Capybara

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Documentation

Capybara is a desktop **GUI application** for solving the *Phylogenetic tree reconciliation problem*.

Its key features are also available as a **Python package**.

Keywords: Cophylogeny reconstruction, phylogenetic tree reconciliationm, enumeration.

To cite Capyabra

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CHAPTER 1

Installation

Here we show how to download the GUI application.

For the installation process of the Python package, see the *Installation* section in the relevant page *Python package*.

1.1 Download

Click here to get Capybara.

You can find the binary executables of Capybara for the following OS:

- Microsoft Windows 10
- macOs
- Linux (Ubuntu, Fedora, Debian, Arch Linux, Manjaro, etc.)

Please note that no additional installation is required. Just unzip and double-click!

For some Linux versions: you might need to manually make the file executable in a terminal

```
chmod +x Capybara
```

1.2 Build

The source code is available at https://github.com/Helio-Wang/Capybara-app.

You may want to build Capybara from source if

- You are not using one of the supported OS (Windows, macOS, major flavors of Linux), or
- You have made some changes to the source code.

First, clone or create the project directory and

```
cd Capybara-app
```

Capybara includes a `Pipfile` specifying all requirements, generated by the virtual environment management tool Pipenv. Install Pipenv if you don't have it already:

```
pip install pipenv
```

Next, build the Pipenv virtual environment and install the requirements from `Pipfile`. Be sure that you already have Python 3.6 installed on your system. If you have multiple versions of Python, this command will automatically search for Python 3.6.

```
pipenv install
```

Then, you can execute the main script directly:

```
pipenv run python main.py
```

Alternatively, you can build and run the binary:

```
pipenv install -d
pipenv run python -OO -m PyInstaller main.py -F
dist/./main
```

For Windows 10 users: you also need to install pywin32-ctypes with

```
pipenv install pywin32-ctypes
```

Note that, although Pipenv automatically scans for the targeted Python version (Python 3.6), this may not give the desired result if you have multiple implementations of Python (for instance, CPython 3.6.8 and PyPy 3.6.9). In this case, you can specify the path to the correct Python version, for example:

```
pipenv --python /usr/bin/python3.6
```

CHAPTER 2

Optimal enumeration

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2.1 Definitions of tasks

By choosing the option *Standard counting and enumeration* in Capybara, the user can either count or list one of the following:

For a given input file and a given cost vector, let **S** be the set containing all reconciliations of minimum cost (cyclic or acyclic).

2.1.1 Task T1: All solutions

Count: size of **S**.

Enumerate: the set **S**.

2.1.2 Task T2: Event vectors

Count: number of different event vectors in **S**.

Enumerate: all different event vectors in **S**.

The **event vector** of a reconciliation is a vector of four integers representing the number of occurrences of cospeciation, duplication, host-switch, and loss events.

Two reconciliations have the same event vectors if the numbers of each event are the same.

2.1.3 Task T3: Event partitions

Count: number of different event partitions in **S**.

Enumerate: all different event partitions in **S**.

The **event partition** of a reconciliation is a partition of the internal nodes of the symbiont tree into three subsets: cospeciation, duplicaiton, and host-switch nodes.

Two reconciliations have the same event partitions if, for each node in the symbiont tree, the assigned events (cospeciation, duplication, host-switch) are the same, regardless of the hosts.

2.1.4 Task T4: Cospeciation-Duplication Equivalence classes

Count: number of equivalence classes in **S**.

Enumerate: all equivalence classes in **S**.

Two reconciliations are considered **CD-equivalent** if, for each node in the symbiont tree, the assigned events (cospeciation, duplication, host-switch) are the same, moreover, the assigned hosts are also the same except when the event is a host-switch.

