# bg Documentation

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**BG** is a python based package that provides a comprehensive implementation of comparative genomics combinatorial object named breakpoint graph [1].

Code is written with the philosophy of TDD and requires Python v3.3+ for correct work.

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Author is very grateful for thoughtful and dedicated leadership of Dr. Max A. Alekseyev, Associate Professor at Department of Mathematics & CBI, GWU.

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# Installation

Package is distributed by pypi online repository of software for the Python programming language.

To install execute the following simple command

>>> pip install bg

## **Contents:**

# 2.1 Contributing

This page will show the basic principals, that are used during the development of this package.

The project is hosted on the github.

### 2.1.1 Test Driven Development

Whole project is written with a test-driven development paradigm. This is especially important, since this project provides an implementation of a complex combinatorial object, which must be reliable in use during research projects.

Project uses unittest framework for implementing TDD paradigm.

### 2.1.2 Issues reporting

Any found bugs, miss-citations, mistakes in documentation, questions, etc. shall be reported to the issue-tracking system, powered by github.

### 2.1.3 Code incorporation

There are several rules for new code to be incorporated into this library:

- 1. All code has to written using the Sphinx style
- 2. All code must be covered by tests
- 3. All algorithms and data structures code must have proper citations

### 2.2 API documentation

### **2.2.1** grimm.py

class bg.grimm.GRIMMReader

Bases: object

Class providing a staticmethod based implementation of reading GRIMM formatted data file-like object and obtain a bg.breakpoint\_graph.BreakpointGraph instance.

There are no private methods implementations for all public methods so inheritance shall be performed with caution. For now GRIMM format is a bit simplified and straightened from the version provided at http://grimm.ucsd.edu/GRIMM/grimm\_instr.html

#### Supported GRIMM format:

- 1.all strings are stripped from both sides for tabs, spaces, etc. Below when said "string", stripped string is assumed
- 2.genome declaration is specified on a string that starts with >
  - (a)genome name is everything, that follows > sign
- 3.all input data before the next genome declaration (or EOF) will be attributed to this genome by its genome name
- 4.a data string (containing information about gene orders) is a string that is not a genome declaration, comment, empty string
  - (a)every new genomic fragments (chromosome/scaffold/contig/etc) must be specified on a new string
  - (b)every data string must contain a \$ (for linear case) or @ (for circular case) gene order terminator, that indicates the end of current genomic fragment
  - (c) everything after the gene order terminator is ignored
  - (d)if no gene order before gene order terminator is specified an error would be raised

#### (e)gene order:

- i. gene order is a sequence of space separated block name strings with optional orientation declaration
- ii. block can be described by a regular expression ^ ((-|\+) .+\$) | ([^-\+]+\$) and viewed as follows: if the sign (+ or -) is present as a first character, then it must be followed by a nonempty block name string if sign is not present, everything is assumed to be a block name, and + orientation is assigned to it automatically

5.comment string starts with # sign and is ignored during data processing

### Main operations:

- GRIMMReader.is\_genome\_declaration\_string(): checks if supplied string after stripping corresponds to genome declaration
- GRIMMReader.is\_comment\_string(): checks if supplied string after stripping corresponds to comment and shall thus be ignored in data processing
- •GRIMMReader.parse\_genome\_declaration\_string(): parses a string marked as genome declaration and returns a corresponding genome name
- GRIMMReader.parse\_data\_string(): parses a string assumed to contain gene order data, retrieving information about fragment type, gene order, blocks names and their orientation
- GRIMMReader.get\_edges\_from\_parsed\_data(): taking into account fragment type (circularllinear) and retrieved gene order information translates adjacencies between blocks into edges for addition to the bg.breakpoint\_graph.BreakpointGraph
- GRIMMReader.get\_breakpoint\_graph(): taking a file-like object transforms supplied gene order data into the language of BreakpointGraph

#### static \_GRIMMReader\_\_assign\_vertex\_pair(block)

Assigns usual BreakpointGraph type vertices to supplied block.

Vertices are labeled as "block\_name" + "h" and "block\_name" + "t" according to blocks orientation.

**Parameters block** ((str, str)) – information about a genomic block to create a pair of vertices for in a format of (+|-, block\_name)

**Returns** a pair of vertices labeled according to supplied blocks name (respecting blocks orientation)

Return type (str, str)

#### static get\_breakpoint\_graph (stream, merge\_edges=True)

Taking a file-like object transforms supplied gene order data into the language of

#### **Parameters**

- merge\_edges (bool) a flag that indicates if parallel edges in produced breakpoint graph shall be merged or not
- **stream** (iterable ver str) any iterable object where each iteration produces a str object

**Returns** an instance of a BreakpointGraph that contains information about adjacencies in genome specified in GRIMM formatted input

Return type bg.breakpoint\_graph.BreakpointGraph

### static get\_edges\_from\_parsed\_data(parsed\_data)

Taking into account fragment type (circularllinear) and retrieved gene order information translates adjacencies between blocks into edges for addition to the bg.breakpoint\_graph.BreakpointGraph

In case supplied fragment is linear (\$) special artificial vertices (with \_\_infinity suffix) are introduced to denote fragment extremities

```
Parameters parsed_data (tuple(str, list((str, str), ...))) - ($ | @, [(+ | -, block_name),...]) formatted data about fragment type and ordered list of oriented blocks
```

**Returns** a list of vertices pairs that would correspond to edges in bg.breakpoint\_graph.BreakpointGraph

Return type list((str, str), ...)

#### static is comment string(data string)

Checks if supplied string after stripping corresponds to comment and shall thus be ignored in data processing

**Parameters data string** (str) – a string to check if it is a pure comment string

Returns a flag indicating if supplied string is a pure comment string

Return type Boolean

### static is\_genome\_declaration\_string(data\_string)

Checks if supplied string after stripping corresponds to genome declaration

**Parameters data\_string** (str) – a string to check genome name declaration in

**Returns** a flag indicating if supplied string corresponds to genome name declaration

Return type Boolean

### static parse\_data\_string (data\_string)

Parses a string assumed to contain gene order data, retrieving information about fragment type, gene order, blocks names and their orientation

First checks if gene order termination signs are present. Selects the earliest one. Checks that information preceding is not empty and contains gene order. Generates results structure by retrieving information about fragment type, blocks names and orientations.

**NOTE:** comment signs do not work in data strings. Rather use the fact that after first gene order termination sign everything is ignored for processing

Parameters data string (str) - a string to retrieve gene order information from

**Returns** (\$ | @, [(+ | -, block\_name),...]) formatted structure corresponding to gene order in supplied data string and containing fragments type

Return type tuple(str, list((str, str), ...))

#### static parse\_genome\_declaration\_string (data\_string)

Parses a string marked as genome declaration and returns a corresponding bg.genome.BGGenome

Parameters data\_string (str) - a string to retrieve genome name from

**Returns** genome name from supplied genome declaration string

Return type bg.genome.BGGenome

### 2.2.2 breakpoint\_graph.py

class bg.breakpoint\_graph.BreakpointGraph(graph=None)
 Bases: object

Class providing implementation of breakpoint graph data structure and most utilized operations on it.

BreakpointGraph anticipates to work with bg.vertex.BGVertex, bg.edge.BGEdge and bg.multicolor.Multicolor classes instances, but is not limited to them. Extreme caution has to be assumed when working with non-expected classes.

