Spectra of tree ensembles

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Abstract

This paper is devoted to spectra of sparse macromolecular clusters. We suggest such clusters to be modeled by unweighed undirected tree ensembles with size distributed in a certain known way. The goal of this work is to compute spectra of such ensembles analytically as spectra of their adjacency matrices. The motivation to the problem investigated is computing spectra of Bernoulli noise in sparse matrices which is essential in cases when the scale of the data and the noise is the same. We solve the special cases of star trees and full binary trees interpreting them as generalized Bethe trees. The target function of an individual tree is supposed to depend on the size of the tree and of an ensemble - on size distribution.
Keywords: binary trees; star trees; spectrum

1. Introduction

The issue of tree ensemble spectra emerged in the context of sparse macromolecular clusters spectra analysis. Macromolecules are suggested to be modeled by unweighed undirected acyclic graphs - trees [1], and for clusters Erdős–Rényi random graph model is used.

There are several reasons to this choice of model. First of all, a macromolecule, which has no cycles, is truly a tree. Second, the degree of a vertex is not too high (very unlikely more than three if the ensemble is random and sparse), which again corresponds with biological context. Finally, the size distribution of macromolecules, for example, exponential, can be included into the model.

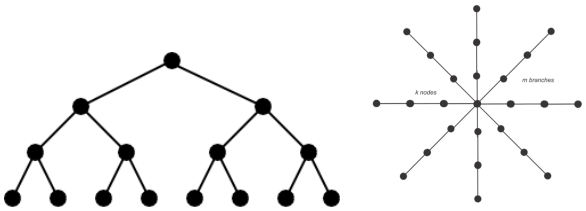
The spectrum of a graph is defined either by the spectrum of its adjacency matrix or its Laplacian, depending on the field of study and application[7]. In physical models the adjacency matrix spectrum is interpreted as the set of resonance frequencies and the Laplacian spectrum defines relaxation of the system. Other applications in graph theory and optimization are thoroughly described in [8] and [9].

In recent studies there was noticed that some properties of macromolecular structures such as its spectrum envelope and spectrum inner structure hierarchy, regardless of their initial context, are inherent generally to tree ensembles, which resulted into reasonable desire to find these spectra analytically.

Another approach to this question is that in sparse matrices, for example, a DNA contact map, the noise is Bernoulli and also sparse. If the matrix is interpreted as an adjacency matrix, the noise is unlikely to join any already existing connected component, which means that the spectrum of the whole matrix is the sum of the investigated spectrum and the spectrum of the noise. The problem is that their scale can be nearly the same. In this case the peculiar shape of noise spectrum can be misinterpreted or at least can make the data incomprehensible [10, 11, 2]. The question is how to tell apart the noise and the initial data and distinguish their properties.

In a recent paper [3] linear chains ensemble spectrum and its properties were thoroughly discussed. Some of the results concerning the maximal eigenvalue were obtained in [4].

In this paper we investigate branching trees. We particularly look into the case of full binary trees and star graphs with respect to their adjacency matrices as these types of trees are most common in described ensembles. To solve these cases we use the method, based on interpreting them as a generalized Bethe trees [5, 6], and compute all their eigenvalues and their multiplicities. We also look into ensembles of trees of particular structure and compute the envelope of spectral density.



(a) A full binary tree (b) A star

Figure 1: A full binary tree and a star with m branches of k nodes.

2. Problem statement

Suppose we have an ensemble of trees and size of a tree is distributed in a certain known way, for example, exponentially. Our aim is to find the spectrum of an individual tree and an ensemble.

2.1. Full binary trees

Let $\mathscr{T}_k$ be a full binary tree of level k (see 1a). This means that length of a path from the root to an external vertex is k. Such tree has 2^k-1 vertices. Let $\mathbf{T}_k$ be its adjacency matrix.

