topsbm Documentation

Release 0.2dev0

topsbm developers

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Contents

Martin Gerlach, Tiago P. Peixoto, and Eduardo G. Altmann, "A network approach to topic models," Science Advances (2018)

Software ported to Scikit-learn format by the Sydney Informatics Hub at the University of Sydney.

CHAPTER 1

Installation

The latest release can be installed from PyPi using:

```
$ pip install topsbm
```

Install the development version from GitHub using:

```
$ pip install https://github.com/TopSBM/topsbm/archive/master.zip
```

or by cloning the source code:

```
$ git clone https://github.com/TopSBM/topsbm
$ cd topsbm
$ pip install .
```

1.1 Installing dependencies

topsbm requires graph-tool to already be installed, as it cannot be installed with *pip*.

A simple way to install graph-tool and its dependencies is to use conda:

```
$ conda install -c conda-forge -c flyem-forge scikit-learn graph-tool pygobject cairo␣
↪gtk3
```

or simply:

```
$ git clone https://github.com/TopSBM/topsbm
$ cd topsbm
$ conda env create
```

1.2 Check your installation

Check the installation has worked with:

```
$ python -m topsbm.check_install
```

or run the full test suite:

```
$ pip install pytest
$ pytest --pyargs topsbm
```

CHAPTER 2

API Documentation

CHAPTER 3

Example: Introduction to topsbm

Topic modelling with hierarchical stochastic block models

[1]:
```
from sklearn.feature_extraction.text import CountVectorizer
import pandas as pd
from topsbm import TopSBM
```

3.1 Setup: Load a corpus

1. We have a list of documents, each document contains a list of words.
2. We have a list of document titles (optional)

The example corpus consists of 63 articles from Wikipedia taken from 3 different categories (Experimental Physics, Chemical Physics, and Computational Biology).

We use scikit-learn's CountVectorizer to turn this text into a feature matrix.

[2]:
```
# Load texts and vectorize
with open('corpus.txt', 'r') as f:
    docs = f.readlines()

vec = CountVectorizer(token_pattern=r'\S+')
X = vec.fit_transform(docs)

# X is now a sparse matrix of (docs, words)

# titles corresponding to docs
with open('titles.txt', 'r') as f:
    x = f.readlines()
titles = [h.split()[0] for h in x]
```

[3]:
```
# view the data for document 0
print(titles[0])
print(docs[0][:100])
```

```
Nuclear_Overhauser_effect
 the nuclear overhauser effect noe is the transfer of nuclear spin polarization from␣
↪one nuclear spi
```

3.2 Fit the model

Calling `TopSBM.fit_transform` will: * construct the bipartite graph between documents and words (samples and features) * perform Hierarchical Stochastic Block Model inference over the graph * return an embedding of the samples in the block level with finest granularity

[18]:
```
model = TopSBM(random_state=9)
Xt = model.fit_transform(X)
```

3.3 Plotting the graph and block structure

The following plot shows the (hierarchical) community structure in the word-document network as inferred by the stochastic block model:

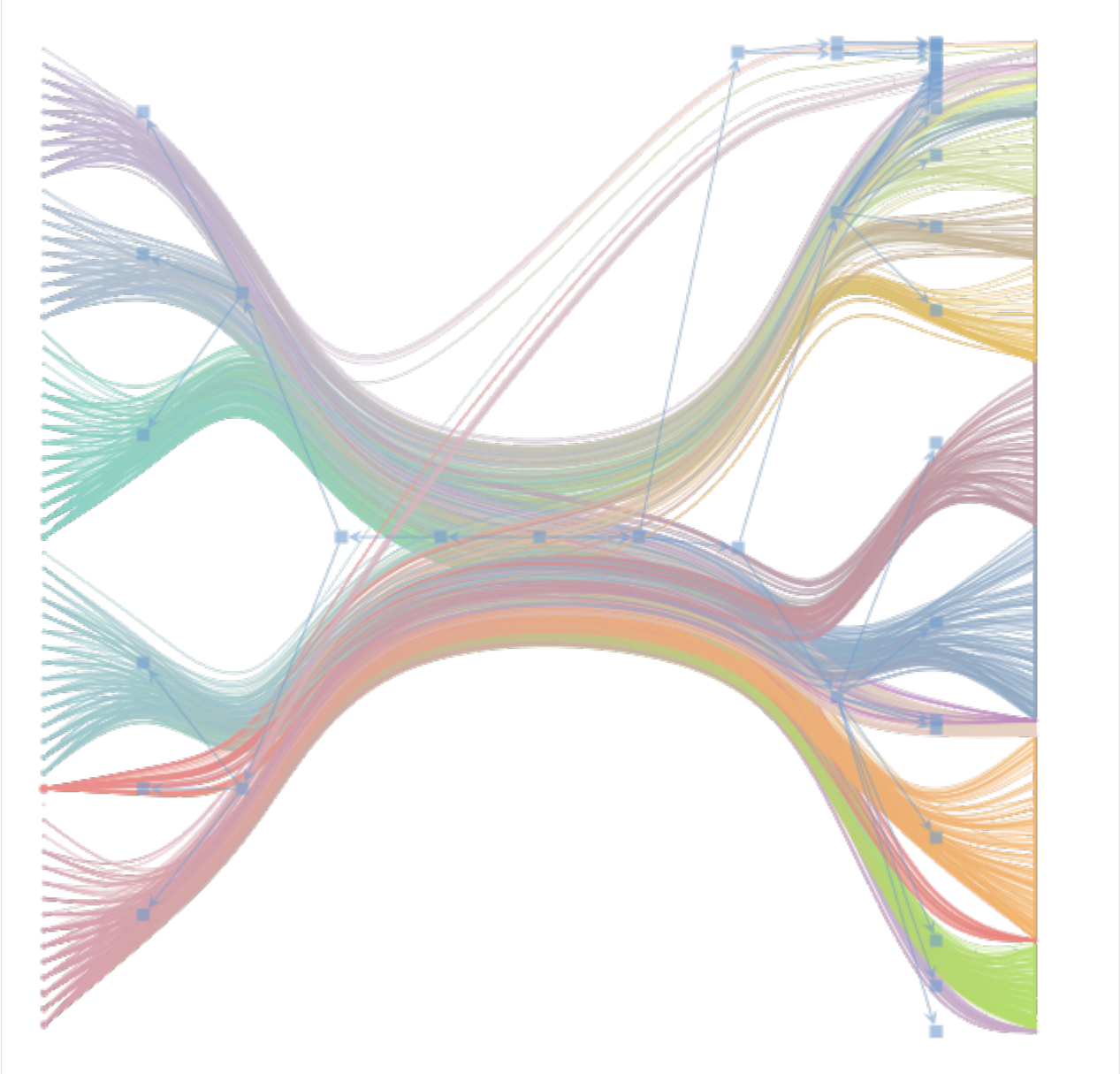
- document-nodes are on the left
- word-nodes are on the right
- different colors correspond to the different groups

The result is a grouping of nodes into groups on multiple levels in the hierarchy:

- on the uppermost level, each node belongs to the same group (square in the middle)
- on the next-lower level, we split the network into two groups: the word-nodes and the document-nodes (blue sqaures to the left and right, respectively). This is a trivial structure due to the bipartite character of the network.
- only next lower levels constitute a non-trivial structure: We now further divide nodes into smaller groups (document-nodes into document-groups on the left and word-nodes into word-groups on the right)

In the code, the lowest level is known as level 0, with coarser levels 1, 2, ...

[19]:
```
model.plot_graph(n_edges=1000)
```



3.4 Topics

For each word-group on a given level in the hierarchy, we retrieve the n most common words in each group – these are the topics!

[20]:
```
topics = pd.DataFrame(model.groups_[1]['p_w_tw'],
                      index=vec.get_feature_names())
```

[21]:
```
for topic in topics.columns:
    print(topics[topic].nlargest(10))
    print()
```

```
the     0.006768
of      0.006661
a       0.006554
in      0.006446
is      0.006446
to      0.006339
and     0.006124
for     0.005372
an      0.005264
as      0.005264
Name: 0, dtype: float64

when        0.008921
where       0.008058
first       0.006619
given       0.006331
if          0.006331
field       0.006043
applied     0.005755
because     0.005755
e           0.005468
energy      0.005468
Name: 1, dtype: float64

computational    0.060606
development      0.055556
proteins         0.045455
open             0.040404
protein          0.040404
software         0.040404
community        0.035354
researchers      0.035354
core             0.025253
identify         0.025253
Name: 2, dtype: float64

point       0.217391
formula     0.188406
must        0.144928
wave        0.115942
spectrum    0.086957
air         0.072464
plane       0.057971
flow        0.043478
q           0.043478
mode        0.028986
Name: 3, dtype: float64
```

3.5 Topic-distribution in each document

Which level-1 topics contribute to each document?

[22]:
```
pd.DataFrame(model.groups_[1]['p_tw_d'],
             columns=titles)
```

[22]:

	Nuclear_Overhauser_effect	Quantum_solvent	Rovibrational_coupling	\
0	0.608392	0.856	0.523529	
1	0.391608	0.144	0.458824	
2	0.000000	0.000	0.000000	
3	0.000000	0.000	0.017647	

	Effective_field_theory	Chemical_physics	Rotational_transition	\
0	0.804651	0.82	0.648649	
1	0.190698	0.16	0.337838	
2	0.000000	0.00	0.000000	
3	0.004651	0.02	0.013514	

	Dynamic_nuclear_polarisation	Knight_shift	Polarizability	\
0	0.584192	0.582418	0.493274	
1	0.412371	0.406593	0.500000	
2	0.000000	0.010989	0.002242	
3	0.003436	0.000000	0.004484	

	Anisotropic_liquid	...	\
0	0.645161	...	
1	0.354839	...	
2	0.000000	...	
3	0.000000	...	

