Discussion Paper

Elastic energy of networks

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1 Introduction

The present paper[1)] is about invariants of networks by labeling and relabeling its nodes or arcs. These can be used to classify networks as to their complexity, or to distinguish non-isomorphic networks.

In (10) complexity measures for networks have been defined, distinguishing graphs from digraphs. The distinction came from the use of directedness (or not) of arcs and edges. An edge can be viewed as a nondirected arc, or a bi-directed link, representing both an arc and its counter-arc. The complexity measure for graphs is based on the average degree of the nodes in the graph. For directed graphs, reachability of the nodes in a graph from some node in the graph is the key issue.

The present paper discusses an idea from physics applied to networks. This idea is to associate an elastic energy with a network, using permutations of the labels associated with the nodes and average these over all such permutations. It has also been applied in the area of graph representation: to represent graphs in the plane $\mathbb{R}^2$ (or space $\mathbb{R}^3$) as dots and line segments connecting them. The problem is to achieve a representation that is not too cluttered.[2)]

The quantity we are interested in concerns a distribution over the energy spectrum, that is the different energy levels obtained for a particular permutation. It depends on the topological structure of the network and is a topological invariant. This would make them useful to distinguish networks that are not isomorphic (they have a different distribution over the energy spectrum, and possibly a different spectrum). [3)]

The energy distributions can be used to characterize networks. It would be nice if such topological invariants would characterize (isomorphic) networks uniquely. But the ones proposed do not: networks with the same characteristics just mentioned may be not be isomorphic.

The remainder of the paper is organized as follows. In Section 2 the elastic energy of networks (EE) is derived from a (random) labeling the points of the network from 1 to the number of nodes in the network. The labels can be viewed as corresponding to equidistant points on the line. So we can view the labeling as an embedding of the network (in particular the nodes) in a certain subset of $\mathbb{Z}$ or $\mathbb{N}$.[4)]. We stick to calling the process an 'embeding' rather than defining a 'representation'. Then the labels can be used to define the total elastic energy (TEE) or the average elastic energy (AEE) for the network. TEE is the sum of the elastic energies of the network when all permutations of the labels are considered. AEE is the average of the EEs per permutation, or, AEE $=$ TEE$/n!$, where n is the number of nodes in the network considered. The terminology is clarified if we look at the embedded network and assume that pegs that correspond to connected nodes in the graph are actually connected by rubber bands, one for each arc. An edge is viewed as a pair of arcs: an arc and its counter-arc. And so an edge is represented by two rubber bands. Section 3 is about sub-networks and their behavior with

1) The author is grateful to Frank Pijpers for reviewing a mature concept of the present paper.
2) Points that are near should also be plotted. But this is not always possible and may require making compromises.
3) However, if the characteristics are the same for two networks, one cannot conclude that they are isomorphic.
4) In terms of the vocabulary of (5) this node labeling would be called defining a representation. The generalizations in Section 4.3 either coincide with the definition given in (5) or go beyond it.

respect to EE, which is linear concerning the total contributions of the energy terms per arc or edge. This property is exploited to derive some useful insights concerning elastic energy and subgraphs or subbdigraphs. Rewriting the expression for EE yields a relationship with the so-called graph Laplacian, This is shown in Section 4. The graph Laplacian is studied in graph theory. It can be viewed as an adoption of the Laplace operator in classical analysis. The aim of Section 4 is mainly to point out this link of elastic energy with the graph Laplacian. There is no opportunity to study the relationship in depth. To give a better feeling for the concept of elastic energy in Section 5 some examples of graphs are considered for which the elastic energy (TEE and AEE) is computed. It is shown that TEE is the weighted sum of EE values for certain labelings of the graph in question. The EE values form the EE spectrum, and the weights are the multiplicities. This leads to the concept of S&M, spectrum and multiplicities, which is also a characteristicfor a network, although two non-isomorphic networks may have the same S&M. In Section 6 some problems for further research are mentioned. Section 7, finally, contains a discussion of the main insights of the present paper and some of the perspectives it offers for future research. The paper closes with a list of references.

2 Node labeling, embedding and elastic energy

The elastic energy associated with a network is defined. It is - in the first instance -based on a labeling of the nodes of the network by numbers $1, \dots, n$, where n is the number of nodes in the network. More generally, the labeling of the nodes can be based on n real numbers $\xi_1, \dots, \xi_n$, assumed to be all different. The elastic energy is a quadratic form which is the sum of m quadratic terms, each associated with one of the m arcs or edges of the network. The elastic energy depends on how the nodes are labelled. However, the average elastic energy can be defined by taking the arithmical average of the elastic energy over all possible numberings of the edges. It is explained why the quadratic form used is called 'elastic energy'. It is possible to define a more refined quantity than the total or average elastic energy, called spectrum and multiplicities (S&M). Furthermore it is indicated how 'elastic energy' can be generalized using embeddings of the node set in normed or metric spaces.

2.1 Node labeling

The idea is to consider a network (digraph or graph) $G = (V, E)$ and label its nodes from 1 to $n = |V|$ in one way or another. The only condition is that this mapping $V \to N_n$, where $N_n = \{1, \dots, n\}$ is injective: different nodes should get different labels. Of course, there is much freedom of choice for the labeling of the nodes. In fact, if the number of nodes is n, so there are $n!$ ways of labeling them. There is no particular reason to prefer one labeling to another. But in a sense the labeling chosen is irrelevant as some important properties are independent of it. They are invariant quantities. As shown in Subsection 2.5 this is true for the size of the spectrum, as well as the multiplicities of spectral values.

Remark The labeling of nodes in a graph $G = (V, E)$ using labels $1, 2, \dots, n$, where $n = |V|$, the number of nodes in G, is the standard one. However, in this paper we will also consider more

general labelings. They are all of the following type: Let $\lambda : V \to \mathbb{N}$ be an injection. The set of labels is then $f(V)$, with $|f(V)| = n$, since λ is an injective function ($i \neq j$ implies $\lambda(i) \neq \lambda(j)$). □

2.2 Elastic energy

Let G be a graph with n nodes. Suppose that these nodes are numbered $1, \dots, n$ is some way. We define the expression

$$\mathcal{E}_G = \sum_{(i,j)\in E} (i-j)^2 \tag{1}$$

and interpret as an elastic energy (EE) of G, for the particular numbering of the nodes chosen. This will become clear if we consider embedding of the graph in a linear structure to which Hooke's law is applied.

The following matrix

$$E_n = \begin{pmatrix} 0 & 1^2 & 2^2 & \cdots & (n-1)^2 \\ 1^2 & 0 & 1^2 & \cdots & (n-2)^2 \\ \vdots & \vdots & \vdots & & \vdots \\ (n-1)^2 & (n-2)^2 & (n-3)^2 & \cdots & 0 \end{pmatrix}, \tag{2}$$

where entry i, j has the value $(i-j)^2$, is convenient to separate energy information from information about a particular graph. (2) can be interpreted as the energy matrix of the complete graph with n points, G^k. Any (di)graph on n points is a subgraph of G^k with n points and so will have less elastic energy associated with it.

So the EE is linear in the energy component delivered by each arc (or edge), whereas each component itself is a quadratic form.

We now come back to the expression for the elastic energy of a graph G in (1) We can rewrite it as:

$$\mathcal{E}_G = \sum_{(i,j)\in E} (i-j)^2 = \sum_{i\in V} \text{iodeg}(i) \cdot i^2 - 2 \sum_{(i,j)\in E} i \cdot j, \tag{3}$$

where

$$\text{iodeg}(i) = \text{indeg}(i) + \text{outdeg}(i), \tag{4}$$

for a node $i \in V$. Here 'indeg' and 'outdeg' denote the indegree and outdegree functions, respectively, defined for each node in G. The function'iodeg' defined in (4) for digraphs is not a standard function in graph theory. In case G is a graph, we have

$$\text{iodeg} = 2 \cdot \text{deg}, \tag{5}$$

where 'deg' is the degree function, counting for a node i the number of edges in G connected to i.

$\mathcal{E}_G$ is an absolute value of the elastic energy and it can be arbitrarily large. A relative version of $\mathcal{E}_G$ can be defined as

$$\mathcal{E}_G^r = \frac{\sum_{(i,j)\in E}(i-j)^2}{\sum_{i\in V}\deg(i)\cdot i^2} = 1 - 2\frac{\sum_{(i,j)\in E} i\cdot j}{\sum_{i\in V}\deg(i)\cdot i^2} \tag{6}$$

Obviously $0 < \mathcal{E}_G^r \leq 1$.

In case the digraph is actually a graph, each edge $\{i,j\}$ consists of two arcs, namely (i,j) and (j,i), which each contribute a value $(i-j)^2$. In this case the sum (1) can be written as

$$\mathcal{E}_G = 2\sum_{\{i,j\}\in E}(i-j)^2. \tag{7}$$

If we have a d-regular graph, that is, a graph with $\deg(i) = d \in \mathbb{N}$ for each node i, the first part of (3) equals the expression

$$d(n^3/3 + n^2/2 + n/6). \tag{8}$$

Note that (8) does not depend on the numbering of the nodes of G. So for $\mathcal{E}_G$ in (3) the variable part (that is, depending on the numbering of the nodes) is the second term

$$-2\sum_{(i,j)\in E} i\cdot j. \tag{9}$$

The numbering of the nodes, or rather their renumbering, is an important issue for the sequel (see Sections 2.4 and 2.5).

2.3 Physical interpretation

Geometrically the labeling of the nodes of a network by numbers $1, \ldots, n$ can be viewed as a realization (or embedding) of the network on n points in $\mathbb{Z}$, that can be thought to be situated on a line. Mapping the nodes of the network to these points implies a mapping of the arcs or edges as well, as they are defined by pairs of nodes (their ordering is irrelevant). The elastic energy of each edge is the distance of the embedded nodes squared. The total elastic energy is the sum of the elastic energy per edge.[5)] The arcs symbolize the edges in the embedded graph. It is more useful to think of them made of rubber. In case of an edge there are two such bands, one for each of the arcs it represents. If we would draw these the resulting picture would not be very informative as the springs would have quite some overlap and it would be unclear which pegs (nodes) are actually connected.

