HYPERGRAPH LAPLACE OPERATORS FOR CHEMICAL REACTION NETWORKS

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ABSTRACT. We generalize the normalized combinatorial Laplace operator for graphs by defining two Laplace operators for hypergraphs that can be useful in the study of chemical reaction networks. We also investigate some properties of their spectra.

1. INTRODUCTION

This paper is a part of a project with the chemist Guillermo Restrepo and his students for a systematic analysis of chemical reaction networks. At an abstract level, such networks can be modelled as directed hypergraphs in which each vertex represents a chemical element and each hyperedge represents a chemical reaction involving the elements that it contains as vertices. In this paper, we therefore define and study a normalized combinatorial Laplace operator for hypergraphs, with the aim of investigating reaction networks through the spectrum of that operator, that is, its collection of eigenvalues. We already know that the spectrum of the normalized combinatorial Laplace operator (that from now on we will just call Laplace operator) for graphs encodes important information about the graphs. For example, we know that the multiplicity of the eigenvalue 0 for the Laplacian on vertices $L^0$ is equal to the number of connected components of the graph; we know that the multiplicity of the eigenvalue 0 for the Laplacian on edges $L^1$ is equal to the number of cycles; the largest eigenvalue reaches its maximum value exactly for bipartite graphs and its minimum value exactly for complete graphs. While a graph is not completely determined by its spectrum – there exist isospectral graphs, that is, different graphs with the same spectrum –, the spectrum does capture the important qualitative properties of a graph. That is, classifying graphs by their spectrum may ignore some little details, but seems to be quite useful in the presence of big data, in particular since eigenvalue computations can be performed with tools from linear algebra.

In Section 2 we define the basic definitions regarding the hypergraphs that represent chemical reaction networks and we make some important assumptions motivated by the chemical interpretation. In Section 3 we construct our Laplace operators for hypergraphs by generalizing, in the most natural way, the construction of the graph Laplace operators. We also prove that their restriction to graphs coincides with the well-known graph Laplace operators. In Section 4 we prove the first basic properties of our Laplace operators; in Section 5 we talk about the multiplicity of the eigenvalue 0 for our two Laplacians. In Section 6 we recall and apply the Courant-Fischer-Weyl min-max principle in order to get more insight about the spectra of our Laplacians and,
in particular, in Section 6.1 we study the largest eigenvalue: we prove that it reaches its maximum value exactly for bipartite hypergraphs and we see when exactly it reaches its minimum value, which is in this case 0. Finally, in Section 7 we talk about isospectral hypergraphs.

2. Basic definitions and assumptions

As already mentioned in the introduction, chemical reaction networks can be modelled by directed hypergraphs. Each reaction is a directed hyperedge, mapping a collection of vertices, its educts or inputs, to another collection, its products or outputs. We could therefore define a suitable Laplace type operator for a directed hypergraph and study its spectrum, as pioneered by F. Bauer [2] for directed graphs. Since such an operator is not self-adjoint w.r.t. some scalar product, however, in general its eigenvalues will not be real, but have nonzero imaginary parts. Here, however, we prefer to work with symmetric operators and real eigenvalues. That would suggest to work with undirected hypergraphs. Nevertheless, we preserve an important bit of additional structure from the chemical reaction networks, the fact that the vertex set of a hyperedge is partitioned into two classes. In the directed case, they correspond to inputs and outputs, but in the setting that we wish to adopt, we do not distinguish these two roles and simply keep the partitioning of the vertices of a hyperedge into two classes. Thus, we are working with hypergraphs with an additional piece of structure, the partitioning of the vertex sets of each hyperedge into two classes. We will call these chemical hypergraphs.

Definition. A chemical hypergraph is a pair $\Gamma = (V, H)$ such that $V = \{v_1, \ldots, v_N\}$ is a finite set of vertices and $H$ is a multiset such that every element $h$ in $H$ is a pair of elements $(V_h, W_h)$ (input and output, not necessarily disjoint) in $\mathcal{P}(V) \setminus \{\emptyset\}$. The elements of $H$ are called the oriented hyperedges. Changing the orientation of a hyperedge $h$ means exchanging its input and output, leading to the pair $(W_h, V_h)$.

Since every chemical reaction has both educts and products, we consider only hyperedges that have at least one input and at least one output (and these may also coincide, as we will see in the next definition).

Definition. A catalyst in a hyperedge $h$ is a vertex that is both an input and an output for $h$. 

\[ \begin{array}{c}
+ \\
v_1 \\
+ \\
v_2 \\
+ \\
v_3 \\
- \\
v_3
\end{array} \]

Figure 1. An hyperedge $h$ that has two inputs and one catalyst.
Remark 1. The above definition comes from the fact that, in chemistry, a catalyst is an element that participates in a reaction but is not changed by that reaction. Our theory thus includes also oriented graphs with self-loops, i.e. graphs that may have edges whose two endpoints coincide.

While according to our definition, we shall not work with directed hyperedges, we shall nevertheless have to work with oriented hyperedges. Let us arbitrarily call the two orientations of a hyperedge \( h^+ \) and \( h^- \). Analogously to differential forms in Riemannian geometry, see for instance [4], we shall consider functions \( \gamma \) from the set of oriented hyperedges that satisfy
\[
\gamma(h, -) = -\gamma(h, +),
\]
that is, changing the orientation of \( h \) produces a minus sign. Importantly, neither of the two orientations that a hyperedge carries plays a preferred role. Thus, an oriented hyperedge should not be confused with a directed hyperedge.

**Definition.** We say that a hypergraph \( \Gamma = (V, H) \) is connected if, for every pair of vertices \( v, w \in V \), there exists a path that connects \( v \) and \( w \), i.e. there exist \( v_1, \ldots, v_m \in V \) and \( h_1, \ldots, h_{m-1} \in H \) such that:
- \( v_1 = v \);
- \( v_m = w \);
- \( \{v_i, v_{i+1}\} \subseteq h_i \) for each \( i = 1, \ldots, m - 1 \).

**Definition.** We say that \( \Gamma = (V, H) \) has \( k \) connected components if there exist \( \Gamma_1 = (V_1, H_1), \ldots, \Gamma_k = (V_k, H_k) \) such that:
1. For every \( i \in \{1, \ldots, k\} \), \( \Gamma_i \) is a connected hypergraph with \( V_i \subseteq V \) and \( H_i \subseteq H \);
2. For every \( i, j \in \{1, \ldots, k\}, i \neq j \), \( V_i \cap V_j = \emptyset \) and therefore also \( H_i \cap H_j = \emptyset \).

**Definition.** Let \( \Gamma = (V, H) \) be a hypergraph. We say that \( S = (V', H') \) is a closed system of reactions in \( \Gamma \) if:
1. \( \emptyset \neq H' \subseteq H \);
2. \( V' = \{ v \in h : h \in H' \} \);
3. Each \( v \in V' \) appears in \( S \) as often as input as as output.

