which edges are rewired with probability \( p_r \). The spectrum \( \{\lambda_1, \lambda_2, \ldots, \lambda_N\} \) of the Watts-Strogatz graph without a link rewiring, i.e., the 1-d lattice with circular boundary condition, can be computed by \( \lambda_m = \frac{\sin(\pi m/N)}{\sin(\pi m/(N-k))} \) where \( m = 1, 2, \ldots, N \). This relation leads to \( \lambda = -1 \) if and only if the following constraint is fulfilled:

\[
\sin(\pi m/(N-k)) = 0 \quad \text{and} \quad \sin(\pi m/k) \neq 0.
\]

In other terms, if \( \lambda_m^\pm_1 \) is an integer and \( q_m^\pm_1 \) is not, then \( \lambda_m = -1 \). The same reasoning applies in the case of 0 the eigenvalue which leads to

\[
n_m^0 = \frac{kN - (m-1)}{2} \quad \text{with} \quad n_m^0 \text{ integer}.
\]

Table 2: 0 and \(-1\) degeneracy in small-world network without link rewiring with \( N = 1000 \). Multiplicity of the \( \lambda \) eigenvalue equals the number of times that \( n_m^\pm \) is an integer, for \( m = 1, 2, \ldots, N \).

| \( k \) | 10 | 20 | 30 | 40 | 50 | 60 |
|-------|----|----|----|----|----|----|
| \( \lambda_0 \) | 5 | 10 | 5 | 20 | 25 | 5 |
| \( \lambda_{-1} \) | 0 | 0 | 0 | 0 | 0 | 0 |

Fig. 3: (Color online) (a) and (b) illustrate the effect of the average degree \( \langle k \rangle \) on the \(-1\) degeneracy for different sizes \( N \) in ER and SF networks, respectively. All values are averaged over 20 random realizations of the network. (c) represents the number of \( 0 \) eigenvalues depending on the link rewiring probability for a 1000 nodes small-world network. The regular graph has degree \( k = 20 \). All values are averaged over 20 random realizations of the network.
Table 3: Statistical properties for all the normal and disease networks. The total number of nodes is $N$, the average degree $\langle k \rangle$, the probability $p$ of two nodes to be connected by an edge and the threshold of $3$-complete percolation $p_c(3)$. $\lambda$ represents the number of eigenvalues in the cancer networks, $\langle CC \rangle$ the average clustering coefficient and $r$ the assortativity value.

| Network   | $N$   | $\langle k \rangle$ | $p$     | $p_c(3)$ | $\lambda_1$ | $\lambda_0$ | $\lambda_{-1}$ | $\langle CC \rangle$ | $r$  |
|-----------|-------|----------------------|---------|----------|-------------|-------------|----------------|----------------|------|
| Breast$_N$ | 2443  | 12.38                | 0.0051  | 0.0143   | 0           | 72          | 21             | 0.28            | 0.08 |
| Breast$_D$ | 2046  | 13.83                | 0.0068  | 0.0156   | 0           | 71          | 12             | 0.29            | 0.19 |
| Colon$_N$  | 4849  | 16.05                | 0.0033  | 0.0102   | 0           | 164         | 19             | 0.25            | 0.18 |
| Colon$_D$  | 3423  | 21.23                | 0.0062  | 0.0121   | 0           | 44          | 10             | 0.23            | 0.09 |
| Oral$_N$   | 2105  | 20.66                | 0.0098  | 0.0154   | 0           | 60          | 13             | 0.31            | 0.19 |
| Oral$_D$   | 1542  | 34.75                | 0.0225  | 0.0180   | 0           | 15          | 1              | 0.35            | 0.03 |
| Ovarian$_N$| 1748  | 7.77                 | 0.0044  | 0.0169   | 4           | 129         | 31             | 0.25            | 0.01 |
| Ovarian$_D$| 2022  | 7.95                 | 0.0039  | 0.0157   | 2           | 116         | 19             | 0.26            | 0.10 |
| Prostate$_N$|2304 | 9.57                 | 0.0042  | 0.0147   | 2           | 125         | 47             | 0.29            | 0.08 |
| Prostate$_D$|4938 | 7.62                 | 0.0015  | 0.0101   | 4           | 340         | 135            | 0.30            | 0.10 |

