Bipartite Configuration Model for Python - Documentation

Release 1.1

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The Bipartite Configuration Model (BiCM) is a statistical null model for binary bipartite networks [Squartini2011], [Saracco2015]. It offers an unbiased method for analyzing node similarities and obtaining statistically validated monopartite projections [Saracco2016].

The BiCM belongs to a series of entropy-based null models for binary bipartite networks, see also

- BiPCM Bipartite Partial Configuration Model
- BiRG Bipartite Random Graph

Please consult the original articles for details about the underlying methods and applications to user-movie and international trade databases [Saracco2016], [Straka2016].

An example case is illustrated in the *Tutorial*.

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CHAPTER

ONE

HOW TO CITE

If you use the bicm module, please cite its location on Github and the original articles [Saracco2015] and [Saracco2016].

1.1 References

Bipartite Configuration Model for Python - Documentation, Release 1.1				

CHAPTER

TWO

GETTING STARTED

2.1 Overview

The bicm module is an implementation of the Bipartite Configuration Model (BiCM) as described in the article [Saracco2016]. The BiCM can be used as a statistical null model to analyze the similarity of nodes in undirected bipartite networks. The similarity criterion is based on the number of common neighbors of nodes, which is expressed in terms of Λ -motifs in the original article [Saracco2016]. Subsequently, one can obtain unbiased statistically validated monopartite projections of the original bipartite network.

The construction of the BiCM, just like the related BiPCM and BiRG models, is based on the generation of a grand canonical ensemble of bipartite graphs subject to certain constraints. The constraints can be of different types. For instance, in the case of the BiCM the average degrees of the nodes of the input network are fixed. In the BiRG, on the other hand, the total number of edges is constrained. In general, these models are referred to as entropy-based null models.

The average graph of the ensemble can be calculated analytically using the entropy-maximization principle and provides a statistical null model, which can be used for establishing statistically significant node similarities. For more information and a detailed explanation of the underlying methods, please refer to [Saracco2016].

By using the bicm module, the user can obtain the BiCM null model which corresponds to the input matrix representing an undirected bipartite network. To address the question of node similarity, the p-values of the observed numbers of common neighbors (i.e. of the Λ -motifs) can be calculated and used for statistical verification. For an illustration and further details, please refer to [Saracco2016] and [Straka2016].

2.1.1 Dependencies

bicm is written in Python 2.7 and uses the following modules:

- poibin Module for the Poisson Binomial probability distribution
- scipy
- numpy
- · multiprocessing
- ctypes
- · doctest For unit testing

2.2 BiCM Quickstart

The bicm module encompasses essentially two steps for the validation of node similarities in bipartite networks:

- 1. given an input matrix, create the biadjacency matrix of the BiCM null model
- 2. calculate the p-values of the observed similarities of nodes in the same bipartite layer

Subsequently, a multiple hypothesis testing of the p-values can be performed. The statistically validated node similarities give rise to a unbiased monopartite projection of the original bipartite network, as illustrated in [Saracco2016].

For more detailed explanations of the methods, please refer to [Saracco2016], the *Tutorial* and the API.

2.2.1 Obtaining the biadjacency matrix of the BiCM null model

Be mat a two-dimensional binary NumPy array, which describes the biadjacency matrix of an undirected bipartite network. The nodes of the two bipartite layers are ordered along the columns and rows, respectively. In the algorithm, the two layers are identified by the boolean values True for the **row-nodes** and False for the **column-nodes**.

Import the module and initialize the Bipartite Configuration Model:

```
>>> from src.bicm import BiCM
>>> cm = BiCM(bin_mat=mat)
```

To create the biadjacency matrix of the BiCM, use:

```
>>> cm.make_bicm()
```

The biadjacency matrix of the BiCM null model can be saved in *<filename>*:

```
>>> cm.save_biadjacency(filename=<filename>, delim='\t')
```

By default, the file is saved in a human-readable .csv format. The information can also be saved as a binary NumPy file .npy by using:

```
>>> cm.save_biadjacency(filename=<filename>, binary=True)
```

If the file is not binary, it should end with, e.g., .csv. If it is binary instead, NumPy automatically appends the ending .npy.

