THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 20: Contextual Bandits and ML Agents

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Definitions:

- **Objective:** overall goal that we aim to achieve. Not available during or immediately after experiment.

- **Reward:** the measure of success available at the end of experiment

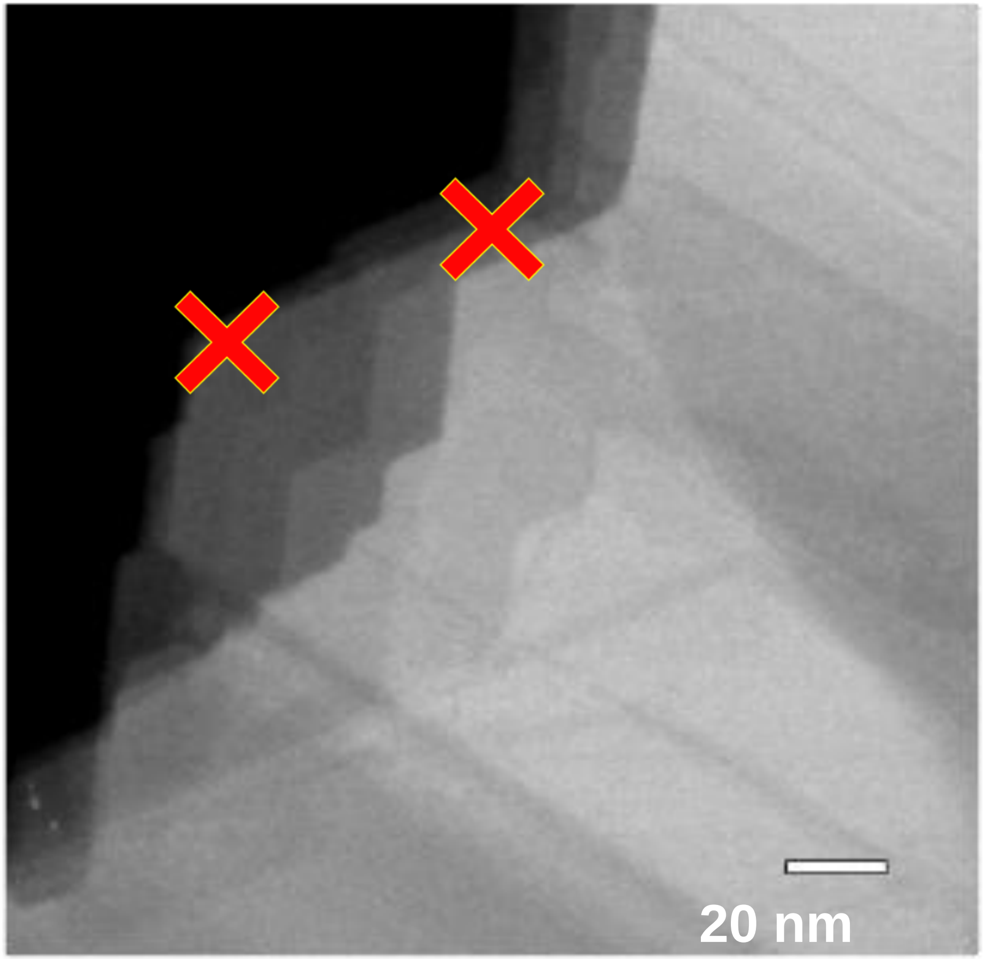
- **Value:** expected reward. Difference between reward and value is a feedback signal for multiple types of active learning

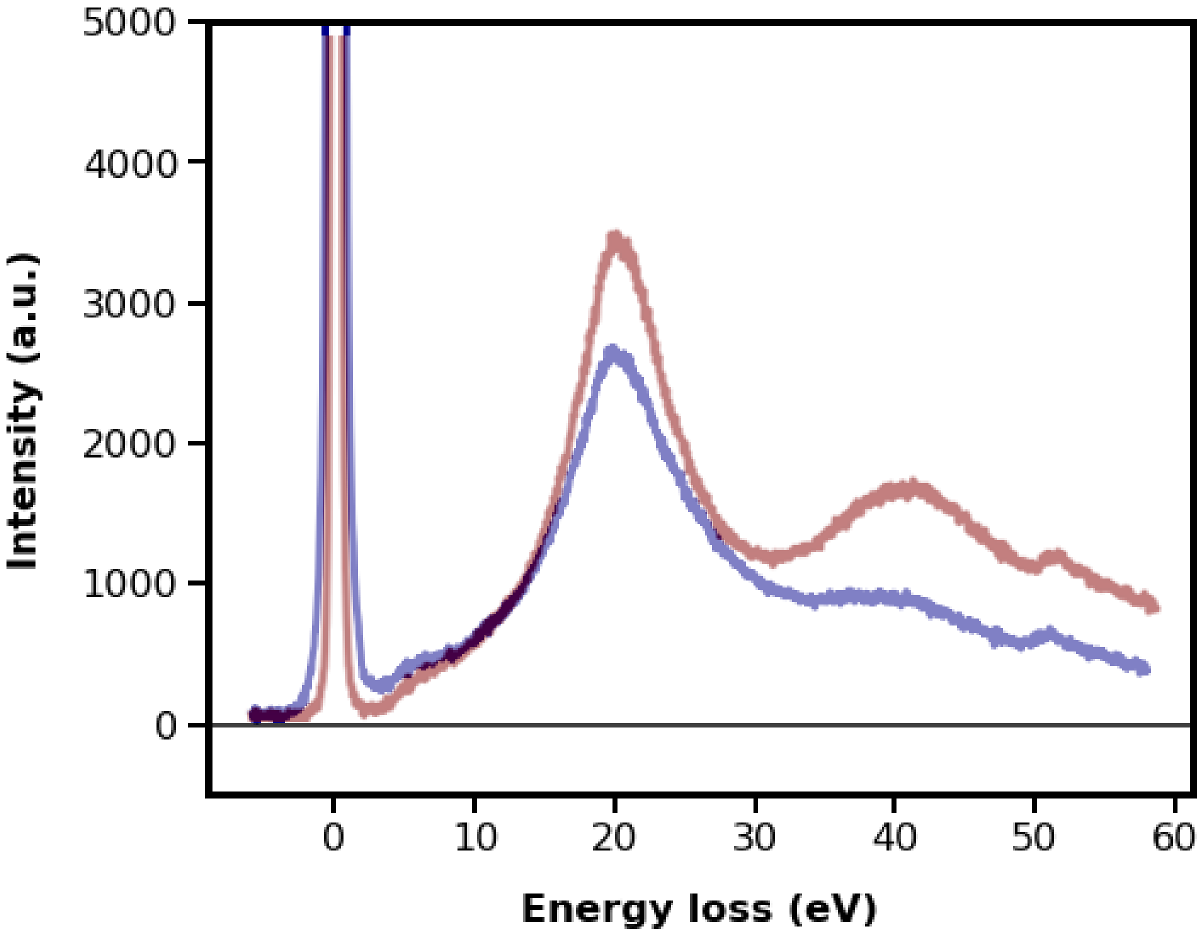
- **Action:** how can ML agent interact with the system

