

A quick guide to PartitionFinder

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PartitionFinder is a Python program for simultaneously choosing partitioning schemes and models of molecular evolution for DNA sequence data. It is useful to use before running a phylogenetic analysis of DNA sequence data, in order to decide how to divide up your sequence data into separate blocks before analysis, and to simultaneously perform model selection on each of those blocks. Currently, PartitionFinder will only work on Intel Macs. We hope to extend this to PPC Macs and to Windows machines soon.

Quick Start

If these instructions don't make sense, there are much more detailed instructions and usage examples below. Have a look at the example file to get your input files in order.

1. Open Terminal and cd to the directory with PartitionFinder in it
2. Run PartitionFinder by typing at the command prompt:

```
python PartitionFinder.py <foldername>
```

where '`<foldername>`' is the full file path to a folder containing a Phylip alignment and a PartitionFinder configuration file called 'partition_finder.cfg'. E.g.

```
python PartitionFinder.py /Users/Rob/new_analysis
```

The results will be in new subfolder called "analysis" within the original folder. The most important files are "best_schemes.txt" and "all_schemes.txt".

Before You Start

Make sure you have Python 2.7 or later installed. To check which ver, open Terminal and type "python". It will tell you the version you have. If you have anything before 2.7, update python using the appropriate installer from here:

<http://www.python.org/getit/>

Input Files

There are two input files, a Phylip alignment and a configuration file.

Alignment

Your DNA alignment needs to be in non-interleaved Phylip format. We use the same version of Phylip that PhyML uses, which is described in detail here <http://www.atgc-montpellier.fr/phyml/usersguide.php?type=phylip>

Configuration File

PartitionFinder gets all of its information on the analysis you want to do from a configuration file. This file should always be called “partition_finder.cfg”. The best thing to do is to base your own .cfg on the example file provided in the “example” folder. Here’s an exhaustive list of everything in that file.

In the configuration file, white spaces, blank lines and lines beginning with a “#” (comments) don’t matter. You can add or remove these as you wish. However, the order of the variables in the file is important, and all variables must be kept in the file.

The configuration file looks like this:

```
# ALIGNMENT FILE #
alignment = test.phy

# BRANCHLENGTHS #
branchlengths = linked

# MODELS OF EVOLUTION #
models = all
model_selection = bic

# PARTITIONS #
[partitions]
Gene1_pos1 = 1-789\3
Gene1_pos2 = 2-789\3
Gene1_pos3 = 3-789\3

# SCHEMES #
[schemes]
search = user

# user schemes
allsame = (Gene1_pos1, Gene1_pos2, Gene1_pos3)
1_2_3   = (Gene1_pos1) (Gene1_pos2) (Gene1_pos3)
12_3    = (Gene1_pos1, Gene1_pos2) (Gene1_pos3)
```

The options in the file are described below. Where an option has a limited set of possible commands, they are listed on the same line as the option, separated by vertical bars like this “[”

alignment

The name of your DNA sequence alignment. If the alignment is in the same file as the partition_finder.cfg file, all you need is the name here, e.g. “alignment = alignment.phy”. If your alignment is in a different file you will need to

supply a full filepath, e.g. `alignment = Users/Rob/analysis/alignment.phy`.

models: all | <list>

This setting tells PartitionFinder which models of molecular evolution to consider during model selection. PartitionFinder performs model selection (in much the same way as other programs like ModelTest, MrModelTest, or ModelGenerator) on each subset of sites. Your results therefore tell you not only the best partitioning scheme, but also which model of molecular evolution is most appropriate for each subset of sites in that scheme. So you don't need to do any further model selection after PartitionFinder is done. For most people, `models=all` will be the most useful setting.

models = all tells PartitionFinder to compare 56 models of molecular evolution for each subset. These comprise the usual 12 models of molecular evolution (JC, K80, TrNef, K81, TVMef, TIMef, SYM, F81, HKY, TrN, K81uf, TVM, TIM, and GTR), each of which comes in four flavours: on its own, with invariant sites (+I), with gamma distributed rates across sites (+G), or with both gamma distributed rates and invariant sites (+I+G).

models = <list>, e.g. **models = GTR+G, GTR+I+G**

If you want to restrict the list of models considered, you can do that by specifying any particular list of models from the above 56 (use the terminology as given above). Each model in the list should be separated by a comma. This option can be particularly useful if the program you will use for your final phylogenetic analysis only implements a few models. For instance, both MrBayes 3.1.2 and RaxML have a limited model implementation. If you were intending to use RaxML to do your final phylogenetic analysis, there would be little point making PartitionFinder analyse all 56 models of molecular evolution on all possible partitions, because your final analysis you will be restricted to choosing between just two models, GTR+G and GTR+I+G. PartitionFinder will have to do a lot less work (and so run a lot more quickly) if you restrict the list of models to only those which are relevant.

model_selection: AIC | AICc | BIC

This setting tells PartitionFinder which method to use for model selection. It also defines the metric that is used for partition selection if you use `search=greedy` (see below).

