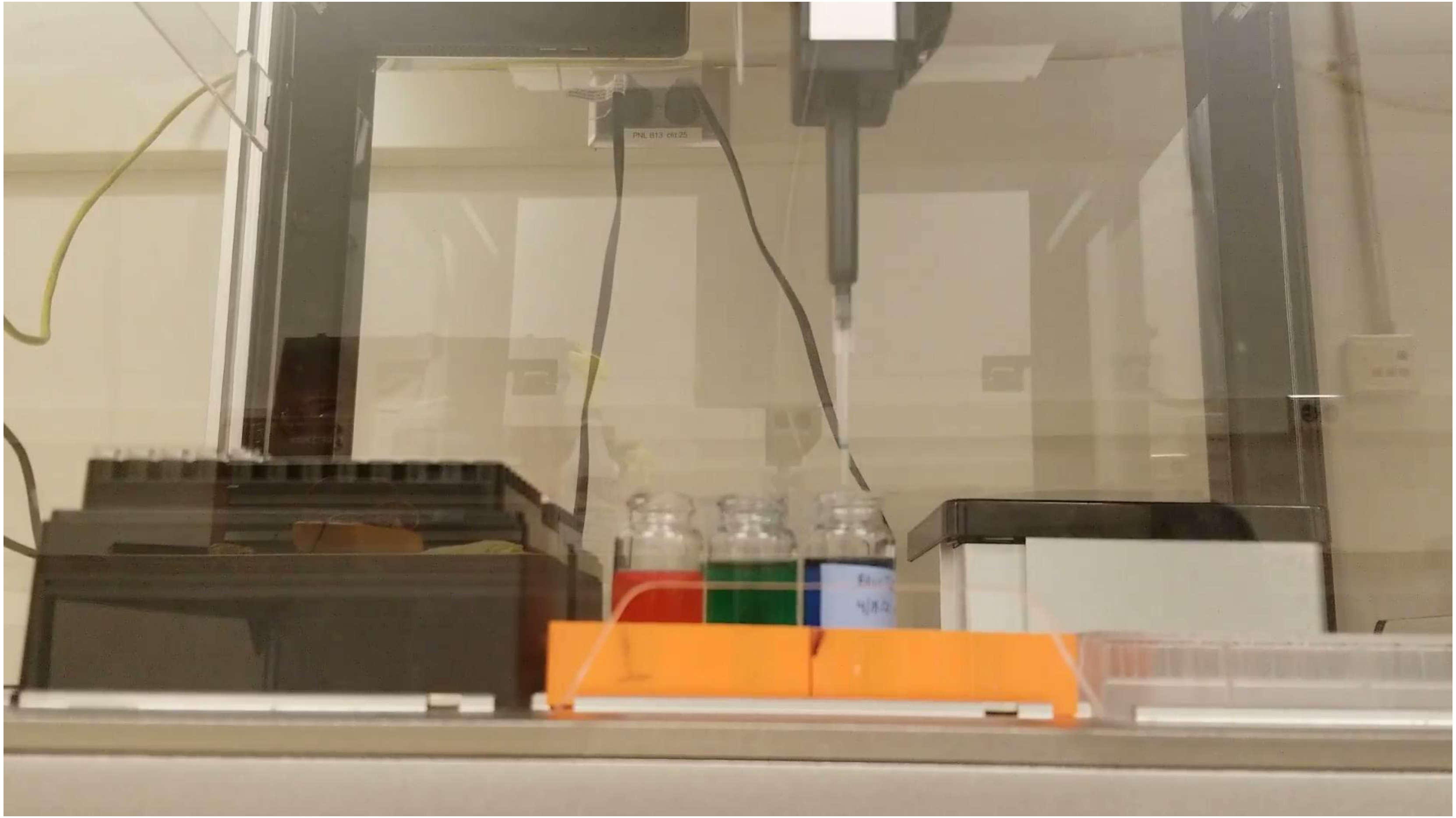
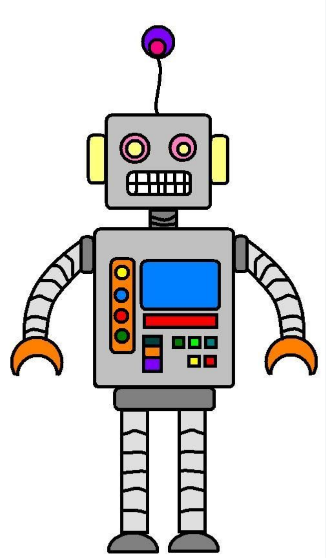
OT2 Pipetting Robots & Reinforcement Learning