- **State:** information about the system available to ML agent

- **Policy:** rulebook that defines actions given the observed state

From Static to Active Learning

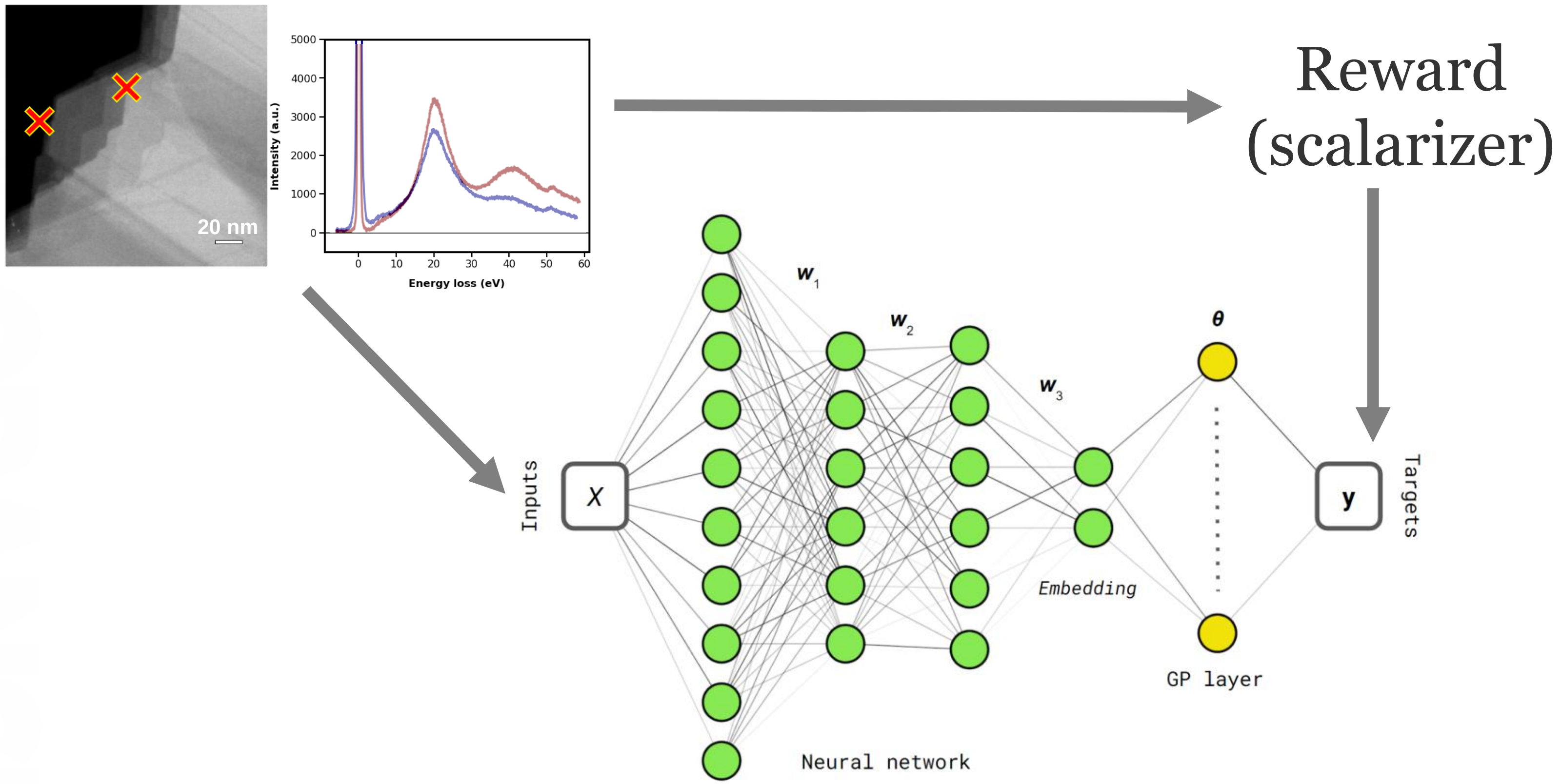




1. What if we have full access to structural information
2. And want to choose locations for (EELS, 4D STEM, CL, EDX) measurements
3. So as to **learn** relationship between structure and spectrum fastest
4. Or **discover** which microstructural elements give rise to specific **desired** spectral features?

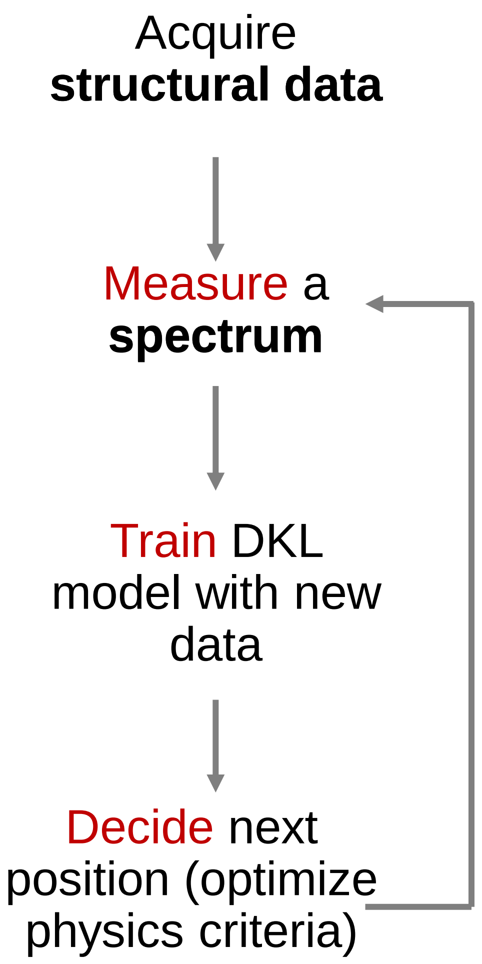
Deep Kernel Learning

- All image patches are available in the beginning of the experiment
- We measure spectra one by one
- And are interested in some specific aspect of spectra
- We aim to learn the relationship between structure and this aspect



Reward (scalarizer)

<u>Specify physics criteria</u>



Acquire **structural data**

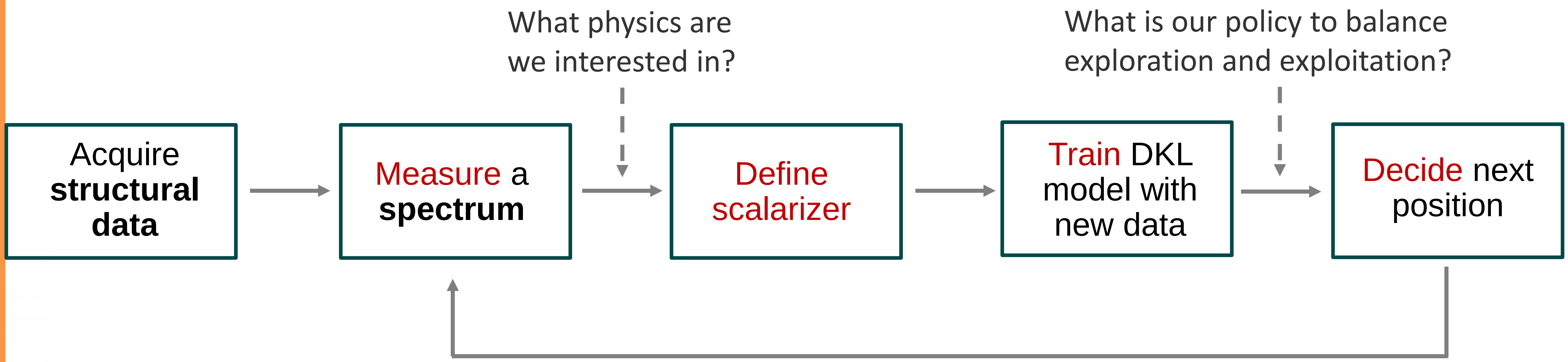
Measure a **spectrum**

Train DKL model with new data

Decide next position (optimize physics criteria)

Allows navigation of the system to search for physics

Deep Kernel Learning based BO


What physics are we interested in?
What is our policy to balance exploration and exploitation?
Acquire **structural data**
Measure a **spectrum**
Define scalarizer
Train DKL model with new data
Decide next position

Key concepts:

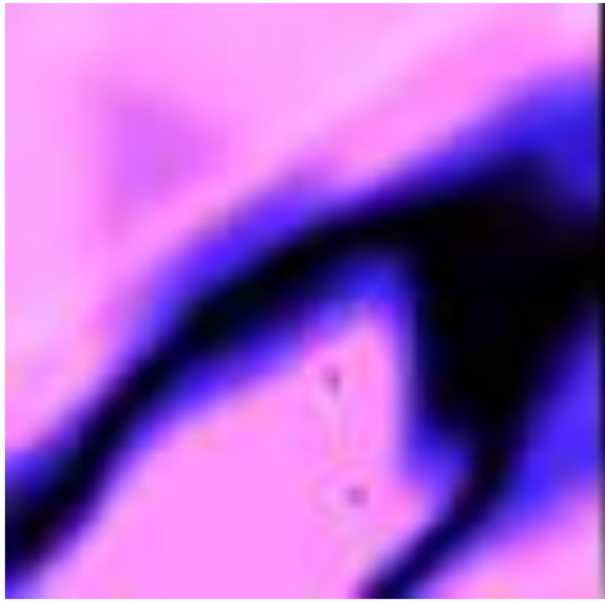
- **Scalarizer:** (any) function that transforms spectrum into measure of interest. Can be integration over interval, parameters of a peak fit, ration of peaks, or more complex analysis

- **Experimental trace:** collection of image patches and associated spectra acquired during experiment. Note that we collect spectra, not only scalarizers

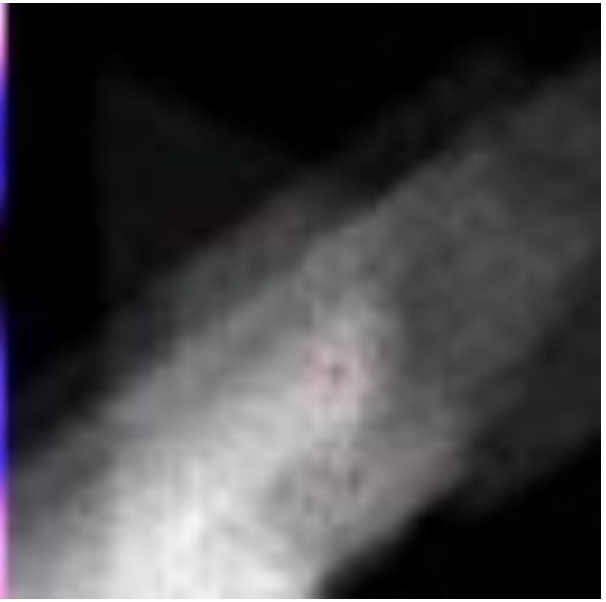
Discovering Regions with Interesting Physics

