Pharmahacks 2025
Error 404 Team Name Not Found

Multiple Sequence Alignment

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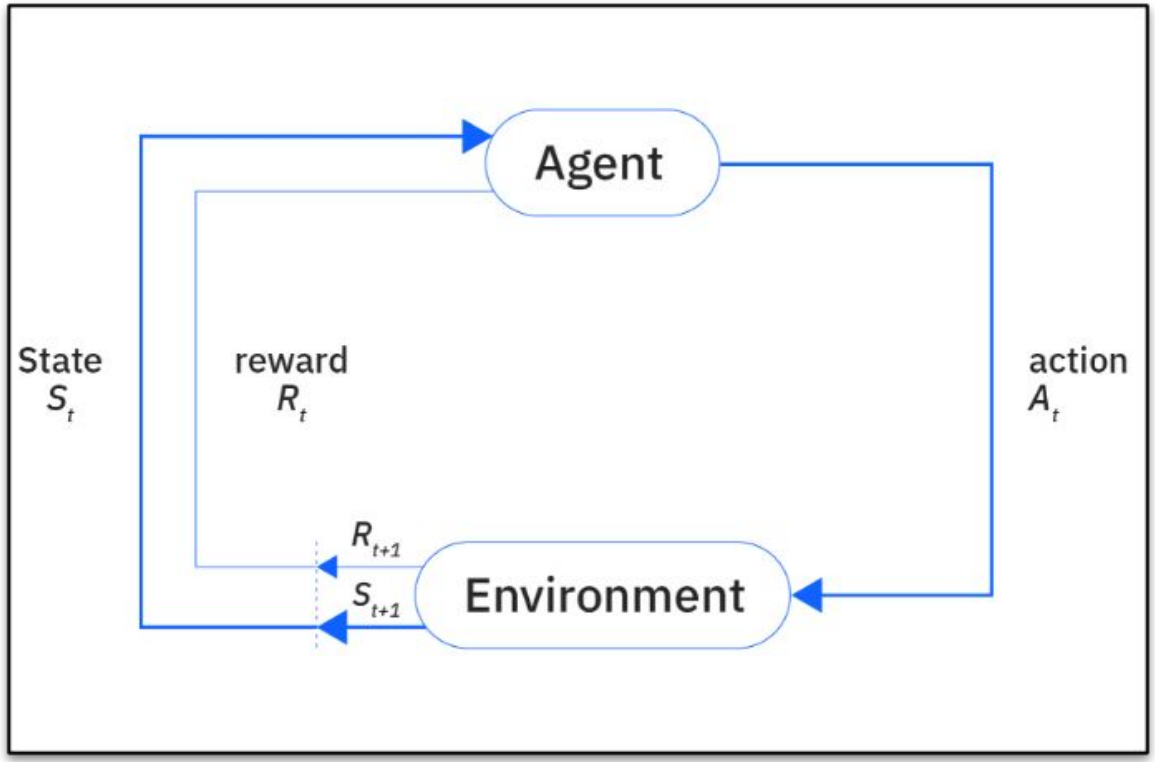
01 Explorations

Reinforcement Learning

Agent: Model
Action: Step
Environment: Sequence Alignment
State: Score calculation for current alignment
Reward:
<u>Positive</u>
Score(New) > Score(Old)
- Step is made

