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Modern Computational Harmonic Analysis on Graphs and Networks

4. Calculating uncertainty principles on graphs

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Outline of this presentation

Goal: description and computation of uncertainty principles on graphs.

- How can space and frequency localization be defined on graphs
- How can uncertainty principles be defined
- How can we calculate the shapes of the uncertainties
- Some applications in space-frequency analysis of signals

Prerequisites: graph Fourier transform and graph convolution

Remember: the graph convolution of two signals y and x is defined as

$$y * x := \mathbf{U}\mathbf{M}_{\hat{y}}\hat{x} = \underbrace{\mathbf{U}\mathbf{M}_{\hat{y}}\mathbf{U}^*}_{\mathbf{C}_y} x, \quad \text{where } \mathbf{M}_{\hat{y}} = \operatorname{diag}(\hat{y}_1, \ldots \hat{y}_n).$$

Uncertainty principles in harmonic analysis

Uncertainty principles describe the following phenomenon encountered in different settings of harmonic analysis:

"A function and its Fourier transform can not both be well-localized"

One famous examples is Heisenberg's uncertainty principle:

Theorem 1 (Heisenberg-Pauli-Weyl)

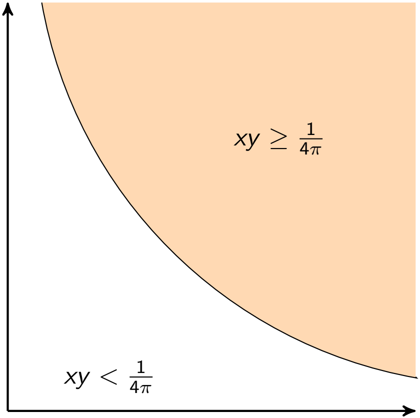
For any $f \in L^2(\mathbb{R})$ and any $a, b \in \mathbb{R}$, we have

$$\int_{\mathbb{R}} (t-a)^2 |f(t)|^2 \mathrm{d}t \int_{\mathbb{R}} (\omega - b)^2 |\hat{f}(\omega)|^2 \mathrm{d}\omega \geq \frac{\|f\|_2^4}{(4\pi)^2}$$

Equality holds if and only if $f(x) = Ce^{2\imath bt} e^{-\gamma(t-a)^2}$, with $C \in \mathbb{C}$, $\gamma > O$.

Normalizing f such that $\|f\|_2 = 1$, we can visualize this uncertainty as:

$$y = \left(\int_{\mathbb{R}} (\omega - b)^2 |\hat{f}(\omega)|^2 \mathrm{d}\omega \right)^{1/2}$$



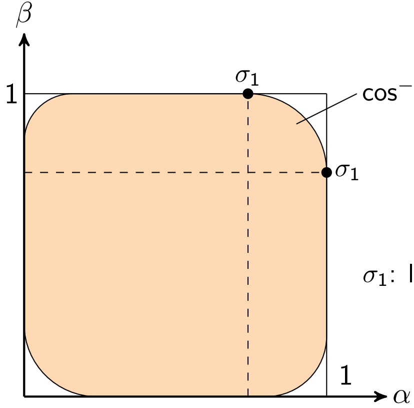
$$x = \left(\int_{\mathbb{R}} (t - a)^2 |f(t)|^2 \mathrm{d}t \right)^{1/2}$$

Landau-Pollak-Slepian uncertainty principle

Assume that $\|f\|_2 = 1$ and that the time and frequency localization of f in the intervals $[-a, a]$ and $[-b, b]$ is described through the values

$$\alpha^2 = \int_{-a}^{a} |f(t)|^2 \mathrm{d}t, \quad \beta^2 = \int_{-b}^{b} |\hat{f}(\omega)|^2 \mathrm{d}\omega.$$

Then the pairs (α, β) can attain only the following values in $[0, 1]^2$:



$\cos^{-1}\alpha + \cos^{-1}\beta \geq \cos^{-1}\sqrt{\sigma_1}$

σ_1: largest possible α for $\beta = 1$

Vertex-frequency localization on graphs

For a vertex-frequency analysis of a signal x on G we use spatial and spectral filter functions $f, g \in \mathbb{R}^n$ with the properties

$$0 \leq f \leq 1,\ 0 \leq \hat{g} \leq 1, \quad \text{and} \quad \|f\|_\infty = \|\hat{g}\|_\infty = 1. \tag{1}$$

