On Graph Uncertainty Principle and Eigenvector Delocalization

***Abstract*—Uncertainty principles present an important theoretical tool in signal processing, as they provide limits on the time-frequency concentration of a signal. In many real-world applications the signal domain has a complicated irregular structure that can be described by a graph. In this paper, we focus on the global uncertainty principle on graphs and propose new connections between the uncertainty bound for graph signals and graph eigenvectors delocalization. We also derive uncertainty bounds for random d-regular graphs and provide numerically efficient upper and lower approximations for the uncertainty bound on an arbitrary graph.**

I. Introduction and background

In many modern signal processing applications, such as social networks and coauthorship studies, brain imaging, epidemiology, and traffic networks, data has complicated relational structures. Such data can be naturally represented by signals defined on a (possibly weighted) graph, edges of which represent the relations between data points. The emerging field of *signal processing on graphs* merges algebraic graph theory and computational harmonic analysis with the purpose to build tools for processing and analyzing such signals on graphs. Even though the theory of signal processing on graphs is very young, it develops rapidly [Shu+13; Ort+18].

One of the cornerstone results in the classical time-frequency signal processing and harmonic analysis is the *uncertainty principle*. It limits the degree to which a function can be simultaneously localized in time and frequency. Generalizations of such a principle to the graph setting, that is, establishing a trade-off between the spread of a signal in the vertex domain and in the frequency domain, is an important problem in signal processing on graphs. In particular, graph uncertainty bounds are used to study sampling properties on graphs [Per+18; TBD16] and to analyse space-frequency and wavelet decompositions [AL13; SRV13].

In this paper, we study how the uncertainty principle for signals on graphs is linked with the structure of the graph eigenvectors. More specifically, we (a) show that more refined localization results for the graph eigenvectors lead to better estimates of the uncertainty bound, and (b) propose the ways to quantify uncertainty bounds for particular graphs numerically.

To formally define uncertainty bound on graphs, we start with reviewing some relevant definitions. Let $G = (V, E)$ be a connected graph with the set of vertices V, set of edges E, and let A be its adjacency matrix. For simplicity, let us assume that G is undirected and thus A is symmetric. All the discussion (with slight modifications) can be extended to the case of directed graphs.

Let $\Lambda = \{\lambda_j\}_{j=1}^{|V|}$ be the multiset of eigenvalues of the graph adjacency matrix A. Since A is real and symmetric, there exists an orthonormal basis $\Phi = \{\varphi_\ell\}_{\ell\in\Lambda}$ consisting of eigenvectors φ_ℓ of A. By slight abuse of notation, we identify a basis Φ with the matrix Φ that has basis vectors as its columns. In some other works, Φ is chosen to be an orthonormal eigenbasis of the (normalized) graph Laplacian, see for instance [SS19].

Consider a signal $f : V \to \mathbb{C}$ defined on the vertex set V of the graph G. Treating f as a vector in $\mathbb{C}^{|V|}$, one can use representation of f in the orthonormal eigenbasis Φ to define the graph Fourier transform (see, for example, [Shu+13]).

Definition I.1. We define the *graph Fourier transform* $\hat{f}$ of a signal $f : V \to \mathbb{C}$ as

$$\hat{f}(\ell) = \langle f, \varphi_\ell \rangle = \sum_{v\in V} f(v)\varphi_\ell^*(n),\ \ell \in \Lambda.$$

Since Φ is an orthonormal basis, the *inverse Fourier transform* is given by $f(v) = \sum_{\ell\in\Lambda} \hat{f}(\ell)\varphi_\ell(v),\ v \in V$.