First, we need to find the spectrum of a single tree of level k with 2^k-1 eigenvalues in it. Its function of spectral density we call $f_k(\lambda)$.

$$f_k(\lambda) : \mathbb{R} \to \mathbb{N}^0,$$

where λ is an eigenvalue and $f_k(\lambda)$ is its frequency which is multiplicity divided by the number or eigenvalues.

Second, we consider an ensemble of such trees, where k is distributed as

$$P(k) = Ce^{-\mu k},$$

where $C = e^{\mu} - 1$ and μ is a parameter. This distribution is normalized:

$$\sum_{k=1}^{\infty} P(k) = \sum_{k=1}^{\infty} Ce^{-\mu k} = 1.$$

Then spectral density of the ensemble is represented as

$$\sum_{k=1}^{\infty} P(k) f_k(\lambda) = f(\lambda).$$

2.2. Star trees

For a star tree (see 1b) the problem is introduced similarly. Let $\mathscr{S}_{k,m}$ be a star of m chains of level k with $m(k-1)+1$ vertices and adjacency matrix $\mathbf{S}_{k,m}$. Its function of spectral density we call $g_{k,m}(\lambda)$.

$$g_{k,m}(\lambda) : \mathbb{R} \to \mathbb{N}^0,$$

where λ is an eigenvalue and $g_{k,m}(\lambda)$ is its frequency which is multiplicity divided by the number or eigenvalues.

The probability of a star to have parameters k and m is normalized:

$$\sum_{k=1}^{\infty} P(k|m) = 1,$$

$$\sum_{m} P(m) = 1.$$

We consider an ensemble of stars with particular m, where k is distributed as

$$P(k|m) = Ce^{-\mu k},$$

where $C = e^{\mu} - 1$ and μ is a parameter. And the target function of spectral density of the ensemble is

$$\sum_{k=1}^{\infty} P(k|m) g_{k,m}(\lambda) = g_m(\lambda).$$

We investigate $m \geq 3$ as $m = 1,2$ corresponds to linear chains.

3. Simulation

The computational experiment is carried out for artificially generated data. Its aim is to generate spectral distribution of a particular tree and an ensemble. The results allow us to make some assumptions about the target functions and visualize the investigated spectra.

3.1. Description of the algorithm

Suppose we have an adjacency matrix of $\mathbf{T}_k$ or $\mathbf{S}_{k,m}$, introduced in the previous section. First, we calculate its eigenvalues, which are real. Second, we construct a histogram. It means that we divide the real axis into segments of equal length $\Delta\lambda$ and construct a piece-wise constant function $\hat{f}_k$:

$$\hat{f}_k(\lambda) : \mathbb{R} \to \mathbb{N}^0,$$

Here by $\mathbb{N}^0$ we mean all non-negative integers. On a segment $[l\Delta\lambda; (l+1)\Delta\lambda]$ function $\hat{f}_k(\lambda)$ is equal to the number of eigenvalues, which got into this segment.

$$\hat{f}_k(\lambda) = \sum_i \#\{\lambda_i \in [l\Delta\lambda; (l+1)\Delta\lambda]\}, \forall \lambda \in [l\Delta\lambda; (l+1)\Delta\lambda],$$

where λ_i is an eigenvalue, l is an integer. As mentioned in the introduction, the maximal eigenvalue is bound [4]:

$$|\lambda_{\max}^{\text{tree}}| \leq 2\sqrt{p-1}. \quad (1)$$

It means that we can actually only consider the segment $[-|\lambda_{\max}^{\text{tree}}|; |\lambda_{\max}^{\text{tree}}|]$ and instead of using $\Delta\lambda$ as a parameter stick to the number of segments N in the histogram. It seems to be reasonable to investigate the results for big enough L and small enough $\Delta\lambda$, or big enough N. Finding the optimal value of $\Delta\lambda$ or N is a separate problem as our estimation needs to be robust and informative.

