New Bounds on the Clique Number of Graphs Based on Spectral Hypergraph Theory

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Abstract. This work introduces new bounds on the clique number of graphs derived from a result due to Sós and Straus, which generalizes the Motzkin-Straus Theorem to a specific class of hypergraphs. In particular, we generalize and improve the spectral bounds introduced by Wilf in 1967 and 1986 establishing an interesting link between the clique number and the emerging spectral hypergraph theory field. In order to compute the bounds we face the problem of extracting the leading H-eigenpair of supersymmetric tensors, which is still uncovered in the literature. To this end, we provide two approaches to serve the purpose. Finally, we present some preliminary experimental results.

1 Introduction

Let $G = (V, E)$ be a (undirected) graph, where $V = \{1, \ldots, n\}$ is the vertex set and $E \subseteq \binom{V}{2}$ is the edge set, with $\binom{V}{k}$ denoting the set of all k-element subsets of V. A *clique* of G is a subset of mutually adjacent vertices in V. A clique is called *maximal* if it is not contained in any other clique. A clique is called *maximum* if it has maximum cardinality. The maximum size of a clique in G is called the *clique number* of G and is denoted by $\omega(G)$.

The problem of finding the clique number of a graph is one of the most famous NP-complete problems, and turns out to be even intractable to approximate [1]. An interesting field of research consists in trying to bound the clique number of a graph. In the literature we find several bounds on the clique number, but, in this paper, our attention will be on bounds that employ spectral graph theory, since our new bounds are obtained using spectral hypergraph theory. However, it is worth noting that there is another very promising class of bounds, which will not be covered in this work, based on semidefinite programming [2,3].

In 1967, Wilf [4] used for the first time spectral graph theory for computing bounds on the clique number of graphs. His result was inspired by a theorem due to Motzkin and Straus [5], which establishes a link between the problem of finding the clique number of a graph G and the problem of optimizing the Lagrangian of G over the simplex Δ, where the Lagrangian of a graph $G = (V, E)$ is the function $L_G : \mathbb{R}^n \to \mathbb{R}$ defined as

$$L_G(\mathbf{x}) = \sum_{\{i,j\} \in E} x_i x_j \,,$$

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and the *standard simplex* Δ is the set of nonnegative n-dimensional real vectors that sum up to 1, i.e., $\Delta = \{\mathbf{x} \in \mathbb{R}^n_+ : \sum_{i=1}^n x_i = 1\}$.

Theorem 1 (Motzkin-Straus). *Let G be a graph with clique number $\omega(G)$, and $\mathbf{x}^*$ a maximizer of L_G over Δ then*

$$L_G(\mathbf{x}^*) = \frac{1}{2}\left[1 - \frac{1}{\omega(G)}\right].$$

Assuming S a maximum clique of G, Motzkin and Straus additionally proved that the *characteristic vector* $\mathbf{x}^S$ of S defined as

$$\mathbf{x}^S_i = \begin{cases} \frac{1}{|S|} & i \in S \\ 0 & i \notin S \end{cases}$$

is a global maximizer of L_G over Δ.

Before introducing the bounds of Wilf, we introduce some notions from spectral graph theory, namely, a discipline that studies the properties of graphs in relationship to the eigenvalues and eigenvectors of its adjacency matrix or Laplacian matrix. The *spectral radius* $\rho(G)$ of a graph G is the largest eigenvalue of the adjacency matrix of G. An eigenvector of unit length having $\rho(G)$ as eigenvalue is called *Perron eigenvector* of G. The Perron eigenvector is always nonnegative and it may not be unique unless the multiplicity of the largest eigenvalue is exactly 1. By definition, the spectral radius ρ and an associated Perron eigenvector $\mathbf{x}_P$ of a graph G satisfy the eigenvalue equation

$$A_G\mathbf{x}_P = \rho\mathbf{x}_P\,,$$

which can be equivalently expressed in terms of the graph Lagrangian L_G as

$$\nabla L_G(\mathbf{x}_P) = \rho\mathbf{x}_P\,,$$

where ∇ is the standard gradient operator. Since G is undirected and hence, A_G is symmetric, a useful variational characterization of ρ and $\mathbf{x}_P$ is given by the following constrained program,

$$\rho = \max_{\mathbf{x}\in S_2} \mathbf{x}^T A_G \mathbf{x} = 2 \max_{\mathbf{x}\in S_2} L_G(\mathbf{x})\,, \tag{1}$$

where $S_k = \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_k^k = 1\}$. Note that the eigenvectors of A_G are the critical points of this maximization problem. A further alternative characterization of the spectral radius and Perron eigenvector, that will be useful in the sequel, consists in maximizing the *Rayleigh quotient*, i.e.,

$$\rho = \max_{\mathbf{x}\in\mathbb{R}^n} \frac{\mathbf{x}^T A_G \mathbf{x}}{\mathbf{x}^T\mathbf{x}} = 2 \max_{\mathbf{x}\in\mathbb{R}^n} \frac{L_G(\mathbf{x})}{\mathbf{x}^T\mathbf{x}}\,. \tag{2}$$

Note that every eigenvector associated to ρ is a maximizer in (2), whereas in (1) only a Perron eigenvector is a global maximizer.

