The dependence of graph energy on network structure

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Abstract. In this paper, we aim at investigating how the energy of a graph depends upon its underlying topological structure for regular and sparse scale free networks. Firstly, the spectra and energies of some simple regular graphs are calculated exactly and an exact expression is derived for the eigenvalues of adjacency matrix of regular graphs with degree $k$ being given by $k = 2^a (a = 1, 2, 3, \ldots)$. It is also found that a graph with $k$ being about $0.8N$ owns the largest energy for the regular graphs with the same size and the same generating method used in this paper. Furthermore, we investigate the energy of sparse scale-free networks with different average degree $< k >$ and degree distribution exponent $\gamma$. While $\gamma$ is specified, the energy is a power-law function of $< k >$ with exponent being about 0.5. And while $< k >$ is fixed, energy will be obviously proportional to $\gamma$. Otherwise, we also find that the energy is a power-law function of the variance of degree sequence with exponent weakly depending on the size of network. Interestingly, while both $< k >$ and $\gamma$ are specified, there will be a terrific linear fit to the relationship between energy and the size of system.

1. Introduction

The graph energy $E$, defined as the sum of the absolute values of eigenvalues of adjacency matrix, is coming from chemistry where it used to approximate the total $\pi$-electron energy of molecules\cite{1}. This definition form was first stated in the 1970s\cite{2} and later proposed in the book\cite{3} and paper\cite{4}. Researches related to the graph energy can be traced back to the 1930s when a German scholar Erich Hückel proposed a method to approximately solve the Schrödinger equation of a class of organic molecules\cite{5, 6, 7}. Erich Hückel obtained an expression for the total energy of all $\pi$-electrons. According to this expression, I. Gutman calculated that the energy is equal to two times the sum of the positive eigenvalues. By considering the symmetry of eigenvalues of all graphs, he changed the expression of graph energy to the sum of absolute values of all eigenvalues which is just formal and does not have a clear physical meaning.

For the classification of graphs according to the energy, a finite and undirected graph $G$ with $N$ nodes is denoted to be "hyper-energetic" if its energy is larger than $2(N - 1)$\cite{8}, which corresponds to the energy of a complete graph on $N$ vertices. And if the energy of a connected graph $G$ is less than $N$(which relates to the graph generated by $N/2$ isolated edges or $N/4$ isolated quadrangles), then the graph will be labeled as "hypo-energetic" graph\cite{9}. Another one
that regards to the "hypo-energetic" graph is the strongly "hypo-energetic" graph with energy being less than \((N - 1)[10]\). It is particular noteworthy that the star graph with \(N\) nodes owns the lowest energy \(2\sqrt{N - 1}\) comparing with all the other connected graphs with the same vertices.

Until now, most researches on graph energy still remain at determining the bounds of energy for some particular graphs. For instance, J. H. Koolen and V. Moulton proved that the energy of graph \(G\) on \(N\) vertices was not larger than \(\frac{N}{2}(1 + \sqrt{N})[11]\). While both \(N\) and edges \(m\) are given, the graph energy will less than or equal to \(\sqrt{2mN}[12]\). Other bounds of graph energy can be found in references [13, 14, 15, 16, 17, 18, 19, 20, 21]. However, even though some bounds of energy for graphs are well developed, relatively little is known regarding to the relationship between energy and the structure of graphs.

In this paper, we aim at exploring the dependence of graph energy on the graph’s underlying structure. In the next section, we first calculate exactly the spectra and energies of some simple \(k\)-regular graphs. And the relation among energy and degree \(k\) for regular graphs is also studied in this part. Some distributions of energy regarding to some topological parameters of sparse scale free networks are displayed in section 3. And Section 4 presents our conclusions.

2. Graph spectra for some regular graphs
We begin with the investigation of some simple regular graphs, which are generated with all nodes being located in a ring and all edges being formed by nearest neighbor connections. In this part, we strictly calculated the eigenvalue spectra of adjacency matrix for some regular graphs with node’s degree \(k\) being small. Furthermore, an exact function of eigenvalue spectra for some regular graphs with \(k\) being an exponential function of 2 is deduced.