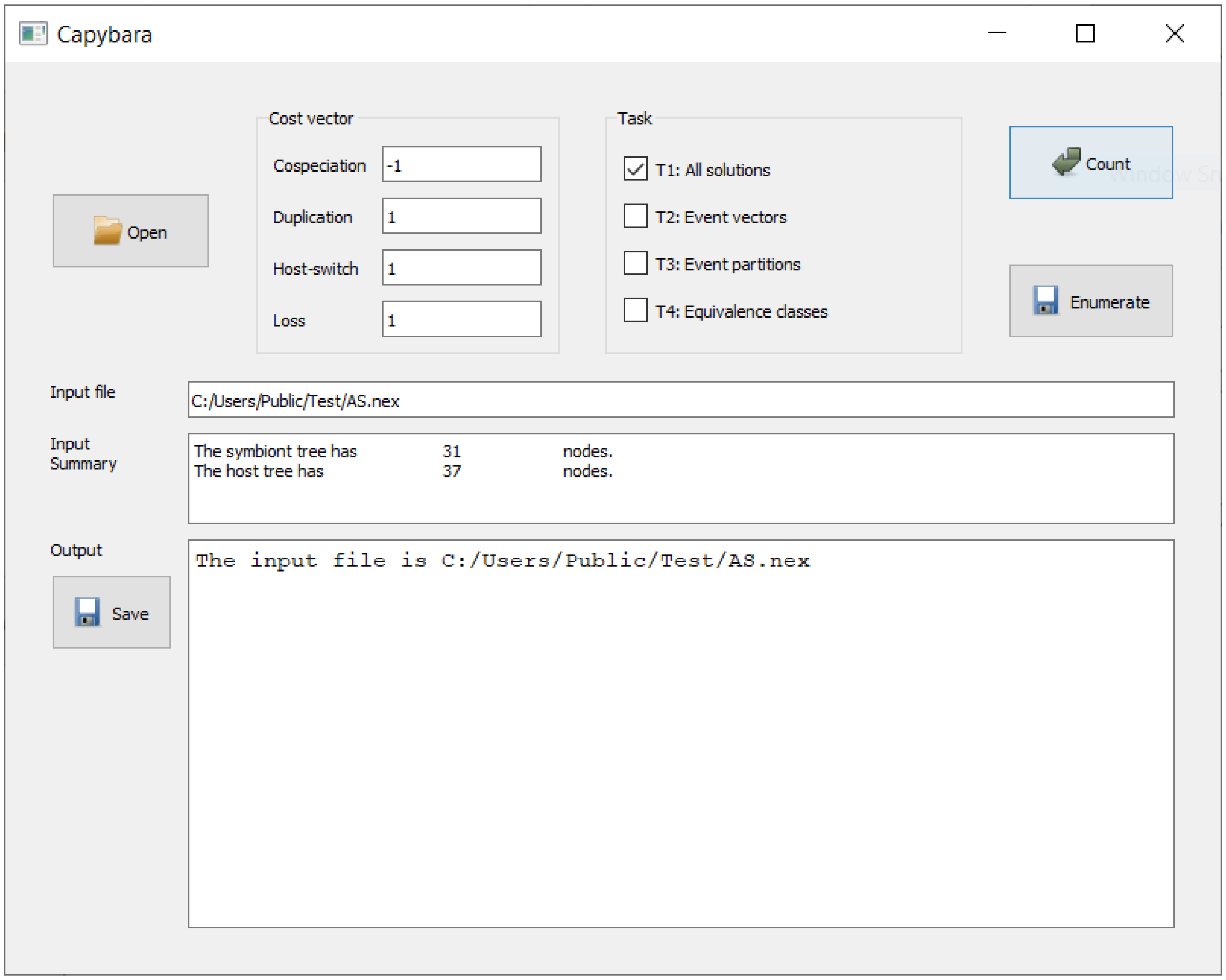
2.2 Loading an input file

The input format is the same as for EUCALYPT. `Here is an example input file`. Note that the symbiont tree can be also introduced in a block starting with *BEGIN SYMBIONT* instead of *BEGIN PARASITE*.

After loading a file with the *Open* button, the input file information is displayed, and the other buttons become available:

Cost vector

- Before clicking on the *Count* or *Enumerate* button, choose the desired cost vector.



Cost vector

Cospeciation -1

Duplication 1

Host-switch 1

Loss 1

Task

[✓ T1: All solutions]

T2: Event vectors

T3: Event partitions

T4: Equivalence classes

Input file C:/Users/Public/Test/AS.nex

Input Summary

```
The symbiont tree has      31          nodes.
The host tree has          37          nodes.
```

```
The input file is C:/Users/Public/Test/AS.nex
```

- All four numbers must be **integers**.
- Floating point numbers will be rounded towards zero (3.6 becomes 3, -3.6 becomes -3).
- Different cost vectors can be used, for example, across differents runs of the counting tasks, without needing to re-load the input file.

Tip:

- The file openning and saving dialogs have their own application-wide favorites list. The user can add a folder to the favorites list using drag and drop to have quicker access in the future.
- Not sure what an option means? Most buttons and boxes have help messages (tooltip). These will appear when the mouse cursor moves over an item.

2.3 Counting

2.3.1 Basic usage

The user can check multiple boxes in **Task** then click on the *Count* button for the results to be printed directly in the **Output** area.

It is possible to save the on-screen text output to a file using the *Save* button.

2.3.2 Example

Here is the output of all four counting tasks on the `example input`:

```
===============
Job started at 2019-09-20 15:24:52
Cost vector: (-1, 1, 1, 1)
------
Task 1: Counting the number of solutions (cyclic or acyclic)...
Total number of solutions = 18
------
Task 2: Counting the number of solutions grouped by event vectors...
1: [8, 1, 6, 2] of size 4
2: [9, 1, 5, 4] of size 2
3: [9, 0, 6, 4] of size 4
4: [8, 0, 7, 2] of size 8
Total number of event vectors = 4
Total number of solutions = 18
------
Task 3: Counting the number of event partitions...
Total number of event partitions = 4
------
Task 4: Counting the number of CD equivalence classes...
Total number of strong equivalence classes = 4
------
Optimal cost = 1.0
------
Job finished at 2019-09-20 15:24:52
```