- **Discovering physics in a “new” material $MnPS_3$**
- **Curve fitting** to help enforce physical processes

“Acquisition function”

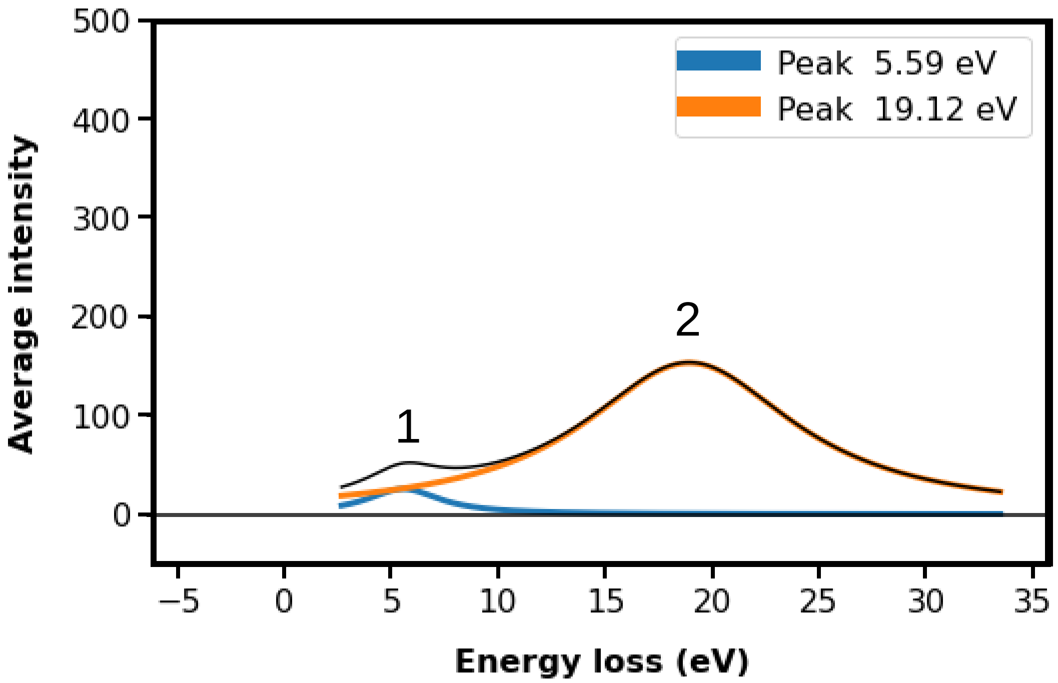


HAADF-STEM



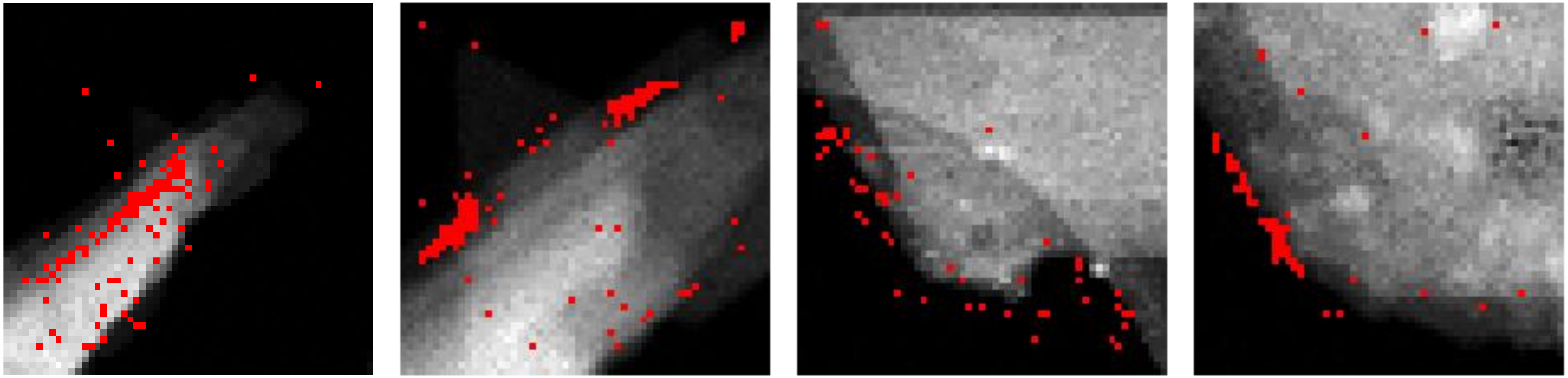
Physics search criteria:

$$\boldsymbol{Ratio = Peak\,1\,/\,peak\,2}$$



More Examples of Physics Discovery

- Very similar behavior when searching for the same criteria!
- Success!



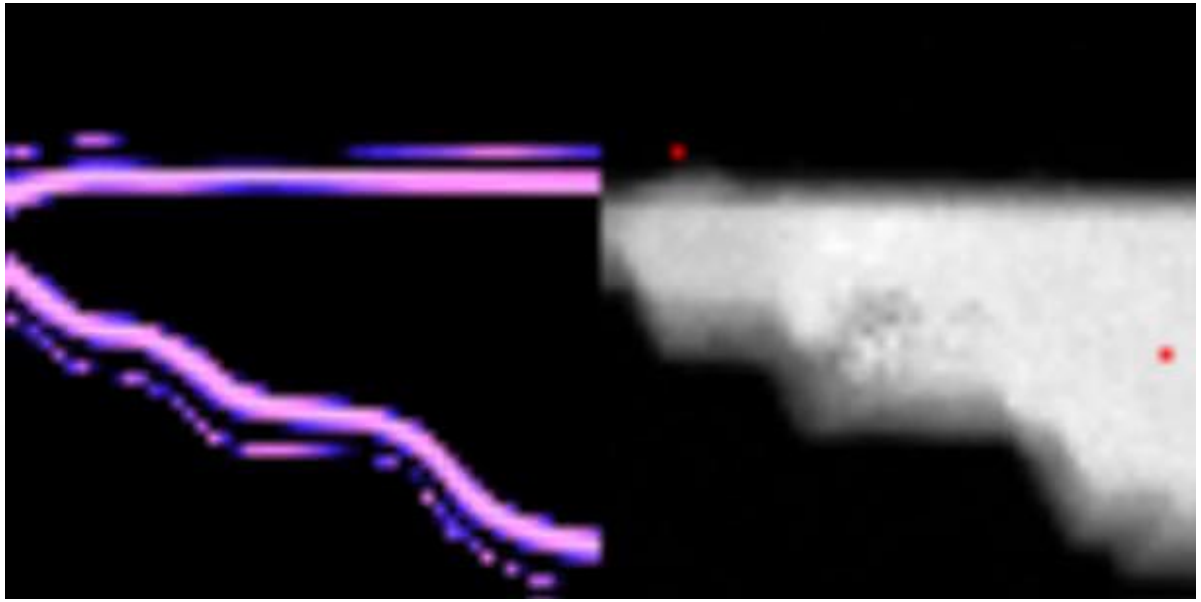
Discovery pathway depends on the reward structure (scalarizer that defines signature of physics we want to discover)!

Changing the scalarizer

- (Same region) **Simple physics search:** peak max in selected region

“Acquisition function”

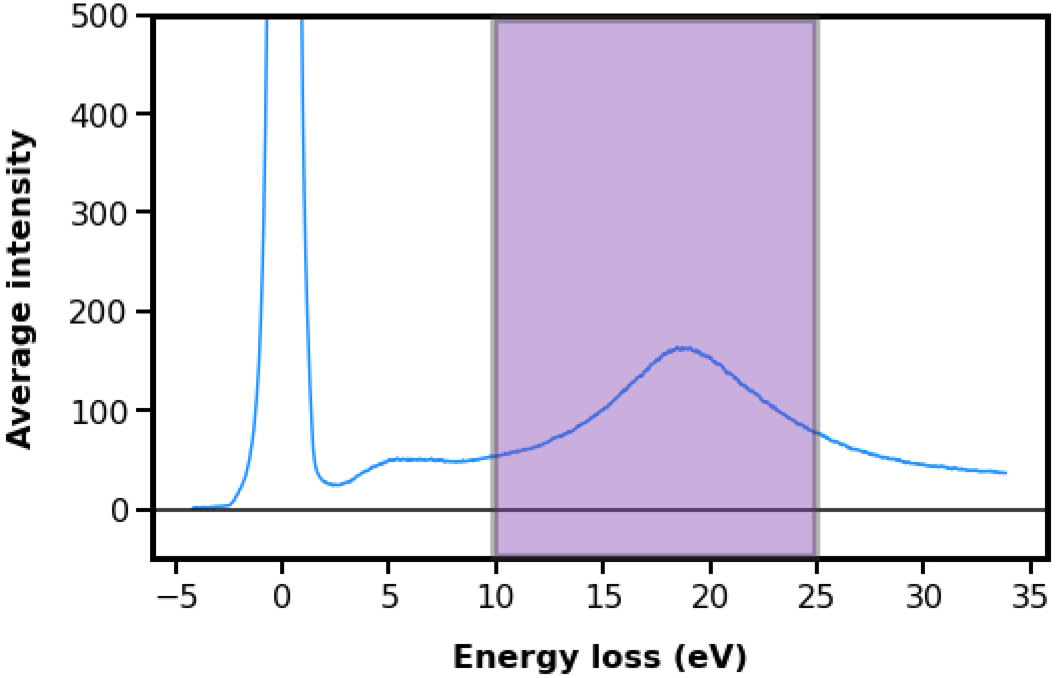
HAADF-STEM
+ points visited



Physics search criteria:

$$\boldsymbol{Maximize(f)}$$

(Specific peak intensity)



What were we doing?

