# Graph topology inference benchmarks for machine learning

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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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# Outline

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

# 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 o ers the best performance?

**Example of graph inference:**

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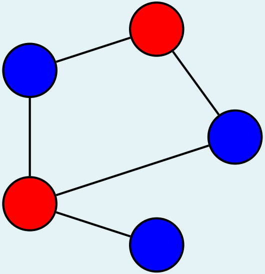
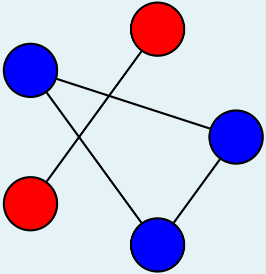
## Example of graph inference:

# Graph Inference

## Limitations of existing works

- Techniques are developed using speci c priors;
- Those priors might or might not be aligned with various tasks;
- Benchmarking graph inference requires to be able to showcase these di erent 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;
  - Re ect the pros and cons of proposed methods.

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# Proposed benchmark
## Main contribution

### Tasks

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

### Datasets for tasks 1 and 2

Graphs encode relationship between observations:

- Images - owers102
- Audio - ESC-50
- Text - cora

### Dataset for task 3

Graph of relationship between features

- Vehicule tra c volume denoising - Toronto.

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# Task 1

## Unsupervised Clustering of Vertices

### 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 Classi cation 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 -  owers102 [Nilsback and Zisserman 2008]

- Flower identi cation;
- From  owers102 [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 classi cation 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]

- Scienti c article classi cation;
- Has a citation graph that we do not use;
- Medium di culty 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]

## Objective

Performance of the inferred graph on graph signal denoising.

## Evaluation

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

$$f_l = \begin{cases} 1 & \text{if } {}_l \quad \frac{}{2} \\ \cos\left(\frac{}{2}\frac{\log({}_l)}{\log(2)}\right) & \text{if } \frac{}{2} < {}_l \\ 0 & \text{if } {}_l > \end{cases};$$

## Dataset

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

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## Denoising of Graph Signals

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# Proposed baselines

## Naive baselines

Baselines based on four steps:

1. Similarity: Cosine, RBF and Covariance;
2. Sparsity: Di erent 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 | owers102 |
|---|---|---|---|---|
| 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 Classi cation of Vertices - labels only

| Method | Inference/Dataset | ESC-50 | | cora | | owers102 | |
|---|---|---|---|---|---|---|---|
| Logistic Regression | | 52.92% | 1:9 | 46.84% | 1:6 | 33.51% | 1:7 |
| Label Propagation | Naive | 59.05% | 1:8 | 58.86% | 2:9 | 36.73% | 1:6 |
| | NNK | 57.44% | 2:2 | 58.66% | 2:9 | 33.57% | 1:6 |
| | Kalofolias | 59.16% | 1:8 | 58.60% | 3:4 | 37.01% | 1:7 |

# Results

## Task 2: Semi-Supervised Classi cation of Vertices - labels and features

| Method | Inference/Dataset | ESC-50 | | cora | | owers102 | |
|---|---|---|---|---|---|---|---|
| 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  ndings

Graph-based methods: Outperform the non-graph baselines;

Similarity choice: When possible use the cosine similarity;

Sparsity : Method and dataset dependant. NNK and Kalofolias are more stable;

Normalization: As expected, normalized graphs perform better;

Naive baselines vs. optimization approaches: No clear winner, NNK and Kalofolias are less hyperparameter dependant;

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


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