2.2.2 Calculating the p-values of the node similarities

In order to analyze the similarities of the **row-nodes** and to save the p-values of the observed numbers of shared neighbors (i.e. of the Λ -motifs [Saracco2016]) in *spilename*, use:

```
>>> cm.lambda_motifs(True, filename=<filename>)
```

By default, the file is saved as binary NumPy file to reduce disk space, and the format suffix .npy is appended. If the file should be saved in a human-readable .csv format, use:

```
>>> cm.lambda_motifs(True, filename=<filename>, delim='\t', binary=False)
```

Analogously for the **column-nodes**, use:

```
>>> cm.lambda_motifs(False, filename=<filename>)
or:
>>> cm.lambda_motifs(False, filename=<filename>, delim='\t', binary=False)
```

Note: The p-values are saved as a one-dimensional array with index $k \in \left[0, \dots, {N \choose 2} - 1\right]$ for a bipartite layer of N nodes. Please check the section A *Note on the Output Format* for details regarding the indexing.

Subsequently, the p-values can be used to perform a multiple hypotheses testing of the node similarities and to obtain statistically validated monopartite projections [Saracco2016]. The p-values are calculated in parallel by default, see *Parallel Computation and Memory Management* for details.

2.3 Tutorial

The tutorial will take you step by step from the biadjacency matrix of a real-data network to the calculation of the p-values. Our example bipartite network will be the following:

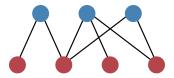


Figure 2.1: Figure 1: Example network.

The structure of the network can be captured in a biadjacency matrix. In our case, the matrix is

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

Note that the nodes of the layers of the bipartite network are ordered along the rows and the columns, respectively. In the algorithms, the two layers are identified by the boolean values True for the **row-nodes** and False for the **column-nodes**. In our example image, the row-nodes are colored in blue (True, top layer) and the column-nodes in red (False, bottom layer).

Let's get started by importing the necessary modules:

```
>>> import numpy
>>> from src.bicm import BiCM
```

The biadjacency matrix of our toy network will be saved in the two-dimensional NumPy array mat

```
>>> mat = np.array([[1, 1, 0, 0], [0, 1, 1, 1], [0, 1, 0, 1]])
```

and we initialize the Bipartite Configuration Model with:

```
>>> cm = BiCM(bin_mat=mat)
```

2.3.1 Biadjacency matrix

In order to obtain the biadjacency matrix of the BiCM null model corresponding to the input network, a number of equations have to be solved. This is done automatically by running

```
>>> cm.make_bicm()
```

In our example graph, the BiCM biadjacency matrix should be:

If necessary, we could now save the matrix in the file *<filename>* with

2.3. Tutorial 7

```
>>> cm.save_biadjacency(filename=<filename>, delim='\t')
```

Note that the default delimiter is \t and does not have to be specified. Other delimiters such as , or ; work fine as well. The matrix can either be saved as a human-readable .csv or as a binary NumPy .npy file, see save_biadjacency() in the API. In the latter case, we would run:

```
>>> cm.save_biadjacency(filename=<filename>, binary=True)
```

If binary == True, the file ending .npy is appended automatically.

2.3.2 P-values

Each entry in the biadjacency matrix of the null model corresponds to the probability of observing a link between the corresponding row- and column-nodes. If we take two nodes in the same layer, we can count the number of common neighbors that they share in the original input network and calculate the probability of observing the same or more common neighbors according to the BiCM [Saracco2016]. This corresponds to calculating the p-values for a right-sided hypothesis testing.

The number of common neighbors can be described in terms of Λ -motifs [Saracco2016], as shown in Figure 2.



Figure 2.2: Figure 2: Illustration of a Λ -motif between the two central red nodes.

