RNA-RNA interaction prediction using seed-extension

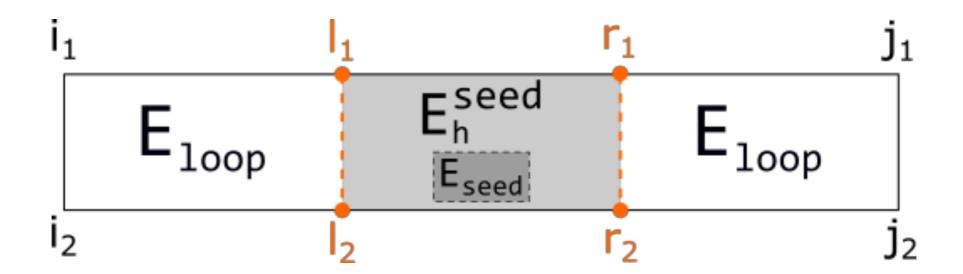
Frank Gelhausen

Motivation

- RNA-RNA interaction prediction computationally expensive
- Idea: compute seed regions and extend interactions starting from seeds to find interaction with minimum energy
- This talk: focus on different seed-extension strategies

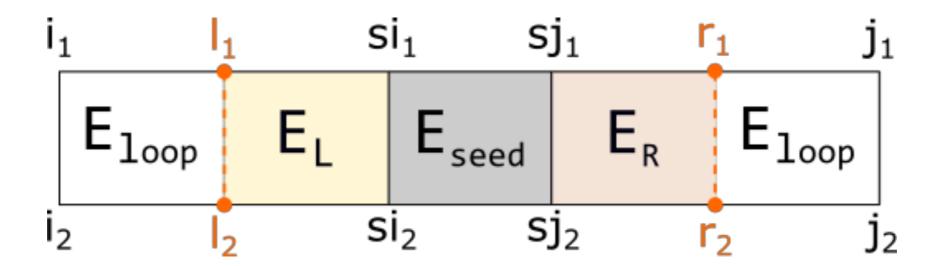
Exact naive method

- O(N⁴) space and time
- Find minimum of all combinations of I₁, I₂, r₁, r₂

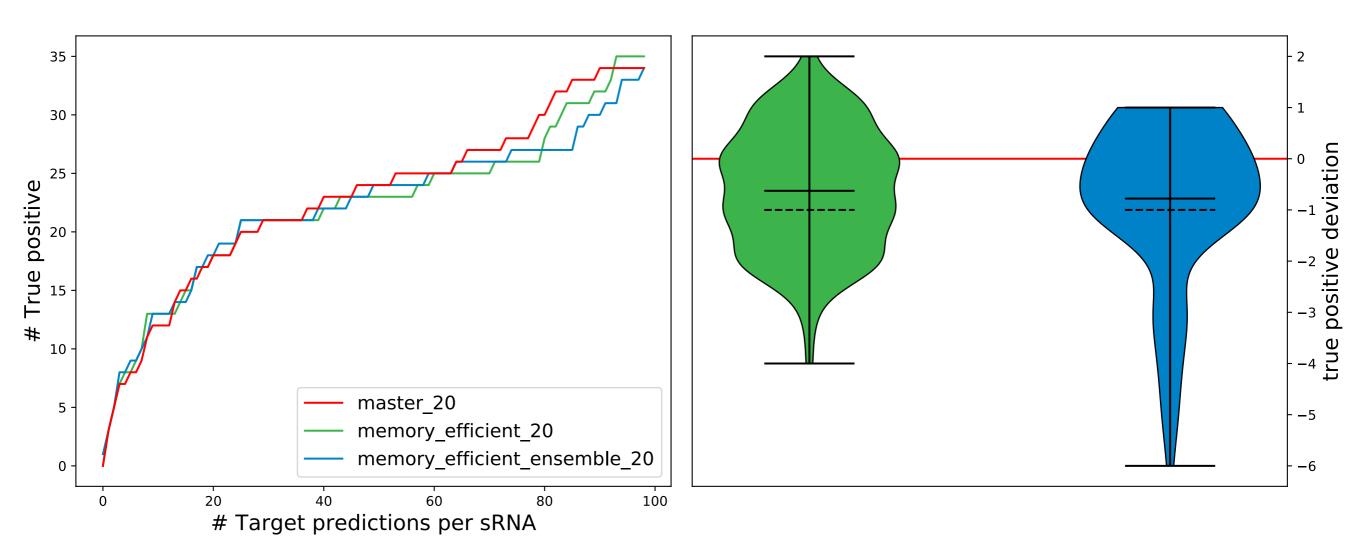


Exact memory efficient method

- O(N²) space and O(N³) time
- Extend to the left (E_L), then to the right (E_R)
- Find minimum of all combinations of E_L and E_R