- **Objective(s):**
  - Understanding the emergence of the nanoplasmonic behaviors
  - For understanding physics, optical interfaces to quantum devices, etc.
  - … and so on. For fundamental research, vey often impact is clear later!

- **Reward:**
  - Minimizing uncertainty in structure-property relationships (can we predict expensive EELS from cheap structure)
  - Discovering structures that maximize certain aspect of nanophotonic behavior (have maximal intensity of certain peak, peak area ratio, etc.)

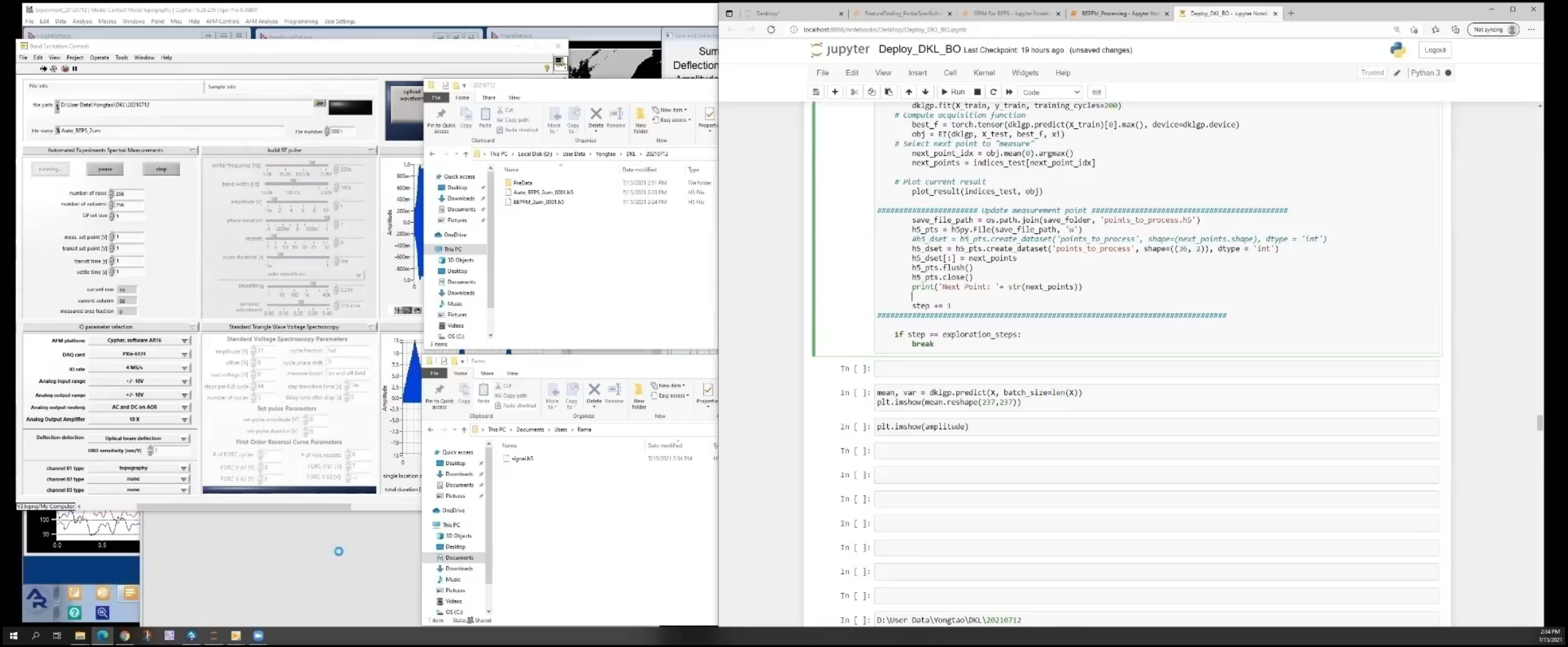
- **Value:** expected reward. Here – predicted scalarizer

- **Action:** position STEM probe at a given location, take EELS spectrum

- **State:** image patch

- **Policy:** myopic optimization (actually, upper confidence bound) with defined exploration-exploitation balance

Deep Kernel Learning AE SPM



Band Excitation Controls
File Edit View Project Operate Tools Window Help
Automated Experiments Spectral Measurements
running...
pause
stop
build BE pulse
IO parameter selection
Standard Triangle Wave Voltage Spectroscopy
Amplitude
Jupyter
File Edit View Insert Cell Kernel Widgets Help
Trusted
Python 3
Run
Code
Logout
Home Share View
Clipboard Organize New

File info
file path: D:\User Data\Yongtao\DKL\20210712
file name: Auto_BEPS_2um
file number: 0001

number of rows: 256
number of columns: 256
GP set size: 1
meas. set point [V]: 1
transit set point [V]: 1
transit time [s]: 1
settle time [s]: 1
current row: 55
current column: 56
measured area fraction: 0

center frequency [Hz]: 330k
band width [Hz]: 100k
amplitude [V]: 1
phase variation: 1
repeats: 4
pulse duration [s]: 4m
auto smooth on
smoothing: 3.21k
window adjustment: 215.63m

AFM platform: Cypher, software AR16
DAQ card: PXIe-6124
IO rate: 4 MS/s
Analog input range: +/- 10V
Analog output range: +/- 10V
Analog output routing: AC and DC on AO0
Analog Output Amplifier: 10 X
Deflection detection: Optical beam deflection
OBD sensitivity (nm/V): 1
channel 01 type: topography
channel 02 type: none
channel 03 type: none

Standard Voltage Spectroscopy Parameters
amplitude [V]: 12
offset [V]: 0
read voltage [V]: 0
steps per full cycle: 64
number of cycles: 3
cycle fraction: full
cycle phase shift: 0
measure loops: on and off field
step transition time [s]: 1m
delay time after step [s]: 0

Set-pulse Parameters
set-pulse amplitude [V]: 0
set-pulse duration [s]: 0

First Order Reversal Curve Parameters
# of FORC cycles: 1
# of Forc repeats: 0
FORC V A1 [V]: 8
FORC V A2 [V]: 8
FORC V B1 [V]: 7
FORC V B2 [V]: -7

This PC > Local Disk (D:) > User Data > Yongtao > DKL > 20210712

Name	Date modified	Type
PreData	7/13/2021 2:51 PM	File folder
Auto_BEPS_2um_0001.h5	7/15/2021 2:33 PM	H5 File
BEPFM_2um_0001.h5	7/15/2021 2:24 PM	H5 File