There are multiple ways to define uncertainty principle. In the continuous setup when $f \in L^2(\mathbb{R})$, the *Heisenberg uncertainty principle* is defined using the notion of time and frequency spread [FS97]. This notion has been generalized to the graph setup by Agaskar and Lu [AL11; AL13]. In this paper we are going to focus on a different, *global version of the uncertainty principle* that generalizes the one proposed by Donoho and Stark [DS89]. They showed that a signal and its Fourier transform cannot be simultaneously sparse. More precisely, $\|f\|_0\|\hat{f}\|_0 \geq N$, where $\|f\|_0$ denotes the support size of f. A similar bound for graph signals, however, does not hold for all graphs G and not only on the graph structure, but also on the choice of Φ. For example, it is easy to check that for a full graph K_N, one can choose an eigenbasis Φ so that there exists a signal f with $\|f\|_0\|\hat{f}\|_0 = 2$, while for a different eigenbasis $\tilde{\Phi}$, $\|f\|_0\|\hat{f}\|_0 \geq N$ for all f. At the same time, for a cycle graph C_N, any choice of Φ leads to the uncertainty bound $\|f\|_0\|\hat{f}\|_0 \geq N/2$.

Motivated by the graph- and basis-dependency of graph uncertainty bounds, we are motivated by the following two questions in the current work:

1) For which G do we have that $\|f\|_0\|\hat{f}\|_0 \geq h(|V|)$ for any choice of Φ and some function h, s.t. $h(n) \to_{n\to\infty} \infty$?
2) For given G and Φ, how can one estimate the bound for $\|f\|_0\|\hat{f}\|_0$?

The first question has been partially answered in [TV17]. In particular, the following connection between the uncertainty

bound on a graph G and the properties of Φ has been shown.

Theorem I.2 ([TV17]). *Let $G = (V, E)$ be a weighted graph and Φ be an orthonormal basis of the eigenvectors of its adjacency matrix A. Then, for any graph signal $f : V \to \mathbb{C}$,*

$$\|f\|_0 \|\hat{f}\|_0 \geq \|\Phi\|_\infty^{-2}$$

where $\|\Phi\|_\infty = \max_{\ell \in \Lambda,\ i \in V} |\varphi_\ell(i)|$.

This bound is only tight if Φ consists of the elements with the same absolute values, although in some models it gives correct asymptotic dependence on the size of the graph. In Section II, we establish a better link between graph uncertainty bound and the distribution of the eigenvectors coefficients. In Section III, we discuss the uncertainty bound on a well-studied model of random d-regular graphs. In Section IV, we propose efficiently computable lower and upper bounds for the global uncertainty bound on an arbitrary graph and test their performance on different random graph models.

II. Global graph uncertainty and eigenvector delocalization

First, we give a generalization of Theorem I.2 that quantifies global uncertainty via the subblocks of the eigenvector matrix.

Theorem II.1. *Let $G = (V, E)$ be a weighted graph and Φ be an orthonormal eigenbasis of its adjacency matrix A. Then, for any graph signal $f : V \to \mathbb{C}$,*

$$\|f\|_0 \|\hat{f}\|_0 \geq \min_{S \subset \Lambda, K \subset V} \left\{ |K||S| \colon \|\Phi_{K \times S}\|_F \geq 1 \right\},$$

where $\Phi_{K \times S}$ is the restriction of the matrix Φ to the rows indexed by K and columns indexed by S, and $\|\cdot\|_F$ denotes the Frobenious norm.

Proof. Without loss of generality, assume that the signal f is normalized so that $\|f\|_2 = 1$. Then, since Φ forms an orthonormal basis $\|\hat{f}\|_2 = \|f\|_2 = 1$. Denote $K = \operatorname{supp}(f)$, $S = \operatorname{supp}(\hat{f})$. Using Cauchy-Schwartz inequality, we obtain

$$\begin{aligned}\|\hat{f}\|_2^2 &= \sum_{\ell \in S} \left| \sum_{i \in K} f(i) \varphi_\ell^*(i) \right|^2 \leq \sum_{\ell \in S} \left[\sum_{i \in K} |f(i)|^2 \sum_{i \in K} |\varphi_\ell^*(i)|^2 \right] \\ &= \sum_{\ell \in S, i \in K} |\varphi_\ell(i)|^2 = \|\Phi_{K \times S}\|_F^2.\end{aligned}$$

That is, $\|\Phi_{\operatorname{supp}(\hat{f}) \times \operatorname{supp}(f)}\|_F \geq 1$ for any graph signal $f : V \to \mathbb{C}$. The claim follows. □

Note that both Theorem I.2 and Theorem II.1 link the global uncertainly bound on a graph to the distribution of the coefficients of its eigenvectors. Informally, good uncertainty bound requires the absolute values of the eigenvector entries to be of similar order. This property is also known as the *delocalization* of (graph) eigenvectors.