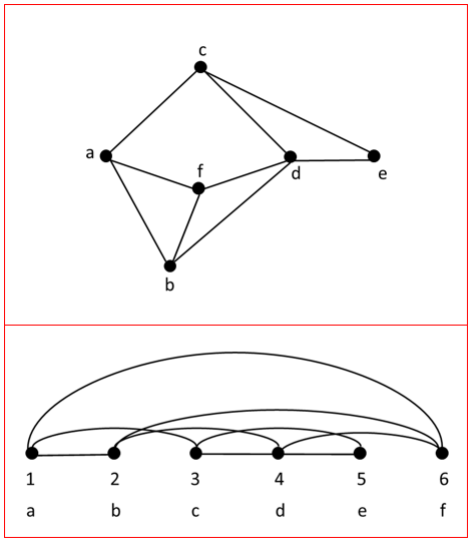


Figure 2.1 A graph (top) and an embedding (bottom). The edges are in fact not bows, as the picture suggests, but tight stretches, like rubber bands.

Another embedding of the graph in Figure 2.1 (top) is shown in Figure 2.2 (bottom).

In Figure 2.3 an example of a digraph is shown with an embedding. The example is derived from Figure 2.1. Arcs are colored red edges black. Each edge represents a pair of arcs, an arc and its counter-arc.

It should be stressed that the original graph carries only topological information, describing which nodes are connected and how (that is in which direction arcs are pointing, in case of a digraph). The picture of the original (di)graph suggests an embedding in the plane. Although that may formally be true, it does not mean that any geometric information is relevant. The numbers associated with the nodes of the original graph are only labels and do not carry any geometric information about the positions of the nodes.

5) Of course, one could use other distance measures (such as the absolute value) just as well. The choice of a quadratic function has the advantage of being easier to handle in practice.

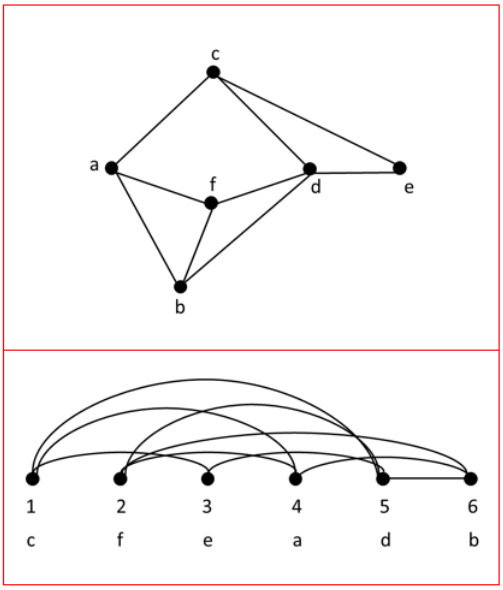


Figure 2.2 Another embedding of the graph in Figure 2.1.

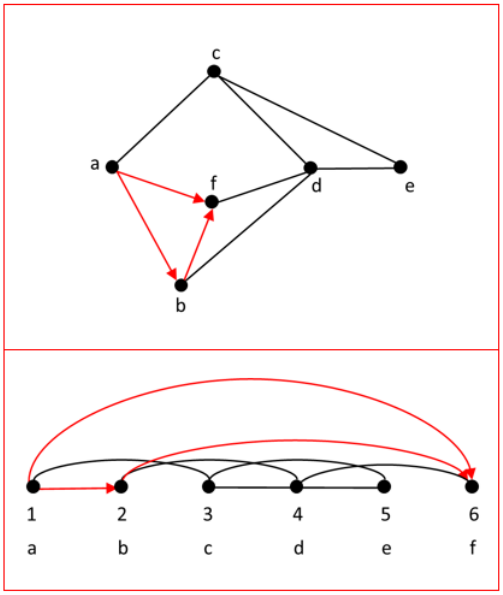


Figure 2.3 An embedding of a digraph (top). Arcs are colored red, edges black.

2.4 Total and average elastic energy

The view that we favor is that of networks with the nodes labeled rather than embed networks on a line. We may assume that the original node labels have been replaced with numbers from V_n, bijectively. If the nodes are relabeled, we have a bijection $V_n \to V_n$ describing the change, that is, a permutation. The advantage of this approach is that we can keep the original picture of the network and only alter the labels of the nodes. Such a permutation could be written as a $2 \times n$ matrix, for instance if $n = 6$ like

$$\tau = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 5 & 6 & 4 & 2 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 5 & 6 & 4 & 2 & 1 & 3 \end{pmatrix}, \tag{10}$$

for a graph with 6 nodes. This notation means that $\tau(1) = 5$, $\tau(2) = 6$, etc. The second expression in (10) is a shorter notation that is handy in case the number of items to be permuted is small.

The idea is to number the nodes of G randomly and compute the elastic energy. We assume this to be repeated many times and are interested in the distribution of this quantity. So we consider a permutation τ of $V_n = \{1, \dots, n\}$. Let Π_n denote the set of permutations of V_n. From (1) we derive the EE in case permutation τ is used:

$$\mathcal{E}_{G,\tau} = \sum_{(i,j)\in E} (\tau(i) - \tau(j))^2, \tag{11}$$

where $\tau \in \Pi_n$. Expression (11) is the elastic energy associated with G_τ, which is the graph that one obtains after renumbering the nodes of G using the permutation τ, and the corresponding adaptation of the arcs of G. Using (3) equation (11) can be written as

$$\mathcal{E}_{G,\tau} = \sum_{i\in V} \text{iodeg}(i) \cdot i^2 - 2 \sum_{(i,j)\in E} \tau(i)\tau(j), \tag{12}$$

where the function 'iodeg' is defined in (4). Note that the first term of (12) does not depend on the permutation τ, as the the second term does.

From (11) we can derive a relative elasticity measure, like $\mathcal{E}_G^r$ in (6), in case the nodes are relabeled by τ:

$$\mathcal{E}_{G,\tau}^r = \frac{\sum_{(i,j)\in E} (\tau(i) - \tau(b))^2}{\sum_{i\in V} \text{iodeg}(\tau(i)) \cdot \tau(i)^2} = 1 - \frac{2\sum_{(i,j)\in E} \tau(i)\tau(j)}{\sum_{i\in V} \text{iodeg}(i) \cdot i^2}, \tag{13}$$

where it was used that the term in the denominator is independent of τ.

So far we have considered the EE of a graph for a particular embedding of the nodes on a line (equidistant points). It is, however, attractive to consider an elastic energy measure that does not

depend on a particular embedding of the graph. So we consider the total elastic energy (TEE), $\mathcal{E}_G^+$, and the average elastic energy (AEE), $\overline{\mathcal{E}}_G$, respectively:

$$\mathcal{E}_G^+ = \sum_{\tau \in \Pi_n} \mathcal{E}_{G,\tau}, \tag{14}$$

$$\overline{\mathcal{E}}_G = \frac{1}{n!}\mathcal{E}_G^+, \tag{15}$$

where $V_n = \{1, \dots, n\}$. The expressions in (14) and (15) can be rewritten in matrix form, using the so-called graph Laplacian (see Section 4.2). This expression neatly separates the topology of the network and the geometry of the location of the nodes on the line.

2.5 Spectrum and multiplicities, ground state and top state

The EE of a network G takes values in a finite set of energies. These values are the spectrum of G. An energy value for G may occur multiple times. The spectral values and their multiplicities are the objects considered in this section. They are characteristic for the graph G. If we have another graph H which is isomorphic to G then it will have the same energy values and corresponding multiplicities. And if these values or multiplicities are different for networks G and H are different, G and H are not isomorphic. However two non-isomorphic networks may have the same spectrum and corresponding multiplicities. S&M is used as an abbreviation as an abbreviation for 'spectrum and multiplicities'.

2.5.1 Spectrum and multiplicities

A concise way to represent S&M is as the formal expression $\mathcal{E}_1^{f_1} \cdots \mathcal{E}_k^{f_k}$, where the $\mathcal{E}_i$'s are the spectral values, with $\mathcal{E}_1 \leq \cdots \leq \mathcal{E}_k$. f_i is the multiplicity of $\mathcal{E}_i$ for $i = 1, \dots, k$. As it is the case, k and $f_1, \dots, f_k$ are invariants of the corresponding network, independent of the node labeling chosen, but not the spectral values $\mathcal{E}_1, \dots, \mathcal{E}_k$.

2.5.2 Ground state

The ground state for a network G is the smallest value in the spectrum of the EE of G. We now consider the problem how to find the ground state. That is, we want to identify the permutation τ such that the expression (1) is minimized. So, formally, we have the following optimization problem:

$$\mathcal{E}_G^\wedge = \min_{\tau \in \Pi_n} \mathcal{E}_G^\tau, \tag{16}$$

For graphs with a small number of nodes the ground state can be easily determined by considering all possible permutations of the labels. However, for graphs with a large number of nodes one cannot hope to find a ground state in this way, because there are far too many possibilities. Instead one should lower one's expectations and settle for finding an acceptable local minimum, as a proxy for a global one. For instance, one could use simulated annealing.

The network in or near the ground state can expected to have an adjacency matrix with a narrow band around the main diagonal containing most of the entries equal to 1. To express the degree of concentration of arcs, or 'bandedness' of the adjacency matrix A, one can use the relative number of entries equal to 1 in a band around the main diagonal of A compared to the total number of entries in this band. So, formally, we are dealing with a function $\beta : \{0, \dots, n-1\} \to [0,1]$, where n the order of A, and

$$\beta(k) = \frac{\text{\# entries 1 in band of width k}}{\text{\# entries in band of width k}} \tag{17}$$

for $k = 0, 1, \dots, n-1$. We have that $\beta(0) = 0$, as the main diagonal of any adjacency matrix A has no entries 1 only entries 0s, and $\beta(n-1) = 1$.

2.5.3 Complete graphs

Let G_n^C be the complete graph on n points. This means that the set of arcs/nodes is maximal: between each pair of nodes there is an edge. Suppose that the nodes are numbered in the standard way (in which each label is used exactly once) using labels $1, \dots, n$. What is the EE of G_n^C? The first thing to remark is that it is not important to know how each node is labeled.