This PC > Documents > Users > Rama

Name	Date modified
signal.h5	7/15/2021 2:34 PM

localhost:8888/notebooks/Desktop/Deploy_DKL_BO.ipynb

Deploy_DKL_BO Last Checkpoint: 19 hours ago (unsaved changes)

```python
        dklgp.fit(X_train, y_train, training_cycles=200)
    # Compute acquisition function
        best_f = torch.tensor(dklgp.predict(X_train)[0].max(), device=dklgp.device)
        obj = EI(dklgp, X_test, best_f, xi)
    # Select next point to "measure"
        next_point_idx = obj.mean(0).argmax()
        next_points = indices_test[next_point_idx]

    # Plot current result
        plot_result(indices_test, obj)

####################### Update measurement point ##############################################
        save_file_path = os.path.join(save_folder, 'points_to_process.h5')
        h5_pts = h5py.File(save_file_path, 'w')
        #h5_dset = h5_pts.create_dataset('points_to_process', shape=(next_points.shape), dtype = 'int')
        h5_dset = h5_pts.create_dataset('points_to_process', shape=((36, 2)), dtype = 'int')
        h5_dset[:] = next_points
        h5_pts.flush()
        h5_pts.close()
        print('Next Point: '+ str(next_points))

        step += 1
##############################################################################################

    if step == exploration_steps:
        break
```

```
In [ ]:

In [ ]: mean, var = dklgp.predict(X, batch_size=len(X))
        plt.imshow(mean.reshape(237,237))

In [ ]: plt.imshow(amplitude)

In [ ]:

In [ ]:

In [ ]:

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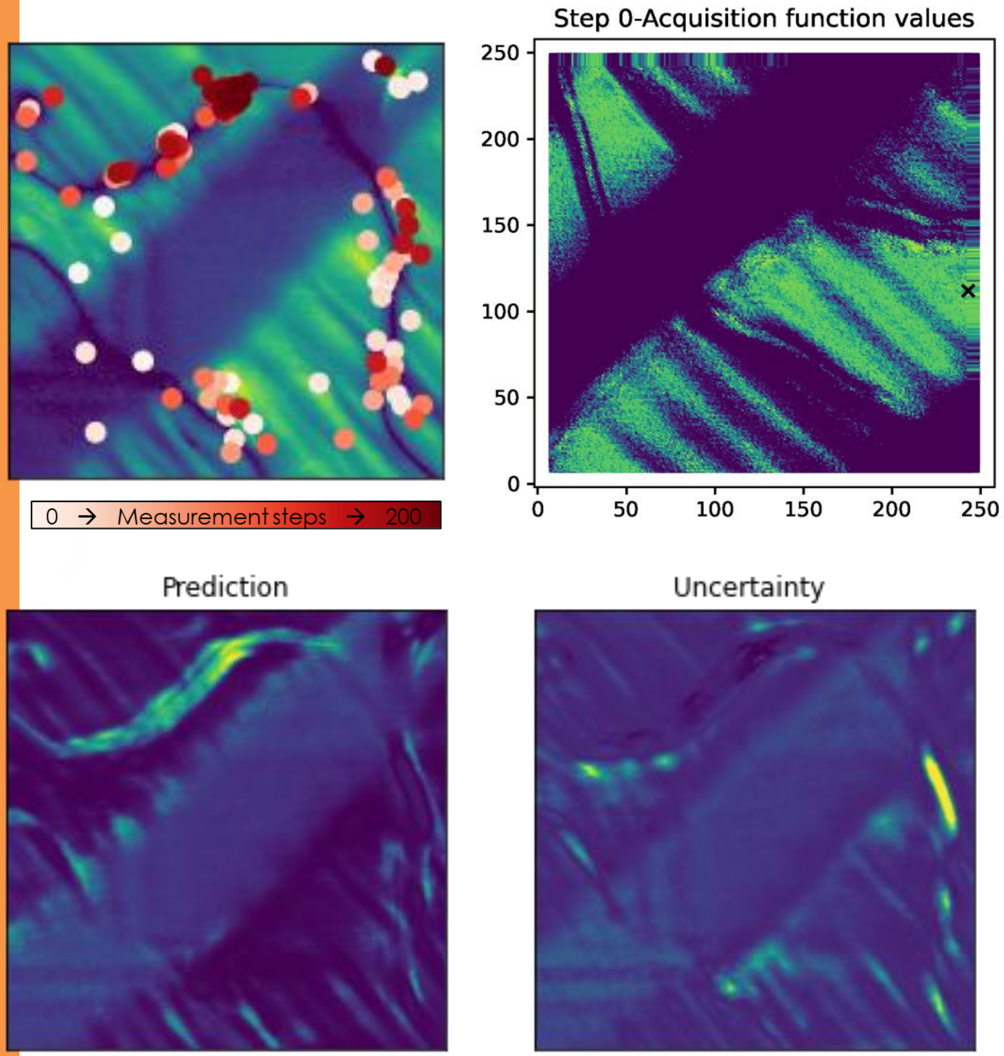
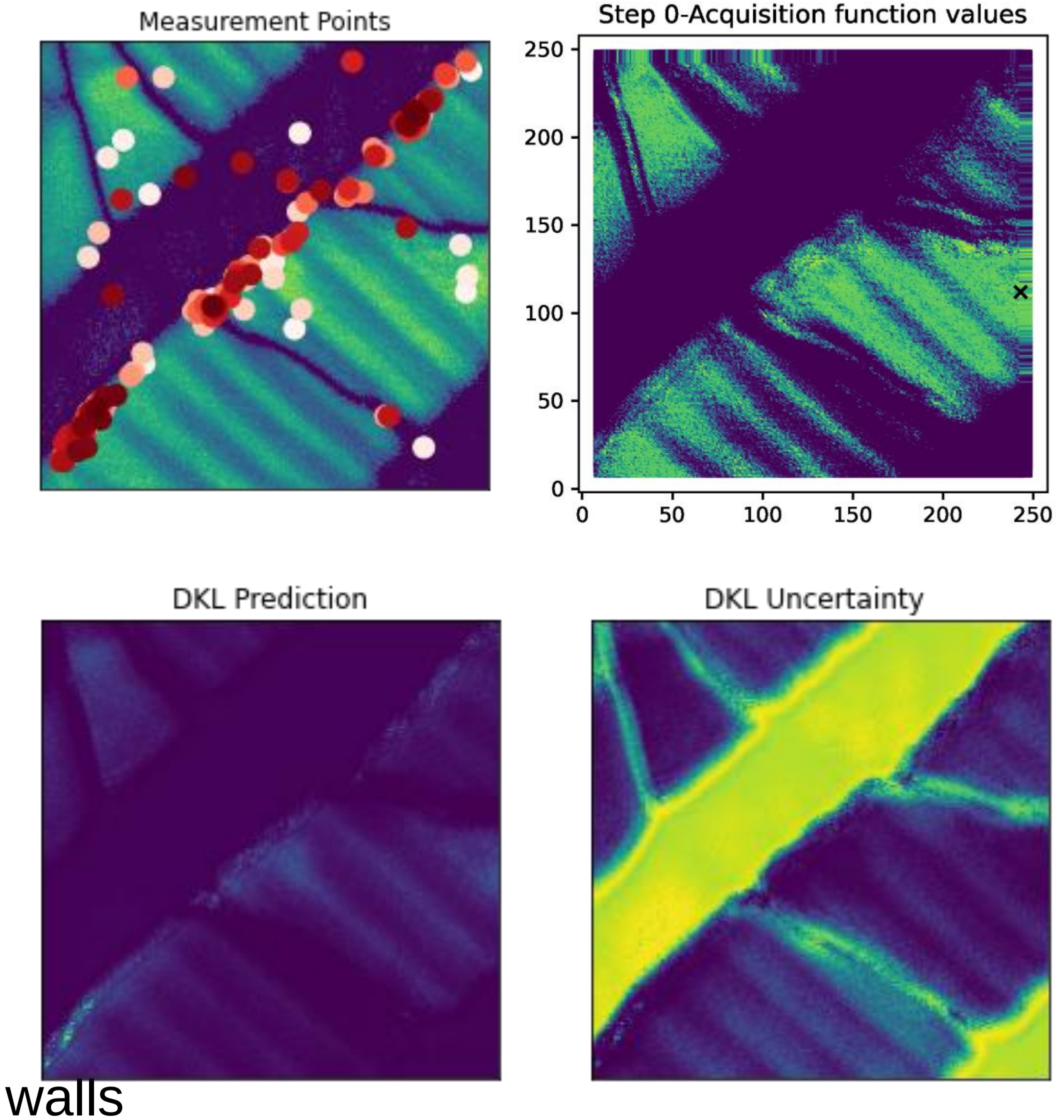
7/15/2021

DKL SPM

Guided by: On field loop area



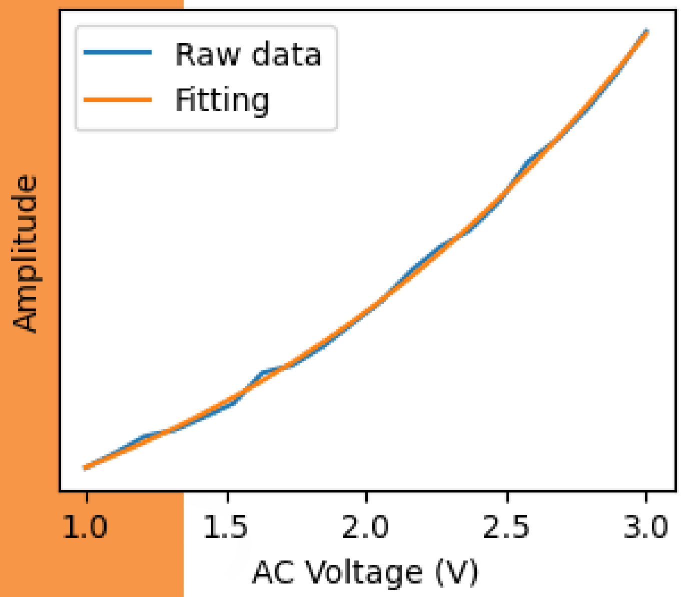
Guided by: Off field loop area



- ➢ Large loop opening corresponding 180º domain walls
- ➢ This behavior can be attributed to the large polarization mobility of 180º walls

Liu, Yongtao, et al, Nature Machine Intelligence 4, 4 (2022): 341-350.

Exploring Non-Linearity



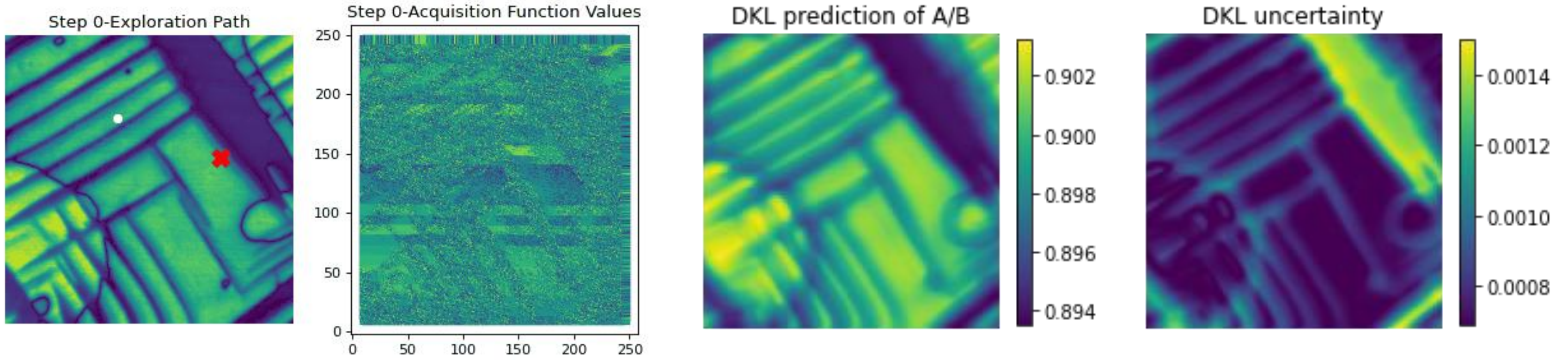
V_{AC} sweep curve at each location was fitted as $y = Ax^3 + Bx^2 + Cx$

