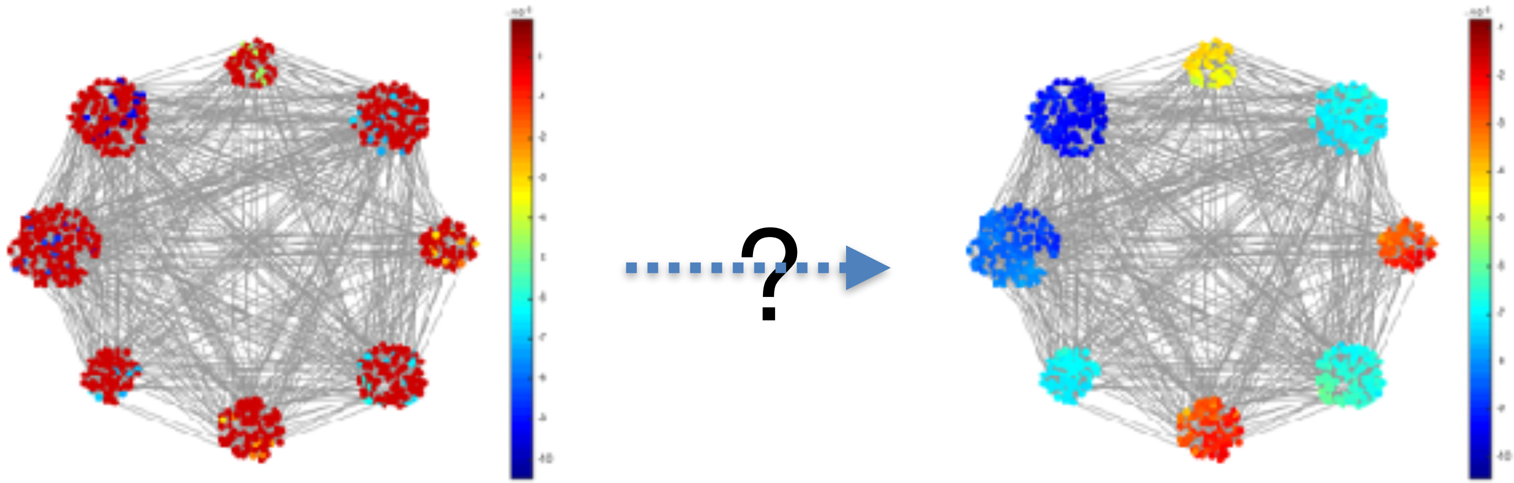
Sampling, Inference and Clustering for Data on Graphs

Joint work with Gilles Puy, Nicolas Tremblay and Rémi Gribonval

Goal

Given partially observed information at the nodes of a graph



Can we robustly and efficiently infer missing information ?

What signal model ?

How many observations ?

Influence of the structure of the graph ?

Notations

$\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathsf{W}\}$ weighted, undirected

$\mathcal{V}$ is the set of n nodes

$\mathcal{E}$ is the set of edges

$\mathsf{W} \in \mathbb{R}^{n \times n}$ is the weighted adjacency matrix

$\mathsf{L} \in \mathbb{R}^{n \times n}$

combinatorial graph Laplacian $\mathsf{L} := \mathsf{D} - \mathsf{W}$

normalised Laplacian $\mathsf{L} := \mathsf{I} - \mathsf{D}^{-1/2}\mathsf{W}\mathsf{D}^{-1/2}$

diagonal degree matrix D has entries $d_i := \sum_{i \neq j} \mathsf{W}_{ij}$

SP on Graphs Cheat Sheet

$$\boldsymbol{x} \in \mathbb{R}^n \quad \text{a (scalar valued) signal}$$

Laplacian

$$\mathsf{L} \in \mathbb{R}^{n \times n} \longrightarrow -\Delta$$

$$\mathsf{L} = \mathsf{U} \Lambda \mathsf{U}^\mathsf{T} \longrightarrow -\Delta = \mathcal{F}^T \omega^2 \mathcal{F}$$

Graph Fourier Frequencies

Filter and Filtering

$$g(\mathsf{L}) = \mathsf{U} g(\Lambda) \mathsf{U}^\mathsf{T}$$

$$g(\mathsf{L})\boldsymbol{x} \longrightarrow g \star \boldsymbol{x}$$

$$\widehat{g(\mathsf{L})\boldsymbol{x}}(k) = g(\lambda_k)\hat{\boldsymbol{x}}(k) \longrightarrow \widehat{g \star \boldsymbol{x}}(\omega) = \hat{g}(\omega)\hat{\boldsymbol{x}}(\omega)$$

Notations

L is real, symmetric PSD

orthonormal eigenvectors $\mathsf{U} \in \mathbb{R}^{n \times n}$ Graph Fourier Matrix

non-negative eigenvalues $\boldsymbol{\lambda}_1 \leqslant \boldsymbol{\lambda}_2 \leqslant \ldots, \boldsymbol{\lambda}_n$