We next remark that the problem can be solved recursively. We start with a graph with two arcs, then look at the one with three arcs, then with four arcs, etc. We look at the corresponding matrices with the energies per arc, which for arc (i,j) is $(i-j)^2$. [6] We obtain successively:

$$\left(\begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array}\right), \left(\begin{array}{cc|c} 0 & 1 & 4 \\ 0 & 0 & 1 \\ \hline 0 & 0 & 0 \end{array}\right), \left(\begin{array}{ccc|c} 0 & 1 & 4 & 9 \\ 0 & 0 & 1 & 4 \\ 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 \end{array}\right), \left(\begin{array}{cccc|c} 0 & 1 & 4 & 9 & 16 \\ 0 & 0 & 1 & 4 & 9 \\ 0 & 0 & 0 & 1 & 4 \\ 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 0 & 0 \end{array}\right), \dots \tag{18}$$

At each stage, the added energy values are, respectively $1+4=5$, $1+4+9=14$, $1+4+9+16=30$, etc. In case we have the $(n+1)\times(n+1)$ case, the added value to the previous case is

$$\sum_{i=1}^{n} i^2 = \frac{1}{6} n(n+1)(2n+3). \tag{19}$$

So if T_n denotes the EE of G_n^C, we have the following recursion:

$$\begin{aligned} T_2 &= 1, \\ T_{n+1} &= T_n + \frac{1}{6} n(n+1)(2n+3). \end{aligned} \tag{20}$$

[6] A similar matrix was considered before, namely (2), in a graph context.

From (20) we can compute:

$$T_n = \frac{1}{4}n(n+2)^2(n+4), \tag{21}$$

using the well-known expressions for $\sum_{i=1}^{n} i$, $\sum_{i=1}^{n} i^2$, and $\sum_{i=1}^{n} i^3$ and some rearrangement of the resulting expression.

The above applies to digraphs. For graphs we simply have to double the values.

2.5.4 Top state

Apart from the ground state of the EE for a network G we also have the top state, corresponding with the highest energy in the spectrum of G.

$$\mathcal{E}_G^{\vee} = \max_{\tau \in \Pi_n} \mathcal{E}_G^{\tau}, \tag{22}$$

Ground state $\mathcal{E}_G^{\wedge}$ and top state$\mathcal{E}_G^{\vee}$ are related, in the sense that if can compute one of then we can compute the other one as well. This is via the duality of a network and its complement, relative to the complete graph with the same number of nodes as G.

We use (26) to link the EE of the top state of a digraph G with n vertices to the ground state of the complementary digraph G^c. Expression (21) gives the energy of the complete graph.

So the EE of the top state of G is given by the following identity:

$$\mathcal{E}_G^{\vee} = \frac{1}{4}n(n+2)^2(n+4) - \mathcal{E}_{G^c}^{\wedge}. \tag{23}$$

This duality between the EE of the top state of a digraph G and of the ground state of its complement G^c is quite insightful and handy and relates the two concepts.

3 Sub-networks

3.1 Splitting networks and EE

The EE is a linear function of the energy components per edge. The implies that for subgraphs whose edge sets form a partitioning of the edge set of the given graph the associated eleastic energies can be added. We illustrate this property in a specific example. For digraphs similar results hold.

Example

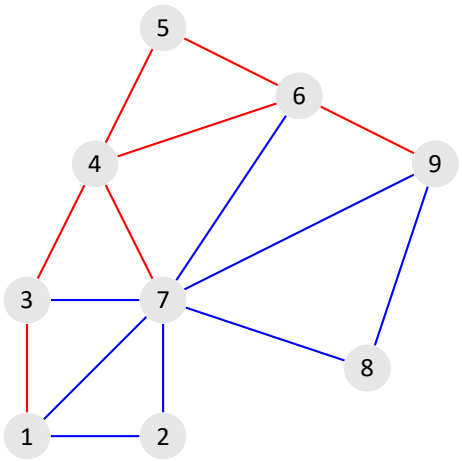


Figure 3.1 Two edge disjoint subgraphs, one with red edges and the other with blue edges that combined form the original graph.

Figure 3.1 shows a graph with two edge-disjoint subgraphs, one $G_1 = (V_1, E_1)$, with edges colored red, the other, $G_2 = (V_2, E_2)$, with edges colored blue. We have:

- G_1:
  - $V_1 = \{1, 3, 4, 5, 6, 7\}$
  - $E_1 = \{\{1, 3\}, \{3, 4\}, \{4, 5\}, \{4, 6\}, \{4, 7\}, \{5, 6\}\}$
- G_2:
  - $V_2 = \{1, 2, 6, 7, 8, 9\}$
  - $E_2 = \{\{1, 2\}, \{1, 7\}, \{2, 7\}\{6, 7\}, \{7, 8\}, \{7, 9\}, \{8, 9\}\}$

So $E_1 \cap E_2 = \emptyset$ and $E_1 \cup E_2 = E$, whereas $V_1 \cap V_2 = \{1, 6, 7\}$ and $V_1 \cup V_2 = V$. In particular, the edge set of G is partioned, but the node set is covered by overlapping sets of nodes. Because the edge set of G is partitioned into two sets, the EE of G neatly splits into two parts along the lines of G_1 and G_2:

$$\mathcal{E}_G = \mathcal{E}_{G_1} + \mathcal{E}_{G_2}. \tag{24}$$

Decomposition results like (24) hold generally for networks. □

3.2 Complementary graph

If G is a graph or digraph with adjacency matrix A, the complementary (di)graph of G, denoted as G^c, has as its adjacency matrix matrix A^c, the complementary matrix of A, defined as

$$A^c = J_0 - A, \tag{25}$$

where $J_0 = J - I$ and J is the $n \times n$ all 1s matrix, i.e. with all entries equal to 1, and I, where all these matrices have the same order as A. Matrix (25) is the adjacency matrix obtained from A by

interchanging all 0s and 1s, except at the main diagonal where the entries remain 0. Then we have

$$\mathcal{E}_G + \mathcal{E}_{G^c} = \mathcal{E}_{G^k}, \tag{26}$$

where G_k is the complete graph on n points, defined above.[7)]

These examples show that the elastic energy associated with a graph can vary quite a bit, depending on the relabeling of the nodes that is used. However, if we average the elastic energies of the various graphs obtained after applying all possible permutations of the nodes, we obtain a measure (AEE) that is less discriminating. In Section 5.4 two non-isomorphic graphs are shown with the same TEE (and hence AEE).

4 Alternative expressions for the elastic energy

We consider the quadratic form expressing the elastic energy and rewrite it using matrices. This rewriting is done in two ways. In the first one a direct product of the adjacency matrix and an energy matrix is used, which separates the geometry dependent energy terms and the topology of the network. In the second way graph Laplacians are used, which are generalizations of the Laplacian operator in mathematical analysis. Also discussed is how to generalize our approach by embedding the network in a normed space or a metric space.

4.1 Separating geometry and topology

Let the following matrix be the adjacency matrix A of some graph

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix} \tag{27}$$

Corresponding to (27) is the following matrix with elastic energy components:

7) We could have defined $A^c = A$ which can be interpreted as the adjacency matrix of a digraph with loops, as it has 1s on the main diagonal. This would be a kind of digraph deviating from the loopless digraphs that we consider in the present paper. However, these loops do not contribute to the elastic energy of the digraph. So in this case the equality (26) would still hold.

$$A \odot E_5 = \begin{pmatrix} 0 & 1 & 4 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 4 & 1 & 0 & 1 & 4 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 4 & 1 & 0 \end{pmatrix}, \tag{28}$$

where

$$E_5 = \begin{pmatrix} 0 & 1 & 4 & 9 & 16 \\ 1 & 0 & 1 & 4 & 9 \\ 4 & 1 & 0 & 1 & 4 \\ 9 & 4 & 1 & 0 & 1 \\ 16 & 9 & 4 & 1 & 0 \end{pmatrix}, \tag{29}$$

is a special case of (2) for $n = 5$. The operator $\odot$ denotes the matrix product that multiplies matrices of the same order element-wise. As (28) shows, there is a clean separation between the structural information of the graph (embodied in the adjacency matrix) and the energy matrix E_5 If another energy would be associated with a graph we would only have to modify the energy matrix and keep the adjacency matrix.

The elastic energy associated with (28) can be expressed as

$$\iota' A \odot E_5 \iota = 24, \tag{30}$$

where where $\iota = (1, 1, 1, 1, 1)'$.

The decomposition of the elastic energy matrix associated with a network into a part that defines the elastic energy for any pair of nodes and a part that consists of the adjacency matrix of the network is insightful. Permuting the labels associated with the nodes of a graph affects the elastic energy only via the adjacency matrix part and not via the energy part.

4.2 Using the graph Laplacian

Suppose we map the nodes of a graph G to the points $\xi_1, \dots, \xi_n$ in $\mathbb{R}$ instead of on $1, \dots, n$ as in (1). In this case the EE would be expressed as

$$\mathcal{E}_G = \sum_{(i,j)\in E} (\xi_i - \xi_j)^2. \tag{31}$$

We can write (31) in matrix form as

$$\mathcal{E}_G = \xi'(\Delta - A)\xi, \tag{32}$$

where $\xi' = (\xi_1, \ldots, \xi_n)$ and Δ is the degree matrix of G, which is a diagonal matrix, with the i-th entry Δ_{ii} equal to the degree of node i of G and A the adjacency matrix of G. The matrix

$$\mathcal{L} = \Delta - A, \tag{33}$$

is the graph Laplacian, which is the equivalent of the Laplacian operator in mathematical analysis. In Cartesian coordinates this operator in $\mathbb{R}^n$ can be expressed as:

$$L_n = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}. \tag{34}$$

From (32) it is clear that the essence of the EE is the graph Laplacian. The vector ξ contains information on the location of the points on the line onto which the nodes of the network are mapped. There is no compelling argument why the nodes of a network G should be mapped on the first n integer values. Other points on the line ($\mathbb{R}$) could be chosen just as well.

