Finite Frames and Graph Theoretical Uncertainty Principles

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Norbert Wiener Center for Harmonic Analysis and Applications

Outline

1. Motivation
2. Definitions
3. Results

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Uncertainty Principles

In the context of harmonic analysis, the Heisenberg uncertainty principle (HUP) states that for an L^2 function $f : \mathbb{R} \to \mathbb{C}$:

$$\|f\|^2_{L^2(\mathbb{R})} \leq 4\pi \, \|tf(t)\|_{L^2(\mathbb{R})} \, \|\gamma \hat{f}(\gamma)\|_{L^2(\widehat{\mathbb{R}})}. \tag{1}$$

If $f \in \mathcal{S}(\mathbb{R})$, the space of Schwartz functions, then inequality (1) is equivalent to

$$\|f\|^2_{L^2(\mathbb{R})} \leq \left\|f'(t)\right\|_{L^2(\mathbb{R})} + \left\|\widehat{f'}(\gamma)\right\|^2_{L^2(\widehat{\mathbb{R}})}.$$

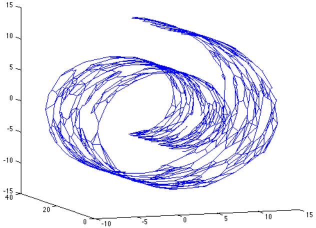
Uncertainty Principles

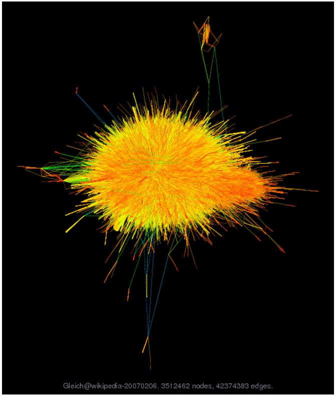
- The study of uncertainty principles is of general interest to analysts.
- In the quantum settings, these principles are of great importance.
- In signal processing, uncertainty principles dictate the trade off between high spectral and high temporal accuracy.

Graph Theory

- Graph theory has a well studied and rich theory associated with pure mathematics.
- Problems grounded in computer science and big data have contributed to recent interest in graph theory in the applied sciences.
- So called "big data" problems are, in many cases, rooted in graph strucures.
- Data fusion of hyperspectral images employs many graph theoretic techniques.

Graphs Visualized





A graph representation of the swiss roll (left) and Gleich's representation of Wikipdedia as of 2007 (right)

Our Goals

- The nascent field of harmonic analysis on graphs looks to further analytic understanding of graphs.
- We look to the recently defined graph Fourier transform, and try to determine which uncertainty principles can be extended into the graph theoretic setting.
- We show the celebrated principle of Donoho and Stark [1], which, due to the loss of the cyclic structure associated with the discrete Fourier transform, no longer holds in the graph setting.[1]

[1] This result is omitted in this talk.

Outline

Graph Defined

- A graph $G = \{V, \mathbf{E} \subseteq V \times V, w\}$ is a set V of vertices, a set $\mathbf{E}$ of edges, and a weight function $w : V \times V \to \mathbb{R}^+$ where $\mathbb{R}^+$ denotes the nonnegative reals.
- We represent $V = \{v_j\}_{j=0}^{N-1}$ and keep the indexing fixed, but arbitrary[2].

[2] For many of our results, changing indexing can have an effect on the values of our results but not the qualitative meanings. We discuss this in our future considerations section.

Weight Function

- For $(v_i, v_j) \in V \times V$ we have that

$$w(v_i, v_j) = \begin{cases} 0 & \text{if } (v_i, v_j) \in \mathbf{E}^c \\ c > 0 & \text{if } (v_i, v_j) \in \mathbf{E}. \end{cases}$$

- We assume that the graph is undirected, such that (v_i, v_j) and (v_j, v_i) are equivalent, and $w(v_i, v_j) = w(v_j, v_i)$.
- We say that a graph is unit weighted if w takes only the values 0 and 1.