$$\mathsf{L} = \mathsf{U}\Lambda\mathsf{U}^\intercal$$

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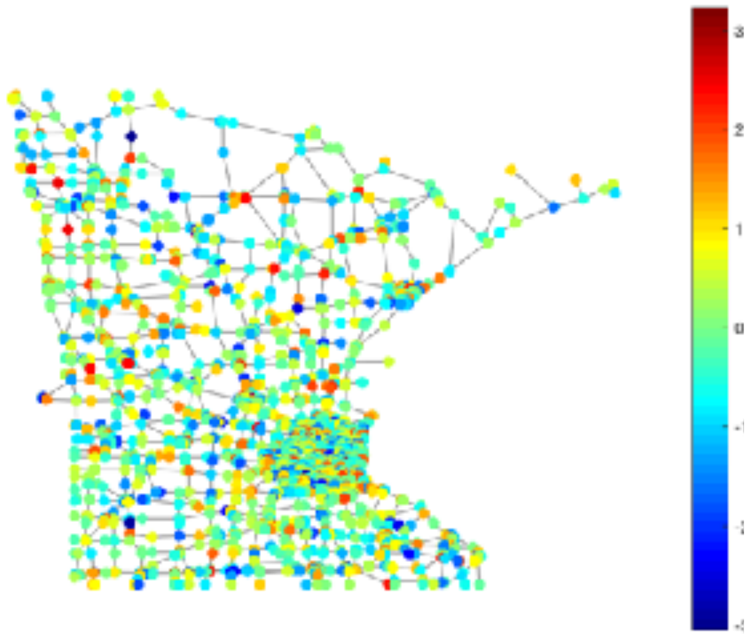
k-bandlimited signals $\boldsymbol{x} \in \mathbb{R}^n$

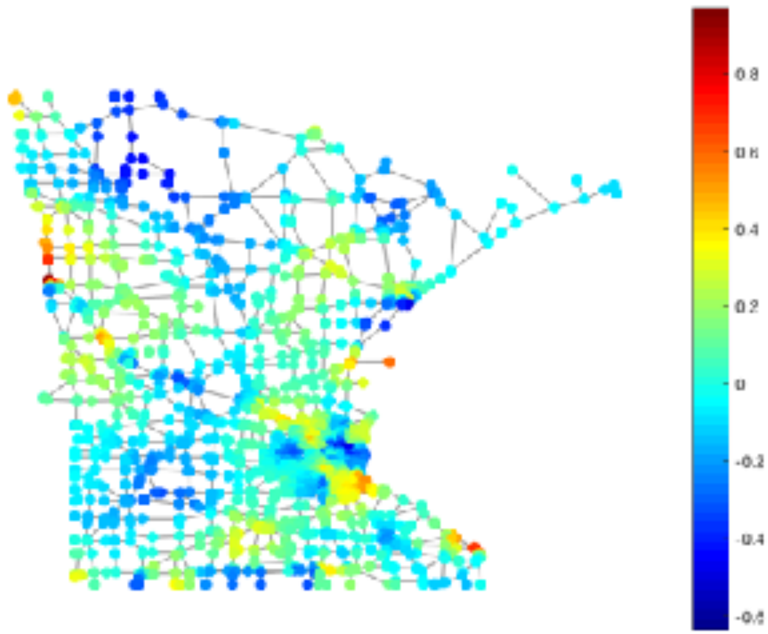
Fourier coefficients $\hat{\boldsymbol{x}} = \mathsf{U}^\intercal \boldsymbol{x}$

$$\boldsymbol{x} = \mathsf{U}_k \hat{\boldsymbol{x}}^k \qquad \hat{\boldsymbol{x}}^k \in \mathbb{R}^k$$

$\mathsf{U}_k := (\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k) \in \mathbb{R}^{n \times k}$ first k eigenvectors only



white noise



band-limited approximation

Sampling Model

$$\boldsymbol{p} \in \mathbb{R}^n \qquad \boldsymbol{p}_i > 0 \qquad \|\boldsymbol{p}\|_1 = \sum_{i=1}^{n} \boldsymbol{p}_i = 1$$

$$\mathsf{P} := \mathrm{diag}(\boldsymbol{p}) \in \mathbb{R}^{n \times n}$$

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Draw independently m samples (random sampling)

$$\mathbb{P}(\omega_j = i) = \boldsymbol{p}_i, \quad \forall j \in \{1, \ldots, m\} \text{ and } \forall i \in \{1, \ldots, n\}$$

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$$\boxed{\begin{gathered} \boldsymbol{y}_j := \boldsymbol{x}_{\omega_j}, \quad \forall j \in \{1, \ldots, m\} \\ \boldsymbol{y} = \mathsf{M}\boldsymbol{x} \end{gathered}}$$

Sampling Model

$$\frac{\|\mathsf{U}_k^{\mathsf{T}}\boldsymbol{\delta}_i\|_2}{\|\mathsf{U}^{\mathsf{T}}\boldsymbol{\delta}_i\|_2} = \frac{\|\mathsf{U}_k^{\mathsf{T}}\boldsymbol{\delta}_i\|_2}{\|\boldsymbol{\delta}_i\|_2} = \|\mathsf{U}_k^{\mathsf{T}}\boldsymbol{\delta}_i\|_2$$

How much a perfect impulse can be concentrated on first k eigenvectors

Carries interesting information about the graph

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Graph Coherence

$$\nu_{\boldsymbol{p}}^k := \max_{1 \leqslant i \leqslant n} \left\{ \boldsymbol{p}_i^{-1/2} \|\mathsf{U}_k^\intercal \boldsymbol{\delta}_i\|_2 \right\}$$