The calculation of the p-values is computationally intensive and should be performed in parallel, see *Parallel Computation and Memory Management* for details. It can be executed by simply running

```
>>> cm.lambda_motifs(<bool>, filename=<filename>)
```

where <bool> is either True of False depending on whether one wants to address the similarities of the rowor column-nodes, respectively. The results are written to <filename>. By default, the file is a binary NumPy file to
reduce disk space, and the format suffix .npy is appended. If the file should be saved in a human-readable .csv
format, provide an appropriate name ending with .csv and use:

```
>>> cm.lambda_motifs(<bool>, filename=<filename>, delim='\t', binary=False)
```

Again the default delimiter is \t.

Note: The p-values are saved as a one-dimensional array with index $k \in \left[0, \dots, {N \choose 2} - 1\right]$ for a bipartite layer of N nodes. Please check the section A *Note on the Output Format* for details regarding the indexing.

Having calculated the p-values, it is possible to perform a multiple hypothesis testing of the node similarities and to obtain an unbiased monopartite projection of the original bipartite network. In the projection, only statistically significant edges are kept.

For further information on the post-processing and the monopartite projections, please refer to [Saracco2016].

2.4 Testing

The methods in the bicm module have been implemented using doctests. To run the tests, execute:

```
>>> python -m doctest bicm_tests.txt
```

from the folder src in the command line. If you want to run the tests in verbose mode, use:

```
>>> python -m doctest -v bicm_tests.txt
```

Note that bicm.py and bicm_tests.txt have to be in the same directory to run the test.

2.5 Parallel Computation and Memory Management

The calculation of the p-values of the Λ -motifs demands computation power as well as working memory which grow quickly with the number of nodes. To address this problem, the calculation is split into chunks and the Python multiprocessing package is used.

2.5.1 Parallel Computation

By default the computation is performed in parallel using the multiprocessing packge. The number of parallel processes depends on the number of CPUs of the work station and is defined by the variable num_procs in the method BiCM.get_pvalues_q() (see API).

If the calculation should **not** be performed in parallel, use:

```
>>> cm.lambda_motifs(<bool>, parallel=False)
instead of:
```

>>> cm.lambda_motifs(<bool>)

2.5.2 Memory Management

In order to calculate the p-values, information on the Λ -motifs and their probabilities has to be kept in the working memory. This can lead to memory allocation errors for large networks due to limited resources. To avoid this problem, the total number of p-value operations is split into chunks which are processed sequentially. The number of chunks can be defined when calling the motif function:

```
>>> cm.lambda_motifs(<bool>, num_chunks=<number_of_chunks>)
```

The default value is num_chunks = 4. As an example, for N nodes in a bipartite layer, $\binom{N}{2}$ p-values have to be computed. If num_chunks = 4, each chunk processes therefore about $\frac{1}{4}\binom{N}{2}$ p-values in parallel.

Note: Increasing num_chunks decreases the required working memory, but leads to longer processing times. For $N \le 15$, num_chunks = 1 by default.

2.5.3 A Note on the Output Format

A layer composed of N vertices requires the computation of $\binom{N}{2}$ p-values to assess the node similarities. They are saved in the output file as a one-dimensional array when running the method *:func: 'BiCM.get_pvalues_q' 'cm.lambda_motifs'*. However, a more intuitive matrix representation can be easily recovered using some helper functions, since each element in the array can be mapped on an element in the matrix and vice versa.

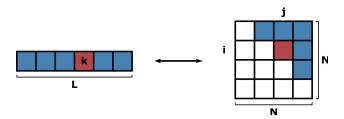


Figure 2.3: Figure 1: Mapping of the one-dimensional array of length L onto a square matrix of dimension $N \times N$. Note that the matrix is symmetric.