Based on the filters f and g we introduce the localization operators

$$\begin{aligned} \mathbf{M}_f x\,(\mathrm{v}) &:= f(\mathrm{v}) x(\mathrm{v}) && \text{(pointwise product)}, \\ \mathbf{C}_g x\,(\mathrm{v}) &:= (g * x)\,(\mathrm{v}) = \mathbf{U}\mathbf{M}_{\hat{g}}\mathbf{U}^* x\,(\mathrm{v}) && \text{(graph convolution)}. \end{aligned}$$

- We call $\mathbf{M}_f$ with the filter f space localization operator;
- We call $\mathbf{C}_g$ with the filter g frequency localization operator;
- $\mathbf{M}_f$ and $\mathbf{C}_g$ are symmetric and positive semidefinite;
- $\mathbf{M}_f$ and $\mathbf{C}_g$ have spectral norm equal to 1.

Vertex-frequency localization on graphs

For $\mathbf{M}_f$ and $\mathbf{C}_g$ we define the expectation values

$$\bar{\mathbf{m}}_f(x) := \frac{\langle \mathbf{M}_f x, x \rangle}{\|x\|^2}, \qquad \bar{\mathbf{c}}_g(x) := \frac{\langle \mathbf{C}_g x, x \rangle}{\|x\|^2}.$$

- x is called space-localized with respect to f if $\bar{\mathbf{m}}_f(x)$ is close to one.
- x is called frequency-localized with respect to g if $\bar{\mathbf{c}}_g(x)$ approaches 1.

We define the set of admissible values related to $\mathbf{M}_f$ and $\mathbf{C}_g$ as

$$\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g) := \left\{ (\bar{\mathbf{m}}_f(x), \bar{\mathbf{c}}_g(x)) \ : \ \|x\| = 1 \right\} \subset [0,1]^2. \tag{2}$$

We call $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ the numerical range of the pair $(\mathbf{M}_f, \mathbf{C}_g)$. All studied uncertainty principles are linked to the boundaries of $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$.

Space-frequency operators

To investigate the joint localization with respect to both filters f and g and to describe the set $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$, we consider the two operators

$$\mathbf{R}_{f,g}^{(\theta)} := \cos(\theta)\, \mathbf{M}_f + \sin(\theta)\, \mathbf{C}_g \quad \text{and} \quad \mathbf{S}_{f,g} := \mathbf{C}_g^{1/2} \mathbf{M}_f \mathbf{C}_g^{1/2},$$

where $\mathbf{C}_g^{1/2}$ is the square root of the positive semidefinite matrix $\mathbf{C}_g$.

- $\mathbf{R}_{f,g}^{(\theta)}$ as combination of $\mathbf{M}_f$ and $\mathbf{C}_g$ is symmetric for any $0 \leq \theta < 2\pi$.
- $\mathbf{S}_{f,g} \in \mathbb{R}^{n \times n}$ is positive semi-definite with norm bounded by 1.

Space-frequency operators

Related to the operators $\mathbf{R}_{f,g}^{(\theta)}$, $\mathbf{S}_{f,g}$, we consider the expectation values:

$$\bar{\mathbf{r}}_{f,g}^{(\theta)}(x) := \frac{\langle \mathbf{R}_{f,g}^{(\theta)} x, x \rangle}{\|x\|^2} = \cos(\theta)\bar{\mathbf{m}}_f(x) + \sin(\theta)\bar{\mathbf{c}}_g(x),$$
$$\bar{\mathbf{s}}_{f,g}(x) := \frac{\langle \mathbf{S}_{f,g} x, x \rangle}{\|x\|^2}.$$

To formulate uncertainty principles, the largest eigenvalues $\rho_1^{(\theta)}$ and σ_1 and eigenvectors $\phi_1^{(\theta)}$ and ψ_1 are of major importance.