Edge Assumptions

- We assume $w(v_i, v_i) = 0$, that is, there are no loops in the graph.
- We assume the graph is simple and connected, i.e., given any two vertices v_i and v_j, there exist at most one edge between them, and there exists a sequence of vertices $\{v_k\}$ for $k = 0, ..., d \leq N - 1$ such that $(v_i, v_0), (v_0, v_1), ..., (v_d, v_j) \in \mathbf{E}$

Adjacency Matrix

The adjacency matrix $A = (A_{ij})$ for G is the symmetric $N \times N$ matrix, where

$$A_{ij} = w(v_i, v_j).$$

Degree Matrix

The degree matrix D is the $N \times N$ diagonal matrix

$$D = diag\left(\sum_{j=0}^{N-1}(A_{0j}), \sum_{j=0}^{N-1}(A_{1j}), \ldots, \sum_{j=0}^{N-1}(A_{(N-1)j})\right)$$

where the i^{th} diagonal entry is the sum of the weights of edges connected to vertex v_i.

Graph Laplacian

- The graph Laplacian L is the symmetric $N \times N$ matrix given by

$$L = D - A.$$

- The normalized graph Laplacian $\mathcal{L}$ is the symmetric $N \times N$ matrix given by

$$\mathcal{L} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} A D^{-1/2}.$$

Incidence and Weight Matrix

- The $|\mathbf{E}| \times N$ incidence matrix $M = (M_{kj})$ with element M_{kj} for edge $\mathbf{e}_k$ and vertex v_j is given by:

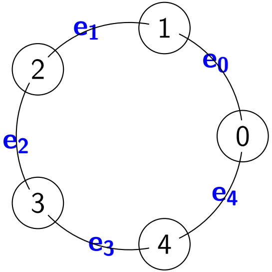
$$(M_{kj}) = \begin{cases} 1, & \text{if } \mathbf{e}_k = (v_j, v_l) \text{ and } j < l \\ -1, & \text{if } \mathbf{e}_k = (v_j, v_l) \text{ and } j > l \\ 0, & \text{otherwise.} \end{cases}$$

- The $|\mathbf{E}| \times |\mathbf{E}|$ weight matrix, W, is the diagonal matrix,

$$W = diag(w(\mathbf{e}_0), ..., w(\mathbf{e}_{|\mathbf{E}|-1}))$$

with the weight of the k^{th} edge on the k^{th} diagonal.

Circulant Graph



A circulant graph with 5 vertices.

$$M = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 1 & 0 & 0 & 0 & -1 \end{bmatrix}$$

$$W = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Decomposition of L and $\mathcal{L}$

It is straightforward, albeit tedious, to show that

$$L = (W^{1/2}M)^*((W^{1/2}M))$$

and

$$\mathcal{L} = (W^{1/2}MD^{-1/2})^*(W^{1/2}MD^{-1/2}).$$

Hence the Laplacian, respectively, the normalized Laplacian, is symmetic, positive semi-definite and has real ordered eigenvalues $0 \leq \lambda_0 \leq ... \leq \lambda_{N-1}$, respectively, $0 \leq \mu_0 \leq ... \leq \mu_{N-1}$.

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Diagonalization of the Laplacians

- By the spectral theorem, L, respectively, $\mathcal{L}$, has an orthonormal eigenbasis, $\{\chi_j\}_{j=0}^{N-1}$ of $\mathbb{R}^N$, respectively, $\{F_j\}_{j=0}^{N-1}$.
- The Laplacian has the diagonalization

$$\Delta = \chi^* L \chi = diag(\lambda_0, \lambda_1, ..., \lambda_{N-1}),$$

where $\chi = [\chi_0, \chi_1, ..., \chi_{N-1}]$ where each χ_j is a column vector.

- The normalized Laplacian has the diagonalization

$$\mathcal{D} = F^* \mathcal{L} F = diag(\mu_0, \mu_1, ..., \mu_{N-1}),$$

where $F = [F_0, F_1, ..., F_{N-1}]$ where each F_j is a column vector.

