Pylogeny Documentation

Release 0.3.4.6

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CHAPTER

ONE

PYLOGENY PACKAGE

1.1 Submodules

1.1.1 pylogeny.JSONWriter module

Serialize a phylogenetic landscape into a JSON object.

```
class pylogeny.JSONWriter.JSONWriter(ls, name)
    Bases: pylogeny.landscapeWriter.landscapeWriter
    __init__(ls, name)
    getCompleteLandscape()
    getJSON()
    getOnlyImprovements(groups=None)
    nodeToJSON(node)
```

1.1.2 pylogeny.alignment module

Handle input biological sequence alignment files for the purposes of phylogenetic inference. Will read all types of alignment files by utilizing the P4 python phylogenetic library.

```
class pylogeny.alignment.alignment (inal=None)
     Bases: object
```

Wrap a biological sequence alignment to enable functionality necessary for phylogenetic inference. Makes use of temporary files; requires to be closed once no longer needed.

```
init (inal=None)
```

Instantiate an object intended to wrap an alignment for the purposes of running phylogenetic inference.

Parameters inal – An alignment file path (most formats are accepted).

```
bootstrap()
```

Perform bootstrapping on the alignment data.

```
close()
```

Delete all temporary files and clear data.

```
getAlignment()
```

Acquire the alignment data structure (P4 module).

getApproxMLNewick()

Get a tree in newick format via use of FastTree that serves as an approximation of the maximum likelihood tree for this data.

getApproxMLTree()

Get a tree object for an approximation of the maximum likelihood tree for this data using FastTree.

getDim()

Return the dimensionality of the sequence alignment (how many different types of characters).

qetFASTA()

Get (and create if not already) a path to a temporary FASTA file. This will be deleted upon closure of the alignment instance.

getFastTreeNewick()

Alias for the "getApproxMLNewick()" function.

getNumSeqs()

Return the number of sequences that are present in the sequence alignment.

getSequence(i)

Acquire the ith sequence.

getSize()

Return the size of the alignment, or how many characters there are in each respective item in the alignment.

getStateModel()

getTaxa()

Return taxa names.

toStrList()

Get all sequences as a list of strings.

class pylogeny.alignment.phylipFriendlyAlignment (inal=None)

```
Bases: pylogeny.alignment.alignment
```

An alignment object that renames all comprising taxa in order to be able to be written as a strict Phylip file.

```
___init___(inal=None)
```

getPhylip()

Get a path to a temporary Phylip file. This will be deleted upon closure of the alignment instance.

getProperName(n)

Return the actual name for an integer-based sequence name that was reassigned at initialization.

getTaxa()

Return current taxa names in the alignment.

reassignFromReinterpretedNewick (tr)

Replace all proper names with reassigned names in Newick tree.

recreateObject()

Reintializes the object.

reinterpretNewick(tr)

Replaces all reassigned names to proper names in Newick tree.

writeProperNexus (wri)

Write a Nexus file with proper names.

1.1.3 pylogeny.base module

label = None
parent = None

```
Definitions for generalized containers and objects used by other structures in this framework.
pylogeny.base.longest_common_substring(s1, s2)
     Simplified, traditional LCS algorithm implementation.
class pylogeny.base.patriciaTree
     Bases: pylogeny.base.trie
     Defines a PATRICIA tree (condensed trie) across a range of strings.
     delete (seq)
          Remove a sequence from the PATRICIA tree. Will not remove added characters to alphabet.
          Dynamically insert a sequence into the PATRICIA tree. Returns the unique index in the tree for that string.
     search (seq)
          Search for a sequence in the PATRICIA tree. Returns its position in addition sequence if it exists. Else,
class pylogeny.base.treeBranch (parent=None, child=None, label='')
     Bases: object
     A branch in a tree.
     __init__ (parent=None, child=None, label='')
     child = None
     getChild()
     getLabel()
     getParent()
     label = "
     parent = None
class pylogeny.base.treeNode (lbl=None, children=None, parent=None)
     Bases: object
     A node in a tree.
     ___init___(lbl=None, children=None, parent=None)
     addChild(item)
     children = None
     getChildByIndex(i)
     getChildren()
     getLabel()
     getParent()
     isInternalNode()
     isLeaf()
```

```
class pylogeny.base.treeStructure (root=None)
     Bases: abcoll.Container
     Defines a base collection of treeNodes and treeBranches in a hierarchical tree structure.
      ___init___(root=None)
     qetAllLeaves()
     getAllNodes()
     getPostOrderTraversal()
     getRoot()
          Return the top-level, root, node of the tree.
     static leaves (root)
     static nodes (root)
     static postOrderTraversal (root)
     root = None
class pylogeny.base.trie
     Bases: _abcoll.Sized, pylogeny.base.treeStructure
     Defines a trie across a range of strings.
     ___init___()
     alphabet = None
     count = 0
     delete (seq)
          Remove a sequence from the trie. Will not remove added characters to alphabet.
     getAlphabet()
     getRoot()
     insert (seq)
          Dynamically insert a sequence into the trie.
     nextLabel = 1
     root = None
     search (seq)
          Search for a sequence in the trie. Returns true if it exists.
class pylogeny.base.trieNode (lbl=None, children=None, parent=None)
     Bases: pylogeny.base.treeNode
     A subclass of treeNode that allows for checking non-zero members amongst children branches and other con-
     veniences.
     getNonEmptyChildrenBranchLabels()
     getNonEmptyChildrenBranches()
          Acquire a list of all non-empty children.
     getNonEmptyChildrenNodes()
          Acquire a list of all non-empty children.
     getParentNode()
```

```
Iterate over all children that are not empty.
     numEmptyChildrenNodes()
          Acquire the number of children nodes that are marked 0 or nonexistent.
     setChildNode (child, newchild)
1.1.4 pylogeny.database module
Connect, access, + manipulate external tree data from a remote SQL server or from a sqlite file.
class pylogeny.database.DatabaseLandscape (ali,
                                                      starting_tree=None,
                                                                            root=True,
                                                                                         opera-
                                                  tor = 'SPR')
     Bases: pylogeny.landscape.landscape
     Abstract the landscape to one comprising a landscape.
     getNode(i)
class pylogeny.database.SQLDatabase(host, user, pw, db)
     Bases: pylogeny.database.database
     Database object to allow reading from a MySQL database.
     ___init___(host, user, pw, db)
     close()
     connect()
     getColumns (table)
         Return column information for a given table.
     getTables()
     \mathtt{query}\left(q\right)
     querymany(q, i)
class pylogeny.database.SQLExhaustiveLandscape (dbobj, aliname)
     Bases: pylogeny.database.DatabaseLandscape
     __init__ (dbobj, aliname)
     exploreRandomTree(i)
     exploreTree (i)
     getDatabaseNode(i)
class pylogeny.database.SQLiteDatabase (filepath)
     Bases: pylogeny.database.database
     __init__(filepath)
     close()
     getColumns (table)
          Return column information for a given table.
     getTables()
     query (q)
     querymany(q, i)
```