Rem: $\nu_{\boldsymbol{p}}^k \geqslant \sqrt{k}$

Stable Embedding

Theorem 1 (Restricted isometry property)**.** *Let* M *be a random subsampling matrix with the sampling distribution* $\boldsymbol{p}$*. For any* $\delta, \epsilon \in (0,1)$*, with probability at least* $1-\epsilon$*,*

$$(1-\delta)\left\|\boldsymbol{x}\right\|_2^2 \leqslant \frac{1}{m}\left\|\mathsf{MP}^{-1/2}\,\boldsymbol{x}\right\|_2^2 \leqslant (1+\delta)\left\|\boldsymbol{x}\right\|_2^2 \tag{1}$$

for all $\boldsymbol{x} \in \mathrm{span}(\mathsf{U}_k)$ *provided that*

$$m \geqslant \frac{3}{\delta^2}\,(\nu_{\boldsymbol{p}}^k)^2\,\log\left(\frac{2k}{\epsilon}\right). \tag{2}$$

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Proof similar to CS in bounded ONB but simpler since model is a subspace (not a union)

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Can we reduce to optimal amount ?

Variable Density Sampling $\quad \boldsymbol{p}_i^* := \dfrac{\|\mathsf{U}_k^\intercal \boldsymbol{\delta}_i\|_2^2}{k}, \quad i = 1, \dots, n$

is such that: $\quad (\nu_{\boldsymbol{p}}^k)^2 = k \quad$ and depends on structure of graph

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Corollary 1. *Let* M *be a random subsampling matrix constructed with the sampling distribution* $\boldsymbol{p}^*$. *For any* $\delta, \epsilon \in (0, 1)$, *with probability at least* $1 - \epsilon$,

$$(1-\delta)\,\|\boldsymbol{x}\|_2^2 \leqslant \frac{1}{m}\left\|\mathsf{MP}^{-1/2}\,\boldsymbol{x}\right\|_2^2 \leqslant (1+\delta)\,\|\boldsymbol{x}\|_2^2$$

for all $\boldsymbol{x} \in \mathrm{span}(\mathsf{U}_k)$ *provided that*

$$m \geqslant \frac{3}{\delta^2}\, k\, \log\left(\frac{2k}{\epsilon}\right).$$

Recovery Procedures (Inference)

$$\boldsymbol{y} = \mathsf{M}\boldsymbol{x} + \boldsymbol{n} \qquad \boldsymbol{y} \in \mathbb{R}^m$$

$$\boldsymbol{x} \in \mathrm{span}(\mathsf{U}_k) \quad \text{stable embedding}$$

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Standard Decoder

$$\min_{\boldsymbol{z} \in \mathrm{span}(\mathsf{U}_k)} \left\| \mathsf{P}_\Omega^{-1/2} \left(\mathsf{M}\boldsymbol{z} - \boldsymbol{y} \right) \right\|_2$$

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re-weighting for RIP

need projector

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Efficient Decoder:

$$\min_{\boldsymbol{z} \in \mathbb{R}^n} \left\| \mathsf{P}_\Omega^{-1/2} \left(\mathsf{M}\boldsymbol{z} - \boldsymbol{y} \right) \right\|_2^2 + \gamma \, \boldsymbol{z}^\intercal g(\mathsf{L}) \boldsymbol{z}$$

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soft constrain on frequencies

efficient implementation

Analysis of Standard Decoder

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Theorem 1. *Let Ω be a set of m indices selected independently from $\{1, \dots, n\}$ with sampling distribution $\boldsymbol{p} \in \mathbb{R}^n$, and M the associated sampling matrix. Let $\epsilon, \delta \in (0,1)$ and $m \geqslant \frac{3}{\delta^2} \, (\nu_{\boldsymbol{p}}^k)^2 \, \log\left(\frac{2k}{\epsilon}\right)$. With probability at least $1 - \epsilon$, the following holds for all $\boldsymbol{x} \in \mathrm{span}(\mathsf{U}_k)$ and all $\boldsymbol{n} \in \mathbb{R}^m$.*

i) Let $\boldsymbol{x}^*$ be the solution of Standard Decoder with $\boldsymbol{y} = \mathsf{M}\boldsymbol{x} + \boldsymbol{n}$. Then,

$$\|\boldsymbol{x}^* - \boldsymbol{x}\|_2 \leqslant \frac{2}{\sqrt{m\,(1-\delta)}} \left\| \mathsf{P}_{\Omega}^{-1/2} \boldsymbol{n} \right\|_2 . \tag{1}$$

ii) There exist particular vectors $\boldsymbol{n}_0 \in \mathbb{R}^m$ such that the solution $\boldsymbol{x}^*$ of Standard Decoder with $\boldsymbol{y} = \mathsf{M}\boldsymbol{x} + \boldsymbol{n}_0$ satisfies

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Efficient Decoder:

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non-negative

Filter reshapes Fourier coefficients

$h : \mathbb{R} \to \mathbb{R}$

$$\boldsymbol{x}_h := \mathsf{U}\, \mathrm{diag}(\hat{\boldsymbol{h}})\, \mathsf{U}^{\mathsf{T}} \boldsymbol{x} \in \mathbb{R}^n$$

$$\hat{\boldsymbol{h}} = (h(\boldsymbol{\lambda}_1), \ldots, h(\boldsymbol{\lambda}_n))^{\mathsf{T}} \in \mathbb{R}^n$$

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$$p(t) = \sum_{i=0}^{d} \alpha_i\, t^i \qquad \boldsymbol{x}_p = \mathsf{U}\,\mathrm{diag}(\hat{\boldsymbol{p}})\,\mathsf{U}^{\mathsf{T}}\boldsymbol{x} = \sum_{i=0}^{d} \alpha_i\, \mathsf{L}^i \boldsymbol{x}$$