**Remark 2.** Closed systems for hypergraphs generalize the oriented cycles that we have for graphs, so they are interesting from the mathematical point of view, and they are also clearly interesting from the chemical point of view.
Figure 3. A closed system of reactions.

Definition. We say that a closed system of reactions $S$ in $\Gamma$ is *minimal* if it is not contained in any other closed system of reactions in $\Gamma$.

Remark 3. The definition of *minimal* closed system of reactions makes sense since it is easy to see that:

1. $S, S'$ closed systems $\implies S \cup S'$ closed system;
2. $S, S'$ closed systems with $S \subseteq S' \implies S' \setminus S$ closed system.

Therefore, if we know the minimal closed systems we know all of them.

Definition. We say that two closed systems $S = (V', H')$ and $S = (V'', H'')$ are *disjoint* if $H \cap H' = \emptyset$.

Remark 4. Disjoint systems don’t have common hyperedges but they may have common vertices.

3. Generalized Laplace Operators

In order to define the Laplace operator for hypergraphs, we will generalize the construction of the Laplace operator for graphs in the most natural way. In particular, we will:

1. Give weight 1 to the hyperedges (as we do for edges in the case of graphs) and therefore give weight $\deg i := |\text{hyperedges containing } i|$ to each vertex $i$;
2. Define a scalar product for functions defined on hyperedges and a scalar product for functions defined on vertices, based on the weights we gave;
3. Define the boundary operator for functions defined on the vertex set;
4. Find the coboundary operator based on the scalar product we defined;
5. Define the Laplace operators as the two different compositions of the boundary and the coboundary operator.

Definition (Scalar product for functions defined on hyperedges). Given $\omega, \gamma : H \to \mathbb{R}$, let

$$(\omega, \gamma)_H := \sum_{h \in H} \omega(h) \cdot \gamma(h).$$
**Definition** (Scalar product for functions defined on vertices). Given \( f, g : V \to \mathbb{R} \), let
\[
(f,g)_V := \sum_{i \in V} \deg i \cdot f(i) \cdot g(i).
\]

**Definition** (Boundary operator for functions defined on vertices). Given \( f : V \to \mathbb{R} \) and \( h \in H \), let
\[
\delta f(h) := \sum_{h_i \text{ input of } h} f(h_i) - \sum_{h^j \text{ output of } h} f(h^j).
\]

**Remark 5.** Note that
\[
\delta : \{ f : V \to \mathbb{R} \} \to \{ \gamma : H \to \mathbb{R} \}
\]
where the \( \gamma \) are always supposed to satisfy (II). In particular, \( \delta f \) also satisfies (II).

**Definition** (Adjoint operator of the boundary operator). Let \( \delta^* : \{ \gamma : H \to \mathbb{R} \} \to \{ f : V \to \mathbb{R} \} \) be defined as
\[
\delta^*(\gamma)(i) := \frac{\sum_{h_{i \text{ input}}} \gamma(h_{i \text{ input}}) - \sum_{h_{i \text{ output}}} \gamma(h_{i \text{ output}})}{\deg i}.
\]

**Lemma 6.** \( \delta^* \) is such that \((\delta f, \gamma)_H = (f, \delta^* \gamma)_V\), therefore it is the (unique) adjoint operator of \( \delta \).

**Proof.**
\[
(\delta f, \gamma)_H = \sum_{h \in H} \gamma(h) \cdot \left( \sum_{h_i \text{ input of } h} f(h_i) - \sum_{h^j \text{ output of } h} f(h^j) \right)
\]
\[
= \sum_{i \in V} f(i) \cdot \left( \sum_{h_{i \text{ input}}} \gamma(h_{i \text{ input}}) - \sum_{h_{i \text{ output}}} \gamma(h_{i \text{ output}}) \right)
\]
\[
= \sum_{i \in V} \deg i \cdot f(i) \cdot \left( \frac{\sum_{h_{i \text{ input}}} \gamma(h_{i \text{ input}}) - \sum_{h_{i \text{ output}}} \gamma(h_{i \text{ output}})}{\deg i} \right)
\]
\[
= \sum_{i \in V} \deg i \cdot f(i) \cdot \delta^*(\gamma)(i)
\]
\[
= (f, \delta^* \gamma)_V.
\]

**Definition** (Laplace operators). Given \( f : V \to \mathbb{R} \) and given \( i \in V \), let
\[
L^V f(i) := \delta^*(\delta f)(i)
\]
\[
= \frac{\sum_{h_{i \text{ input}}} \delta f(h_{i \text{ input}}) - \sum_{h_{i \text{ output}}} \delta f(h_{i \text{ output}})}{\deg i}
\]
\[
= \frac{\sum_{h_{i \text{ input}}} \left( \sum_{i' \text{ input of } h_{i \text{ input}}} f(i') - \sum_{j' \text{ output of } h_{i \text{ input}}} f(j') \right)}{\deg i}.
\]
\[
\sum_{h_{\text{out}}:i \text{ output of } h_{\text{out}}} \left( \sum_i \text{ input of } h_{\text{out}} f(i) - \sum_j \text{ output of } h_{\text{out}} f(j) \right) \div \deg i.
\]

Analogously, given \( \gamma : H \to \mathbb{R} \) and \( h \in H \), let
\[
L^H \gamma(h) := \delta(\delta^* \gamma)(h)
\]
\[
= \sum_{h_{\text{in}}:i \text{ input of } h_{\text{in}}} \delta^* \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}:j \text{ output of } h_{\text{out}}} \delta^* \gamma(h_{\text{out}}) + \frac{\sum_{h_{\text{in}}:i \text{ input of } h_{\text{in}}} \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}:j \text{ output of } h_{\text{out}}} \gamma(h_{\text{out}})}{\deg h_{\text{in}}} + \frac{\sum_{h_{\text{out}}:j \text{ output of } h_{\text{out}}} \gamma(h_{\text{out}}) - \sum_{h_{\text{in}}:i \text{ input of } h_{\text{in}}} \gamma(h_{\text{in}})}{\deg h_{\text{out}}}.
\]

**Proposition 7.** Let \( \Gamma \) be a graph with vertex set \( V \) and edge set \( E \), with the convention for orientations as introduced above for hypergraphs. Then
\[
L^V f(i) = f(i) - \frac{1}{\deg i} \sum_{i \to j} f(j),
\]
which is exactly the Laplace operator of graphs for functions defined on vertices.

Analogously, if \( \gamma : E \to \mathbb{R} \) is such that \( \gamma(-e) = -\gamma(e) \) and \( e = [v_0, v_1] \),
\[
L^H \gamma(e) = \frac{1}{\deg v_0} \cdot \sum_{v_0 \in f=[v_0,w]} \gamma(f) - \frac{1}{\deg v_1} \cdot \sum_{v_1 \in g=[v_1,w]} \gamma(g),
\]
which is equal to \( L^1 \) for graphs.