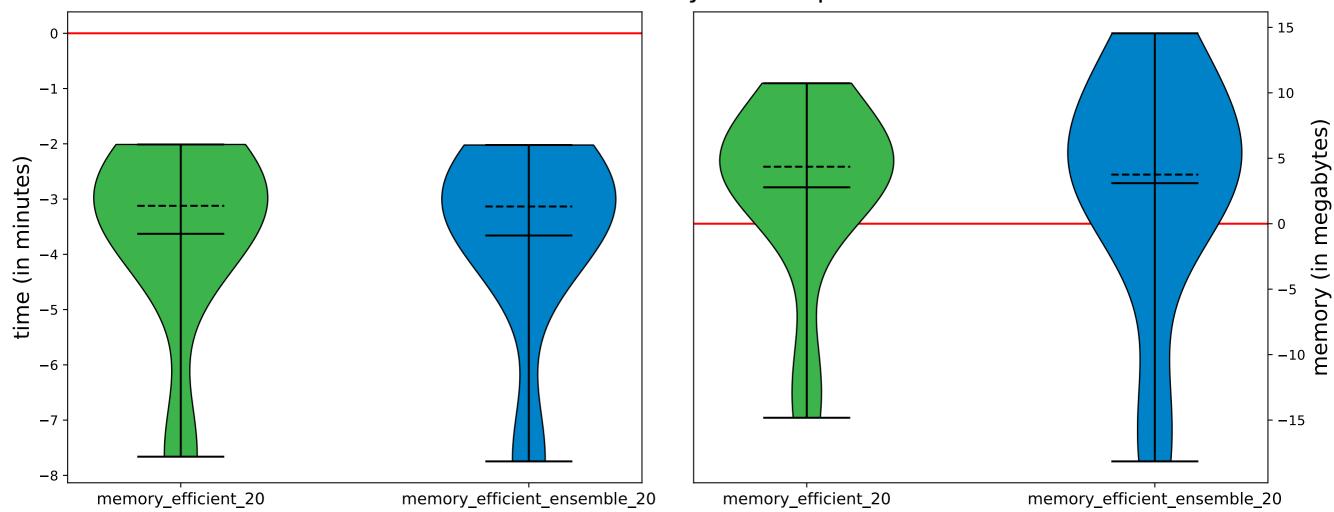
Results



master_20: --qIntLenMax 20 --tIntLenMax 20 --threads 8
memory_efficient_20: -pred X -m M --qIntLenMax 20 --tIntLenMax 20 --threads 8
memory_efficient_ensemble_20: -pred E -m M —qIntLenMax 20 --tIntLenMax 20 --threads 8

Results (time + mem)