Pick special polynomials and use e.g. recurrence relations for fast filtering (with sparse matrix-vector multiply only)

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non-decreasing $=$
penalizes high-frequencies

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Favours reconstruction of approximately band-limited signals

Ideal filter yields Standard Decoder

$$i_{\lambda_k}(t) := \begin{cases} 0 & \text{if } t \in [0, \lambda_k], \\ +\infty & \text{otherwise,} \end{cases}$$

Analysis of Efficient Decoder

Theorem 1. *Let* Ω, M, P, m *as before and* $M_{\max} > 0$ *be a constant such that* $\left\|\mathsf{M}\mathsf{P}^{-1/2}\right\|_2 \leqslant M_{\max}$. *Let* $\epsilon, \delta \in (0,1)$. *With probability at least* $1-\epsilon$, *the following holds for all* $\boldsymbol{x} \in \operatorname{span}(\mathsf{U}_k)$, *all* $\boldsymbol{n} \in \mathbb{R}^n$, *all* $\gamma > 0$, *and all nonnegative and nondecreasing polynomial functions* g *such that* $g(\boldsymbol{\lambda}_{k+1}) > 0$.

Let $\boldsymbol{x}^*$ *be the solution of Efficient Decoder with* $\boldsymbol{y} = \mathsf{M}\boldsymbol{x} + \boldsymbol{n}$. *Then,*

$$\|\boldsymbol{\alpha}^* - \boldsymbol{x}\|_2 \leqslant \frac{1}{\sqrt{m(1-\delta)}} \left[\left(2 + \frac{M_{\max}}{\sqrt{\gamma g(\boldsymbol{\lambda}_{k+1})}} \right) \left\| \mathsf{P}_\Omega^{-1/2} \boldsymbol{n} \right\|_2 + \left(M_{\max} \sqrt{\frac{g(\boldsymbol{\lambda}_k)}{g(\boldsymbol{\lambda}_{k+1})}} + \sqrt{\gamma g(\boldsymbol{\lambda}_k)} \right) \|\boldsymbol{x}\|_2 \right], \tag{1}$$

and

$$\|\boldsymbol{\beta}^*\|_2 \leqslant \frac{1}{\sqrt{\gamma g(\boldsymbol{\lambda}_{k+1})}} \left\| \mathsf{P}_\Omega^{-1/2} \boldsymbol{n} \right\|_2 + \sqrt{\frac{g(\boldsymbol{\lambda}_k)}{g(\boldsymbol{\lambda}_{k+1})}} \|\boldsymbol{x}\|_2, \tag{2}$$

where $\boldsymbol{\alpha}^* := \mathsf{U}_k \mathsf{U}_k^\intercal \boldsymbol{x}^*$ *and* $\boldsymbol{\beta}^* := (\mathsf{I} - \mathsf{U}_k \mathsf{U}_k^\intercal)\, \boldsymbol{x}^*$.

Analysis of Efficient Decoder

Noiseless case:

$$\|\boldsymbol{x}^* - \boldsymbol{x}\|_2 \leqslant \frac{1}{\sqrt{m(1-\delta)}} \left(M_{\max} \sqrt{\frac{g(\boldsymbol{\lambda}_k)}{g(\boldsymbol{\lambda}_{k+1})}} + \sqrt{\gamma g(\boldsymbol{\lambda}_k)} \right) \|\boldsymbol{x}\|_2 + \sqrt{\frac{g(\boldsymbol{\lambda}_k)}{g(\boldsymbol{\lambda}_{k+1})}} \|\boldsymbol{x}\|_2$$

$g(\boldsymbol{\lambda}_k) = 0$ + non-decreasing implies perfect reconstruction

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$g(\boldsymbol{\lambda}_k) = 0$ + non-decreasing implies perfect reconstruction

Otherwise:

choose γ as close as possible to 0 and seek to minimise the ratio $g(\boldsymbol{\lambda}_k)/g(\boldsymbol{\lambda}_{k+1})$

Choose filter to increase spectral gap ?

Clusters are of course good

Noise: $\|\mathsf{P}_\Omega^{-1/2}\boldsymbol{n}\|_2 / \|\boldsymbol{x}\|_2$

Estimating the Optimal Distribution

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$$\boxed{\text{Need to estimate} \quad \|\mathsf{U}_k^\intercal \boldsymbol{\delta}_i\|_2^2}$$

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Filter random signals with ideal low-pass filter:

$$\boldsymbol{r}_{b_{\boldsymbol{\lambda}_k}} = \mathsf{U}\,\mathrm{diag}(\boldsymbol{\lambda}_1, \ldots, \boldsymbol{\lambda}_k, 0, \ldots, 0)\,\mathsf{U}^\intercal\,\boldsymbol{r} = \mathsf{U}_k \mathsf{U}_k^\intercal\,\boldsymbol{r}$$

$$\mathbb{E}\left(\boldsymbol{r}_{b_{\boldsymbol{\lambda}_k}}\right)_i^2 = \boldsymbol{\delta}_i^\intercal \mathsf{U}_k \mathsf{U}_k^\intercal\,\mathbb{E}(\boldsymbol{r}\boldsymbol{r}^\intercal)\,\mathsf{U}_k \mathsf{U}_k^\intercal \boldsymbol{\delta}_i = \|\mathsf{U}_k^\intercal \boldsymbol{\delta}_i\|_2^2$$

