```
ronny@bled:/$ more ViennaRNAPackage-2.0
```

More notes about the Vienna RNA Package 2.0

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Changes in the new distribution

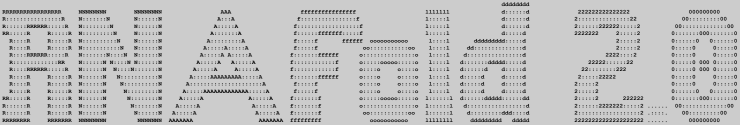
- extended nearest neighbor model (Turner ’04)
- additional energy parameter sets
  (Andronescu ’07, Turner ’99, Mathews DNA)
- FASTA, ClustalW and STOCKHOLM format support
- new programs
  (e.g. RNA2Dfold, RNALfoldz, RNALalifold)
- command line options according to GNU standard
- detailed help

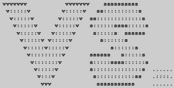
Changes in RNAlib

New

- function and function wrapper design
- algorithms (e.g. findpath, maximum matching)
- utility functions
- OpenMP parallel computation support
- API code documentation with doxygen → reference manual

Performance Measurements





RNAfold 1.8.4
UNAFold 3.8
RNAstructure 5.2

Runtime Performance

Test environment:

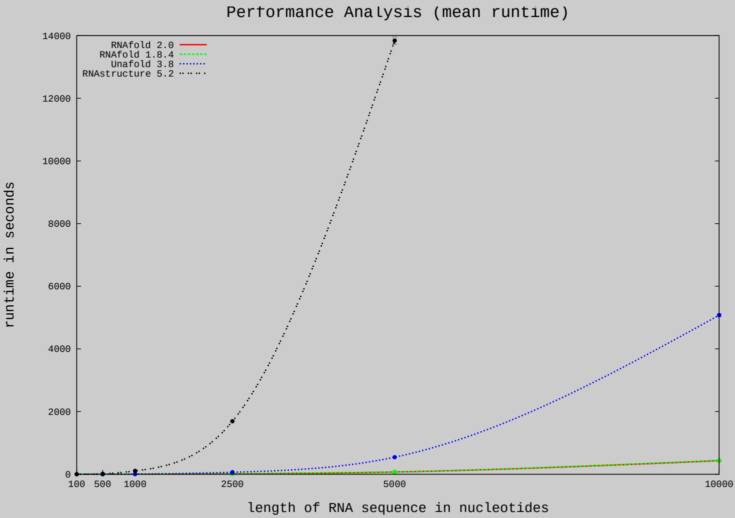
- Random RNA sequences of length:
  100(100)
  500(100)
  1000(100)
  2500(20)
  5000(16)
  10000(16)
- programs run with default parameters
- Intel(R) Core(TM)2 CPU 6600 @ 2.40GHz

Runtime Performance

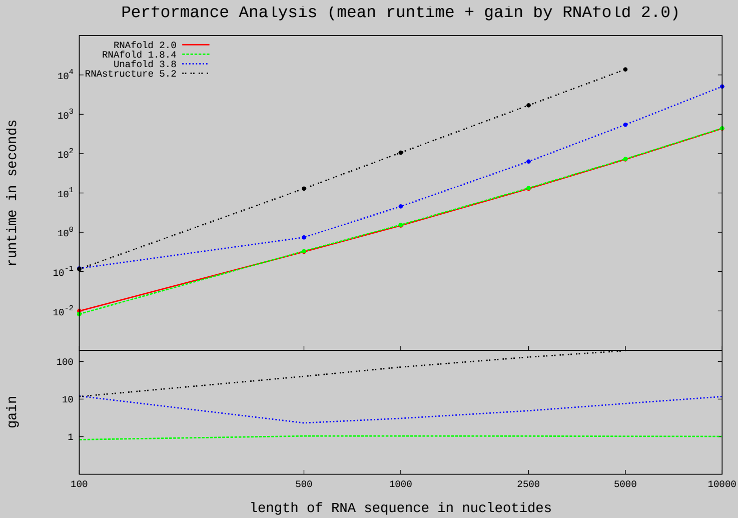
Mean runtimes:

	RNAfold 2.0	**RNAfold 1.8.4**	**UNAFold 3.8**	**RNAstructure 5.2**
100nt	0.01s	0.01s	0.12s	0.117s
500nt	0.32s	0.33s	0.74s	12.89s
1000nt	1.48s	1.54s	4.55s	105.72s
2500nt	12.83s	13.32s	62.96s	1691.32s
5000nt	71.31s	73.15s	543.66s	13842.10s
10000nt	434.10s	441.00s	5076.25s	NA

