Sparse Partial Least Squares for Coarse Noisy Graph Alignment

Michael Weylandt

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IC Postdoctoral Research Fellow
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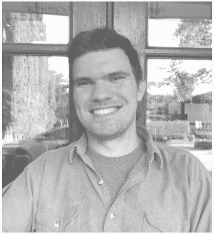
Acknowledgements

Co-Authors: George Michailidis (UF) and Mitch Roddenberry (Rice ECE)

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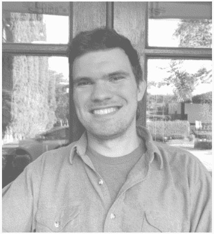

US Intelligence Community Postdoctoral Research Fellowship

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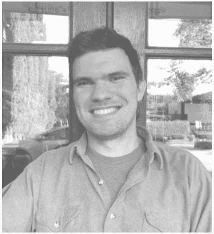

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Discussions: Genevera Allen (Rice U)

Ubiquitous Network Data: telecommunications, social media, neuroscience, sensor networks, transportation, *etc.*

Network Data

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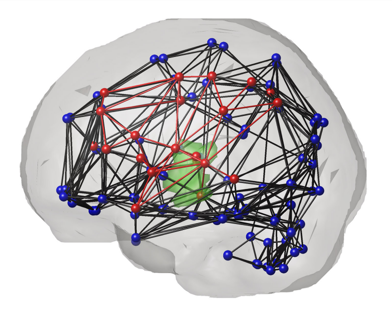
Three types of network data:

- Networks as models of complex phenomena ("graphical models")



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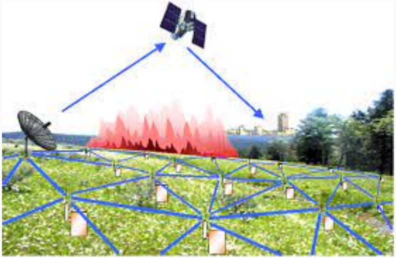

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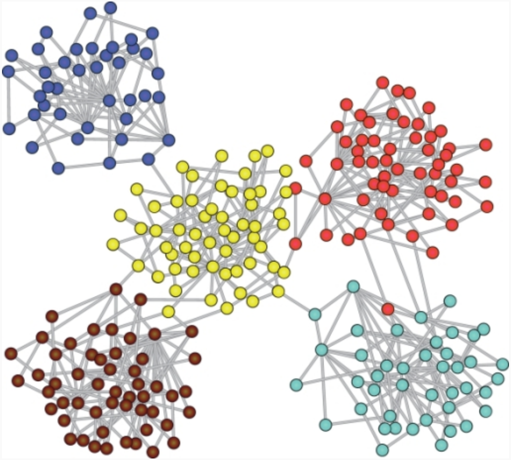
Today: contributions to **network science** and **graph signal processing**

Community Detection

Community detection - dividing an observed network into meaningful groups ("communities")



Very well studied problem (Levina, Zhu, Amini, Vershynin, Bickel ...)

Coarse Alignment via Graph Signal Processing

Graph alignment:

- Input: two graphs $\mathcal{G}_1, \mathcal{G}_2$
- Output: Mapping between $\mathcal{V}_1, \mathcal{V}_2$ so that the graphs are (nearly) "the same" under some metric

Can require exact alignment or allow inexact matching (possibly on different size graphs)

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Goal: Coarse graph alignment using noisy graph signals on $\mathcal{G}_1, \mathcal{G}_2$