**Proof.** Every oriented edge has exactly one input and exactly one output. Therefore, if \( h_{\text{in}} \) is an edge with input \( i \), then
\[
\{i' : i' \text{ input of } h_{\text{in}}\} = \{i\}
\]
and
\[
\left| \{j' : j' \text{ output of } h_{\text{in}}\} \right| = 1.
\]
If \( h_{\text{out}} \) is an edge with output \( i \), then
\[
\{j : j \text{ output of } h_{\text{out}}\} = \{i\}
\]
and
\[
\left| \{\hat{i} : \hat{i} \text{ input of } h_{\text{out}}\} \right| = 1.
\]
Therefore,
\[
L^V f(i) = \frac{\sum_{h_{\text{in}}:i \text{ input of } h_{\text{in}}} \left( \sum_{i'} \text{ input of } h_{\text{in}} f(i') - \sum_{j'} \text{ output of } h_{\text{in}} f(j') \right)}{\deg i} + \frac{\sum_{h_{\text{out}}:i \text{ output of } h_{\text{out}}} \left( \sum_i \text{ input of } h_{\text{out}} f(i) - \sum_{j} \text{ output of } h_{\text{out}} f(j) \right)}{\deg i}.
\]
\[
\sum_{h_{\text{in}:i}} \text{input} \left( f(i) - \sum_{j'} \text{output of } h_{\text{in}} f(j') \right) \frac{1}{\deg i} + \\
- \frac{\sum_{h_{\text{out}:i}} \text{output} \left( \sum_{i'} \text{input of } h_{\text{out}} f(i') - f(i) \right)}{\deg i} \\
= \frac{f(i)}{\deg i} \left( |h_{\text{in}} : i \text{ input}| + |h_{\text{out}} : i \text{ output}| \right) + \\
- \frac{1}{\deg i} \left( \sum_{h_{\text{in}:i}} \sum_{j'} f(j') + \sum_{h_{\text{out}:i}} f(i) \right) \\
= f(i) - \frac{1}{\deg i} \sum_{i \to j} f(j),
\]

where the last equality is due to the properties of orientation for graphs. Analogously, if \( e = [v_0, v_1] \), then

\[
L^H \gamma(e) = \sum_{h_{i, \text{input of } e}} \frac{\sum_{h_{\text{in}}:h_{i}} \text{input } \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}:h_{i}} \text{output } \gamma(h_{\text{out}})}{\deg h_{i}} + \\
- \sum_{h_{j, \text{output of } e}} \frac{\sum_{h'_{\text{in}}:h_{j}} \text{input } \gamma(h'_{\text{in}}) - \sum_{h'_{\text{out}}:h_{j}} \text{output } \gamma(h'_{\text{out}})}{\deg h_{j}} \\
= \frac{\sum_{h_{\text{in}}:v_0} \text{input } \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}:v_0} \text{output } \gamma(h_{\text{out}})}{\deg v_0} + \\
- \frac{\sum_{h'_{\text{in}}:v_1} \text{input } \gamma(h'_{\text{in}}) - \sum_{h'_{\text{out}}:v_1} \text{output } \gamma(h'_{\text{out}})}{\deg v_1} \\
= \frac{1}{\deg v_0} \sum_{v_0 \in f = [v_0, w]} \gamma(f) - \frac{1}{\deg v_1} \sum_{v_1 \in g = [v_1, w]} \gamma(g),
\]

where the last equality is due to the fact that \(-\gamma(h_{\text{out}}) = \gamma(-h_{\text{out}})\) and \(-\gamma(h'_{\text{out}}) = \gamma(-h'_{\text{out}})\). \(\square\)

**Remark 8.** \(L^H \gamma(h)\) counts what flows out at the inputs - what flows in at the inputs - what flows out at the outputs + what flows in at the outputs.

### 4. First properties

**Lemma 9.** \(L^V\) and \(L^H\) are both self-adjoint.

**Proof.** Use the fact that \(L^V\) and \(L^H\) are the two compositions of \(\delta\) and \(\delta^*\), which are adjoint to each other. \(\square\)

**Lemma 10.** \(L^V\) and \(L^H\) are non-negative operators.

**Proof.** Let \( f : V \to \mathbb{R} \). Then

\[
(L^V f, f)_V = (\delta^* \delta f, f)_V = (\delta f, \delta f)_H \geq 0.
\]  
(2)
Analogously, for $\gamma : H \to \mathbb{R}$,
\[
(L^H \gamma, \gamma)_H = (\delta \delta^* \gamma, \gamma)_H = (\delta^* \gamma, \gamma)_V \geq 0.
\] (3)

A direct consequence of Lemmas 9 and 10 is

**Corollary 11.** The eigenvalues of $L^V$ and $L^H$ are real and non-negative.

**Notation.** Let $N := |V|$ and let $M := |H|$. Since the space of real functions on a set with cardinality $k$ is $k$-dimensional, an operator on this space has precisely $k$ eigenvalues, counted with their multiplicities. Therefore $L^V$ has $N$ eigenvalues that we will arrange as
\[\lambda_1 \leq \ldots \leq \lambda_N.\]

Analogously, $L^H$ has $M$ eigenvalues that we will arrange as
\[\lambda_1^H \leq \ldots \leq \lambda_M^H.\]

**Lemma 12.** If $A$ and $B$ are linear operators, then the non-zero eigenvalues of $AB$ and $BA$ are the same.

**Proof.** Let $\lambda$ be a non-zero eigenvalue of $AB$ for a non-zero eigenvector $v$. Then
\[\lambda Bv = B\lambda v = B(ABv) = (BA)Bv.\]
Therefore, $\lambda$ is an eigenvalue of $BA$ for the eigenvector $Bv$. \qed

**Corollary 13.** The non-zero eigenvalues of $L^V$ and $L^H$ are the same. In particular, if $f$ is an eigenfunction of $L^V$ with eigenvalue $\lambda \neq 0$, then $\delta f$ is an eigenfunction of $L^H$ with eigenvalue $\lambda$; if $\gamma$ is an eigenfunction of $L^H$ with eigenvalue $\lambda' \neq 0$, then $\delta^* \gamma$ is an eigenfunction of $L^V$ with eigenvalue $\lambda'$.

This corollary is quite important because it offers us two alternative ways to control or estimate the nonvanishing eigenvalues, either through $L^V$ or through $L^H$. In particular, we shall see in Section 6 below that these eigenvalues can therefore be expressed in two different ways by Rayleigh quotients.

As another important consequence of Cor. 13, the two operators only differ in the multiplicity of the eigenvalue 0. Let $m_V$ and $m_H$ be the multiplicity of the eigenvalue 0 of $L^V$ and $L^H$, resp. Then Cor. 13 implies

**Corollary 14.**
\[m_V - m_H = |V| - |H|.\] (4)

5. **The eigenvalue 0**

In this section, we want to control the multiplicity of the eigenvalue 0 for our two Laplacians. They are related by Cor. 14. In order to see the principle, let us start with the simple situation where we only have a set $V$ of vertices, but no (hyper)edges connecting them. Then 14 tells us that $m_V = |V|$, which of course can be trivially verified. Now let us add edges. As long as these edges do not form cycles, that is, as long as the graph is a forest, i.e., a collection of trees, we have $m_H = 0$, and therefore,
each new edge reduces the number of components as well as $m_V = |V| - |H|$ by 1. When, however, a new edge closes a cycle, then $m_H$ increases by 1, and consequently, $m_V$ is left unchanged. A special case of this is when we add a loop to a vertex. A loop induces a new eigenvalue 0 of $L^H$ and thus lets $m_V$ unchanged. The general formula says that $m_V - m_H$ equals the number of connected components minus the number of independent cycles, including self-loops.