As mentioned, in 1967 Wilf [4] obtained a spectral upper bound to the clique number exploiting both the Motzkin-Straus theorem and (2).

Theorem 2. *Let G be an undirected graph with clique number $\omega(G)$ and spectral radius ρ. Then*

$$\omega(G) \leq \rho + 1\,.$$

Proof. Let $\mathbf{x}_\omega$ be the characteristic vector of a maximum clique of G, then $\mathbf{x}_\omega^T \mathbf{x}_\omega = 1/\omega(G)$ and by the Motzkin-Straus theorem $\mathbf{x}_\omega^T A_G \mathbf{x}_\omega = 1 - 1/\omega(G)$. By (2) we have that

$$\frac{\mathbf{x}_\omega^T A_G \mathbf{x}_\omega}{\mathbf{x}_\omega^T \mathbf{x}_\omega} = \frac{1 - \frac{1}{\omega(G)}}{\frac{1}{\omega(G)}} = \omega(G) - 1 \leq \rho\,,$$

from which the property derives.

Later in 1986, Wilf [6] introduced also a lower bound again combining the Motzkin-Straus theorem and (2), but this time also the Perron eigenvector is involved in the result.

Theorem 3. *Let G be an undirected graph with spectral radius ρ and Perron eigenvector $\mathbf{x}_P$. Then*

$$\omega(G) \geq \frac{s_P^2}{s_P^2 - \rho}\,,$$

where $s_P = \|\mathbf{x}_P\|_1$.

Proof. Let $\mathbf{y} = \mathbf{x}_P / s_P$. Clearly $\mathbf{y} \in \Delta$. By the Motzkin-Straus theorem we have that

$$\mathbf{y}^T A_G \mathbf{y} = \frac{\mathbf{x}_P^T A_G \mathbf{x}_P}{s_P^2} = \frac{\rho}{s_P^2} \leq 1 - \frac{1}{\omega(G)}\,,$$

from which the result derives.

For a review of further spectral bounds we refer to [7]. We also refer to [8] for bounds that employ spectral graph theory based on the Laplacian of the graph.

In this paper, we introduce new classes of upper and lower bounds on the clique number of graphs, generalizing the Wilf's ones. More precisely, we achieve our goal combining a reformulation of a theorem due to Sós and Straus in terms of hypregraphs, and the emerging spectral hypergraph theory field. Further, we tackle the computational aspects of our new bounds and, finally, we present some preliminary experiments on random graphs.

2 A Reformulation of the Sós and Straus Theorem

In this section, we provide a reformulation of a generalization of the Motzkin-Straus theorem due to Sós and Straus [9], by explicitly establishing a connection to hypergraph theory, which will form the basis of our new bounds.To this end we start introducing hypergraphs.

A *k-uniform hypergraph*, or simply a *k-graph*, is a pair $G = (V, E)$, where $V = \{1, \ldots, n\}$ is a finite set of *vertices* and $E \subseteq \binom{V}{k}$ is a set of k-subsets of V, each of which is called a *hyperedge*. 2-graphs are typically called *graphs*. The *complement* of a k-graph G is given by $\bar{G} = (V, \bar{E})$ where $\bar{E} = \binom{V}{k} \setminus E$. A subset of vertices $C \subseteq V$ is called a *hyperclique* if $\binom{C}{k} \subseteq E$. To improve readability, in the sequel we will drop the prefix "hyper" when referring to edges and cliques of a k-graph. A clique is said to be *maximal* if it is not contained in any other clique, while it is called *maximum* if it has maximum cardinality. The *clique number* of a k-graph G, denoted by $\omega(G)$, is defined as the cardinality of a maximum clique. The *Lagrangian* of a k-graph G with n vertices is the following homogeneous multilinear polynomial in n variables:

$$L_G(\mathbf{x}) = \sum_{e \in E} \prod_{i \in e} x_i \ . \tag{3}$$

Given an undirected graph G and a positive integer k not exceeding the clique number $\omega(G)$, we can build a hypergraph H, that we call the *k-clique* $(k+1)$*-graph* of G having k-cliques of G as vertices and $(k+1)$-cliques of G as edges. Note that each $(k+1)$-clique of G has exactly $(k+1)$ different k-cliques as subsets. By shrinking each k-clique of G into a vertex in H, each $(k+1)$-clique of G can be transformed into an edge of H containing exactly $k+1$ vertices. Before addressing a more formal definition we provide an example. Figure 1 shows an undirected graph G on the left and the related 3-clique 4-graph H on the right. Each vertex in H is associated to the 3-clique of G reported in red over it. For each 4-clique C in G, there exists an edge in H containing the vertices associated to 3-subsets of C. For example, the clique $\{1, 2, 3, 4\}$ in G is associated to the edge $\{1, 2, 3, 4\}$ in H, and the vertices $1, 2, 3, 4$ of H are associated to the 3-cliques $\{1, 2, 3\}, \{2, 3, 4\}, \{1, 2, 4\}, \{1, 3, 4\}$ of G respectively. It is worth noting that the construction of the k-clique $(k+1)$-graph of a graph G depends on how we label the vertices in H, i.e., an enumeration of the set of k-cliques of G. Therefore, we provide also a more formal definition. Let G be an undirected graph G, $\mathcal{C}_k(G)$ the set of all k-cliques of G, and let Φ_k^G be the set of possible enumerations of $\mathcal{C}_k(G)$, i.e., one-to-one mappings from $\{1, \ldots, |\mathcal{C}_k(G)|\}$ to $\mathcal{C}_k(G)$. The *k-clique* $(k+1)$*-graph* of G with respect to $\phi \in \Phi_k^G$ is the $(k+1)$-graph $H = (V, E)$, where $V = \{1, \ldots, |\mathcal{C}_k(G)|\}$, and $E = \left\{ e \in \binom{V}{k+1} : \bigcup_{i \in e} \phi(i) \in \mathcal{C}_{k+1}(G) \right\}$.

Let G be an undirected graph with clique number ω and let H be its k-clique $(k+1)$-graph with respect to an enumeration $\phi \in \Phi_k^G$. Sós and Straus provided a characterization of the clique number of a graph G in terms of the maximum of the Lagrangian of H over Δ_k, where

$$\Delta_k = \{\mathbf{x} \in \mathbb{R}_+^n : \|\mathbf{x}\|_k^k = 1\} \, ,$$

leading to the following result.

Theorem 4. *Let G be an undirected graph with clique number ω and let H be its k-clique $(k+1)$-graph with respect to any $\phi \in \Phi_k^G$. The Lagrangian of H attains its maximum over Δ_k at $\binom{\omega}{k+1} / \binom{\omega}{k}^{(k+1)/k}$.*

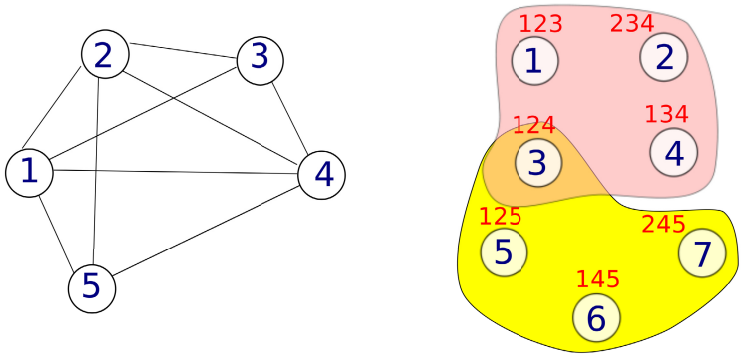


Fig. 1. Example of a 3-clique 4-graph (right) of an undirected graph (left)

Moreover, a subset of vertices C is a maximum clique of G if and only if the vector $\mathbf{x} \in \Delta_k$ defined as

$$x_i = \begin{cases} \binom{\omega}{k}^{-1/k} & \text{if } \phi(i) \subset C \\ 0 & \text{otherwise}, \end{cases} \tag{4}$$

is a global maximizer of L_H over Δ_k.

Proof. See [9].

If we consider $k = 1$, then Theorem 4 is the Motzkin-Straus theorem.

As the Motzkin-Straus theorem inspired new bounds on the clique number of graphs, Theorem 4 prompted our new bounds by combining it with spectral hypergraph theory.

3 Spectral Hypergraph Theory

Opposed to spectral graph theory, which has a long history, spectral hypergraph theory is a novel field roughed out by Drineas and Lim [10]. Clearly, spectral hypergraph theory includes spectral graph theory as a special case, but this generality introduces some ambiguities. For example, the adjacency matrix for graphs becomes an adjacency tensor for hypergraphs, for which there are several possible notions of eigenvalues and eigenvectors that can be taken into account for studying the properties of the hypergraph [10,11].

For our purposes, we will employ spectral hypergraph theory in a transversal way, as we will use the spectral properties of the adjacency tensor of the k-clique $(k+1)$-graph of a graph G to study properties of G. This means that we do not want to study the properties of the hypergraph by itself, but those of the graph it is constructed from.

A real kth-order n-dimensional *tensor* A consists of n^k real entries, $A_{i_1,\ldots,i_k} \in \mathbb{R}$, where $i_j = 1,\ldots,n$ for $j = 1,\ldots,k$. The tensor A is called *supersymmetric* if its entries are invariant under any permutation of their indices.

