Kinetic Folder Update

Harry LaBollita

Arizona State University

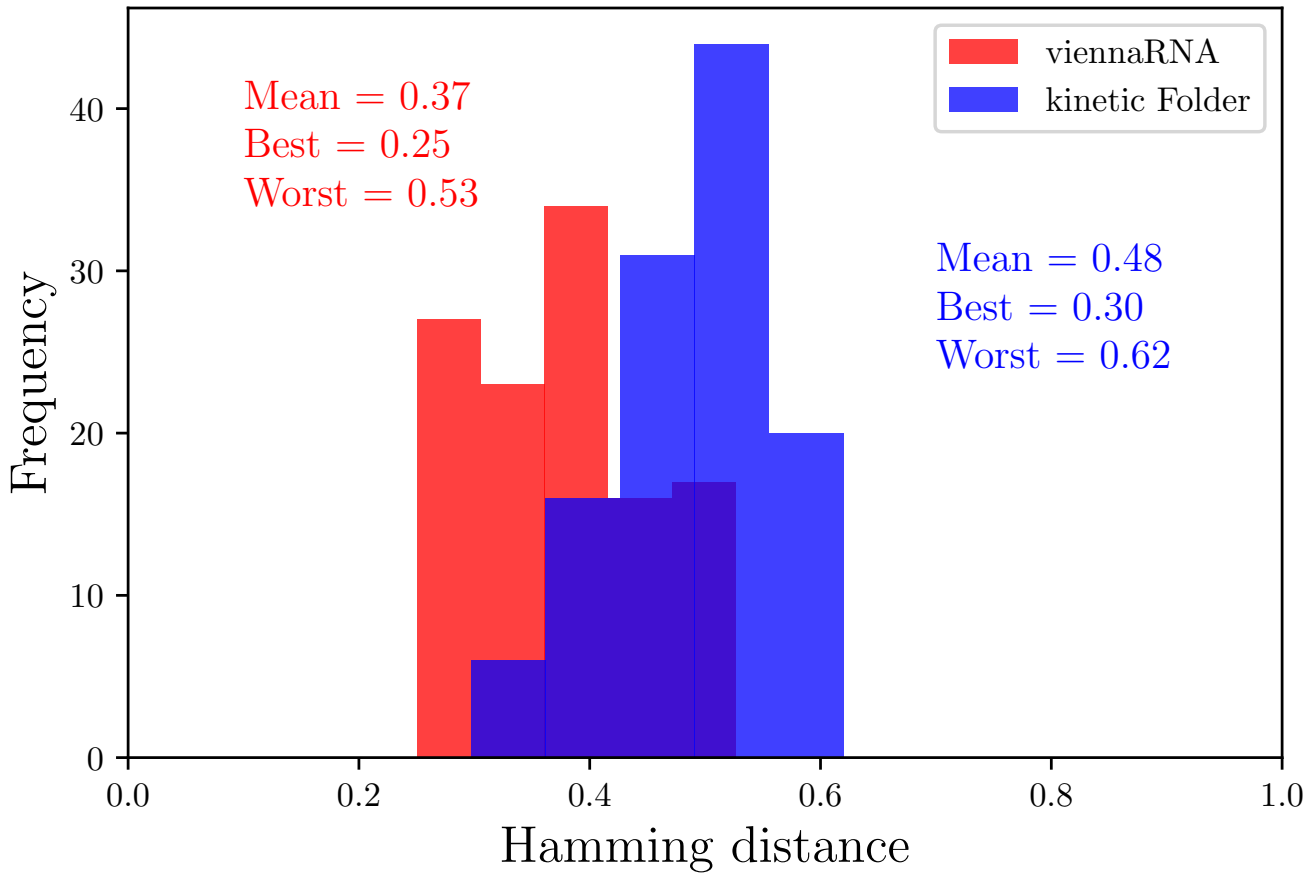
February 12, 2020

"Bad Seq" Dataset

- 117 sequences
- Variable length (max: 80 ntds)

Stats	Kinetic Folder	viennaRNA
Mean	0.48	0.37
Best	0.30	0.25
Worst	0.62	0.53

Results


viennaRNA
kinetic Folder
Mean = 0.37
Best = 0.25
Worst = 0.53
Mean = 0.48
Best = 0.30
Worst = 0.62
Frequency
Hamming distance
0
10
20
30
40
0.0
0.2
0.4
0.6
0.8
1.0