Firstly, for the regular graph with \(k = 2\) (see Fig.1(a)), the eigenvalues of adjacency matrix can be expressed by

\[
\{\lambda_i\}_0^{N-1} = 2 \cos\left(\frac{2\pi i}{N}\right),
\]

where \(N\) is the number of nodes. Therefore, according the definition of graph energy, we can strictly obtain the energy \(E\):

\[
E = \sum_{i=0}^{N-1} 2|\cos\left(\frac{2\pi i}{N}\right)| = \frac{4N}{\pi}.
\]

And for the regular graph with \(k = 4\) (see Fig.1(b)), the eigenvalues are

\[
\{\lambda_i\}_0^{N-1} = 4 \cos\left(\frac{\pi i}{N}\right) \cos\left(\frac{3\pi i}{N}\right),
\]

and graph energy is \(\frac{3\sqrt{3}N}{\pi}\).

For the cases of \(k = 6\) and \(k = 8\), whose topological structures are showed in Fig.1(c) and Fig.1(d), the eigenvalues are

\[
\{\lambda_i\}_0^{N-1} = 2 \cos\left(\frac{6\pi i}{N}\right) + 4 \cos\left(\frac{\pi i}{N}\right) \cos\left(\frac{3\pi i}{N}\right),
\]

and

\[
\{\lambda_i\}_0^{N-1} = 8 \cos\left(\frac{\pi i}{N}\right) \cos\left(\frac{2\pi i}{N}\right) \cos\left(\frac{5\pi i}{N}\right).
\]

And the corresponding graph energies are \(\frac{32\sqrt{3} - 6\sqrt{3}}{6\pi}\) and \(\frac{(5\sin\left(\frac{\pi}{3}\right) + 25\sin\left(\frac{3\pi}{2}\right) - 8)N}{3\pi}\) respectively.
So, for the specified regular graphs with $k = 2^a$, where $a$ is an integer, we have derived an exact expression for the eigenvalues of adjacency matrix. That is

$$\{\lambda_i\}_{0}^{N-1} = k \cos\left(\frac{\pi i}{N}\right) \cos\left(\frac{2\pi i}{N}\right) \cos\left(\frac{4\pi i}{N}\right) \cdots \cos\left(\frac{(k/2 + 1)\pi i}{N}\right),$$

(6)
in which, the number of $\cos[...]$ function is $a$.

Figure 1. Topological structures of some regular graphs generated with all vertices being located in a ring and all edges being formed by nearest connections.

In 1978, I. Gutman put forward a conjecture to describe that a complete graph would have maximal energy[2]. However, soon thereafter, this conjecture was shown to be false by means of counterexamples[22]. So in this part, we will investigate whose energy will rank first for those regular graphs with the same generating method. Fig. 2(a) shows the distribution of graph energy $E$ in the variation of $k$ for different values of $N$. It can be obviously noticed that there exist a peak in the change curve of graph energy for each $N$. When the network is very sparse, graph energy $E$ will be monotonically increasing with $k$. With slow increase of intensity, energy $E$ will be still proportional to $k$ but with appearing of some weak fluctuations. However, while the network is becoming highly dense, the graph energy will drop sharply. And the value of $k$ that corresponds to the largest graph energy is about $0.8N$. Fig. 2(b) presents the normalized result for the increasing part of the left one. It displays that while the regular network is very sparse, the normalized graph energy follows a power-law function of $k$, which can be expressed by $E/E(k = 2) = 0.977k^{0.214}$. And the two parameters in this function are almost independent of the size of system. Particularly it is worth mentioning that the graph energy corresponding to complete graph ($k = N - 1$) or sub-complete graph ($k = N - 2$) is equal to $2k$.

3. Some results in sparse scale free networks

The correlation between energy and average degree, denoted by $< k >$, is also explored firstly in this part, as it is depicted in Fig. 3, which plots the normalized energy as a function of $< k >$ for two different situations with $\gamma$ being 2.5 and 6.0 ($\gamma$ is the exponent of degree distribution of network considered). The fitting line suggests a power law function between $E$ and $< k >$, which can be expressed as follows.

$$E/E(< k >= 3) = 0.570 < k >^{0.502},$$

(7)
in which, the three parameters are almost independent of the value of $\gamma$ as long as $< k >$ is small.

Furthermore, the effect of degree exponent $\gamma$ on graph energy is also studied. Plots presenting normalized graph energy distribution for different network sizes are shown in Fig. 4, which provides an intuitive perspective to realize the proportional relationship between $\gamma$ and $E$ when $\gamma$ is not so large. After $\gamma$ gets to 7, the plateau in the energy distribution is presented obviously, especially for the smaller systems. Plateau corresponds to the network with a regular structure. Apparently, for larger systems, the value of $\gamma$ resulting in a regular structure network will be
Figure 2. (Color online) (a) shows the dependence of graph energy $E$ on degree $k$ for different values of $N$. (b) with a solid power law fitting line describes the normalized results for the increasing part of left plot without any fluctuations. It shows a power law correlation between $E$ and $k$ while $k$ is small.