<u>Negative</u>
Score(New) < Score(Old)
- Step is not made
- Model is penalized

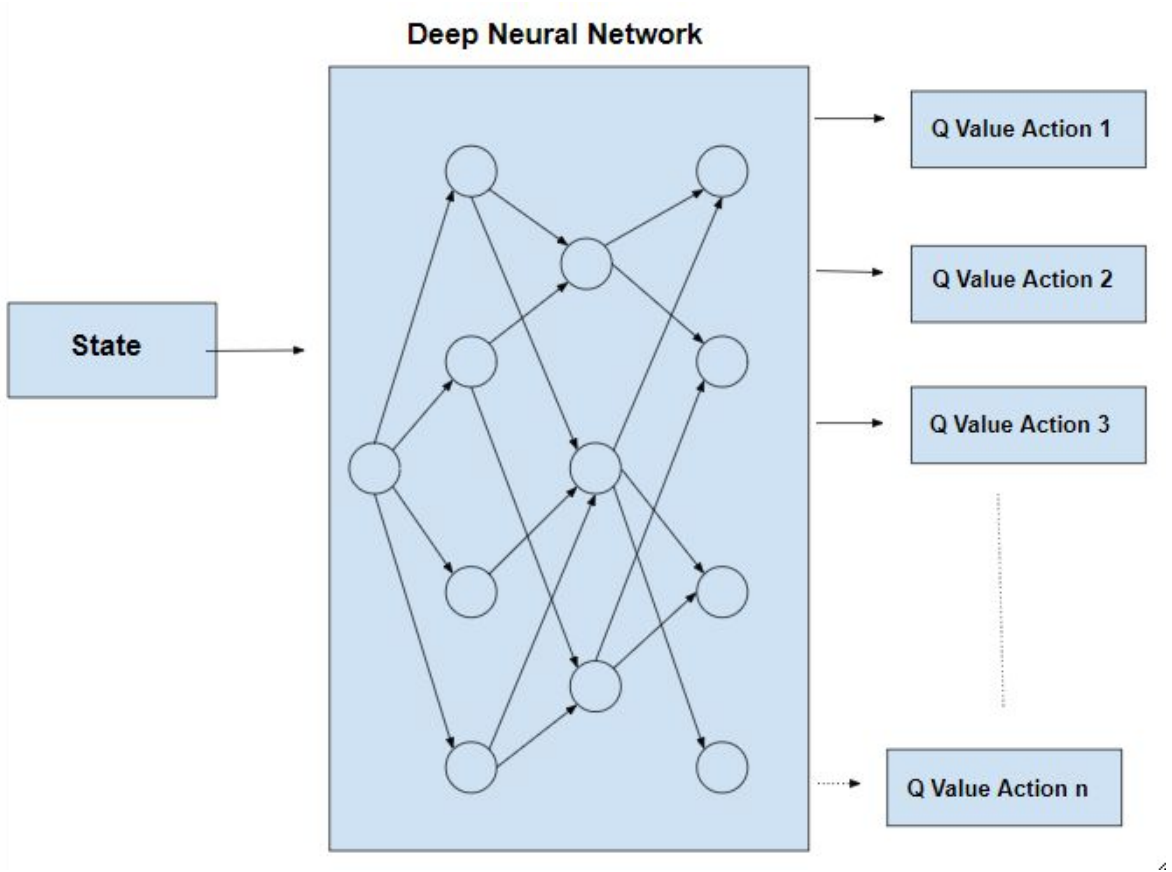


Challenge: Exponential number of possible steps