Estimating the Optimal Distribution

$$\boxed{\text{Need to estimate} \quad \|\mathsf{U}_k^\intercal \boldsymbol{\delta}_i\|_2^2}$$

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In practice, one may use a polynomial approximation of the ideal filter and:

$$\tilde{\boldsymbol{p}}_i := \frac{\sum_{l=1}^{L} \left(\boldsymbol{r}^l_{c_{\lambda_k}}\right)_i^2}{\sum_{i=1}^{n} \sum_{l=1}^{L} \left(\boldsymbol{r}^l_{c_{\lambda_k}}\right)_i^2}$$

$$L \geqslant \frac{C}{\delta^2} \log\left(\frac{2n}{\epsilon}\right)$$

Estimating the Eigengap

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Again, low-pass filtering random signals:

$$(1-\delta)\sum_{i=1}^{n}\left\|\mathsf{U}_{j*}^{\mathsf{T}}\boldsymbol{\delta}_i\right\|_2^2 \leqslant \sum_{i=1}^{n}\sum_{l=1}^{L}(\boldsymbol{r}_{b_\lambda}^{l})_i^2 \leqslant (1+\delta)\sum_{i=1}^{n}\left\|\mathsf{U}_{j*}^{\mathsf{T}}\boldsymbol{\delta}_i\right\|_2^2$$

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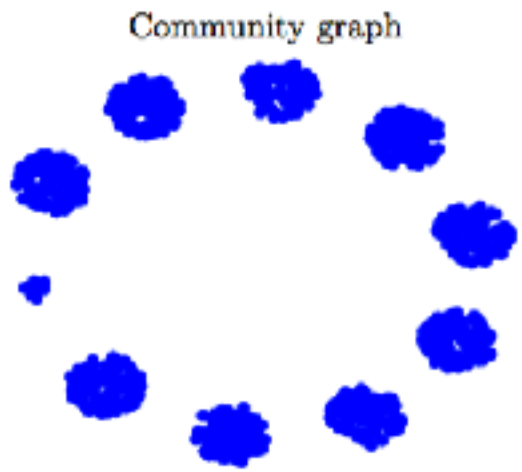
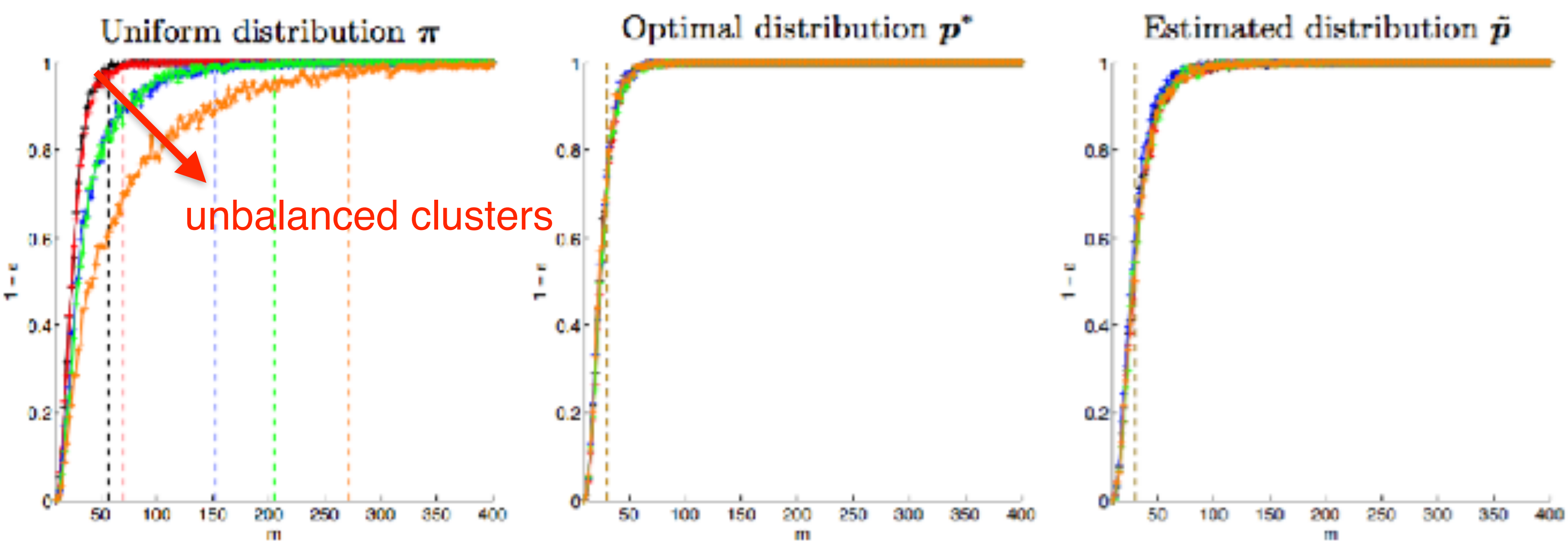
Since: $$\sum_{i=1}^{n}\left\|\mathsf{U}_{j^*}^{\mathsf{T}}\boldsymbol{\delta}_i\right\|_2^2 = \|\mathsf{U}_{j^*}\|_{\text{Frob}}^2 = j^*$$

We have: $$(1-\delta)\,j^* \leqslant \sum_{i=1}^{n}\sum_{l=1}^{L}(\boldsymbol{r}_{b_\lambda}^{l})_i^2 \leqslant (1+\delta)\,j^*$$

