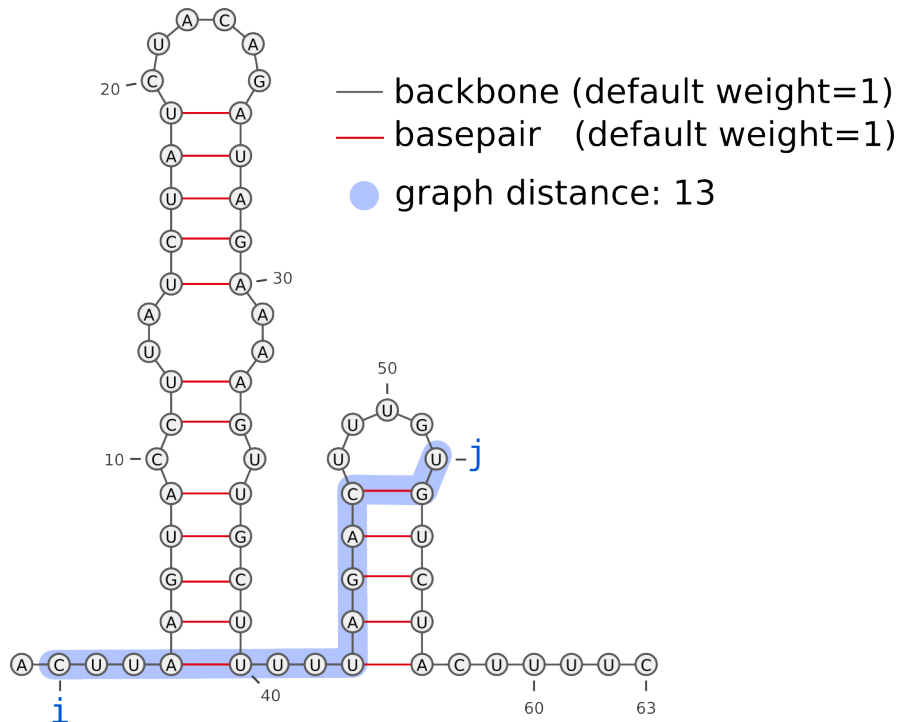


RNAgraphdist v.1.0

DESCRIPTION

The RNAgraphdist calculates the equilibrium distribution of graph-distances between arbitrary pair of nucleotides in an RNA molecule. The program reads RNA structures generated from RNAsubopt, calculates their equilibrium distribution and outputs the graph-distances in a tab delimited list or in the terminal.



REQUIREMENTS for full functionality

Please install OPENMP (<http://openmp.org/wp/>) for multicore usage and Gnuplot (<http://www.gnuplot.info/>) for plotting. Both programs are **not** mandatory for RNAgraphdist, but very helpful.

INSTALL

extract RNAgraphdist.tar.gz and type:

```
cd ./RNAgraphdist
make
```

Would you use RNAgraphdist distance with multiple cores type (requires OPENMP <http://openmp.org/wp/>):

```
make 'OPENMP=1'
```

Would you plot your results type (requires Gnuplot <http://www.gnuplot.info/>):

```
make 'GNUPLOT=1'
```

For both options type:

```
make 'OPENMP=1' 'GNUPLOT=1'
```

GENERAL OPTIONS

Usage: RNAgraphdist -f <File> [options]

-f	--file	STRING	Input File
-o	--out	[STRING]	Output File
-i	--start	[INT]	Start position (default=1)
-j	--end	[INT]	End position (default=N, N = constraint length)
-m	--mode	[INT]	0 = static i,j; 1 = running i; 2 = running j; 3 = running i and j (default=0)
-s		[INT]	Weight of backbone (default=1)
-b		[INT]	Weight of basepair (default=1)
-t		[INT]	Number of cpu's (default=1)
-p	--plot		Plot results (requires Gnuplot)
-q	--quiet		Silent mode
-h			Print help

To run RNAgraphdist you need a list of folding constraints generated from RNAsubopt -p (requires ViennaRNA Package 2.0 <http://www.tbi.univie.ac.at/~ronny/RNA/vrna2.html>):

>Example

> Example [100]

```

.....((((((.((((.(((((((.....)))))).)))..((((.....)))))).....
.....((((((.((((.(((((((.....)))))).)))..((((.....)))))).....
.....((..(((.(((((((.....)))))).)))..)).....((.....)).....

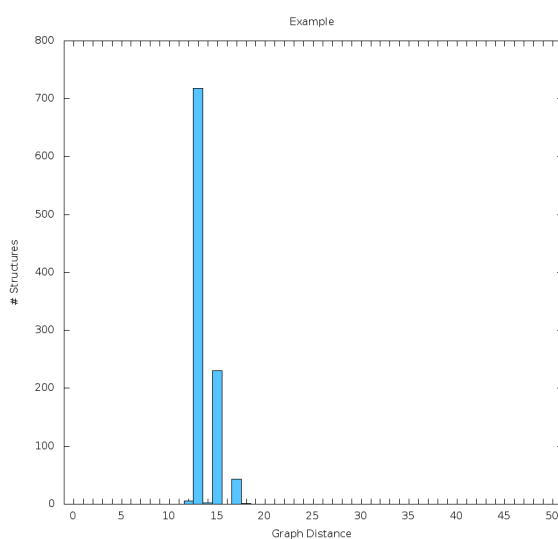
```

In RNAgraphdist you can choose between four modes. All modes return 2 files (and a plot)¹. The *.plot file contains a tab delimited list with the results, the *.gp file contains a executable Gnuplot file to plot the results.