Let's consider an array of length L as shown in Figure 1. The dimension N of the matrix, i.e. the number of nodes in the original bipartite network layer, can be obtained as:

```
>>> N = cm.flat2triumat_dim(L)
```

To convert an array index k to the corresponding matrix index couple (i, j) in the upper triangular part, use:

```
>>> (i, j) = cm.flat2triumat_idx(k, N)
```

Note: As illustrated in Figure 1, the output array contains the **upper triangular part** of the symmetric square matrix, excluding the diagonal. Thus

- $k \in [0, \dots, N(N-1)/2-1]$
- $i \in [0, ..., N-1]$
- $j \in [i+1, ..., N-1]$

The inverse operations are given by:

```
>>> L = cm.triumat2flat_dim(N)
>>> k = cm.triumat2flat_idx(i, j, N)
```

2.6 API

API for the methods in the bicm module.

```
class bicm.BiCM(bin_mat)
```

Bipartite Configuration Model for undirected binary bipartite networks.

This class implements the Bipartite Configuration Model (BiCM), which can be used as a null model for the analysis of undirected and binary bipartite networks. The class provides methods for calculating the biadjacency matrix of the null model and for quantifying node similarities in terms of p-values.

add2inqueue (nprocs, plam_mat, nlam_mat, k1, k2)

Add elements to the in-queue to calculate the p-values.

Parameters

- **nprocs** (*int*) number of processes running in parallel
- plam_mat (numpy.array (square matrix)) array containing the list of probabilities for the single observations of Λ -motifs
- **nlam_mat** (numpy.array (square matrix)) array containing the observations of Λ -motifs
- **k1** (*int*) lower interval limit

• **k2** (*int*) – upper interval limit

check_input_matrix_is_binary()

Check that the input matrix is binary, i.e. entries are 0 or 1.

Raises AssertionError raise an error if the input matrix is not binary

equations (xx)

Return the equations of the log-likelihood maximization problem.

Note that the equations for the row-nodes depend only on the column-nodes and vice versa, see [Saracco2015].

Parameters xx (numpy.array) – Lagrange multipliers which have to be solved

Returns equations to be solved (f(x) = 0)

Return type numpy.array

static flat2triumat_dim(k)

Return the dimension of the matrix hosting k triangular elements.

Parameters k (*int*) – the number of elements in the upper triangular part of the corresponding square matrix, exluding the diagonal

Returns dimension of the corresponding square matrix

Return type int

static flat2triumat idx(k, n)

Convert an array index into the index couple of a triangular matrix.

k is the index of an array of length $\binom{n}{2}$ 2, which contains the elements of an upper triangular matrix of dimension n excluding the diagonal. The function returns the index couple (i,j) that corresponds to the entry k of the flat array.

Note:

•
$$k \in \left[0, \ldots, \binom{n}{2} - 1\right]$$

•returned indices:

$$-i \in [0, \ldots, n-1]$$

$$-j \in [i+1,\ldots,n-1]$$

Parameters

- **k** (*int*) flattened array index
- **n** (*int*) dimension of the square matrix

Returns matrix index tuple (row, column)

Return type tuple

get_biadjacency_matrix(xx)

Calculate the biadjacency matrix of the null model.

The biadjacency matrix describes the BiCM null model, i.e. the optimal average graph $< G >^*$ with the average link probabilities $< G >^*_{rc} = p_{rc}$, $p_{rc} = \frac{x_r \cdot x_c}{1 + x_r \cdot x_c}$. x are the solutions of the equation system which has to be solved for the null model. Note that r and c are taken from opposite bipartite node sets, thus $r \neq c$.

Parameters xx (numpy.array) – solutions of the equation system (Lagrange multipliers)

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Returns biadjacency matrix of the null model

Return type numpy.array

Raises ValueError raise an error if $p_{rc} < 0$ or $p_{rc} > 1$ for any r, c

get_lambda_motif_block (mm, k1, k2)

Return a subset of Λ -motifs as observed in mm.

Given the binary input matrix mm, count the number of Λ -motifs for all the node couples specified by the interval $[k_1, k_2]$.