Something analogous happens when we more generally add hyperedges. In contrast to the case of graphs, however, by adding hyperedges, we can potentially eliminate all eigenvalues 0 of $L^V$. For a graph, $L^V$ always has the eigenvalue 0, as should be clear from the preceding or also follows from Lemma 23 below. We shall see examples of hypergraphs where $L^V$ has only positive eigenvalues. But let us first make some obvious observations.

**Lemma 15.** On a hypergraph with a single hyperedge, $L^V$ has 0 as an eigenvalue. More precisely, $m_V = |V| - 1$ if not every vertex is a catalyst and $m_V = |V|$ if every vertex is a catalyst.

**Proof.** In Example 3 we shall see that, on a hypergraph with a single hyperedge, the only eigenvalue of $L^H$ is non-zero if and only if not every vertex is a catalyst. Therefore, by (4), $m_V = |V| - 1$ if not every vertex is a catalyst and $m_V = |V|$ otherwise. □

In order to investigate this in more detail, we observe that by (2), a function $f$ on the vertex set satisfies $L^V f = 0$ if and only for every $h \in H$,

$$\sum_{h_i \text{ input of } h} f(h_i) = \sum_{h_j \text{ output of } h} f(h_j). \quad (5)$$

Thus, to create an eigenvalue 0 of $L^V$, we need a function $f : V \to \mathbb{R}$ such that is not identically 0 and satisfies (5). For instance, this already implies

**Lemma 16.** If a hypergraph has a vertex $v_0$ that is a catalyst for every hyperedge that it is contained in, then $L^V$ has 0 as an eigenvalue.

**Proof.** Let $f(v_0) = 1$ and $f(v) = 0$ for $v \neq v_0$. This then satisfies (5). □

**Remark 17.** Any function $f : V \to \mathbb{R}$ is an eigenfunction for the eigenvalue 0 in some hypergraph that has vertex set $V$. Construct a hypergraph $\Gamma$ in which all the vertices $v_1, \ldots, v_k$ of $V$ are always catalysts. Then $f$ satisfies (5) for $\Gamma$.

In fact, we have

**Proposition 18.** If $k$ vertices are always catalysts, then $m_V \geq k$.

And $m_V = N$, or equivalently, $\lambda_N = 0$, that is, 0 is the only eigenvalue $\iff$ all vertices are always catalysts.

**Proof.** The first part and the implication $\iff$ are clear from the proof of Lemma 16. Let’s prove $\implies$. In particular, let’s assume that there exists at least one vertex $i \in \hat{h}$ which is not a catalyst for $\hat{h}$ (without loss of generality, we can assume that it is an input). We want to prove that $\lambda_N > 0$. Let $f : V \to \mathbb{R}$ such that $f(j) = 0$ for all $j \neq i$.
and such that

\[ f(i) = \frac{1}{\sqrt{\deg i}}. \]

Then \( \sum_{i \in V} \deg i \cdot f(i)^2 = 1 \) and

\[
\sum_{h \in H} \left( \sum_{h_i \text{ input of } h} f(h_i) - \sum_{h_j \text{ output of } h} f(h_j) \right)^2 \\
\geq \left( \sum_{h_i \text{ input of } h} f(h_i) - \sum_{h_j \text{ output of } h} f(h_j) \right)^2 \\
= \left( \frac{1}{\sqrt{\deg i}} \right)^2 > 0.
\]

Therefore, \( \lambda_N > 0. \)

**Remark 19.** The previous proposition implies that, unlike the case of the graphs, the multiplicity of the eigenvalue 0 for \( L^V \) is in general not equal to the number of connected components of the hypergraph (in particular, we don’t have that \( \lambda_2 > 0 \) for every connected hypergraph) and, analogously, the multiplicity of the eigenvalue 0 for \( L^H \) does not count, in general, the cycles of the hypergraph.

Similarly, by (3), in order to get an eigenvalue 0 of \( L^H \), we need \( \gamma : H \to \mathbb{R} \) satisfying (1) and

\[
\sum_{h_{\text{in};i \text{ input}}} \gamma(h_{\text{in}}) = \sum_{h_{\text{out};i \text{ output}}} \gamma(h_{\text{out}}) \quad (6)
\]

for every vertex \( i \).

And the multiplicity of the eigenvalue 0 of \( L^V \) and \( L^H \) then is given by the number of linearly independent, or since we have scalar products, equivalently by the number of orthogonal \( f \) and \( \gamma \), resp., satisfying these equations. Conversely, if there is no such \( f \) or \( \gamma \), then the corresponding multiplicity is 0.

Now let us see how to apply this. First, when we have a closed system of reactions, we can take a \( \gamma \) that has the same nonzero value on all hyperedges involved in that system and vanishes on all other hyperedges. Such a \( \gamma \) then satisfies (6) because every vertex in such a system appears the same number of times as input as output for hyperedges belonging to that system. This is formalized in the next Lemma.

**Lemma 20.** If \( \Gamma \) has a closed system of reactions, then \( \lambda_1^H = 0. \)

**Proof.** Let \( S = (V', H') \) be a closed system in \( \Gamma \). Let \( \gamma : H \to \mathbb{R} \) be defined as

\[ \gamma(h') := 1 \text{ for all } h' \in H' \text{ and } \gamma(h) := 0 \text{ for all } h \in H \setminus H'. \]

Then \( \gamma \) satisfies (6). Therefore \( \lambda_1^H = 0. \)

**Remark 21.** The claim of Lemma 20 is actually an if and only if for both the case of graphs (for which we know that the multiplicity of 0 for \( L^H \) is equal to the number
of oriented cycles) and the case of $\Gamma$ containing only a single hyperedge. In fact, as we shall see in Example 3 in this case $\lambda_1^H = 0$ if and only if all vertices are catalysts, that is, if and only if there is a closed system of reactions in $\Gamma$ (which is $\Gamma$ itself). But Example 2 will show that the converse of Lemma 20 does not hold.