The eigenvector delocalization is one of the central topics in modern random matrix theory. It is possible to show that certain classes of random matrices exhibit eigenvector universality: their eigenvector matrices are distributed similarly to those of the Gaussian Orthogonal Ensemble (i.e., like a sample of Haar measure on the orthogonal group $O(n)$), see, e.g., [AGZ10; OVW16]. Various measures of distribution similarity were studied; among the most popular in non-asymptotic context are the following

- *Supremum delocalization* (studied in a variety of papers staring from [ESY09]) gives a bound of the largest coordinates $\|\varphi_\ell\|_\infty$ of the eigenvectors in Φ;
- *No-gap delocalization* (first introduced in [RV16]) ensures that any sufficiently large set of coordinates of an eigenvector carries a non-negligible portion of its Euclidean norm.

These two types of delocalization measure complementary properties of the distribution of an eigenvector coefficients, as one of them rules out peaks while the other one rules out gaps. It is easy to see that neither of these two properties implies the other. For example, a presence of a few large outlier entries in the matrix fails supremum delocalization but a no-gap localization can still hold.

While Theorem I.2 gives a direct link between supremum delocalization and the uncertainty bound (see Corollary III.2 below), Theorem II.1 can be used to deduce the uncertainty bound from other types of delocalization.

Corollary II.2. *(Uncertainty from no-gap delocalization) Let $G = (V, E)$ be a graph. Suppose for any $\varepsilon \in (0, 1)$ and any unit eigenvector φ of G, $\|(\varphi)_K\|^2 \geq \varepsilon$ implies $|K| \geq g(\varepsilon, |V|)$ for any $K \subset V$. Then, for any signal f defined on G,*

$$\|f\|_0 \|\hat{f}\|_0 \geq \min_{S \subset \Lambda} g\left(\frac{1}{|S|}, |V|\right) |S|.$$

Proof. Suppose that for $K \subset V$ and $S \subset \Lambda$, $\|\Phi_{K \times S}\|_F^2 \geq 1$. Then there exists $\ell \in S$, such that $\|(\varphi_\ell)_K\| \geq \frac{1}{|S|}$. Choosing $\varepsilon = \frac{1}{|S|}$, we deduce that $|K| \geq g\left(\frac{1}{|S|}, |V|\right)$, and the claim of the corollary follows from Theorem II.1. □

Note that no-gap delocalization results are restricted to individual columns in the eigenvector matrix and do not address how many eigenvectors can be localized on the same index set. New non-asymptotic delocalization results addressing submatrices of the eigenvector matrix would lead to the tighter bounds for the uncertainty. An example of a delocalization of this type is *box delocalization* we define in the following corollary.

Corollary II.3. *(Uncertainty from box delocalization) Suppose that the eigenvectors of a graph $G = (V, E)$ have box delocalization. That is, for $\varepsilon \in (0, 1)$, $k \in \{1, \ldots |V|\}$, and any coordinate subset $K \subset V$ with $|K| \leq k$, we have $\left|\left\{\ell \in \Lambda \colon \|(\varphi_\ell)_K\|_2^2 \geq \varepsilon\right\}\right| \leq L(k, \varepsilon)$, for some function L. Then, for any signal f defined on G,*

$$\|f\|_0 \|\hat{f}\|_0 \geq \max_{k, \varepsilon} \left\{ kL(k, \varepsilon) \colon \varepsilon L(k, \varepsilon) < 1 \right\}.$$