The engine of graph information storage, low-level algorithms implementation is powered by NetworkX package MultiGraph data structure. This class provides a smart wrapping around it to perform most useful, from combinatorial bioinformatics stand point, operations and manipulations.

Class carries following attributes carrying information about graphs structure:

•BreakpointGraph.bg: instance of NetworkX MultiGraph class

#### Main operations:

- •BreakpointGraph.add\_bgedge(): adds an instance of bg.edge.BGEdge to the current BreakpointGraph
- •BreakpointGraph.add\_edge(): adds a new bg.edge.BGEdge, constructed from a pair of supplied vertices instances and bg.multicolor.Multicolor object, to the current BreakpointGraph
- •BreakpointGraph.get\_vertex\_by\_name(): returns a bg.vertex.BGVertex instance by provided name argument
- •BreakpointGraph.get\_edge\_by\_two\_vertices(): returns a first edge (order is determined by key NetworkX MultiGraph edge attribute) between two supplied bg.vertex.BGVertex
- •BreakpointGraph.get\_edges\_by\_vertex(): returns a generator yielding bg.edge.BGEdge
- •BreakpointGraph.edges\_between\_two\_vertices(): returns a generator yielding bg.edge.BGEdge between two supplied vertices

- •BreakpointGraph.connected\_components\_subgraphs(): returns a generator of BreakpointGraph object, that represent connected components of a current BreakpointGraph object, deep copying(by default) all information of current BreakpointGraph
- •BreakpointGraph.delete\_edge(): deletes and edge from perspective of multi-color substitution of supplied vertices
- •BreakpointGraph.delete\_bgedge(): deletes a supplied bg.edge.BGEdge instance from perspective of substituting multi-colors.
- •BreakpointGraph.split\_edge(): deletes a supplied bg.multicolor.Multicolor instance in identifies edge from two supplied vertices.
- •BreakpointGraph.split\_bgedge(): splits a bg.edge.BGEdge with respect to provided guidance
- •BreakpointGraph.split\_all\_edges\_between\_two\_vertices(): splits all edges between two supplied vertices with respect to provided guidance.
- •BreakpointGraph.split\_all\_edges(): splits all edge in BreakpointGraph with respect to provided guidance.
- •BreakpointGraph.delete\_all\_edges\_between\_two\_vertices(): deletes all edges between two given vertices, by plain deleting them from MultiGraph underling structure.
- •BreakpointGraph.merge\_all\_edges\_between\_two\_vertices(): merges all edge between two given vertices creating a single edge containing information about multi-colors in respective edges.
- •BreakpointGraph.merge all edges (): merges all edges in current BreakpointGraph.
- •BreakpointGraph.merge(): merges two BreakpointGraph instances with respect to vertices, edges, and multicolors.
- •BreakpointGraph.update(): updates information in current BreakpointGraph instance by adding new bg.edge.BGEdge instances form supplied BreakpointGraph.

### \_BreakpointGraph\_\_add\_bgedge(bgedge, merge=True)

Adds supplied bq.edge.BGEdge object to current instance of BreakpointGraph.

Checks that vertices in supplied bg.edge.BGEdge instance actually are present in current BreakpointGraph if merge option of provided. Otherwise a new edge is added to the current BreakpointGraph.

#### **Parameters**

- **bgedge** (bg.edge.BGEdge) instance of bg.edge.BGEdge infromation form which is to be added to current BreakpointGraph
- merge (Boolean) a flag to merge supplied information from multi-color perspective into a first existing edge between two supplied vertices

Returns None, performs inplace changes

\_BreakpointGraph\_\_delete\_all\_bgedges\_between\_two\_vertices (vertex1, vertex2)

Deletes all edges between two supplied vertices

#### **Parameters**

- **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) a first out of two vertices edges between which are to be deleted
- **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) a second out of two vertices edges between which are to be deleted

**Returns** None, performs inplace changes

### \_BreakpointGraph\_\_delete\_bgedge(bgedge, key=None, keep\_vertices=False)

Deletes a supplied bg.edge.BGEdge from a perspective of multi-color substitution. If unique identifier key is not provided, most similar (from perspective of bg.multicolor.Multicolor.similarity\_score() result) edge between respective vertices is chosen for change.

If no unique identifier for edge to be changed is specified, edge to be updated is determined by iterating over all edges between vertices in supplied bg.edge.BGEdge instance and the edge with most similarity score to supplied one is chosen. Once the edge to be substituted from is determined, substitution if performed form a perspective of bg.multicolor.Multicolor substitution. If after substitution the remaining multicolor of respective edge is empty, such edge is deleted form a perspective of MultiGraph edge deletion.

#### **Parameters**

- **bgedge** (*bg.edge.BGEdge*) an edge to be deleted from a perspective of multi-color substitution
- **key** unique identifier of existing edges in current *BreakpointGraph* instance to be changed

**Type** any python object. int is expected.

Returns None, performed inplace changes.

### \_BreakpointGraph\_\_edges (nbunch=None, keys=False)

Iterates over edges in current BreakpointGraph instance.

Returns a generator over the edges in current *BreakpointGraph* instance producing instances of *bg.edge.BGEdge* instances wrapping around information in underlying MultiGraph object.

#### **Parameters**

- **nbunch** a vertex to iterate over edges outgoing from, if not provided, iteration over all edges is performed.
- **keys** (Boolean) a flag to indicate if information about unique edge's ids has to be returned alongside with edge

Returns generator over edges in current BreakpointGraph

Return type generator

### \_BreakpointGraph\_\_edges\_between\_two\_vertices(vertex1, vertex2, keys=False)

Iterates over edges between two supplied vertices in current BreakpointGraph

Checks that both supplied vertices are present in current breakpoint graph and then yield all edges that are located between two supplied vertices. If keys option is specified, then not just edges are yielded, but rather pairs (edge, edge\_id) are yielded

#### **Parameters**

- **vertex1** (any hashable object, bg.vertex.BGVertex is expected) a first vertex out of two, edges of interest are incident to
- vertex2 (any hashable object, bg.vertex.BGVertex is expected) a second vertex out of two, edges of interest are incident to
- **keys** (Boolean) a flag to indicate if information about unique edge's ids has to be returned alongside with edge

**Returns** generator over edges (tuples edge, edge\_id if keys specified) between two supplied vertices in current *BreakpointGraph* wrapped in bg.vertex.BGVertex

Return type generator

### \_BreakpointGraph\_\_get\_edge\_by\_two\_vertices(vertex1, vertex2, key=None)

Returns an instance of bg.edge.BBGEdge edge between to supplied vertices (if key is supplied, returns a bg.edge.BBGEdge instance about specified edge).

Checks that both specified vertices are in current <code>BreakpointGraph</code> and then depending on key argument, creates a new <code>bg.edge</code> . <code>BBGEdge</code> instance and incorporates respective multi-color information into it.

#### **Parameters**

- vertex1 (any hashable object) first vertex instance out of two in current BreakpointGraph
- vertex2 (any hashable object) second vertex instance out of two in current BreakpointGraph
- **key** (any python object. None or int is expected) unique identifier of edge of interested to be retrieved from current *BreakpointGraph*

**Returns** edge between two specified edges respecting a key argument.

Return type bg.edge.BGEdge

### \_BreakpointGraph\_\_get\_edges\_by\_vertex(vertex, keys=False)

Iterates over edges that are incident to supplied vertex argument in current BreakpointGraph

Checks that the supplied vertex argument exists in underlying MultiGraph object as a vertex, then iterates over all edges that are incident to it. Wraps each yielded object into bg.edge.BGEdge object.