More information on graph Laplacians can be found in e.g. (5) (chapter 13), (3) and (9). For instance, the graph Laplacian $\mathcal{L}$ in (33) can alternatively be expressed as[8)]

$$\mathcal{L} = DD', \tag{35}$$

where D is the incidence matrix of an arbitrary orientation σ of the graph G.[9)] We denote this digraph derived from G using σ as G^σ. So D is the incidence matrix of G^σ. In general, rk($\mathcal{L}$) equals the number of connected components of G, where rk(·) is the function that yields the rank of a matrix. Another result is the following. If $\lambda_1, \ldots, \lambda_n$ denote the eigenvalues of $\mathcal{L}$ then the number of spanning trees in G equals $\frac{1}{n}\prod_{i=1}^{n}\lambda_i$. These results (and several more) can be found in (3), Section 13.2.

4.3 Embeddings in normed or metric spaces

It is straightforward to extend the idea underlying our approach to EE to other spaces, such as Euclidean spaces. Instead of mapping the nodes of a network to points on a line (e.g. $\mathbb{N}$ or $\mathbb{Z}$) we can map them to points in different metric spaces, or normed spaces, from which a metric can be derived from the norm. Instead of (1) we could get as an energy function

$$\mathcal{E}_G^n = \sum_{(i,j)\in E} || \tau(i) - \tau(j) ||^2, \tag{36}$$

8) See e.g. (5), Lemma 8.3.2.

9) Which means that each edge of G should be replaced by an arcs. So if an edge is thought of as a pair of arcs (an arc and its counter-arc) one of them should be picked. Which one is chosen is not important. The incidence matrix of an oriented graph is not a complicated concept but takes some space to define. To save this space we choose to refer to the definition in (5), Section 8.3.

where $||\cdot||$ is the norm in a normed linear space $(X, ||\cdot||)$ with $\tau : V \to X$ an injective map.[10] For instance we could take $X = \mathbb{R}^2$, with $||(x, y)|| = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}$ where $x = (x_1, x_2) \in \mathbb{R}^2$ and $y = (y_1, y_2) \in \mathbb{R}^2$. Let $\Sigma \subset \mathbb{R}^2$ be a finite subset with the same number of elements as the number of nodes in V, that is, $|\Sigma| = |V|$.

Even more general is the following expression for an energy function:

$$\mathcal{E}_G^d = \sum_{(i,j)\in E} d(\tau(i), \tau(j))^2, \tag{37}$$

where d is the metric in a metric space (Y, d) with $\tau : V \to Y$ an injective map.[11]

Although these extensions are obvious in a theoretical sense, technically they are much more demanding. We therefore shall not delve into them in the present paper. For embeddings in $\mathbb{R}^m$, for some m, the interested reader is referred to (5).[12]

4.4 AEE and the graph Laplacian

Note that the permutation operation that changes G into G_τ does not change the topology of G. However, it (generally) will change the elastic energy of G, i.e. (1). There are a few exceptions: if G has no arcs but only nodes and in case G is a full graph, we have $\overline{\mathcal{E}}_G = \mathcal{E}_{G,\tau}$ for all $\tau \in \Pi_n$.

Instead of (32) we have the following expression for the elastic energy for the graph G with relabeled nodes using τ:

$$\mathcal{E}_G^\tau = \tau(\xi)'(\Delta - A)\tau(\xi), \tag{38}$$

where $\tau(\xi)' = (\tau(1), \ldots, \tau(n)) = T\xi$, where T is the permutation matrix representing τ, so that

$$\mathcal{E}_G^\tau = \xi' T \mathcal{L} T \xi, \tag{39}$$

where we have used $T' = T$.

The distribution of the elastic energy for all permutations τ of the node set of G is a topological invariant of G, and of each G_τ. We call the different energies that are obtained by applying all possible permutations τ, the spectrum of the elastic energy of G. This set is the carrier for the distribution of the elastic energy. Multiplicities for each value indicate how often these energies occur when permutations are applied.

[10] Strictly speaking there is no compelling reason why the map should be injective. The original map from the nodes to the line has this property, and we borrowed it. But this restriction could be dropped and one still would have an energy function, although a degenerated one because different nodes are assigned to the same point in the co-domain.

[11] Again, injectivity is not really a requirement, as explained in footnote 10.

[12] As mentioned before, (5) uses 'representation' instead of 'embedding'.

Computing this invariant may be difficult, as the number of terms increases rapidly with increasing n. See Section 6.1 for a discussion of these issues.

Using the graph Laplacian $\mathcal{L}$ we can express the AEE of G (see (15)) as

$$\overline{\mathcal{E}}_G = \frac{1}{n!}\sum_{T\in\Pi_n} \xi' T\mathcal{L}T\xi = \xi'(\frac{1}{n!}\sum_{T\in\Pi_n} T\mathcal{L}T)\xi, \tag{40}$$

where ξ and T are as in (39). Now Π_n is interpreted as the set of permutation matrices of order n. The second expression in (40) contains the averaging operator

$$\frac{1}{n!}\sum_{T\in\Pi_n} T\mathcal{L}T. \tag{41}$$

.

which is the operator associated with AEE.

Computing an average such as (41) directly may be prohibitive if the number of edges or arcs in the network is huge. The best one can hope for is to estimate of $\mathcal{E}_G$ based on a sample of permutations $\tau \in \Pi_n$. The question is what sample size should be chosen in order to obtain a sufficiently accurate estimate.

4.5 Discrete harmonic functions

This section is somewhat of a sidestep, in order to get a bit more familiar with the concept of a graph Laplacian. It links this concept to the more familiar concept of the Laplacian in mathematical analysis.

Let $G = (V, E)$ be a connected graph, with $|V| = n$ and with graph Laplacian $\mathcal{L}$. Let $x = (x_1, \dots, x_n)'$ be a column vector that satisfies

$$\mathcal{L}x = 0, \tag{42}$$

that is, $x \in$ Ker($\mathcal{L}$), the kernel of $\mathcal{L}$. As $\iota' = (1, \dots, 1)$ satisfies (42), Ker($\mathcal{L}$) is not empty.

Now, (42) can be seen as the discrete equivalent of Laplace's equation $L_2 f = 0$, with L_2 is the Laplacian in (34) for $n = 2$. This can be expressed in Cartesian coordinates as

$$\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2} = 0, \tag{43}$$

The solutions to (43) are so-called harmonic functions.

We now turn back to the network case. Using (33) we obtain from (42):

$$x = \Delta^{-1}Ax, \tag{44}$$

where Δ is the degree matrix as defined in (32). The inverse of Δ exists because Δ is a nonsingular matrix:G is connected, so the degree of each node is at least 1. Hence all diagonal element of Δ are strictly positive. Note that (44) expresses the condition that the value at any node is the average of the values associated with its adjacent nodes:

$$x_i = \frac{1}{d_i}\sum_{j\sim i} x_j, \tag{45}$$

where $i, j \in V$, d_i is the degree of i and $j \sim i$ means that j is an adjacent node to i, or, alternatively expressed, that $\{i, j\} \in E$. If we define a function $x : V \to \mathbb{R}$ with $x(i) = x_i$ then x satisfying (42) is a discrete harmonic function. Note that $\Delta^{-1}A$ in (44) is a Markov matrix. The digraph G represents it: its nodes are the states, and each arc denotes a possible jump from one state to another (in the direction of the arc). If transition probabilities are attached to the arcs, the Markov chain is completely defined. Each of the d_i arcs emanating from node i have associated probability $1/d_i$.

Property (45) can be viewed as the discrete analogue of the property of continuous harmonic functions f stating that the value at any point x in its domain is the average of the values over a contour Γ that encloses x:

$$f(x) = \frac{1}{2\pi i}\oint_{\Gamma}\frac{f(z)}{z-x}dz \tag{46}$$

There is a close connection between harmonic functions and holomorphic functions in complex analysis, which are the central objects of study in this subfield of mathematical analysis.

4.6 Eigenvalues of graph Laplacians

Note that the graph Laplacian $\mathcal{L}$ associated with the EE of a graph $G = (V, E)$ is a matrix of order $|V| = n$, that is a symmetric, positive semi-definite (as the energy values are ≥ 0), and singular (as the row (and column) totals are 0). Therefore $\mathcal{L}$ can be diagonalized and its eigenvalues are ≥ 0. If $|E| = m$, we have

$$\mathrm{Tr}(\mathcal{L}) = \mathrm{Tr}(\Delta - A) = \mathrm{Tr}(\Delta) = \sum_{i=1}^{n} d_i = 2m, \tag{47}$$

as each edge in G is counted twice. Also we have

$$Tr(\mathcal{L}) = \sum_{i=1}^{n} \lambda_i, \tag{48}$$

where λ_i, for $i = 1, \dots, n$, denote the eigenvalues of $\mathcal{L}$. From (47) and (48) we conclude

$$\sum_{i=1}^{n} \lambda_i = 2m = \sum_{i=1}^{n} d_i. \tag{49}$$

It is possible to define graph Laplacians as analogues in graph theory of Laplace equations in analysis. In fact, one can go even further in translating problems defined in the are of analysis to the area of graph theory. This applies, for instance, to certain problems concerning vibrating membranes suspended over domains and fixed at their boundaries. This leads to so-called boundary value problems involving a Laplace operator. These turn out to be eigenvalue problems for the Laplace equation, where the function values at the boundary of the membrane are fixed to 0. In particular one focuses on the smallest eigenvalue, which turns out to depend on the area of the membrane, and ask for the shape of the membrane with a fixed area and boundary length, for which this smallest eigenvalue is minimal.[13)] The English physicist Lord Rayleigh conjectured that this is the case for a circular area, which was later proved to be correct by the mathematicians Georg Faber and Edgar Krahn, independently of each other (see e.g. (7), chapter 6).

Now one can try to emulate the setup of the vibrating membranes in terms of graphs. One then looks at functions defined on the nodes of the graph, which are 0 at the boundary nodes of the graph. A boundary node is a node of degree 1. The concept 'Area of the membrane' is translated into the concept 'the number of interior nodes', where an interior node is a node of degree at least 2. The concept 'length of the boundary of the membrane' is translated into the concept 'the number of boundary nodes'. The operator used in the translated problem is the graph Laplacian. The interested reader is referred to e.g. (3) for several results concerning this type of problem.