In order to prepare that example, we shall first present another example of a closed system of reactions

**Example 1.** Consider a hypergraph with three vertices $v_1, v_2, v_3$, with a hyperedge $h_1$ with input $v_1$ and output $v_1, v_2$ and another hyperedge $h_2$ with input $v_2, v_3$ and output $v_3$. Thus, $v_1$ and $v_3$ are catalysts. In this system, $v_2$ is created in $h_1$ with the help of $v_1$, without using up $v_1$, and it is destroyed in $h_2$ with the help of $v_3$, without creating anything. Each vertex appears once as input and once as output, and thus, this hypergraph represents a closed system of reactions in the sense of the definition. We shall call this a *source-sink system.*

![Figure 4. The hypergraph in Example 1.](image)

We shall now use this principle to create another example that is no longer a closed system of reactions, but makes use of the possibility demonstrated in the previous example to create and destroy products independently. And this will allow us to let the system branch and reunite in between.

**Example 2.** Let $\Gamma$ be the hypergraph with 4 vertices $v_1, \ldots, v_4$ and 3 hyperedges $h_1, h_2, h_3$ such that:

1. $h_1$ has $v_1$ as input and $v_2$ as output;
2. $h_2$ has $v_1$ as output and $v_3$ as catalyst;
3. $h_3$ has $v_1$ as input, $v_2$ as input and $v_4$ as catalyst.

This $\Gamma$ does not contain any closed system. Now, let $\gamma : H \to \mathbb{R}$ such that $\gamma(h_1) := \gamma(h_3) := \frac{1}{2}$ and $\gamma(h_2) := 1$. Then $\gamma$ satisfies (6), therefore $\lambda_1^H = 0$.

**Proposition 22.** If $\Gamma$ has $k$ pairwise disjoint closed systems, then

$$\lambda_1^H = \ldots = \lambda_k^H = 0,$$

i.e. the multiplicity of the eigenvalue 0 for $L^H$ is at least $k$.

**Proof.** Let $S_1, \ldots, S_k$ be pairwise disjoint closed systems in $\Gamma$. For each $S_i = (V_i, H_i)$, let $\gamma_i : H \to \mathbb{R}$ be defined as $\gamma_i(h_i) := 1$ for all $h_i \in H_i$ and $\gamma_i(h) := 0$ for all $h \in H \setminus H_i$. Then the $\gamma_i$’s are all orthogonal to each other (since the $H_i$’s are pairwise disjoint) and they all satisfy (6). Therefore,

$$\lambda_1^H = \ldots = \lambda_k^H = 0.$$
Analogously to constructions that satisfy (6) and thereby produce an eigenvalue 0 for $L^H$, we can also construct situations where we can find a function satisfying (5) and obtain an eigenvalue 0 for $L^V$. We have

**Lemma 23.** Let $\Gamma$ satisfy

$$|\text{inputs of } h| = |\text{outputs of } h| \text{ for each } h \in H.$$ (7)

Then $L^V$ has the eigenvalue 0.

This holds in particular for graphs, because there, every edge has precisely one input and one output.

**Proof.** When (7) holds, then any constant function satisfies (5). □

**Remark 24.** In fact, some such condition is necessary. More precisely, the fact that $\lambda_1 = 0$ for a hypergraph means that we can give a weight $f : V \to \mathbb{R}$ to the vertices such that, in each hyperedge, inputs and outputs have in total the same weight. We shall now see two examples of hypergraphs with $\lambda_1 > 0$, that is, where $L^V$ does not have 0 as an eigenvalue.

**Lemma 25.** Let $\Gamma$ be the union of a connected graph $\Gamma'$ with a hyperedge $h$ that involves only vertices of $\Gamma'$ and such that $|\text{inputs of } h| \neq |\text{outputs of } h|$. Then $\lambda_1 > 0$.

**Proof.** We know that $f$ satisfies (5) on a connected graph $\Gamma'$ if and only if $f$ is a constant function. But a constant function $f$ can clearly not satisfy (5) for a hyperedge $h$ such that $|\text{inputs of } h| \neq |\text{outputs of } h|$. Therefore, $\lambda_1$ cannot be 0 in this case. □

**Lemma 26.** Let $\Gamma$ be the hypergraph on $N > 2$ vertices $v_1, \ldots, v_N$ with $N$ hyperedges $h_1, \ldots, h_N$ such that, for each $i \in \{1, \ldots, N\}$, $h_i$ has:

- $v_i$ as input, and
- every $v_j$ with $j \neq i$ as output.

Then $\lambda_1 > 0$. 

**Figure 5.** The hypergraph in Example 2.
Proof. Let \( f : V \to \mathbb{R} \) be a function that satisfies (5). Then for every \( i, l \in \{1, \ldots, N\} \),
\[
f(v_i) = \sum_{j \neq i} f(v_j) = f(v_i) + \sum_{j \neq i, l} f(v_j) = f(v_i) + 2 \cdot \sum_{j \neq i, l} f(v_j).
\]
Therefore \( \sum_{j \neq i, l} f(v_j) = 0 \) and \( f(v_i) = f(v_i) \). Since this is true for every \( i, l \in \{1, \ldots, N\} \), \( f \) must be the zero function. This implies that \( \lambda_1 > 0 \). \( \square \)

We conclude this section with some further special cases of hypergraphs with \( \lambda_1 = 0 \).

**Proposition 27.** If \( \Gamma \) is one of the following hypergraphs, then \( \lambda_1 = 0 \):

1. \( \Gamma \) has at least two vertices \( v_1, v_2 \) such that, for every \( (i, j) \in \{(1, 2), (2, 1)\} \) and for every \( h \in H \), if \( v_i \in h \) then:
   - either \( v_i \) is a catalyst for \( h \)
   - or \( v_i \) is only an input (respectively only an output) for \( h \) and \( v_j \) is only an output (respectively only an input) for \( h \);
2. \( \Gamma \) has at least two vertices \( v_1, v_2 \) such that, for every \( (i, j) \in \{(1, 2), (2, 1)\} \) and for every \( h \in H \), if \( v_i \in h \) then:
   - either \( v_i \) is a catalyst for \( h \)
   - or \( v_i \) is only an input (respectively only an output) for \( h \) and \( v_j \) is also only an input (respectively only an output) for \( h \);
3. \( \Gamma \) is given by the union of a hypergraph \( \Gamma' \) with \( \chi_1 = 0 \) together with a hyperedge \( h \) such that there exists at least one \( v \in h \setminus \Gamma' \);
4. \( \Gamma \) is given by the union of a hypergraph \( \Gamma' \) with \( \chi_1 = 0 \) together with a hyperedge \( h \) that involves only vertices of \( \Gamma' \) and has only catalysts.

**Proof.** Let’s consider the different cases of the proposition:

1. Assume that \( \Gamma \) has two vertices \( v_1, v_2 \) such that, for every
   \[
   (i, j) \in \{(1, 2), (2, 1)\}
   \]
   and for every \( h \in H \), if \( v_i \in h \) then:
   - either \( v_i \) is a catalyst for \( h \)
   - or \( v_i \) is only an input (respectively only an output) for \( h \) and \( v_j \) is only an output (respectively only an input) for \( h \).

   Let \( f : V \to \mathbb{R} \) defined as \( f(v_1) := f(v_2) := 1 \), \( f(v) := 0 \) otherwise. Then \( f \) satisfies (5).