Given a n-dimensional vector $\mathbf{x}$, we denote by X^k the kth-order n-dimensional rank-one tensor with entries $x_{i_1}\cdots x_{i_k}$, and by $\mathbf{x}^k$ the n-dimensional vector with entries x_i^k. Finally, if A is a kth-order n-dimensional tensor and $\mathbf{x} \in \mathbb{R}^n$, then AX^k is the real scalar given by

$$AX^k = \sum_{i_1,\ldots,i_k=1}^{n} a_{i_1,\ldots,i_k} x_{i_1}\cdots x_{i_k}\,,$$

and AX^{k-1} is the n-dimensional vector, whose ith entry is given by

$$\left(AX^{k-1}\right)_i = \sum_{i_2,\ldots,i_k=1}^{n} a_{i,i_2,\ldots,i_k} x_{i_2}\cdots x_{i_k}\,.$$

The *adjacency tensor* of a k-graph $H = (V,E)$ with n vertices is the kth-order n-dimensional tensor A_H, whose entry indexed by $(i_1,\ldots,i_k)$ is 1, if $\{i_1,\ldots,i_k\} \in E$, 0 otherwise. Clearly, A_H is supersymmetric.

As mentioned before, there are several notions of eigenvalue/eigenvector for tensors, but only one fits our needs. In 2005, Lim [10] and Qi [11] independently introduced the same notion of eigenvalue, which they called ℓ^p-eigenvalue and H-eigenvalue respectively. Given a kth-order n-dimensional tensor A, a real value λ and a vector $\mathbf{x} \in \mathbb{R}^n$ are an *eigenvalue* and an *eigenvector* of A respectively, if they satisfy the following equation

$$AX^{k-1} = \lambda \mathbf{x}^{k-1}\,. \tag{5}$$

The eigenvalues derived from (5) reflect many properties of the eigenvalues of matrices [11]. In fact, Drineas and Lim [10] successfully generalize some results from spectral graph theory to hypergraphs employing this notion of eigenvalue.

The *spectral radius* $\rho(H)$ of a k-graph H is the largest eigenvalue of the adjacency tensor of H. An eigenvector of unit k-norm having $\rho(H)$ as eigenvalue is called *Perron eigenvector* of H. As it happens for graphs, the Perron eigenvector may not be unique unless the multiplicity of the largest eigenvalue is 1. In the sequel, a *leading eigenpair* of a k-graph will be a pair comoposed by the spectral radius and a Perron eigenvector.

The eigenvalue equation for hypergraphs can be rewritten in terms of the Lagrangian as follows,

$$(k-1)!\nabla L_H(\mathbf{x}) = \lambda \mathbf{x}^{k-1}\,, \tag{6}$$

and there is a variational characterization of the spectral radius and a related Perron eigenvector of H derived from the following constrained program,

$$\rho(H) = \max_{\mathbf{x}\in S_k} A_H X^k = k! \max_{\mathbf{x}\in S_k} L_H(\mathbf{x})\,, \tag{7}$$

which has the Perron eigenvector as maximizer. Note that all the eigenvalues of A_H are the critical points of (7).

By a generalization of the Perron-Frobenius theory to nonnegative tensors [12], it turns out that a Perron eigenvector of H is always nonnegative. This allows us to add a non negativity constraint to (7) without affecting the solution, i.e. we can replace S_k with Δ_k, yielding

$$\rho(H) = \max_{\mathbf{x}\in\Delta_k} A_H X^k = k! \max_{\mathbf{x}\in\Delta_k} L_H(\mathbf{x})\,, \tag{8}$$

Alternatively, a further characterization is obtained by maximizing a generalization of the Rayleigh quotient, namely

$$\rho(H) = \max_{\mathbf{x}\in\mathbb{R}^n} \frac{A_H X^k}{\|\mathbf{x}\|_k^k} = k! \max_{\mathbf{x}\in\mathbb{R}^n} \frac{L_H(\mathbf{x})}{\|\mathbf{x}\|_k^k}\,, \tag{9}$$

where all eigenvectors associated to ρ are global maximizers.

4 New Bounds Based on Spectral Hypergraph Theory

In this section, we provide new classes of upper and lower bounds that generalize those introduced by Wilf [4,6] for graphs. The basic idea is to combine the Sós and Straus theorem with spectral hypergraph theory.

Theorem 5 (New Upper Bound). *Let G be an undirected graph with clique number $\omega(G)$ and H a k-clique $(k+1)$-graph of G with spectral radius $\rho(H)$. Then*

$$\omega(G) \le \frac{\rho(H)}{k!} + k\,.$$

Proof. Let C be a maximum clique of G and $\mathbf{x}_\omega$ the vector defined as (4). We write ω for $\omega(G)$. By (9) and Theorem 4,

$$(k+1)!\frac{L_H(\mathbf{x}_\omega)}{\|\mathbf{x}_\omega\|_{k+1}^{k+1}} = (k+1)!\frac{\binom{\omega}{k+1}\binom{\omega}{k}^{-(k+1)/k}}{\binom{\omega}{k}^{-1/k}} = \\ = (k+1)!\frac{\binom{\omega}{k+1}}{\binom{\omega}{k}} = k!(\omega-k) \le \rho(H)\,,$$

from which the result derives.