REinforced Automaton Learning (REAL) Pipetting



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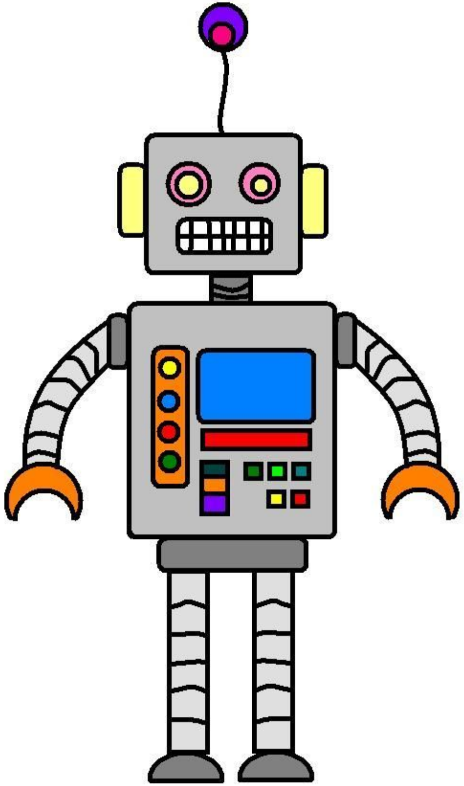
Overview

1. Background and Motivation
    a. Robots in the lab
    b. Reinforcement learning
2. Methods
    a. Virtual Testing
    b. In-lab Testing
3. Results
    a. Genetic Algorithm
    b. Gaussian Process - Batch Upper Confidence Bound
4. Future directions

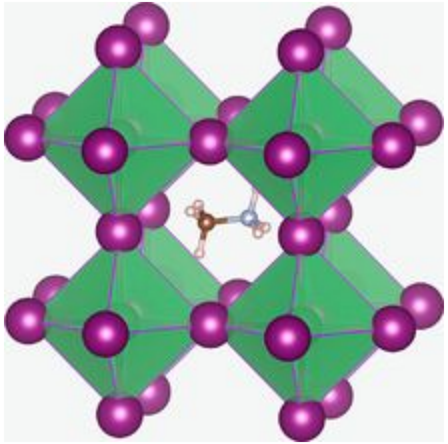


Robots are being increasingly used in the lab

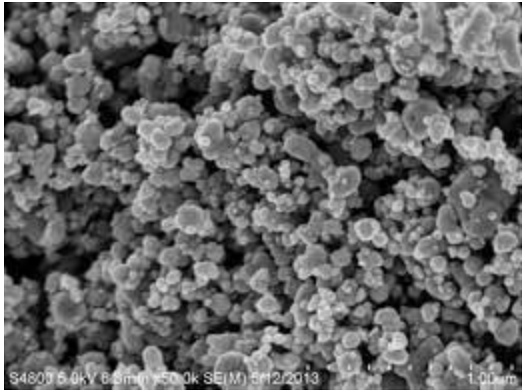
HTE + Reinforcement learning

Quantum Dots

Perovskites



Nanoparticles



We will demonstrate these concept by combining food dyes to reach a desired UV/ Vis spectra

REAL Pipetting

- Incorporated reinforcement learning algorithms that
    1. Interface with the OT2 robot
    2. Can be implemented in any high-throughput experiments
    3. Autonomously plan and execute experiments in **batch** mode
- All code (and preliminary results) are available on GitHub

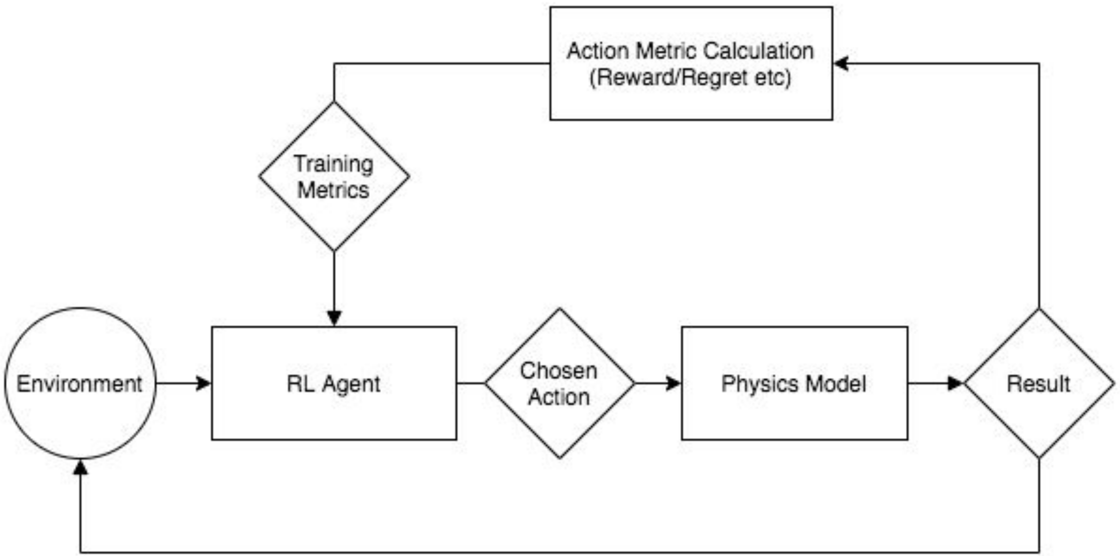
REinforced-Automaton-Learning-REAL-Pipetting

