Learning parsimonious ensembles for biomedical prediction problems and DREAM challenges

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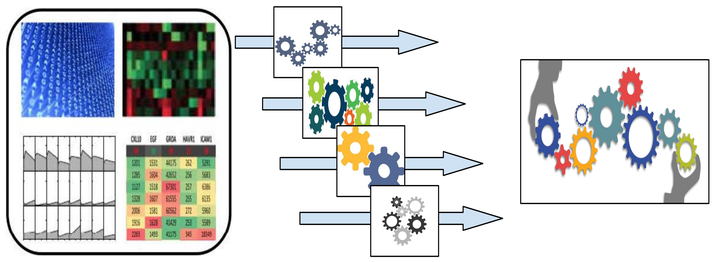
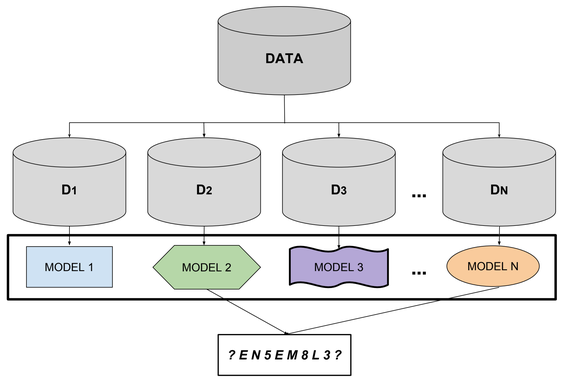
HETEROGENEOUS ENSEMBLES FOR DREAM CHALLENGES:

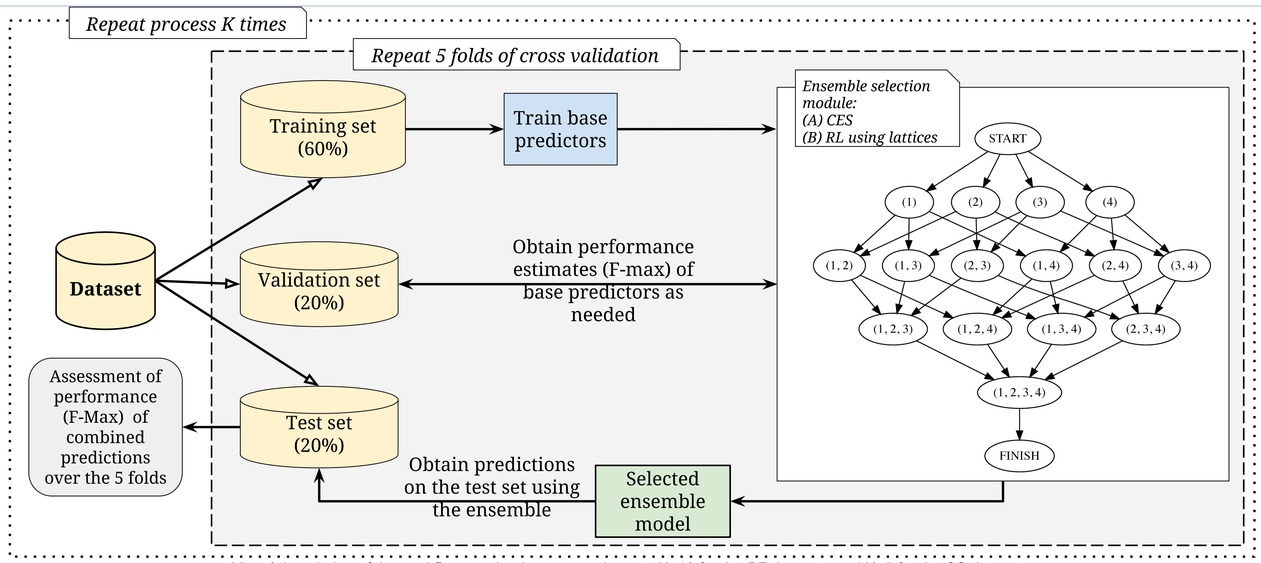
- DREAM challenges are a great mechanism for identifying the most effective solution(s) for challenging biomedical problems.
- Can we improve the (predictive) ability of DREAM challenges by considering the contributions of non-winning submissions/ models also?



