EVALUATING POLICY PERFORMANCE IN SCREENING PIPELINES

Filtering Policies and Stage Covariance Structures

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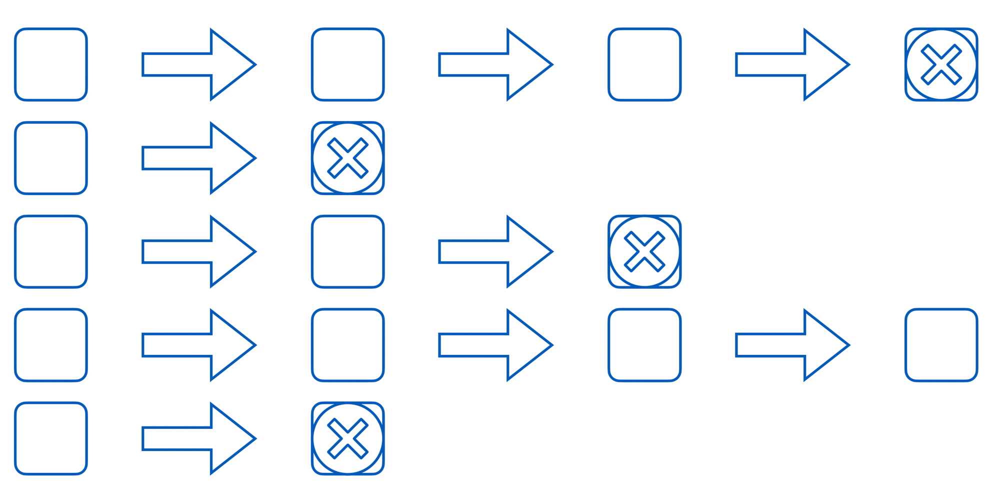
Introduction

The theoretical study of screening pipelines has not been researched much. They are used to take candidates, such as potentially successful drugs or materials, and find the best ones by screening out the others along the way. More specifically, at every stage, each candidate receives a reward, which updates the prior beliefs of the candidates' Gaussian distribution through Bayes' theorem, and then a mathematical filtering policy determines which candidates survive.



Methods

Using Python and SLURM, simulation studies were run with varying hyperparameters such as differing policies. With the simulation data loaded into Python and subsequently split up by policy, the exploratory data analysis covered three main topics.

MAIN TOPICS

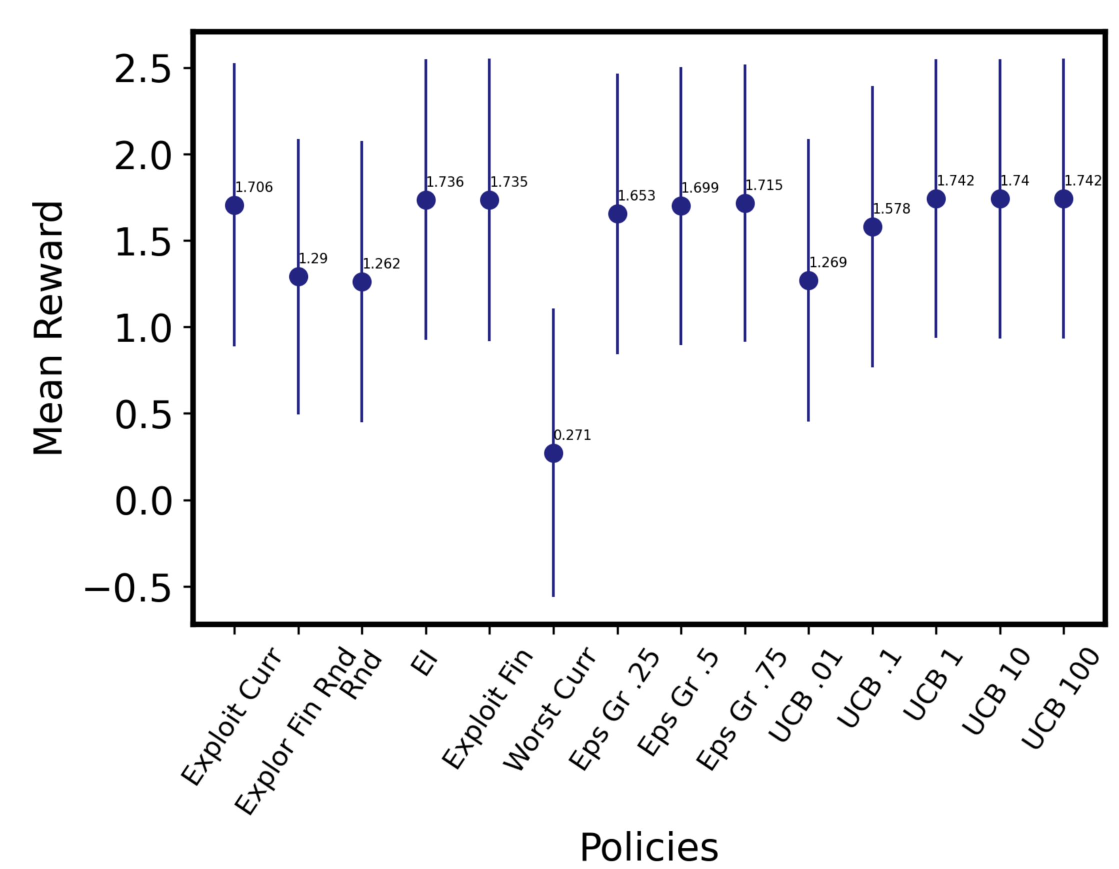
A. Take the average mean and standard deviation for each policy and plot the respective error bars.