iterNonEmptyChildrenNodes()

```
class pylogeny.database.SQLiteLandscape (dbobj)
     Bases: pylogeny.landscape.landscape
     Allow random access of all landscape data from an sqlite file found on the hard disk.
     ___init___(dbobj)
class pylogeny.database.database
     Bases: object
     Allow interfacing with a SQL/sqlite database.
     close()
     cursor = None
     filterRecords (table, condn)
          Get all records from a given table following a condition.
     getColumns (table)
     getHeaders (table)
          Get only header names for a given table's columns.
     getRecords (table)
          Get all records from a given table in the database.
     getRecordsAsDict(table)
          Acquires records using getRecords() and then leverages access using a dictionary data structure.
     getRecordsColumn (table, col)
          Get all data for a single colmun from records for a table.
     getTables()
     insertRecord(tablename, record)
     insertRecords (tablename, items)
     isEmpty()
          Determine if the database is empty.
     iterRecords (table)
          Get a record, one at a time, from a table in the database.
     newTable (tablename, *args)
     query(q)
     querymany(q, i)
```

1.1.5 pylogeny.executable module

Defines an interface to manage interfacing with the system for respective application calls and implements some of these for executables such as FastTree and RAxML. Currently requires a UNIX-like environment (e.g., Mac OS X or a Linux-based environment).

```
class pylogeny.executable.aTemporaryDirectory (dir=None)
    Bases: object
A class intended to be used as a context manager that allows Python to run in a temporary directory for a finite period of time.
    __init__(dir=None)
```

```
class pylogeny.executable.consel (treeset, alignment, name)
     Bases: pylogeny.executable.executable
     Denotes a single run of the CONSEL workflow in order to acquire a confidence interval and perform an AU test
     on a set of trees. Requires CONSEL to be installed.
      init (treeset, alignment, name)
     getInstructionString()
     getInterval()
          Compute the AU test. Return the interval of trees.
pylogeny.executable.exeExists(cmd)
     Determines whether a function exists in a UNIX environment.
class pylogeny.executable.executable
     Bases: object
     An abstract class for the instantation and running of a single instance for a given application.
     exeName = None
     getInstructionString()
     run()
          Perform a run of this application.
class pylogeny.executable.fasttree(inp align, out file=None, isProtein=True)
     Bases: pylogeny.executable.executable
     Denotes a single run of the FastTree executable in order to acquire an approximate maximum likelihood tree for
     the input alignment. See http://www.microbesonline.org/fasttree/ for more information on FastTree. Requires
     FastTree to be installed.
     ___init___(inp_align, out_file=None, isProtein=True)
     exeName = 'fasttree'
     getInstructionString()
                                                   out_file, model=None,
class pylogeny.executable.raxml (inp_align,
                                                                            is_Protein=True,
                                       terTrees=False, alg=None, startingTree=None, rapid=False,
                                       slow=False, optimizeBootstrap=False, numboot=100, log=None,
                                       wdir=None)
     Bases: pylogeny.executable.executable
     Denotes a single run of the RAxML executable. See http://sco.h-its.org/exelixis/software.html for more infor-
     mation on RAxML. Requires RAxML to be installed.
     __init__(inp_align, out_file, model=None, is_Protein=True, interTrees=False, alg=None, start-
                 ingTree=None, rapid=False, slow=False, optimizeBootstrap=False, numboot=100,
                 log=None, wdir=None)
     exeName = 'raxmlHPC'
     getInstructionString()
     runFunction (alg)
class pylogeny.executable.rspr(treeA, treeB, algorithm='', overlap=True)
     Bases: pylogeny.executable.executable
     Denotes a single run of the rSPR executable by Dr. Chris Whidden (2014), a software package for comput-
     ing rooted subtree-prune-and-regraft (SPR) distances. See http://kiwi.cs.dal.ca/Software/RSPR. Requires the
```

