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Generating a Dataset for Deep Reinforcement Learning

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Generating Datasets for Opentrons Flex protocols

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Abstract

Reinforcement Learning (RL), is a subfield of Machine Learning where a computational agent interacts with the environment, learning an optimal course of action by trial and error. Deep Reinforcement Learning (Deep RL) uses neural networks to learn to perform tasks directly from raw data, such as images or text, without hard-coding task-specific knowledge. In this context, datasets are collections of data used as a single unit for analytic and prediction purposes. Datasets are made for specific tasks with raw data specific to the task or machine being used. There is a need for increasingly robust datasets to increase the use and effectiveness of these tasks. The purpose of this work is to generate a dataset designed specifically for Opentrons Flex, a pipetting robot designed for high throughput and laboratory experiments. For this purpose, an attempt to generate a dataset using Opentrons API, and its protocols was done. This attempt was to use Gazebo to simulate and acquire image data for Deep RL. However, the limitations on this action were finding proper documentation and files to run gazebo simulations with. Opentrons API has no documentation that works to recreate its machines in gazebo's virtual environment, without this, simulations for which data can be extracted cannot be done.

Introduction

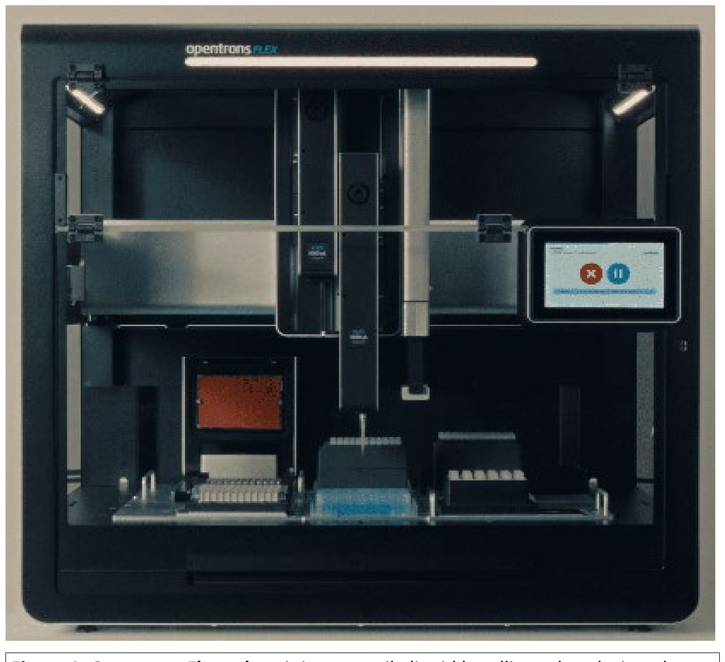

Figure 1. Opentrons Flex robot. it is a versatile liquid handling robot designed to automate laboratory tasks. It's part of the Opentrons line of lab automation tools, known for making automation accessible and affordable.

Methods

Opentrons API has a module available to download for simulating its protocols. This allows for a text-based simulation to generated with Opentrons API. Generate a full sample and create a trajectory for a dataset, gazebo is required to simulate a machine within its environment. Fiting the scene with virtual cameras and sensors can allow for data collection on the different states as the simulation is taken. These states make up the sample that can used to create a trajectory for a dataset. Repeating this process with different opentrons protocols in mind would allow for a dataset with many samples to be created. The pipetting machine's simulation be used to test more trial and error to create an even better dataset thereafter.

```
Belt calibration not found.
Transferring 100.0 from A1 of NEST 12 Well Reservoir 15 mL on slot D2 to A1 of NEST 96 Well Plate 200 µL Flat on slot D3
        Picking up tip from A1 of Opentrons Flex 96 Tip Rack 200 µL on slot D1
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into A1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into B1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into C1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into D1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into E1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into F1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into G1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into H1 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into A2 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into B2 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into C2 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into D2 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot D2 at 716.0 uL/sec
        Dispensing 100.0 uL into E2 of NEST 96 Well Plate 200 µL Flat on slot D3 at 716.0 uL/sec
```

Figure 2. This screen shot is am example of a Opentrons text simulation for an Opentrons flex robot. The activity described is a dilution protocol.

Results

There are unfortunately no results for this project, as the Opentrons API documentation doesn't support gazebo. To further explain. One can import a robot into gazebo for simulations with a urdf file. The model and make-up of the robot would be accurate, and simulations would be useful, however, there is no URDF file in opentrons documentation that I can find, without it, a simulation cannot be run, and a true dataset cannot be created.

I had a plan to put a picture here to fill the empty space but I don't have any ideas, I'll return it when I think of something, inaddition to the changed you'd like me to make.

Summary

- While Opentrons does have documentation for its text simulations, ones for gazebo do exist
- Creating the files needed to run gazebo with opentrons machines is not within my ability

Conclusions

- Without a URDF file, or a suitable substitute available, Opentrons Flex robot cannot be simulated, and data cannot be extracted. In the future, show such documentation become available, the next steps would be to learn how to use Deep RL on the data accrued through the agent and compare it with other models.