Runtime Performance



Runtime Performance

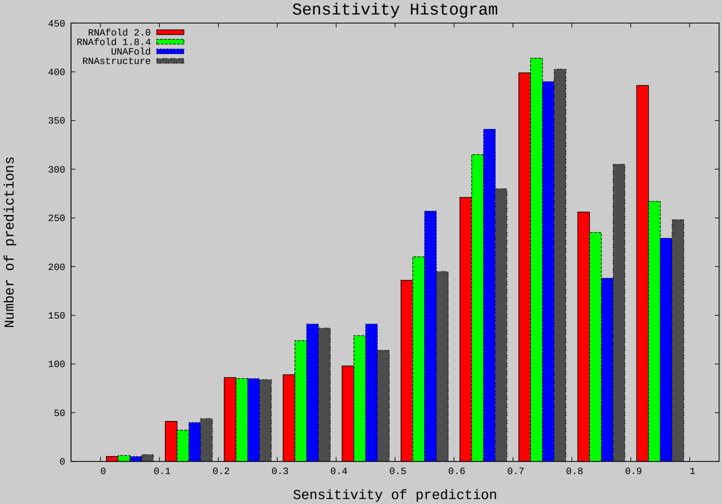


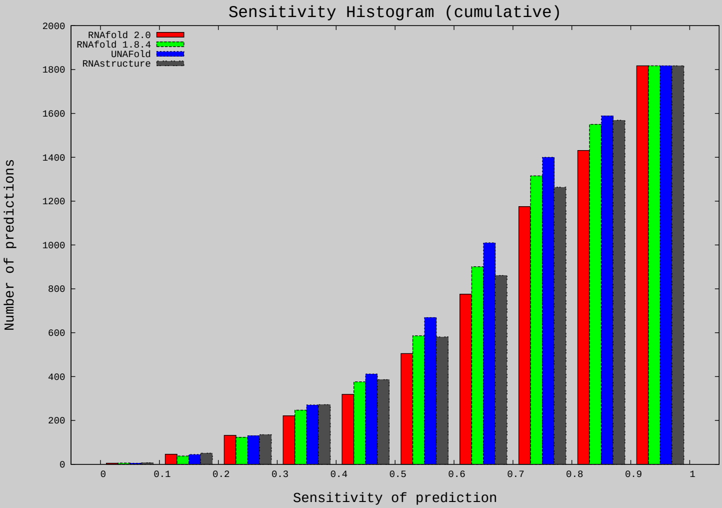
Prediction Performance

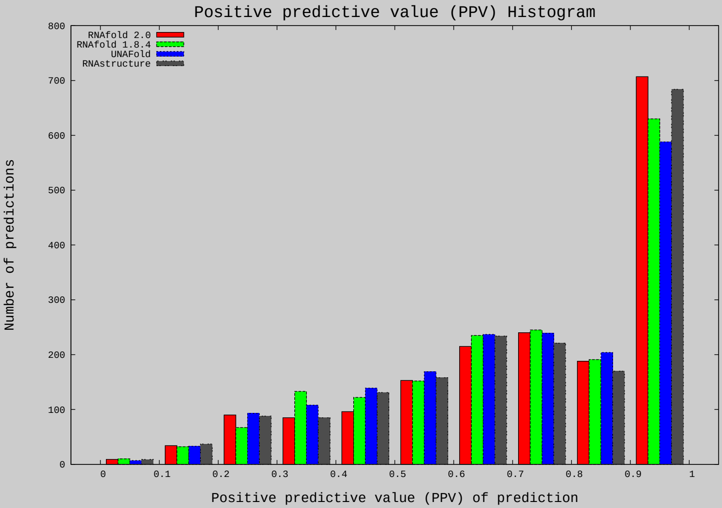
- RNAstrand database test set
- Single RNA sequences w/o pseudoknots
- Non-standard nucleotides substituded by ’N’
- Non-canonical base pairs discarded
- Total: 1817 sequence/structure pairs

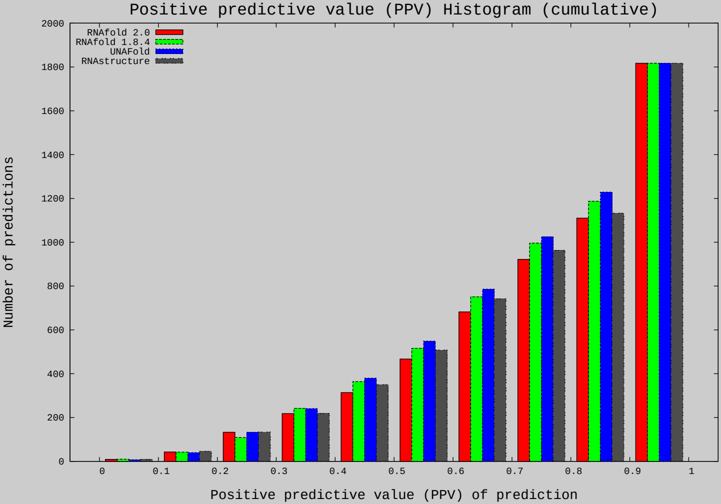
Prediction Performance

Program	**Sensitivity**	**PPV**	**MCC**	**F-measure**
RNAfold 2.0	0.760	0.795	0.776	0.775
RNAfold 1.8.4	0.731	0.776	0.752	0.750
UNAFold 3.8	0.710	0.769	0.737	0.735
RNAstructure 5.2	0.733	0.783	0.756	0.755