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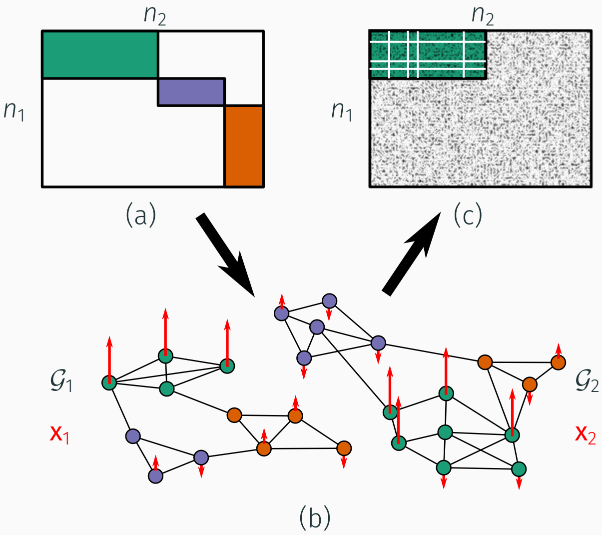
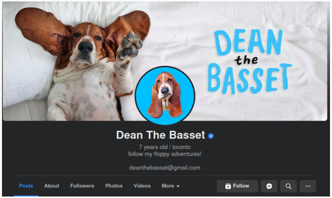
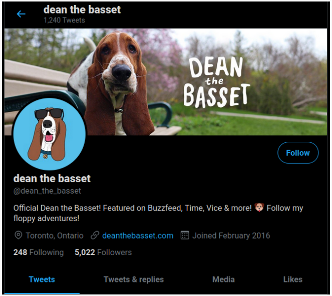
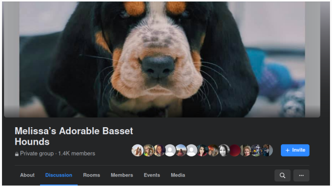


Example: Coarse Alignment via Graph Signal Processing







CONGA via Sparse Graph PLS

Model: two graphs $\mathcal{G}_1$, $\mathcal{G}_2$ with corresponding signals

- Graphs have "paired" community structure
- If community of $\mathcal{G}_1$ reflects signal, so does corresponding in $\mathcal{G}_2$
- No other structural assumptions on $\mathcal{G}_1, \mathcal{G}_2$

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Solution: Graph-Regularized Sparse Multi-Rank PLS

$$\underset{\mathbf{U},\mathbf{V}\in\mathcal{V}_{n_1\times K}^{\mathbf{I}_{n_1}+\alpha_1\mathbf{L}_1}\times\mathcal{V}_{n_2\times K}^{\mathbf{I}_{n_2}+\alpha_2\mathbf{L}_2}}{\arg\max}\ \mathrm{Tr}(\mathbf{U}^\top\mathbf{X}_1^\top\mathbf{X}_2\mathbf{V}) - \lambda_1 P_1(\mathbf{U}) - \lambda_2 P_2(\mathbf{V})$$

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Decompose $X_1^T X_2$ into two parts U, V such that:

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$$\mathop{\arg\max}_{\mathbf{U},\mathbf{V} \in \mathcal{V}_{n_1 \times K}^{\mathbf{I}_{n_1}+\alpha_1 \mathbf{L}_1} \times \mathcal{V}_{n_2 \times K}^{\mathbf{I}_{n_2}+\alpha_2 \mathbf{L}_2}} \mathrm{Tr}(\mathbf{U}^\top \mathbf{X}_1^\top \mathbf{X}_2 \mathbf{V}) - \lambda_1 P_1(\mathbf{U}) - \lambda_2 P_2(\mathbf{V})$$

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Decompose $X_1^T X_2$ into two parts U, V such that:

- correlation between signals
- in a way that respects graph structure

$$\mathbf{U} \in \mathcal{V}^{\mathbf{I}_{n_1} + \alpha_1 \mathbf{L}_1} \Leftrightarrow \mathbf{U}^T (\mathbf{I}_{n_1} + \alpha_1 \mathbf{L}_1) \mathbf{U} = \mathbf{I}$$

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Decompose $X_1^T X_2$ into two parts U, V such that:

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- and selects a sparse set of nodes

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Sparsity + Orthogonality $\approx$ Non-overlapping support

Paired columns of $\mathbf{U}, \mathbf{V}$ give corresponding community membership