Note that for each choice of $0 < k \le \omega(G)$, we have a new bound. In particular, by taking $k = 1$, we have $H = G$ obtaining Wilf's upper bound (Theorem 2). Note also that if we take $k = \omega(G)$, then H is a hypergraph consisting only of vertices (one per maximum clique of G) and no edges. In this case, the bound gives trivially $\omega(G)$.

Theorem 6 (New Lower Bound). *Let G be an undirected graph with clique number $\omega(G)$ and H a k-clique $(k+1)$-graph of G with spectral radius $\rho(H)$ and Perron eigenvector $\mathbf{x}_P$. Then*

$$\omega(G) \geq \psi_k^{-1}\left(\frac{\rho(H)}{k!\|\mathbf{x}_P\|_k^{k+1}}\right) \qquad \psi_k(x) = (x-k)\binom{x}{k}^{-\frac{1}{k}}.$$

Before proving this result we prove that $\psi_k(x)$ is monotonically increasing for $x \geq k$.

Lemma 1. *$\psi_k(x)$ is monotonically increasing for $x \geq k$.*

Proof. For all $x \geq k$,

$$\psi_k'(x) = \binom{x}{k}^{-\frac{1}{k}}\left[1 - \frac{1}{k}\sum_{j=0}^{k-1}\frac{x-k}{x-j}\right],$$

which is positive for $x \geq k$. Hence, $\psi_k(x)$ is monotonically increasing for $x \geq k$.

Proof (Theorem 6). Let $\mathbf{y} = \mathbf{x}_P/\|\mathbf{x}_P\|_k$. Clearly, $\mathbf{y} \in \Delta_k$. We write ω for $\omega(G)$. By (7) and Theorem 4,

$$L_H(\mathbf{y}) = \frac{L_H(\mathbf{x}_P)}{\|\mathbf{x}_P\|_k^{k+1}} = \frac{\rho(H)}{(k+1)!\|\mathbf{x}_P\|_k^{k+1}} \leq$$
$$\leq \binom{\omega}{k+1}\Big/\binom{\omega}{k}^{\frac{k+1}{k}} = \frac{\omega-k}{k+1}\binom{\omega}{k}^{-\frac{1}{k}} = \frac{\psi_k(\omega)}{k+1}.$$

Since by Lemma 1, $\psi_k(x)$ is monotonically increasing and $\omega \geq k$, the result follows.

Theorem 6 introduces a class of lower bounds, one for each choice of $0 < k \leq \omega(G)$. Again, by taking $k = 1$, we obtain the Wilf's lower bound (Theorem 3). Moreover, by taking $k = \omega(G)$, the bound trivially returns $\omega(G)$.

By Lemma 1, $\psi_k(x)$ is invertible for $x \geq k$, however, it is difficult, and maybe not possible, to find a general analytical inverse. It is straightforward to find the inverse for $k = 1, 2$ analytically. In fact we obtain,

$$\psi_1^{-1}(y) = \frac{1}{1-y} \qquad \psi_2^{-1}(y) = \frac{8 - y^2 + y\sqrt{y^2+16}}{2(2-y^2)},$$

but, in general, the best way for computing the inverse is numerically through some kind of section search, like the dicotomic search.

The computational complexity of our bounds is dominated by the construction of the k-clique $(k+1)$-graph. This, in fact, increases exponentially with the parameter k, that can be chosen between 1 and the clique number. This fact

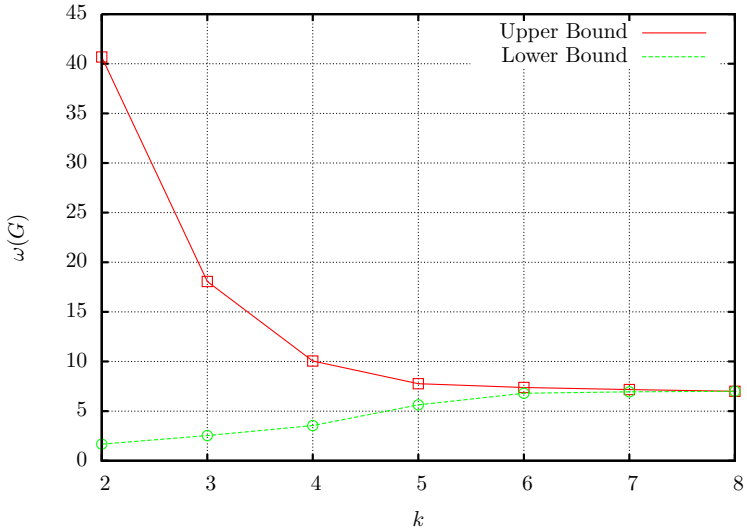


Fig. 2. Application of our classes of upper and lower bounds to a random graph $[n = 100; \delta = 0.4]$. We conjecture that, by increasing k, the upper bound is monotonically non increasing and our lower bound is monotonically non decreasing.

intuitively suggests that also the tightness of the bound should increase with k, as we require more computational effort for its calculation. Although we have no prove by now, we conjecture that, by increasing k, our new upper and lower bounds are monotonically non increasing and non decreasing respectively. This fact is also supported by all the experiments that we conducted. As an example of this monotonicity, Figure 2 plots our bounds on the clique number of a random graph $[n = 100; \delta = 0.4]$ at varying values of k.