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```
Time elapsed: 0.71 s
===============
```

2.4 Listing

2.4.1 Basic usage

Use the *Enumerate* button for listing solutions to a file that can be used for analysis or visualization. Unlike the *Count* button, it allows only one task box to be checked at a time.

After choosing the output file name, the user selects additional options, depending on the task. Once the additional options are confirmed, the computation starts automatically, and a progress bar pops out. It is possible to stop the computation at anytime by closing the progress bar (the program may freeze for a few seconds).

Note that the on-screen text output (human-readable trace of computational tasks) can still be saved using the *Save* button.

2.4.2 Options for tasks T1 and T2

The output is in the same format as the output of EUCALYPT. And just like in EUCALYPT, the user can choose the maximum number of solutions that she likes to generate.

For the task T1 (all optimal reconciliations) only, it is possible to keep only the acyclic reconciliations.

Here is an example of the on-screen output when this option is chosen, for `another input file` and cost vector (0,1,1,1):

```
===============
Job started at 2019-09-20 19:40:04
Cost vector: (0, 1, 1, 1)
Task 1: Enumerate acyclic solutions...
------
Number of acyclic solutions = 144 out of 184
Optimal cost = 11.0
Output written to C:/Users/Public/Test/output.txt
------
Job finished at 2019-09-20 19:40:05
Time elapsed: 0.63 s
===============
```

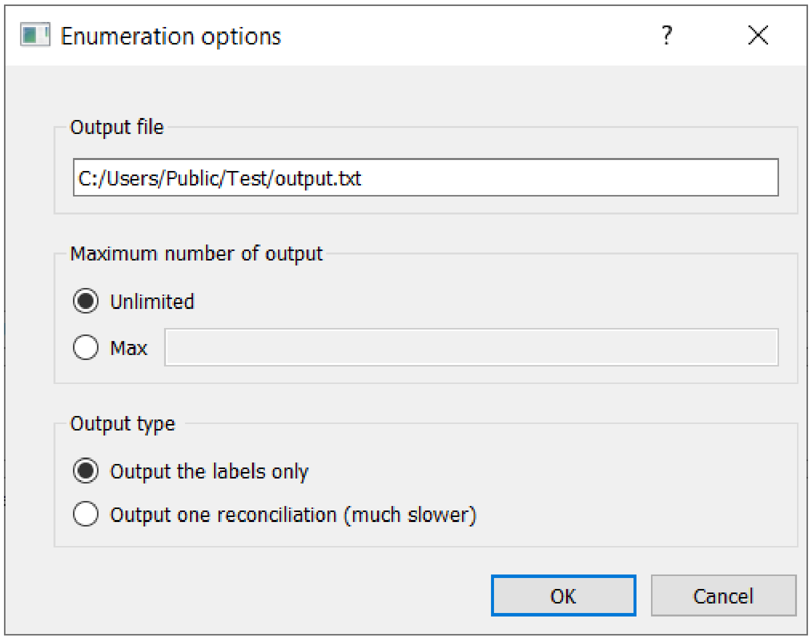
2.4.3 Options for tasks T3 and T4

There are two output types:

Labels only

If the first output type *"labels only"* is chosen, the result will be compatible with the new visualization tool Capybara Viewer.

Task T3: Each event partition is represented by the assignment, to each internal symbiont node, of one of the three events.



Output file: C:/Users/Public/Test/output.txt

Maximum number of output: [✓ Unlimited] Max

Output type: [✓ Output the labels only] Output one reconciliation (much slower)