2. Assume that \( \Gamma \) has two vertices \( v_1, v_2 \) such that, for every
   \[
   (i, j) \in \{(1, 2), (2, 1)\}
   \]
   and for every \( h \in H \), if \( v_i \in h \) then:
   - either \( v_i \) is a catalyst for \( h \)
   - or \( v_i \) is only an input (respectively only an output) for \( h \) and \( v_j \) is also only an input (respectively only an output) for \( h \).

   Let \( f : V \to \mathbb{R} \) defined as \( f(v_1) := 1 \), \( f(v_2) := -1 \), \( f(v) := 0 \) otherwise. Then \( f \) satisfies (5).

3. Assume that \( \Gamma \) is given by the union of a hypergraph \( \Gamma' \) with \( \chi_1 = 0 \) together with a hyperedge \( h \) which involves at least one vertex that is not in \( \Gamma' \). Since
If \( \lambda_1' = 0 \), there exists a function \( f' \) for \( \Gamma' \) that satisfies (3). If there is a vertex in \( h \setminus \Gamma' \) which is a catalyst, we can apply Lemma [16]. If \( h \) involves at least one vertex \( v \notin \Gamma' \) which is not a catalyst, let

\[
f(i) := f'(i)
\]

for every \( i \in \Gamma' \);

\[
f(j) := 0
\]

for every vertex \( j \in h \setminus \Gamma', j \neq v \);

\[
f(v) := \sum_{h^j \in \Gamma', h^j \text{ output of } h} f'(h^j) - \sum_{h^i \in \Gamma', h^i \text{ input of } h} f'(h^i)
\]

if \( v \) is an input and not an output;

\[
f(v) := \sum_{h^i \in \Gamma', h^i \text{ input of } h} f'(h^i) - \sum_{h^j \in \Gamma', h^j \text{ output of } h} f'(h^j)
\]

if \( v \) is an output and not an input.

Then \( f \) satisfies (3).

(4) Assume that \( \Gamma \) is given by the union of a hypergraph \( \Gamma' \) with \( \lambda_1' = 0 \) together with a hyperedge \( h \) which involves only vertices of \( \Gamma' \) and which has only catalysts. Since \( \lambda_1' = 0 \), there exists a function \( f' \) for \( \Gamma' \) that satisfies (5). Such \( f' \) satisfies (3) also for \( \Gamma \).

□

Corollary 28. The function \( f : V \to \mathbb{R} \) such that \( f(v_1) = f(v_2) = 1 \) and \( f(v) = 0 \) otherwise is an eigenfunction for the eigenvalue 0 if and only if \( v_1 \) and \( v_2 \) satisfy the condition in Point 1 of Prop. [27].

Proof. We have already proved the if in the first point of Prop. [27]. The other implication follows easily from the fact that \( f \) has to satisfy (3) and that it has non-zero values only \( v_1 \) and \( v_2 \). □

Corollary 29. The function \( f : V \to \mathbb{R} \) such that \( f(v_1) = 1 \), \( f(v_2) = -1 \) and \( f(v) = 0 \) otherwise is an eigenfunction for the eigenvalue 0 if and only if \( v_1 \) and \( v_2 \) satisfy the condition in Point 2 of Prop. [27].

6. Applications of the Min-max Principle

In this section, we will apply the following theorem in order to get more insight about the spectra of \( L^V \) and \( L^H \).

Theorem 30 (Courant-Fischer-Weyl min-max principle). Let \( V \) be an \( N \)-dimensional vector space with a positive definite scalar product \((.,.)\). Let \( V_k \) be the family of all \( k \)-dimensional subspaces of \( V \). Let \( A : V \to V \) be a self adjoint linear operator. Then the eigenvalues \( \lambda_1 \leq \ldots \leq \lambda_N \) of \( A \) can be obtained by

\[
\lambda_k = \min_{V_k \in \mathcal{V}_k} \max_{g(\neq 0) \in V_k} \frac{(Ag, g)}{(g, g)} = \max_{V_{N-k+1} \in \mathcal{V}_{N-k+1}} \min_{g(\neq 0) \in V_{N-k+1}} \frac{(Ag, g)}{(g, g)}.
\]
The vectors $g_k$ realizing such a min-max or max-min then are corresponding eigenvectors, and the min-max spaces $V_k$ are spanned by the eigenvectors for the eigenvalues $\lambda_1, \ldots, \lambda_k$, and analogously, the max-min spaces $V_{N-k+1}$ are spanned by the eigenvectors for the eigenvalues $\lambda_k, \ldots, \lambda_N$. Thus, we also have

$$\lambda_k = \min_{g \in V, (g,g_j)=0 \text{ for } j=1,...,k-1} \frac{(Ag,g)}{(g,g)} = \max_{g \in V, (g,g_l)=0 \text{ for } l=k+1,...,N} \frac{(Ag,g)}{(g,g)}.$$  \hfill (8)

In particular,

$$\lambda_1 = \min_{g \in V} \frac{(Ag,g)}{(g,g)}, \quad \lambda_N = \max_{g \in V} \frac{(Ag,g)}{(g,g)}.$$  

**Definition.** $\frac{(Ag,g)}{(g,g)}$ is called the Rayleigh quotient of $g$.

**Remark 31.** Without loss of generality, we may assume $(g,g) = 1$ in (8).

6.1. **Largest eigenvalue.** Since $LV$ and $LH$ are self-adjoint operators, we can apply the Courant-Fischer-Weyl min-max Principle and find, in particular, two alternative ways of computing $\lambda_N$:

(1)

$$\lambda_N = \max_f \frac{(\delta f, \delta f)_H}{(f,f)_V} = \max_f \frac{\sum_{h \in H} \delta f(h)^2}{\sum_{i \in V} \deg i \cdot f(i)^2} = \max_f \frac{\sum_{i \in V} \deg i \cdot f(i)^2 = 1} \sum_{h \in H} \delta f(h)^2 \sum_{h \in H} f(h) \left( \sum_{h \text{ input of } h} f(h) - \sum_{h \text{ output of } h} f(h) \right)^2 \sum_{h \in H} \gamma(h)^2.$$

and

(2)

$$\lambda_N = \max_\gamma \frac{(\delta^* \gamma, \delta^* \gamma)_H}{(\gamma, \gamma)_H} = \max_\gamma \frac{\sum_{i \in V} \deg i \cdot \delta^* \gamma(i)^2}{\sum_{h \in H} \gamma(h)^2} = \max_\gamma \frac{\sum_{i \in V} \deg i \cdot \delta^* \gamma(i)^2}{\sum_{h \in H} \gamma(h)^2 = 1} \sum_{i \in V} \frac{1}{\deg i} \left( \sum_{\text{input } i} \gamma(h) - \sum_{\text{output } i} \gamma(h) \right)^2.$$

**Example 3.** Consider a hypergraph with only one hyperedge $h$ that involves $N$ vertices: $k$ inputs and $m$ outputs, with $N \leq k + m \leq 2N$, so that there are $k + m - N$ catalysts.
Then
\[
\lambda_N = \max_{\gamma} \sum_{i \in V} \left( \sum_{h \text{ input}} \gamma(h) - \sum_{h \text{ output}} \gamma(h) \right)^2
\]
\[
= |\text{inputs that are not outputs}| + |\text{outputs that are not inputs}|
\]
\[
= |\text{inputs}| + |\text{outputs}| - 2 \cdot |\text{catalysts}|
\]
\[
= k + m - 2k - 2m + 2N
\]
\[
= 2N - k - m.
\]
In particular, this is the only eigenvalue of $L^H$. Observe that $\lambda_N$ is equal to 0 if and only if $2N = k + m$, i.e. if and only if all vertices are catalysts, while $\lambda_N$ achieves the largest value $N$ exactly when $k + m = N$, i.e. when there are no catalysts.