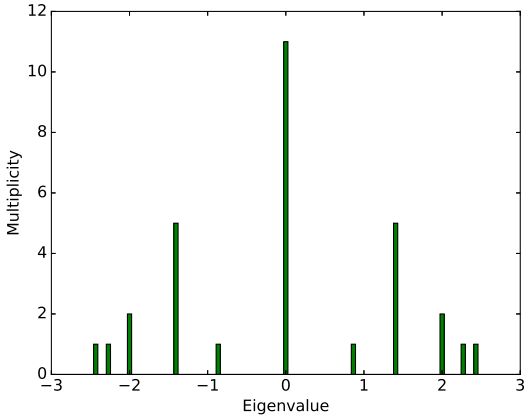


Figure 2: Eigenvalue distribution of a full binary tree with level $k = 6$.

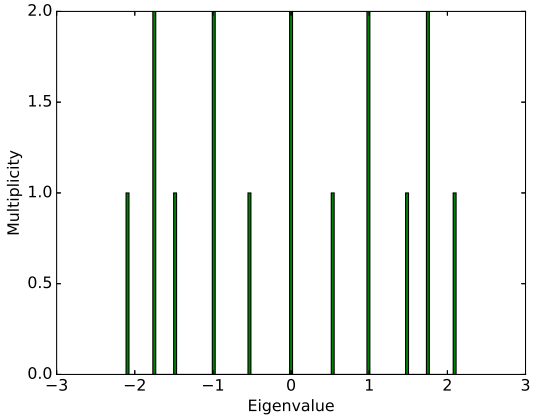


Figure 3: Eigenvalue distribution of a star with $m = 3$, $k = 6$.

3.2. Full binary trees

For full binary trees we calculate spectra for sizes up to 12 as bigger sizes are rare according to exponential distribution with small expectation. What is more, as the complexity of eigenvalue computation is $O(n^3)$, it takes much time yet the results are not informative. The number of segments should be odd in order to avoid irregularities near $\lambda = 0$ as this point should belong to a segment, symmetric in respect to zero. Small computational errors can lead to calculating eigenvalues very close to zero, both positive and negative, when in fact all of them are equal to zero. Also the number of segments near one hundred seems to be most informative from subjective point of view.

Maximal vertex degree for a full binary tree is $p = 3$, so, according to inequality 1:

$$|\lambda_{\max}^{\text{tree}}| \leq 2\sqrt{2} < 3.$$

This is true for any size k of a full binary tree. For $k \geq 6$ the spectrum changes insignificantly and seems to be distinctively discrete. The peaks of local maxima for different sizes coincide. As for the maximal eigenvalue, the bigger k is, the bigger $\lambda_{\max}^{k}$. The tail of the distribution, which is the series of the highest eigenvalues, behaves like:

$$\varphi(\lambda) = A \exp\left(-\frac{1}{\sqrt{|\lambda_{\max}^{\text{tree}}| - \lambda}}\right),$$

where A is a constant, $|\lambda_{\max}^{\text{tree}}| = 2\sqrt{2}$. This fact is known as Anderson localization.

3.3. Star trees

Most of the calculations are made for $m = 3$ and $m = 4$, where m is the number of chains. The reason to this choice of m is that in random ensembles vertex degrees are rarely more than 3. The length of a chain k is distributed exponentially, so large sizes are also rare.

It was noticed that the number of original eigenvalues of an individual star is $(2k-1)$ regardless of chain number, and the multiplicity is either 1 or $m-1$.

The spectrum of a single star and of an ensemble are quite different. The Anderson localization does not take place.