Task T4: Each CD-equivalence class is represented by the assignment, to each internal symbiont node, of one of the three events, and the assignment of a host hame to each symbiont node with non-host-switch event.

Reconciliation

If the second output type *"reconciliation"* is chosen, the result will be compatible with the the original viewer for EUCALYPT.

Note that in this case, the output is only one reconciliation chosen arbitrarily among the potentially many (cyclic or acyclic) reconciliations having the same event partition or belonging in the same CD-equivalence class.

CHAPTER 3

Suboptimal enumeration

The input format is the same as for *Optimal enumeration* (see *Loading an input file*).

3.1 Basic usage

Consider all reconciliations of a given input **ordered by cost** in a list, then the K-best solutions is the first K element of this list.

Note that the ordering between solutions having the same cost is arbitrary.

K-best solution enumeration allows to obtain sub-optimal solutions if the number K is fixed to be larger than the number of optimal solutions.

3.2 Example

For `this input file` and cost vector (0,1,2,1), there are 40 solutions having the optimal cost 21 (none of which is acyclic), and 396 solutions having the second-optimal cost 22 (146 are acyclic).

By fixing K = 100 (without filtering by cyclicity), the output will contain 100 solutions. The first 40 are the optimal solutions, and the next 60 are chosen arbitrarily among the 396 second-optimal solutions.

The choice of these 60 solutions are arbitrary, meaning that if the user closes and restarts the program, the output may be different in spite of using exactly the same input.

If the cyclicity filter is applied, the output will contain a certain number of acyclic solutions: it's the number of acyclic solutions among the 60 second-optimal solutions. This number varies each time the program restarts, and it might be zero.

CHAPTER 4

Output visualization