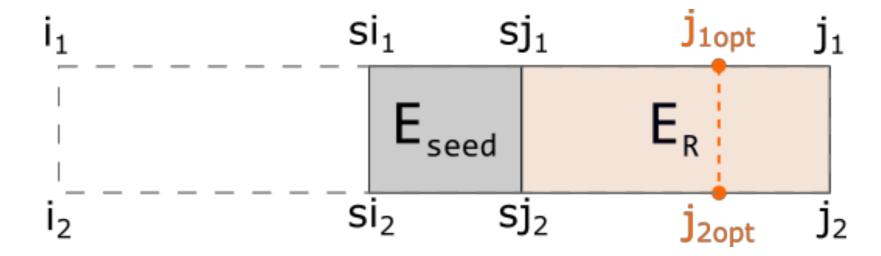
Time and memory consumption



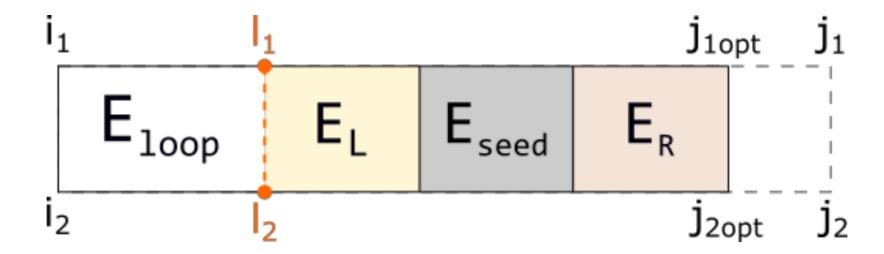
master_20: --qIntLenMax 20 --tIntLenMax 20 --threads 8
memory_efficient_20: -pred X -m M --qIntLenMax 20 --tIntLenMax 20 --threads 8
memory_efficient_ensemble_20: -pred E -m M —qIntLenMax 20 --tIntLenMax 20 --threads 8

Heuristic method

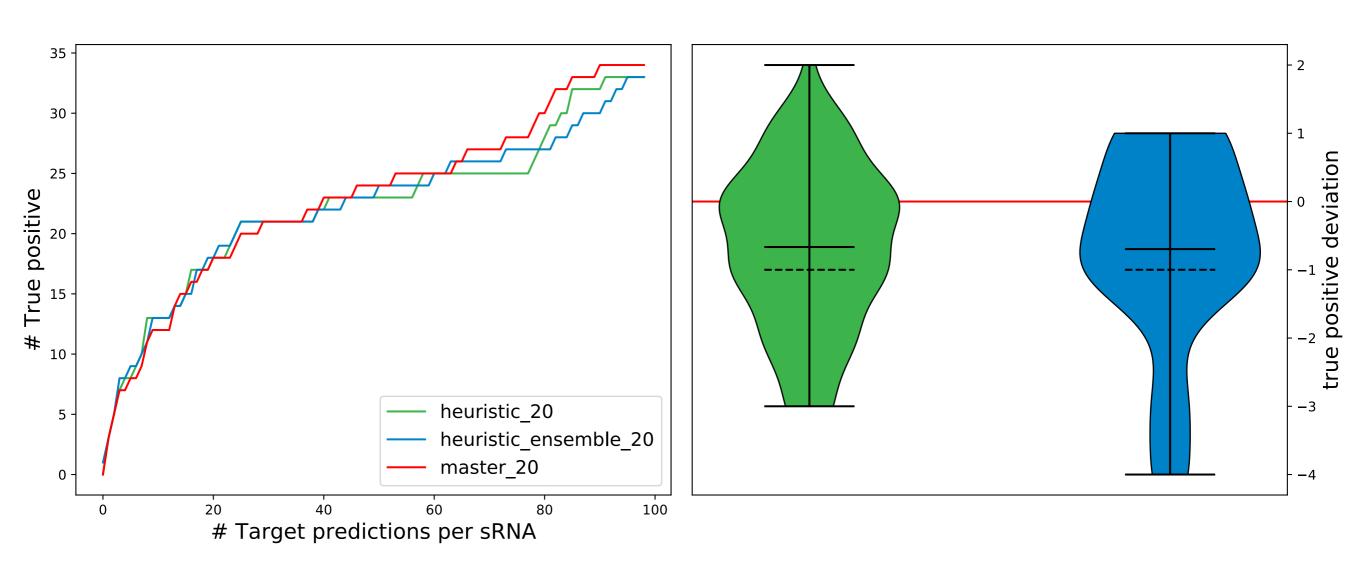
- O(N²) space and O(N²) time
- First find j₁ and j₂ that minimalize E_R



