de.NBI and its Galaxy interface for RNA folding

Jörg Fallmann, Jan Engelhardt

Institute for Bioinformatics University of Leipzig

September 28, 2017

You can download the pdfs you will need today here http://www.bioinf.uni-leipzig.de/~fall/RNA_folding_workshoppresentation.pdf http://www.bioinf.uni-leipzig.de/~fall/Exercises.pdf

Goal: Use RNAfold to do a simple structure prediction.

- Upload the file rna.fa into your Galaxy session.
- Start RNAfold with standard parameters
- ► Look into the output

Goal: Use RNAfold to do a structure prediction using the partition function

- ► Start RNAfold using --partfunc
- ► Look into the output

Goal: Use SHAPE-directed RNAfold to do a structure prediction

- Upload the file rna.shape into your Galaxy session.
- ► Start RNAfold using the shape file and --shapeMethod=D
- Look into the output

Goal: Use RNAcofold to predict the cofolding of two sequences.

- Upload the file cofold.txt into your Galaxy session. (Look at it)
- ► Start RNAcofold using cofold.txt with the --partfunc option
- Look at the output.

Goal: Use RNAduplex to predict *only* intermolecular base pairs of two sequences.

- Upload the file duplex.txt into your Galaxy session. (Look at it)
- ► Start RNAduplex using duplex.seq with standard parameter
- Look at the output.

Goal: Use RNAup to test the RNAduplex result.

- Start RNAup using duplex.txt with --include_both
- ▶ Look at the output and compare it with the RNAduplex result.

Bonus exercises:

Use RNAcofold for duplex.seq, as well (you have to edit the file)

Goal: Use RNAalifold to predict the consensus structure

- ▶ Upload the clustal file alifold.aln into your Galaxy session.
- Edit the data type of alifold.aln to 'clustal'
- ► Use RNAalifold with the alifold.aln and --partfunc (Calculate partition function: 1)
- (Download the output) and look at it
- Bonus: Fold the sequences (alifold.fa) individually (RNAfold) and compare the results.

Goal: Use RNAalifold to predict *and visualize* the consensus structure

- ▶ Use RNAalifold with alifold.aln and --color and --aln
- ▶ (Download the output) and look at it

Goal: Use RNAcode to predict coding sequences in a MAF alignment.

- ▶ Upload the file oskar.27way.rnacode.maf into your Galaxy session.
- (Change its data type to maf)
- Use RNAcode with the maf file
- ▶ (Download the output) and look at it

Goal: Use RNAz

- ▶ Upload the file oskar.27way.rnaz.maf into your Galaxy session.
- Use RNAz with the maf file
- ▶ (Download the output) and look at it