5 Spectral properties of some networks

So far the discussion was general and abstract. Now we want to look at some concrete examples to obtain more feeling for the concept of elastic energy of networks. To this end we consider some tiny networks for which it is easy to compute the EE and related quantities.

We start with the tiny networks called Trident, Triad and Filament, respectively. They are discussed in this order in Sections 5.1 , 5.2 and 5.3. These networks have in common that they

[13)] Problems concerning the quest for a plane figure possessing the largest possible area whose boundary has a specified length, are called isoperimetric problems.

have four nodes and three edges. They are different topologically, however. In Section 5.4 we compare the results for these graphs. In Section 5.5 we consider all graphs with four nodes. The number of edges for these graphs ranges from 0 to 6. For all these graphs TEE, AEE and S&M are computed and compared. In Section 5.6, finally, we look at the graph Laplacians of some networks. In particular we compare these matrices for three types of networks: general digraphs, graphs (where each arc has its counter-arc) and mixed digraphs (where some arcs have their counter-arcs, but some arcs do not).

5.1 Trident

The EE expression for the Trident in Figure 5.1 is:

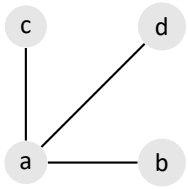


Figure 5.1 Trident with 'general' node labeling.

$$\mathcal{E}_\Psi/2 = (a-b)^2 + (a-c)^2 + (a-d)^2. \tag{50}$$

We now expand the right hand sides of (50). The advantage of an expanded EE expression is that it is easy to add EE- components, to compute the TEE or AEE; it can be done term-wise. We obtain

$$\mathcal{E}_\Psi/2 = 3a^2 + b^2 + c^2 + d^2 - 2ab - 2ac - 2ad. \tag{51}$$

So the coefficients of (51) of the terms a^2, b^2, c^2, d^2,ab, ac, ad, bc, bd and cd are presented in the in the row labeled 1 in Table 5.1. The coefficients for the remaining permutations of the nodes can be found in the rows below. The relevant permutation for each row is in the final column of the table.

We can express (51) in matrix form as

$$\mathcal{E}_\Psi/2 = (a,b,c,d)\begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}, \tag{52}$$

where the matrix in (52) is the graph Laplacian of the Trident, which is the difference of the diagonal degree matrix Δ_T and the adjacency matrix A_T:

$$\begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \Delta_T - A_T. \tag{53}$$

no	a^2	b^2	c^2	d^2	ab	ac	ad	bc	bd	cd	permutation
1	3	1	1	1	-2	-2	-2	0	0	0	(abcd)
2	3	1	1	1	-2	-2	-2	0	0	0	(abdc)
3	3	1	1	1	-2	-2	-2	0	0	0	(acbd)
4	3	1	1	1	-2	-2	-2	0	0	0	(acdb)
5	3	1	1	1	-2	-2	-2	0	0	0	(adbc)
6	3	1	1	1	-2	-2	-2	0	0	0	(adcb)
7	1	3	1	1	-2	0	0	-2	-2	0	(bacd)
8	1	3	1	1	-2	0	0	-2	-2	0	(badc)
9	1	3	1	1	-2	0	0	-2	-2	0	(bcad)
10	1	3	1	1	-2	0	0	-2	-2	0	(bcda)
11	1	3	1	1	-2	0	0	-2	-2	0	(bdac)
12	1	3	1	1	-2	0	0	-2	-2	0	(bdca)
13	1	1	3	1	0	-2	0	-2	0	-2	(cabd)
14	1	1	3	1	0	-2	0	-2	0	-2	(cadb)
15	1	1	3	1	0	-2	0	-2	0	-2	(cbad)
16	1	1	3	1	0	-2	0	-2	0	-2	(cbda)
17	1	1	3	1	0	-2	0	-2	0	-2	(cdab)
18	1	1	3	1	0	-2	0	-2	0	-2	(cdba)
19	1	1	1	3	0	0	-2	0	-2	-2	(dabc)
20	1	1	1	3	0	0	-2	0	-2	-2	(dacb)
21	1	1	1	3	0	0	-2	0	-2	-2	(dbac)
22	1	1	1	3	0	0	-2	0	-2	-2	(dbca)
23	1	1	1	3	0	0	-2	0	-2	-2	(dcab)
24	1	1	1	3	0	0	-2	0	-2	-2	(dcba)
tot	36	36	36	36	-24	-24	-24	-24	-24	-24	

Table 5.1 For the Trident: coefficients of $\mathcal{E}_\Psi/2$, for all permutations of the node labels.

Now we consider a particular choice of the labels, namely $a = 1$, $b = 2$, $c = 3$, $d = 4$. Table 5.1 was used to compute Tables 5.2, in which these values for the labels a, b, c and d have been used. This gives an insight into which labeling of the nodes leads to the most efficient embedding and which to the worst, in each case. And also into the spectrum and their multiplicities (S&M). Note that the last column of Table 5.1 lists half of the values of the respective EEs. This is because we are dealing with graphs where each edge counts double.

We have chosen $a = 1$, $b = 2$, $c = 3$ and $d = 4$ as the standard labeling for the nodes. But alternative labelings for the nodes are also possible, of course. For instance, if one would choose the labeling $a = 1$, $b = 2$, $c = 3$ and $d = 4$, one would find the TEE spectrum to consist of two values, namely 24 and 56, each with multiplicity 12. So the size of the spectrum (2 in the case of the Trident) and the multiplicities of the spectral values (12 and 12 in this case) have not changed. The spectral values, depend on the labeling, however. For other labelings (with different labels) one would find the same result.

5.2 Triad

This graph is on right-hand side on the one but last row in Figure 5.5. It is the dual of the Trident, which is in the same row, and which has the same characteristics (TEE/AEE and S&M) as the 'Triangle-and-dot' graph, for short 'Triad'.

In Figure 5.3 the Triad and the Trident are shown together, as dual graphs, with complementary edges.

no	a^2 = 1	b^2 = 4	c^2 = 9	d^2 = 16	ab = 2	ac = 3	ad = 4	bc = 6	bd = 8	cd = 12	$\mathcal{E}_\Psi/2$
1	3	4	9	16	-4	-6	-8	0	0	0	14
2	3	4	9	16	-4	-6	-8	0	0	0	14
3	3	4	9	16	-4	-6	-8	0	0	0	14
4	3	4	9	16	-4	-6	-8	0	0	0	14
5	3	4	9	16	-4	-6	-8	0	0	0	14
6	3	4	9	16	-4	-6	-8	0	0	0	14
7	1	12	9	16	-4	0	0	-12	-16	0	6
8	1	12	9	16	-4	0	0	-12	-16	0	6
9	1	12	9	16	-4	0	0	-12	-16	0	6
10	1	12	9	16	-4	0	0	-12	-16	0	6
11	1	12	9	16	-4	0	0	-12	-16	0	6
12	1	12	9	16	-4	0	0	-12	-16	0	6
13	1	4	27	16	0	-6	0	-12	0	-24	6
14	1	4	27	16	0	-6	0	-12	0	-24	6
15	1	4	27	16	0	-6	0	-12	0	-24	6
16	1	4	27	16	0	-6	0	-12	0	-24	6
17	1	4	27	16	0	-6	0	-12	0	-24	6
18	1	4	27	16	0	-6	0	-12	0	-24	6
19	1	4	9	48	0	0	-8	0	-16	-24	14
20	1	4	9	48	0	0	-8	0	-16	-24	14
21	1	4	9	48	0	0	-8	0	-16	-24	14
22	1	4	9	48	0	0	-8	0	-16	-24	14
23	1	4	9	48	0	0	-8	0	-16	-24	14
24	1	4	9	48	0	0	-8	0	-16	-24	14

Table 5.2 For the Trident: $\mathcal{E}_\Psi/2$ for all permutations of the node labels, with the node labeling: $a = 1, b = 2, c = 3, d = 4$.

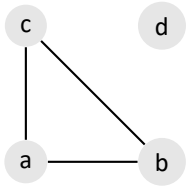


Figure 5.2 Triad with 'general' node labeling.

The properties just mentioned of the triad graph can be deduced by using the duality of the Triad and the Trident. See Section 2.2, the example discussing the splitting of the elastic energies for subgraphs. However, in the present section we want to use direct calculation, as in case of the Trident and the Filament.

We can write down the expression for the elastic energy of the triad, which we denote by $\mathcal{E}_\Delta$. We have

$$\mathcal{E}_\Delta/2 = (a-b)^2 + (b-c)^2 + (c-a)^2, \tag{54}$$

which we can expand as

$$\mathcal{E}_\Delta/2 = 2a^2 + 2b^2 + 2c^2 - 2ab - 2ac - 2bc. \tag{55}$$

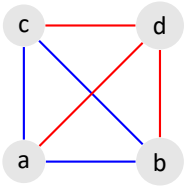


Figure 5.3 Trident (red) and Triad (blue) as dual graphs.