build passing coverage 97%

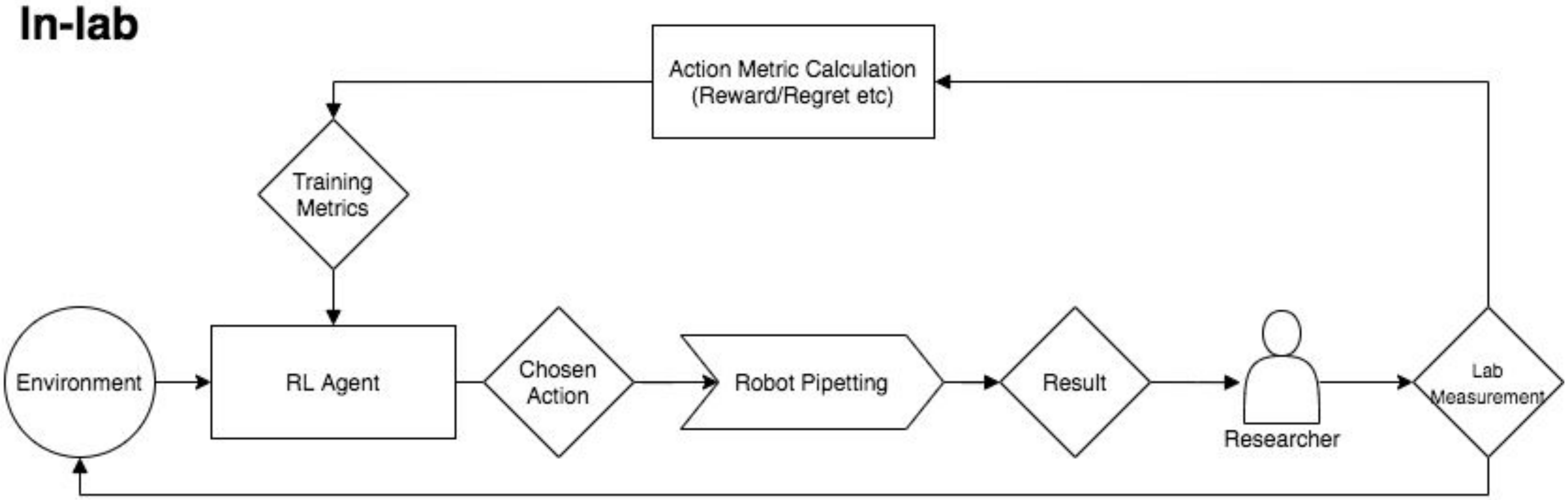
This project integrates reinforcement learning with the open source pipetting robots from Opentrons (OT2) to guide future batched trials in high throughput experiments. We utilize two reinforcement learning algorithms:

REAL Pipetting

Virtual Testing



REAL Pipetting



REAL Pipetting

Gaussian Process Batch Upper Confidence Bound (GP-BUCB)

Strengths:

- Has “memory”
- Converges to a final solution
- Takes only a few batches to arrive at answer

Weaknesses:

- Discrete experimental space that scales exponentially
- Slower computation time

Genetic Algorithm (GA)

Strengths:

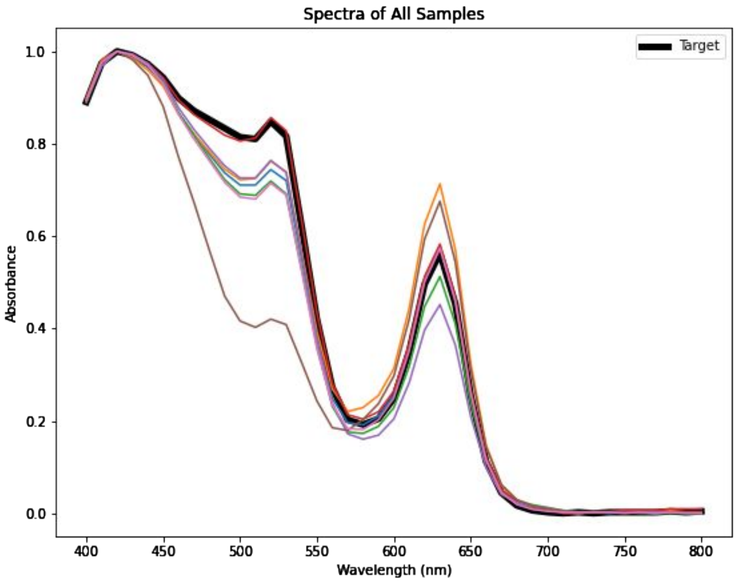
- Operates in continuous space
- Faster computation time
- Iterations are independent of each other