Model: Deep-Q Learning

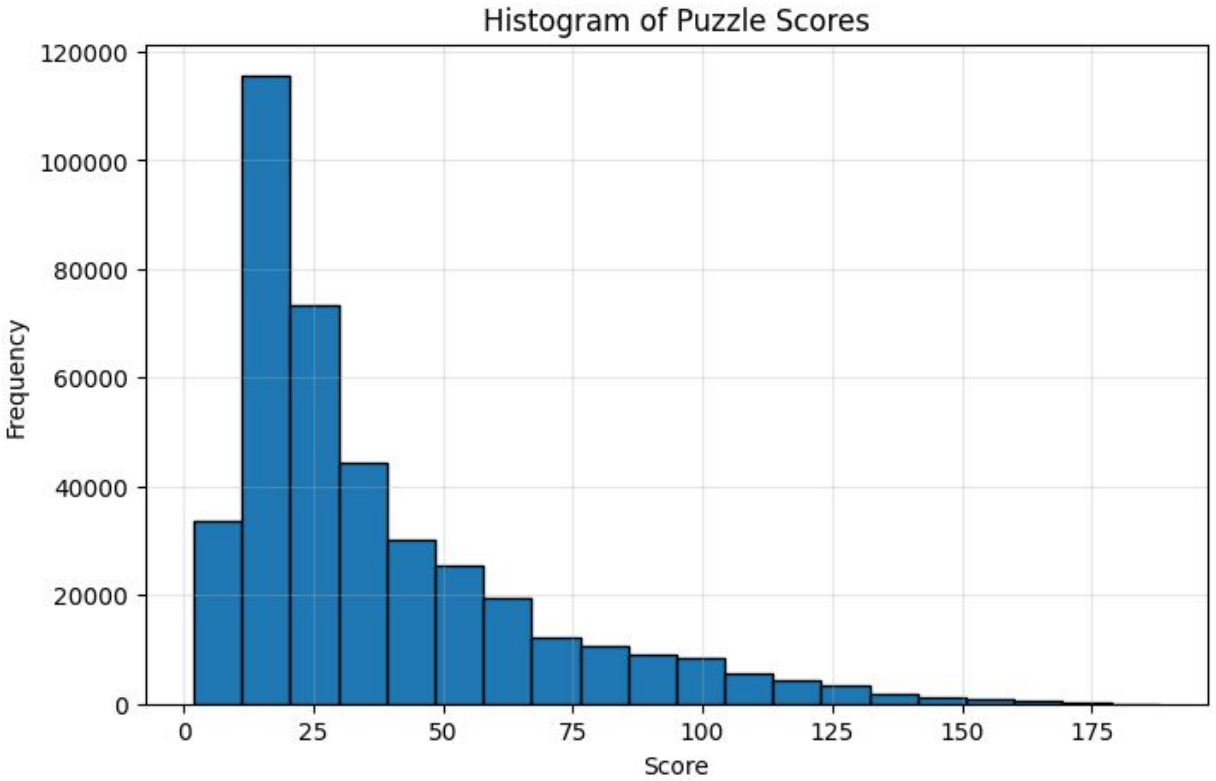
Mathematical approximation of all the possible steps given a state

Neural Network chooses the best action (step)