Proof. For each $k \in \{1, \ldots |V|\}$, let us fix $\varepsilon \in (0, 1)$, such that $\varepsilon L(k, \varepsilon) < 1$. Then, for each fixed $K \subset V$ with $|K| = k$, the box delocalization assumption implies that for any $S \subset \Lambda$ with $|S| \leq L(k, \varepsilon)$, we have $\|\Phi_{K \times S}\|_F^2 < 1$. Thus, $\|\Phi_{K \times S}\|_F^2 \geq 1$

implies that $|S||K| \geq kL(k,\varepsilon)$, and the claim follows from Theorem II.1. $\square$

III. Uncertainty bounds for d-regular graphs

In this section, we focus on (random) d-regular graphs and show how some known (de)localization results can be applied to obtain uncertainty bounds. Let $G_{n,d}$ denote a random d-regular graph chosen uniformly from all d-regular graphs on $|V| = n$ vertices. Delocalization properties of d-regular graphs were extensively studied over the recent years, e.g., [BKY17; Lit+19; HY21]. The following supremum delocalization result was established in [HY21].

Theorem III.1 ([HY21])**.** *For each $d > 3$, there exist a constant $\omega_d \in \mathbb{N}$ and $c \in (0,1)$, such that any eigenvector φ of the adjacency matrix of $G_{n,d}$ satisfies*

$$\|\varphi\|_\infty \leq \frac{\log^{\Omega(1)} n}{\sqrt{n}} \|\varphi\|_2$$

with probability at least $1 - O\left(n^{-(1-c)\omega_d}\right)$.

Using this result and Theorem I.2, we obtain the following uncertainty principle for d-regular graphs.

Corollary III.2. *For each $d > 3$, the following uncertainty bound holds for any signal f on $G_{n,d}$ with high probability*

$$\|f\|_0 \|\hat{f}\|_0 \geq \frac{n}{\log^{\Omega(1)} n}.$$

Remark III.3. We note that Theorem III.1 indicates that, with high probability, random d-regular graphs enjoy strong supremum delocalization, in the sense that, up to a poly-log factor, the maximal coordinate of the eigenvectors has the same absolute value as its average coordinate. For this reason, more refined Theorem II.1 used together with different type delocalization results would not allow to significantly improve the n-dependence in the obtained uncertainty bound for $G_{n,d}$.

The following theorem shows that, while most of the d-regular graphs have nice delocalization properties, there exist infinite families of such graphs with localized eigenvectors.

Theorem III.4 ([AGS21])**.** *For every $d = p+1$, with p prime, and parameter $\alpha \in (0, 1/6)$, there are infinitely many integers n, such that there exists a $(d+1)$-regular graph G_n on n vertices with the following property. There are sets $T_n \subset V_n$ with $|T_n| = O(n^\alpha)$ and $S_n \subset \Lambda_n$ with $|S_n| = \lfloor \alpha \log_d(n) \rfloor$, such that $\operatorname{supp}(\varphi_\ell) \subset T_n$ for all $\ell \in S_n$.*

By selecting $\alpha = \frac{1}{\log_d(n)}$, so that $|S_n| = 1$, we obtain that for any signal f defined on a graph G_n described in Theorem III.4,

$$\|f\|_0 \|\hat{f}\|_0 \gtrsim n^{\frac{1}{\log_d(n)}} = d,$$

and this bound is attained when $f = \varphi_\ell$ with $\ell \in S_n$. We note that the proof of Theorem III.4 produces eigenvectors φ_ℓ, $\ell \in S_n$ with the additional property of partial localization on the same index set. That is, these graphs also do not enjoy box delocalization.

IV. Numerical bounds on graph uncertainty

Another approach to quantifying uncertainty via Theorem II.1 is by directly estimating the quantity

$$B = \min_{S \subset \Lambda,\ K \subset V} \{|K||S| \colon \|\Phi_{K \times S}\|_F \geq 1\} \tag{1}$$

for a given (non-random) graph. It is a binary non-convex quadratic optimizartion problem that can be formulated as

$$\begin{aligned} &\min_{x_i, y_j} \sum_{i,j=1}^n x_i y_j \\ &\text{s.t.} \sum_{i,j=1}^n \Phi_{ij}^2 x_i y_j \geq 1, \\ &\quad x_i, y_j \in \{0,1\} \text{ for } i,j = 1,\dots,n \end{aligned} \tag{2}$$

Note that the problem above reduces to n^2 decision problems of the existence of a submatrix of given size with Frobenious norm at least 1. In turn, this is equivalent to the Weighted Edge Biclique Decision Problem on complete bipartite graphs that is known to be NP-complete [PSJ20].