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executable to be on PATH.

```
RSPR ALG APPROX = '-approx'
     RSPR ALG BB = '-bb'
     RSPR ALG DEFAULT = "
     RSPR_ALG_FPT = '-fpt'
      init (treeA, treeB, algorithm='', overlap=True)
          Algorithm choices are defined in this class. If overlap is set to True, will attempt to consolidate taxa names
          such that they are overlapping (otherwise, RSPR will return an error if they do not match).
     exeName = 'rspr'
     getInstructionString()
     getSPRDistance()
class pylogeny.executable.treepuzzle(ali, treefile)
     Bases: pylogeny.executable.executable
     Wrap TREE-PUZZLE in order to create an intermediate file for CONSEL to read and assign confidence to a set
     of trees. Requires TREE-PUZZLE to be installed.
     ___init___(ali, treefile)
     exeName = 'puzzle'
     getInstructionString()
     getSiteLikelihoodFile()
```

1.1.6 pylogeny.heuristic module

Define the interface for a heuristic in order to implement any manner of heuristic for a combinatorial problem that can be abstracted into a state graph. In this case, a phylogenetic tree space.

```
class pylogeny.heuristic.RAxMLIdentify(ls, startNode, workdir='.rxml')
     Bases: pylogeny.heuristic.phylogeneticLinearHeuristic
     RAxML-driven landscape evaluation of intermediate checkpoint trees output from the RAxML executable.
     __init__ (ls, startNode, workdir='.rxml')
     explore()
class pylogeny.heuristic.heuristic(G=None, start=None)
     Bases: object
     A base interface for a heuristic that explores a state graph.
     ___init___(G=None, start=None)
     explore()
     getStartState()
     getStateGraph()
class pylogeny.heuristic.likelihoodGreedy (ls, startNode)
     Bases: pylogeny.heuristic.phylogeneticLinearHeuristic
     Greedy (hill-climbing) landscape exploration by comparsion of likelihood.
     ___init___(ls, startNode)
```

```
explore()
          Perform greedy search of the landscape using a method of greed via likelihood.
class pylogeny.heuristic.parsimonyGreedy (ls, startNode)
     Bases: pylogeny.heuristic.phylogeneticLinearHeuristic
     Greedy (hill-climbing) landscape exploration by comparsion of parsimony.
     ___init___(ls, startNode)
     explore()
          Perform greedy search of the landscape using a method of greed via parsimonious criterion.
class pylogeny.heuristic.phylogeneticLinearHeuristic(ls, startNode)
     Bases: pylogeny.heuristic.heuristic
     A base class for a heuristic that works on a phylogenetic landscape and only possesses a single path (of search).
     ___init___(ls, startNode)
     bestTree = None
     getBestTree()
     getPath()
     path = []
class pylogeny.heuristic.smoothGreedy (ls, startNode)
     Bases: pylogeny.heuristic.phylogeneticLinearHeuristic
     Parsimony-driven greedy landscape exploration by comparsion of likelihoods.
      __init___(ls, startNode)
     explore()
          Perform greedy search of the landscape using a method of greed via parsimonious criterion and then
          performing final smoothing via likelihood on top 10% of 1-SPR neighbors ranked on basis of parsimony.
```

1.1.7 pylogeny.landscape module

Encapsulate a phylogenetic tree space. A phylogenetic landscape or tree space refers to the entire combinatorial space comprising all possible phylogenetic tree topologies for a set of n taxa. The landscape of n taxa can be defined as consisting of a finite set T of tree topologies. Tree topologies can be associated with a fitness function $f(t_i)$ describing their fit. This forms a discrete solution search space and finite graph (T, E) = G. E(G) refers to the neighborhood relation on E(G). Edges in this graph are bidirectional and represent transformation from one tree topology to another by a tree rearrangement operator. An edge between E(G) would be notated as E(G).

```
class pylogeny.landscape.graph (gr=None)
    Bases: object

Define an empty graph object.
__init__(gr=None)
    Instantiate a graph.

Parameters gr - A networkx graph object, if already exists.
clearEdgeWeights()
getCenter()
    Get the centre of the graph.
```

```
getCliqueNumber()
    Get the clique number of the graph.
getCliques()
    Get the cliques present in the graph.
getCliquesOfNode(i)
    Get the clique that a node corresponds to.
getComponentOfNode(i)
    Get the graph component of a given node.
getComponents()
    Get the connected components in the graph.
getDegreeFor (i)
    Return in- and out-degree for node named i.
getDiameter()
    Acquire the diameter of the graph.
getEdge(i, j)
getEdges()
getEdgesFor(i)
getMST()
    Acquire the minimum spanning tree for the graph.
getNeighborsFor(i)
getNode(i)
getNodeNames()
    Return the names of nodes in the graph.
getNodes()
getNumCliques()
    Get the number of cliques found in the graph.
getNumComponents()
    Get the number of components of the graph.
getShortestPath (nodA, nodB)
    Get the shortest path between two nodes.
getShortestPathLength (nodA, nodB)
    Get the shortest path length between two nodes.
getSize()
    Return the number of nodes in the graph.
hasPath(nodA, nodB)
    See if a path exists between two nodes.
isEdge(i, j)
iterNodes()
    Iterate over all node keys.
setDefaultWeight(w)
```