Source: https://www.geeksforgeeks.org/deep-q-learning/

Visualize Data Spread



Trend's from Top Scorers

No strong trends between number of moves or gameplay time and high scores

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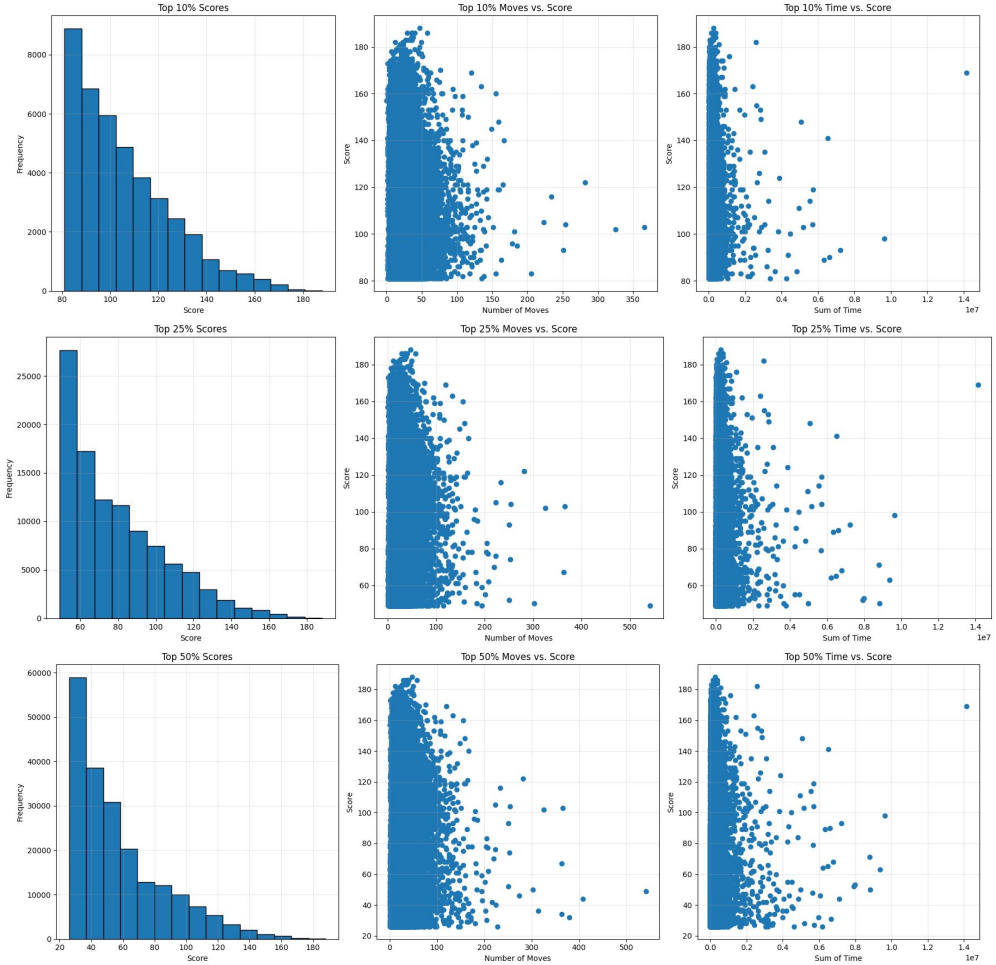