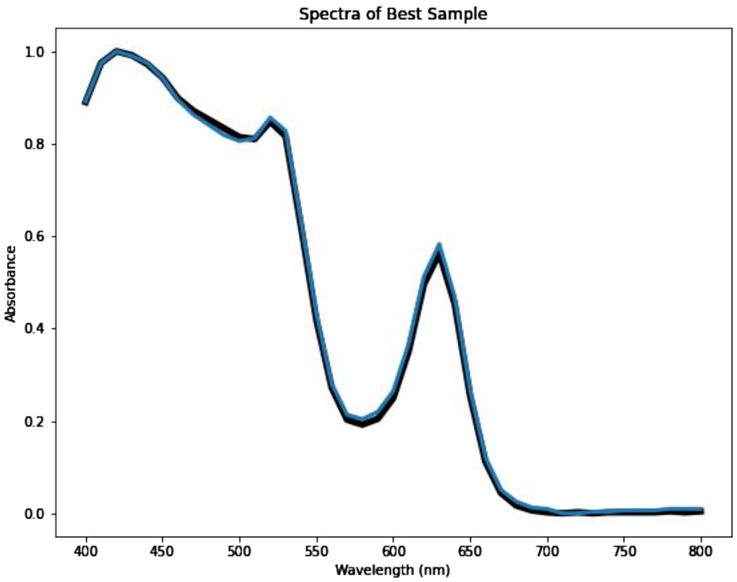
Weaknesses:

- Converges to local minimum
- May take too long to converge

Results

Results: In the lab

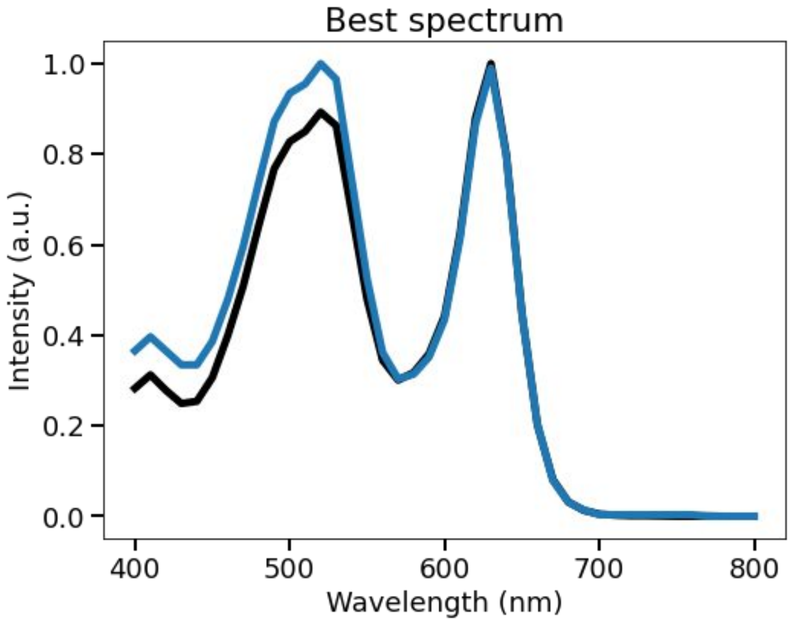


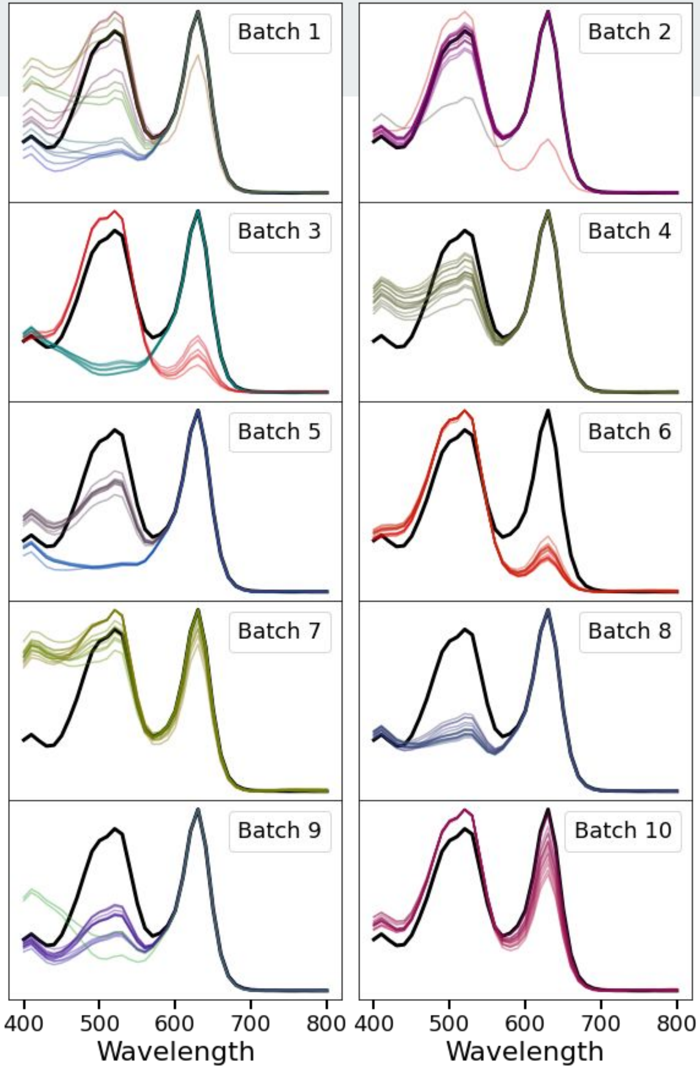


Genetic Algorithm

Results: In the lab

GP-BUCB





Conclusion & Future directions

- Develop stopping criteria instead of relying on human interference to end
- Full integration with OT2 Pipetting Robot
    - Currently relies on file I/O
- GP-BUCB Optimization
    - Sequential Gaussian Process Regression
    - Lazy Variance Calculation
    - Optimize parameter space and constraints
- Parallel Deep Learners
- Use on discrete and continuous variables
- Continuous experimentation