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Graph Fourier transform

- The inverse Fourier transform of an integrable function f may be thought of as the expansion of f in the complex exponentials. These are eigenfunctions of the Laplacian operator.
- Motivated by this, we define the graph Fourier transform $\widehat{f}$ of a function $f \in l^2(G)$ as coefficients of the expansion in the eigenbasis of the graph Laplacian:

$$\widehat{f}[j] = \langle \chi_j, f \rangle, \; j = 0, ..., N-1.$$

- We define the normalized graph Fourier transform $\overset{*}{f}$ as the as coefficients of the expansion in the eigenbasis of the normalized graph Laplacian:

$$\overset{*}{f} = \langle F_j, f \rangle, \; j = 0, ..., N-1.$$

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Matrix Version

If

$$\chi = [\chi_0, \chi_1, ..., \chi_{N-1}]$$

then we have $\widehat{f} = \chi^* f$, and since χ is unitary we may invert the transform with χ. That is

$$f = \chi\chi^* f = \chi\hat{f}.$$

Similarly, let $F = [F_0, F_1, ..., F_{N-1}]$ such that $\overset{*}{f} = F^* f$ and

$$f = FF^* f = F\overset{*}{f}.$$

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Difference Operator

Define the difference operator

$$D_r = W^{1/2}M \text{ such that } D_r f[k] = (f[j] - f[i])\,(w(\mathbf{e}_k))^{1/2},$$

where $\mathbf{e}_k = (v_j, v_i)$ and $j < i$.
This operator maps from $l^2(G) \to \mathbb{R}^{|\mathbf{E}|}$ with coordinate values representing the weighted change in a function f over each edge.

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Normalized Difference Operator

Define the normalized difference operator

$$D_{nr} = W^{1/2} M D^{-1/2}$$

such that

$$D_{nr} f[k] = \left(\frac{f[j]}{(deg(v_j))^{1/2}} - \frac{f[i]}{(deg(v_i))^{1/2}} \right) (w(\mathbf{e}_k))^{1/2},$$

where $\mathbf{e}_k = (v_j, v_i)$ and $j < i$. This operator maps from $l^2(G) \to \mathbb{R}^{|\mathbf{E}|}$ with coordinate values representing the normalized, weighted change in a function f over each edge.

Outline

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Differential Uncertainty Principle

Motivated by the additive form of the Heisenberg uncertainty principle, and by the discrete Heisenberg uncertainty principle due to Grünbaum [2] we introduce a graph differential uncertainty principle.

Theorem

Let G be a simple connected, and undirected graph. Then, for any non-zero function $f \in l^2(G)$, the following inequalities hold:

$$0 < \|f\|^2 \tilde{\lambda}_0 \leq \|D_r f\|^2 + \left\|D_r \widehat{f}\right\|^2 \leq \|f\|^2 \tilde{\lambda}_{N-1}, \qquad (2)$$

where $0 < \tilde{\lambda}_0 \leq \tilde{\lambda}_1 \leq \ldots \leq \tilde{\lambda}_{N-1}$ are the ordered real eigenvalues of $L + \Delta$. Furthermore, the bounds are sharp.

Proof

Noting that

$$\|D_r f\|^2 = \langle D_r f, D_r f\rangle$$
$$= \langle f, \chi\Delta\chi^* f\rangle$$
$$= \left\langle \widehat{f}, \Delta\widehat{f}\right\rangle$$

and, similarly, that $\left\|D_r \widehat{f}\right\|^2 = \left\langle \widehat{f}, L\widehat{f}\right\rangle$, we have

$$\|D_r f\|^2 + \left\|D_r \widehat{f}\right\|^2 = \left\langle \widehat{f}, (L+\Delta)\widehat{f}\right\rangle.$$ [3]

[3] One should note that $D_r f$ is a vector with dimension not usually equal to N as there are usually more edges than vertices. However, using properties of the inner product, we are able to translate our problem into one involving N dimensional vectors.

The operator $L + \Delta$ is symmetric positive semidefinite so applying the properties of the Rayleigh quotient for symmetric operators we have

$$0 \leq \|f\|^2 \tilde{\lambda}_0 \leq \|D_r f\|^2 + \left\|D_r \widehat{f}\right\|^2 \leq \|f\|^2 \tilde{\lambda}_{N-1}.$$

The minimum, respectively, the maximum, values are attained by setting $\widehat{f}$ equal to the first, respectively, the last, eigenfunction for $L + \Delta$.