Model Theory

Accepted Pairs

-	C
T	G
G	T
A	C
A	C
A	C
-	T
T	G

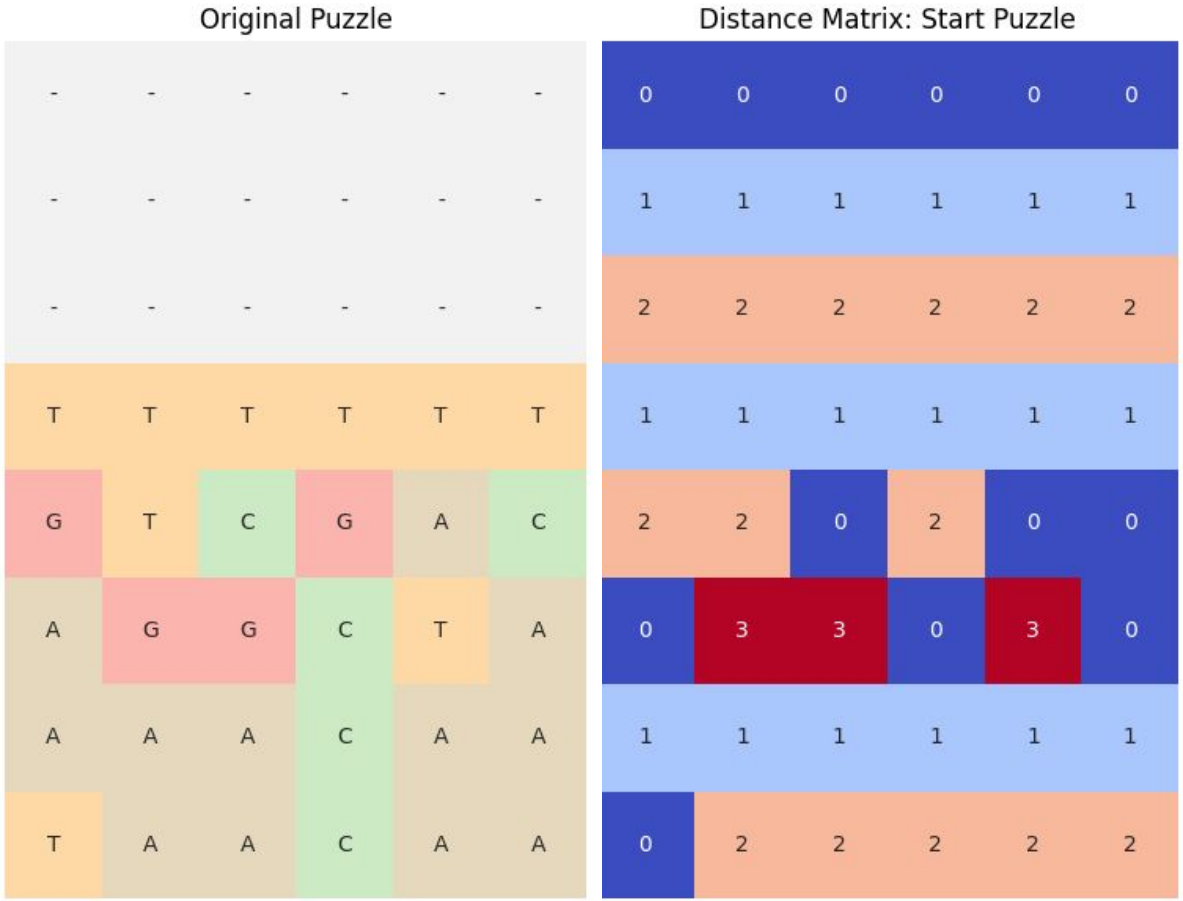
Original Puzzle

-	-	-	-	-	-
-	-	-	-	-	-
-	-	-	-	-	-
T	T	T	T	T	T
G	T	C	G	A	C
A	G	G	C	T	A
A	A	A	C	A	A
T	A	A	C	A	A

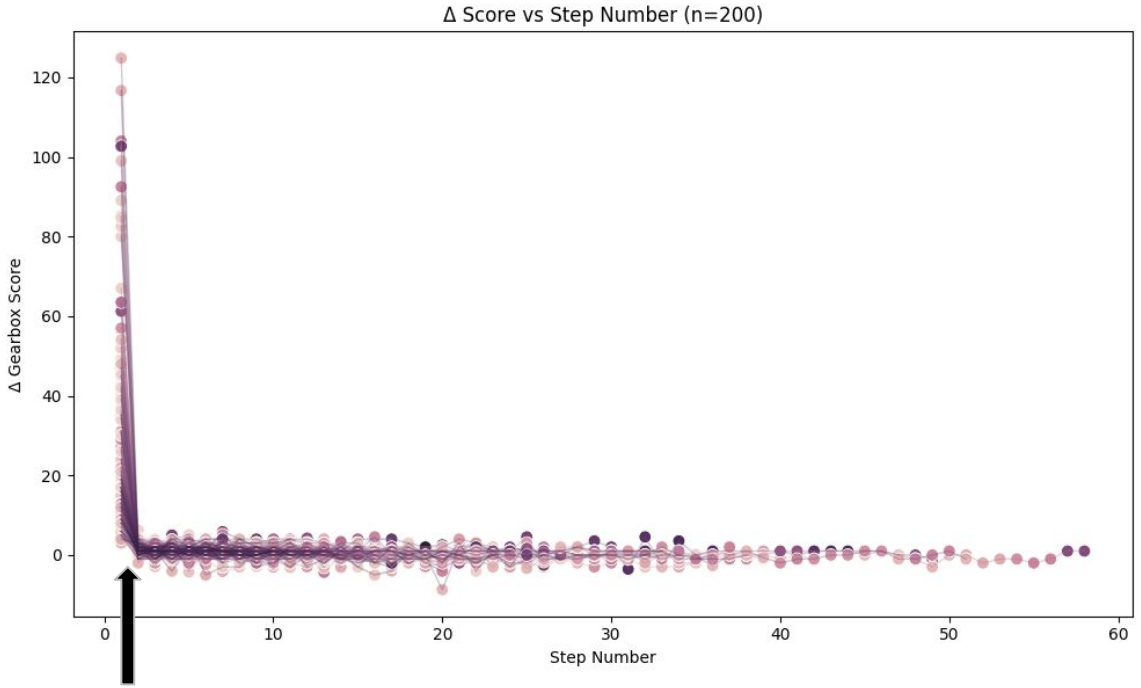
Distance Algorithm

Calculate how far each base pair is from alignment

Spatial awareness task component enhances model accuracy and efficiency

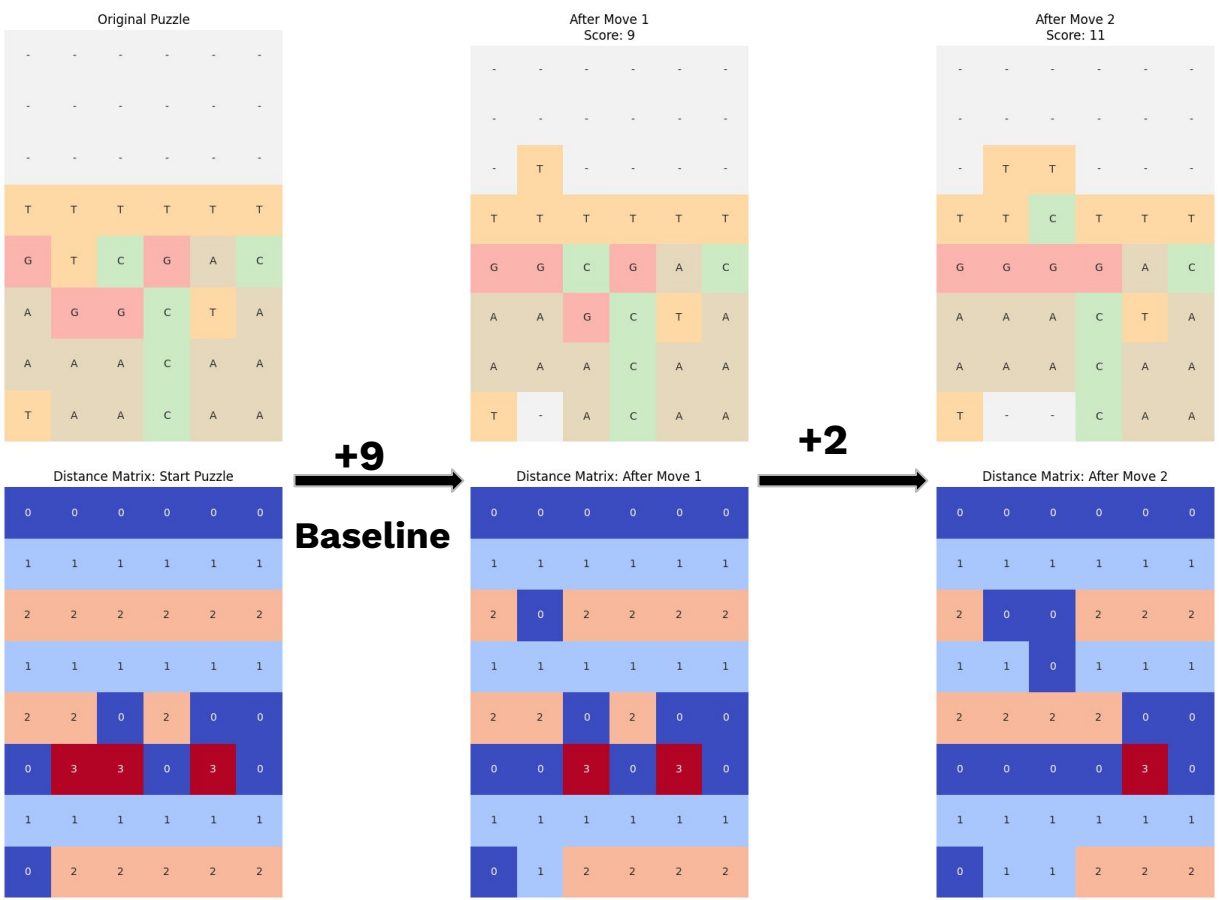


Importance of first steps



Baseline gearbox

Algorithm input: Correlate changes in distance matrix to gearbox score