- **GOAL**: build **heterogeneous ensembles**
- **Parsimony** of such an ensemble can be of even greater value for DREAM challenges due to enhanced interpretability
- Ensemble Selection(ES)/Pruning is a potential approach for this, but popular algorithms like Caruana's ES (CES) are ad-hoc (sub-optimal) and non-exhaustive

- **IDEA**: A novel ensemble selection approach based on reinforcement learning (RL), which provides a systematic way of exhaustively exploring the many possible combinations of base predictors that can be selected into an ensemble



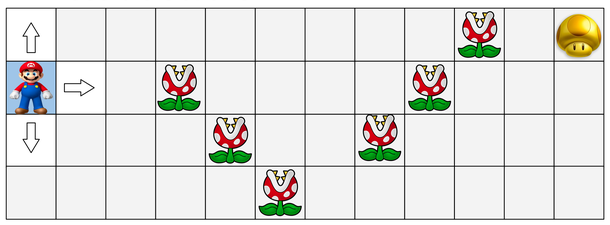


Visual description of the workflow used to in our experiments. K=10 for the PF datasets and K=5 for the SS datasets.

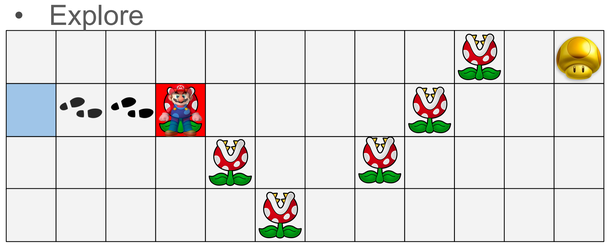
MATERIALS and METHODS:

Reinforcement Learning (RL)

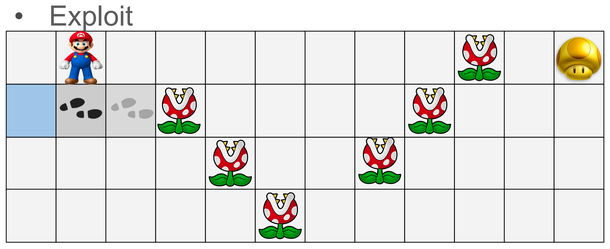
- Possible actions



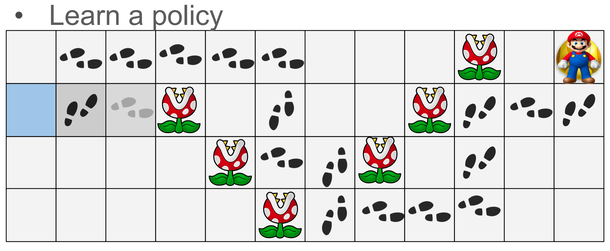
- Explore

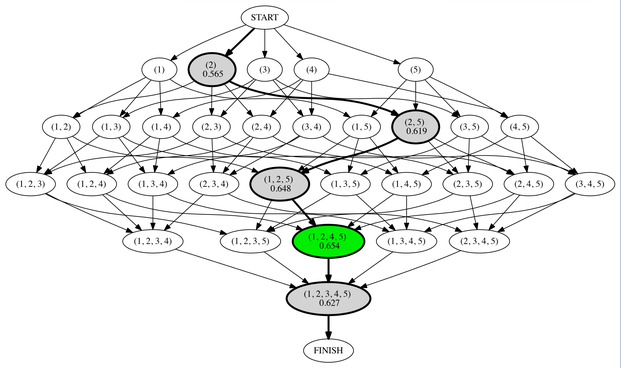


- Exploit



- Learn a policy





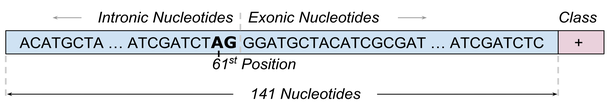
RL Strategies for ES

- **RL_greedy**
  - Reward is given by ensemble performance
- **RL_pessimistic**
  - Reset to start as soon as performance drops
- **RL_backtrack**
  - Go back one position when performance drops