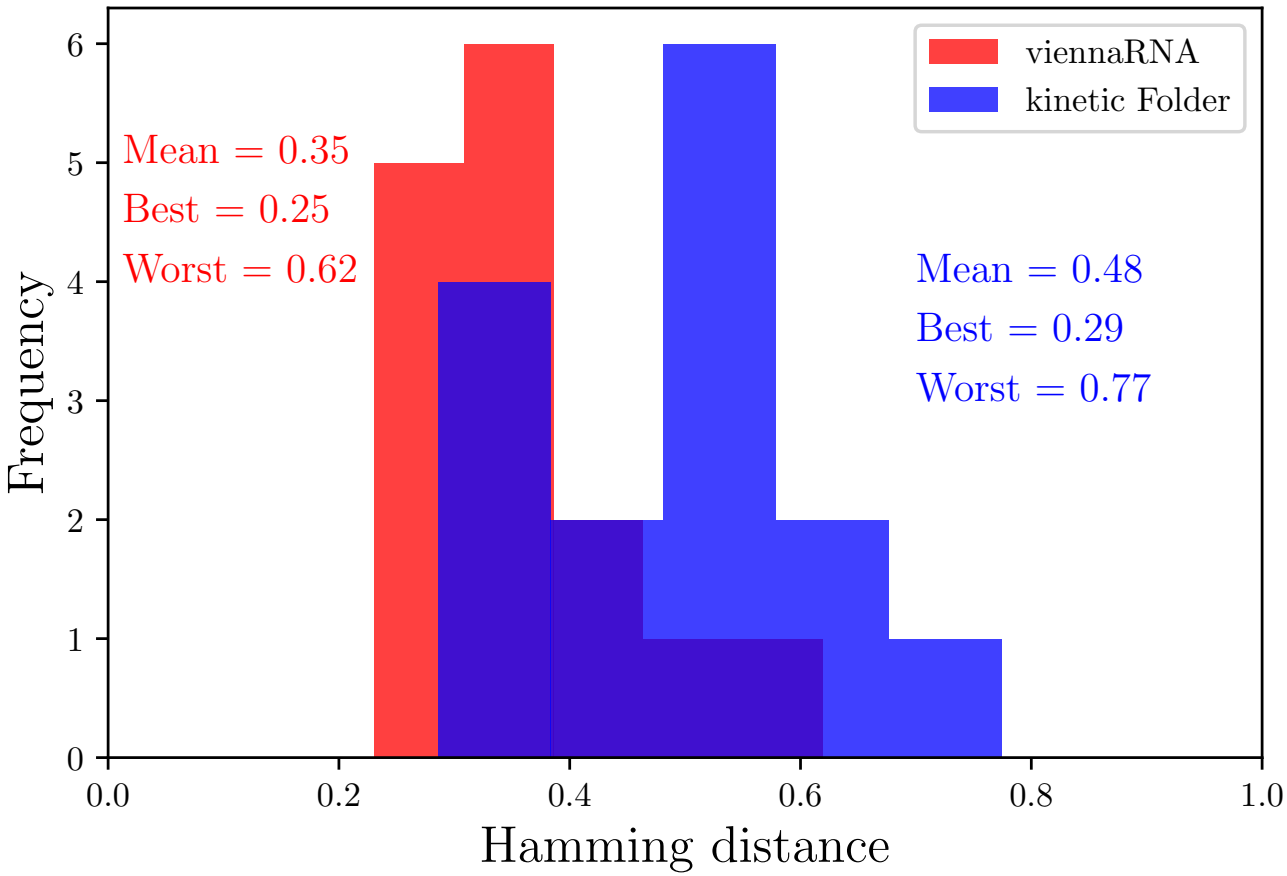
pseudoknotted

- 15 sequences with pseudoknotted secondary structures[1]
- Mean length: 29 ntds

Stats	Kinetic Folder	viennaRNA
Mean	0.48	0.35
Best	0.29	0.25
Worst	0.77	0.62

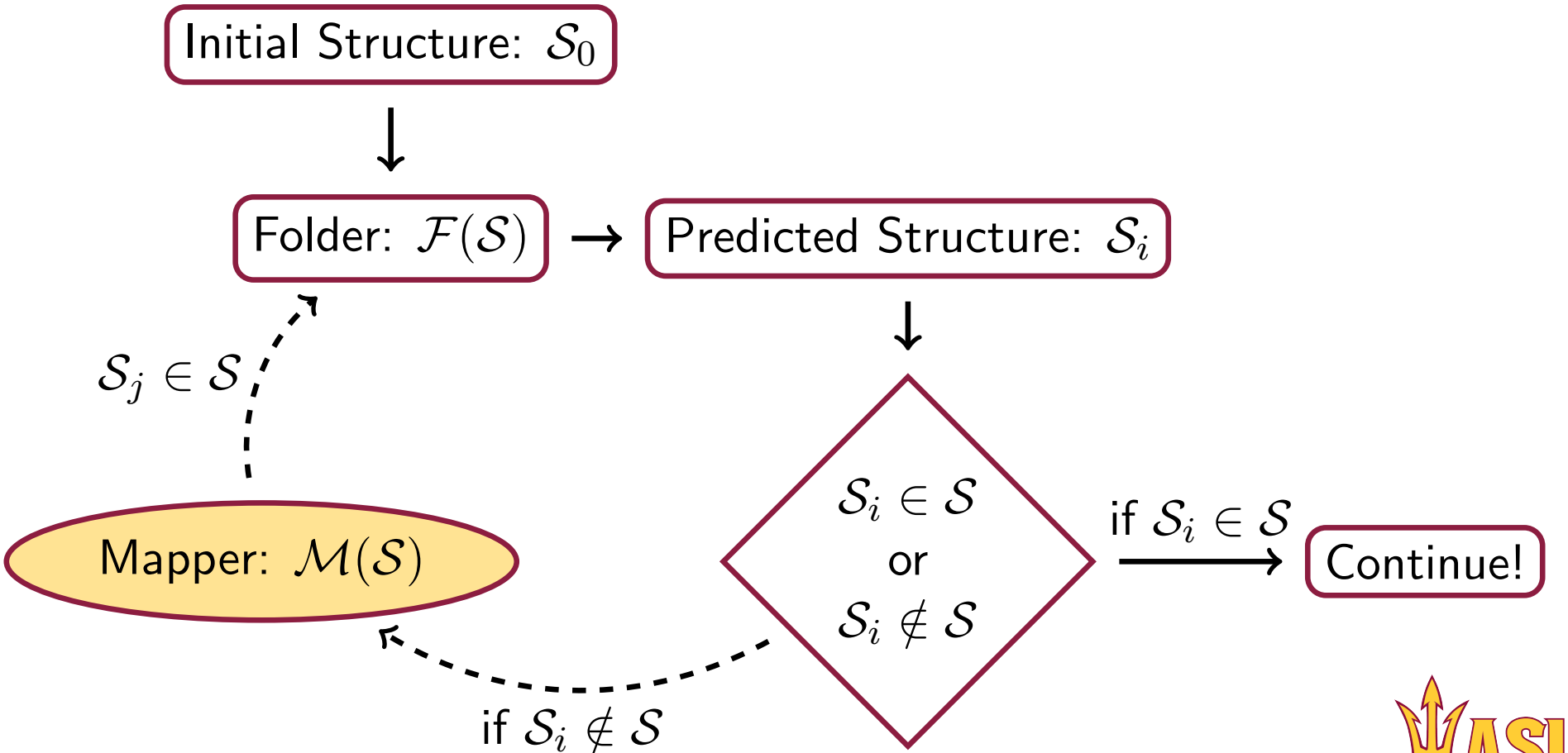
[1] Sequences from Pseudobase++

Results


viennaRNA
kinetic Folder
Mean = 0.35
Best = 0.25
Worst = 0.62
Mean = 0.48
Best = 0.29
Worst = 0.77
Frequency
Hamming distance
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0

Mapping function

A schematic of where the mapping function $\mathcal{M}(\mathcal{S})$ will be implemented in the roll-out algorithm.



Mapping function

Mapping function features:

- Checks that constraints are within the possible move space; if this condition is not met prints error.
- Two mapping features:
  1. Re-run algorithm until constraints are satisfied (Max iterations = 1000).
  2. Find the list of moves that satisfy the constraints enforce these moves to happen.

Note: By enforcing certain moves to exist the move space shrinks to essentially allow one move.

Mapping function

Examples from Folder

Constraints are $\mathcal{C} = [[0, (], [1, (]]$

Correct first try

```
All constraints are within the move space!
+ | [[0, 12], [1, 11], [2, 10]] | (((.......)))).....
+ | [[5, 26], [6, 25], [7, 24]] | (((..[[[..)))......]]]
Structure meets constraints!
```

Mapping function

Examples from Folder

Constraints are $\mathcal{C} = [[0, (], [1, (]]$

Option 1

```
All constraints are within the move space!
Structure fails! Using option 1 to fix!
fixedStructure: ((((((((.......))))))))........
```

Mapping function

Examples from Folder

Constraints are $\mathcal{C} = [[0, (], [1, (]]$

Option 2

```
All constraints are within the move space!
Structure fails! Using option 2 to fix!
ERROR: No structure found using option 2
```