We can write (55) in matrix form as

$$\mathcal{E}_\Delta/2 = (a,b,c,d)\begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}. \tag{56}$$

Using (56) we can compute the coefficients of the quadratic forms that we obtain when applying all possible permutations of the nodes. The results are collected in Table 5.3. The bottom line contains the column totals. We find for the Triad the same column totals as for the Trident and the Filament.

no	a^2	b^2	c^2	d^2	ab	ac	ad	bc	bd	cd	permutation
1	2	2	2	0	-2	-2	0	-2	0	0	(abcd)
2	2	2	0	2	-2	0	-2	0	-2	0	(abdc)
3	2	2	2	0	-2	-2	0	-2	0	0	(acbd)
4	2	0	2	2	0	-2	-2	0	0	-2	(acdb)
5	2	2	0	2	-2	0	-2	0	-2	0	(adbc)
6	2	0	2	2	0	-2	-2	0	0	-2	(adcb)
7	2	2	2	0	-2	-2	0	-2	0	0	(bacd)
8	2	2	0	2	-2	0	-2	0	-2	0	(badc)
9	2	2	2	0	-2	-2	0	-2	0	0	(bcad)
10	0	2	2	2	0	0	0	-2	-2	-2	(bcda)
11	2	2	0	2	-2	0	-2	0	-2	0	(bdac)
12	0	2	2	2	0	0	0	-2	-2	-2	(bdca)
13	2	2	2	0	-2	-2	0	-2	0	0	(cabd)
14	2	0	2	2	0	-2	-2	0	0	-2	(cadb)
15	2	2	2	0	-2	-2	0	-2	0	0	(cbad)
16	0	2	2	2	0	0	0	-2	-2	-2	(cbda)
17	2	0	2	2	0	-2	-2	0	0	-2	(cdab)
18	0	2	2	2	0	0	0	-2	-2	-2	(cdba)
19	2	2	0	2	-2	0	-2	0	-2	0	(dabc)
20	2	0	2	2	0	-2	-2	0	0	-2	(dacb)
21	2	2	0	2	-2	0	-2	0	-2	0	(dbac)
22	0	2	2	2	0	0	0	-2	-2	-2	(dbca)
23	2	0	2	2	0	-2	-2	0	0	-2	(dcab)
24	0	2	2	2	0	0	0	-2	-2	-2	(dcba)
tot	36	36	36	36	-24	-24	-24	-24	-24	–24	

Table 5.3 For the Triad: coefficients of $\mathcal{E}_\Delta/2$, for all permutations of the node labels.

Using Table 5.3 we can compute the elastic energies for each permutation of the nodes. The results can be found in Table 5.4. Note that the spectrum consist of two values, namely 6 and 14, each with multiplicity 12.

no	a^2 = 1	b^2 = 4	c^2 = 9	d^2 = 16	ab = 2	ac = 3	ad = 4	bc = 6	bd = 8	cd = 12	$\mathcal{E}_\Delta/2$
1	2	8	18	0	-4	-6	0	-12	0	0	6
2	2	8	0	32	-4	0	-8	0	-16	0	14
3	2	8	18	0	-4	-6	0	-12	0	0	6
4	2	0	18	32	0	-6	-8	0	0	-24	14
5	2	8	0	32	-4	0	-8	0	-16	0	14
6	2	0	18	32	0	-6	-8	0	0	-24	14
7	2	8	18	0	-4	-6	0	-12	0	0	6
8	2	8	0	32	-4	0	-8	0	-16	0	14
9	2	8	18	0	-4	-6	0	-12	0	0	6
10	0	8	18	32	0	0	0	-12	-16	-24	6
11	2	8	0	32	-4	0	-8	0	-16	0	14
12	0	8	18	32	0	0	0	-12	-16	-24	6
13	2	8	18	0	-4	-6	0	-12	0	0	6
14	2	0	18	32	0	-6	-8	0	0	-24	14
15	2	8	18	0	-4	-6	0	-12	0	0	6
16	0	8	18	32	0	0	0	-12	-16	-24	6
17	2	0	18	32	0	-6	-8	0	0	-24	14
18	0	8	18	32	0	0	0	-12	-16	-24	6
19	2	8	0	32	-4	0	-8	0	-16	0	14
20	2	0	18	32	0	-6	-8	0	0	-24	14
21	2	8	0	32	-4	0	-8	0	-16	0	14
22	0	8	18	32	0	0	0	-12	-16	-24	6
23	2	0	18	32	0	-6	-8	0	0	-24	14
24	0	8	18	32	0	0	0	-12	-16	-24	6

Table 5.4 For the Triad: $\mathcal{E}_\Delta/2$ for all permutations of the node labels, with the node labeling: $a = 1, b = 2, c = 3, d = 4$.

5.3 Filament

We now consider the filament as labeled in Figure 5.4. We repeat the same kind of computations as in Section 5.1, so we can compare the results. The actual comparison will do done in Section 5.4.

For the Filament in Figure 5.4 we have the following polynomial expression for its EE:

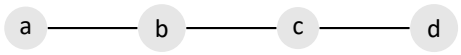


Figure 5.4 Filament with 'general' node labeling.

$$\mathcal{E}_F/2 = (a-b)^2 + (b-c)^2 + (c-d)^2, \tag{57}$$

and expand it to yield:

$$\mathcal{E}_F/2 = a^2 + 2b^2 + 2c^2 + d^2 - 2ab - 2bc - 2cd. \tag{58}$$

The coefficients of the terms in the polynomial expressions for the EE for the Filament, for each permutation of the nodes, can be found is Table 5.5.

$$\mathcal{E}_F/2 = (a,b,c,d)\begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}, \tag{59}$$

where the matrix is the graph Laplacian of the filament, which is the difference of the diagonal degree matrix Δ_F and the adjacency matrix A_F:

$$\begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \Delta_F - A_F. \tag{60}$$

no	a^2	b^2	c^2	d^2	ab	ac	ad	bc	bd	cd	permutation
1	1	2	2	1	-2	0	0	-2	0	-2	(abcd)
2	1	2	1	2	-2	0	0	0	-2	-2	(abdc)
3	1	2	2	1	0	-2	0	-2	-2	0	(acbd)
4	1	1	2	2	0	-2	0	0	-2	-2	(acdb)
5	1	2	1	2	0	0	-2	-2	-2	0	(adbc)
6	1	1	2	2	0	0	-2	-2	0	-2	(adcb)
7	2	1	2	1	-2	-2	0	0	0	-2	(bacd)
8	2	1	1	2	-2	0	-2	0	0	-2	(badc)
9	2	1	2	1	0	-2	-2	-2	0	0	(bcad)
10	1	1	2	2	0	0	-2	-2	0	-2	(bcda)
11	2	1	1	2	0	-2	-2	0	-2	0	(bdac)
12	1	1	2	2	0	-2	0	0	-2	-2	(bdca)
13	2	2	1	1	-2	-2	0	0	-2	0	(cabd)
14	2	1	1	2	0	-2	-2	0	-2	0	(cadb)
15	2	2	1	1	-2	0	-2	-2	0	0	(cbad)
16	1	2	1	2	0	0	-2	-2	-2	0	(cbda)
17	2	1	1	2	-2	0	-2	0	0	-2	(cdab)
18	1	2	1	2	-2	0	0	0	-2	-2	(cdba)
19	2	2	1	1	-2	0	-2	-2	0	0	(dabc)
20	2	1	2	1	0	-2	-2	-2	0	0	(dacb)
21	2	2	1	1	-2	-2	0	0	-2	0	(dbac)
22	1	2	2	1	0	-2	0	-2	-2	0	(dbca)
23	2	1	2	1	-2	-2	0	0	0	-2	(dcab)
24	1	2	2	1	-2	0	0	-2	0	-2	(dcba)
tot	36	36	36	36	-24	-24	-24	-24	-24	-24	

Table 5.5 For the filament: coefficients of $\mathcal{E}_F/2$, for all permutations of the node labels.

Now we consider a particular choice of the labels a, b, c, d, namely $a = 1$, $b = 2$, $c = 3$, $d = 4$. Tables 5.1 and 5.5 were used to compute Tables 5.2 and 5.6, in which these values for the labels a, b, c and d have been used. This gives an insight into which labeling leads to the most efficient embedding and which to the worst, in each case. And also, in the distribution of the EE values, i.e. the spectrum and the multiplicities (S&M). Note that the last column of Tables 5.1 and 5.5 lists half of the values of the respective EEs. This is because we are dealing with graphs and each edge is counted twice (as it is assumed to consist of two arcs).

no	a^2 = 1	b^2 = 4	c^2 = 9	d^2 = 16	ab = 2	ac = 3	ad = 4	bc = 6	bd = 8	cd = 12	$\mathcal{E}_F/2$
1	1	8	18	16	-4	0	0	-12	0	-24	3
2	1	8	9	32	-4	0	0	0	-16	-24	6
3	1	8	18	16	0	-6	0	-12	-16	0	9
4	1	4	18	32	0	-6	0	0	-16	-24	9
5	1	8	9	32	0	0	-8	-12	-16	0	14
6	1	4	18	32	0	0	-8	-12	0	-24	11
7	2	4	18	16	-4	-6	0	0	0	-24	6
8	2	4	9	32	-4	0	-8	0	0	-24	11
9	2	4	18	16	0	-6	-8	-12	0	0	14
10	1	4	18	32	0	0	-8	-12	0	-24	11
11	2	4	9	32	0	-6	-8	0	-16	0	17
12	1	4	18	32	0	-6	0	0	-16	-24	9
13	2	8	9	16	-4	-6	0	0	-16	0	9
14	2	4	9	32	0	-6	-8	0	-16	0	17
15	2	8	9	16	-4	0	-8	-12	0	0	11
16	1	8	9	32	0	0	-8	-12	-16	0	14
17	2	4	9	32	-4	0	-8	0	0	-24	11
18	1	8	9	32	-4	0	0	0	-16	-24	6
19	2	8	9	16	-4	0	-8	-12	0	0	11
20	2	4	18	16	0	-6	-8	-12	0	0	14
21	2	8	9	16	-4	-6	0	0	-16	0	9
22	1	8	18	16	0	-6	0	-12	-16	0	9
23	2	4	18	16	-4	-6	0	0	0	-24	6
24	1	8	18	16	-4	0	0	-12	0	-24	3

Table 5.6 For the filament: $\mathcal{E}_F/2$, for all permutations of the node labels, with the node labeling: $a = 1$, $b = 2$, $c = 3$, $d = 4$.

If we would use a different labeling of the nodes, say $a = 1$, $b = 3$, $c = 5$ and $d = 7$, we would find the TEE-spectrum: 24, 48, 72, 88, 112, 136 with multiplicities 2, 4, 6, 6, 4, 2, respectively. So the size of the spectrum (6) and the corresponding multiplicities[14)] are the same, as in case of the original labeling. The spectral values are different from the ones based on the original labeling $a = 1$, $b = 2$, $c = 3$, $d = 4$. We also have pairs of spectral values, namely $(24, 136)$, $(48, 112)$ and $(72, 88)$, each of which has the total value of 160.