Algorithm: Manifold Optimization

Sparse Graph-Smooth PLS Algorithm

1. Construct Graph Laplacians $\mathsf{L}_1, \mathsf{L}_2$ and associated smoothing matrices $\mathsf{S}_1 = \mathsf{I}_{n_1} + \alpha_1 \mathsf{L}_1$, $\mathsf{S}_2 = \mathsf{I}_{n_2} + \alpha_2 \mathsf{L}_2$
2. Initialize $\hat{\mathsf{U}}, \hat{\mathsf{V}}$ to the leading K singular vectors of $\mathsf{X}_1^\top \mathsf{X}_2$
3. Repeat until convergence:

$$\hat{\mathsf{U}} = \underset{\mathsf{U} \in \text{conv}\, \mathcal{V}^{\mathsf{S}_1}_{n_1 \times K}}{\arg\min} - \text{Tr}(\mathsf{U}^\top \mathsf{X}_1^\top \mathsf{X}_2 \hat{\mathsf{V}}) + \lambda_1 P_1(\mathsf{U})$$

$$\hat{\mathsf{V}} = \underset{\mathsf{V} \in \text{conv}\, \mathcal{V}^{\mathsf{S}_2}_{n_2 \times K}}{\arg\min} - \text{Tr}(\mathsf{V}^\top \mathsf{X}_2^\top \mathsf{X}_1 \hat{\mathsf{U}}) + \lambda_2 P_2(\mathsf{V})$$

4. Return $\hat{\mathsf{U}}$ and $\hat{\mathsf{V}}$

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Application of Multi-Rank Regularized PCA (Weylandt, 2019) to PLS

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4. Return $\hat{\mathbf{U}}$ and $\hat{\mathbf{V}}$

Application of Multi-Rank Regularized PCA (Weylandt, 2019) to PLS

Solve $\hat{\mathbf{U}}, \hat{\mathbf{V}}$-subproblems via Manifold ADMM (Kovnatsky *et al.*, 2016)

Sparse Graph-Smooth PLS Algorithm (Greedy Variant for Large Graphs)

1. Construct Graph Laplacians and smoothing matrices with leading eigenvalues $\ell_1 = \lambda_{\max}(\mathsf{S}_1)$ and $\ell_2 = \lambda_{\max}(\mathsf{S}_2)$
2. Initialize $\mathbf{C}_1 := \mathsf{X}_1^\top \mathsf{X}_2$
3. For $k = 1, \dots K$:
   - 3.1 Initialize $\hat{\mathbf{u}}_k, \hat{\mathbf{v}}_k$ to the leading singular vectors of $\mathbf{C}_k$
   - 3.2 Repeat until convergence:
     - 3.2.1 iterate $\mathbf{u}$-update: $\hat{\mathbf{u}}_k \propto \text{prox}_{\frac{\lambda_1}{\ell_1} P_1(\cdot)}\left(\mathbf{u}_k + \ell_1^{-1}\left(\mathbf{C}_k\hat{\mathbf{v}}_k - \mathsf{S}_1\mathbf{u}_k\right)\right)$
     - 3.2.2 iterate $\mathbf{v}$-update: $\hat{\mathbf{v}}_k \propto \text{prox}_{\frac{\lambda_2}{\ell_2} P_2(\cdot)}\left(\mathbf{v}_k + \ell_2^{-1}\left(\mathbf{C}_k^\top\hat{\mathbf{u}}_k - \mathsf{S}_2\mathbf{v}_k\right)\right)$
   - 3.3 Set $\mathbf{C}_{k+1} := \mathbf{C}_k - \frac{\mathbf{C}_k\hat{\mathbf{v}}_k\hat{\mathbf{u}}_k^T\mathbf{C}_k}{\hat{\mathbf{u}}_k^T\mathbf{C}_k\hat{\mathbf{v}}_k}$
4. Return $\{\hat{\mathbf{u}}_k\}_{k=1}^K$ and $\{\hat{\mathbf{v}}_k\}_{k=1}^K$

Combines Rank-1 Sparse and Functional PCA (Allen and Weylandt, 2019) with Schur Deflation (Weylandt, 2019)

Regularity and Optimality Guarantees

The CONGA problem is well-posed

1. $|\mathbf{U}^*_{\cdot k}\|_{S_1}$ is either 0 or 1 for all k. Similarly for $\mathbf{V}^*$.
2. If $(\mathbf{U}^*, \mathbf{V}^*) \neq (0, 0)$, the SGPLS solution $(\mathbf{U}^*, \mathbf{V}^*)$ depends smoothly on all (non-zero) regularization parameters.