#### **Parameters**

- **vertex** (any hashable object. bg.vertex.BGVertex object is expected.) a vertex object in current *BreakpointGraph* object
- **keys** (Boolean) a flag to indicate if information about unique edge's ids has to be returned alongside with edge

**Returns** generator over edges (tuples edge, edge\_id if keys specified) in current BreakpointGraph wrapped in bg.vertex.BGEVertex

 $Return \ type \ \texttt{generator} \\$ 

### \_BreakpointGraph\_\_get\_vertex\_by\_name(vertex\_name)

Obtains a vertex object by supplied label

Returns a bg. vertex.BGVertex or its subclass instance

**Parameters vertex\_name** (any hashable python object. str expected.) – a vertex label it is identified by.

**Returns** vertex with supplied label if present in current *BreakpointGraph*, None otherwise

#### \_BreakpointGraph \_ merge\_all\_bgedges\_between\_two\_vertices(vertex1, vertex2)

Merges all edge between two supplied vertices into a single edge from a perspective of multi-color merging.

### **Parameters**

• **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) – a first out of two vertices edges between which are to be merged together

• **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) – a second out of two vertices edges between which are to be merged together

Returns None, performs inplace changes

```
_BreakpointGraph__split_all_edges_between_two_vertices(vertex1, vertex2, guidance=None, sorted_guidance=False, ac-
```

Splits all edges between two supplied vertices in current *BreakpointGraph* instance with respect to the provided guidance.

Iterates over all edges between two supplied vertices and splits each one of them with respect to the guidance.

#### **Parameters**

- **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) a first out of two vertices edges between which are to be split
- **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) a second out of two vertices edges between which are to be split
- guidance (iterable where each entry is iterable with colors entries) a guidance for underlying bg.multicolor.Multicolor objects to be split

Returns None, performs inplace changes

```
_BreakpointGraph__split_bgedge (bgedge, guidance=None, sorted_guidance=False, account_for_colors_multiplicity_in_guidance=True, key=None)
```

Splits a bg.edge. BGEdge in current Breakpoint Graph most similar to supplied one (if no unique identifier key is provided) with respect to supplied guidance.

If no unique identifier for edge to be changed is specified, edge to be split is determined by iterating over all edges between vertices in supplied bg.edge.BGEdge instance and the edge with most similarity score to supplied one is chosen. Once the edge to be split is determined, split if performed form a perspective of bg.multicolor.Multicolor split. The originally detected edge is deleted, and new edges containing information about multi-colors after splitting, are added to the current BreakpointGraph.

#### **Parameters**

- **bgedge** (bg.edge.BGEdge) an edge to find most "similar to" among existing edges for a split
- guidance (iterable where each entry is iterable with colors entries) a guidance for underlying bg.multicolor.Multicolor object to be split
- duplication\_splitting (Boolean) flag (not currently implemented) for a splitting of color-based splitting to take into account multiplicity of respective colors
- **key** (any python object. int is expected) unique identifier of edge to be split

Returns None, performs inplace changes

```
_BreakpointGraph__update(breakpoint_graph, merge_edges=False)
```

Updates a current :class'BreakpointGraph' object with information from a supplied :class'BreakpointGraph' instance.

count for colors multiplicity in guidance=T

Depending of a merge\_edges flag, while updating of a current :class'BreakpointGraph' object is occuring, edges between similar vertices can be merged to already existing ones.

#### **Parameters**

- breakpoint\_graph (:class 'BreakpointGraph') a breakpoint graph to extract information from, which will be then added to the current
- merge\_edges (Boolean) flag to indicate if edges to be added to current :class'BreakpointGraph' object are to be merged to already existing ones

**Returns** None, performs inplace changes

#### \_\_\_init\_\_\_(graph=None)

Initialization of a BreakpointGraph object.

Parameters graph (instance of NetworkX MultiGraph is expected.) — is supplied, BreakpointGraph is initialized with supplied or brand new (empty) instance of NetworkX MultiGraph.

### add\_bgedge (bgedge, merge=True)

Adds supplied bg.edge.BGEdge object to current instance of BreakpointGraph.

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_add\_bgedge() method.

#### **Parameters**

- **bgedge** (bg.edge.BGEdge) instance of bg.edge.BGEdge infromation form which is to be added to current BreakpointGraph
- merge (Boolean) a flag to merge supplied information from multi-color perspective into a first existing edge between two supplied vertices

Returns None, performs inplace changes

### add\_edge (vertex1, vertex2, multicolor, merge=True, data=None)

Creates a new bg.edge.BGEdge object from supplied information and adds it to current instance of BreakpointGraph.

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_add\_bgedge() method.

#### **Parameters**

- **vertex1** (any hashable object) first vertex instance out of two in current BreakpointGraph
- **vertex2** (any hashable object) second vertex instance out of two in current BreakpointGraph
- multicolor (bg.multicolor.Multicolor) an information about multi-colors of added edge
- merge (Boolean) a flag to merge supplied information from multi-color perspective into a first existing edge between two supplied vertices

Returns None, performs inplace changes

#### apply\_kbreak (kbreak, merge=True)

Check validity of supplied k-break and then applies it to current BreakpointGraph

Only bg.kbreak.KBreak (or its heirs) instances are allowed as kbreak argument. KBreak must correspond to the valid kbreak and, since some changes to its internals might have been done since its creation, a validity check in terms of starting/resulting edges is performed. All vertices in supplied KBreak (except for paired infinity vertices) must be present in current BreakpointGraph. For all supplied pairs

of vertices (except for paired infinity vertices), there must be edges between such pairs of vertices, at least one of which must contain a multicolor matching a multicolor of supplied kbreak.

Edges of specified in kbreak multicolor are deleted between supplied pairs of vertices in kbreak.start\_edges (except for paired infinity vertices). New edges of specified in kbreak multicolor are added between all pairs of vertices in kbreak.result\_edges (except for paired infinity vertices). If after the kbreak application there is an infinity vertex, that now has no edges incident to it, it is deleted form the current <code>BreakpointGraph</code>.

#### **Parameters**

- **kbreak** (*bg.kbreak*.*KBreak*) a k-break to be applied to current *BreakpointGraph*
- merge (Boolean) a flag to indicate on how edges, that will be created by a k-break, will be added to current *BreakpointGraph*

**Returns** nothing, performs inplace changes

Return type None

Raises ValueError, TypeError

#### connected\_components\_subgraphs (copy=True)

Iterates over connected components in current *BreakpointGraph* object, and yields new instances of *BreakpointGraph* with respective information deep-copied by default (week reference is possible of specified in method call).

**Parameters copy** (Boolean) – a flag to signal if graph information has to be deep copied while producing new *BreakpointGraph* instances, of just reference to respective data has to be made.

**Returns** generator over connected components in current *BreakpointGraph* wrapping respective connected components into new *BreakpointGraph* objects.