A, B, C, and A/B were us as the target function to guide DKL-V_{AC} measurement.

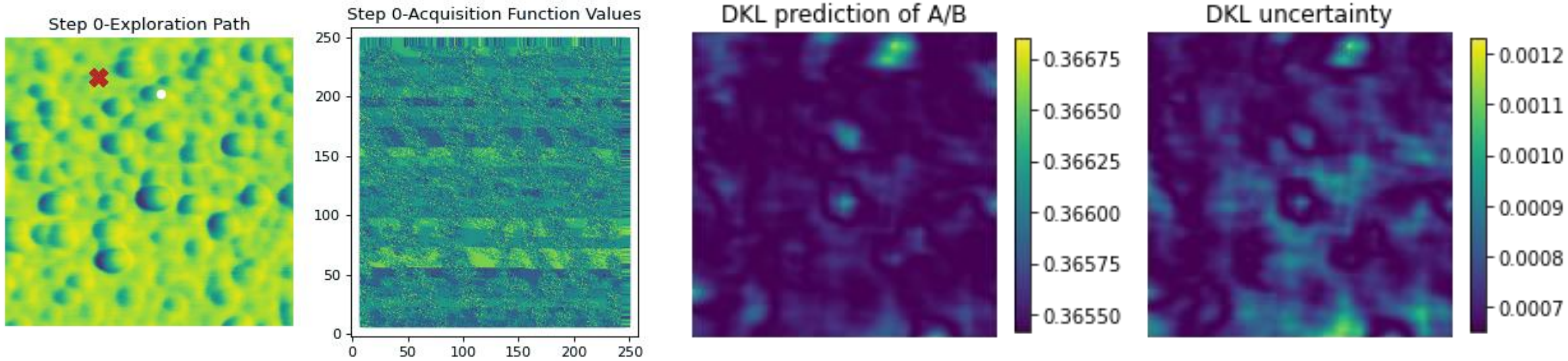
PTO and HZO thin films were studied.

- Shown are 200-step measurements of PTO and HZO thin films
- PFM amplitude was used as structure image; A/B was used to guide the measurement.

PTO experiment process and results



HZO experiment process and results



- In conventional microscopy experiment, human runs everything directly – defines scan, positions the probe, defines measurement parameters.

- In AE SPM, the policies are defined before the experiment and do not change. Sometimes it works – but not always.

- How would we:
  - (a) explain the AE progression after the experiment and
  - (b) control it during the experiment ?

Is there a problem with this type of automated experiment?

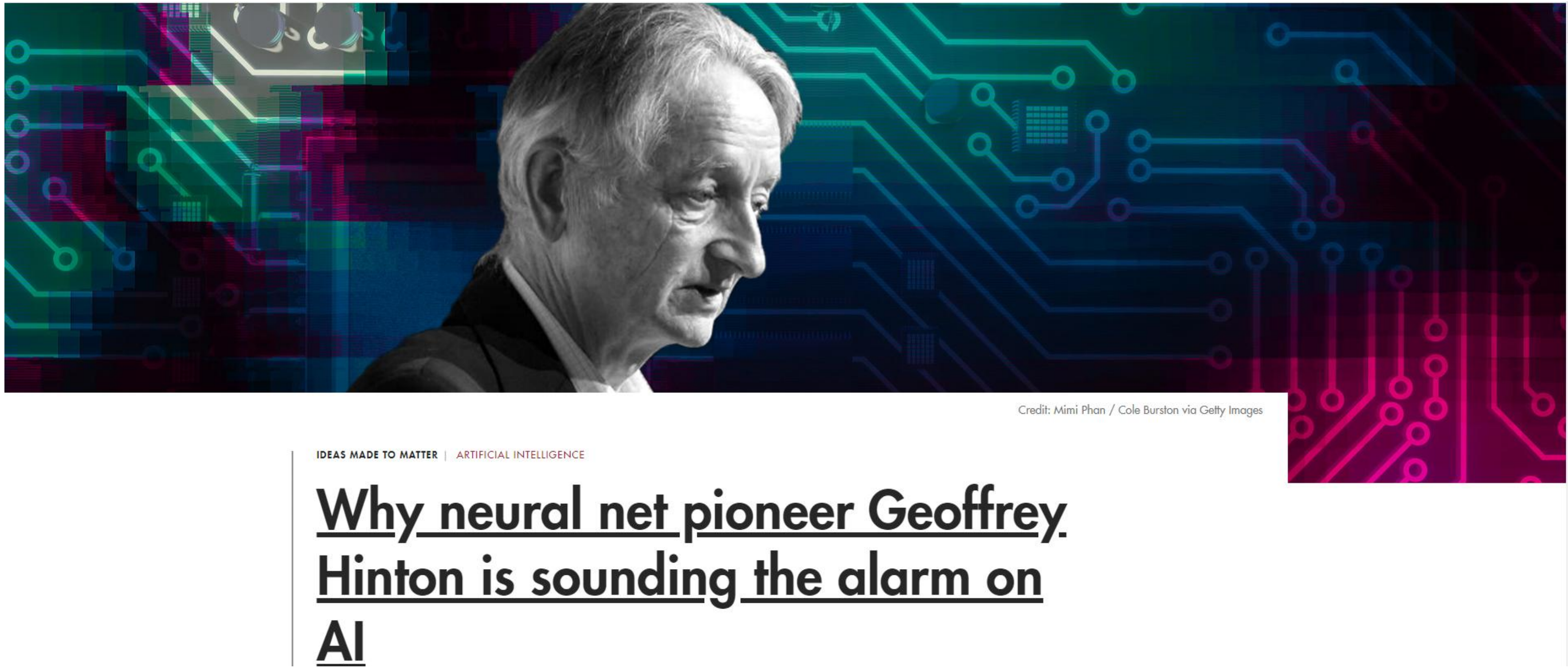
Taking the Human Out of the Loop: A Review of Bayesian Optimization

Citation

Shahriari, Bobak, Kevin Swersky, Ziyu Wang, Ryan P. Adams, and Nando de Freitas. 2016. "Taking the Human Out of the Loop: A Review of Bayesian Optimization." Proc. IEEE 104 (1) (January): 148–175. doi:10.1109/jproc.2015.2494218.

Published Version

doi:10.1109/JPROC.2015.2494218



Credit: Mimi Phan / Cole Burston via Getty Images

IDEAS MADE TO MATTER | ARTIFICIAL INTELLIGENCE

Why neural net pioneer Geoffrey Hinton is sounding the alarm on AI

Solution: if we can monitor in real time, we can adjust rewards and policies!

Interactive AI

Human-in-the-loop Automated Experiment

Policies:

- **A/B testing:** separate exploration and exploitation
- **Epsilon-greedy:** dedicate part of the budget to exploration
- **UCB:** balance exploration and exploitation giving preference to selections that are more likely to be positive/are less explored
- **Thompson sampling:** draw from probability distribution

Thompson sampling

$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)}$$

- Initially, we don't have any reason to believe that the parameter is high or low for a given ad. Therefore, it makes sense to assume that $\boldsymbol{\theta_k}$ has a uniform distribution [0,1].