B. Compare the reward of each policy to that of the baseline and plot the respective samples in relation to their stage covariance structure.

C. Repeat the first main topic but further divide by each stage covariance structure class.

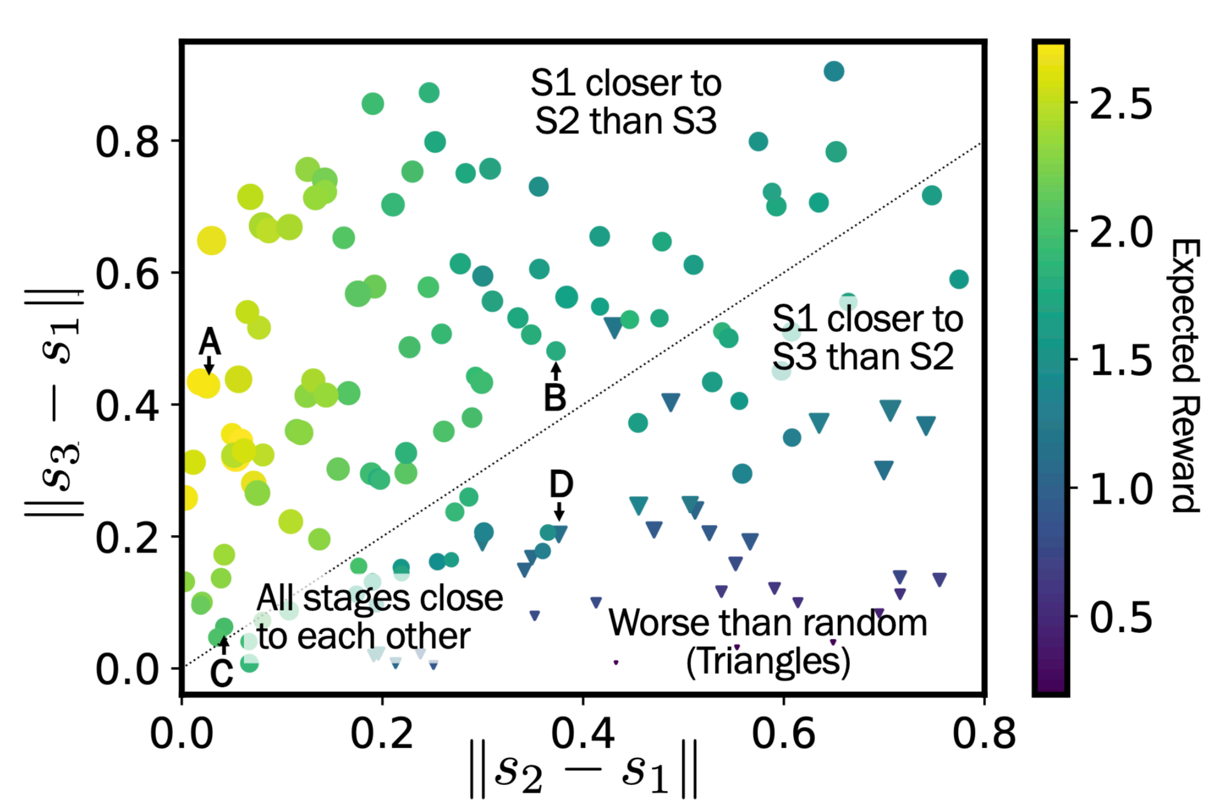
Results

(A) Mean Reward with Standard Deviation for Different Policies