Return type generator

### delete\_all\_edges\_between\_two\_vertices (vertex1, vertex2)

Deletes all edges between two supplied vertices

 $\begin{array}{l} \textbf{Proxies a call to } \textit{BreakpointGraph.\_BreakpointGraph} \underline{\quad } \textit{delete\_all\_bgedges\_between\_two\_vertice} \\ \textbf{method.} \end{array}$ 

### **Parameters**

- **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) a first out of two vertices edges between which are to be deleted
- **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) a second out of two vertices edges between which are to be deleted

**Returns** None, performs inplace changes

### delete\_bgedge (bgedge, key=None)

Deletes a supplied bg.edge.BGEdge from a perspective of multi-color substitution. If unique identifier key is not provided, most similar (from perspective of bg.multicolor.Multicolor.similarity\_score() result) edge between respective vertices is chosen for change.

Proxies a call to  $BreakpointGraph._BreakpointGraph_{delete_bgedge}$  method.

### **Parameters**

 bgedge (bg.edge.BGEdge) – an edge to be deleted from a perspective of multi-color substitution • **key** – unique identifier of existing edges in current *BreakpointGraph* instance to be changed

**Type** any python object. int is expected.

**Returns** None, performed inplace changes.

#### delete\_edge (vertex1, vertex2, multicolor, key=None)

Creates a new bg.edge.BGEdge instance from supplied information and deletes it from a perspective of multi-color substitution. If unique identifier key is not provided, most similar (from perspective of bg.multicolor.Multicolor.similarity\_score() result) edge between respective vertices is chosen for change.

Proxies a call to  $BreakpointGraph._BreakpointGraph_{delete,gedge}$  method.

#### **Parameters**

- **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) a first vertex out of two the edge to be deleted is incident to
- **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) a second vertex out of two the edge to be deleted is incident to
- multicolor (bg.multicolor.Multicolor) a multi-color to find most suitable edge to be deleted
- **key** unique identifier of existing edges in current *BreakpointGraph* instance to be changed

**Type** any python object. int is expected.

**Returns** None, performed inplace changes.

#### edges (nbunch=None, keys=False)

Iterates over edges in current BreakpointGraph instance.

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_edges().

#### **Parameters**

- **nbunch** a vertex to iterate over edges outgoing from, if not provided, iteration over all edges is performed.
- **keys** (Boolean) a flag to indicate if information about unique edge's ids has to be returned alongside with edge

Returns generator over edges in current BreakpointGraph

Return type generator

#### edges\_between\_two\_vertices (vertex1, vertex2, keys=False)

Iterates over edges between two supplied vertices in current BreakpointGraph

Proxies a call to Breakpoint.\_Breakpoint\_\_edges\_between\_two\_vertices() method.

#### **Parameters**

- **vertex1** (any hashable object, bg.vertex.BGVertex is expected) a first vertex out of two, edges of interest are incident to
- **vertex2** (any hashable object, bg.vertex.BGVertex is expected) a second vertex out of two, edges of interest are incident to
- **keys** (Boolean) a flag to indicate if information about unique edge's ids has to be returned alongside with edge

**Returns** generator over edges (tuples edge, edge\_id if keys specified) between two supplied vertices in current <code>BreakpointGraph</code> wrapped in bg.vertex.BGVertex

Return type generator

A JSON descrialization operation, that recovers a breakpoint graph from its JSON representation

as information about genomes, that are encoded in breakpoint graph might be available somewhere else, but not the json object, there is an option to provide it and omit encoding information about genomes.

#### get\_edge\_by\_two\_vertices (vertex1, vertex2, key=None)

Returns an instance of bg.edge.BBGEdge edge between to supplied vertices (if key is supplied, returns a bg.edge.BBGEdge instance about specified edge).

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_get\_edge\_by\_two\_vertices().

#### **Parameters**

- **vertex1** (any hashable object) first vertex instance out of two in current BreakpointGraph
- vertex2 (any hashable object) second vertex instance out of two in current BreakpointGraph
- **key** (any python object. None or int is expected) unique identifier of edge of interested to be retrieved from current *BreakpointGraph*

**Returns** edge between two specified edges respecting a key argument.

Return type bg.edge.BGEdge

#### get\_edges\_by\_vertex (vertex, keys=False)

Iterates over edges that are incident to supplied vertex argument in current BreakpointGraph

Proxies a call to Breakpoint.\_Breakpoint\_\_get\_edges\_by\_vertex() method.

#### **Parameters**

- **vertex** (any hashable object. bg.vertex.BGVertex object is expected.) a vertex object in current *BreakpointGraph* object
- **keys** (Boolean) a flag to indicate if information about unique edge's ids has to be returned alongside with edge

**Returns** generator over edges (tuples edge, edge\_id if keys specified) in current BreakpointGraph wrapped in bg.vertex.BGEVertex

Return type generator

#### get\_vertex\_by\_name (vertex\_name)

Obtains a vertex object by supplied label

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_get\_vertex\_by\_name().

**Parameters vertex\_name** (any hashable python object. str expected.) – a vertex label it is identified by.

**Returns** vertex with supplied label if present in current BreakpointGraph, None otherwise

Return type bg. vertices. BGVertex or None

 $\textbf{classmethod merge} \ (breakpoint\_graph1, breakpoint\_graph2, merge\_edges=False)$ 

Merges two given instances of :class'BreakpointGraph' into a new one, that gather all available information from both supplied objects.

Depending of a merge\_edges flag, while merging of two dat structures is occurring, edges between similar vertices can be merged during the creation of a result :class'BreakpointGraph' obejct.

Accounts for subclassing.

#### **Parameters**

- breakpoint\_graph1 (:class 'BreakpointGraph') a first out of two :class'BreakpointGraph' instances to gather information from
- breakpoint\_graph2 (:class 'BreakpointGraph') a second out of two :class'BreakpointGraph' instances to gather information from
- merge\_edges (Boolean) flag to indicate if edges in a new merged :class'BreakpointGraph' object has to be merged between same vertices, or if splitting from supplied graphs shall be preserved.

**Returns** a new breakpoint graph object that contains all information gathered from both supplied breakpoint graphs

Return type :class'BreakpointGraph'

#### merge\_all\_edges()

Merges all edges in a current :class'BreakpointGraph' instance between same pairs of vertices into a single edge from a perspective of multi-color merging.

Iterates over all possible pairs of vertices in current *BreakpointGraph* and merges all edges between respective pairs.

Returns None, performs inplace changes

#### merge\_all\_edges\_between\_two\_vertices (vertex1, vertex2)

Merges all edge between two supplied vertices into a single edge from a perspective of multi-color merging.

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_merge\_all\_bgedges\_between\_two\_verts

#### **Parameters**

- **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) a first out of two vertices edges between which are to be merged together
- **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) a second out of two vertices edges between which are to be merged together

Returns None, performs inplace changes

#### nodes()

Iterates over nodes in current *BreakpointGraph* instance.

**Returns** generator over nodes (vertices) in current *BreakpointGraph* instance.

Return type generator

Splits all edge in current BreakpointGraph instance with respect to the provided guidance.

Iterate over all possible distinct pairs of vertices in current *BreakpointGraph* instance and splits all edges between such pairs with respect to provided guidance.

```
Parameters guidance (iterable where each entry is iterable with colors entries) - a guidance for underlying bg.multicolor.Multicolor objects to be split
```

2.2. API documentation

**Returns** None, performs inplace changes

Splits all edges between two supplied vertices in current *BreakpointGraph* instance with respect to the provided guidance.

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_split\_all\_edges\_between\_two\_vertices() method.