Q-Learning

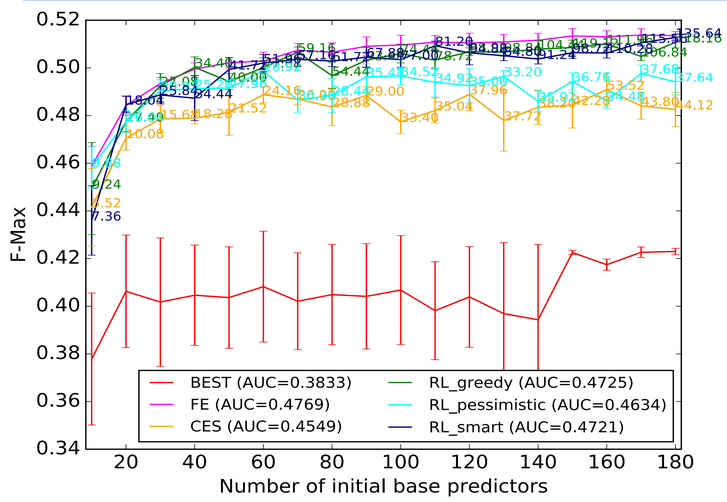
- Algorithm to find an optimal action-selection policy.
- Proven to converge to an optimal solution (i.e. find an optimal action-selection policy) under certain constraints.

Target problem: Splice Site Prediction



Problem	*C. elegans*	*D. melanogaster*	*P. pacificus*	*C. remanei*	*A. thaliana*
#Features	141	141	141	141	141
#Positives	1,598	997	1,596	1,600	1,600
#Negatives	158,150	99,003	156,326	157,542	158,377
Total	159,748	100,000	157,922	159,142	159,977

RESULTS:

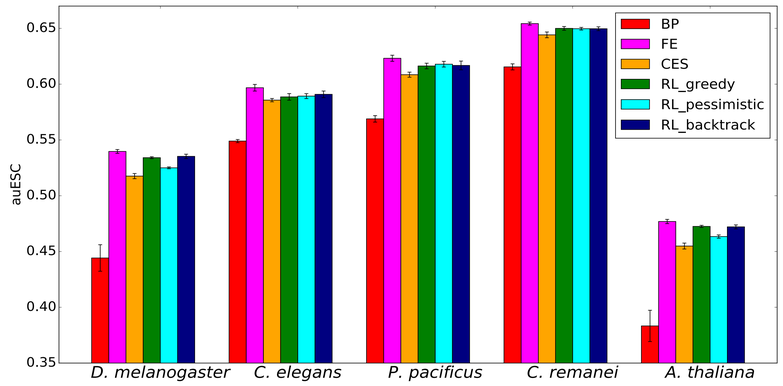


- RL able to better capture predictive performance close to the full ensembles with a much smaller number of base predictors.
  - More capable of achieving this balance than CES, especially for larger datasets.
- The downstream performance or sizes of the RL selected ensembles is not sensitive to RL parameters (*e.g.*, exploitation/exploration probability), showing **robustness to parameters** as compared to other, more ad-hoc ES methods.

A. thaliana	auESC	size_ratio@60	size_ratio@120	size_ratio@180	perf_ratio@60	per_ratio@120	perf_ratio@180
BP	0.3833	0.0167	0.0083	0.0056	0.8118	0.7912	0.8237
FE	0.4769	1	1	1	1	1	1
CES	0.4549	0.4	0.31	0.24	0.9710	0.9577	0.9379
RL_greedy	0.4725	0.5	0.5	0.51	0.9946	0.9927	0.9945
RL_pessimistic	0.4634	0.48	0.29	0.21	0.9919	0.9649	0.9623
RL_backtrack	0.4721	0.87	0.79	0.75	0.9983	0.9919	0.9985

- **Our approach can help extract more useful knowledge from DREAM challenges by constructing predictive and parsimonious ensembles of the submissions.**
  - Will be applied in the DREAM Respiratory Viral challenge
- **Implementation available:**

https://github.com/GauravPandeyLab/lens



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