4. Theoretical part

Following [6] denote $\mathscr{B}_k$ a generalized Bethe tree of k levels (see fig.6), a rooted unweighed and undirected tree with vertices of equal degree at one level. The root is at level 1 and for level $j = 1,\ldots,k$ the number of the vertices is n_{k-j+1}, of degree d_{k-j+1}. Particularly, d_k is the degree of the root, $n_k = 1$ and n_1 is the number of

Table 1: Peak heights for different k, normalized

peak#	ensemble	$k = 8$	$k = 9$	$k = 10$
0	1.000	1.000	1.000	1.000
1	0.420	0.435	0.427	0.428
2	0.190	0.200	0.199	0.200
3	0.090	0.094	0.099	0.097
4	0.042	0.047	0.047	0.047

Table 2: Peak heights for different k, non-normalized

peak#	ensemble	$k = 8$	$k = 9$	$k = 10$
0	17259	85	171	341
1	7267	37	73	146
2	3283	17	34	68
3	1545	8	17	33
4	721	4	8	16

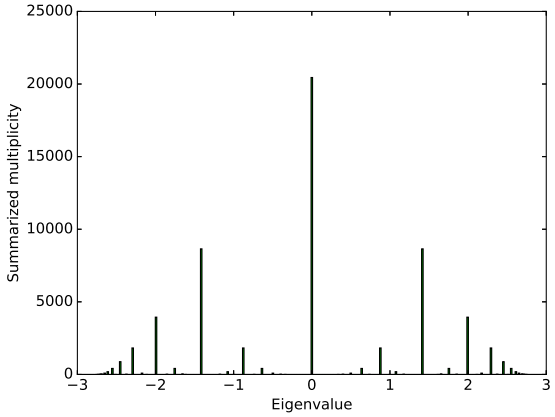


Figure 4: Eigenvalue distribution of a full binary tree ensemble with level distributed exponentially, $\mu = 0.5$.

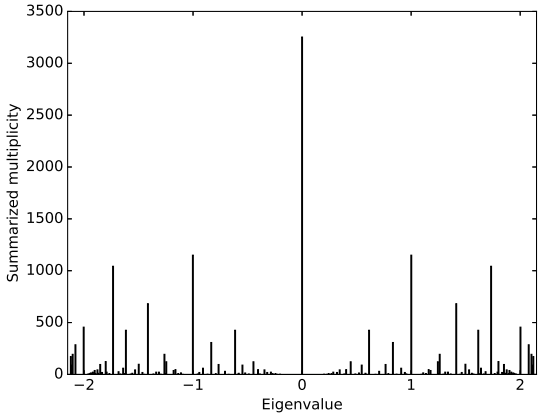


Figure 5: Eigenvalue distribution of a star ensemble with level distributed exponentially, $m = 3$, $\mu = 0.5$.

external vertices. Let $\mathbf{A}(\mathscr{B}_k)$ be an adjacency matrix of a Bethe tree and $\sigma(\mathscr{B}_k)$ its spectrum. Recall that a full binary tree adjacency matrix we note $\mathbf{T}_k$ and a star $\mathbf{S}_{k,m}$.

Theorem 1 [6]. If $\mathbf{A}_j(d)$ is the $j \times j$ leading principal submatrix of the $k \times k$ symmetric tridiagonal matrix

$$\mathbf{A}_k(d) = \begin{bmatrix} 0 & \sqrt{d_2-1} & & & & \\ \sqrt{d_2-1} & 0 & \sqrt{d_3-1} & & & \\ & \sqrt{d_3-1} & 0 & & & \\ \dots & \dots & \dots & \dots & \dots & \dots \\ & & & 0 & \sqrt{d_k-1} & \\ & & & \sqrt{d_k-1} & 0 & \sqrt{d_k} \\ & & & & \sqrt{d_k} & 0 \end{bmatrix}$$

then

1. $\sigma(\mathbf{A}(\mathscr{B}_k)) = \left(\bigcup_{j=1}^{k-1} \sigma(\mathbf{A}_j(d)) \right) \cup \sigma(\mathbf{A}_k(d))$.
2. The multiplicity of an eigenvalue of the matrix $\mathbf{A}_j(d)$ as an eigenvalue of $\mathbf{A}(\mathscr{B}_k)$ is $(n_j - n_{j+1})$ for $j \in 1, \dots, k-1$, and eigenvalues of $\mathbf{A}_k(d)$, as eigenvalues of $\mathbf{A}(\mathscr{B}_k)$, are simple.