Although our new bounds are intuitively simple, their computation is not obvious, in particular we refer to the extraction of the Perron vector and spectral radius of a k-graph. Therefore the next section is devoted to the computational aspects of our new spectral bounds.

5 Computing the Bounds

As mentioned, the computational complexity of our approach is dominated by the construction of the k-clique $(k + 1)$-graph, which increases exponentially with k. Despite the complexity, the construction of the hypergraph is a fairly simple task. Indeed, the computation of the bounds involves more interesting problems such as the computation of the spectral radius and Perron eigenvector of a k-graph.

We have seen that a useful characterization of the leading eigenpair of a k-graph derives from the maximization in (7), whose critical points are those

satisfying Equation (6). From this, we can derive a primal method for the optimization of (7) consisting in the following update rules:

$$\mathbf{y}^{(t+1)} = \nabla L_H\left(\mathbf{x}^{(t)}\right)^{\frac{1}{k-1}} \quad \mathbf{x}^{(t+1)} = \frac{\mathbf{y}^{(t+1)}}{\|\mathbf{y}^{(t+1)}\|_k} \quad \rho^{(t+1)} = k! L_H\left(\mathbf{x}^{(t+1)}\right), \quad (10)$$

where $\mathbf{x}^{(0)} \in \Delta_k$ and $\mathbf{x}^{(0)} > \mathbf{0}$ and where we remind the notation $\mathbf{x}^k$, for representing a vector with entries x_i^k. Note that the fixed points of this iterative process satisfy equation (6). Hence, the solution at convergence is a nonnegative eigenvector with the related eigenvalue. This approach can be straightforwardly extended to the extraction of the leading eigenpair of any nonnegative tensor, yielding a Generalization to nonnegative tensors of the known Power Method, which is a method for extracting the leading eigenpair of matrices (case $k = 2$). Thereby, we call GPM the method governed by (10). Although, we achieved this method autonomously, it was already proposed in [12,13], in a more general setting, for optimizing nonnegative generalized polynomials under ℓ^p constraints. There is still no prove of convergence for this approach, except for the case $k = 2$, however, supported by the experimental results, we conjecture that it always converges.

Another interesting method (called GBE) that we developed for extracting the leading eigenpair of k-graphs, and more in general of nonnegative tensors, derives from a Generalization of the Baum-Eagon Theorem [14] to nonnegative generalized homogeneous polynomials.

A *generalized polynomial* is a function $P : \mathbb{R}^n \to \mathbb{R}$ of the form:

$$P(\mathbf{x}) = \sum_{\boldsymbol{\alpha}} c_{\boldsymbol{\alpha}} \prod_{i=1}^{n} x_i^{\alpha_i}$$

where $\boldsymbol{\alpha}$ ranges over a finite set of $\mathbb{R}_+^n$. By definition, the degree of P is $h = \max_{\boldsymbol{\alpha}} h_{\boldsymbol{\alpha}}$, where $h_{\boldsymbol{\alpha}} = \sum_i \alpha_i$. If $h_{\boldsymbol{\alpha}} = h$ for all $\boldsymbol{\alpha}$, we call P a *homogeneous* generalized polynomial of degree h. We say that P is *nonnegative* if $c_{\boldsymbol{\alpha}} \geq 0$ for all $\boldsymbol{\alpha}$.

Theorem 7. *Let $P(\mathbf{x})$ be a nonnegative generalized homogeneous polynomial in the variables x_i, and let $\mathbf{x} \in \Delta$. Define the mapping $\mathbf{z} = \mathcal{M}(\mathbf{x})$ as follows:*

$$z_i = x_i \partial_i P(\mathbf{x}) \Big/ \sum_{j=1}^{n} x_j \partial_j P(\mathbf{x}), \quad i = 1, \ldots, n.$$