Check out our Github at: https://github.com/REAL-Pipetting/REinforced-Automaton-Learning-REAL-Pipetting

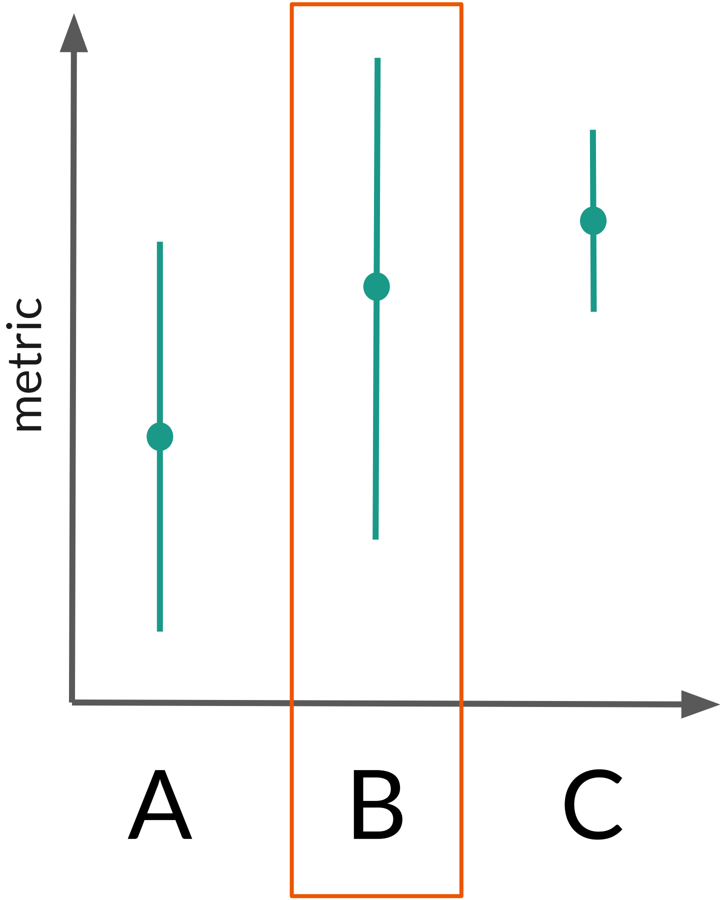
Conclusion: *It works!*

The algorithms

The Algorithms

1. Gaussian Process Batch Upper Confidence Bound

(GP-BUCB)



The Algorithms

1. Gaussian Process Batch Upper Confidence Bound

(GP-BUCB)

Major limitation:

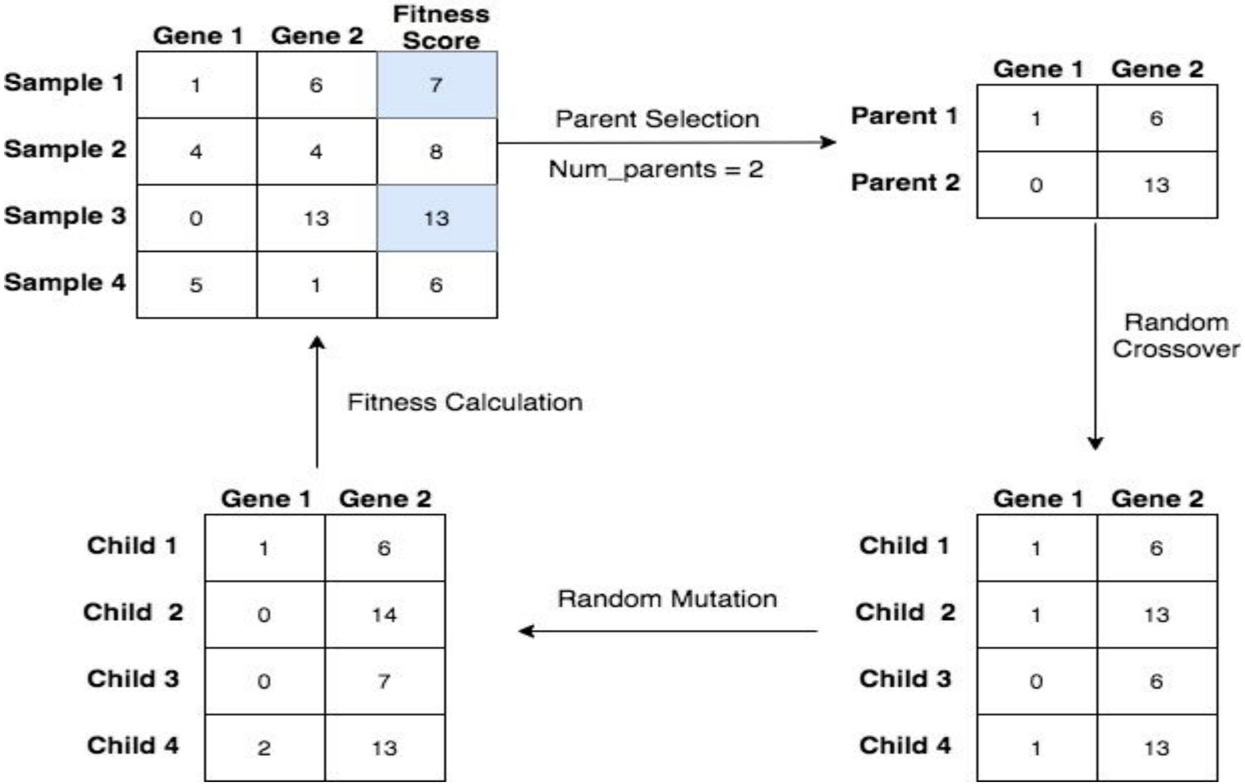
1. Parameter space is discretized
   a. Scales with complexity
   b. Not all options available