You can calculate the shortest distance between:

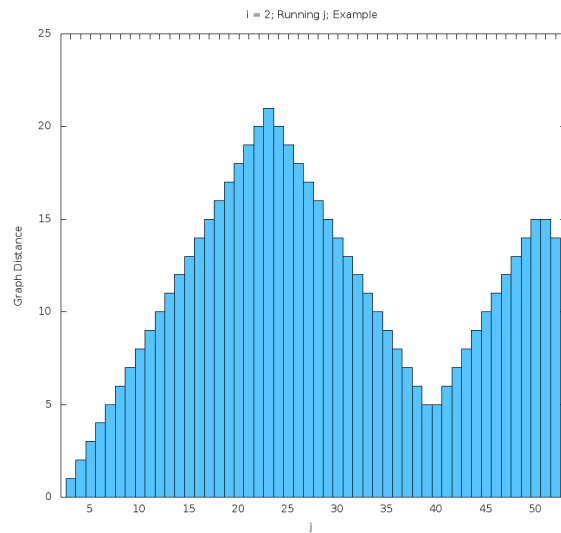
1. the start position *i* and the end position *j* [mode 0]

=> returns the mean, standard deviation and distribution of the graph distance between *i* and *j*. (and the resulting plot)¹



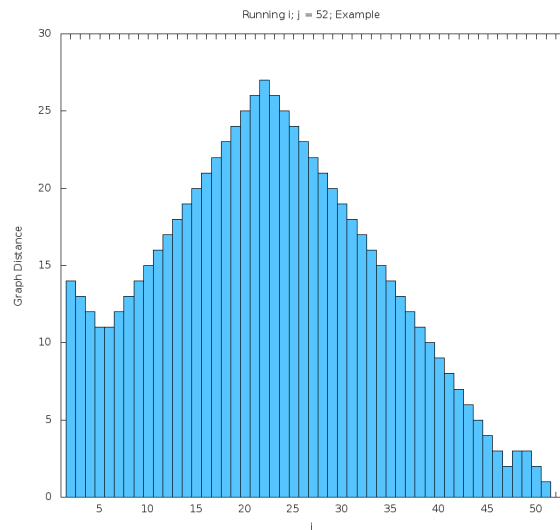
2. the start position *i* to all end positions *t* ($i+1 \leq t \leq j$) [mode 2]

=> returns a list of results for each *t* (and the resulting plot)¹



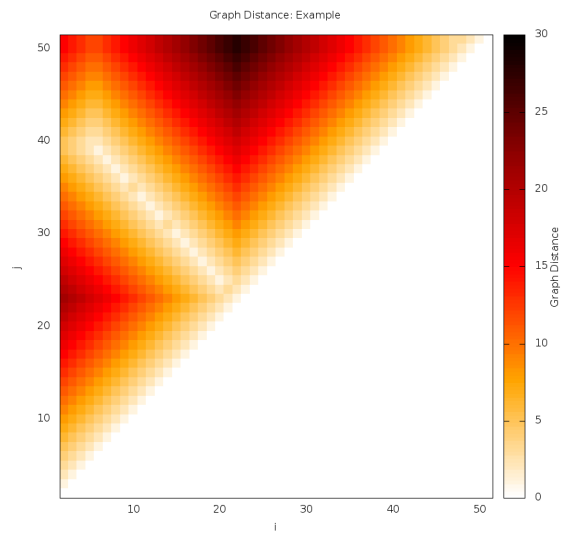
3. all start positions k ($i \leq k \leq j-1$) to the end position j [mode 1]

=> returns a list of results for each k (and the resulting plot)¹



4. all start positions k ($i \leq k \leq j-1$) to all end positions t ($i+1 \leq t \leq j$) [mode 3]

=> returns a list of results for each combination kt (and the resulting plot)¹



¹ if you have used the gnuplot compiling option and the `-p` option

EXAMPLE

```
cd ./RNAgraphdist
./RNAgraphdist -f sample.fold -i 2 -j 52 -m 1
```

HOW TO CREATE INPUT FILES (requires ViennaRNA Package 2.0)

```
cd ./RNAgraphdist
RNAsubopt -p 1000 < sample.fa > sample.fold
```