#### **Parameters**

- **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) a first out of two vertices edges between which are to be split
- **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) a second out of two vertices edges between which are to be split
- guidance (iterable where each entry is iterable with colors entries) a guidance for underlying bg.multicolor.Multicolor objects to be split

Returns None, performs inplace changes

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_split\_bgedge() method.

#### **Parameters**

- **bgedge** (bg.edge.BGEdge) an edge to find most "similar to" among existing edges for a split
- guidance (iterable where each entry is iterable with colors entries) a guidance for underlying bg.multicolor.Multicolor object to be split
- **duplication\_splitting** (Boolean) flag (**not** currently implemented) for a splitting of color-based splitting to take into account multiplicity of respective colors
- key (any python object. int is expected) unique identifier of edge to be split

**Returns** None, performs inplace changes

Proxies a call to BreakpointGraph.\_BreakpointGraph\_\_split\_bgedge() method.

#### **Parameters**

- **vertex1** (any python hashable object. bg.vertex.BGVertex is expected) a first vertex out of two the edge to be split is incident to
- **vertex2** (any python hashable object. bg.vertex.BGVertex is expected) a second vertex out of two the edge to be split is incident to
- multicolor (bg.multicolor.Multicolor) a multi-color to find most suitable edge to be split

- duplication\_splitting (Boolean) flag (not currently implemented) for a splitting of color-based splitting to take into account multiplicity of respective colors
- key (any python object. int is expected) unique identifier of edge to be split

Returns None, performs inplace changes

#### to\_json (schema\_info=True)

JSON serialization method that account for all information-wise important part of breakpoint graph

```
update (breakpoint_graph, merge_edges=False)
```

Updates a current :class'BreakpointGraph' object with information from a supplied :class'BreakpointGraph' instance.

Proxoes a call to BreakpointGraph.\_BreakpointGraph\_update() method.

#### **Parameters**

- **breakpoint\_graph** (*BreakpointGraph*) a breakpoint graph to extract information from, which will be then added to the current
- merge\_edges (Boolean) flag to indicate if edges to be added to current :class'BreakpointGraph' object are to be merged to already existing ones

Returns None, performs inplace changes

### 2.2.3 tree.py

```
class bg.tree.BGTree (newick=None, newick_format=1, dist=1, leaf_wrapper=<class
    'bg.genome.BGGenome'>)
```

Bases: object

Class that is designed to store information about phylogenetic information and relations between multiple genomes

Class utilizes a ete3. Tree object as an internal storage This tree can store information about:

edge lengths

•tree topology

### \_BGTree\_\_get\_node\_by\_name (name)

Returns a first TreeNode object, which name matches the specified argument

Raises ValueError (if no node with specified name is present in the tree)

#### \_BGTree\_\_get\_v\_tree\_consistent\_leaf\_based\_hashable\_multicolors()

Internally used method, that recalculates VTree-consistent sets of leaves in the current tree

```
_BGTree__has_edge (node1_name, node2_name, account_for_direction=True)
```

Returns a boolean flag, telling if a tree has an edge with two nodes, specified by their names as arguments

If a account\_for\_direction is specified as True, the order of specified node names has to relate to parent - child relation, otherwise both possibilities are checked

```
_BGTree__has_node(name)
```

Check is the current Tree has a node, matching by name to the specified argument

### \_BGTree\_\_update\_consistent\_multicolors()

Internally used method, that recalculates T-consistent / VT-consistent multicolors for current tree topology

#### \_BGTree\_\_vertex\_is\_leaf(node\_name)

Checks if a node specified by its name as an argument is a leaf in the current Tree

**Raises** ValueError (if no node with specified name is present in the tree)

```
add_edge (node1_name, node2_name, edge_length=1)
```

Adds a new edge to the current tree with specified characteristics

Forbids addition of an edge, if a parent node is not present Forbids addition of an edge, if a child node already exists

#### **Parameters**

- node1\_name name of the parent node, to which an edge shall be added
- node2\_name name of newly added child node
- edge\_length a length of specified edge

**Returns** nothing, inplace changes

**Raises** ValueError (if parent node IS NOT present in the tree, or child node IS already present in the tree)

```
append (node_name, tree, copy=False)
```

Append a specified tree (represented by a root TreeNode element) to the node, specified by its name

**Parameters** copy (Boolean) – a flag denoting if the appended tree has to be added as is, or is the deepcopy of it has to be used

**Raises** ValueError (if no node with a specified name, to which the specified tree has to be appended, is present in the current tree)

#### bgedge\_is\_tree\_consistent(bgedge)

Checks is supplied BGEdge (from the perspective of its multicolor is T-consistent)

#### bgedge\_is\_vtree\_consistent(bgedge)

Checks is supplied BGEdge (from the perspective of its multicolor is VT-consistent)

### edges()

Returns iterator over edges in current tree.

Return type iterator

#### get\_distance (node1\_name, node2\_name)

Returns a length of an edge / path, if exists, from the current tree

#### **Parameters**

- node1\_name a first node name in current tree
- node2\_name a second node name in current tree

**Returns** a length of specified by a pair of vertices edge / path

**Return type** Number

Raises ValueError, if requested a length of an edge, that is not present in current tree

#### get\_node\_by\_name (name)

Proxies the call to the <u>\_\_get\_node\_by\_name</u> method

#### get\_tree\_consistent\_multicolors()

Returns a copy of the list of T-consistent multicolors from current tree

#### get\_vtree\_consistent\_multicolors()

Returns a copy of the list of VT-consistent multicolors from current tree

```
has_edge (node1_name, node2_name, account_for_direction=True)
```

Proxies a call to the \_\_has\_edge method

#### has\_node (name)

Proxies a call to \_\_has\_node method

#### multicolor is tree consistent(multicolor)

Checks is supplied multicolor is T-consistent

#### multicolor is vtree consistent(multicolor)

Checks is supplied multicolor is VT-consistent

#### nodes()

Proxies iteration to the underlying Tree.iter\_descendants iterator, but first yielding a root element

**Returns** iterator over all descendants of a root, starting with a root, in current tree

Return type iterator

#### root

A property based call for the root pointer in current tree

#### tree\_consistent\_multicolors

Property based getter, that checks for consistency in terms of precomputed T-consistent multicolors, recomputes all consistent multicolors if tree topology has changed and returns internally stored list of T-consistent multicolors

#### tree\_consistent\_multicolors\_set

Property based getter, that checks for consistency in terms of precomputed T-consistent multicolors, recomputes all consistent multicolors if tree topology has changed and returns internally stored set of hashable representation of T-consistent multicolors

#### vtree\_consistent\_multicolors

Property based getter, that checks for consistency in terms of precomputed VT-consistent multicolors, recomputes all consistent multicolors if tree topology has changed and returns internally stored list of VT-consistent multicolors

#### vtree\_consistent\_multicolors\_set

Property based getter, that checks for consistency in terms of precomputed VT-consistent multicolors, recomputes all consistent multicolors if tree topology has changed and returns internally stored set of hashable representation of VT-consistent multicolors

### 2.2.4 kbreak.py

class bg.kbreak.KBreak(start\_edges, result\_edges, multicolor, data=None)

Bases: object

A generic object that can represent any k-break ( $k \ge 2$ )

A notion of k-break arises from the bioinformatics combinatorial object BreakpointGraph and is first mentioned in http://home.gwu.edu/~maxal/ap\_tcs08.pdf A generic k-break operates on k specified edges of spisific multicolor and replaces them with another set of k edges with the same multicolor on the same set of vertices in way, that the degree of vertices is kept intact.