For σ_1, we have

$$\sigma_1 = \|\mathbf{S}_{f,g}\| = \|\mathbf{M}_f^{1/2}\mathbf{C}_g^{1/2}\|^2 = \|\mathbf{C}_g^{1/2}\mathbf{M}_f^{1/2}\|^2 = \|\mathbf{M}_f^{1/2}\mathbf{C}_g\mathbf{M}_f^{1/2}\|.$$

Example 1, projection-projection filters

Let $\chi_{\mathcal{A}}$ denote the indicator function of a set $\mathcal{A}$, i.e.

$$\chi_{\mathcal{A}}(\mathrm{v}) := \begin{cases} 1 & \text{if } \mathrm{v} \in \mathcal{A}, \\ 0 & \text{if } \mathrm{v} \notin \mathcal{A}. \end{cases}$$

For a subset $\mathcal{A}$ of the node set V and a subset $\mathcal{B}$ of the frequencies, we define the filter functions f and g as

$$f = \chi_{\mathcal{A}} \quad \hat{g} = \chi_{\mathcal{B}}. \tag{3}$$

- $\mathbf{M}_f$ and $\mathbf{C}_g$ are in this case orthogonal projectors satisfying

$$\mathbf{M}_f^2 = \mathbf{M}_f \quad \text{and} \quad \mathbf{C}_g^2 = \mathbf{C}_g.$$

- $\mathbf{S}_{f,g}$ is in this case equivalently given as $\mathbf{S}_{f,g} = \mathbf{C}_g \mathbf{M}_f \mathbf{C}_g$.

References:

- Studied by Landau, Pollak and Slepian in the 60's for signals on $\mathbb{R}$.
- General theory for projection operators in Hilbert spaces (Havin & Jöricke).
- Studied for graphs by Tsitsivero, Barbarossa, Di Lorenzo.

Example 2, distance-projection filters

Consider the graph geodesic distance $\mathrm{d}(\mathrm{v}, \mathrm{w})$ on G. We set

$$\mathrm{d}_{\mathrm{w}}(\mathrm{v}) := \mathrm{d}(\mathrm{v}, \mathrm{w}), \quad \mathrm{d}_{\mathrm{w}}^{\infty} := \max_{\mathrm{v} \in V} \mathrm{d}(\mathrm{v}, \mathrm{w}).$$

Then, as spatial filter f and frequency filter g, we define

$$f(v) = 1 - \frac{\mathrm{d}_{\mathrm{w}}(\mathrm{v})}{\mathrm{d}_{\mathrm{w}}^{\infty}}, \quad \text{and} \quad \hat{g} = \chi_{\mathcal{B}}, \tag{4}$$

i.e., the spatial filter f incorporates the distance d_{w} to a reference node w. For this distance filter f we have

$$\mathbf{M}_f x = x - \tfrac{1}{\mathrm{d}_{\mathrm{w}}^{\infty}} \mathbf{M}_{\mathrm{d}_{\mathrm{w}}} x, \quad \bar{\mathbf{m}}_f(x) = 1 - \frac{x^* \mathbf{M}_{\mathrm{d}_{\mathrm{w}}} x}{\mathrm{d}_{\mathrm{w}}^{\infty} \|x\|^2}.$$

References:

- Similar distance-projection filters have been used also in a continuous setting on the real line and on the sphere (Erb, Mathias).

Example 3, Distance-Laplace filter

Another spectral filter $\hat{g} = (\hat{g}_1 \; \cdots \; \hat{g}_n)$ on $\hat{G}$ can be defined as

$$\hat{g}_j = 1 - \lambda_j/2, \tag{5}$$

where λ_j denotes the j-th. smallest eigenvalue of the graph Laplacian $\mathbf{L}$. In this case, we get

$$\mathbf{C}_g x = \mathbf{U}(\mathbf{I}_n - \tfrac{1}{2}\mathbf{M}_\lambda)\mathbf{U}^* x = (\mathbf{I}_n - \tfrac{1}{2}\mathbf{L})x.$$

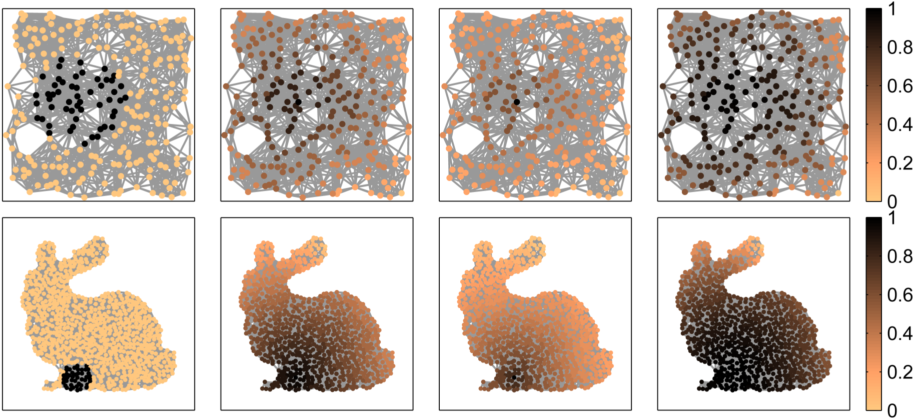
Using a (modified) distance filter as a spatial filter, we get