For positivity of the lower bound, we note that $\|D_r f\|^2 = 0$ if and only if $\widehat{f} = [c, 0, ..., 0]'$, however this implies

$$\left\|D_r \widehat{f}\right\|^2 = c^2 deg(v_0) > 0.$$

We conclude inequality (2) holds, as desired. ■

Normalized Differential Uncertainty Principle

Theorem

Let G be a simple connected, and undirected graph. Then, for any non-zero function $f \in l^2(G)$, the following inequalities hold:

$$0 < \|f\|^2 \tilde{\mu}_0 \leq \|D_{nr} f\|^2 + \left\| D_{nr} \overset{*}{f} \right\|^2 \leq \|f\|^2 \tilde{\mu}_{N-1}, \tag{3}$$

where $0 < \tilde{\mu}_0 \leq \tilde{\mu}_1 \leq \ldots \leq \tilde{\mu}_{N-1}$ are the ordered real eigenvalues of $\mathcal{L} + \mathcal{D}$. Furthermore, the bounds are sharp.

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Future Directions

- Proving similar results for directed graphs and graphs with disconnected components.
- Effect of permuting graph labels.

Frames

- A set $\{e_j\}$ of N vectors in $\mathbb{C}^d$ is said to be a frame for $\mathbb{C}^d$ if there exist $0 < A \leq B$ such that for all $f \in \mathbb{C}^d$ the following bounds hold:

$$0 < A \|f\|^2 \leq \sum_{j=0}^{N-1} |\langle f, e_j \rangle|^2 \leq B \|f\|^2 .$$

- If $A = B = 1$ then the frame is called a Parseval frame.
- Define the matrix $E = [e_0, e_1, ..., e_{N-1}]$ to be a $d \times N$ matrix where the set of N $d-$vectors $\{e_k\}$ forms a Parseval frame for $\mathbb{C}^d$, i.e., $EE^* = I_{d \times d}$.

Finite Frame Differential Uncertainty Principle

We extend the finite frame uncertainty principle due to Lammers and Maeser [3] to the graph theoretic setting.

Theorem

Let G be a simple connected and undirected graph. The following inequalities hold for all $d \times N$ Parseval frames E:

$$\sum_{j=0}^{d-1} \tilde{\lambda}_j \leq \|D_r \chi^* E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2 \leq \sum_{j=N-d}^{N-1} \tilde{\lambda}_j, \qquad (4)$$

where $\left\{\tilde{\lambda}_j\right\}$ is the ordered set of real, positive eigenvalues of $L + \Delta$. Furthermore, these bounds are sharp.

Proof

Writing out the Frobenius norms as trace operators yields:

$$\|D_r \chi^* E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2 = tr(E\chi D_r^* D_r \chi^* E^*) + tr(D_r E^* E D_r^*). \tag{5}$$

Using the invariance of the trace when reordering products, we have $\|D_r \chi^* E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2$

$$= tr(L\chi^* E^* E\chi) + tr(LE^* E)$$
$$= tr(L\chi^* E^* E\chi) + tr(\chi\Delta\chi^* E^* E)$$
$$= tr((L+\Delta)\chi^* E^* E\chi).$$

The operator $\Delta + L$ is real, symmetric, and positive semidefinite. By the spectral theorem, it has an orthonormal eigenbasis P that, upon conjugation, diagonalizes $\Delta + L$:

$$P^*(\Delta + L)P = \tilde{\Delta} = \mathrm{diag}(\tilde{\lambda}_0, \tilde{\lambda}_1, ..., \tilde{\lambda}_{N-1}).$$

Hence, we have

$$\begin{aligned} \|D_r \chi E^*\|_{fr}^2 + \|D_r E^*\|_{fr}^2 &= tr((\Delta + L)\chi^* E^* E \chi) \\ &= tr(P\tilde{\Delta}P^*\chi^* E^* E\chi) \\ &= tr(\tilde{\Delta}P^*\chi^* E^* E\chi P) \\ &= \sum_{j=0}^{N-1} (K^* K_{jj})\, \tilde{\lambda}_j, \end{aligned}$$

where $K = E\chi P$.