Initialization of the instance of KBreak is performed with a validity check of supplied data, which must comply with the definition of k-break.

Class carries following attributes carrying information about k-break structure:

•KBreak . start\_edges: a list of edges (in terms of paired vertices) that are to be removed by current KBreak

- •KBreak . result\_edges: a list of edges (in terms of paired vertices) that are to be created by current KBreak
- •KBreak.multicolor: a bg.multicolor.Multicolor instance, that specifies the multicolor of edges that are to be removed / created by current KBreak

#### Main operations:

• KBreak.valid\_kbreak\_matchings(): a method that checks if provided sets of started / resulted edges comply with the notions ob k-break definition

```
__init__ (start_edges, result_edges, multicolor, data=None)
Initialization of KBreak object.
```

The initialization process consists of multiple checks, before any assignment and initialization itself is performed.

First checks the fact, that information about start / result edges is supplied in form of paired vertices. Then check is performed to make sure, that degrees of vertices, that current KBreak operates on, is preserved.

#### **Parameters**

- **start\_edges** (list (tuple (vertex, vertex), ...)) a list of pairs of vertices, that specifies where edges shall be removed by current *KBreak*
- result\_edges (list(tuple(vertex, vertex), ...)) a list of pairs of vertices, that specifies where edges shall be created by current KBreak
- multicolor (bg.multicolor.Multicolor) a multicolor, that specifies which edges between specified pairs of vertices are to be removed / created

**Returns** a new instance of Kbreak

Return type KBreak
Raises ValueError

#### static valid\_kbreak\_matchings (start\_edges, result\_edges)

A staticmethod check implementation that makes sure that degrees of vertices, that are affected by current KBreak

By the notion of k-break, it shall keep the degree of vertices in bg.breakpoint\_graph.BreakpointGraph the same, after its application. By utilizing the Counter class, such check is performed, as the number the vertex is mentioned corresponds to its degree.

#### **Parameters**

- **start\_edges** (list (tuple (vertex, vertex), ...)) a list of pairs of vertices, that specifies where edges shall be removed by *KBreak*
- result\_edges (list(tuple(vertex, vertex), ...)) a list of pairs of vertices, that specifies where edges shall be created by KBreak

**Returns** a flag indicating if the degree of vertices are equal in start / result edges, targeted by KBreak

Return type Boolean

### 2.2.5 multicolor.py

```
class bg.multicolor.Multicolor(*args)
    Bases: object
```

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Class providing implementation of multi-color notion for edges in bg.breakpoint\_graph.BreakpointGraph.

Multi-color is a specific property of edges in Breakpoint Graph combinatorial object which represents similar adjacencies between genomic material in multiple genomes.

This class supports the following attributes, that carry information colors and their multiplicity of edges in bg.breakpoint\_graph.BreakpointGraph.

- •Multicolor.multicolors: a python Counter object which contains information about colors and their multiplicity for a given *Multicolor* instance
- •Multicolor.colors: a property attribute providing a set of colors in Multicolor.multicolors attribute, hiding information about colors multiplicity

#### Main operations:

- •+, -, +=, -=, ==, >, >=, <, <=
- $\bullet$  Multicolor.update(): updates information in Multicolor.multicolors attribute of respective instance
- •Multicolor.merge(): creates a new Multicolor object out of a list of provided Multicolor objects, gathering respective information about colors and their multiplicity
- •Multicolor.left\_merge(): updates respective Multicolor instance with information from supplied Multicolor object
- •Multicolor.delete(): reduces information in respective instance Multicolor.multicolors attribute by iterating over supplied data
- •Multicolor.similarity\_score() computes how similar two supplied Multicolor object are
- •Multicolor.split\_colors() produces several new instances of Multicolor object by splitting information about colors by using provided guidance iterable set-like object

### \_Multicolor\_\_delete(multicolor)

Reduces information Multicolor attribute by iterating over supplied colors data.

In case supplied argument is a *Multicolor* instance, multi-color specific information to de deleted is set to its Multicolor.multicolors. In other cases multi-color specific information to de deleted is obtained from iterating over the argument.

Colors and their multiplicity is reduces with a help of – method of python Counter object.

**Parameters multicolor** (any iterable with colors object as entries or *Multicolor*) – information about colors to be deleted from *Multicolor* object

**Returns** None, performs inplace changes

#### static \_Multicolor\_\_left\_merge (multicolor1, multicolor2)

Updates first supplied Multicolor instance with information from second supplied Multicolor instance.

First supplied instances attribute Multicolor.multicolors is updated with a help of + method of python Counter object.

#### **Parameters**

- multicolor1 (Multicolor) instance to update information in
- multicolor2 (Multicolor) instance to use information for update from

**Returns** updated first supplied Multicolor instance

Return type Multicolor

#### classmethod \_Multicolor\_\_merge (\*multicolors)

Produces a new *Multicolor* object resulting from gathering information from all supplied *Multicolor* instances.

New Multicolor is created and its Multicolor.multicolors attribute is updated with similar attributes of supplied Multicolor objects.

Accounts for subclassing.

Parameters multicolors (Multicolor) – variable number of Multicolor objects

**Returns** object containing gathered information from all supplied arguments

Return type Multicolor

```
__add___(other)
```

Implementation of + operation for Multicolor

Invokes a private Multicolor.\_Multicolor\_\_merge() method to implement addition of two Multicolor instances.

**Parameters other** (*Multicolor*) – object, whose multi-color information has to be added to current one

**Returns** new *Multicolor* object, colors in which and their multiplicity result from addition of current Multicolor.multicolors and supplied Multicolor.multicolors

Return type Multicolor

Raises TypeError, if not Multicolor instance is provided

\_\_\_eq\_\_(other)

Implementation of == operation for Multicolor

Two Multicolor objects are called to be equal if colors that both of them contain and respective colors multiplicity are equal. Multicolor instance never equals to non-Multicolor object. Performs Multicolors comparison with a help of == method of python Counter object.

Parameters other (any python object) – an object to compare to

**Returns** a flag of equality between current Multicolor instance and supplied object

Return type Boolean

**\_\_ge**\_\_(other)

Implementation of ">=" operation for Multicolor

One Multicolor instance is said to be "greater than" the other Multicolor instance, if it contains greater or equal number of colors, as the other Multicolor object does, and multiplicity of all of them is greater or equal than in the other multicolor. Multicolor instance is never less, than non-Multicolor object.

**Parameters other** (any python object) – an object to compare to

**Returns** a flag if current Multicolor object is greater or equal than supplied object

Return type Boolean

\_\_\_gt\_\_\_(other)

Implementation of > operation for Multicolor

One Multicolor instance is said to be "greater than" the other Multicolor instance, if it contains greater os equal number of colors, as the other Multicolor object does, and multiplicity of all of them is greater or equal than in the other multicolor, and at least one color has multiplicity greater, than in the other multicolor. Multicolor instance is never less, than non-Multicolor object.

Parameters other (any python object) – an object to compare to

**Returns** a flag if current Multicolor object is less than supplied object

Return type Boolean

```
__iadd__(other)
```

Implementation of += operation for Multicolor

Invokes a private Multicolor.\_Multicolor.\_merge() method to implement addition of two Multicolor instances.