Figure 3. The normalized graph energy as a function of average degree $<k>$ for the cases of $\gamma = 2.5$ (squares) and $\gamma = 6.0$ (circles) with $N = 1000$. The solid line is a power law fitting line for the case of $\gamma$ being 2.5.

larger. And on the whole, the dependence of graph energy on degree exponent $\gamma$ will be stronger with the increasing of $N$.

Describing it differently, the correlations between graph energy and degree distribution can be interpreted by the relations between it and the variance of degree sequence. The variance, denoted by $D$, is defined as

$$D = \frac{1}{N} \sum_{i=1}^{N} (k_i - <k>)^2,$$  \hspace{1cm} (8)

where $k_i$ means the degree of $i^{th}$ agent.
To analyze the impacts of the variance of degree sequence on the variability of graph energy, we propose the relative variation of energy, labeled as $\delta E$. $\delta E$ is defined by $\frac{(E - E_{\text{max}})}{E_{\text{max}}}$, where $E_{\text{max}}$ denotes the graph energy with the condition of $D$ being close to 0 which corresponds to a uniform degree distribution. Fig. 5 shows how the relative variation of graph energy relies on the degree variance for different values of $N$. This shape of energy distribution represents a power-law correlation between $\delta E$ and $D$, that can be fitted by the following function.

$$\delta E = -yD^\beta. \quad (9)$$

Fig. 6 displays the dependence of parameters $y$ and $\beta$ in equation (9) on the size of system $N$. There exists a smooth power law fitting line to the relationship between parameter $\beta$ and $N$, which can be described by $\beta = 1.251N^{-0.075}$. And according to Fig. 6(b), it can be obviously noticed that parameter $y$ almost does not change with increasing of $N$ but owns a fixed value close to 0.013. So, we can draw easily that the dependence of variability of graph energy on the variance of degree sequence will be weak with the increasing of $N$.

We have known about the linear relationship between graph energy and the size of system for the regular graphs (all nodes are located in a ring and all edges are generated by nearest connections) with specified degree $k$ from theoretical view. Similarly, we study the distribution of graph energy over $N$ with specified average degree $<k>$ and degree exponent $\gamma$, see Fig. 7. It indicates that the energy is also linearly increasing with $N$ for each value of $\gamma$, that is

$$E \propto \alpha N, \quad (10)$$

and $\alpha$ will increase with $\gamma$ while $\gamma$ is small according to Fig. 7. And the overlap of the results under the conditions of $\gamma = 6.0$ and $\gamma = 8.0$ is simply on account of the uniform degree distribution (i.e, the corresponding network is regular) after $\gamma$ gets to 6.0. With the increasing of $\gamma$ from 6.0, the structure of network will hardly change.

4. Conclusions
We first calculated exactly the energy of regular graphs for node’s degree $k$ being small. And an exact formula for the eigenvalues spectra of regular graphs with $k = 2^a \ (a = 1, 2, 3, \ldots)$ is

Figure 4. (Color online) The distribution of normalized graph energy with the variation in $\gamma$ for some specified values of $N$. Inset shows the distributions of graph energy before being normalized.
Figure 5. The relative variation $\delta E$ of graph energy as a function of $D$ for systems with different size and average degree $<k>$ being 4. The solid lines are obtained by power-law fitting.

Figure 6. (a). The distribution of exponent $\beta$ in equation (9) with the variation in $N$ for average degree $<k>$ being 4. And the solid line is fitted by a power law function. (b). The dependence of another parameter $y$ in equation (9) on $N$. As can be seen on the plot, parameter $y$ has barely anything to do with $N$.

deduced. We also find that the graph with $k$ being about 0.8$N$ owns the largest energy for
regular graphs (generated in such a way that all nodes are positioned on a ring and edges are formed by nearest neighbor connections) with specified $N$. Subsequently, we investigated the dependence of energy on the structure of graph, such as the average degree, the degree exponent and degree variance for sparse scale free networks. The results illustrate that graph energy is a power-law function of average degree $<k>$ when degree exponent $\gamma$ is fixed and is also a power-law function of degree variance $D$ while $<k>$ is specified. And the dependence of graph energy on degree exponent will be stronger with the increasing of $N$ while the case is opposite for its dependence on degree variance. It is worth mentioning that the energy is always linearly increasing with the size of system in regular and scale free graphs.

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