The following policies perform the best: exploitation current stage, EI, exploitation final stage, the higher end of epsilon-greedy, and the higher end of UCB. Moreover, they all seem to have similar standard deviations.

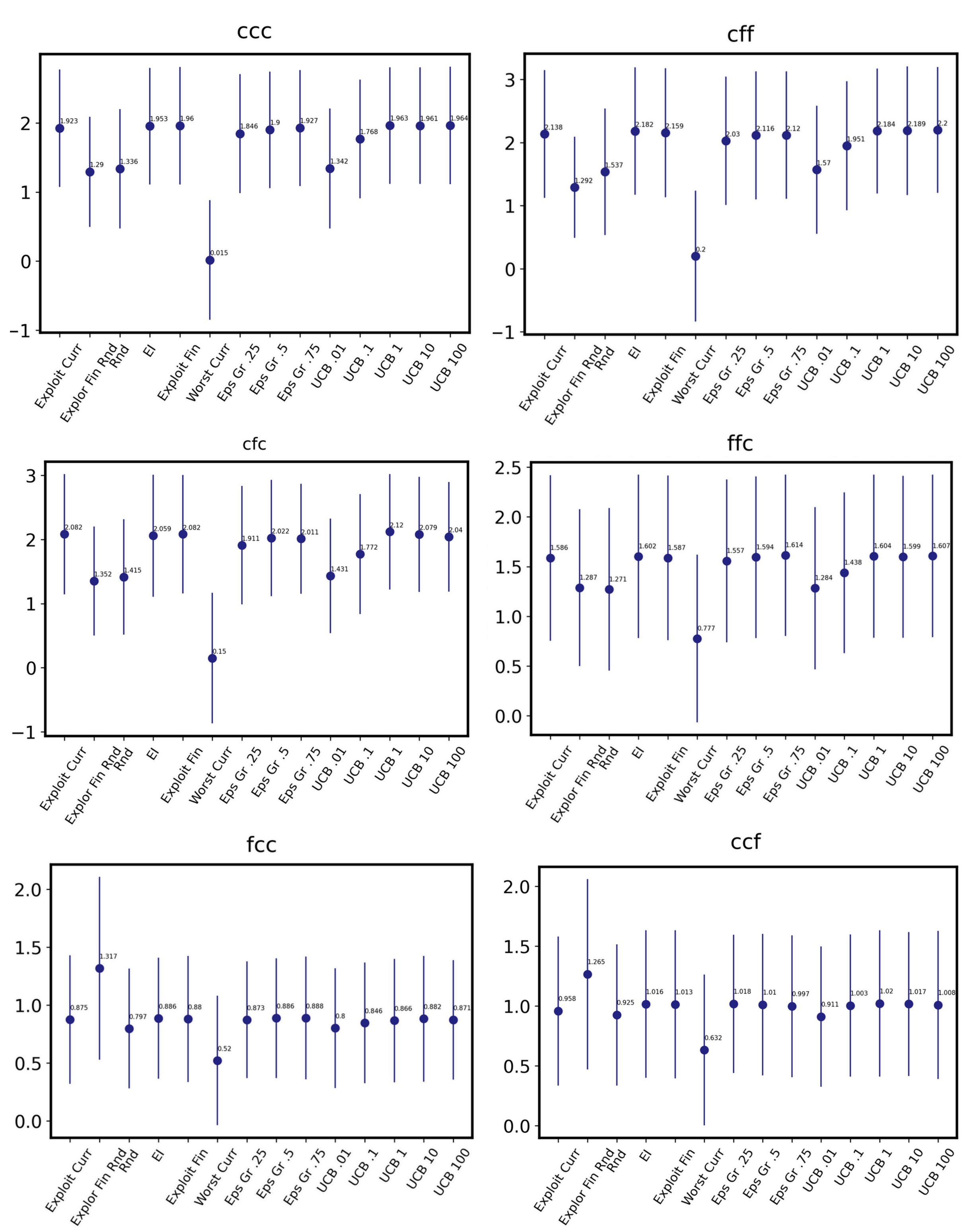
(B) Relative Reward Compared to Baseline



