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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Graphs are ubiquitous in machine learning

What is the best graph for my considered task?
Outline

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

2. Proposed benchmark framework

3. Baseline, results and findings

4. Conclusion
Graphs

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

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Key question: what method offers the best performance?

Example of 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.
Proposed benchmark

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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.
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 [Nilsson and Zisserman 2008]

- Flower identification;
- From flowers102 [Nilsson 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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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

<table>
<thead>
<tr>
<th>Method</th>
<th>Inference/Dataset</th>
<th>ESC-50</th>
<th>cora</th>
<th>flowers102</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-means</td>
<td></td>
<td>0.59</td>
<td>0.10</td>
<td>0.36</td>
</tr>
<tr>
<td>Spectral clustering</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Naive</td>
<td></td>
<td>0.66</td>
<td>0.34</td>
<td>0.45</td>
</tr>
<tr>
<td>NNK</td>
<td></td>
<td>0.66</td>
<td>0.34</td>
<td>0.44</td>
</tr>
<tr>
<td>Kalofolias</td>
<td></td>
<td>0.65</td>
<td>0.27</td>
<td>0.44</td>
</tr>
</tbody>
</table>

C. Lassance, V. Gripon and G. Mateos

Graph inference benchmarks

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## Results

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

<table>
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<tr>
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<th>flowers102</th>
</tr>
</thead>
<tbody>
<tr>
<td>Logistic Regression</td>
<td></td>
<td>52.92% ±1.9</td>
<td>46.84% ±1.6</td>
<td>33.51% ±1.7</td>
</tr>
<tr>
<td>Label Propagation</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Naive</td>
<td></td>
<td>59.05% ±1.8</td>
<td>58.86% ±2.9</td>
<td>36.73% ±1.6</td>
</tr>
<tr>
<td>NNK</td>
<td></td>
<td>57.44% ±2.2</td>
<td>58.66% ±2.9</td>
<td>33.57% ±1.6</td>
</tr>
<tr>
<td>Kalofolias</td>
<td></td>
<td>59.16% ±1.8</td>
<td>58.60% ±3.4</td>
<td>37.01% ±1.7</td>
</tr>
</tbody>
</table>
Results

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

<table>
<thead>
<tr>
<th>Method</th>
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<tr>
<td>Logistic Regression</td>
<td></td>
<td>52.92% ±1.9</td>
<td>46.84% ±1.6</td>
<td>33.51% ±1.7</td>
</tr>
<tr>
<td>SGC</td>
<td>Naive</td>
<td>60.48% ±2.0</td>
<td><strong>67.19% ±1.5</strong></td>
<td><strong>37.73% ±1.5</strong></td>
</tr>
<tr>
<td></td>
<td>NNK</td>
<td><strong>61.38% ±2.0</strong></td>
<td>66.58% ±1.5</td>
<td>36.81% ±1.5</td>
</tr>
<tr>
<td></td>
<td>Kalofolias</td>
<td>59.36% ±2.0</td>
<td>66.28% ±1.5</td>
<td>37.5% ±1.5</td>
</tr>
</tbody>
</table>
Results
Task 3: Denoising of Graph Signals

<table>
<thead>
<tr>
<th>Best SNR</th>
<th>Road graph</th>
<th>Kalofolias</th>
<th>RBF NNK</th>
<th>RBF $k$-NN</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10.32</td>
<td>10.41</td>
<td>9.99</td>
<td>9.80</td>
</tr>
</tbody>
</table>
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](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.
Conclusion

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Thank you for your attention

Benchmarks available at:
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References

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- Sen et al 2008 “Automated flower classification over a large number of classes” ICVGIP;
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- 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;