Upper Confidence Sampling

-22.8	-21.2	-18.6	-15.2	-11.4	-7.6	-4.5	-2.8	-3.1	-6.1	-11.6
-31.7	-29.0	-24.9	-19.8	-14.1	-8.6	-4.0	-1.3	-1.0	-3.6	-9.1
-42.7	-39.3	-33.9	-27.0	-19.3	-11.9	-5.5	-1.3	0.0	-1.8	-6.7
-55.1	-51.4	-45.0	-36.6	-27.1	-17.6	-9.4	-3.6	-0.8	-1.3	-4.9
-67.5	-64.0	-57.2	-47.7	-36.7	-25.6	-15.8	-8.2	-3.7	-2.5	-4.5
-78.6	-75.7	-69.0	-59.0	-47.3	-35.1	-23.9	-14.8	-8.6	-5.5	-5.6
-86.7	-84.8	-78.7	-69.1	-57.3	-44.8	-32.8	-22.6	-14.9	-10.2	-8.3
-90.8	-90.0	-85.0	-76.4	-65.3	-53.1	-41.1	-30.4	-21.9	-15.6	-12.0
-90.3	-90.7	-87.1	-79.9	-70.2	-59.0	-47.6	-37.1	-28.3	-21.1	-16.1
-85.5	-86.9	-84.7	-79.3	-71.2	-61.6	-51.4	-41.7	-33.0	-25.5	-19.8
-77.1	-79.4	-78.5	-74.6	-68.4	-60.6	-52.0	-43.4	-35.4	-28.2	-22.3