The matrix K is a Parseval frame because unitary transformations of Parseval frames are Parseval frames . Therefore, $tr(K^*K) = tr(KK^*) = d$. K^*K is also the product of matrices with operator norm ≤ 1. Therefore, each of the entries, (K^*K_{jj}), satisfies $0 \leq (K^*K_{j,j}) \leq 1$. Hence, minimizing (maximizing) $\sum_{j=0}^{N-1} (K^*K_{jj})\,\tilde{\lambda}_j$ is achieved if

$$(K^*K_{jj}) = \begin{cases} 1 & j < d \ (j \geq N-d) \\ 0 & j \geq d \ (j < N-d). \end{cases}$$

Choosing E to be the first (last) d rows of $(\chi P)^*$ accomplishes this. The positivity of the bounds follows from the proof of Theorem 3.1

Normalized Finite Frame Differential Uncertainty Principle

Theorem

Let G be a simple, connected and undirected graph. The following inequalities hold for all $d \times N$ Parseval frames E:

$$\sum_{j=0}^{d-1} \tilde{\mu}_j \leq \|D_{nr}\mathcal{F}^* E^*\|_{fr}^2 + \|D_{nr} E^*\|_{fr}^2 \leq \sum_{j=N-d}^{N-1} \tilde{\mu}_j, \qquad (6)$$

where $\{\tilde{\mu}_j\}$ is the ordered set of real, non-negative eigenvalues of $\mathcal{L} + \mathcal{D}$. Furthermore, these bounds are sharp.

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Feasibility Results

- We introduce analysis on the region of all possible pairs,

$$(\|D_r f\|^2, \left\|D_r \widehat{f}\right\|^2).$$

- This work is highly motivated by the work of Agaskar and Lu [4]

Feasibility Results

Define the difference operator feasibility region FR as follows:

$$FR = \{(x,y) : \exists f \in l^2(G) \setminus \{0\} \text{ such that } \|f\| = 1,\ \|D_r f\|^2 = x \text{ and } \left\|D_r \widehat{f}\right\|^2 = y$$

Convexity of *FR*

Proposition

Let FR be the difference operator feasibility region for a simple and connected graph G with N vertices. Then, the following properties hold.

a) *FR is a closed subset of $[0, \lambda_{N-1}] \times [0, \lambda_{N-1}]$ where λ_{N-1} is the maximal eigenvalue of the Laplacian L.*

b) *$y = 0$ and $x = \frac{1}{N}\sum_{j=0}^{N-1} \lambda_j$ is the only point on the horizontal axis in FR. $x = 0$ and $y = L_{0,0}$ is the only point on the vertical axis in FR.*

c) *FR is in the half plane defined by $x + y \geq \tilde{\lambda}_0 > 0$ with equality if and only if $\widehat{f}$ is in the eigenspace associated with $\tilde{\lambda}_0$.*

d) *If $N \geq 3$ then FR is a convex region.*

Complete Graph

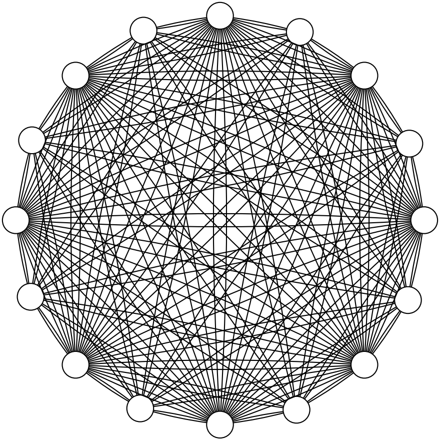
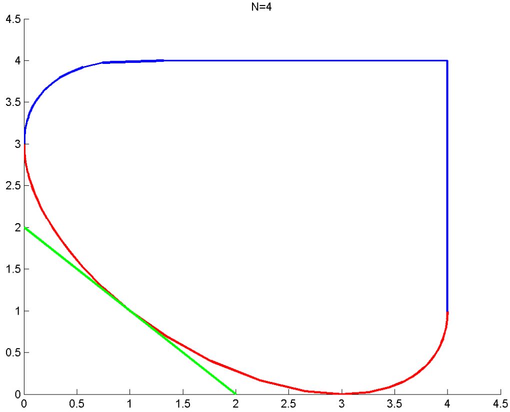


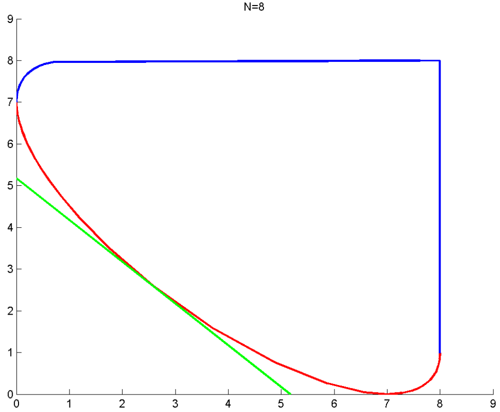
Figure: A unit weighted complete graph with 16 vertices.