class pylogeny.landscape (ali, starting_tree=None, root=True, operator='SPR')

Bases: pylogeny.landscape.graph, pylogeny.tree.treeSet

Defines an entire phylogenetic tree space.

Parameters

- ali An alignment alignment object.
- starting_tree An optional tree object to start

the landscape with. :param root: Whether or not to acquire an approximate maximum likelihood tree (FastTree) or start the landscape with a given starting tree. :param operator: A string that describes what operator the landscape is mostly comprised of.

```
___init__ (ali, starting_tree=None, root=True, operator='SPR')
```

```
addTree (tr, score=True, check=True, newick=None, struct=None)
```

Add a tree to the landscape. Will return its index.

addTreeByNewick (newick, score=True, check=True, struct=None)

Add tree to the landscape by Newick string. Will return index.

exploreRandomTree(i, type=1)

Acquire a single neighbor to a tree in the landscape by performing a random rearrangement of type SPR (by default), NNI, or TBR – this is done by performing a rearrangement on a random branch in the topology. Rearrangement type is provided as a rearrangement module type definition of form, for example, TYPE SPR, TYPE NNI, etc.

exploreTree(i, type=1)

Get all neighbors to a tree named i in the landscape using a respective rearrangement operator as defined in the rearrangement module. Rearrangement type is provided as a rearrangement module type definition of form, for example, TYPE_SPR, TYPE_NNI, etc. By default, this is TYPE_SPR.

findTree(newick)

Find a tree by Newick string, taking into account branch lengths. Returns the index of this tree in the landscape.

findTreeTopology (newick)

Find a tree by topology, not taking into account branch lengths.

findTreeTopologyByStructure(struct)

Find a tree by topology, not taking into account branch lengths, given the topology.

getAlignment()

Acquire the alignment object associated with this space.

getAllPathsOfBestImprovement()

Return all paths of best improvement as a dictionary.

getBestImprovement(i)

For a tree in the landscape, investigate neighbors to find a tree that leads to the best improvement of fitness function score on the basis of likelihood.

getBipartitionFoundInTreeByIndex(tr, brind, topol=None)

Given a tree node and a branch index, return the associated bipartition.

getGlobalOptimum()

Get the global optimum of the current space.

getLocalOptima()

Get all trees in the landscape that can be labelled as a local optimum.

getLocks()

getNumberTaxa()

Return the number of different taxa present in any respective tree in the landscape.

getPathOfBestImprovement(i)

For a tree in the landscape, investigate neighbors iteratively until a best path of score improvement is found on basis of likelihood.

getPossibleNumberRootedTrees()

Assuming all of the trees in the space are rooted, return the maximum possible number of unrooted trees that can possibly be generated for the number of taxa of trees in the landscape.

getPossibleNumberUnrootedTrees()

Assuming all of the trees in the space are unrooted, return the maximum possible number of unrooted trees that can possibly be generated for the number of taxa of trees in the landscape.

getRoot()

Returns the index to the root (starting) tree of the space.

getRootTree()

Acquire the first tree that was placed in this space.

getTree(i)

Get the object for a tree by its name.

getVertex(i)

Acquire a vertex object from the landscape; this is a high-level representation of a tree in the landscape with additional functionality. Object created upon invocation of this function.

indexOf(tr)

Acquire the index/name in this landscape of a tree object. Returns -1 if not found.

isLocalOptimum(i)

Determine if a tree is a local optimum. This means it has the following properties:

- 1.Possesses a likelihood score.
- 2.Local neighborhood completely enumerated (and scored).
- 3. None of its neighbors is a better improvement.

isViolating(i)

Determine if a tree is violating any locks intrinsic to the landscape.

iterAllPathsOfBestImprovement()

Return an iterator for all paths of best improvement.

lockBranchFoundInTree(tr, br)

Given a tree node and a branch object, add a given bipartition to the bipartition lock list. Returns bipartition if locked.

lockBranchFoundInTreeByIndex(tr, brind)

Given a tree node and a branch index, add an associated bipartition to the bipartition lock list. Returns the bipartition if locked.