5.4 Comparing the EE of Trident, Triad and Filament

In Tables 5.1 and 5.5 the coefficients of the base terms a^2, b^2, c^2, d^2, ab, ac, ad, bc, bd and cd of all TEEs that are obtained after permutation of the labels are shown, for the Trident en the Filament, respectively. The bottom line in each of these tables is the sum of the coefficients for each base term. If we divide these values by 24 (the number of permutations of four elements), we obtain the AEE. We see that the TEE (and hence the AEE) is the same in both cases. However, the coefficients for the polynomials obtained in both cases are quite different.

Note that for Tables 5.1 and 5.5 column totals are equal, implying that the TEE and AEE are the same. So these measures fail to discriminate between these graphs. However, if we look at the spectra and their multiplicities of the Trident and the Filament we see that they are different. The

[14)] Dependent on the ranking of the spectral values

Trident only has two spectral values, namely 12 and 28, each with multiplicity 12 whereas the Filament has as spectral values 6, 12, 18, 22, 28, 34 with multiplicities 2, 4, 6, 6 , 4 and 2 respectively.

It should be noted that the spectral values come in pairs: in the Trident case there is only one pair of values in the spectrum.

We now consider the spectral values and their multiplicities (S&M) for the Trident, Triad and Filament. From Table 5.7 we learn, for the Trident, that the two spectral values are 6 and 14, and the corresponding multiplicities 12, in each case.

TEE	no	permutation	TEE	no	permutation
6	1	(abcd)	14	7	(bacd)
6	2	(abdc)	14	8	(badc)
6	3	(acbd)	14	9	(bcad)
6	4	(acdb)	14	10	(bcda)
6	5	(adbc)	14	11	(bdac)
6	6	(adcb)	14	12	(bdca)
6	19	(dabc)	14	13	(cabd)
6	20	(dacb)	14	14	(cadb)
6	21	(dbac)	14	15	(cbad)
6	22	(dbca)	14	16	(cbda)
6	23	(dcab)	14	17	(cdab)
6	24	(dcba)	14	18	(cdba)

Table 5.7 For the Trident: permutations of the node labels that yield the same spectral value for $\mathcal{E}_\Psi/2$.

From Table 5.8 we learn, for the Triad, that the two spectral values are 6 and 14 as well, and with multiplicities 12 as well, as in case of Figure 5.7. So this is an example of two topologically different (non-isomorphic) graphs with the same S&M.

TEE	no	permutation	TEE	no	permutation
6	1	(abcd)	14	2	(abdc)
6	3	(acbd)	14	4	(acdb)
6	7	(bacd)	14	5	(adbc)
6	9	(bcad)	14	6	(adcb)
6	10	(bcda)	14	8	(badc)
6	12	(bdca)	14	11	(bdac)
6	13	(cabd)	14	14	(cadb)
6	15	(cbad)	14	17	(cdab)
6	16	(cbda)	14	19	(dabc)
6	18	(cdba)	14	20	(dacb)
6	22	(dbca)	14	21	(dbac)
6	24	(dcba)	14	23	(dcab)

Table 5.8 For the Triad: permutations of the node labels that yield the same spectral value for $\mathcal{E}_\Delta/2$.

From Table 5.9 we learn, for the Filament, that the spectral values are: 3, 6 9, 11, 14 and 17, and their respective multiplicities: 2, 4, 6, 6, 4 and 2. Also the pairing of the spectral values is clear: 3 and 17, 6 and 14, 9 and 11. The sum of the values of each pair is the same, namely 20.

It is clear that the S&M of a network is related to the symmetries of the associated network, more in particular concerning the permutations of the nodes. This brings us to the area of group

TEE	no	permutation	TEE	no	permutation
3	1	(abcd)	17	11	(bdac)
3	24	(dcba)	17	14	(cadb)
6	2	(abdc)	14	5	(adbc)
6	7	(bacd)	14	9	(bcad)
6	18	(cdba)	14	16	(cbda)
6	23	(dcab)	14	20	(dacb)
9	3	(acbd)	11	6	(adcb)
9	4	(acdb)	11	8	(badc)
9	12	(bdca)	11	10	(bcda)
9	13	(cabd)	11	15	(cbad)
9	21	(dbac)	11	17	(cdab)
9	22	(dbca)	11	19	(dabc)

Table 5.9 For the Filament: permutations of the node labels that yield the same spectral value for $\mathcal{E}_F/2$.

theory, applied to graph theory. We do not wish to go into this topic in the present paper, but only dip our toe into it, by noting that certain permutations in the Tables 5.7, 5.8 and 5.9 form subgroups of the group of permutations of (a, b, c, d). In Tables 5.7 and 5.8 these are the permutations in the first column (both corresponding to TEE$= 6$. In Table 5.9 these are the permutations corresponding to the value 3. We leave it at this minor observation. This topic is, however, interesting for further pursuit elsewhere.

5.5 Graphs with four nodes

So far we considered three tiny graphs with four nodes in the present subsection, namely Trident, Triad and Filament. Now we extend the scope a bit and consider all graphs with four nodes. The number of edges for these graphs varies from 0 to 6. The graphs in question are shown in Figure 5.5. Each row of this picture contains graphs that are mutual complements. At the bottom row a self-complementary graph is shown in different guises.

For each graph, some characteristics are shown, namely TEE, AEE and S&M. Note that both TEE and AEE are simple functions of the number of edges m:

$$\text{TEE} = 160 \cdot m, \tag{61a}$$

$$\text{AEE} = 6\frac{2}{3} \cdot m, \tag{61b}$$

So this shows that TEE and AEE are rather crude as complexity measures, as they do not distinguish these networks. Two graphs with the same number of edges and nodes have the same TEE and AEE values. But topologically these networks need not be the same.

The spectrum of the graphs (in the column S&M) in Figure 5.5 does sometimes distinguish graphs that TEE/AEE do not. For instance in case of the graphs in the left column presented in the 4-th and 5-th row, and the one in this column in the final and one but final row. However, it does not distinguish the graphs on the one but last row. In this case the graphs have the same spectrum

and multiplicities, but they are not isomorphic graphs.[15] So S&M yields a finer measure to distinguish non-isomorphic graphs. But it is also not a perfect one.

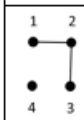
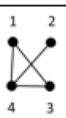
Network	TEE	AEE	S&M	Network	TEE	AEE	S&M
	0	0	S: 0 M.: 24		960	40	S: 40 M: 24
	160	$6\frac{2}{3}$	S: 2, 8, 18 M: 12, 8, 4		800	$33\frac{1}{3}$	S: 22, 32, 38 M: 4, 8, 12
	320	$13\frac{1}{3}$	S: 4, 16, 20 M: 8, 8, 8		640	$26\frac{2}{3}$	S: 20, 24, 36 M: 8, 8, 8
	320	$13\frac{1}{3}$	S: 4, 10, 20, 26 M: 4, 12, 4, 4		640	$26\frac{2}{3}$	S: 14, 20, 30, 36 M: 4, 4, 12, 4
	480	20	S: 12, 28 M: 12, 12		480	20	S: 12, 28 M: 12, 12
	480	20	S: 6, 12, 18, 22, 28, 34 M: 2, 4, 6, 6, 4, 2		480	20	S: 6, 12, 18, 22, 28, 34 M: 2, 4, 6, 6, 4, 2

Figure 5.5 Some graphs with 4 nodes and some characteristics: Total elastic energy (TEE), average elastic energy (AEE) and the spectrum and the corresponding multiplicities (S&M). Each row contains dual graphs.

5.6 Comparison of (di)graph Laplacians

Consider the graph G_4 in Figure 5.6. Imagine for the moment that the label associated with node i is x_i, for $i = 1, \dots, 4$. Then the elastic energy associated with G_4 is

$$\mathcal{E}_{G_4}/2 = (x_1 - x_2)^2 + (x_1 - x_3)^2 + (x_1 - x_4)^2 + (x_3 - x_4)^2, \tag{62}$$

where each term has a factor 2 because we are dealing with edges and not arcs without counter-arcs..

We can expand the quadratic forms and reassemble them. We then obtain

[15] Isomorphism would preserve the distribution of the degrees of the nodes in a graph. Both graphs have different degree distributions of the nodes.

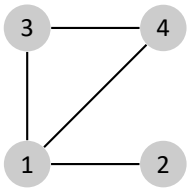


Figure 5.6 Graph G_4.

$$\mathcal{E}_{G_4}/2 = 3x_1^2 + x_2^2 + 2x_3^2 + 2x_4^2 - 2x_1x_2 - 2x_1x_3 - 2x_1x_4 - 2x_3x_4. \tag{63}$$

which in matrix form can be expressed as

$$\mathcal{E}_{G_4}/2 = (x_1, x_2, x_3, x_4)\begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = x' L_{G_4} x. \tag{64}$$

.

The matrix L_{G_4} in (64) can be recognized as the graph Laplacian of G_4. In (5), p.281, Lemma 13.1.5. the same kind of derivation can be found as given above, but for a more general quadratic form.

The graph Laplacian is defined $\Delta - A$, where Δ is the diagonal matrix with the degrees of the nodes of G on the main diagonal and A is its adjacency matrix. It is symmetric and $(\Delta - A)\iota = 0$, for $\iota = (1, 1, 1, 1)'$, which shows that it is a singular matrix.

More generally, it holds that an expression like (62) for a graph G can be written in the form

$$x' \mathcal{L} x, \tag{65}$$

with $x' = (x_1, \ldots, x_n)$ and $\mathcal{L}$ is the graph Laplacian for G.

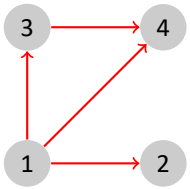


Figure 5.7 Digraph DG_4.

In case of the digraph in Figure 5.7 we find as the expression for the EE:

$$\mathcal{E}_{DG_4} = (x_1 - x_2)^2 + (x_1 - x_3)^2 + (x_1 - x_4)^2 + (x_3 - x_4)^2, \tag{66}$$

which is half the amount of $\mathcal{E}_{G_4}$ in (62).

Now consider the mixed digraph HDG_4 in Figure 5.8, which has some arcs and their counter-arcs, which together can be viewed as edges, and some arcs without their counter-arcs.