$$\bar{\mathbf{m}}_f(x) = 1 - \frac{x^* \mathbf{M}_{\mathrm{d}_\mathrm{w}^2} x}{(\mathrm{d}_\mathrm{w}^\infty)^2 \|x\|^2}, \qquad \bar{\mathbf{c}}_g(x) = 1 - \frac{x^* \mathbf{L} x}{2\|x\|^2}.$$

References:

- Agaskar, Lu used such filters to obtain uncertainties on graphs based on spatial and spectral spreads.

Examples of spatial filters



From left to right the following spatial filters:

$$f_1(\mathrm{v}) = \chi_{\mathcal{A}}(\mathrm{v}) \quad \text{(Example 1)}, \qquad f_2(\mathrm{v}) = 1 - \frac{\mathrm{d_w}(\mathrm{v})}{\mathrm{d_w^\infty}} \quad \text{(Example 2)},$$

$$f_3(\mathrm{v}) = 1 - \left(\frac{\mathrm{d_w}(\mathrm{v})}{\mathrm{d_w^\infty}}\right)^{\frac{1}{2}}, \qquad f_4(\mathrm{v}) = 1 - \left(\frac{\mathrm{d_w}(\mathrm{v})}{\mathrm{d_w^\infty}}\right)^{2} \quad \text{(Example 3)}.$$

Uncertainty principle related to the operator $\mathbf{S}_{f,g}$

Theorem 2

The range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ *is contained in the domain* $\mathcal{W}_\gamma^{(f,g)}$ *given by*

$$\mathcal{W}_\gamma^{(f,g)} = \left\{ (t,s) \in [0,1]^2 \;\middle|\; \begin{array}{ll} s \leq \gamma_{f,g}(t) & \text{if } ts \geq \sigma_1^{(f,g)}, \\ 1-s \leq \gamma_{f,g^*}(t) & \text{if } t(1-s) \geq \sigma_1^{(f,g^*)}, \\ s \leq \gamma_{f^*,g}(1-t) & \text{if } (1-t)s \geq \sigma_1^{(f^*,g)}, \\ 1-s \leq \gamma_{f^*,g^*}(1-t) & \text{if } (1-t)(1-s) \geq \sigma_1^{(f^*,g^*)} \end{array} \right\}$$

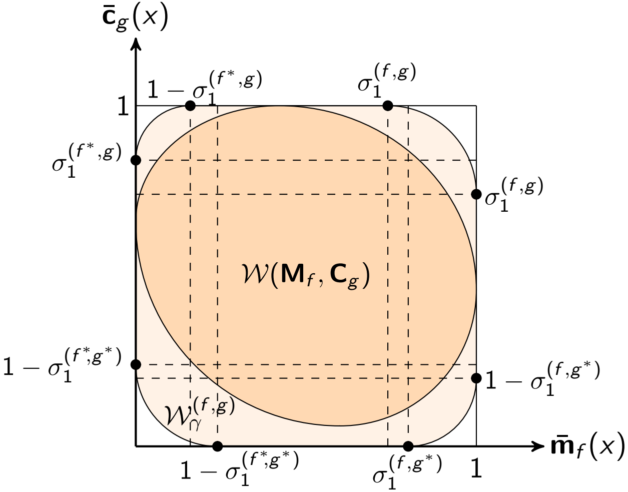
where $\sigma_1^{(f,g)}$ *is the largest eigenvalue of* $\mathbf{S}_{f,g}$*,*

$$\gamma_{f,g} : [\sigma_1^{(f,g)}, 1] \to \mathbb{R} : \quad \gamma_{f,g}(t) := \left((t\, \sigma_1^{(f,g)})^{\frac{1}{2}} + ((1-t)(1-\sigma_1^{(f,g)}))^{\frac{1}{2}} \right)^2.$$

and $f^* = 1 - f$, $g^* = 1 - g$.

Uncertainty principle related to the operator $\mathbf{S}_{f,g}$

Graphical version of Theorem 2.