${\tt removeTree}\ (tree)$

Remove a tree from the landscape by object.

removeTreeByIndex(i)

Remove a tree from the landscape by index.

setAlignment (ali)

Set the alignment present in this landscape. WARNING; will not modify existing scores.

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```
setOperator(op)
          Set the operator assigned to this landscape.
     toProperNewickTreeSet()
          Convert this landscape into an unorganized set of trees where taxa names are transformed to their original
          form (i.e. not transformed to a state friendly for the Phylip format).
     toTreeSet()
          Convert this landscape into an unorganized set of trees.
     toggleLock(lock)
          Add a biparition to the list of locked bipartitions if not present; otherwise, remove it. Return status of lock.
class pylogeny.landscape.vertex (obj, ls)
     Bases: object
     Encapsulate a single vertex in the landscape and add convenient functionality to alias parent landscape functions.
     __init__(obj, ls)
     approximatePossibleNumNeighbors()
          Approximate the possible number of neighbors to this vertex by considering the type of tree rearrangement
          operator.
     getBestImprovement()
          Alias function for function of same name in parent landscape.
     getBipartitionScores()
          Get all corresponding bipartition vectors of SPR scores.
     getBipartitions()
          Get all bipartitions for this vertex.
     getDegree()
     getDict()
     getIndex()
     getNeighbors()
     getNeighborsOfBipartition(bi)
          Get corresponding neighbors of a bipartition in this vertex's tree.
     getNeighborsOfBranch(br)
          Get corresponding neighbors of a branch in this vertex's tree.
     getNewick()
     getObject()
     getOrigin()
     getPathOfBestImprovement()
          Alias function for function of same name in parent landscape.
```

Get the proper Newick string for a tree. :returns: A string.

Check to see if this vertex is a best move for another node.

getProperNewick()

isBestImprovement()

getScore()
getTree()

```
isExplored()
isFailed()
isLocalOptimum()
isViolating()
    Alias function for function of same name in parent landscape.
iterBipartitions()
    Return a generator to iterate over all bipartitions for this vertex.
scoreLikelihood()
    Acquire the log-likelihood for this vertex.
setExplored(exp)
    Sets the "explored" flag of this node in the landscape.
```

1.1.8 pylogeny.landscapeWriter module

Serialize a phylogenetic landscape into an SQLlite database file made up of three components: all tree IDs and respective scores, the alignment file as a set of sequences, and a representation of the graph as an edge list.

```
class pylogeny.landscapeWriter.landscapeParser(path)
    Bases: object

Encapsulates the construction of a landscape object from a sqlite landscape file.
    __init__(path)

getName()
    Acquire the name of the parsed landscape.

parse()
    Parse the file.

class pylogeny.landscapeWriter.landscapeWriter(landscape, name)
    Bases: object

Encapsulate the writing of a landscape to a file format.
    __init__(landscape, name)

writeFile(path='.')
    Write the landscape serialized file to given path.
```

1.1.9 pylogeny.model module

Phylogenetic tree scoring models; intended to be coupled with the use of pytbeaglehon (BEAGLE) high-performance library.

```
class pylogeny.model.DiscreteStateModel (alignment)
    Bases: object
    Initialize a discrete state model for phylogenetic data. State frequencies and character time are determined from the given alignment object.
    __init__(alignment)
    getAlignment()
    getAlignmentAsStateList()
```

```
getCharType()
     getFrequencyOfState(i)
     getRawFrequencyOfState(i)
     getRawStateFreqs()
     getRawStateFreqsAsDict()
     getRawStateFreqsAsList()
     getSequenceMatrix()
     getStateFreqs()
exception pylogeny.model.PhyloModelError(v)
     Bases: exceptions. Exception
     ___init___(v)
1.1.10 pylogeny.newick module
Newick string parsing and object interaction. A Newick string can represent a phylogenetic tree.
exception pylogeny.newick.ParsingError(val)
     Bases: exceptions. Exception
     ___init___(val)
pylogeny.newick.assignParents(top)
     Should be a one-time use function. Goes through and assigns parents to the parsed newick tree structure nodes
     and branches to allow for up-traversal.
class pylogeny.newick.branch(chi, l, parent=None, s=None)
     Bases: pylogeny.base.treeBranch
     Newick branch.
     ___init___(chi, l, parent=None, s=None)
pylogeny.newick.getAllBranches(br)
     Given a branch, traverse subtree and return comprising branches as a list.
pylogeny.newick.getBalancingBracket (newick, i)
     Given a position of an opening bracket in a newick string, i, output the closing bracket's position that corresponds
     to this opening bracket.
pylogeny.newick.getBranchLength (newick, i)
     Given a position of a colon symbol (indicating a branch length), return the branch length.
pylogeny.newick.getLeafName(newick, i)
     Given the position of a leaf, find its complete name.
pylogeny.newick.invertAlongPathToNode(target, top)
     DANGEROUS: Reverses all directionality to a given node from a top-level node. Intended as a low-level
     function for rerooting a tree.
pylogeny.newick.isSibling(br, other)
     Given a branch, determine if that branch is adjacent to another branch.
class pylogeny.newick.newickParser(newick)
     Parsing object for Newick strings.
```

1.1. Submodules

init (newick)