Feasibility Region



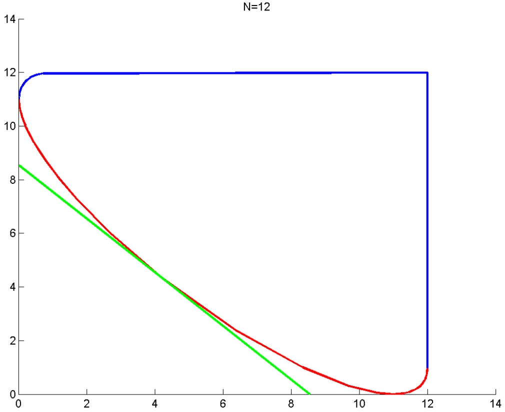
The green line intersects the red boundary at $\|D+rf\|^2+\left\|D_r\widehat{f}\right\|^2=\tilde{\lambda}_0$ according to differential uncertainty bounds

Feasibility Region



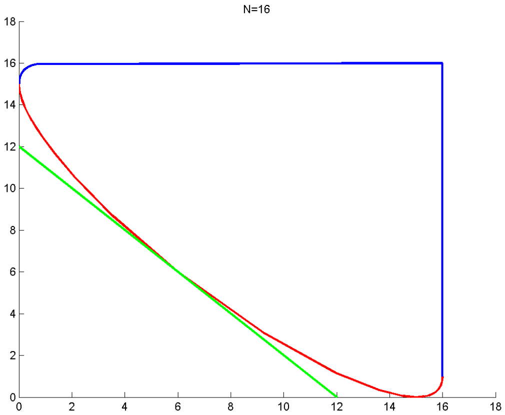
The green line intersects the red boundary at $\|D+rf\|^2 + \left\|D_r\widehat{f}\right\|^2 = \tilde{\lambda}_0$ according to differential uncertainty bounds

Feasibility Region



The green line intersects the red boundary at $\|D + rf\|^2 + \left\|D_r \widehat{f}\right\|^2 = \tilde{\lambda}_0$ according to differential uncertainty bounds.

Feasibility Region



The green line intersects the red boundary at $\|D+rf\|^2 + \left\|D_r\widehat{f}\right\|^2 = \tilde{\lambda}_0$ according to differential uncertainty bounds.

Differential Uncertainty Curve

We now turn our attention the lower boundary of FR: the differential uncertainty curve (DUC) $\omega(x)$ is defined as

$$\forall x \in [0, \lambda_{N-1}],\ \omega(x) = \inf_{g \in l^2(G,\ \|g\|=1)} \langle g, Lg \rangle \text{ subject to } \langle g, \Delta g \rangle = x.$$

Given a fixed $x \in [0, \lambda_{N-1}]$, we say g' attains the DUC if for all unit normed g with $\langle g, \Delta g \rangle = x$ we have

$$\|g\| = 1 \text{ and } \left\langle g', Lg' \right\rangle \leq \langle g, Lg \rangle \,.$$

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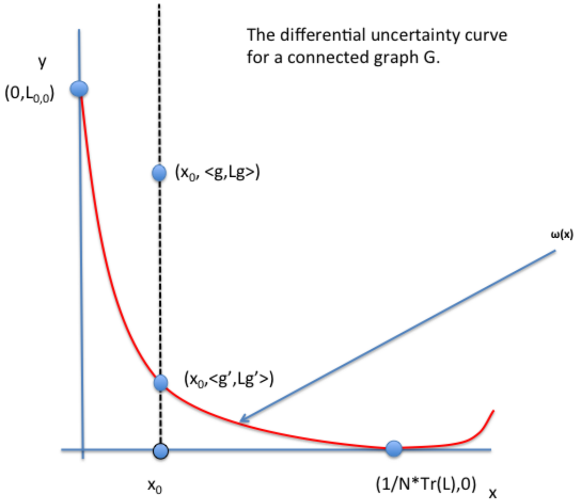
The differential uncertainty curve
for a connected graph G.
y
(0,L0,0)
(x0, <g,Lg>)
ω(x)
(x0,<g',Lg'>)
x0
(1/N*Tr(L),0)
x