For visualizating reconciliations (symbiont tree drawn on top of the host tree), use the original viewer for EUCALYPT.

For visualizating event partitions or equivalence classes (colorings of the parasite tree with animation), use the new animated web tool Capybara Viewer.

Next we present the usage of the new visualization tool.

4.1 Input format

The Capybara visualizer tool takes two input formats generated from the third tab *Convert enumeration files for visualization* of the main Capybara tool:

- File input (DOT format) can be saved into the filesystem by clicking the *Save* button. This file needs to be uploaded into Capybara viewer after selecting the first upload method.
- Plain text input can be copied into the user's clipboard by clicing the *Copy* button. Then the clipboard content can be pasted into Capybara viewer.

  Note that the text area for copy-and-paste is hidden by default, and will only appear after the user selects the second upload method *Copy and paste text*.

Note: When the Capybara app closes, the clipboard content will also be cleared. Therefore, if you choose the second upload method, *do not* close the main app while using the viewer.

4.2 Graphical elements

One event partition or equivalence class will be drawn as a colored symbiont tree.

Texts The names of the nodes in the symbiont tree are shown.

Colors The internal nodes of the symbiont tree are colored according to the event. The correspondance between color and event is shown in the legend on top of the graphic area.

🟧 cospeciation 🟩 duplication 🟦 host-switch

Hover texts When the mouse hovers over a node, the corresponding host name, if known, is shown in small tag. This applies to all leaf nodes of the symbiont tree, or, in an equivalence class, those internal nodes with non-host-switch event.

4.3 Visualization methods

One **frame** of the animation corresponds to one event partition, or one equivalence class.

The user can:

- Either **play the animation**, i.e., a continous transition of images from one frame to another. The transition time can be adjusted. This method is interesting because it can provide a quick global view on multiple solutions. Combined with a screen-recording tool, it can also produce a video output.