Sensitivity Histogram
RNAfold 2.0
RNAfold 1.8.4
UNAFold
RNAstructure
Number of predictions
0
50
100
150
200
250
300
350
400
450
Sensitivity of prediction
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Sensitivity Histogram (cumulative)
RNAfold 2.0
RNAfold 1.8.4
UNAFold
RNAstructure
Number of predictions
0
200
400
600
800
1000
1200
1400
1600
1800
2000
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Sensitivity of prediction


Positive predictive value (PPV) Histogram
RNAfold 2.0
RNAfold 1.8.4
UNAFold
RNAstructure
Number of predictions
0
100
200
300
400
500
600
700
800
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Positive predictive value (PPV) of prediction


Positive predictive value (PPV) Histogram (cumulative)
RNAfold 2.0
RNAfold 1.8.4
UNAFold
RNAstructure
Number of predictions
0
200
400
600
800
1000
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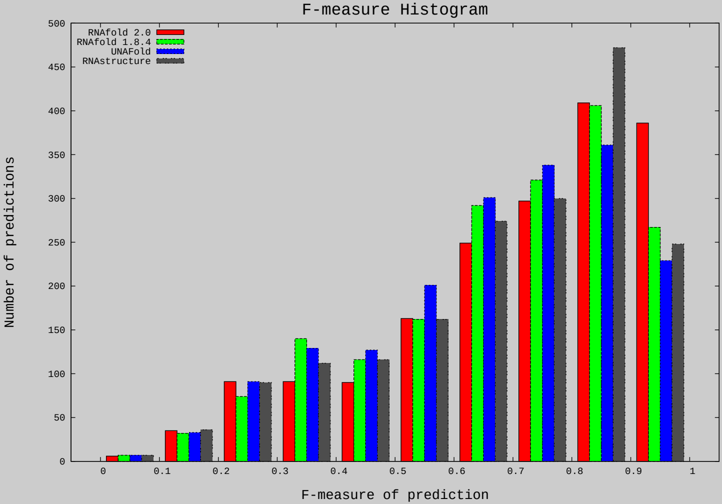
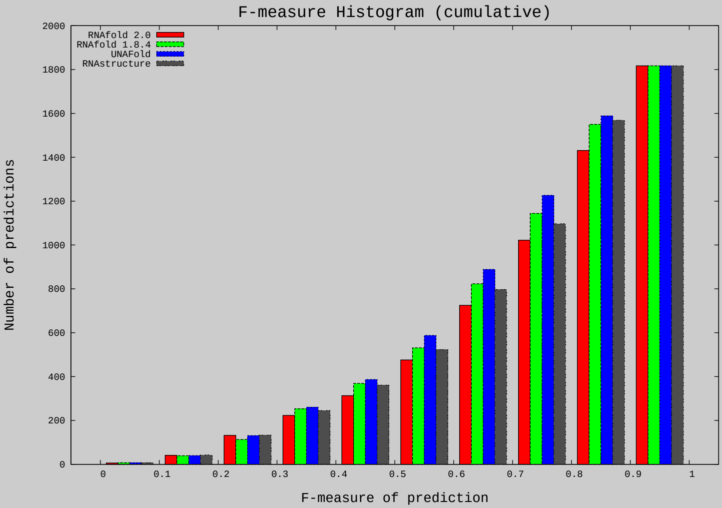
1400
1600
1800
2000
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Positive predictive value (PPV) of prediction


F-measure Histogram
RNAfold 2.0
RNAfold 1.8.4
UNAFold
RNAstructure
Number of predictions
500
450
400
350
300
250
200
150
100
50
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
F-measure of prediction


F-measure Histogram (cumulative)
RNAfold 2.0
RNAfold 1.8.4
UNAFold
RNAstructure
Number of predictions
2000
1800
1600
1400
1200
1000
800
600
400
200
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
F-measure of prediction

Summary

Advantages only!

- Highly accurate predictions
- Very high speed performance
- Perfectly fits into scripting pipelines
- All algorithms available through RNAlib

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Could be even used for games ;)