Model + Task

Adding the distance algorithm task as a parameter in the neural network helps refine learning to make it more MSA-specific

Features:
- Steps
- Accepted Pairs
- Start
- Distance Matrix

Target Variable:
- Score

Goal:
- Model solution score should beat test solution score

Moves variable omitted for simplicity

Model

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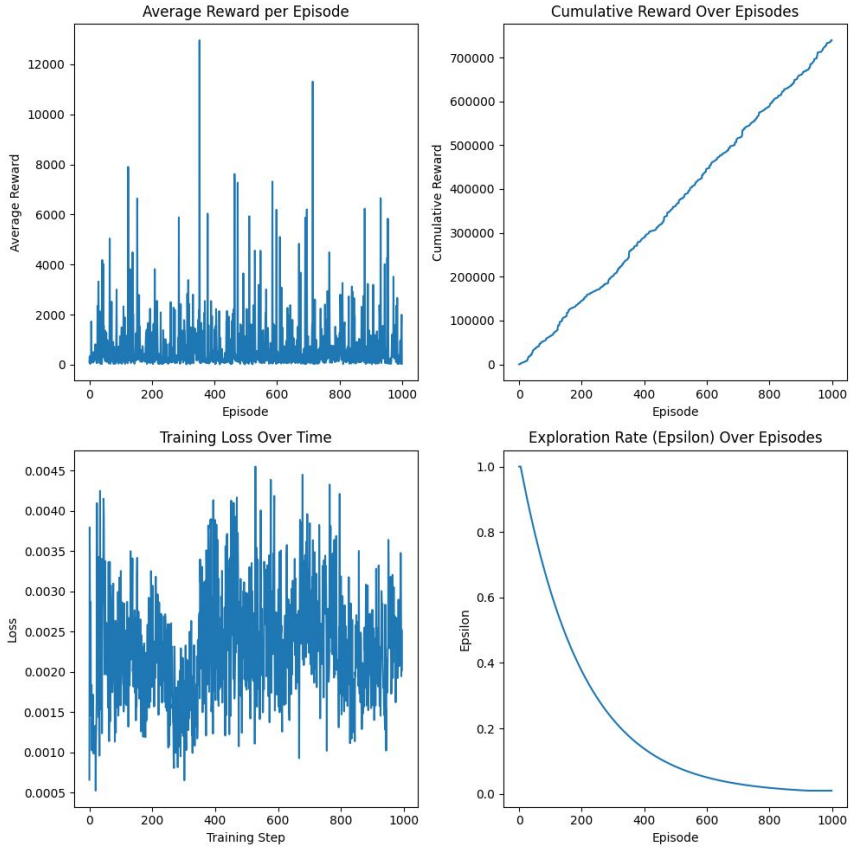
02
Results

Evaluation Metrics



Evaluation Metrics

Model Metrics currently in queue as of submission deadline

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Conclusions

Biological Significance

- This algorithm is a starting point for small sequences
- Much more complicated to apply to large sequences
- Could be refined to be more biology-specific with the integration of the spatial task algorithm

Future Directions

- Increasing models layers and episodes
- Evaluate carbon footprint
- Use Leave-One-Out cross validation to refine algorithm
- Expand on distance matrix calculations to refine efficiency