Note: If $\mathbf{M}_f$ and $\mathbf{C}_g$ are projectors, we have $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g) = \mathcal{W}_\gamma^{(f,g)}$.

Uncertainty principle related to the operator $\mathbf{R}_{f,g}^{(\theta)}$

Theorem 3

For every $0 \leq \theta < 2\pi$*, we have the inclusion*

$$\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g) \subseteq [0,1]^2 \cap \mathcal{H}^{(\theta)},$$

with the half-plane

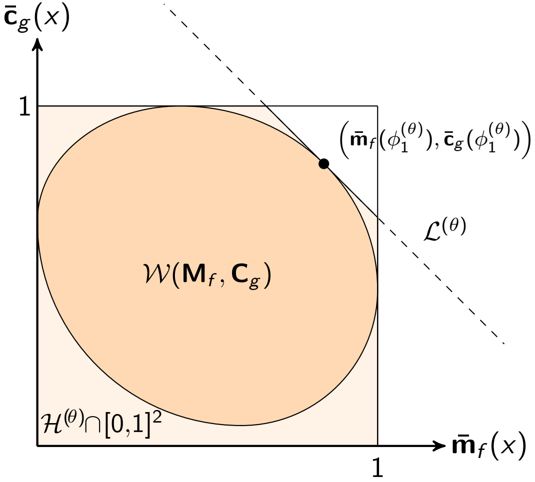
$$\mathcal{H}^{(\theta)} := \{(t,s) \mid \cos(\theta)\, t + \sin(\theta)\, s \leq \rho_1^{(\theta)}\}$$

having a supporting line $\mathcal{L}^{(\theta)}$ *that intersects the boundary of* $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$*. On the other hand, for every point* p *on the boundary of* $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ *we have an angle* $0 \leq \theta < 2\pi$ *such that* $p \in \mathcal{L}^{(\theta)}$*. For this angle, we get an eigenvector* $\phi_1^{(\theta)}$ *(not necessarily unique) corresponding to the largest eigenvalue* $\rho_1^{(\theta)}$ *of* $\mathbf{R}_{f,g}^{(\theta)}$ *such that*

$$p = (\phi_1^{(\theta)*}\mathbf{M}_f \phi_1^{(\theta)}, \phi_1^{(\theta)*}\mathbf{C}_g \phi_1^{(\theta)}).$$

Uncertainty principle related to the operator $\mathbf{R}_{f,g}^{(\theta)}$

Graphical version of Theorem 3.



Note: for $n \geq 3$, the numerical range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ is convex.

Numerical calculation of $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$

Using a set $\Theta = \{\theta_1, \ldots \theta_K\} \subset [0, 2\pi)$ of $K \geq 3$ different angles, we approximate the numerical range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ with the two K-gons

$$\mathcal{P}_{\mathrm{out}}^{(\Theta)}(\mathbf{M}_f, \mathbf{C}_g) := \bigcap_{k=1}^{K} \mathcal{H}^{(\theta)} = \bigcap_{k=1}^{K} \left\{(t, s) \mid \cos(\theta_k)\, t + \sin(\theta_k)\, s \leq \rho_1^{(\theta_k)}\right\},$$

$$\mathcal{P}_{\mathrm{in}}^{(\Theta)}(\mathbf{M}_f, \mathbf{C}_g) := \mathrm{conv}\{p^{(\theta_1)}, p^{(\theta_2)}, \ldots p^{(\theta_K)}\}.$$

The convexity of the numerical range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ (for $n \geq 3$) combined with the statements of Theorem 3 imply the following result.

Theorem 4

Let $\Theta = \{\theta_1, \ldots \theta_K\} \subset [0, 2\pi)$ be a set of $K \geq 3$ different angles and $n \geq 3$. Then,

$$\mathcal{P}_{\mathrm{in}}^{(\Theta)}(\mathbf{M}_f, \mathbf{C}_g) \subseteq \mathcal{W}(\mathbf{M}_f, \mathbf{C}_g) \subseteq \mathcal{P}_{\mathrm{out}}^{(\Theta)}(\mathbf{M}_f, \mathbf{C}_g).$$

Algorithm 1: Calculation of polygonal approximation to $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$

Input: $\mathbf{M}_f$, $\mathbf{C}_g$, angles $0 \leq \theta_1 < \theta_2 < \cdots < \theta_K < 2\pi$, with $K \geq 3$. Set $\theta_0 = \theta_K$.