Characterization of the DUC

Theorem

A unit normed function $f \in l^2(G)$ *with* $\|D_r \hat{f}\|^2 = x \in (0, \lambda_{N-1})$ *achieves the uncertainty curve if and only if* f *is a nonzero eigenfunction for* $K(\alpha) = L - \alpha\Delta$ *associated with the minimal eigenvalue of* $K(\alpha)$ *where* $\alpha \in (-\infty, \infty)$.

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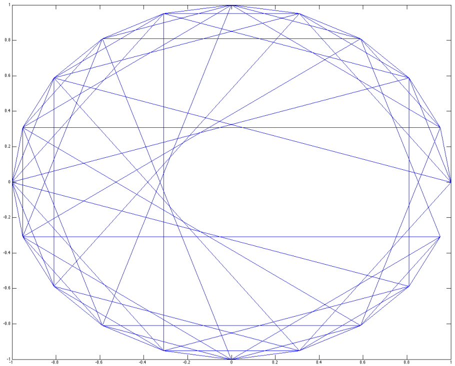
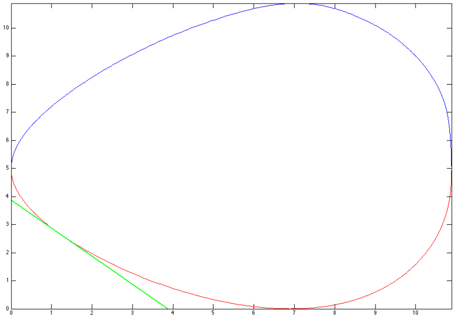
The UF-Trefethen 20 Graph



This graph was used to facilitate solving the Problem 7 of the Hundred-dollar, Hundred-digit Challenge Problems,

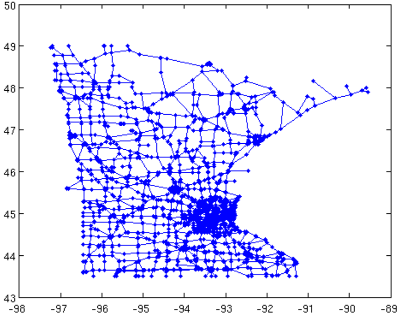
SIAM News, vol 35, no. 1.

The Trefethen 20 FR



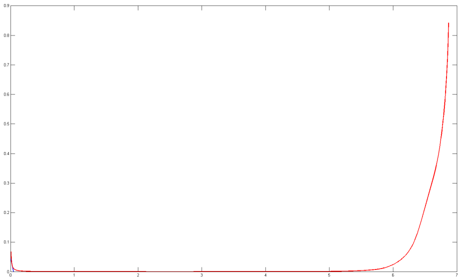
The DUC is in red, and the green is the lower bound from the Differential UP theorem.

The Minnesota Road Graph



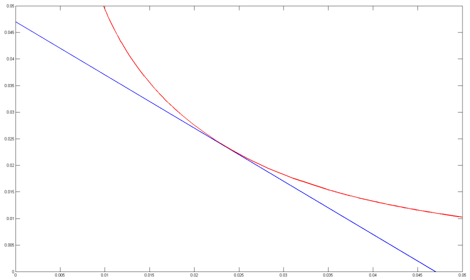
The road graph of Minnesota due to Gleich. It has 2640 vertices, and only 3,003 edges.

The Minnesota Road Graph



The DUC for the Minnesota road graph.

The Minnesota Road Graph



A magnification of the DUC in the region near the origin.

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Future Considerations

- Examine feasibility region for the normalized Laplacian
- Directed graphs approach
- Explore the connection with the Bell labs feasibility results in [5] and [6]

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