**Remark 32.** The previous example implies that $\lambda_N$ can not be bounded from above by a quantity that does not depend on the number of vertices $N$ (while, for graphs, we always have $\lambda_N \leq 2$). One should also compare this with Prop. 18.

### 6.1.1. Bipartite hypergraphs

We know that the following theorem holds for graphs:

**Theorem 33.** Let $\Gamma$ be a graph. Then $\lambda_N \leq 2$ and the equality holds if and only if $\Gamma$ is bipartite.

**Recall 34.** Recall that a graph is bipartite if one can decompose the vertex set as a disjoint union $V = V_1 \sqcup V_2$ such that every edge has one of its endpoints in $V_1$ and the other in $V_2$.

We will now generalize the notion of bipartite graph and extend it to hypergraphs, then we will generalize Theorem 33.

**Definition.** We say that a hypergraph $\Gamma$ is bipartite if one can decompose the vertex set as a disjoint union $V = V_1 \sqcup V_2$ such that, for every hyperedge $h$ of $\Gamma$, either $h$ has all its inputs in $V_1$ and all its outputs in $V_2$, or vice versa.

![Figure 6. A bipartite hypergraph with $V_1 = \{v_1, v_2, v_3\}$ and $V_3 = \{v_4, v_5, v_6\}$.](image)

**Remark 35.** It is clear from the definition that:
- If a hypergraph is bipartite it does not contain catalysts;
- The definition of bipartite hypergraph applied to graphs gives exactly the definition of bipartite graph that we already know.
Lemma 36. Let $\Gamma$ be a bipartite hypergraph. Then

$$\lambda_N \geq \frac{\sum_{h \in H} |h|^2}{\sum_{h \in H} |h|}.$$  

Proof. Since $\Gamma$ is bipartite, we can write

$$\lambda_N = \max_{f: \sum_{i \in V} \deg i \cdot f(i)^2 = 1} \sum_{h \in H} \left( \sum_{\text{input of } h} f(h_i) - \sum_{\text{output of } h} f(h_j) \right)^2$$

$$= \max_{f: \sum_{i \in V} \deg i \cdot f(i)^2 = 1} \sum_{h \in H} \left( \sum_{h_i \in h, f(h_i) > 0} f(h_i) - \sum_{h_j \in h, f(h_j) < 0} f(h_j) \right)^2.$$  

Now, let

$$f(i) := \frac{1}{\sqrt{\sum_i \deg i}}$$

for every $i \in V_1$ and

$$f(j) := -\frac{1}{\sqrt{\sum_i \deg i}}$$

for every $j \in V_2$. Then

$$\sum_{i \in V} \deg i \cdot f(i)^2 = 1$$

and

$$\sum_{h \in H} \left( \sum_{h_i \in h, f(h_i) > 0} f(h_i) - \sum_{h_j \in h, f(h_j) < 0} f(h_j) \right)^2$$

$$= \sum_{h \in H} \left( \frac{1}{\sqrt{\sum_i \deg i}} \cdot |h| \right)^2$$

$$= \frac{\sum_{h \in H} |h|^2}{\sum_{h \in H} |h|},$$

where the last equality is due to the fact that $\sum_i \deg i = \sum_{h \in H} |h|$.

Therefore

$$\lambda_N \geq \frac{\sum_{h \in H} |h|^2}{\sum_{h \in H} |h|}.$$

Remark 37. The quantity

$$h' := \frac{\sum_{h \in H} |h|^2}{\sum_{h \in H} |h|}$$

appearing in Lemma 36 has the biggest value $N$ exactly when every $h \in H$ has the biggest possible cardinality, which is $N$.

Remark 38. Recall from Example 3 that, for bipartite hypergraphs with only one hyperedge, $\lambda_N = N$, therefore in this case $\lambda_N = h'$. 

Remark 39.

Let’s apply Lemma 36 to a bipartite graph $\Gamma$. Since $|e| = 2$ for every edge, the lemma tells us that
\[
\lambda_N \geq \frac{\sum_{e \in E} 4}{\sum_{e \in E} 2} = \frac{|E| \cdot 4}{|E| \cdot 2} = 2
\]
and, as we know, this is actually an equality.

Proposition 40. Let $\Gamma$ be a hypergraph with largest eigenvalue $\lambda_N$. Then
\[
\lambda_N \leq \lambda'_N
\]
where $\lambda'_N$ is the largest eigenvalue of a bipartite hypergraph that has the same number of hyperedges as $\Gamma$ and also the same number of inputs and the same number of outputs in each hyperedge (catalysts are not included).
The equality holds if and only if $\Gamma$ is bipartite.

Proof. Let $\Gamma$ be a hypergraph with largest eigenvalue $\lambda_N$. Then
\[
\lambda_N = \max_{f: \sum_i \deg_i f(i)^2 = 1} \sum_{h \in H} \left( \sum_{h_i \text{ input of } h} f(h_i) - \sum_{h_j \text{ output of } h} f(h_j) \right)^2
\]
\[
\leq \max_{f: \sum_i \deg_i f(i)^2 = 1} \sum_{h \in H} \left( \sum_{h_i \in h: f(h_i) > 0} f(h_i) - \sum_{h_j \in h: f(h_j) < 0} f(h_j) \right)^2,
\]
where the last inequality is due to the fact that, for every $f$,
\[
\left| \sum_{h_i \text{ input of } h} f(h_i) - \sum_{h_j \text{ output of } h} f(h_j) \right| \leq \left| \sum_{h_i \in h: f(h_i) > 0} f(h_i) - \sum_{h_j \in h: f(h_j) < 0} f(h_j) \right|.
\]
It is clear that the inequality for $\lambda_N$ becomes an inequality if and only if, for every $h \in H$, we can let such $f$ be positive in the inputs and negative in the outputs, or vice versa. And this is possible if and only if the hypergraph is bipartite. Therefore
\[
\lambda_N \leq \lambda'_N
\]
and the equality holds if and only if $\Gamma$ is bipartite. \qed

Remark 41. We can put together Lemma 36 and Prop. 40 and say that the largest eigenvalue of $\lambda_N$ is achieved by bipartite hypergraphs and that, in this case, $\lambda_N \geq h'$. In particular, $\lambda_N \geq h'$ becomes an equality for both bipartite graphs and bipartite hypergraphs with only one hyperedge. But it is in general not an equality, as proved by the next example.