for $k \in \{1, 2, \ldots, K\}$ **do**

- Create $\mathbf{R}_{f,g}^{(\theta_k)} = \cos(\theta_k)\mathbf{M}_f + \sin(\theta_k)\mathbf{C}_g$;
- Calculate norm. eigenvector $\phi_1^{(\theta_k)}$ for max. eigenvalue $\rho_1^{(\theta_k)}$;
- Create boundary point $p^{(\theta_k)} = \left(\phi_1^{(\theta_k)*}\mathbf{M}_f\phi_1^{(\theta_k)}, \phi_1^{(\theta_k)*}\mathbf{C}_g\phi_1^{(\theta_k)}\right)$.

Generate interior polygon $\mathcal{P}_{\mathrm{in}}^{(\Theta)}(\mathbf{M}_f,\mathbf{C}_g) = \mathrm{conv}\{p^{(\theta_1)},\ldots,p^{(\theta_K)}\}$ to approximate $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$.

for $k \in \{1, 2, \ldots, K\}$ **do**

- Create the outer vertex $q^{(\theta_k)}$.

Generate $\mathcal{P}_{\mathrm{out}}^{(\Theta)}(\mathbf{M}_f, \mathbf{C}_g) = \mathrm{conv}\{q^{(\theta_1)}, \ldots q^{(\theta_K)}\}$ as a polygon exterior to $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$.

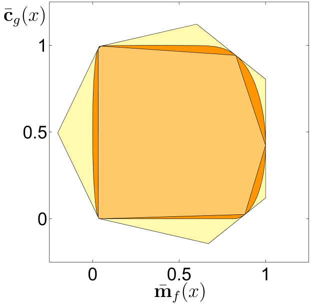
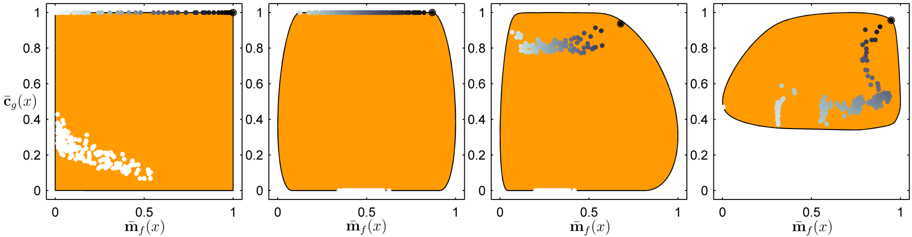


Fig.: Interior and exterior approximation of the numerical range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ based on Algorithm 1 with $K = 7$ vertices.

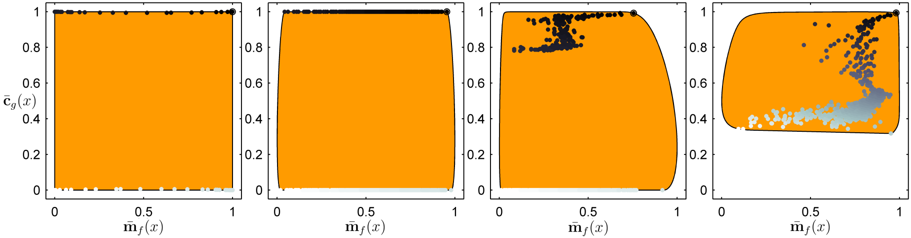
Shapes of uncertainty - illustrations



The numerical range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ for four filter pairs on the sensor network. The first, second and fourth plot correspond to the filters described in Example 1, 2 and 3.

The dots represent the position $(\bar{\mathbf{m}}_f(\psi_k), \bar{\mathbf{c}}_g(\psi_k))$ of the eigenvectors of the operator $\mathbf{S}_{f,g}$. The color (from black to white) of the dots indicates the corresponding eigenvalue σ_k (in the range from 1 to 0).