5. Solution

5.1. Full binary trees

A full binary tree of level k has $n_i = 2^{i-1}$ vertices at level i, all of degree $d_i = 3$ except for the leaves $d_1 = 1$ and the root $d_k = 2$. According to Theorem 1, its spectrum can be computed as:

$$\sigma(\mathscr{T}_k) = \bigcup_{i=1}^{k} \sigma(\mathbf{A}_i),$$

where $\mathbf{A}_i$ is the following:

$$\mathbf{A}_i = \sqrt{2} \begin{bmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ \dots & \dots & \dots & \dots & \dots & \dots \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix}$$

Denote $\hat{\mathbf{A}}_i = \frac{1}{\sqrt{2}} \mathbf{A}_i$ and $\hat{\lambda} = \frac{1}{\sqrt{2}} \lambda$.

Characteristic polynomial $F_i = \det(\hat{\mathbf{A}}_i + \hat{\lambda}\mathbf{E})$ of matrix $\hat{\mathbf{A}}_i$ is found from the following recurrence equation:

$$F_{i+1} = \hat{\lambda} F_i - F_{i-1},$$
$$F_0 = 1, F_1 = \hat{\lambda}.$$

The solution is obtained from another equation:

$$\mu^2 - \mu\hat{\lambda} + 1 = 0,$$

$$\mu_{1,2} = \frac{\hat{\lambda} \pm \sqrt{\hat{\lambda}^2 - 4}}{2}.$$

The solution F_i of this recurrence equation is:

$$F_n = \frac{1}{\sqrt{\hat{\lambda}^2 - 4}} \left(\frac{\hat{\lambda} + \sqrt{\hat{\lambda}^2 - 4}}{2} \right)^{i+1} - \\ - \frac{1}{\sqrt{\hat{\lambda}^2 - 4}} \left(\frac{\hat{\lambda} - \sqrt{\hat{\lambda}^2 - 4}}{2} \right)^{i+1}.$$

The solution to the equation $F_i = 0$ is:

$$\hat{\lambda} = 2 \cos \frac{\pi j}{i+1}, \; j = 1 \dots i.$$

Then the initial eigenvalues of matrix $\mathbf{A}_i$ are:

$$\lambda = 2\sqrt{2} \cos \frac{\pi j}{i+1}, \; j = 1 \dots i.$$

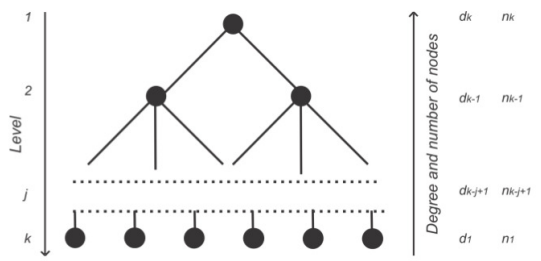


Figure 6: A generalized Bethe tree of k levels.

So, the spectrum of a full binary tree $\mathscr{T}_k$ is the following:

$$\sigma(\mathscr{T}_k) = \bigcup_{n=1}^{k} \bigcup_{j=1}^{n} \left\{ 2\sqrt{2} \cos \frac{\pi j}{n+1} \right\}. \tag{2}$$

As for eigenvalue multiplicities, according to Theorem 1, the contribution of the i-th principal submatrix is:

$$m_i = n_i - n_{i+1} = 2^{k-i-1},\ i = 1 \ldots k-1,\ m_k = 1.$$

Denote multiplicity of eigenvalue λ as an eigenvalue of the initial tree $m(k,\lambda)$, then:

$$m(k,\lambda) = \sum_{i=1}^{k} m_i\ \mathbb{I}(\lambda, i),$$

where $\mathbb{I}(\lambda, i)$ is indicator function, equal to 1 if $\lambda \in \sigma(\mathbf{A}_i)$ and 0 otherwise. The target function f_k is