```
parse()
          Parse the stored newick string into a topological structure.
class pylogeny.newick.node (lbl='', children=None, parent=None)
     Bases: pylogeny.base.treeNode
     Newick node.
      __init__ (lbl='', children=None, parent=None)
pylogeny.newick.parseNewick(newick, i, j, top)
     Parse a newick string into a topological newick structure given a top-level node.
pylogeny.newick.removeBranchLengths(top)
     Goes through and removes any stored branch lengths.
pylogeny.newick.removeUnaryInternalNodes(top)
     Goes through and ensures any degree-2 internal nodes are smoothed into a single degree-3 internal node.
pylogeny.newick.shuffleLeaves(top)
     DANGEROUS: Given a top-level node, shuffle all leaves in this tree.
1.1.11 pylogeny.parsimony module
Toolkit for performance of Parsimonious Criterion (Parsimony) methods of optimization of a phylogenetic topology
with a particular set of data.
pylogeny.parsimony.fitch(topology, alignment)
     Perform the Fitch algorithm on a given tree topology and associated alignment. Deprecated: Python imple-
     mentation of the Fitch algorithm; see fitch C++ module for a C++ implementation that is roughly four times
     faster.
pylogeny.parsimony.fitch_cost (topology, profiles)
     Calculate the cost using Fitch algorithm on profile set and alignment. Deprecated: Python implementation of
     the Fitch algorithm; see fitch C++ module for a C++ implementation that is roughly four times faster.
class pylogeny.parsimony.profile_set (alignment)
     Hold a set of site_profile profiles for an entire alignment.
     __init__ (alignment)
     get (val)
     getForTaxa (val, tax)
     weight (val)
class pylogeny.parsimony.site_profile (alignment, site)
     Consolidate the single-column alignment at a region into a set of components on the basis of similarity alone.
        _init___(alignment, site)
```

1.1.12 pylogeny.pll module

Wrap C extension for libpll library for use in natural Python.

```
class pylogeny.pll.dataModel(topo, alignm, model=None)
```

Encapsulating a phylogenetic tree (as topology) + corresponding alignment into a libpll-associated data structure. Allows for log-likelihood scoring of this model. **MUST BE CLOSED AFTER USE.**

```
__init__ (topo, alignm, model=None)
          Initialize the data model and respective structures.
               Parameters
                   • topo – A topology object.
                   • alignm – A phylipFriendlyAlignment object.
     close()
          If done with this particular problem. Frees associated memory.
     getLogLikelihood()
          Calculates log-likelihood using libpll.
     getNewickString()
          Acquire the Newick string of the problem instance.
class pylogeny.pll.partitionModel (ali)
     A partition model intended for libpll.
      ___init___(ali)
     close()
          Delete file.
     createModel (models, partnames, ranges)
          Establish a more complex model.
     createSimpleModel (protein, pmodel='WAG')
          Establish a simple model (e.g., one type).
     getFileName()
          Get the file name of the model file.
```

1.1.13 pylogeny.rearrangement module

Phylogenetic tree structure encapsulation; allow rearrangement of said structure. Tree rearrangements inducing other topologies include Nearest Neighbor Interchange (NNI), Subtree Pruning and Regrafting (SPR), and Tree Bisection and Reconstruction (TBR). Each of these describe a transfer of one node in phylogenetic trees from one parent of a tree to a new parent. Respectively, these operators describe transformations that are subsets of those possible by the successive operator. For example, an NNI operator can perform transformations that are a subset of the transformations possible by the SPR operator.

```
exception pylogeny.rearrangement.RearrangementError(val)
    Bases: exceptions.Exception
    __init__(val)

pylogeny.rearrangement.dup(topo, where=None)

class pylogeny.rearrangement.rearrangement(struct, type, targ, dest)
    Encapsulates a single rearrangement move of type SPR, NNI, ...
    __init__(struct, type, targ, dest)
        Initialize by providing a pointer to a base topology, a target branch to be moved, and its destination.

doMove()

getType()
    Get the type of movement.

isNNI()
```

isSPR()

isTBR()

toNewick()

Commit the move but do not create a new structure. Only retrieve resultant Newick string; will be more efficient.

toTopology()

Commit the actual move and return the topology.

toTree()

Commit the move and transform to tree object.

class pylogeny.rearrangement.**topology** (t=None, rerootToLeaf=True, toLeaf=None)

```
Bases: pylogeny.base.treeStructure
```

Encapsulate a tree topology, wrapping the newick tree structure. Is immutable.

```
NNI (branch, destination)
```

Perform an NNI move of a branch to a destination, only if that destination branch is a parent's parent or a parent's sibling. Returns a rearrangement structure (not the actual new structure) that can then be polled for the actual move; this is in order to save memory.

```
SPR (branch, destination)
```

Perform an SPR move of a branch to a destination branch, creating a new node there. Returns a rearrangement structure (not the actual new structure) that can then be polled for the actual move; this is in order to save memory.