- Assume that we display the ad $\boldsymbol{k}$ and it results in a click. We take this as a signal to update the probability distribution for $\boldsymbol{\theta_k}$ so that the expected value shifts a little bit towards 1.

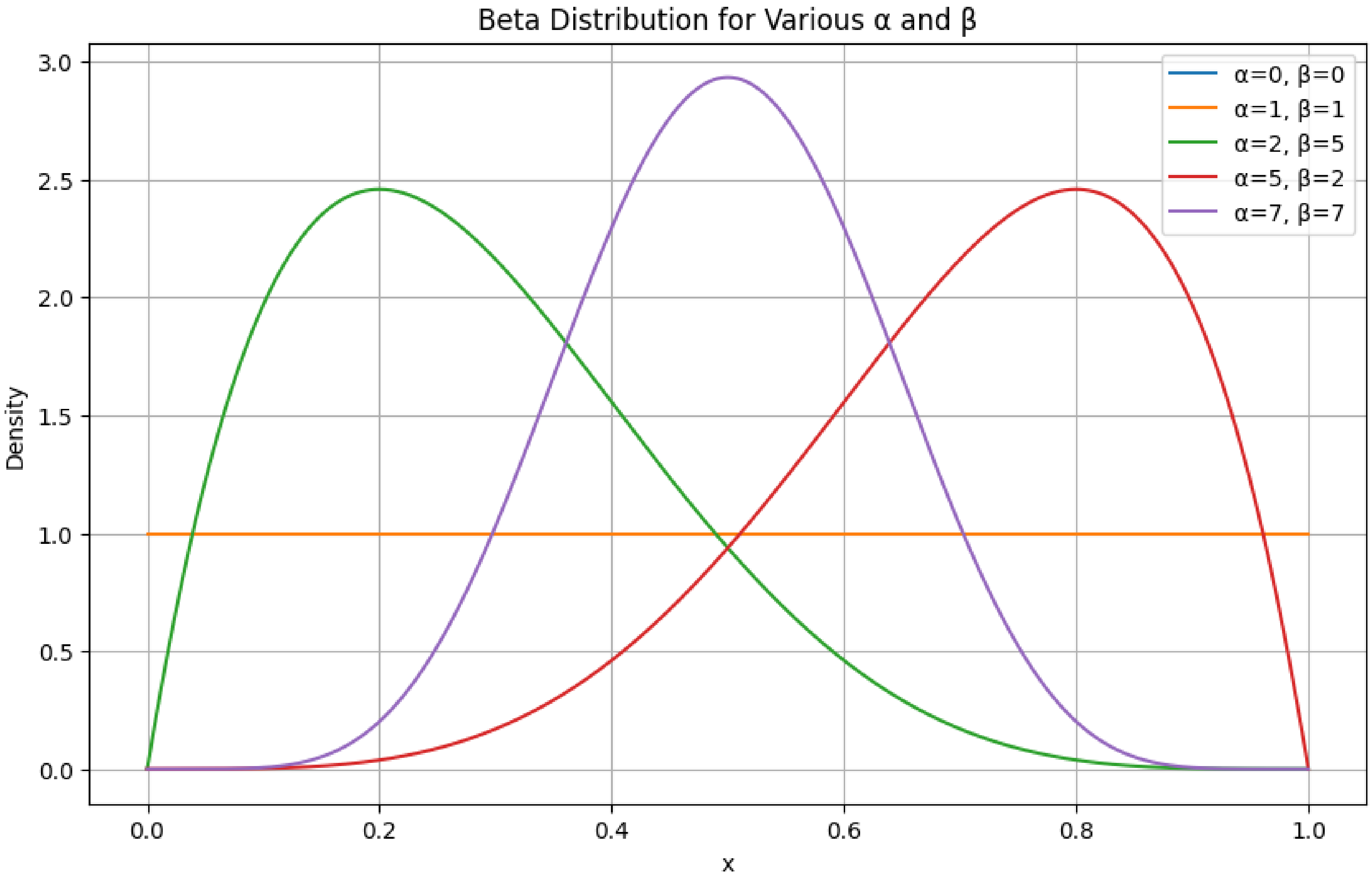
- As we collect more and more data, we should also see the variance estimate for the parameter shrink. Thompson sampling does it using Bayesian inference.

- This method tells us to take a sample from the posterior distribution of the parameter, $\boldsymbol{p(\theta_k|X)}$ If the expected value of $\boldsymbol{\theta_k}$ is high, we are likely to get samples closer to 1. If the variance is high because ad k has not been selected many times that far, our samples will also have high variance, which will lead to exploration.

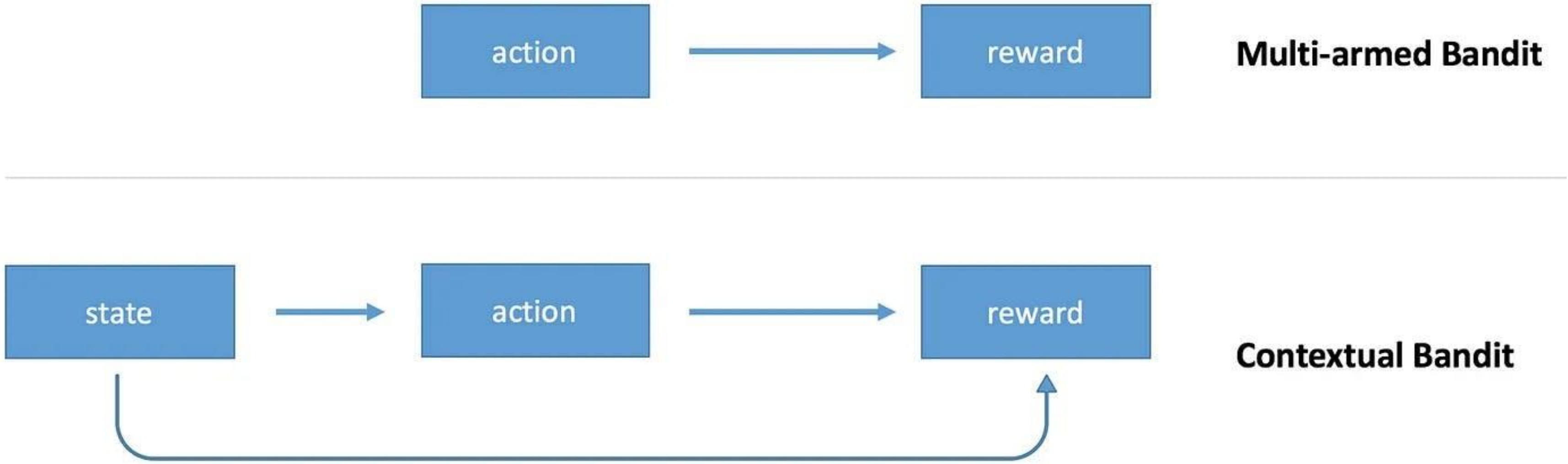
From Enes Bilgin, Mastering Reinforcement Learning with Python, Packt 2020

Thompson sampling: first taste of Bayes

$$p(\theta_k) = \frac{\theta_k^{\alpha_k - 1} \cdot (1 - \theta_k)^{\beta_k - 1}}{B(\alpha_k, \beta_k)}.$$



Contextual Bandits



- In contextual bandits the decision-making process is informed by the context.

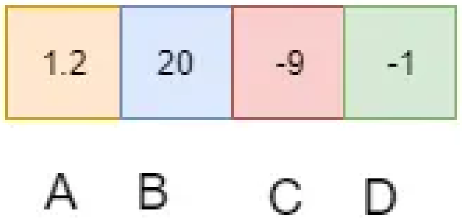
- The context, in this case, refers to a set of observable variables that can impact the result of the action.

- This addition makes the bandit problem closer to real-world applications, such as personalized recommendations, clinical trials, or ad placement, where the decision depends on specific circumstances.

https://hackernoon.com/contextual-multi-armed-bandit-problems-in-reinforcement-learning

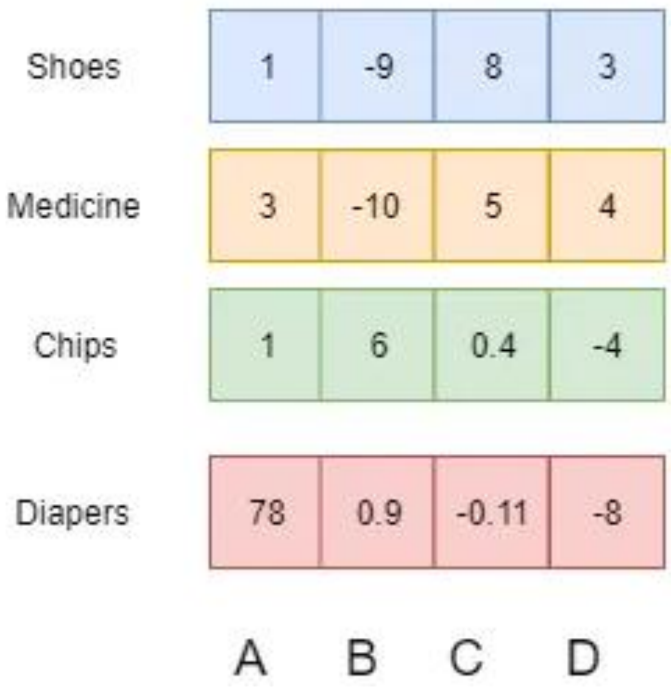
Simple example

Bandit



A	B	C	D
1.2	20	-9	-1

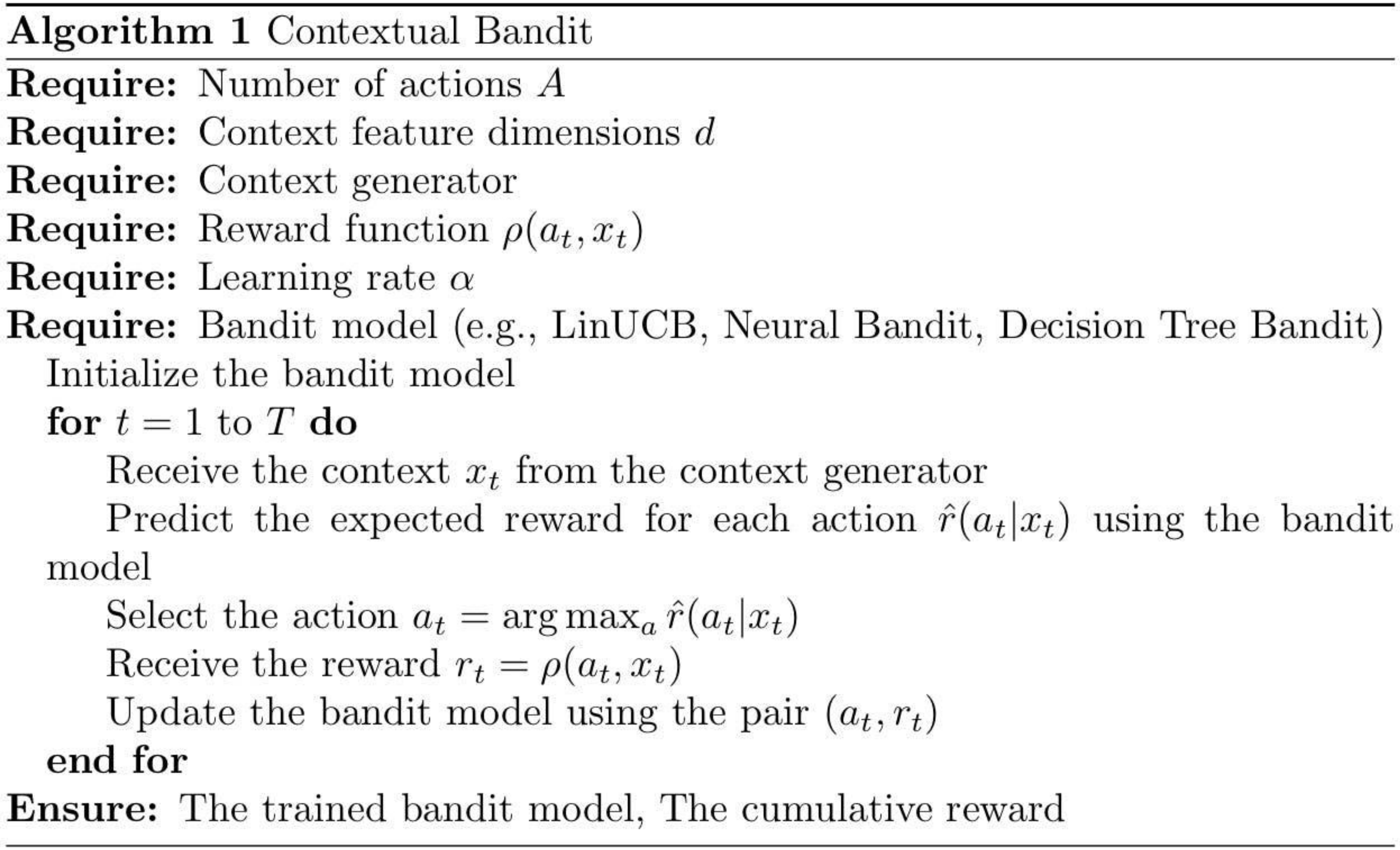
Contextual Bandit



	A	B	C	D
Shoes	1	-9	8	3
Medicine	3	-10	5	4
Chips	1	6	0.4	-4
Diapers	78	0.9	-0.11	-8

https://medium.com/data-science-in-your-pocket/contextual-bandits-in-reinforcement-learning-explained-with-example-and-codes-3c707142437b

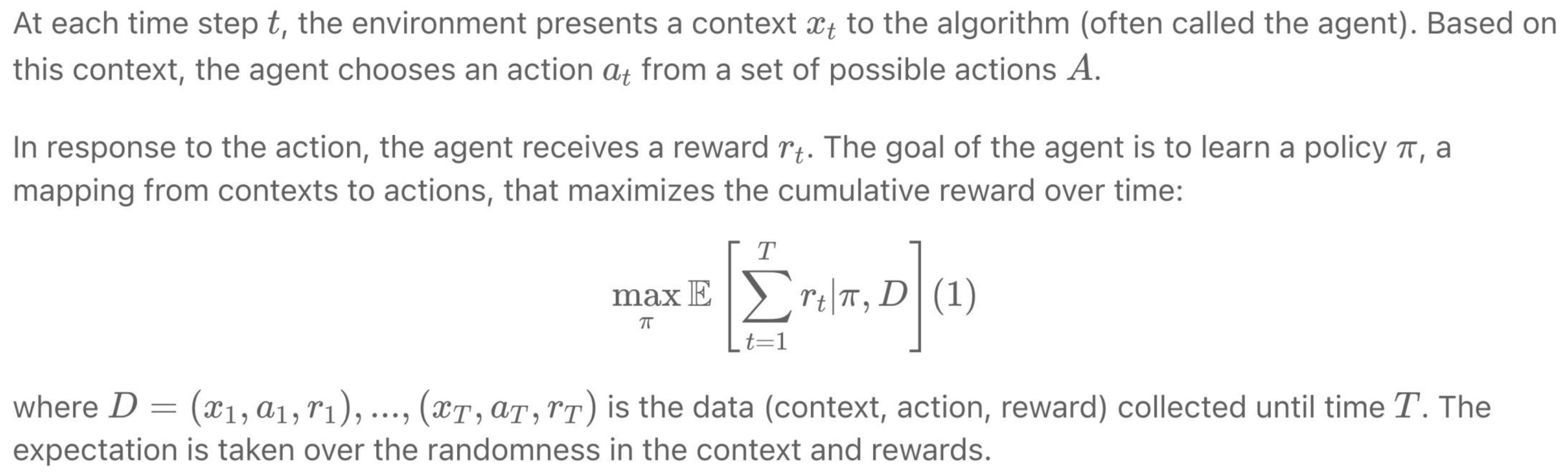
Contextual Bandits