The AIC, AICc, and BIC are all quite similar in spirit – they reward models which fit the data better, but also penalise models depending on how many parameters they have. The idea is find the right balance between including parameters which allow us to model evolution well, but avoiding overparameterisation. In general, the BIC penalises parameters the most, followed by the AICc, and then the AIC is most lenient. Which `model_selection` approach you use will depend on your preference. There are lots of papers comparing the merits of the different metrics, and based on those papers (especially Minin et al Syst. Biol. 52(5):674–683, 2003; and Adbo et al Mol. Biol. Evol. 22(3):691–703. 2004) my own preference is to use the BIC.

[partitions]

On the lines following this statement you define the starting partitions for your analysis. Each partition has a name, followed by an “=” and then a description. The description is built up as in most Nexus formats, and tells PartitionFinder which sites of your original alignment correspond to each partition. The best way to understand this is to look at a couple of examples.

Imagine a DNA sequence alignment with 1000bp of protein-coding DNA, followed by 1000bp of intronic DNA. Let's imagine that some of the intron was unalignable too, so we don't want that included in our analysis.

```
Gene1_codon1 = 1-1000\3      ❶
Gene1_codon2 = 2-1000\3      ❷
Gene1_codon3 = 3-1000\3      ❸
intron       = 1001-1256 1675-2000 ❹
```

❶–❸ are typical of how you might separate out codon positions for a protein coding gene. The numbers either side of the dash define the start and end of the gene, and the number after the backslash defines the spacing of the sites. Every third site will define a codon position, as long as your alignment stays in the same reading frame throughout that gene.

❹ shows how you can include ranges of sites without backslashes, and demonstrates that you can combine >1 range of sites in a single partition. Here, we excluded sites 1257-1674 because they were unalignable.

There are a couple of general points about partitions. First, the total list of partitions does not have to include all the sites in your original alignment. For instance, you might exclude some sites you're not interested in, or that were unalignable. However, you'll get a warning from PartitionFinder if not all of the sites in the original alignment are included in the partitions you've defined. Second, partitions cannot be overlapping. That is, each site in the original alignment can only be included in a single partition.

To help with cutting and pasting from Nexus files (like MrBayes) you can leave “charset” at the beginning of each line, and a semi-colon at the end of each line. Both of these things are ignored. So, the following would be treated exactly the same as the example above:

```
charset Gene1_codon1 = 1-1000\3;
charset Gene1_codon2 = 2-1000\3;
charset Gene1_codon3 = 3-1000\3;
charset intron       = 1001-1256 1675-2000;
```

search: all | user | greedy

This option defines which partitioning schemes PartitionFinder will analyse, and how thorough the search will be. In general ‘all’ is only practical for analyses that start with 10 or fewer partitions defined (see below).

search = all Tells PartitionFinder to analyse all possible partitioning schemes. That is, every scheme that includes all of your partitions in any combination at all. Whether you can analyse all schemes will depend on how

much time you have, and on what is computationally possible. **If you have any more than 12 partitions to start with you should not choose 'all'**. This is because the number of possible schemes can be extremely large. For instance, with 13 starting partitions there are almost 28 million possible schemes, and for 16 partitions the number of possible schemes is over 10 billion. It's just not possible to analyse that many schemes exhaustively. For 12 starting partitions, the number of possible schemes is about 4 million, so it might be possible to analyse all schemes if you have time to wait, and a fast computer with lots of processors.

search = user Use this option to compare only the partitioning schemes that you define by hand. User-defined schemes are simply listed, one-per-line, on the lines following "search=user". A scheme is defined by a name, followed by an "=" and then a definition. To define a scheme, simply use parentheses to join together partitions that you would like to combine. Within parentheses, each partition is separated by a comma. Between parentheses, there is no comma.

