Graph topology inference benchmarks for machine learning

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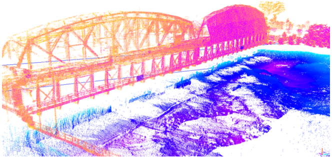
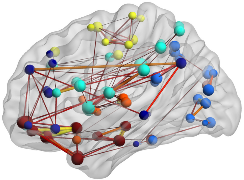
MLSP - September 2020

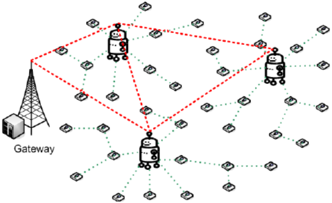
Benchmarks available at:
https://github.com/cadurosar/benchmark_graphinference

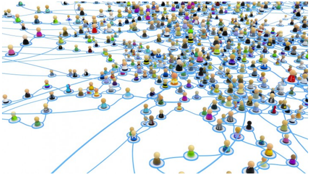
Motivation

Graphs are ubiquitous in machine learning









What is the best graph for my considered task?

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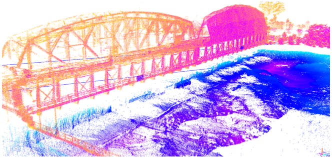

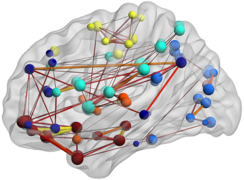

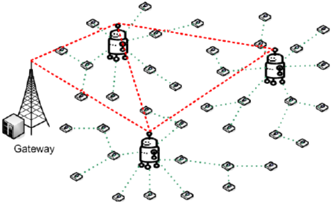

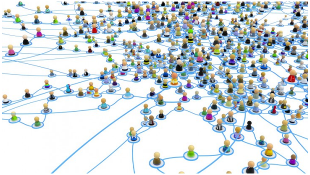

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Outline

1. Graph inference
2. Proposed benchmark framework
3. Baseline, results and findings
4. Conclusion

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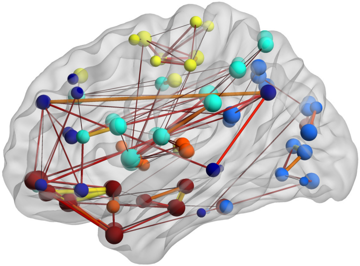
Graphs

- Graphs express relationships between items;
- Ubiquitous in machine learning;
- **Problem:** Not always available;
- *Solution:* Infer a graph from the data.



Graph Inference

- There are numerous ways to infer a graph from data:
  - Stationarity [Pasdeloup et al 2017, Segarra et al 2018];
  - Probabilistic [Egilmez et al 2017];
  - Smoothness [Kalofolias et al 2019];
  - Sparsity [Shekizzar and Ortega 2020].

Key question: what method offers the best performance?

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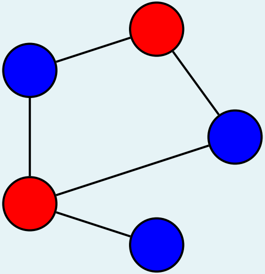

Graph Inference

Limitations of existing works

- Techniques are developed using specific priors;
- Those priors might or might not be aligned with various tasks;
- Benchmarking graph inference requires to be able to showcase these different characteristics;
- Often rely on synthetic data and graphs aligned with their priors.

Our contribution

- We introduce a comprehensive set of benchmarks meant to:
  - Represent a diverse set of cases;
  - Use real data and real tasks;
  - Be easy-to-use and fair for comparison purposes;
  - Reflect the pros and cons of proposed methods.

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Proposed benchmark

Main contribution

Tasks

1. Unsupervised Clustering of Vertices;
2. Semi-Supervised Classification of Vertices;
3. Denoising of Graph Signals.

Datasets for tasks 1 and 2

Graphs encode relationship between observations:

- Images - flowers102
- Audio - ESC-50
- Text - cora

Dataset for task 3

Graph of relationship between features

- Vehicule traffic volume denoising - Toronto.

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Objective

Evaluate how aligned is the inferred graph structure to the unsupervised clustering.

Evaluation

AMI of the Spectral Clustering using the inferred graph.

Task 2

Semi-Supervised Classification of Vertices

Objective

Evaluate the performance of the inferred graph in identifying the class of each vertex.

Evaluation

Two types of evaluation:

- Label only: Test set accuracy using label propagation on the graph;
- Label and Features: Test set accuracy using SGC[Wu et al 2019].

Averaged over 100 runs using 5% of labeled nodes.

Task 1 and 2 Datasets

Image dataset - flowers102 [Nilsback and Zisserman 2008]

- Flower identification;
- From flowers102 [Nilsback and Zisserman 2008]
- InceptionV2 [Szegedy et al 2016] features;
- Very challenging:
  - High amount of classes (102)
  - High signal to items ratio (2)

Task 1 and 2 Datasets

Audio dataset - ESC-50 [Piczak 2015]

- Environment classification via audio;
- Features extracted with [Kumar et al 2018];
- Easier than the image dataset:
  - Medium amount of classes (50)
  - Small signal to items ratio (0.512)

Task 1 and 2 Datasets

Text dataset - Cora [Sen et al 2008]

- Scientific article classification;
- Has a citation graph that we do not use;
- Medium difficulty dataset:
    - Small amount of classes (7);
    - Small signal to items ratio (0.53);
    - Bag of Words -> binary features.