$$f_k(\lambda) = \frac{m(k,\lambda)}{2^k - 1}.$$

Recall that $\lambda \in \sigma(A_i)$ if there exists an integer j such that:

$$\lambda = 2\sqrt{2}\ \cos \frac{\pi j}{i+1}.$$

The i-th value in the series of main peaks which happens to be the series of maximal eigenvalues of levels 1 to k is:

$$\lambda_i^{main} = 2\sqrt{2}\ \cos \frac{\pi}{i+1}. \tag{3}$$

This value contributes to the spectrum as an eigenvalue of every $(i+1)$ principal submatrix:

$$2\sqrt{2}\ \cos \frac{2\ \pi}{2\ (i+1)}, \ldots,\ 2\sqrt{2}\ \cos \frac{n\ \pi}{n\ (i+1)},$$

while $n\ (i+1) \le k+1$. Thus for the i-th main peak the following equation takes place:

$$m_k + \cdots + m_{k+i} = 2^k,$$

where k is the level of the tree. The solution to this equation is

$$m_{i,k}^{main} = \left[\frac{2^k}{2^{i+1} - 1} \right],$$

where $\psi(x) = [x]$ is the function of the closest integer. Then, the envelope of function f_k is the following:

$$f_k\left(2\sqrt{2}\ \cos \frac{\pi}{i+1} \right) = \frac{1}{2^k - 1} \left[\frac{2^k}{2^{i+1} - 1} \right]. \tag{4}$$

The spectrum of the full-binary tree ensemble is

$$\sigma^{\text{ens}} = \bigcup_{k=1}^{\infty} \bigcup_{j=1}^{k} \left\{ 2\sqrt{2} \cos \frac{\pi j}{k+1} \right\}, \tag{5}$$

and the target function $f(\lambda)$ is

$$f(\lambda) = \sum_{k=1}^{\infty} (e^{\mu} - 1)\, e^{-\mu k}\, f_k(\lambda) = \\ = \sum_{k=1}^{\infty} (e^{\mu} - 1)\, e^{-\mu k}\, \frac{m(k,\lambda)}{2^k - 1}.$$

For main peaks:

$$f\left(2\sqrt{2}\ \cos \frac{\pi}{i+1} \right) = \sum_{k} (e^{\mu} - 1)\, e^{-\mu k} \frac{1}{2^k - 1} \left[\frac{2^k}{2^{i+1} - 1} \right] \approx \\ \approx \frac{e^{\mu} - 1}{2^{i+1} - 1} \sum_{k=1}^{\infty} e^{-\mu k}\, \frac{2^k}{2^k - 1} \tag{6}$$

with error δ such that:

$$\delta \le (e^{\mu} - 1)\ \sum_{k=1}^{\infty} e^{-\mu k}\, \frac{1}{2}\, \frac{1}{2^k - 1} \le \\ \le \frac{1}{4} \frac{e^{\mu} - 1}{2e^{\mu} - 1}. \tag{7}$$

5.2. Star trees

For a star of m branches and k levels, following the notation, $n_i = m$ and $d_i = 2$ except for the root $n_k = 1$ and $d_k = m$, and leaves $d_1 = 1$. According to Theorem 1, its spectrum:

$$\sigma(\mathscr{S}_{k,m}) = \bigcup_{i=1}^{k} \sigma(\mathbf{B}_{i,m}),$$

where $\mathbf{B}_{i,m}$ is the following:

$$\mathbf{B}_{i,m} = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & 1 & 0 & \sqrt{m} \\ & & & \sqrt{m} & 0 \end{bmatrix}.$$