Here's an example. If I'm working on my one protein-coding gene plus intron alignment above, I might want to try the following schemes: (i) all partitions analysed together; (ii) intron analysed separately from protein coding gene; (iii) intron separate, 1st and 2nd codon positions analysed separately from 3rd codon positions; (iv) all partitions analysed separately. I could do this as follows, with one scheme on each line:

```
together      = (Gene1_codon1, Gene1_codon2, Gene1_codon3, intron)
intron_123    = (Gene1_codon1, Gene1_codon2, Gene1_codon3) (intron)
intron_12_3   = (Gene1_codon1, Gene1_codon2) (Gene1_codon3) (intron)
separate      = (Gene1_codon1) (Gene1_codon2) (Gene1_codon3) (intron)
```

search = greedy Tells PartitionFinder to implement a greedy algorithm to search for a good partitioning scheme. This is a lot quicker than using search=all, and will often give you the optimal scheme. However, it is not 100% guaranteed to give you the optimal partitioning scheme. When you implement this option, PartitionFinder will start by looking at the most partitioned scheme (e.g. 'separate' in the example above. It will then try all possible ways of joining together two partitions of that scheme, and see if any of them improve on the fully-partitioned model. It will carry on in this way until it can't find a scheme that improves on the current 'best' scheme.

When you use search=greedy, PartitionFinder has to compare models using a scoring system. Which scoring system it uses is defined using the **model_selection** option (see above). Because the greedy algorithm follows a path through the partitions, it will only find a single best-scheme, which will be output to the 'best_schemes.txt' file (see below).

Running PartitionFinder

Once you have your input files set up, to run PartitionFinder you:

1. Open Terminal (on most Macs, this is found in Applications/Utilities)
2. cd to the directory with PartitionFinder in it. The easiest way to do this is to type “cd “ (the space is important) at the command prompt, and then drag-and-drop the PartitionFinder folder icon into terminal. This will fill out all of the filepath for the PartitionFinder file for you. Now hit enter.
3. Run PartitionFinder by typing at the command prompt:

```
python PartitionFinder.py <foldername>
```

where ‘<foldername>’ is the full file path to a folder containing a Phylip alignment and a PartitionFinder configuration file called ‘partition_finder.cfg’. E.g.

```
python PartitionFinder.py /Users/Rob/new_analysis
```

Note that you don’t have to be in the PartitionFinder folder to run PartitionFinder. In fact, you can just open up terminal and run it. To do that, all you need to do is change “PartitionFinder.py” above to the full filepath for PartitionFinder.py. For instance, it might look something like this:

```
python Users/Rob/Applications/PartitionFinder/PartitionFinder.py -p -1  
/Users/Rob/new_analysis
```

There are a couple of additional commandline options that can be useful:

--force-restart

delete all previous output and start afresh. Useful if you have had to quit an analysis halfway through, and the program won’t restart.

-p N

Define the number processors to use, where ‘N’ is an number. Use -1 to match the total number of cpus on your machine (this is the default), or set N to any number to use that many processors. The more processors you can use, the faster PartitionFinder will be.

Output files

All of the output is contained in a folder called “analysis” which appears in the same file as your alignment. There is a lot of output, but in general you are likely to be interested in four things, maybe this order:

best_schemes.txt: has information on the best partitioning scheme(s) found. This includes the name of the best schemes, a detailed description of the schemes, and which model of molecular evolution was selected for each partition each scheme. In addition, it includes the log Likelihood of each scheme, the AIC, AICc and BIC of each scheme, the number of parameters in the scheme, and a lot of other information too.

If you search among all schemes (`search=all`) or some pre-defined user schemes (`search=user`) then this file will contain information on the best scheme under each of the three information-theory metrics: the Akaike Information Criterion (AIC), the corrected Akaike Information Criterion (AICc), and the Bayesian Information Criterion (BIC).

If you use the greedy algorithm (`search=greedy`), there will only be a single scheme in `best_schemes.txt`. This is because the greedy algorithm searches among partitioning schemes using one of the information-theory metrics to guide it (defined using `model_selection`, see above). Because of this, you can only find the best scheme for the metric you’ve used, and not for all three metrics.

all_schemes.txt: contains most of the same information as `best_schemes.txt`, but organised in spreadsheet format, and for all schemes that were compared during the search. This is probably only useful if you’re interested in working on methods of finding good partitioning schemes.

subsets is a folder which contains detailed information on the model selection performed on each partition, or combination of partitions (which we call a ‘subset’). This output is very similar to what you would get from any model-selection program. Each model tested is listed, in order of increasing BIC score (i.e. best model is at the top). There will be some minor differences from other model selection programs, due to the implementation we use, but the results should be broadly similar. This folder also contains alignments for each subset, and a .bin file which allows PartitionFinder to re-load information from previous analyses.

schemes is a folder which contains detailed information on all the schemes that were analysed, each in a separate .txt file which has the same name as the scheme. Most of this information is contained in `all_schemes.txt`, apart from the results of the model-selection on each partition in a scheme.

Citation

There isn't one yet.