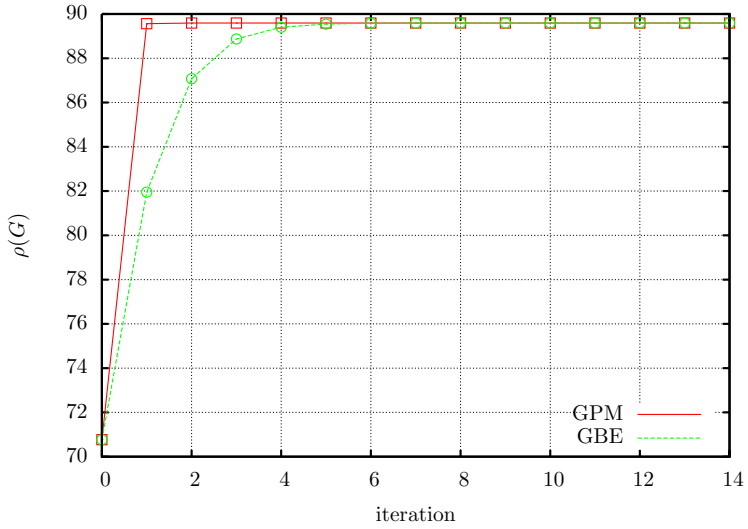
Then $P(\mathcal{M}(\mathbf{x})) > P(\mathbf{x})$, unless $\mathcal{M}(\mathbf{x}) = \mathbf{x}$. In other words, $\mathcal{M}$ is a growth transformation for the polynomial P.

Proof. See [15].

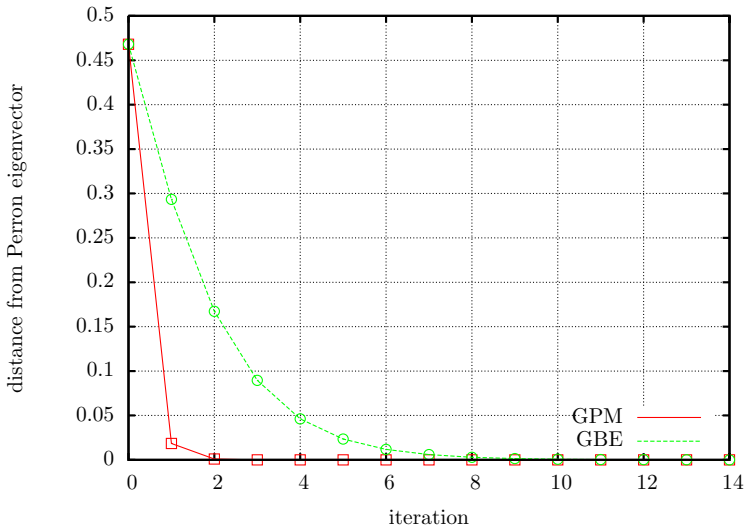
In order to apply this result, we cast (8) into an equivalent optimization problem, which satisfies the conditions of Theorem 7, obtaining in this way a new

optimization approach. We define the diffeomorphism $\varphi_k : \mathbb{R}^n_+ \to \mathbb{R}^n_+$ by putting $\varphi_k(\mathbf{x}) = \mathbf{x}^{\frac{1}{k}}$. By setting $\mathbf{y} = \varphi_k^{-1}(\mathbf{x})$, we have that

$$\rho(H) = k! \max_{\mathbf{x} \in \Delta_k} L_H(\mathbf{x}) = k! \max_{\mathbf{y} \in \Delta} (L_H \circ \varphi_k)(\mathbf{y}) \ . \tag{11}$$



(a) Test on spectral radius



(b) Test on Perron eigenvector

Fig. 3. Comparison of GPM and GBE on the extraction of (a) the spectral radius and (b) the Perron eigenvector, of a random graph $[n = 100; \delta = 0.9]$

Here $L_H \circ \varphi_k$ is a generalized nonnegative homogeneous polynomial of degree 1 and by applying Theorem 7, we obtain the following update rules:

$$x_i^{(t+1)} = \left[\frac{x_i^{(t)} \partial_i L_H(\mathbf{x}^{(t)})}{\sum_j x_j^{(t)} \partial_j L_H(\mathbf{x}^{(t)})} \right]^{\frac{1}{k}} \qquad \rho^{(t+1)} = k! L_H \left(\mathbf{x}^{(t+1)} \right), \tag{12}$$

where $\mathbf{x}^{(0)} \in \Delta_k$ and $\mathbf{x}^{(0)} > \mathbf{0}$.

It is worth noting that this idea can be extended to compute the leading eigenpair of any nonnegative tensor. In particular, it provides us with a new approach for computing the leading eigenpair of nonnegative matrices, which is different to the standard known techniques.

Differently from GPM, it is not obvious that the fixed points of GBE are only those satisfying equation (7). Experimentally, this was always the case and we aim at proving this result in future developments of this work.

The nonnegative eigenvector of A_H that we obtain from one of the two proposed approaches, may unfortunately not be a Perron eigenvector, because our methods are basically local optimizers. However, we can easily overcome this problem, yielding a global solution. In fact, by employing a generalization of the Perron-Frobenious theory to generalized polynomials [12], it can be shown [15] that every nonnegative eigenvector has the positive components indexed by the vertices of a connected component of the hypergraph (or more than one in some special cases). This suggests a simple approach to achieve a global solution. We first find the connected components of the hypergraph H. Then we apply GPE or GBE on each component and keep the best solution. In this way we are able to extract the spectral radius and a Perron eigenvector of H.