	Louis_and_Beatrice_Laufer_Center_for_Physical_and_Quantitative_Biology	\
0	0.907692	
1	0.092308	
2	0.000000	
3	0.000000	

	Law_of_Maximum	Enzyme_Function_Initiative	SnoRNA_prediction_software	\
0	0.851351	0.857143	0.857143	
1	0.121622	0.095238	0.142857	
2	0.027027	0.044218	0.000000	
3	0.000000	0.003401	0.000000	

	Sepp_Hochreiter	Aureus_Sciences	\
0	0.846690	0.822222	
1	0.139373	0.133333	
2	0.013937	0.044444	
3	0.000000	0.000000	

	IEEE/ACM_Transactions_on_Computational_Biology_and_Bioinformatics	\
0	0.84375	
1	0.09375	
2	0.06250	
3	0.00000	

	Knotted_protein	BioUML	De_novo_transcriptome_assembly
0	0.773585	0.870647	0.868932
1	0.169811	0.084577	0.092233
2	0.047170	0.044776	0.038835
3	0.009434	0.000000	0.000000

[4 rows x 63 columns]

3.6 Extra: Clustering of documents - for free.

The stochastic block models clusters the documents into groups. We do not need to run an additional clustering to obtain this grouping.

For a query article, we can return all articles from the same group

[23]:
```
cluster_labels = pd.DataFrame(model.groups_[1]['p_td_d'],
                              columns=titles).idxmax(axis=0)
cluster_idx = cluster_labels['Rovibrational_coupling']
cluster_labels[cluster_labels == cluster_idx]
```

[23]:
```
Nuclear_Overhauser_effect                          0
Rovibrational_coupling                             0
Rotational_transition                              0
Dynamic_nuclear_polarisation                       0
Knight_shift                                       0
Polarizability                                     0
Anisotropic_liquid                                 0
Rotating_wave_approximation                        0
Molecular_vibration                                0
Fuel_mass_fraction                                 0
Electrostatic_deflection_(structural_element)      0
Magic_angle_(EELS)                                 0
Reactive_empirical_bond_order                      0
Photofragment-ion_imaging                          0
Molecular_beam                                     0
McConnell_equation                                 0
Ziff-Gulari-Barshad_model                          0
Empirical_formula                                  0
Newton's_laws_of_motion                            0
Ripple_tank                                        0
Particle-induced_X-ray_emission                    0
Elevator_paradox_(physics)                         0
Wave_tank                                          0
X-ray_crystal_truncation_rod                       0
Faraday_cup_electrometer                           0
Line_source                                        0
X-ray_standing_waves                               0
Point_source                                       0
Fragment_separator                                 0
Dynamic_mode_decomposition                         0
Euler's_laws_of_motion                             0
Quantum_oscillations_(experimental_technique)      0
dtype: int64
```

CHAPTER 4

Maintaining the Package

This document contains information for the software developers and maintainers. Issues can be posted at **'https://github.com/TopSBM/topsbm/issues'_**.

4.1 Travis CI

When a commit is made to any branch of the repository, or a pull request is made, Travis CI pulls in the changes and runs the tests. It will give a green tick if the tests run successfully.

Anyone listed in GitHub as a repository owner can administrate Travis too.

4.2 Building the Documentation

You can build the documentation on your own machine by installing sphinx and nbsphinx. Then, in the `doc/` directory, run `make html`.

Recompiling the documentation will re-run examples in Jupyter notebooks *only if* all cells' output has been cleared. Otherwise, the documentation will show the output already in the notebook.

Note that the ReadTheDocs service currently refuses to re-run the example notebook, as it takes longer than that service allows.

4.3 ReadTheDocs

ReadTheDocs recompiles the documentation when any commit is made to the `master` branch, and publishes it to **'https://topsbm.readthedocs.io'_**.

?Anyone listed in GitHub as a repository owner can administrate ReadTheDocs too.

4.4 Releasing to PyPI

When you are ready to release a new version of the software, you should first make sure that you are authorised to maintain the PyPI package (it lists maintainers on that page).

Then follow these steps:

1. Make sure the version is correct in the `__version__` variable in [`topsbm/__init__.py`](https://github.com/TopSBM/topsbm/blob/master/topsbm/__init__.py). For releases, remove suffixes like `dev0`. Commit that change.
2. Tag the commit with the version number, with a command such as `git tag v0.2`.
3. Push the tags to github. `git push --tags`

4. Make sure setuptools and twine are installed. `pip install setuptools twine` 4. Remove any files from previous releases in the `dist` directory: `rm dist/*.tar.gz` 5. Run `python setup.py sdist` to create new entries in `dist/` 6. Ensure your PyPI credentials are stored in `~/.pypirc`. 7. Run `twine upload dist/*.tar.gz`. 8. If you want, create a corresponding GitHub release

- genindex

Python Module Index

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