Example 4. Let $\Gamma = (\{v_1, v_2, v_3, v_4\}, \{h_1, h_2\})$ be the bipartite hypergraph such that:
1. $h_1$ has $v_1$ and $v_2$ as inputs and $v_3$ as output;
2. $h_2$ has $v_1$ as input and $v_4$ as output.
In this case,
\[ h' = \frac{\sum_{h \in H} |h|^2}{\sum_{h \in H} |h|} = \frac{13}{5} = 2.6. \]

Now, let’s compute \( \lambda_N \) using the Min-max Principle applied to \( L^H \). For simplicity, let \( \gamma(h_1) := x \) and let \( \gamma(h_2) := y \). Then

\[
\lambda_N = \max_{\gamma : \sum_{h \in H} \gamma(h)^2 = 1} \left( \sum_{h \in V} \deg i \left( \sum_{\text{input}} \gamma(h) - \sum_{\text{output}} \gamma(h) \right)^2 \right)
\]

\[
= \max_{x,y \in \mathbb{R} : x^2 + y^2 = 1} \left( x^2 + x^2 + \frac{(x+y)^2}{2} + y^2 \right)
\]

\[
= \max_{x,y \in \mathbb{R} : x^2 + y^2 = 1} \left( \frac{3}{2} + x^2 + xy \right),
\]

where in the last equality we have used the fact that \( x^2 + y^2 = 1 \). Now, let \( x := \cos(t) \) and let \( y := \sin(t) \). Then

\[
\lambda_N = \max_{0 \leq t \leq 2\pi} \left( \frac{3}{2} + \cos^2(t) + \cos(t) \cdot \sin(t) \right).
\]

Now,
\[
\frac{d}{dt} \left( \frac{3}{2} + \cos^2(t) + \cos(t) \cdot \sin(t) \right) = \cos(2t) - \sin(2t),
\]

which has value 0 for \( t = \frac{\pi}{8} \) and \( t = \frac{5\pi}{8} \). In particular, for \( t = \frac{5\pi}{8} \) we get that

\[
\lambda_1^H = \frac{3}{2} + \cos^2 \left( \frac{5\pi}{8} \right) + \cos \left( \frac{5\pi}{8} \right) \cdot \sin \left( \frac{5\pi}{8} \right)
\]

\[
= 2 - \frac{1}{\sqrt{2}}
\]

\[
\approx 1.29.
\]
For $t = \frac{7}{8}$ we get that
\[
\lambda_N = \frac{3}{2} + \cos^2\left(\frac{\pi}{8}\right) + \cos\left(\frac{\pi}{8}\right) \cdot \sin\left(\frac{\pi}{8}\right)
= 2 + \frac{1}{\sqrt{2}}
\approx 2.71.
\]

In particular, $\lambda_N > h'$. This proves that the $\geq$ of Lemma 36 is, in general, not an equality.

Let’s end this section by proving that there is another family of bipartite hypergraphs with $\lambda_N = h'$.

**Lemma 42.** Let $\Gamma$ be a bipartite graph on $N$ nodes such that $|h| = N$ for every $h \in H$. Then
\[
\lambda_N = h' = N.
\]

**Proof.** Let’s first observe that, in this case,
\[
h' = \frac{\sum_h |h|^2}{\sum_h |h|} = \frac{|H| \cdot N^2}{|H|} = N.
\]

Now observe that, for any bipartite hypergraph,
\[
\lambda_N = \max_f \frac{\sum_{h \in H} \left( \sum_{i \in h_{\text{input of } h}} f(h_i) - \sum_{j \in h_{\text{output of } h}} f(h_j) \right)^2}{\sum_{i \in V} \deg i \cdot f(i)^2}
= \max_f \frac{\sum_{h \in H} \left( \sum_{i \in h : f(h_i) > 0} f(h_i) - \sum_{j \in h : f(h_j) < 0} f(h_j) \right)^2}{\sum_{i \in V} \deg i \cdot f(i)^2}
= \max_{f > 0} \frac{\sum_{h \in H} \left( \sum_{i \in h} f(i) \right)^2}{\sum_{i \in V} \deg i \cdot f(i)^2}.
\]

In our particular case, since $\{i \in h\} = \{i \in V\}$ for every $h$ and since $\deg_i = |H|$ for every $i$, we have that
\[
\lambda_N = \max_{f > 0} \frac{|H| \cdot \left( \sum_{i \in V} f(i) \right)^2}{|H| \cdot \sum_{i \in V} f(i)^2}
= \max_{f > 0} \frac{\left( \sum_{i \in V} f(i) \right)^2}{\sum_{i \in V} f(i)^2}
= \lambda_N'.
\]
where $\lambda_N'$ is the largest eigenvalue of a bipartite hypergraph on $N$ nodes with only one hyperedge. As we have seen in Example 3, $\lambda_N' = N$, therefore $\lambda_N = h' = N$.

7. **isospectral hypergraphs**

We already know that two graphs cannot always be distinguished by their spectra, but the spectrum reveals some important properties. *Is the graph bipartite? How many connected components does it have? How many cycles? Is it complete?* – these are all questions that can be answered using the spectrum of the Laplace operator for graphs, so even if it does not distinguish the details of graphs, it does partition them into important families. We expect something similar to happen for hypergraphs.

For instance, the spectrum of $L^V$ of all complete bipartite graphs with the same number of vertices is the same. (The multiplicity of the eigenvalue 0 of $L^H$, however, distinguishes between them.) For hypergraphs, a new phenomenon arises.

**Lemma 43.** The spectrum of $L^H$ doesn’t change if we reverse the role of a vertex in all the hyperedges in which it is contained, i.e. if we let it become an input where it is an output and we let it become an output where it is an input.

**Proof.** By the Min-max Principle, the spectrum of $L^H$ is given by the min-max of the Rayleigh quotient, which is now

$$\sum_{i \in V} \frac{1}{\deg i} \left( \sum_{h_{\text{in}}:i \text{ input}} \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}:i \text{ output}} \gamma(h_{\text{out}}) \right)^2 \sum_{h \in H} \gamma(h)^2.$$

Now, since for each $i \in V$ we have

$$\left( \sum_{h_{\text{in}}:i \text{ input}} \gamma(h_{\text{in}}) - \sum_{h_{\text{out}}:i \text{ output}} \gamma(h_{\text{out}}) \right)^2 = \left( \sum_{h_{\text{out}}:i \text{ output}} \gamma(h_{\text{out}}) - \sum_{h_{\text{in}}:i \text{ input}} \gamma(h_{\text{in}}) \right)^2,$$

the Rayleigh quotient and therefore the spectrum of $L^H$ doesn’t change if we reverse the role of a vertex in all the hyperedges in which it is contained. \qed

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