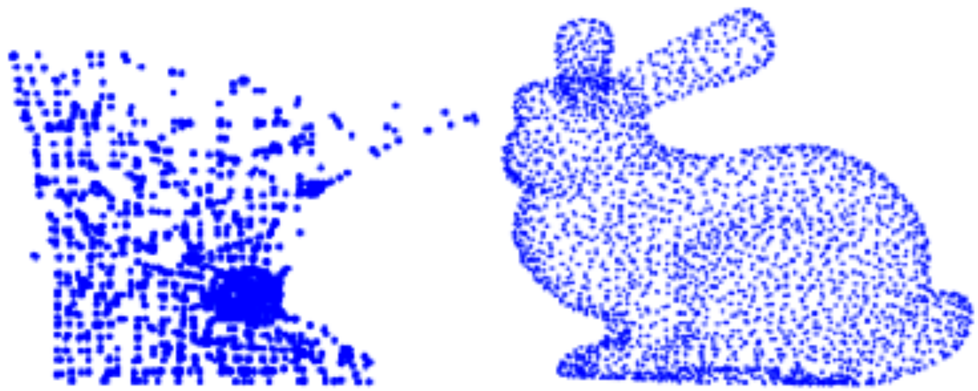
Dichotomy using the filter bandwidth

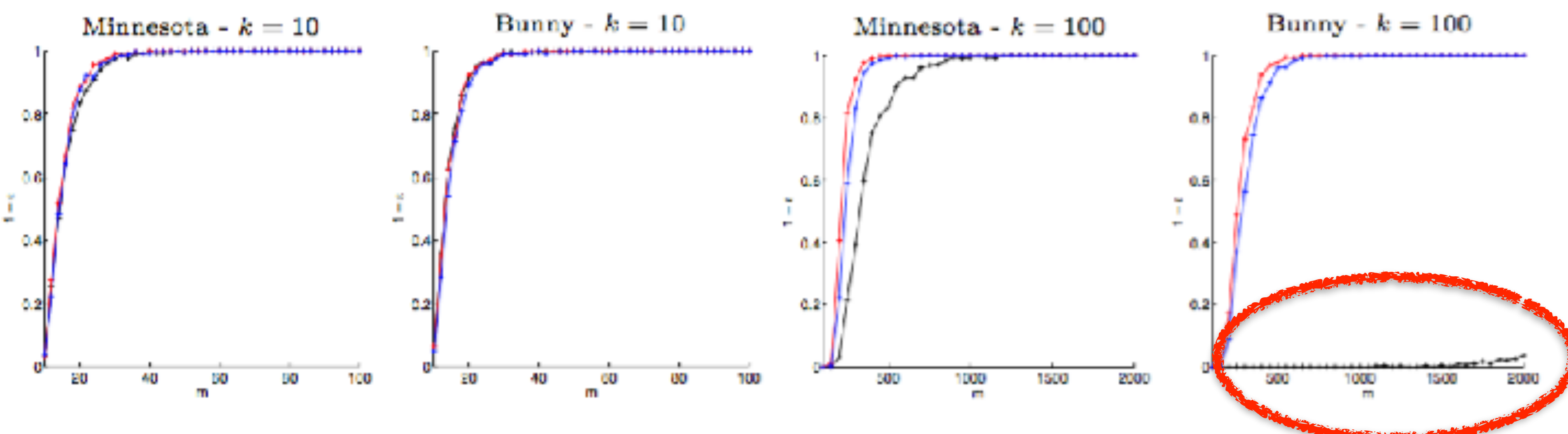
Experiments



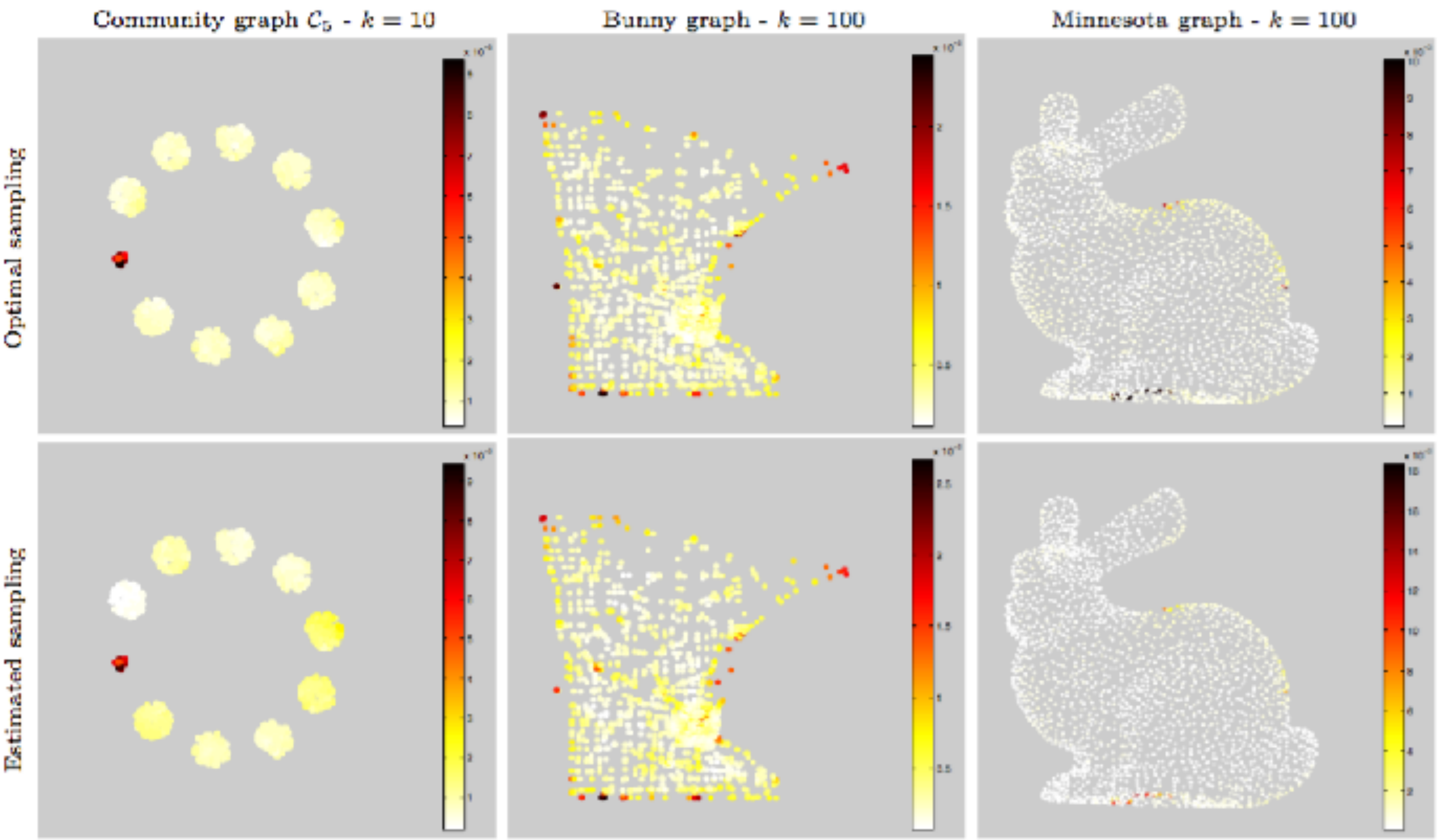


Experiments





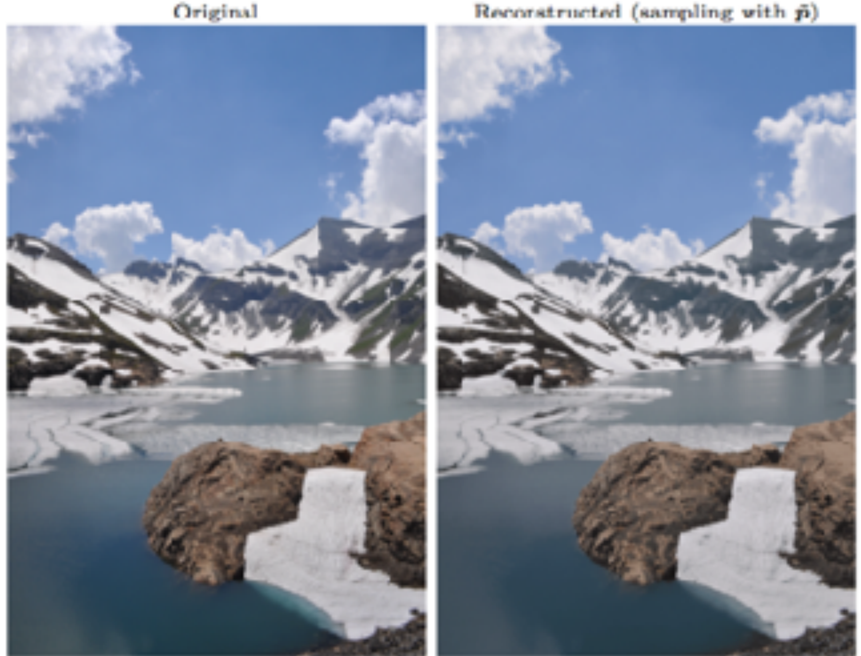
Experiments



Experiments

(a) (b)

Original Reconstructed (sampling with $\bar{p}$)