Below, we employ some simple relaxation techniques to investigate empirically the dependence of B on the graph size n for different graph models. These bounds serve two goals: (a) they form hypotheses about the dependence $B(n)$; and (b) they provide a way to obtain estimates for uncertainty bound for a given graph.

- **Supremum lower bound.** Clearly, the supremum-based lower bound of Theorem I.2 is very weak – it would be tight only if all the entries of the matrix have the same absolute values. We still include it for comparison: for any $K \times S \subset V \times \Lambda$, we have $\|\Phi_{K\times S}\|_F^2 \leq |K||S| \|\Phi\|_\infty^2$. Thus,
$$B \geq \|\Phi\|_\infty^{-2}.$$
- **Greedy lower bound.** Accounting for the sizes of the elements but not their locations, we obtain
$$B \geq \min\left\{ m \colon \sum_{j=1}^m \tilde{\Phi}(j) \geq 1 \right\},$$
where $\tilde{\Phi} \in \mathbb{R}^{n^2}$ consists of the squared elements of Φ in descending order.
- **Linear lower bound.** A standard linear relaxation of a bilinear optimization problem on a bounded domain [McC76] leads to the following problem
$$\begin{aligned} &\min_{U,x,y} \sum_{i,j=1}^n u_{ij} \\ &\text{s.t.} \sum_{i,j=1}^n \Phi_{ij}^2 u_{ij} \geq 1,\ 0 \leq x_i, y_j \leq 1 \\ &\quad \max\{0, x_i + y_j - 1\} \leq u_{ij} \leq \min\{x_i, y_j\} \end{aligned} \tag{3}$$
for the decision variables $U \in \mathbb{R}^{n \times n}$ and $x, y \in \mathbb{R}^n$.
- **Semidefinite lower bound.** Our approach for an SDP relaxation follows [Ans09], after symmetrization of the

problem (2), and leads to the following problem:

$$\begin{aligned}
&\min_{U,x} \sum_{i,j=1}^{2n} J_{ij} u_{ij} \\
&\text{s.t.} \sum_{i,j=1}^{2n} \bar{\Phi}^2_{ij} u_{ij} \geq 1, \\
&\quad u_{ii} - x_i = 0,\ 0 \leq x_i \leq 1 \\
&\quad \max\{0, x_i + x_j - 1\} \leq u_{ij} \leq \min\{x_i, x_j\} \\
&\quad U - xx^T \succcurlyeq 0
\end{aligned} \tag{4}$$

for the decision variables $U \in \mathrm{Sym}(2n \times 2n)$ and $x \in \mathbb{R}^{2n}$. The last constraint is semidefinite by a standard Schur complements representation. The matrices J and $\bar{\Phi}^2$ are symmetrized versions of an all-ones matrix and the matrix Φ^2, respectively.

- **k-width upper bound.** We upper-bound the optimal solution of (2) by a solution of the problem with additional constraint
$$\max\left\{\sum x_i, \sum y_i\right\} \leq k.$$
In other words, we narrow down the set of submatrices in (1) to the submatrices with at most k rows or columns and do an exhaustive search. For each possible subset of k rows (columns), we take as many of the largest partial row-sums as needed to get at least 1 in total. The complexity of this problem is $O(kn^{k+2}\ln(n))$, so it is feasible only for small fixed k. Below, we take $k = 3$ to form an upper bound.