The Algorithms

2. Genetic algorithm

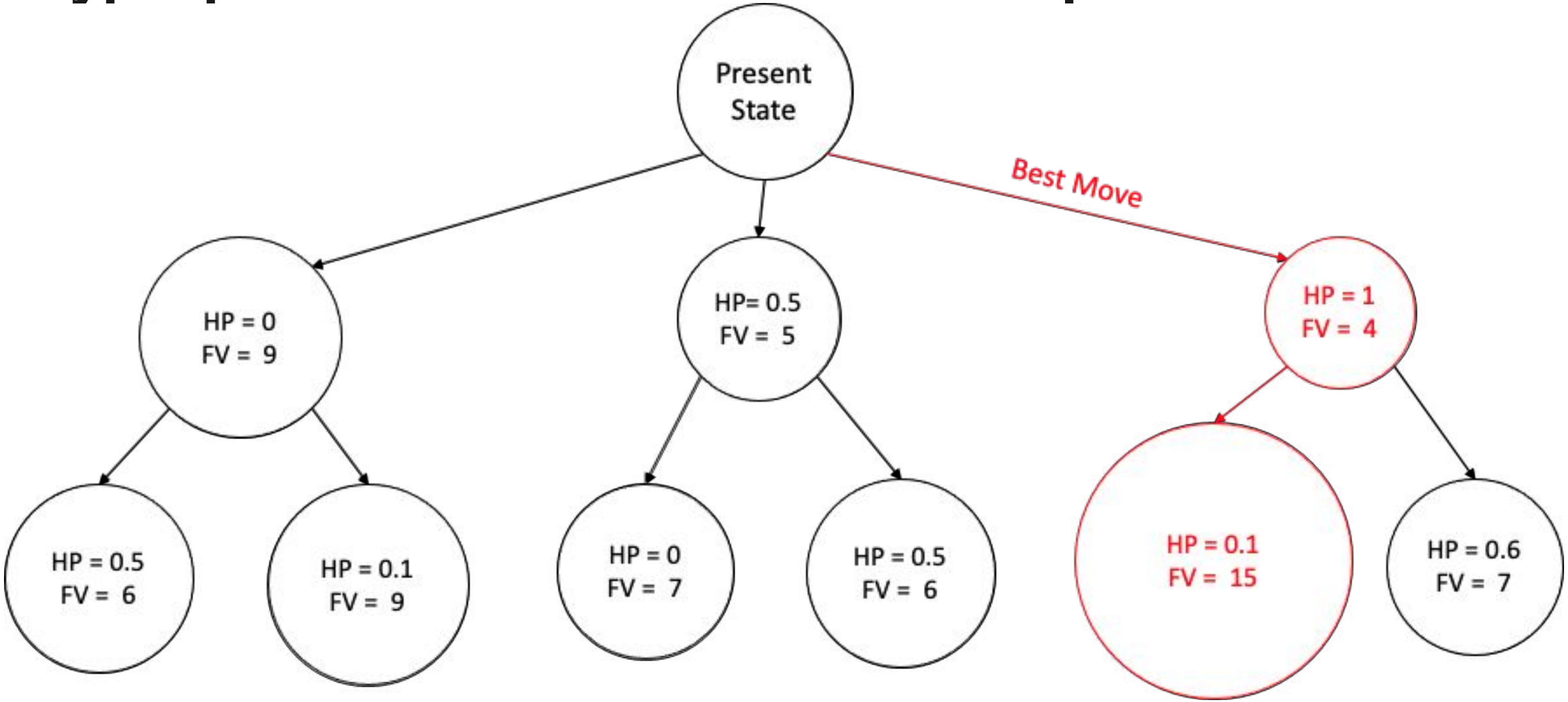


Limitations of the Genetic Algorithm

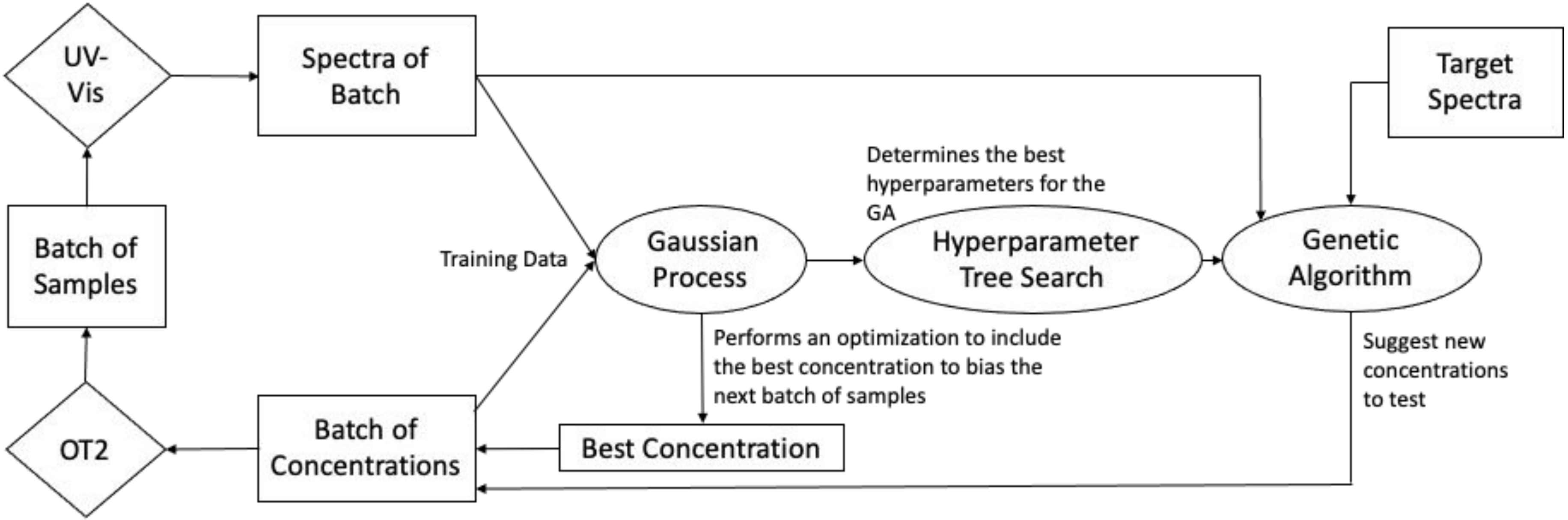
- Can get stuck in local optimums

- Can take many iterations to converge