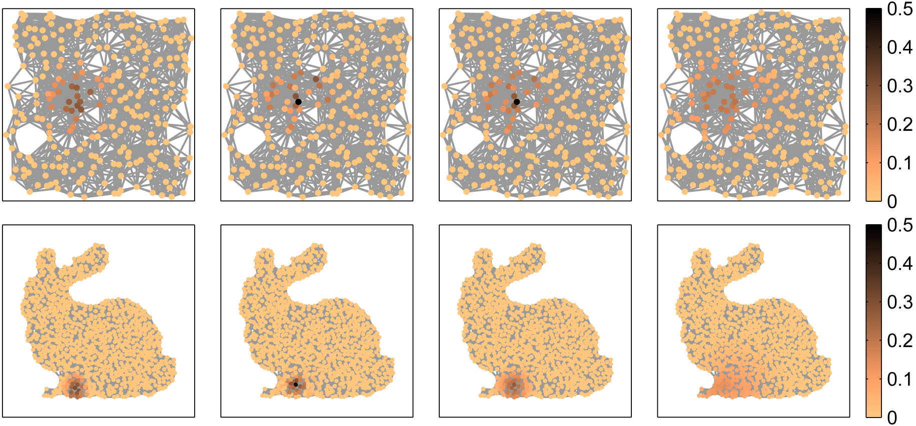
Shapes of uncertainty - illustrations



The numerical range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$ for four filter pairs on the bunny network. The first, second and fourth plot correspond to the filters described in Example 1, 2 and 3.

The dots represent the position $(\bar{\mathbf{m}}_f(\psi_k), \bar{\mathbf{c}}_g(\psi_k))$ of the eigenvectors of the operator $\mathbf{R}_{f,g}^{(\theta)}$ with $\theta = 9\pi/20$. The color (from black to white) of the dots indicates the corresponding eigenvalue $\rho_k^{(\theta)}$ (in the range from 1 to 0).

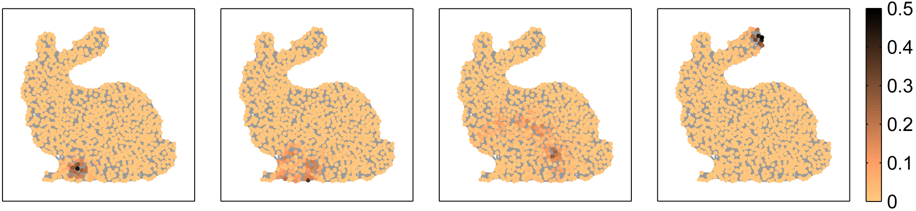
Space-frequency localization of eigenvectors of $\mathbf{S}_{f,g}$, $\mathbf{R}_{f,g}^{(\theta)}$.



Top row: the eigenvector ψ_1 of the operator $\mathbf{S}_{f,g}$ for the sensor graph and four different filter pairs.

Bottom row: the eigenvector $\phi_1^{(\theta)}$ of the operator $\mathbf{R}_{f,g}^{(\theta)}$ with $\theta = \frac{9}{20}\pi$ for the bunny graph and four filter pairs.

Space-frequency localization of eigenvectors of $\mathbf{S}_{f,g}$.



The eigenvectors ψ_1 ψ_{10}, ψ_{50} and ψ_{200} of $\mathbf{S}_{f,g}$ on the bunny graph for the distance-projection filter (Example 2).

Conclusion

Uncertainty relations are useful tool for the development of basis systems/dictionaries on graphs with prescribed space-frequency properties.

- $\mathbf{S}_{f,g}$ and $\mathbf{R}_{f,g}^{(\theta)}$ provide explicit uncertainty principles for graphs;
- The operator $\mathbf{R}_{f,g}^{(\theta)}$ can be used to calculate the shapes of the uncertainties (aka the numerical range $\mathcal{W}(\mathbf{M}_f, \mathbf{C}_g)$);
- The eigendecompositions of the operators $\mathbf{S}_{f,g}$ and $\mathbf{R}_{f,g}^{(\theta)}$ help to construct orthogonal basis systems with a space-frequency behavior determined by the operators $\mathbf{M}_f$ and $\mathbf{C}_g$;
- The shapes of the uncertainties provide useful information on the joint range of the localization operators $\mathbf{M}_f$ and $\mathbf{C}_g$ and on how complementary the two filters f and g are.

Thanks a lot for your attention!

General introduction to Graph Signal Processing:

[1] ORTEGA, A. Introduction to Graph Signal Processing, *Cambridge University Press* (2022)

Article related to this talk:

[2] ERB, W. Shapes of Uncertainty in Spectral Graph Theory, *IEEE Trans. Inform. Theory 67:2* (2021), 1291-1307

Software to create the uncertainty shapes

https://github.com/WolfgangErb/GUPPY