Then minimize over entire interaction up to j_{1opt}, j_{2opt}



Results



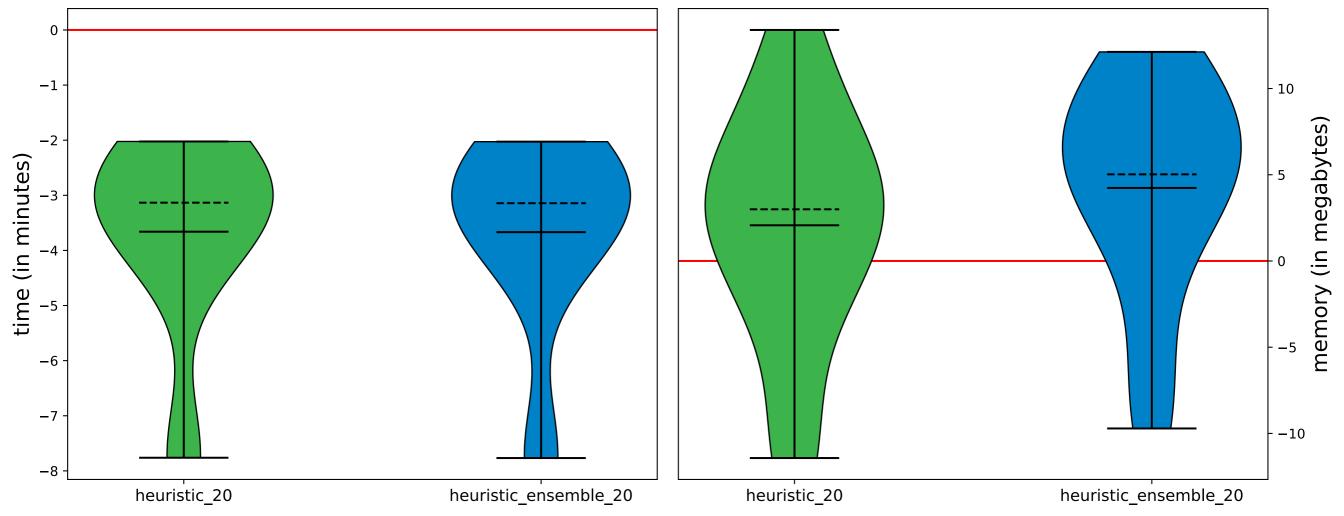
master_20: --qIntLenMax 20 --tIntLenMax 20 --threads 8

heuristic_20: -pred X -m H --qIntLenMax 20 --tIntLenMax 20 --threads 8

heuristic_ensemble_20: -pred E -m H --qIntLenMax 20 --tIntLenMax 20 --threads 8

Results (time + mem)

Time and memory consumption



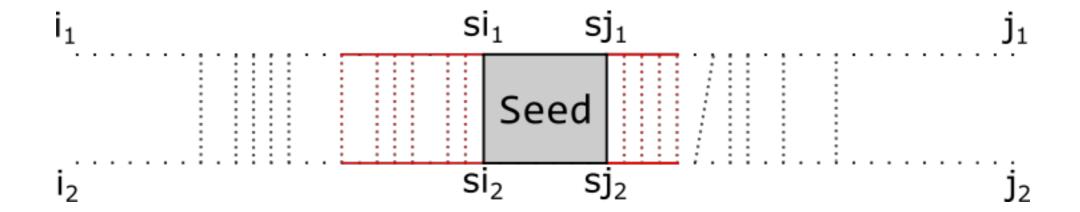
master_20: --qIntLenMax 20 --tIntLenMax 20 --threads 8

heuristic_20: -pred X -m H --qIntLenMax 20 --tIntLenMax 20 --threads 8

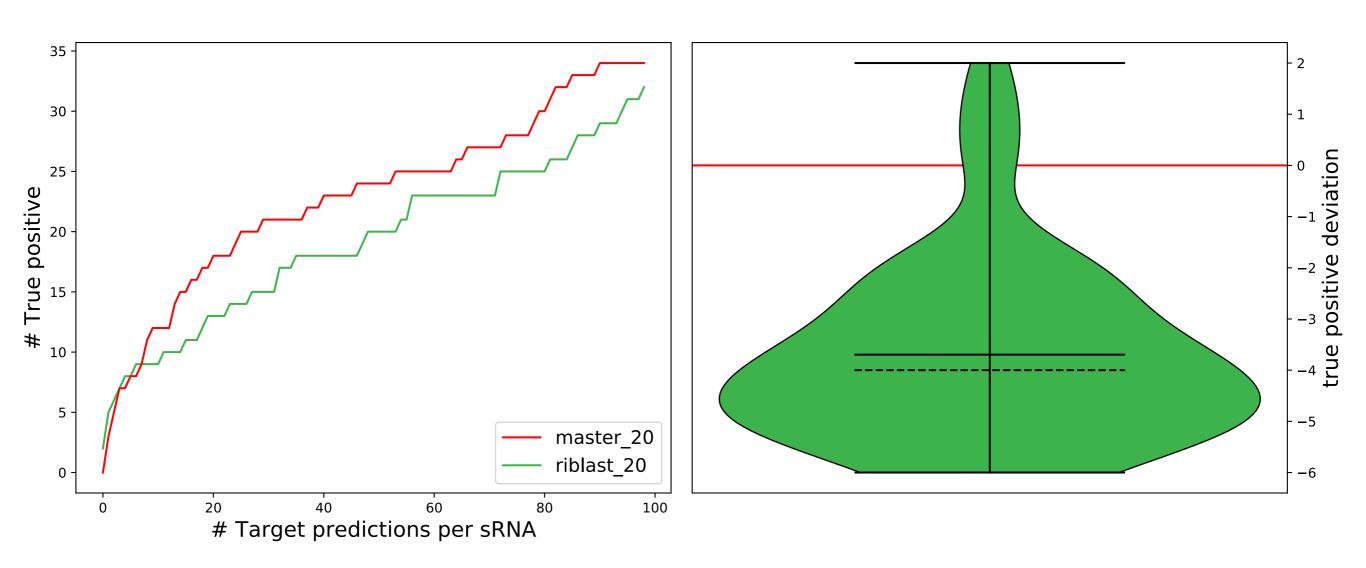
heuristic_ensemble_20: -pred E -m H —qIntLenMax 20 --tIntLenMax 20 --threads 8