- Or **freeze the animation** at one particular frame. This can be useful for checking the host names in equivalence classes.

A single frame can be **saved in a image file**, either by using the save button on top of the legend, or by using the cell menu (this menu appears when clicking the three small dots on the top left corner of the graphic area).

4.4 Example

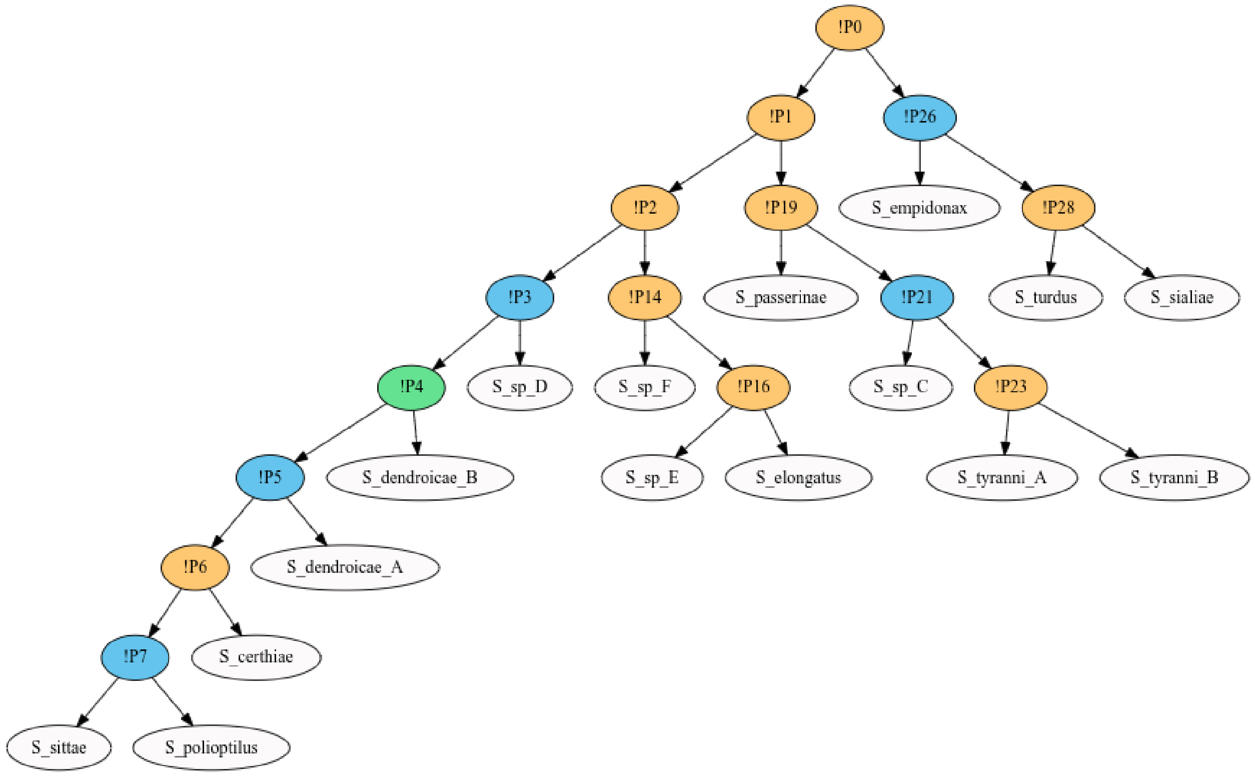
There are 4 event partitions on `this example input file` and cost vector (-1,1,1,1). Thereofre, there are 4 frames in the animation.

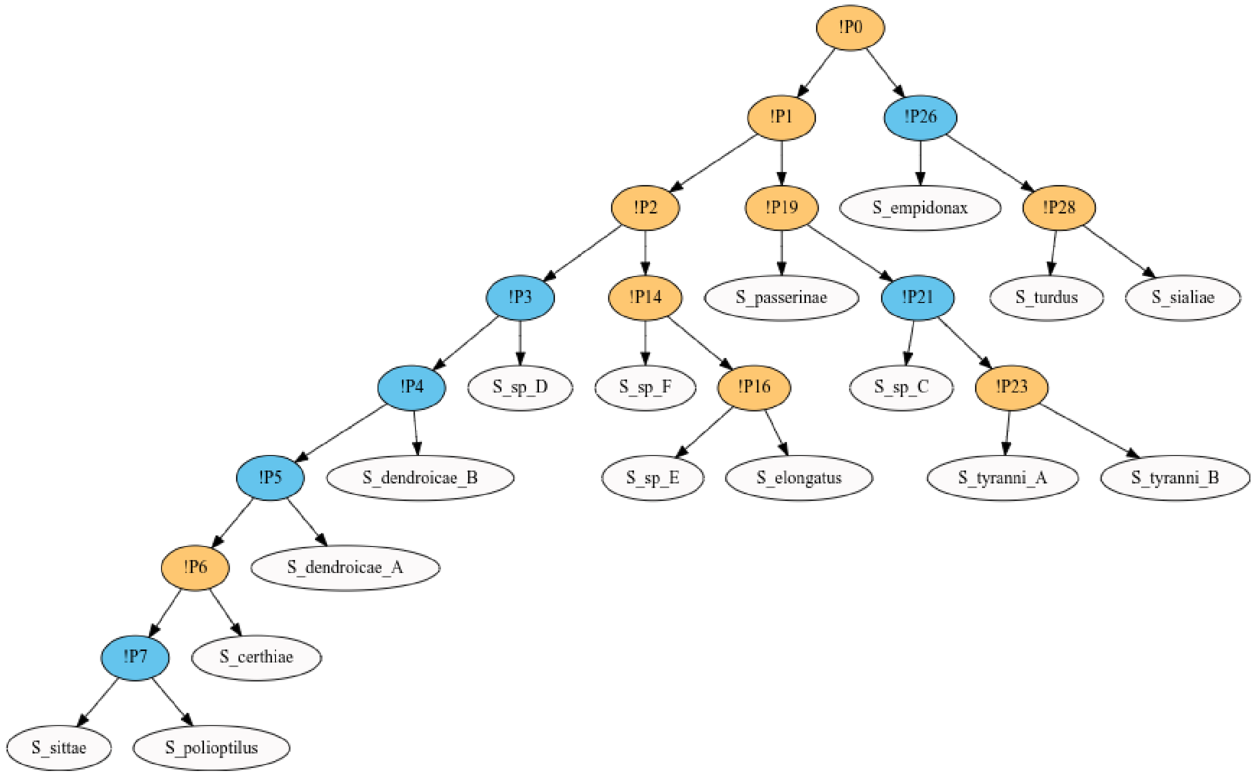
Frame 1:

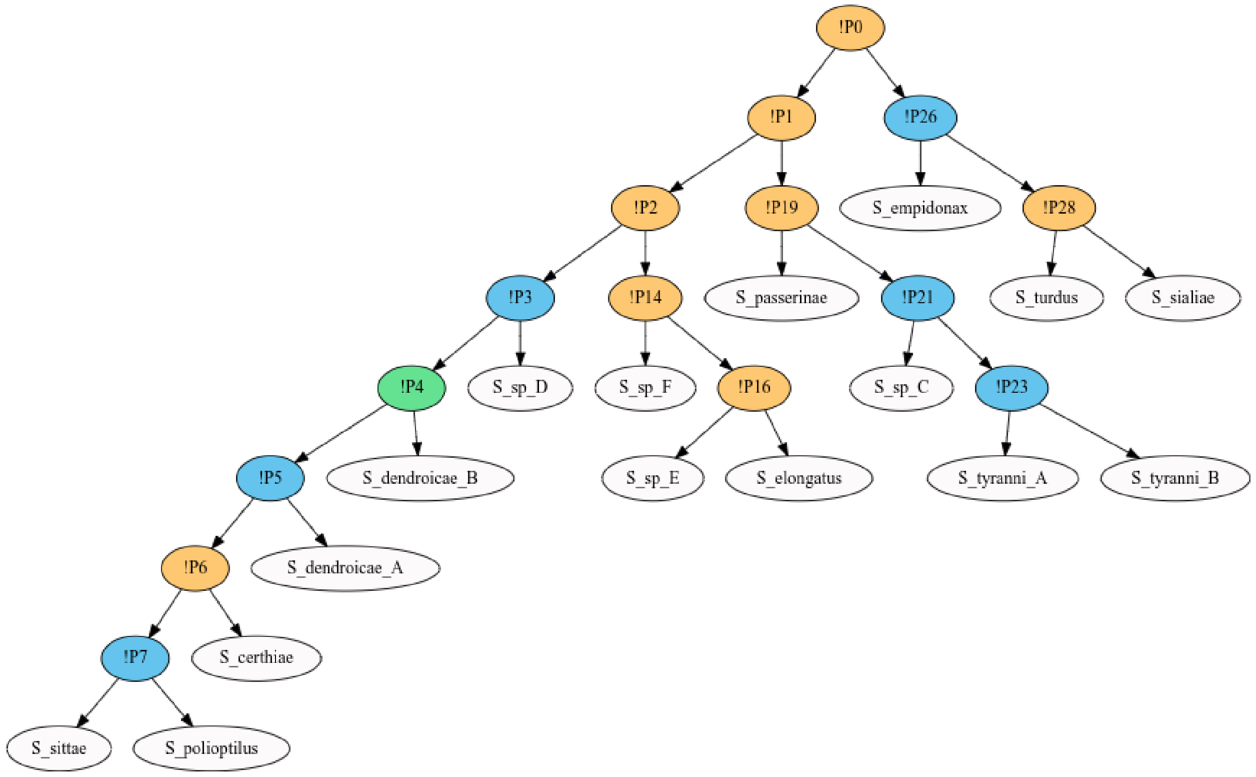
Frame 2:

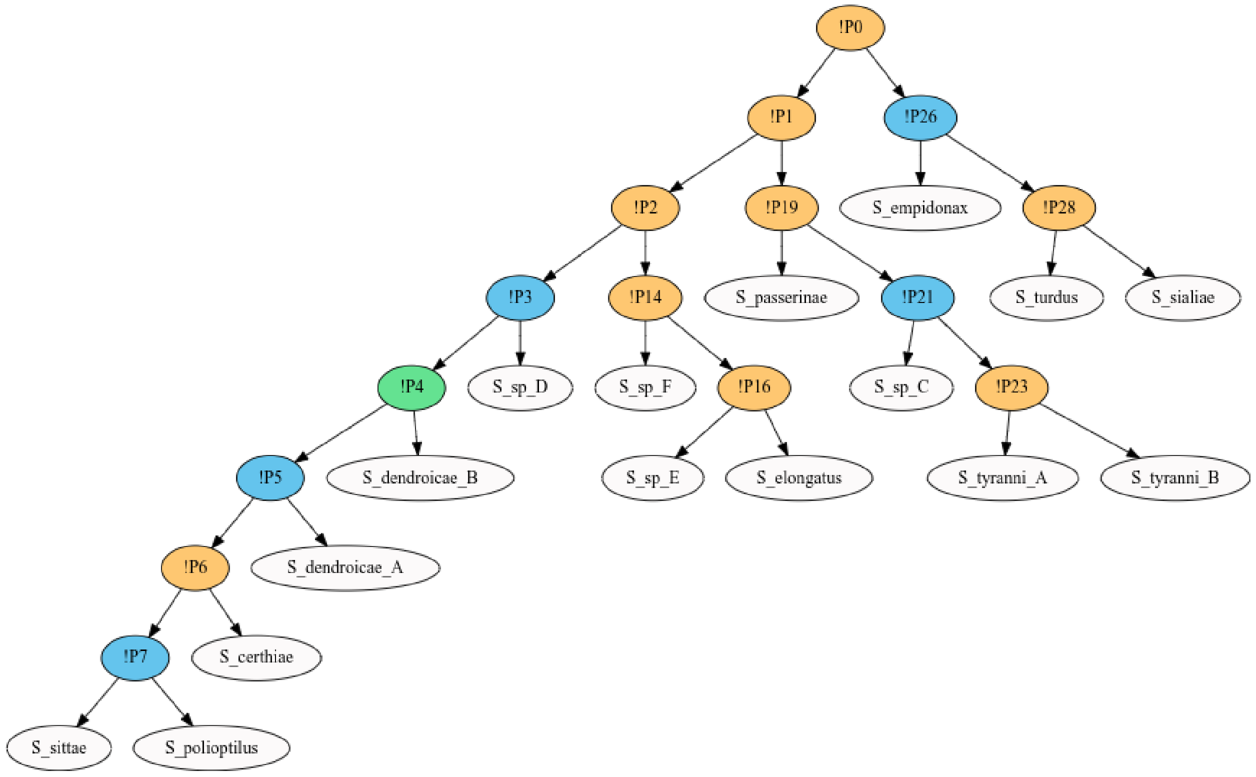
Frame 3:

Frame 4:


!P0
!P1
!P26
!P2
!P19
S_empidonax
!P28
!P3
!P14
S_passerinae
!P21
S_turdus
S_sialiae
!P4
S_sp_D
S_sp_F
!P16
S_sp_C
!P23
!P5
S_dendroicae_B
S_sp_E
S_elongatus
S_tyranni_A
S_tyranni_B
!P6
S_dendroicae_A
!P7
S_certhiae
S_sittae
S_polioptilus


!P0
!P1
!P26
!P2
!P19
S_empidonax
!P28
!P3
!P14
S_passerinae
!P21
S_turdus
S_sialiae
!P4
S_sp_D
S_sp_F
!P16
S_sp_C
!P23
!P5
S_dendroicae_B
S_sp_E
S_elongatus
S_tyranni_A
S_tyranni_B
!P6
S_dendroicae_A
!P7
S_certhiae
S_sittae
S_polioptilus


!P0
!P1
!P26
!P2
!P19
S_empidonax
!P28
!P3
!P14
S_passerinae
!P21
S_turdus
S_sialiae
!P4
S_sp_D
S_sp_F
!P16
S_sp_C
!P23
!P5
S_dendroicae_B
S_sp_E
S_elongatus
S_tyranni_A
S_tyranni_B
!P6
S_dendroicae_A
!P7
S_certhiae
S_sittae
S_polioptilus


!P0
!P1
!P26
!P2
!P19
S_empidonax
!P28
!P3
!P14
S_passerinae
!P21
S_turdus
S_sialiae
!P4
S_sp_D
S_sp_F
!P16
S_sp_C
!P23
!P5
S_dendroicae_B
S_sp_E
S_elongatus
S_tyranni_A
S_tyranni_B
!P6
S_dendroicae_A
!P7
S_certhiae
S_sittae
S_polioptilus

CHAPTER 5

Python package

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5.1 Installation

Important: We strongly recommand installing the Capybara package only in virtual environments.

First, install Pipenv if you don't have it already:

```
pip install pipenv
```

Then, navigate to the project folder, create and activate a virtual environment:

```
cd PATH-TO-THE-PROJECT-FOLDER
pipenv install
pipenv shell
```

Once inside the virtual environment, follow the installation guide below.

Install the package **capybara-cophylogeny** via `pip`:

```
python -m pip install capybara-cophylogeny
```

You can verify whether the installation is successful inside the Python interactive shell:

```
python
```

Import the two Capybara modules:

```
>>> import capybara.counter
>>> import capybara.enumerator
```

The import statements should not yield any error.

Important: Be sure to update to the newest version if you have not used Capybara for a while:

```
python -m pip install capybara-cophylogeny --upgrade
```

Improve performance with PyPy

You can **speed up the computation** by using PyPy3 instead of the standard CPython interpreters. To do this, follow these simple steps:

1. Download and install PyPy3.
2. Create and activate the virtual environment using PyPy3 as interpreter:

   ```
   pipenv install --python=pypy3
   pipenv shell
   ```

3. Already done! Python commands will now use PyPy3. For example, you can write:

   ```
   python -m pip install capybara-cophylogeny
   python MY_SCRIPT.py
   ```

5.2 Usage

The user is assumed to be already familiar with the GUI version of Capybara.

The Python package provides two functions `capybara.counter.run` and `capybara.enumerator.run`, corresponding to the two buttons *Count* and *Enumerate* in *Optimal enumeration*.

5.2.1 Count: `capybara.counter.run`

The function takes 4 parameters (2 optional):

Parameters	
input_name	Name of the input file (or the path)
task	Integer between 1 and 4
cost_vector	List (or tuple) of four integers. **Default**: (-1,1,1,1)
verbose	If set to True, print a message when the computation starts and ends. **Default**: False

The function returns an integer, depending on the chosen task (see also *Definitions of tasks*):

	Return value
task=1	Number of optimal reconciliations
task=2	Number of event vectors
task=3	Number of event partitions
task=4	Number of equivalence classes

5.2.2 Enumerate: `capybara.enumerater.run`

The function takes 7 parameters (4 optional):

Parameters	
input_name	Name of the input file (or the path)
output_name	Name of the output file (or the path)
task	Integer between 1 and 4
cost_vector	List (or tuple) of four integers. Default: (-1,1,1,1)
verbose	If set to True, print a message when the computation starts and ends. **Default**: False
maximum	Maximum number of solutions to be outputted. **Default**: Infinity
acyclic_only	If set to True and task=1, output only acyclic solutions. **Default**: False

The function does not return anything. It writes the output to the specified file, depending on the chosen task (see *Definitions of tasks*).

The output format is the same as in the GUI version, except for task 2: it only enumerates the event vectors, not one reconciliation per event vector.

For tasks 3 and 4, the output format corresponds to the option **Labels only** in the GUI version (see *Options for tasks T3 and T4*).

5.2.3 Log file

With the option **verbose**, only simple messages are printed to the console, at the start and the end of computation.

More detailed information (parameters used, time of computation, cause of error) can be found in the log file **capybara.log** in the working directory.

After a successful job, the user can find messages similar to the following at the end of the log file:

```
2020-04-19 21:50:05,131 - 448c175a865711ea8496b8ca3aced137 - INFO - ===== Job started!
↪ =====
2020-04-19 21:50:05,131 - 448c175a865711ea8496b8ca3aced137 - INFO - Running Capybara␣
↪Counter Task 2
```

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```
2020-04-19 21:50:05,132 - 448c175a865711ea8496b8ca3aced137 - INFO - Input file: /home/
↪user/cophy/data/input1.nex
2020-04-19 21:50:05,132 - 448c175a865711ea8496b8ca3aced137 - INFO - Cost vector: (0,␣
↪1, 1, 1)
2020-04-19 21:50:05,133 - 448c175a865711ea8496b8ca3aced137 - INFO - Reading the input␣
↪file...
2020-04-19 21:50:05,134 - 448c175a865711ea8496b8ca3aced137 - INFO - Successful!␣
↪Computing...
2020-04-19 21:50:05,162 - 448c175a865711ea8496b8ca3aced137 - INFO - Done! The result␣
↪of Counter Task 2 is 8
2020-04-19 21:50:05,166 - 448c175a865711ea8496b8ca3aced137 - INFO - ===== Job␣
↪finished successfully! =====
```