**Parameters other** (Multicolor) – object, whose multi-color information has to be added to current one

**Returns** new *Multicolor* object, colors in which and their multiplicity result from addition of current Multicolor.multicolors and supplied Multicolor.multicolors

Return type Multicolor

Raises TypeError, if not Multicolor instance is provided

\_\_\_init\_\_\_(\*args)

Initialization of Multicolor object.

Initialization is performed by supplied variable number of colors, that respective Multicolor object must contain information about Multiplicity of each color is determined by the number of times it occurs as argument in initialization process.

Parameters args (any hashable python object) - variable number of colors to contain information about

**Returns** a new instance of Multicolor

Return type Multicolor

```
___isub___(other)
```

Implementation of – operation for Multicolor

Updates current Multicolor instance by updating its Multicolor.multicolors attribute information by deleting multi-colors in supplied Multicolor.multicolors attribute. Utilizes – method of python Counter

**Parameters other** (*Multicolor*) – object, whose multi-color information to subtract form current one

Returns updated current Multicolor object

Return type Multicolor

Raises TypeError, if not Multicolor instance is supplied

\_\_\_le\_\_\_(other)

Implementation of "<=" operation for Multicolor

One Multicolor instance is said to be "less or equal than" the other Multicolor instance, if it contains less or equal number colors, as the other Multicolor object does, and multiplicity of all of them is less or equal than in the other multicolor. Multicolor instance is never less or equal, than non-Multicolor object.

**Parameters other** (any python object) – an object to compare to

**Returns** a flag if current Multicolor object is less or equal than supplied object

Return type Boolean

```
lt (other)
```

Implementation of < operation for Multicolor

One Multicolor instance is said to be "less than" the other Multicolor instance, if it contains less or equal number of colors colors, as the other Multicolor object does, and multiplicity of all of them is less or equal than in the other multicolor, and at least one color has multiplicity less, than in the other multicolor. Multicolor instance is never less, than non-Multicolor object.

Parameters other (any python object) – an object to compare to

**Returns** a flag if current Multicolor object is less than supplied object

Return type Boolean

```
__mul__(other)
```

Multicolor can be multiplied by a number and it multiplies multiplicity of each present color respectively

Parameters other – an integer multiplier

**Returns** a new multicolor object resulted from multiplying each colors multiplicity by the multiplier

```
__sub__(other)
```

Implementation of – operation for Multicolor

Creates a new *Multicolor* instance by cloning current *Multicolor* object and updating its Multicolor.multicolors attribute information by deleting multi-colors in supplied *Multicolor* object.

**Parameters other** (*Multicolor*) – object, whose multi-color information to subtract form current one

Returns new Multicolor object, colors in which and their multiplicity result from subtracting of current Multicolor.multicolors and supplied Multicolor.multicolors attributes.

Return type Multicolor

Raises TypeError, if not Multicolor instance is supplied

#### colors

Implements an "attribute" like object to access information about colors only, hiding information about their multiplicity.

Creates a fresh set object every time is accessed.

**Returns** all colors that current *Multicolor* object contains information about.

Return type set

#### delete (multicolor)

Reduces information Multicolor attribute by iterating over supplied colors data.

Works as proxy to respective call to private static method <code>Multicolor.\_Multicolor\_\_delete()</code> for purposes of inheritance compatibility.

**Parameters multicolor** (any iterable with colors object as entries or *Multicolor*) – information about colors to be deleted from *Multicolor* object

Returns None, performs inplace changes

#### hashable\_representation

For a sake of speed check for multicolor presence, each multicolor has a deterministic hashable representation

#### intersect (other)

Computes the multiset intersection, between the current Multicolor and the supplied Multicolor

Parameters other – another Multicolor object to compute a multiset intersection with

Returns

Raises TypeError – an intersection can be computed only between two Multicolor objects

#### classmethod left merge (multicolor1, multicolor2)

Updates first supplied Multicolor instance with information from second supplied Multicolor instance.

Works as proxy to respective call to private static method <code>Multicolor.\_Multicolor\_\_left\_merge()</code> for purposes of inheritance compatibility.

Accounts for subclassing.

#### **Parameters**

- multicolor1 (Multicolor) instance to update information in
- multicolor2 (Multicolor) instance to use information for update from

**Returns** updated first supplied Multicolor instance

Return type Multicolor

#### classmethod merge (\*multicolors)

Produces a new Multicolor object resulting from gathering information from all supplied Multicolor instances.

Works as proxy to respective call to private static method <code>Multicolor.\_Multicolor\_merge()</code> for purposes of inheritance compatibility.

Parameters multicolors (Multicolor) – variable number of Multicolor objects

Returns object containing gathered information from all supplied arguments

Return type Multicolor

### static similarity\_score (multicolor1, multicolor2)

Computes how similar two Multicolor objects are from perspective of information, that they contain.

Two multicolors are called to be similar if they contain same colors (at least one). Multiplicity of colors is taken into account as well.

#### **Parameters**

- multicolor1 (Multicolor) first out of two multi-colors to compute similarity between
- multicolor2 (Multicolor) second out of two multi-colors to compute similarity between

**Returns** the similarity score between two supplied Multicolor object

Return type int

Produces several new instances of Multicolor object by splitting information about colors by using provided guidance iterable set-like object.

Guidance is an iterable type of object where each entry has information about groups of colors that has to be separated for current Multicolor.multicolors chunk. If no Guidance is provided, single-color guidance of Multicolor.multicolors is created. Guidance object is first reversed sorted to iterate

over it from larges color set to the smallest one, as small color sets might be subsets of bigger ones, and shall be utilized only if bigger sets didn't help in separating.

During the first iteration over the guidance information all subsets of Multicolor.multicolors that equal to entries of guidance are recorded. During second iteration over remaining of the guidance information, if colors in Multicolor.multicolors form subsets of guidance entries, such instances are recorded. After this two iterations, the rest of Multicolor.multicolors is recorded as non-tackled and is recorded on its own.

Multiplicity of all separated colors in respective chunks is preserved.

Accounts for subclassing.

#### **Parameters**

- **multicolor** (*Multicolor*) an instance information about colors in which is to be split
- guidance (iterable where each entry is iterable with colors entries) information how colors have to be split in current Multicolor object
- sorted\_guidance a flag, that indicates is sorting of provided guidance is in order

**Returns** a list of new *Multicolor* object colors information in which complies with guidance information

Return type list of Multicolor objects

update (\*args)

Updates information about colors and their multiplicity in respective Multicolor instance.

By iterating over supplied arguments each of which should represent a color object, updates information about colors and their multiplicity in current Multicolor instance.

**Parameters args** (any hashable python object) – variable number of colors to add to currently existing multi colors data

Returns None, performs inplace changes to Multicolor.multicolors attribute

### 2.2.6 edge.py

**class** bg.edge.BGEdge (vertex1, vertex2, multicolor, data=None)

Bases: object

A wrapper class for edges in bg.breakpoint\_graph.BreakpointGraph

Is not stored on its own in the <code>bg.breakpoint\_graph.BreakpointGraph</code>, but is rather can be supplied to work with and is returned if retrieval is performed. BGEdge represents an undirected edge, thus distinction between <code>BGEdge.vertex1</code> and <code>BGEdge.vertex2</code> attributes is just from identities perspective, not from the order perspective.