Riblast method

- by Fukunaga et al.
- First do a parallel extension, then thorough extension
- Parallel Extension:



Results

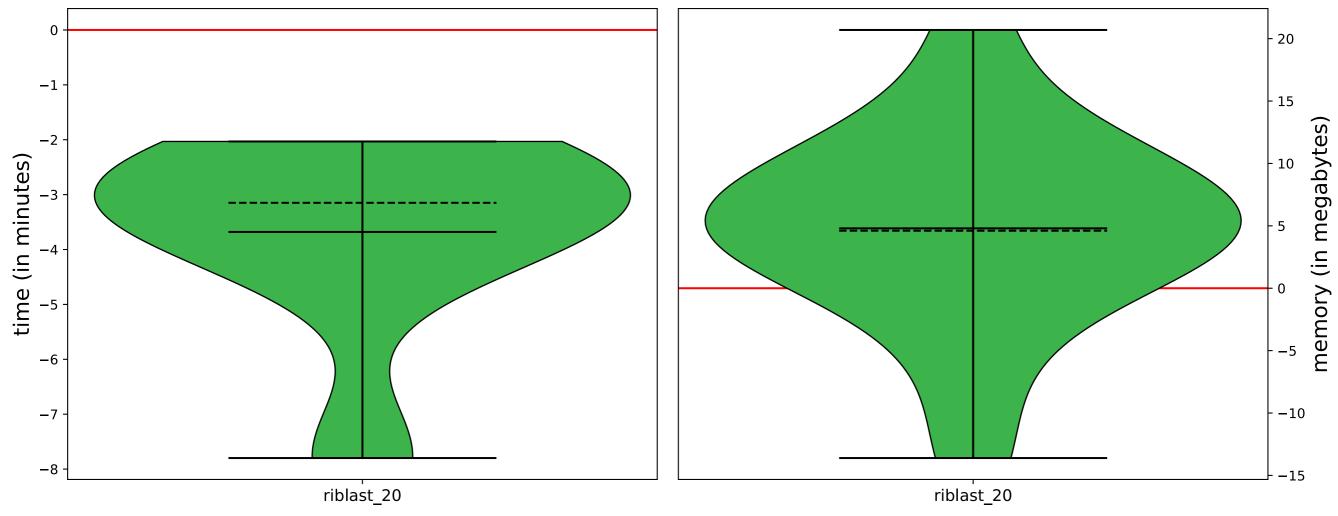


master_20: --qIntLenMax 20 --tIntLenMax 20 --threads 8

riblast_20: -pred X -m R --qIntLenMax 20 --tIntLenMax 20 --threads 8

Results (time + mem)

Time and memory consumption



master_20: --qIntLenMax 20 --tIntLenMax 20 --threads 8
memory_efficient_20: -pred X -m M --qIntLenMax 20 --tIntLenMax 20 --threads 8
memory_efficient_ensemble_20: -pred E -m M--qIntLenMax 20 --tIntLenMax 20 --threads 8

Comparison

Conclusion