Note:

- •The Λ -motifs are counted between the **row-nodes** of the input matrix mm.
- •If $k_2 \equiv \binom{mm.shape[0]}{2}$, the interval becomes $[k_1, k_2]$.

Parameters

- **mm** (*numpy.array*) binary matrix
- **k1** (*int*) lower interval limit
- **k2** (*int*) upper interval limit

Returns array of observed Λ -motifs

Return type numpy.array

get_plambda_block (biad_mat, k1, k2)

Return a subset of the Λ probability matrix.

Given the biadjacency matrix biad_mat with $\mathbf{M}_{rc} = p_{rc}$, which describes the probabilities of row-node r and column-node c being linked, the method returns the matrix

$$P(\Lambda)_{ij} = (M_{i\alpha_1} \cdot M_{j\alpha_1}, M_{i\alpha_2} \cdot M_{j\alpha_2}, \dots),$$

for all the node couples in the interval $[k_1,k_2[.~(i,j)]$ are two **row-nodes** of biad_mat and α_k runs over the nodes in the opposite layer.

Note:

- •The probabilities are calculated between the **row-nodes** of the input matrix biad_mat.
- •If $k_2 \equiv \binom{biad_mat.shape[0]}{2}$, the interval becomes [k1, k2].

Parameters

- biad_mat (numpy.array) biadjacency matrix
- **k1** (*int*) lower interval limit
- **k2** (*int*) upper interval limit

Returns Λ -motif probability matrix

Return type numpy.array

get_pvalues_q (plam_mat, nlam_mat, k1, k2, parallel=True)

Calculate the p-values of the observed Λ -motifs.

For each number of Λ -motifs in nlam_mat for the node interval [k1, k2], construct the Poisson Binomial distribution using the corresponding probabilities in plam_mat and calculate the p-value.

Parameters

- plam_mat (numpy.array (square matrix)) array containing the list of probabilities for the single observations of Λ -motifs
- nlam_mat (numpy.array (square matrix)) array containing the observations of Λ -motifs
- **k1** (*int*) lower interval limit
- **k2** (*int*) upper interval limit
- parallel (bool) if True, the calculation is executed in parallel; if False, only one
 process is started

get_triup_dim(bip_set)

Return the number of possible node couples in bip_set.

Parameters bip_set (bool) – selects row-nodes (True) or column-nodes (False)

Returns return the number of node couple combinations corresponding to the layer bip_set

Return type int

Raises ValueError raise an error if the parameter bip_set is neither True nor False

jacobian(xx)

Return a NumPy array with the Jacobian of the equation system.

Parameters xx (numpy.array) – Lagrange multipliers which have to be solved

Returns Jacobian

Return type numpy.array

lambda_motifs (bip_set , parallel=True, filename=None, delim='t', binary=True, $num_chunks=4$) Calculate and save the p-values of the Λ -motifs.

For each node couple in the bipartite layer specified by bip_set, calculate the p-values of the corresponding Λ -motifs according to the link probabilities in the biadjacency matrix of the BiCM null model.

The results can be saved either as a binary .npy or a human-readable .csv file, depending on binary.

Note:

- •The total number of p-values that are calculated is split into num_chunks chunks, which are processed sequentially in order to avoid memory allocation errors. Note that a larger value of num_chunks will lead to less memory occupation, but comes at the cost of slower processing speed.
- •The output consists of a one-dimensional array of p-values. If the bipartite layer bip_set contains n nodes, this means that the array will contain $\binom{n}{2}$ entries. The indices (i, j) of the nodes corresponding to entry k in the array can be reconstructed using the method BiCM.flat2_triumat_idx(). The number of nodes n can be recovered from the length of the array with BiCM.flat2_triumat_dim()
- •If binary == False, the filename should end with .csv. If binary == True, it will be saved in binary NumPy .npy format and the suffix .npy will be appended automatically. By default, the file is saved in binary format.