This class supports th following attributes, that cary information about multi-color for this edge, as well as vertices, its is attached to:

- •BGEdge.vertex1: a first vertex to be utilized in bg.breakpoint\_graph.BreakpointGraph
- •BGEdge.vertex2: a second vertex to be utilized in bg.breakpoint\_graph.BreakpointGraph

#### Main operations:

•--

•BGEdge.merge(): produces a new BGEdge with multi-color information being merged from them

**class BGEdgeJSONSchema** (*obj=None*, *extra=None*, *only=None*, *exclude=None*, *prefix=''*, *strict=False*, *many=False*, *skip missing=False*, *context=None*)

Bases: marshmallow.schema.Schema

Marshmallow powered JSON schema used for serialization / deserialization of edge object

#### static BGEdge . \_BGEdge \_\_vertex\_json\_id (vertex)

A proxy property based access to vertices in current edge

When edge is serialized to JSON object, no explicit object for its vertices are created, but rather they are referenced by special vertex json\_ids.

BGEdge.\_\_eq\_\_(other)

Implementation of == operation for BGEdge

Checks if current *BGEdge* instance comply in terms of vertices set with the supplied *BGEdge*, and then checks the edebage does not equal to non-*BGEdge* objects

Parameters other (any python object) - object to compare current BGEdge to

Returns flag of equality if current BGEdge object equals to the supplied one

Return type Boolean

BGEdge.\_\_init\_\_(vertex1, vertex2, multicolor, data=None)

Initialization of BGEdge object.

#### **Parameters**

- vertex1 (any hashable python object) vertex the edges is outgoing from
- vertex2 (any hashable python object) vertex the edges is ingoing to
- multicolor (bg.multicolor.Multicolor) multicolor that this single edge shall posses

**Returns** a new instance of BGEdge

Return type BGEdge

#### BGEdge.colors\_json\_ids

A proxy property based access to vertices in current edge

When edge is serialized to JSON object, no explicit object for its multicolor is created, but rather all colors, taking into account their multiplicity, are referenced by their json\_ids.

#### classmethod BGEdge.from\_json(data, json\_schema\_class=None)

JSON deserialization method that retrieves edge instance from its json representation

If specific json schema is provided, it is utilized, and if not, a class specific is used

#### BGEdge.json\_schema\_name

When genome is serialized information about JSON schema of such serialization can be recorded, and this property provides access to it

### classmethod BGEdge.merge(edge1, edge2)

Merges multi-color information from two supplied BGEdge instances into a new BGEdge

Since BGEdge represents an undirected edge, created edge's vertices are assign according to the order in first supplied edge.

Accounts for subclassing.

#### **Parameters**

• edge1 – first out of two edge information from which is to be merged into a new one

• edge2 – second out of two edge information from which is to be merged into a new one

**Returns** a new undirected with multi-color information merged from two supplied *BGEdge* objects

Raises ValueError

BGEdge.to\_json(schema\_info=True)

JSON serialization method that accounts for a possibility of field filtration and schema specification

BGEdge.vertex1\_json\_id

First vertex json id access

BGEdge.vertex2\_json\_id

Second vertex json id access

### 2.2.7 vertices.py

```
class bg.vertices.BGVertex(name)
```

Bases: object

An base class that represents a vertex (node) with all associated information in a breakpoint graph data structure

While class represents a base inheritance point for specific vertex implementations, it does implement most of business logic operations, that vertex shall support.

While different type of vertices are to be represented with different python classes, they all have a string representation, which mainly relies one the *name* attribute.

```
class bg.vertices.BlockVertex(name, mate_vertex=None)
```

Bases: bg.vertices.BGVertex

This class represents a special type of breakpoint graph vertex that correspond to a generic block extremity (gene/ synteny block/ etc.)

```
class BlockVertexJSONSchema (obj=None, extra=None, only=None, exclude=None, prefix='', strict=False, many=False, skip missing=False, context=None)
```

Bases: bg.vertices.BGVertexJSONSchema

JSON schema for this class is redefined to tune the *make\_object* method, that shall return *BlockVertex* instance, rather than *BGVertex* one

```
classmethod BlockVertex.from_json(data, json_schema_class=None)
```

This class overwrites the from\_json method thus, making sure, that if *from\_json* is called from this class instance, it will provide its JSON schema as a default one

```
BlockVertex.is_block_vertex
```

This class implements a property check for vertex to belong to a class of vertices, that correspond to extremities of genomic blocks

```
BlockVertex.is_regular_vertex
```

This class implements a property check for vertex to belong to class of regular vertices

```
class bg.vertices.InfinityVertex(name)
```

Bases: bg.vertices.BGVertex

This class represents a special type of breakpoint graph vertex that correspond to a generic extremity of genomic fragment (chromosome, scaffold, contig, etc.)

```
class InfinityVertexJSONSchema (obj=None, extra=None, only=None, exclude=None, pre-fix='', strict=False, many=False, skip\_missing=False, con-fix='', strict=False, many=False, skip\_missing=False, con-fix='', strict=False, many=False, skip\_missing=False, skip\_missing=False,
```

text=None)

Bases: bg.vertices.BGVertexJSONSchema

JSON Schema for this class is redefined to tune the *make\_object* method, that shall return *InfinityVertex* instance, rather than a *BGVertex* one

```
classmethod InfinityVertex.from_json(data, json_schema_class=None)
```

This class overwrites the from\_json method, thus making sure that if *from\_json* is called from this class instance, it will provide its JSON schema as a default one

```
InfinityVertex.is infinity vertex
```

This class implements a property check for vertex to belong to a class of vertices, that correspond to standard extremities of genomic fragments

```
InfinityVertex.is_irregular_vertex
```

This class implements a property check for vertex to belong to a class of vertices, that correspond to extremities of genomic fragments

```
InfinityVertex.name
```

access to classic name attribute is hidden by this property

### 2.2.8 genome.py

```
class bg.genome.BGGenome (name)
```

Bases: object

A class that represent a genome object for the breakpoint graph

For purposes of breakpoint graph no additional information about genome is needed, except its name, that is used in various algorithmic tasks (multicolor splitting, tree traversing, etc)

```
class BGGenomeJSONSchema (obj=None, extra=None, only=None, exclude=None, prefix='', strict=False, many=False, skip_missing=False, context=None)
```

Bases: marshmallow.schema.Schema

a JSON schema powered by marshmallow library to serialize/deserialize genome object into/from JSON format

```
BGGenome.__eq_ (other)
```

Two genomes a called equal if they are of same class and their hash values are equal to each other

```
BGGenome. hash ()
```

Since for breakpoint graph purposes distinction between genomes is made purely by their name, hash value of genome is proxied to hash value of genomes name

```
BGGenome.__le__(other)
```

Genomes are ordered according to lexicographical ordering of their names

```
BGGenome.__lt__(other)
```

Genomes are ordered according to lexicographical ordering of their names

```
classmethod BGGenome.from_json(data, json_schema_class=None)
```

JSON deserialization method that retrieves a genome instance from its json representation

If specific json schema is provided, it is utilized, and if not, a class specific is used

```
BGGenome.json_id
```

A genome is references multiple times, as for example in multicolor object, and such reference is done by genome unique json id.

```
BGGenome.json schema name
```

When genome is serialized information about JSON schema of such serialization can be recorded, and this property provides access to it

BGGenome.to\_json(schema\_info=True)

JSON serialization method that accounts for a possibility of field filtration and schema specification

# 2.2.9 distances.py

# 2.2.10 util.py

# CHAPTER 3

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