Theoretical Properties

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Furthermore, the proposed algorithms are well-behaved:

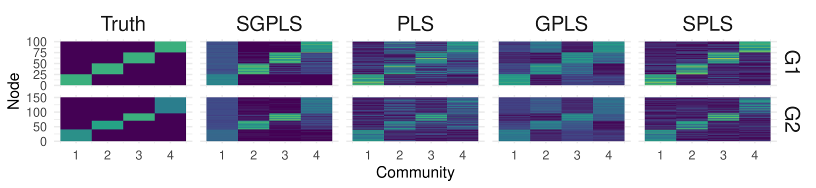
1. Step 3.2.1 of the greedy algorithm converges to a stationary point of

$$\underset{\mathbf{u}:\mathbf{u}^\top(\mathbf{I}+\alpha_1\mathbf{L}_1)\mathbf{u}\leq 1}{\arg\min} \frac{1}{2}\|\mathbf{C}_k\hat{\mathbf{v}}_k - \mathbf{u}\|_2^2 + \lambda_1 P_1(\mathbf{u}) + \frac{\alpha_1}{2}\mathbf{u}^\top\mathbf{L}_1\mathbf{u}$$

   Furthermore, if P_1 is convex, the convergence is monotone, at an $\mathcal{O}(1/K)$ rate, and to a global solution. Similar for Step 3.2.2
2. If P_1, P_2 are both convex, then $(\hat{\mathbf{u}}_k, \hat{\mathbf{v}}_k)$ returned by each step 3(b) of the greedy algorithm is both a coordinate-wise global maximum (Nash point) and a stationary point of SGPLS.

Simulation:

- $\mathcal{G}_1$: 4-block SBM (25, 25, 25, 25) with $p = 0.95, q = 0.2$
- $\mathcal{G}_2$: 4-block SBM (40, 30, 25, 55) with $p = 0.95, q = 0.2$
- m = 1000 signals: $\text{SNR}_{\mathcal{G}_1} = 0.2$, $\text{SNR}_{\mathcal{G}_2} = 0.163$
- Oracle tuning for all methods



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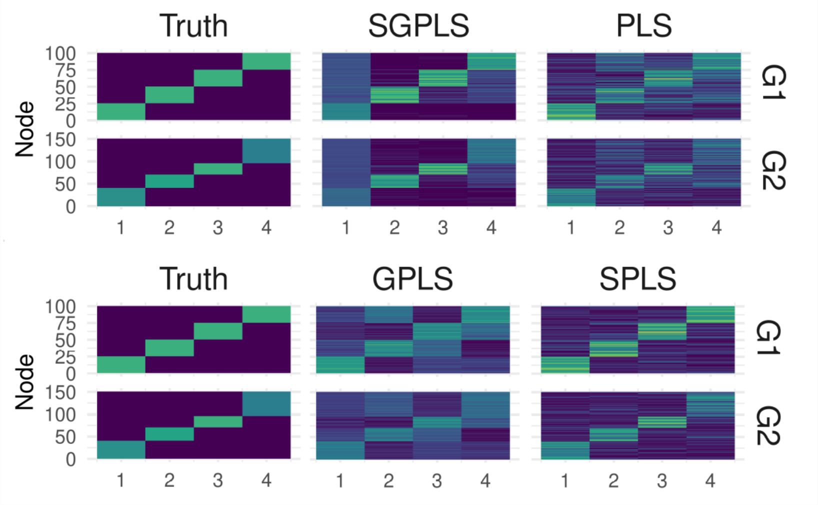

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Coarse Network Alignment: ArXiv 2104.02810

Thank you!

References

Allen, Genevera I. and Michael Weylandt (2019). "Sparse and Functional Principal Components Analysis". In: *DSW 2019: Proceedings of the 2nd IEEE Data Science Workshop*. Ed. by George Karypis, George Michailidis, and Rebecca Willett. Minneapolis, Minnesota: IEEE, pp. 11–16.

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