Trek: a program to retrieve context-dependent core substitution rate constants (Homo sapiens) for DNA sequences and entire genomes

The TREK methodology is described in detail at http://dx.doi.org/10.1101/024257. The name of the package reflects on the fact that we obtained the **Tr**ansposon **E**xposed **k** rate constants (byr⁻¹), using the genomic *treks* of retrotransposon remnants in the human genome.

Installation

- 1. Install the latest version of R programming language or skip to the next step. Some step-wise instructions on R installation and upgrade can be found here: 1, 2.
- **2.** Launch R from the command line and install the R packages *shiny* (required for the graphical user interface), *doMC*, *foreach* and *itertools* (required for a parallel execution of the program) from within R.

```
$ R
```

```
> install.packages("shiny")
> install.packages("doMC")
> install.packages("foreach")
> install.packages("itertools")
```

3. Download the TREK source code from the github repository. You can also do that via a Linux/Unix/OSX command line, given that git is installed, by typing the following:

```
$ git clone https://github.com/aleksahak/Trek
```

The downloaded folder has the following content:

- lib/ the subfolder containing all the source files,
- TrekGUI/ the subfolder containing the graphical user interface,
- \bullet $\ensuremath{\mathbf{Trek.R}}$ the interfacing R script used to execute Trek from command line.
- **4.** Finally, you need to bit compile the package by going into the **lib**/ subfolder and executing **bitcompile.R** code from within R.

```
$ cd lib/
$ R
```

```
> source("bitcompile.R")
```

This generates a single file, **Trek.lib**, which encapsulates (Trek) and all its dependencies. At this stage, the subfolder **lib**/ can be safely removed. You might, however, want to copy the **test.fasta** file from inside **lib**/, in order to test the TREK installation.

Now, the Trek installation folder should contain:

• Trek.lib - the bit-compiled TREK program,

- TrekGUI/ the subfolder containing the graphical user interface,
- Trek.R the interfacing R script used to execute Trek from command line,

and, if the test sequence file is preserved,

• test.fasta - the example DNA sequence fasta file.

Running Trek from R

TREK can be executed as an R program, either from within R, or from the Linux/Unix/OSX command line through R CMD BATCH or Rscript execution. The latter two options allow the usage of TREK from the scripts written via programming languages other than R.

In R, as exemplified in the **Trek.R** interfacing script, one should load the **Trek.lib** bit-compiled file, then execute TREK via the R function Trek(). The latter accepts four arguments:

- FastaFile the relative or absolute path to the fasta file to analyse,
- OutFile the relative or absolute path to the output file to be saved,
- *MutRates* an argument accepting "sym" and "nosym" options for the strand-symmetrised (recommended) and raw parameter usage for substitution rates,
- nCPU the number of CPUs to be used for the calculation, where the larger values can markedly speed up the mapping process for entire genomes.

Alternatively, the **Trek.R** file can be edited to set the desired arguments, and executed from the command line via R CMD BATCH or Rscript.

Running Trek from a GUI

TREK features a browser-based graphical user interface (GUI), written with Shiny that can be executed locally on as many CPUs as desired. To launch the GUI, enter the **TrekGUI**/ subfolder and double click on **TrekGUI** file. If the file fails to open a browser, make sure that the permissions are correctly set for the file (as executable):

```
$ cd TrekGUI/
$ chmod 700 TrekGUI # May require sudo rights.
```

If double clicking on **TrekGUI** does not launch your browser after the above step, then, most probably, your Rscript utility of R is not installed on the default /usr/bin/Rscript path. To correct the TrekGUI setup, first find out the installed path for Rscript by typing from the command line:

```
$ which Rscript
```

then open the **TrekGUI** executable file via a usual plain text editor and correct the Rscript path stated at the first line.

Now double click on **TrekGUI**. As soon as the browser opens, the rest is self explanatory.

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Questions and bug reports to Aleksandr Sahakyan via [as952 at cam dot ac dot uk].