```
init (t=None, rerootToLeaf=True, toLeaf=None)
```

Initialize structure with a top-level internal node OR nothing.

allNNI()

Consider all valid NNI moves for a given topology and return all possible rearrangements.

allNNIForBranch (br, flip=True)

Consider all valid NNI moves for a given branch in the topology and return all possible rearrangements.

allSPR()

Consider all valid SPR moves for a given topology and return all possible rearrangements.

allSPRForBranch (br, flip=True)

Consider all valid SPR moves for a given branch in the topology and return all possible rearrangements.

allType(type=1)

Consider all valid moves of a given rearrangement operator for a given topology. Uses a given rearrangement operator type defined in this module. For example, calling this function by providing TYPE_NNI as the type will iterate over all NNI operations. By default, the type is TYPE SPR.

fromNewick (newickstr)

Alias for parse().

getBipartitions()

Get all bipartitions.

getBranchFromBipartition(bip)

Given a bipartition object, return a branch that creates that partition of taxa.

getBranchFromStrBipartition (bip)

Given a bipartition of taxa, return a branch that creates that partition of tree taxa.

getBranches()

getLeaves()

getStrBipartitionFromBranch(br)

Given a branch, return corresponding bipartition.

iterNNIForBranch (br, flip=True)

Consider all valid NNI moves for a given branch in the topology and and yield all possible rearrangements as a generator.

iterSPRForBranch(br, flip=True)

Consider all valid SPR moves for a given branch in the topology and yield all possible rearrangements as a generator.

iterTypeForBranch (br, type=1, flip=True)

Iterate over all possible rearrangements for a branch using a given rearrangement operator type defined in this module. For example, calling this function by providing TYPE_NNI as the type will iterate over all NNI operations. By default, the type is TYPE_SPR.

lockBranch (branch)

Given a branch, lock it such that no transitions can ever occur across it.

move (branch, destination, returnStruct=True)

Move a branch and attach to a destination branch. Return new structure, or return merely the resultant Newick string.

parse (newickstr)

Parse a newick string and assign the tree to this object. Cannot already be initialized with a tree.

rerootToLeaf (toleaf=None)

PRIVATE: Reroots the given tree structure such that it is rooted nearest the lowest-order leaf.

toNewick()

Return the newick string of the tree.

toTree()

Return the tree object for this topology.

toUnrootedNewick()

Return the newick string of the tree as an unrooted topology with a multifurcating top-level node.

toUnrootedTree()

Return the tree object of the unrooted version of this topology.

1.1.14 pylogeny.scoring module

Functions for phylogenetic tree goodness-of-fit scoring.

```
pylogeny.scoring.beaglegetLogLikelihood(tree, alignment)
```

Acquire log-likelihood via C++ library BEAGLE via use of pybeaglethon wrapper library. Currently uses HKY85 model.

Parameters

- tree A tree object.
- alignment An alignment object.

Returns A floating point value.

pylogeny.scoring.getLogLikelihood (tree, alignment, updateBranchLengths=True)
Acquire log-likelihood via C library libpll.

Parameters

• **tree** – A tree object.

- alignment An alignment object.
- updateBranchLengths Whether or not to update the branch lengths

in the provided tree with optimized ones. :returns: A floating point value.

pylogeny.scoring.getParsimony(newick, alignment)

Acquire parsimony via a C++ implementation.

Parameters

- newick A New Hampshire (Newick) tree string.
- alignment An alignment object.

Returns An integer value.

pylogeny.scoring.getParsimonyForTopology(topo, alignment)

Acquire parsimony via a C++ implementation.

Parameters

- topo A topology object.
- alignment An alignment object.

Returns An integer value.

pylogeny.scoring.getParsimonyFromProfiles (newick, profiles)

Acquire parsimony via a C++ implementation.

Parameters

- newick A New Hampshire (Newick) tree string.
- **profiles** A set of profiles corresponding to an alignment.

Returns An integer value.

 $\verb"pylogeny.scoring.getParsimonyFromProfilesForTopology", \textit{profiles}")$

Acquire parsimony via a C++ implementation.

Parameters

- topo A topology object.
- **profiles** A set of profiles corresponding to an alignment.

Returns An integer value.

1.1.15 pylogeny.tree module

Container definition for (phylogenetic) bifurcating or multifurcating trees defined using Newick strings, collections of them, and for splits of these trees.

```
class pylogeny.tree.bipartition(topol, bra=None)
    Bases: object
```

A tree bipartition. Requires a tree topology. Using the term borrowed from nomenclature of a bipartite graph, a bipartition for a phylogenetic tree coincides with the definition of two disjoint sets U and V. A branch in a phylogenetic tree defines a single bipartition that divides the tree into two disjoint sets U and V. The set U comprises all of the children leaf of the subtree associated with that branch. The set V contains the rest of the leaves or taxa in the tree.