K.G. Reyes et al. (2022), reproduced in this research for other policies

(C) Mean Reward with Standard Deviation for Different Policies, Divided by Stage Covariance Structure Class

Where c means close and f means far, the first letter signifies the relationship between s_1 and s_2, the second signifies s_1 and s_3, and the third s_2 and s_3.



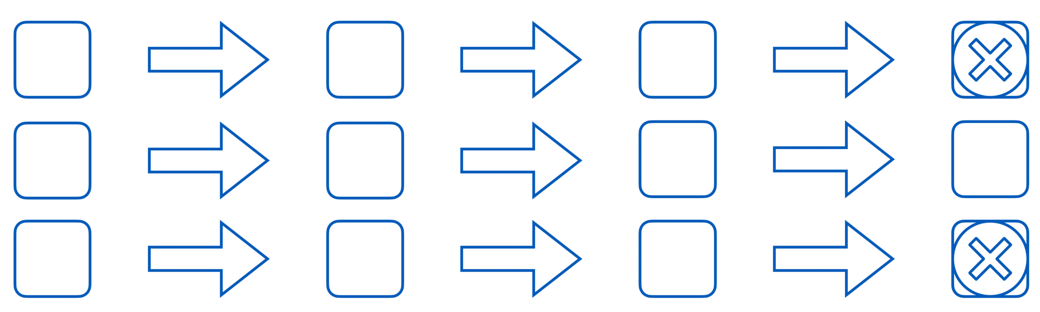
There appear to be only 2 distinct distributions that result from the 6 covariance structures, regardless of sample size.

1. **Distribution 1:** ccc, cfc, cff, ffc. Plot A can also be considered to have this distribution since most samples fall under stage covariance structure classes that belong to this distribution.
2. **Distribution 2:** fcc, ccf. Interestingly enough, in this distribution, the baseline policy performs best.

No sample data for fcf or fff classes.

Discussion & Conclusion

- The baseline performing best for fcc situations explains the presence of triangles at the bottom right corner of plot B. Moreover, with the limited data at hand, it appears that one might use the baseline policy when s_1 and s_3 are close (*c*) except for when they're all close (ccc).
- The low sample size of cfc compared to the other classes seems to not affect it, as it can be still categorized as having distribution 1, which could mean that there is indeed an underlying behavior.
- No fcf or fff samples were used, making them a potential area of research.
- Another potential research idea could be to keep candidates in the pipeline instead of screening them out to maintain covariance structure throughout.



- The baseline and current stage exploitation policies are the ones currently in use; however, there is still much to learn and the aim of this research is to help researchers leverage the known covariance structure by selecting the best screening policy for it.

Acknowledgements & References

1. A special thank you to Professor Kristofer Reyes
2. Supported by NSF Award 1950796
3. K. G. Reyes, Jiaqian Liu, and Carlos Juan Díaz Vargas, "Decision-Making Under Uncertainty for Multi-stage Pipelines: Simulation Studies to Benchmark Screening Strategies," 2022.

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