As multiplicity $m_i = n_i - n_{i+1} = 0$ for any $i = 1, \ldots, k-2$, we only compute the $(k-1)$-th principal submatrix, which is the adjacency matrix of a linear chain, and we have already solved that case with:

$$\lambda = 2\ \cos \frac{\pi j}{k},\ i = 1 \ldots k-1,$$

$$\sigma_k^{lin} = \bigcup_{j=1}^{k-1} \left\{ 2\cos\frac{\pi j}{k} \right\}$$

and multiplicities $m_{k-1} = m-1$. Characteristic polynomial $F_i = \det(\mathbf{B}_{i,m} + \lambda\mathbf{E})$ of matrix $\mathbf{B}_{k,m}$ can be found from the following recursive equation:

$$F_{i+1} = \lambda F_i - F_{i-1},$$

$$F_0 = m, F_1 = \lambda.$$

The solution F_i to the recurrence equation is

$$F_i = \frac{m(\lambda+\sqrt{\lambda^2-4})-2\lambda}{2\sqrt{\lambda^2-4}} \left(\frac{\lambda-\sqrt{\lambda^2-4}}{2} \right)^i - \\ - \frac{m(\lambda-\sqrt{\lambda^2-4})-2\lambda}{2\sqrt{\lambda^2-4}} \left(\frac{\lambda+\sqrt{\lambda^2-4}}{2} \right)^i.$$

For $|\lambda| < 2$ the equation $F_i = 0$ can be transformed into:

$$\tan i\varphi = \frac{m}{m-2}\tan\varphi,$$
$$\tan\varphi = \frac{\sqrt{4-\lambda^2}}{\lambda},$$
$$\lambda = 2\cos\varphi.$$

For $|\lambda| \geq 2$:

$$\tanh i\varphi = \frac{m}{m-2}\tanh\varphi,$$
$$\tanh\varphi = \frac{\sqrt{\lambda^2-4}}{\lambda},$$
$$\lambda = 2\cosh\varphi.$$

Analysis shows that previous equation has no more than 2 roots λ_1, λ_2 such that $\lambda_1 = -\lambda_2 = \lambda_{max}$. What is more, $\lambda_{max} \in (\sqrt{m}; \frac{m}{\sqrt{m-1}})$.

For equation $F_n = 0$ denote its set of roots $\sigma_{n,m}$. Then the spectrum of a star is:

$$\sigma(\mathscr{S}_{n,m}) = \bigcup_{j=1}^{n} \left\{ 2\cos\frac{\pi j}{n+1} \right\} \cup \sigma_{n,m} = \sigma_n^{lin} \cup \sigma_{n,m} \quad (8)$$

with multiplicities:

$$m(n,\lambda) = m-1;\ \lambda \in \sigma_n^{lin},$$
$$m(n,\lambda) = 1;\ \lambda \in \sigma_{n,m}.$$

The target function $g_{k,m}(\lambda)$ is

$$g_{k,m}(\lambda) = \frac{m(k,\lambda)}{m(k-1)+1}. \quad (9)$$

For an ensemble:

$$\sigma_m^{\text{ens}} = \bigcup_{k=1}^{\infty} \sigma_k^{lin} \cup \sigma_{k,m} \quad (10)$$

with target function $g_m(\lambda)$:

$$g_m(\lambda) = \sum_{k=1}^{\infty} (e^{\mu}-1)\, e^{-\mu k}\, g_{k,m}(\lambda) = \\ = (e^{\mu}-1) \sum_{k=1}^{\infty} e^{-\mu k} \frac{m(k,\lambda)}{m(k-1)+1}. \quad (11)$$

6. Conclusion

In this paper we investigated the spectra of sparse macromolecular clusters, modeled by tree ensembles. We particularly looked into the cases of two common tree types: full binary trees and star trees. Interpreting these trees as Bethe trees, we obtained the following results.

We computed the spectrum of an individual full binary tree (see formula 2) and its envelope defined by the series of main peaks (see formulae 3 and 4). After that we computed the spectral density of an ensemble of such trees with size distributed exponentially (see formula 5), and its envelope (see formulae 6 and 7).

We also computed the spectrum of a star, partly in its exact form, partly as the set of roots of a transcendental equation (see formulae 8 and 9). We improved the accuracy of the maximal eigenvalue bound. Finally, we computed the spectrum of star tree ensemble with particular branch number (see formulae 10 and 11).

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