

## Changes from IQPNNI version 2.6 to 3.0

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This text describes what are new and changed from IQPNNI version 2.6 to 3.0. If you already used version 2.6, please read carefully. Information here would also be useful for ones who are new to IQPNNI.

### 1. What changed in menu-driven interface from 2.6 to 3.0 ?

- The option to switch among rate heterogeneity is now 'r' instead of 'w'.
- The checkpoint file will ONLY be loaded if the program detects that the last run was not finished (in case of user's break or runtime crash). If you want IQPNNI not to load the checkpoint file, then specify the option '-sfc'. See below for more details.
- The default stopping rule is now 'No' instead of 'Yes, but at least <n> iterations'.
- The default number of iterations is now increased a bit compared to the old default value.

For the full usage of the text-based menu-driven interface, please read the manual.

### 2. Command line options

This is a new feature of version 3.0. Run './iqpnni -h' to print out a short description of available options. You can specify some options first with the command line, and then change again with the menu-driven interface. The mechanism is follows:

First, the <input\_file>.iqpnni.checkpoint file is read if the '-sfc' option is NOT specified. The program now checks whether the last run on this alignment is finished or not. If NOT, the parameters recorded in the checkpoint file will be used, and all the command line options will be omitted. In this case, you will see some printout like:

```
The program was not done from the last run!  
Load parameters from the checkpoint file...
```

Thus, if the last run was broken (e.g. with Ctrl+C or runtime error), there are two ways to start a new search:

- specify '-sfc' option on the command line, OR
- delete the .iqpnni.checkpoint file before running.

OPTIONS:

**-n <iteration\_count>** set the default number of iterations to *iteration\_count*.

<b>-s &lt;stopping_rule&gt;</b>	either <i>on</i> or <i>off</i> , default is <i>off</i> .
<b>-p &lt;probability&gt;</b>	set the probability of deleting a sequence in the optimization step.
<b>-k &lt;representatives&gt;</b>	set the number of representative leaves.
<b>-w &lt;rate_type&gt;</b>	set the rate heterogeneity type, either <i>uniform</i> , <i>gamma</i> , <i>igamma</i> (invariable sites+gamma distributed rates) or <i>sitespec</i> (site-specific rates).
<b>-m &lt;model&gt;</b>	set the model type for: Nucleotides: HKY85 (default), TN93, GTR. Amino acids: WAG (default), Dayhoff, JTT, VT, REV, Blosum. Protein-coding DNA: GY94, YN98, NY98, CP98, CGTR, CPR.
<b>-u &lt;user_tree&gt;</b>	read the starting tree from <i>user_tree</i> file.
<b>-ni</b>	non-interactive, don't prompt for user option, run directly with the specified options.
<b>-sfc</b>	start from scratch, don't load the check point file.

#### ADVANCED OPTIONS:

<b>-cdm</b>	stop after computing distance matrix.
<b>-ep</b>	stop after estimating paramters.
<b>-nni</b>	stop after nearest neighbor interchange operations.

### 3. Parallel with Message Passing Interface (MPI)

The program can now be run in parallel with MPI. You should download the source code and build it yourself, since it depends on your installed MPI library. See the manual on how to compile the source package.

### 4. Example usage

Run directly with default paramters, do not further prompt for user option:

```
./iqpnni <input_file> -sfc -ni
```

Run the analysis with Tamura-Nei 1993 model of substitution (TN93), gamma rate distribution and ignore the checkpoint:

```
./iqpnni <input_file> -m TN93 -w gamma -sfc
```

Run in parallel with 10 CPUs, 1000 iterations:

```
mpirun -np 10 ./iqpnni <input_file> -n 1000 -sfc
```