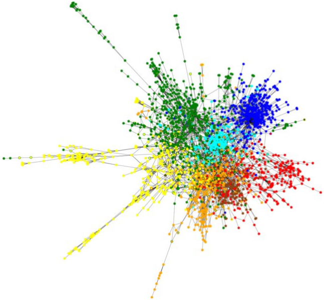

Figure extracted from [Monti et al 2017]

Task 3

Denoising of Graph Signals

Objective

Performance of the inferred graph on graph signal denoising.

Evaluation

Signal-to-noise ratio of the signal denoised by a Simoncelli graph filter.

$$f_l = \begin{cases} 1 & \text{if } \lambda_l \leq \frac{\tau}{2} \\ \cos\left(\frac{\pi}{2}\frac{\log(\lambda_l)}{\log(2)}\right) & \text{if } \frac{\tau}{2} < \lambda_l \leq \tau \\ 0 & \text{if } \lambda_l > \tau \end{cases},$$

Dataset

Toronto traffic data with added noise [Irion and Saito 2016].

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Outline

Proposed baselines

Naive baselines

Baselines based on four steps:

1. Similarity: Cosine, RBF and Covariance;
2. Sparsity: Different values of k-NN;
3. Symmetrize the graph;
4. Normalization: Yes or no.

Prior-based baselines

Baselines based on a prior of a signal property:

- Smoothness prior: Kalofolias method [Kalofolias et al 2019]
- Sparsity prior: NNK method [Shekizzar and Ortega 2020]

Results

Task 1: Unsupervised Clustering of Vertices

Method	Inference/Dataset	ESC-50	cora	flowers102
C-means		0.59	0.10	0.36
Spectral clustering	Naive	**0.66**	**0.34**	**0.45**
	NNK	**0.66**	**0.34**	0.44
	Kalofolias	0.65	0.27	0.44

Results

Task 2: Semi-Supervised Classification of Vertices - labels only

Method	Inference/Dataset	ESC-50	cora	flowers102
Logistic Regression		52.92% $\pm$1.9	46.84% $\pm$1.6	33.51% $\pm$1.7
Label Propagation	Naive	59.05% $\pm$1.8	**58.86%** $\pm$2.9	36.73% $\pm$1.6
	NNK	57.44% $\pm$2.2	58.66% $\pm$2.9	33.57% $\pm$1.6
	Kalofolias	**59.16%** $\pm$1.8	58.60% $\pm$3.4	**37.01%** $\pm$1.7

Results

Task 2: Semi-Supervised Classification of Vertices - labels and features

Method	Inference/Dataset	ESC-50	cora	flowers102
Logistic Regression		52.92% ±1.9	46.84% ±1.6	33.51% ±1.7
SGC	Naive	60.48% ±2.0	**67.19%** ±1.5	**37.73%** ±1.5
	NNK	**61.38%** ±2.0	66.58% ±1.5	36.81% ±1.5
	Kalofolias	59.36% ±2.0	66.28% ±1.5	37.5% ±1.5

Results

Task 3: Denoising of Graph Signals

	Road graph	Kalofolias	RBF NNK	RBF k-NN
Best SNR	10.32	**10.41**	9.99	9.80

Initial findings

1. **Graph-based methods:** Outperform the non-graph baselines;
2. **Similarity choice:** When possible use the cosine similarity;
3. **Sparsity**: Method and dataset dependant. NNK and Kalofolias are more stable;
4. **Normalization:** As expected, normalized graphs perform better;
5. **Naive baselines vs. optimization approaches:** No clear winner, NNK and Kalofolias are less hyperparameter dependant;
6. **Hard task:** sparse graphs in semi-supervised random splits.

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Summary

- Graphs -> natural way to encode relational data;
- Not always available -> **graph inference** is needed;
- Evaluating graph inference is hard -> we introduce a benchmark;
- Easily accessible online:
  - `https://github.com/cadurosar/benchmark_graphinference`;
- Tests with baselines -> encouraging findings.

Future work

- Extend to additional graph-related tasks;
- Include more task-agnostic methods;
- Improve task-specific evaluation.

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Thank you for your attention

Benchmarks available at:

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References

- Nilsback and Zisserman 2008 “Collective classification in network data” AI Magazine;
- Sen et al 2008 “Automated flower classification over a large number of classes” ICVGIP;
- Piczak 2015 “ESC: Dataset for Environmental Sound Classification” ACM on Multimedia;
- Irion and Saito 2016 “Efficient approximation and denoising of graph signals using the multiscale basis dictionaries” IEEE TSIPN;
- Szegedy et al 2016 “Rethinking the inception architecture for computer vision” CVPR;
- Pasdeloup et al 2017 “Characterization and inference of graph diffusion processes from observations of stationary signals” IEEE TSIPN;
- Egilmez et al 2017 “Graph learning from data under Laplacian and structural constraints” IEEE JSTSP;
- Monti et al 2017 “Geometric deep learning on graphs and manifolds using mixture model CNNs” CVPR;
- Kumar et al 2018 “Knowledge transfer from weakly labeled audio using convolutional neural network for sound events and scenes” ICASSP;
- Kalofolias et al 2019 “Large scale graph learning from smooth signals” ICLR;
- Shekizzar and Ortega 2020 “Graph construction from data using non negative kernel regression (NNK graphs)” ICASSP;