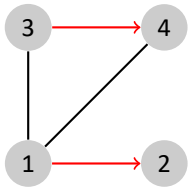


Figure 5.8 Digraph HDG_4.

We have as the expression for the EE in case of HDG_4

$$\mathcal{E}_{HDG_4} = (x_1 - x_2)^2 + 2(x_1 - x_3)^2 + 2(x_1 - x_4)^2 + (x_3 - x_4)^2, \tag{67}$$

Elaborating (67) and writing the result in matrix form yields

$$\mathcal{E}_{HDG_4} = (x_1, x_2, x_3, x_4)\begin{pmatrix} 5 & -1 & -2 & -2 \\ -1 & 1 & 0 & 0 \\ -2 & 0 & 3 & -1 \\ -2 & 0 & -1 & 3 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} \tag{68}$$

.

To understand (68) we recall the definition of the function 'iodeg' in (4). We are dealing here with a generalization of the concept of graph Laplacian to digraphs, which could be called a digraph Laplacian. We can write

$$\begin{pmatrix} 5 & -1 & -2 & -2 \\ -1 & 1 & 0 & 0 \\ -2 & 0 & 3 & -1 \\ -2 & 0 & -1 & 3 \end{pmatrix} = \begin{pmatrix} 5 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 2 & 2 \\ 1 & 0 & 0 & 0 \\ 2 & 0 & 0 & 1 \\ 2 & 0 & 1 & 0 \end{pmatrix}. \tag{69}$$

,

where the first matrix on the right hand side of (69) could be called the io-degree matrix, where each entry an the main diaginal is the iodeg of the corresponding node. It is a generalization of the degree matrix. The second matrix on the right hand side of (69) is a generalization of the adjacency matrix. Each entry (i, j) counts the number of arcs connecting nodes i and j: 1 if there is a single arc connecting them, 2 if there are 2 arcs connecting them, which together comprise and edge. Obviously both matrices are symmetric and so is their difference. Both matrices are positive semi-definite. The matrix on the left-hand side of (69) has 0 row sums and column sums, and hence is singular.

So we see that digraph Laplacians are a generalization of graph Laplacians. They are defined for several classes of digraphs: oriented graphs (where nodes are connected by arcs without the counter-arc), graphs (in which each arc has its counter-arc) and for mixed digraphs (where some arcs are without their counter-arcs and some arcs are with their counter-arcs). These digraph Laplacians appear naturally when defining the EE for the various classes of digraphs mentioned, inclusing graphs.

6 Further research

In this section we have collected some problems that came up during the writing of this paper. Some of them are relevant for practical applications, whereas others are of a more theoretical nature. They may be taken up as challenges for interested readers.

6.1 Big graphs

The number of permutations of the node set of a graph may quickly become enormous. How are we supposed to compute the (average) elastic energy in such cases? Or if exact computations are impossible, how can we find good approximations of the (average) elastic energy?

So far only tiny graphs have been considered, in order to illustrate and motivate certain concepts. But clearly one runs into trouble when applying concepts like TEE/AEE and S&M as the number of permutations one is facing is staggering. It is then simply impossible to compute these quantities exactly. The best one can do is to estimate these quantities, considering random labelings of the nodes. In particular estimates of the AEE are of interest.

The problem is to estimate the average of expressions of the type (11), on the basis of a sample $\mathcal{S}$ of permutations in $\mathcal{I}_n$. An estimate of this average is obtained on the basis of a srswr sample of permutations of size $|\mathcal{S}| = s$, say.[16] So as an estimator of (11) we can take

$$\hat{\hat{\mathcal{E}}}_G = \frac{\sum_{\tau\in\mathcal{S}} \sum_{(i,j)\in E} (\tau(i) - \tau(j))^2}{s}. \tag{70}$$

It remains to be seen to what extent the estimate (70) of AEE is able to distinguish between large non-isomorphic grahs; this depends on the sample size, of course, in relation to the proximity of the AEEs of the networks.

Even more challenging than estimating of AEE of a big graph is estimating its spectrum and the multiplicities of the spectral values, that is, estimating the S&M.

In considering big graphs an approach like the one chosen in statistical mechanics to describe gases seems promising. The nodes in the graphs can be viewed as particles and the edges represent 'interactions' between the 'particles'. By permuting the positions of the particles one does not change the 'particles' that interact with each other, but the 'interaction energies' (elastic energies) are likely to change. As the number of 'particles' and that of'interactions' is big (or even huge), one is forced to use statistical methods to compute macro-properties such as average 'interaction energies', which are elastic energies in this case.

It may also be fruitful to consider random matrix theory for big networks.[17] A classical problem considered in this area is to to find a multivariate probability density of the eigenvalues of certain

[16] We can take a simple random sample with replacement (srswr) because n is supposed to be large, so that the probability that the sample has duplicates is negligible, as the size of the sample s is tiny compared to $|\mathcal{I}_n| = n!$.

[17] This was suggested by Frank Pijpers when he reviewed the present paper.

ensembles of random matrices. In our case such an ensemble consists of all energy matrices under all possible permutations of the labels $1, \dots, n$ of the nodes of a given (big) graph.

Among the physicists that pioneered this area are Freeman Dyson and Eugene Wigner. It is not so easy to suggest pertinent articles in this area that would provide useful entries. However some books have been published that survey this area (such as (8), (2) and (1)) that are useful to get acquainted with the area.

6.2 Computational complexity of the ground state problem

Let a network $G = (V, E)$ be given. Suppose that $V = \{1, \dots, n\}$. The following question is of interest: For which permutation τ of these node values is the TEE minimal? In (16) there is a formal statement of the ground state problem.

With this optimization problem a decision problem is associated: given a bound $b > 0$ is there a permutation of the labels of nodes of G such that the EE is less than b? Even if finding such a permutation τ may be a challenge, verifying that the EE is smaller than b is easy, that is, can be done in polynomial time (in terms of the size of the problem, i.e. the numbers of arcs $|E|$ in the network).

We are interested in the first place in the computational complexity of the problem. Can the corresponding decision problem be solved in polynomial time? Is it NP-complete, that is in the same league as the Traveling Salesman Problem (TSP)? See (6), to which the ground state problem bears some resemblance. A standard reference on NP-completeness is (4).

As in case of TSP, heuristics to find upper bounds of the ground state are not so difficult to find (such as using a greedy algorithm), but that is no guarantee that these are very sharp.

6.3 Existence of networks with a given S&M

So far we have considered problems where a network was given and the S&M was computed. In principle this is straightforward, except when the network is large (in terms of the number of edges/arcs). But what about the inverse problem? If $k \in \mathbb{N}$ values $0 < e_1 < \cdots < x_k$ are given as well as k natural numbers $m_1, \dots, m_k$ is there a network with $e_1^{m_1} \cdots e_k^{m_k}$ as its S&M? If so, how can it be constructed?

6.4 Digraph Laplacians

The concept of graph Laplacian was generalized (in Section 5.6) to that of digraph Laplacian. It is of interest to study digraph Laplacians as they appear naturally when defining EE for digraphs. Several subclasses of digraphs can be distinguised, of which that one consisting of graphs (digraphs with the property that each of its arcs also has its counter-arc) is well-studied. That of oriented graphs and that of mixed digraphs much less so, if at all. In particular one may study the spectral properties of digraph Laplacians. In particular, it is interesting to compare the spectra of digraphs which share the property that their underlying graphs are the same. A special challenge present the big digraphs. This, of course, is an extension of the the kind of problems discussed in Section 6.1.

7 Discussion

Several network invariants have been introduced in this paper, which can be used as measures of their complexity. In (10) also complexity measures are introduced for networks, using different criteria.

The invariants introduced in the present paper are inspired by elasticity theory: by mapping the nodes of a network to a fixed set of equidistant points on a line, each arc/edge is of a certain leng/th and its square is interpreted as an elastic energy, as in classical mechanics, if it is an arc. An edge is considered to consist of two arcs (an arc and its counter-arc) and its elastic energy is twice that of a single arc. The elastic energy of the network is the sum of the elastic energies of each of its arcs/edges.

The n nodes of the network can be mapped in $n!$ ways on the points of the line (assuming that no two nodes are mapped to a single point). If the elastic energies of each of these 'embeddings' is added we obtain the TEE and if they are averaged we obtain the AEE.

It is also possible to group the elastic energies for all 'embeddings' into groups of equal elastic energy. This yields the spectrum (S) of the elastic energies and their multiplicities (M) of a network, combined indicated as S&M. Isomorphic graphs have the same TEE/AEE and S&M. However, these characteristics do not necessarily discriminate classes of isomorphic networks: non-isomorphic graphs may possess the same TEE/AEE and S&M.

The paper explores some properties of the elastic energy of networks and also considers a few small examples of networks to compute TEE, AEE and S&M. It is clear that this is possible only for such small networks. However, it is insightful to see some concrete results.

Some problems concerning the elastic energy of networks may be computationally intractable, such as computing the embedding of the nodes (injectively) in $\mathbb{N}$ yielding the highest (or lowest) elastic energy for the network considered.

Embedding of the nodes in $\mathbb{N}$ is taken as a standard example in the present paper. But it is remarked that an embedding is also possible in other sets (or rather spaces), such as normed or metric spaces, and using the corresponding norms or metrics to measure the distances of the 'embedded' nodes.

The essence of the elastic energy of a graph is contained in the graph Laplacian. A lot is known about graph Laplacians in the literature on algebraic graph theory. This knowledge is useful for a better grasp of the elastic energy of networks, in particular concerning the S&M of the graph. To include various type of digraphs, such as oriented graphs and mixed digraphs, the concept of graph Laplacian needs to be generalized to that of digraph Laplacians, as is suggested in the present paper. This concept does not seem to have been explored before in the litarature; it is left for future exploration.

For small networks it is easy to compute the invariants introduced in this paper. However, for big networks (in terms of the number of edges) it is a challenge to compute these characteristics (unless these networks have a regular structure). It is probably only feasible to provide estimates of AEE, rather than exact calculations. Ideas from statistical mechanics and random matrix theory

are likely to be fruitful in we are dealing with big networks. Again, exploring these ideas are left for future research.

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