We consider two graph models to test the bounds described above: a $2\lceil\sqrt{n}\rceil$-regular graph on n vertices (Figure 1) and the same regular graph modified by adding high-degree vertices. More precisely, $\lceil 0.5n \rceil$ random edges are added to $\lceil 0.1n \rceil$ randomly selected vertices (Figure 2). The first model satisfies theoretical delocalization results outlined in Section III and we expect linear in n (up to a logarithm) bound for uncertainty. The second model is constructed to disrupt the "like-uniform" structure of the entries in the adjacency eigenvector matrix. We use it as an example where the uncertainty bound could grow sublinearly with the graph size.

Let us briefly discuss how these bounds address two goals mentioned above. Asymptotically, our bounds support the conjecture above, showing linear growth of $B(n)$ with n in Figure 1 and sublinear growth of $B(n)$ in Figure 2 for the non-regular (modified) graph. For the individual uncertainty estimates, we see there is still a considerable gap between the lower and upper bounds (illustrated as a cyan region in Figures 1 and 2), but more sophisticated relaxations give better lower bounds. In particular, a supremum-based lower bound, that is used for known asymptotics (see Section III), is not competitive on larger graphs.

V. Discussion

The study of uncertainty principle is not only useful in graph signal processing applications, but it also stems a variety of interesting mathematical questions in spectral graph theory, optimization, and random matrix theory, and promotes connections between these diverse areas. In particular, the findings of this paper motivate the study of different, more refined, types of eigenvector delocalization that rule out simultaneous concentration of different eigenvectors on the same coordinate subsets (see, for instance, Corollary II.3). Moreover, study of the eigenvector delocalization for new families of (random) graphs with varying combinatorial properties, such as degree distribution and girth (e.g. [Sla12; HY21]), would allow to establish a link between these properties and graph uncertainty.

In practice, an important problem is efficient numerical estimation of the uncertainty bound for a given graph. As discussed in Section IV, semidefinite relaxation comes with significant time requirements (the complexity is polynomial of large degree, as the input size is n^2, see (4)). Thus, for larger graphs, scalable approximation techniques (e.g., [Yur+21]) or dual reformulations could be considered in the future work.

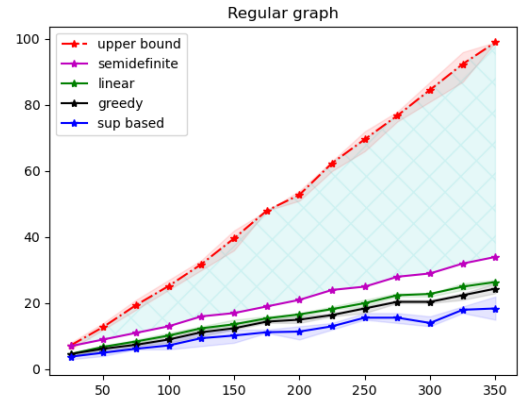

Fig. 1: Upper and lower estimates for the uncertainty bound (1) on $G_{n,2\lceil\sqrt{n}\rceil}$, averaged over 5 runs (semidefinite lower bound from 1 run). True value of B is in the cyan region. All the bounds suggest linear growth of B with n.

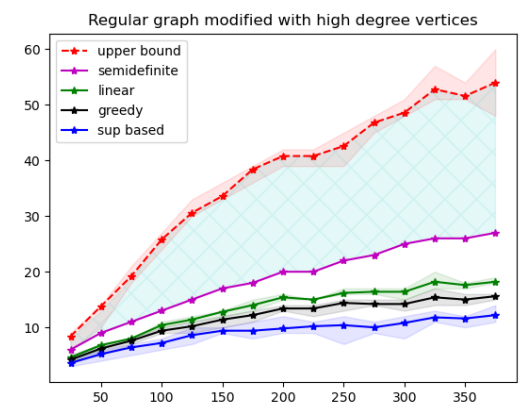

Fig. 2: Upper and lower estimates for the uncertainty bound (1) on $G_{n,2\lceil\sqrt{n}\rceil}$ modified by added high-degree vertices, averaged over 5 runs (semidefinite lower bound from 1 run). True value of B is in the cyan region. The bounds suggest sublinear growth of B with n.

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