Parameters

- **bip set** (*bool*) **select** row-nodes (True) or **column-nodes** (False)
- parallel (bool) select whether the calculation of the p-values should be run in parallel (True) or not (False)

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- **filename** (*str*) name of the output file
- **delim** (str) **delimiter** between entries in the .csv `file, default is ``\t
- binary (bool) if True, the file will be saved in the binary NumPy format .npy, otherwise as .csv
- num_chunks (int) number of chunks of p-value calculations that are performed sequentially

Raises ValueError raise an error if the parameter bip_set is neither True nor False

make_bicm()

Create the biadjacency matrix of the BiCM null model.

Solve the log-likelihood maximization problem to obtain the BiCM null model which respects constraints on the degree sequence of the input matrix.

Raises AssertionError raise an error if the adjacency matrix of the null model has different dimensions than the input matrix

outqueue2pval_mat (nprocs, pvalmat)

Put the results from the out-queue into the p-value array.

pval_process_worker()

Calculate p-values and add them to the out-queue.

static save_array (mat, filename, delim='t', binary=False)

Save the array mat in the file filename.

The array can either be saved as a binary NumPy .npy file or as a human-readable .npy file.

Note:

- •The relative path has to be provided in the filename, e.g. ../data/pvalue_matrix.csv.
- •If binary==True, NumPy automatically appends the format ending .npy to the file.

Parameters

- mat (numpy.array) array
- **filename** (*str*) name of the output file
- **delim** (str) delimiter between values in file
- binary (bool) if True, save as binary .npy, otherwise as a .csv file

save_biadjacency (filename, delim='t', binary=False)

Save the biadjacendy matrix of the BiCM null model.

The matrix can either be saved as a binary NumPy . npy file or as a human-readable . ${\tt csv}$ file.

Note:

- •The relative path has to be provided in the filename, e.g. ../data/pvalue_matrix.csv.
- •If binary==True, NumPy automatically appends the format ending .npy to the file.

Parameters

• **filename** (str) – name of the output file

- **delim** (str) delimiter between values in file
- binary (bool) if True, save as binary .npy, otherwise as a .csv file

set_degree_seq()

Return the node degree sequence of the input matrix.

Returns node degree sequence [degrees row-nodes, degrees column-nodes]

Return type numpy.array

Raises AssertionError raise an error if the length of the returned degree sequence does not correspond to the total number of nodes

solve_equations (eq, jac)

Solve the system of equations of the maximum log-likelihood problem.

The system of equations is solved using scipy's root function. The solutions correspond to the Lagrange multipliers

$$x_i = \exp(-\theta_i).$$

Parameters

- eq (numpy.array) system of equations (f(x) = 0)
- jac (numpy.ndarray) Jacobian of the system

Returns solution of the equation system

$split_range(n, m=4)$

Split the interval $[0, \ldots, n]$ in m parts.

Parameters

- **n** (*int*) upper limit of the range
- m number of part in which range should be split

Returns delimiter indices for the m parts

Return type list

test_average_degrees()

Test the constraints on the node degrees.

Check that the degree sequence of the solved BiCM null model graph corresponds to the degree sequence of the input graph.

static triumat2flat dim(n)

Return the size of the triangular part of a $n \times n$ matrix.

Parameters n (*int*) – the dimension of the square matrix

Returns number of elements in the upper triangular part of the matrix (excluding the diagonal)

Return type int

$static triumat2flat_idx(i, j, n)$

Convert an matrix index couple to a flattened array index.

Given a square matrix of dimension n and the index couple (i, j) of the upper triangular part of the matrix, return the index which the matrix element would have in a flattened array.

Note:

$$\bullet i \in [0, ..., n-1]$$

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$$\bullet j \in [i+1,...,n-1]$$
 •returned index $\in [0,\,n(n-1)/2-1]$

Parameters

- **i** (*int*) row index
- \mathbf{j} (int) column index
- **n** (*int*) dimension of the square matrix

Returns flattened array index

Return type int

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2.8 Contact

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