Hyperparameter Tree Search Example

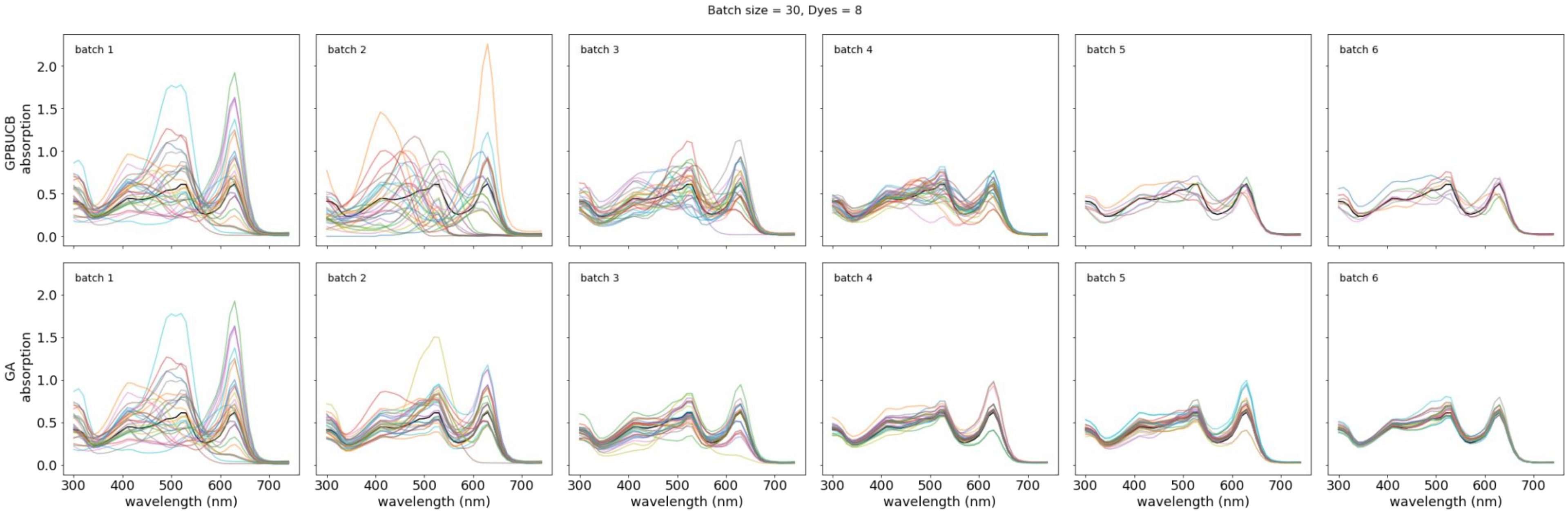


Gaussian Process Assisted Genetic Algorithm

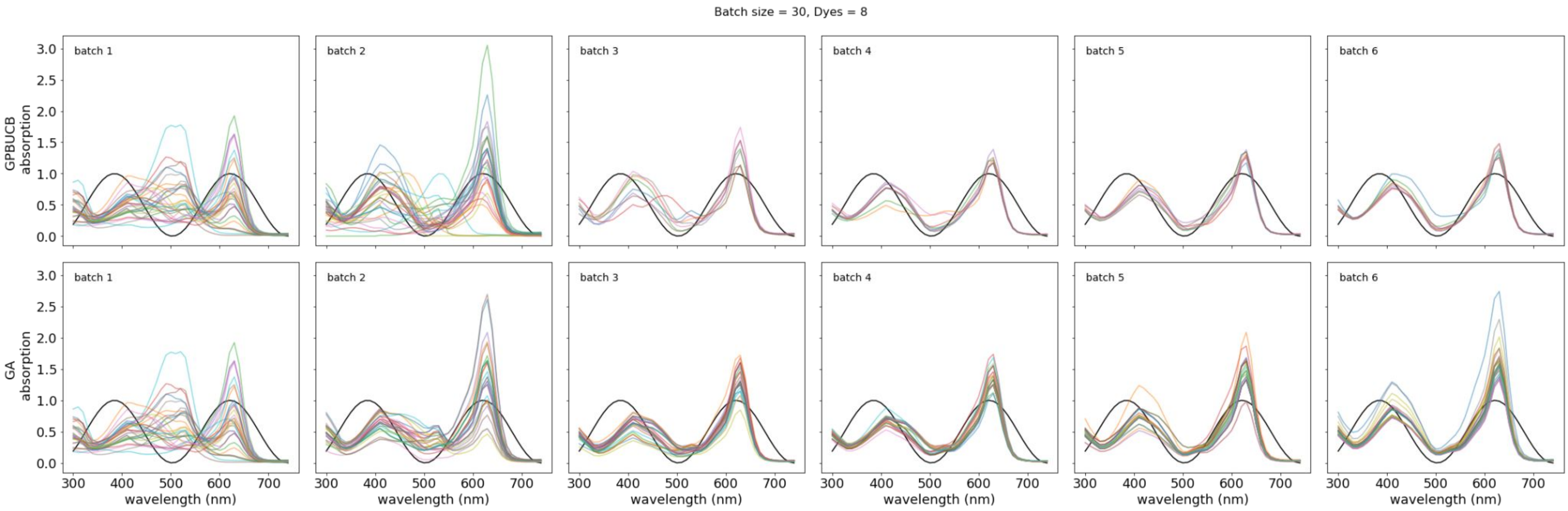


Algorithm comparison

Algorithm Comparison



Algorithm Comparison



Algorithm Comparison