There is experimental evidence that GPM converges faster than GBE. As an example, we calculated through GPM and GBE the spectral radius and a Perron eigenvector of a random graph with $n = 100$ vertices and density $\delta = 0.9$. In Figure 3(a) we plot the evolution of $2L_G(\mathbf{x}^{(t)})$, which has $\rho(G)$ as limit point. It is evident that GPM with just one step reaches a good approximation of the spectral radius, while GBE manifests a smoother curve. Figure 3(b) focuses on the approximation of the Perron eigenvector and plots the distance between $\mathbf{x}^{(t)}$ and the Perron eigenvector, i.e., $\|\mathbf{x}^{(t)} - \mathbf{x}_P\|$. Here, we see that GPM needs 2 steps for a good approximation of the Perron eigenvector, whereas GBE needs about 9 steps. Therefore for the experiments we will use GPM for computing the leading eigenpair of the k-cliques $(k+1)$-graphs.

6 Experiments

In this section, we evaluate only the performances of our 3th-order upper and lower bounds, which have a complexity $O(\gamma n^3)$, where γ is the number of iterations of GPM and can be assumed constant. Clearly, provided that our conjecture holds, by increasing k, we can only improve the results obtained with $k = 3$, but also the computational effort will increase.

Table 1. Experiments on random graphs. The columns n, δ and ω are the order, density and average clique number of the random graphs, respectively. The results, expecting the last row, are expressed in terms of relative error.

Random graphs			Upper bound errors			Lower bound errors		
n	δ	ω	Wilf	Amin	Order 3	Wilf	Budin.	Order 3
100	0.05	3.12	1.25	10.58	**0.13**	0.648	0.641	**0.119**
	0.10	3.96	1.99	9.26	**0.15**	0.714	0.707	**0.363**
	0.20	5.00	3.33	7.84	**0.59**	0.745	0.738	**0.512**
	0.30	6.13	4.17	6.52	**0.91**	0.761	0.753	**0.616**
	0.40	7.51	4.49	5.24	**1.34**	0.775	0.765	**0.664**
	0.50	9.11	4.58	4.19	**2.00**	0.779	0.768	**0.685**
	0.60	11.51	4.28	3.16	**2.29**	0.782	0.769	**0.711**
	0.70	14.55	3.85	**2.33**	2.52	0.772	0.756	**0.714**
	0.80	19.99	3.03	**1.45**	2.30	0.754	0.734	**0.708**
	0.90	30.69	1.94	**0.61**	1.70	0.695	0.662	**0.646**
	0.95	43.50	1.19	**0.16**	1.08	0.606	**0.562**	0.587
200	0.10	4.17	4.25	19.97	**0.29**	0.728	0.725	**0.463**
	0.50	11.00	8.19	7.71	**3.62**	0.817	0.811	**0.746**
	0.90	?	180.10	**99.08**	164.19	9.646	10.330	**10.851**

We compare our 3rd-order bounds against other state-of-the-art spectral bounds, which were the best performing approaches reviewed in the work of Budinich [7]. For the upper bound, we compare against Wilf's upper bound [4] (which is our bound with $k = 2$), that will never perform better than our 3rd order bound according to our conjecture, and we compare also against the Amin's bound [16]. For the lower bound, we compare against Wilf's lower bound [6] and Budinich's lower bound [7].

Table 1 reports the obtained results. The columns n, δ and ω are the order, density and average clique number of the random graphs, respectively. The results, expecting the last row, are expressed in terms of relative error, i.e. if $\bar{\omega}$ is the value of the bound then the relative error for the upper and lower bounds are $(\bar{\omega} - \omega)/\omega$ and $(\omega - \bar{\omega})/\omega$, respectively. In the last row, where the average clique number could not be computed, we reported the absolute value of the bounds. It is clear that, as expected, our 3th-order bounds strictly improve the Wilf's one. It is also evident that our lower bound outperforms the competitors, excepting very dense graphs ($\delta = 0.95$), whereas our upper bound outperforms Amin's one on low and medium densities ($\delta \leq 0.6$). The decrease of the performances with respect to Amin and Budinich on high densities is due to the fact that the advantage of knowing the triangles of the graph becomes irrelevant when approaching the complete graph. However, also the relative error slowly approaches zero, since for the complete graph all our bounds are exact.

7 Conclusions

In this work, we introduce a new class of bounds on the clique number of graphs by employing, for the first time to our knowledge, spectral hypergraph theory.

The bounds are derived from a result due to Sós and Straus and generalize the classic spectral upper and lower bounds of Wilf.

The computation of our new bounds introduces the side problem of establishing the spectral radius and a Perron eigenvector of a k-graph, which is still uncovered. To this end, we introduce two dynamics that serve our purposes. The first is a generalization of the known Power Method, while the second derives from our generalization of the Baum-Eagon result to generalized polynomials.

Finally, we test our 3th-order bounds comparing them against state-of-the-art spectral approaches on random graphs. The results show the superiority of our bounds on all graphs excepting the dense ones, where anyway we achieve low relative errors.

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