Acknowledgements

Dr. Kumar and Swaroop

Funding: McNair Scholars Program

Generating a dataset for Opentrons OT-2 dilution protocols in autonous labs

Davis, Lewis; Kumar, Sathish

Department, Institution, City, Two letter state abbreviation

Abstract

Reinforcement Learning (RL), is a subfield of Machine Learning where a computational agent interacts with the environment, learning an optimal course of action by trial and error. Deep Reinforcement Learning (Deep RL) uses neural networks to learn to perform tasks directly from raw data, such as images or text, without hard-coding task-specific knowledge. In this context, datasets are collections of data used as a single unit for analytic and prediction purposes. Datasets are made for specific tasks with raw data specific to the task or machine being used. There is a need for increasingly robust datasets to increase the use and effectiveness of these tasks. The purpose of this work is to generate a dataset designed specifically for Opentrons Flex, a pipetting robot designed for high throughput and laboratory experiments. For this purpose, an attempt to generate a dataset using Opentrons API, and its protocols was done. This attempt was to use Gazebo to simulate and acquire image data for Deep RL. However, the limitations on this action were finding proper documentation and files to run gazebo simulations with. Opentrons API has no documentation that works to recreate its machines in gazebo's virtual environment, without this, simulations for which data can be extracted cannot be done.

Introduction

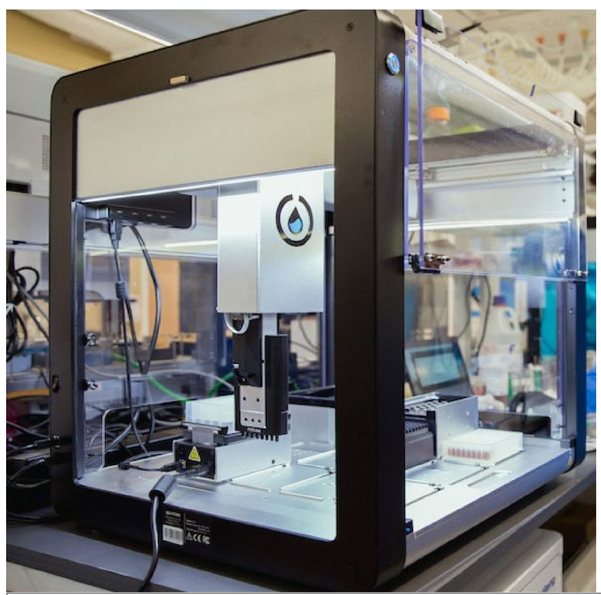

Figure 1. Opentrons OT-2 robot. Is a pipetting robot meant for lab automous labs. The image on the right is the specific pipette used in this robot.

Methods

Opentrons API has a module available to download for simulating its protocols. This allows for a text-based simulation to generated with Opentrons API. Generate a full sample and create a trajectory for a dataset, gazebo is required to simulate a machine within its environment. Fiting the scene with virtual cameras and sensors can allow for data collection on the different states as the simulation is taken. These states make up the sample that can used to create a trajectory for a dataset. Repeating this process with different opentrons protocols in mind would allow for a dataset with many samples to be created. The pipetting machine's simulation be used to test more trial and error to create an even better dataset thereafter.

```
(base) C:\Users\McNair Scholars Prog\Downloads>opentrons_simulate dilution-tutorial.py
C:\Users\McNair Scholars Prog\.opentrons\robot_settings.json not found. Loading defaults
Deck calibration not found.
C:\Users\McNair Scholars Prog\.opentrons\deck_calibration.json not found. Loading defaults
Transferring 100.0 from A1 of NEST 12 Well Reservoir 15 mL on slot 2 to A1 of NEST 96 Well Plate 200 µL Flat on slot 3
        Picking up tip from A1 of Opentrons OT-2 96 Tip Rack 300 µL on slot 1
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
        Dispensing 100.0 uL into A1 of NEST 96 Well Plate 200 µL Flat on slot 3 at 94.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
        Dispensing 100.0 uL into A2 of NEST 96 Well Plate 200 µL Flat on slot 3 at 94.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
        Dispensing 100.0 uL into A3 of NEST 96 Well Plate 200 µL Flat on slot 3 at 94.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
        Dispensing 100.0 uL into A4 of NEST 96 Well Plate 200 µL Flat on slot 3 at 94.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
        Dispensing 100.0 uL into A5 of NEST 96 Well Plate 200 µL Flat on slot 3 at 94.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
        Dispensing 100.0 uL into A6 of NEST 96 Well Plate 200 µL Flat on slot 3 at 94.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
        Dispensing 100.0 uL into A7 of NEST 96 Well Plate 200 µL Flat on slot 3 at 94.0 uL/sec
        Aspirating 100.0 uL from A1 of NEST 12 Well Reservoir 15 mL on slot 2 at 94.0 uL/sec
```

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