```
___init___(topol, bra=None)
```

Construct a bipartition from a branch in a topology.

Parameters

```
• topol – A topology.
```

• bra – An optional argument; can still acquire a bipartition from a

string. :type bra: :class: newick.branch

fromStringRepresentation(st)

Acquire all component elements from a string representation of a bipartition.

Parameters st – A string representation from a bipartition object.

getBestSPRScore (ls, node=None)

Given a landscape, return the best SPR score.

getBranch()

Get branch corresponding to this bipartition.

Returns newick.branch

getBranchIndex()

Return an index of the branch with respect to a post order traversal of the topology.

Returns an integer

getBranchListRepresentation()

Get the tuple of lists of branches that represent this bipartition.

getMedianSPRScore (ls, node=None)

Given a landscape, return the median SPR score.

getSPRRearrangements()

Return the set of all scores related to this bipartition.

getSPRScores (ls, node=None)

Given a landscape, return all possible scores, not actively performing scoring if not done.

getShortStringMappings()

Get the mapping of symbols from taxa names for the shorter string representation.

getShortStringRepresentation()

Get the shorter string representation corresponding to this bipartition.

Returns a string

${\tt getStringRepresentation}\;(\,)$

Get the string representation corresponding to this bipartition.

Returns a string

Defines a single (phylogenetic) tree by newick string; can possess other metadata.

```
__init__ (newi='', check=False, structure=None)
```

If enabled, "check" will force the structure to reroot the given Newick string tree to a lowest-order leaf in order to ensure a consistent Newick string among any duplicate topologies. If a structure is provided and check is disabled, all parsing routines are bypassed and the Newick and Structure fields of this tree are overriden by the appropriate arguments.

Parameters newi – A Newick or New Hampshire string for a tree (unrooted

or rooted). :type newi: string :param check: An optional argument; boolean indicating whether to perform parsing checks on the string. May change what Newick string is assigned without changing tree topology.

getName()

Gets the name of this tree if it has been defined.

Returns a string

getNewick()

Gets the Newick (New Hampshire) string for this tree.

Returns a string

getOrigin()

Gets the "origin" of this tree, or where this tree was acquired or constructed from. Usually set by other code or an interface.

Returns string or None

getRerootedNoBranchLengthNewick()

Returns the tree's "structure", a Newick string without any branch lengths.

Returns a string

getScore()

Gets the score(s) (objective function) for this tree if it/they has/have been defined.

Returns a tuple of floats or integers

getSimpleNewick()

Return a Newick string with all taxa name replaced with successive integers.

Returns a string

getStructure()

Returns the tree's "structure", a Newick string without any branch lengths.

Returns a string

setName(n)

Sets the name of this tree (object).

Parameters n (*a string*) – A string indicating this tree's name.

$\mathtt{setOrigin}\left(o\right)$

Set the "origin" or specification of where this tree was acquired or constructed from.

Parameters o (string or None) – A string indicating where the tree came from.

setScore(s)

Sets the score(s) for this tree. Should be performed by a scorer (see scoring functions in the appropriate module).

Parameters s (a tuple of floats or integers) – A set of objective function scores.

toNewick()

Gets the Newick (New Hampshire) string for this tree.

Returns a string

toTopology()

Return a topology object instance for this tree to allow for rearrangement of the actual structure of the tree.

Returns a :class: rearrangement.topology object

updateNewick (n, reroot=False)

Update the contained Newick string only as long as the structure obtained (after rerooting, which is an optional parameter) is identical to the contained structure.

Parameters

- **n** (*a string*) A Newick or New Hampshire formatted string.
- reroot A boolean indicating whether to reroot the provided

Newick string to a lexicographically lowest-order taxa name to ensure redundant topologies across other trees.

class pylogeny.tree.treeSet

```
Bases: _abcoll.Sized, _abcoll.Iterable
```

Represents an ordered, disorganized collection of trees that do not necessarily comprise a combinatorial space.

```
___init___()
```

addTree(tr)

Add a tree object to the collection.

Parameters tr - A tree object.

addTreeByNewick (newick)

Add a tree to the structure by Newick string.

Parameters newick (a string) – A New Hampshire or Newick string.

static fromTreeFile (fin)

Acquire a file where newlines separate Newick strings, and create an instance of treeSet from those trees.

indexOf(tr)

Acquire the index in this collection of a tree object. Returns -1 if not found.

Parameters tr - A tree object.

Returns an integer [-1,length of collection)

iterTrees()

Iterate over all trees found in this set.

removeTree(tr)

Remove a tree object from the collection if present.

Parameters tr - A tree object (present in the collection).

toTreeFile (fout)

Output this landscape as a series of trees, separated by newlines, as a text file saved at the given path.

Parameters fout (a string) – A string indicating a file system path to a file.

1.2 Module contents

Pylogeny is a Python library and code framework for phylogenetic tree reconstruction and scoring.

Allows one to perform the following tasks: (1) Generate and manage phylogenetic tree landscapes. (2) Build and rearrange phylogenetic trees using preset operators such as NNI, SPR, and TBR. (3) Score phylogenetic trees by Log-likelihood and Parsimony.

Dependencies: Pandas, P4 Phylogenetic Library. Suggested: FastTree, RAxML, PytBEAGLEhon.

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