However, we observe a degeneracy at the 0 eigenvalue. It is interesting to notice that the degeneracy does not increase constantly with an increase in $k$. Let us now attempt to understand how the probability $p_c$ affects the multiplicity of the 0 eigenvalue for a small-world network. Figure 3 reveals that the number of 0 eigenvalues decreases quickly with $p_c$. More particularly, the 0 degeneracy is completely removed for low link rewiring probability. Simulations for different configurations ($N, k$) yield similar results. As a consequence, the introduction of randomness, even small, has strong impacts on the multiplicity of eigenvalues.

We substantiate the previous results by considering examples of few real-world networks. We analyse protein-protein interaction networks (PPI) of five cancers namely breast, colon, oral, ovarian and prostate cancers [23]. The PPI networks have proteins as nodes and the interactions between those proteins as edges. These networks exhibit 0 and $-1$ degeneracies (see table 3). In addition, we find a low degeneracy at $+1$ in few of these networks. The number of 0 eigenvalues being higher than the number of $-1$ eigenvalues indicates that duplication structures are more frequent than the $K \ast S$ structures. It may be tempting to make a causal link between macroscopic properties such as clustering coefficient or assortativity and eigenvalue degeneracy. However, as reported in table 3, the normal oral-cancer network has $\langle CC \rangle = 0.31$ and $\lambda_0 = 60$, whereas for the disease one, $\langle CC \rangle = 0.35$ and $\lambda_0 = 15$. This follows that one can find networks having lesser degeneracy but with high value of $\langle CC \rangle$. Furthermore, let us consider one more macroscopic quantity which consists in degree-degree correlations and let us attempt to find a relation between assortativity (positive degree-degree correlations and degeneracy at $-1$). Again, let us consider the ovarian cancer which for the disease case has $r = 0.10$ and $\lambda_0 = 116$, whereas for the normal case it has $r = -0.01$ and $\lambda_0 = 129$. Therefore, even if assortativities of networks are different, degeneracies may be quite the same.

All these point out that there exists no obvious causal link between these macroscopic properties and degeneracy in networks. Our experiments only indicate that randomness has a strong impact on degeneracy in networks spectra.

Thanks to eqs. (4) and (5), we can go further by using what we know about eigenvectors associated to the $-1$ eigenvalue in order to identify each contribution to degeneracy in the cancer networks. Table 4 reports the number of $-1$ eigenvalues, denoted by $\lambda_{-1}$, and nodes, denoted by $N_{\lambda_{-1}}$, by condition for all the normal and disease networks. The condition ii) is largely at the origin of the $-1$ degeneracy and in a few cases, condition iii) is not met. Therefore, the $K \ast S$ structure mostly contributes to the $-1$ degeneracy in the networks spectra. As a conclusion, real-world networks contain a large number of $K \ast S$ structures whose existence is revealed by high multiplicity of $-1$ eigenvalues. As degeneracy at $-1$ eigenvalue is poorly observed in model networks, this indicates that the resulting structures may have a significance in real-world networks.

As a conclusion, many real-world networks exhibit a very high degeneracy at few eigenvalues such as 0 and...
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−1 as compared to their corresponding random networks. This suggests that the nodes contributing to high multiplicity may play a central role in these networks. This letter has numerically and analytically demonstrated the origin as well as the structures contributing to degeneracy, giving the opportunity to study their impact on real-world networks. In the case of cancer networks, if such structures turn out to have a biological significance, the proposed approach will provide a new and different way to search for drug targets and biomarkers [24].

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