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Compressive Spectral Clustering

Clustering equivalent to recovery of cluster assignment functions

Well-defined clusters -> band-limited assignment functions!

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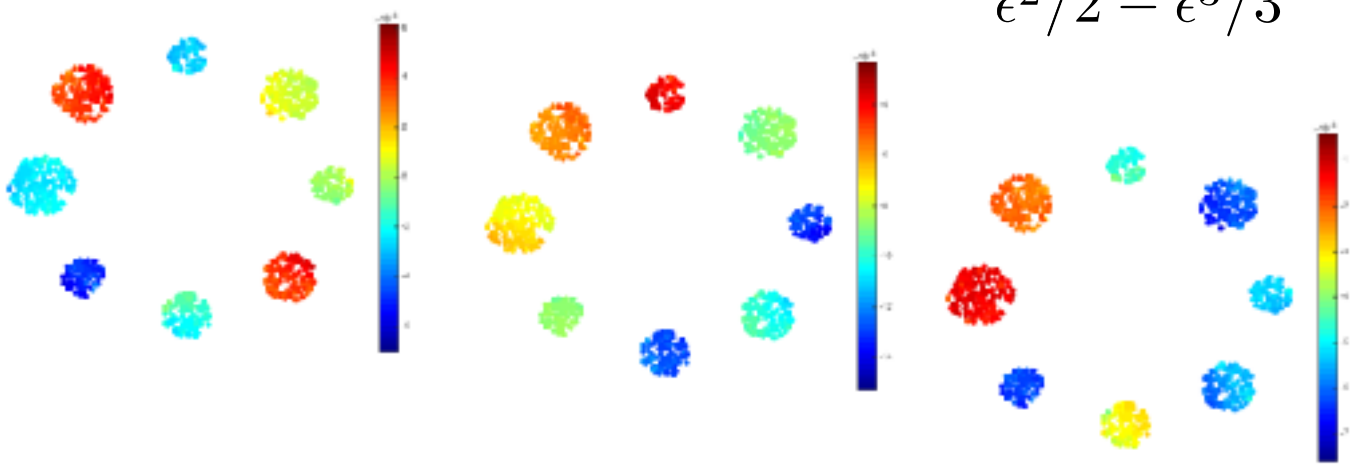
Generate features by filtering random signals