A job interrupted by the user (for example, by pressing Ctrl+C) is also shown in the log file:

```
2020-04-19 22:04:11,600 - 448c175a865711ea8496b8ca3aced137 - INFO - ===== Job started!
↪ =====
2020-04-19 22:04:11,600 - 448c175a865711ea8496b8ca3aced137 - INFO - Running Capybara␣
↪Enumerator Task 4
2020-04-19 22:04:11,601 - 448c175a865711ea8496b8ca3aced137 - INFO - Input file: /home/
↪user/cophy/data/input1.nex
2020-04-19 22:04:11,601 - 448c175a865711ea8496b8ca3aced137 - INFO - Cost vector: (0,␣
↪1, 1, 1)
2020-04-19 22:04:11,601 - 448c175a865711ea8496b8ca3aced137 - INFO - Output file: /
↪home/user/cophy/input1-classes.txt
2020-04-19 22:04:11,601 - 448c175a865711ea8496b8ca3aced137 - INFO - Reading the input␣
↪file...
2020-04-19 22:04:11,602 - 448c175a865711ea8496b8ca3aced137 - INFO - Successful!␣
↪Computing...
2020-04-19 22:04:11,604 - 448c175a865711ea8496b8ca3aced137 - WARNING - Keyboard␣
↪interrupt
2020-04-19 22:04:11,604 - 448c175a865711ea8496b8ca3aced137 - INFO - ===== Job aborted!
↪ =====
```

The log file is automatically cleaned after 48 hours (the old file is renamed as capybara.log.CREATION-DATE).

5.3 Examples

5.3.1 A simple example

Here is a simple script where we print the number of event vectors, for different cost vectors:

```python
import capybara.counter

for cost_vector in [(-1,1,1,1), (0,1,1,1), (0,1,1,0), (0,2,3,1)]:
    num_vectors = capybara.counter.run('input.nex', task=2, cost_vector=cost_vector)

    print("Cost vector =", cost_vector)
    print("Number of event vectors =", num_vectors)
```

5.3.2 Multiprocessing on multiple input files

The user may want to use **more than one CPU unit** when working with a large number of files.

We propose below a script that uses **multiprocessing**. It follows three steps:

- Define a function that applies `capybara.enumerator.run` with parameters *task=4* and *cost_vector=(0,1,1,1)* on the given input file. The output file name is obtained by **adding a suffix** “0111_classes” to the input file name.
- Get the list of all input files, located in the directory **data/**.
- Create a pool of 4 worker processes, and apply the function on the list of input files.

```
import os
from multiprocessing import Pool
import capybara.enumerator

# define my custom function
def my_function(input_name):
    output_name = '{name}_{suffix}.txt'.format(name=os.path.splitext(input_name)[0],
                                               suffix='0111_classes')
    capybara.enumerator.run(input_name, output_name, task=4, cost_vector=(0,1,1,1))

# getting all .nex files in the data folder
nexfiles = [os.path.join('data', fname) for fname in os.listdir('data')
                                        if fname.endswith('.nex')]

# apply the function to the list of files
with Pool(processes=4) as pool:
    pool.map(my_function, nexfiles)
```

CHAPTER 6

Overview

Phylogenetic tree reconciliation is the method of choice in analyzing host-symbiont systems. Despite the many reconciliation tools that have been proposed in the literature, two main issues remain unresolved:

- listing **suboptimal** solutions (i.e., whose score is “close” to the optimal ones), and
- listing only solutions that are **biologically different “enough”**.

The first issue arises because the optimal solutions are not always the ones biologically most significant; providing many suboptimal solutions as alternatives for the optimal ones is thus very useful. The second one is related to the difficulty to analyze an often huge number of optimal solutions.

Capybara addresses both of these problems in an efficient way. Furthermore, it includes a tool for visualizing the solutions that significantly helps the user in the process of analyzing the results.

CHAPTER 7

Features

Capybara has some features in common with its predecessor **EUCALYPT**[1]: counting the number of optimal reconciliations, listing optimal reconciliations to a file, keeping only the acyclic ones (the definition of cyclicity is taken from[2]).

Wow! New features!

[1] Beatrice Donati, Christian Baudet, Blerina Sinaimeri, Pierluigi Crescenzi, and Marie-France Sagot. Eucalypt: efficient tree reconciliation enumerator. *Algorithms for Molecular Biology*, 10(1):3, 2015. doi: 10.1186/s13015-014-0031-3.

[2] Maureen Stolzer, Han Lai, Minli Xu, Deepa Sathaye, Benjamin Vernot, and Dannie Durand. Inferring duplications, losses, transfers and incomplete lineage sorting with nonbinary species trees. *Bioinformatics*, 28(18):i409–i415, 2012. doi: 10.1093/bioinformatics/bts386.

Capybara also has some **exciting new features**:

- Counting and enumeration of even vectors, event partitions, equivalence classes (see the *Definitions of tasks* in *Optimal enumeration*)
- Enumeration of suboptimal reconciliations (see *Suboptimal enumeration*)
- Animated visualization of event partitions and equivalence classes (see *Output visualization*)

The counting and enumeration features of Capybara's *Optimal enumeration* are also avaible as a *Python package*.

CHAPTER 8

References