by Johnson-Lindenstrauss $\eta = \dfrac{4 + 2\beta}{\epsilon^2/2 - \epsilon^3/3} \log n$



Compressive Spectral Clustering

Clustering equivalent to recovery of cluster assignment functions

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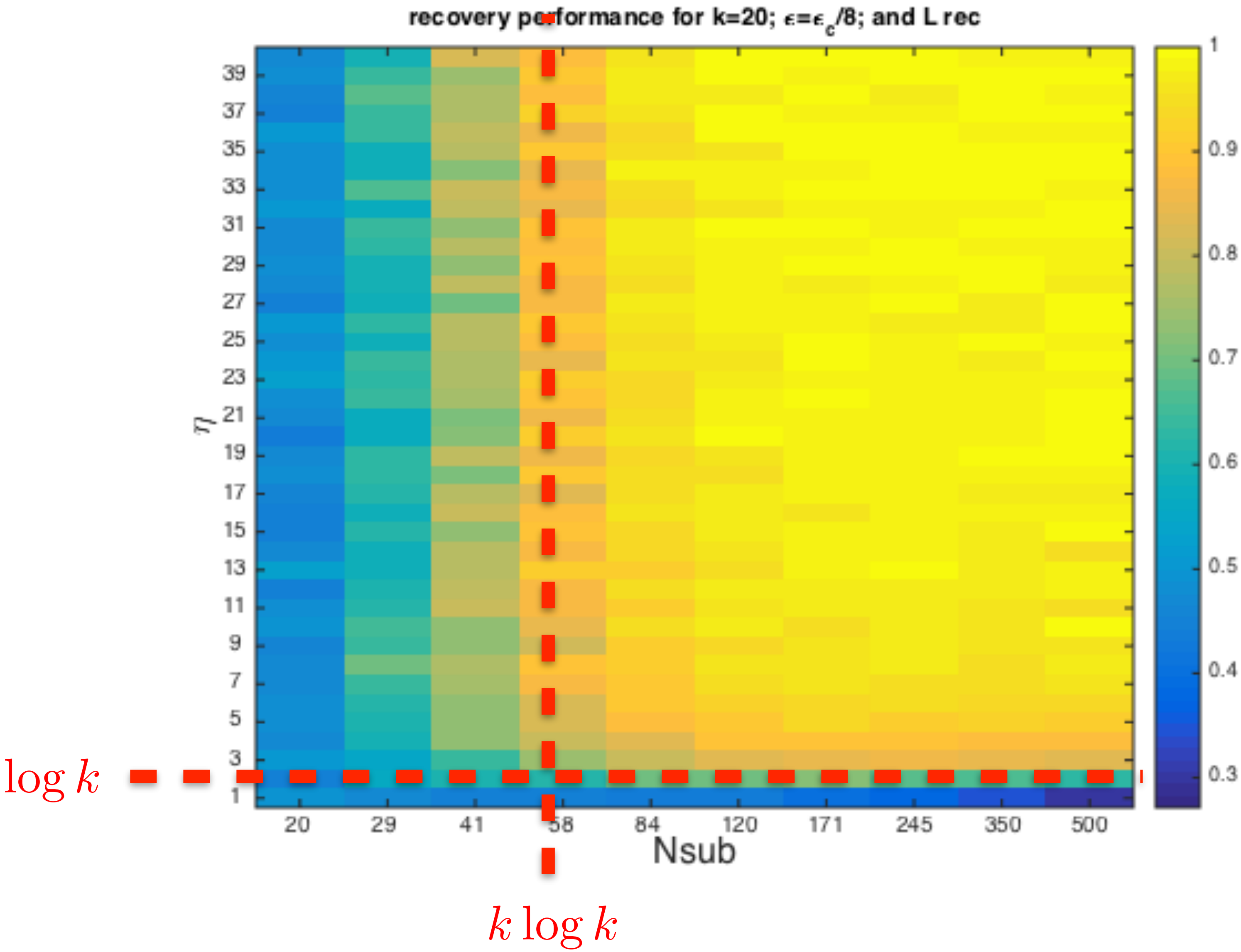
Each feature map is smooth, therefore keep

$$m \geqslant \frac{6}{\delta^2}\, \nu_k^2 \, \log\left(\frac{k}{\epsilon'}\right)$$

Use k-means on compressed data and feed into Efficient Decoder

Compressive Spectral Clustering



Conclusion

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- ***Optimal sampling distribution*** depends on graph structure

- Can be used for inference, (SVD less) compressive clustering

Thank you !