```
Algorithm 1 Contextual Bandit
Require: Number of actions $A$
Require: Context feature dimensions $d$
Require: Context generator
Require: Reward function $\rho(a_t, x_t)$
Require: Learning rate $\alpha$
Require: Bandit model (e.g., LinUCB, Neural Bandit, Decision Tree Bandit)
  Initialize the bandit model
  for $t = 1$ to $T$ do
    Receive the context $x_t$ from the context generator
    Predict the expected reward for each action $\hat{r}(a_t|x_t)$ using the bandit model
    Select the action $a_t = \arg\max_a \hat{r}(a_t|x_t)$
    Receive the reward $r_t = \rho(a_t, x_t)$
    Update the bandit model using the pair $(a_t, r_t)$
  end for
Ensure: The trained bandit model, The cumulative reward
```

https://hackernoon.com/contextual-multi-armed-bandit-problems-in-reinforcement-learning

Contextual Bandits



At each time step t, the environment presents a context x_t to the algorithm (often called the agent). Based on this context, the agent chooses an action a_t from a set of possible actions A.

In response to the action, the agent receives a reward r_t. The goal of the agent is to learn a policy π, a mapping from contexts to actions, that maximizes the cumulative reward over time:

$$\max_{\pi} \mathbb{E}\left[\sum_{t=1}^{T} r_t|\pi, D\right] (1)$$

where $D = (x_1, a_1, r_1), ..., (x_T, a_T, r_T)$ is the data (context, action, reward) collected until time T. The expectation is taken over the randomness in the context and rewards.

- The goal of the algorithm is to maximize the cumulative reward over some time horizon.
- In each round, the reward for only the chosen action is observed.
- This is known as partial feedback, which differentiates bandit problems from supervised learning

https://hackernoon.com/contextual-multi-armed-bandit-problems-in-reinforcement-learning

Linear UCB

$$\mathbb{E}[r|x,a] = x^T\theta_a(1)$$

$\mathbb{E}[r|x,a] = x^T\theta_a$ is the expected reward of action a given context x under the linear model
θ_a is the parameter vector for action a.
The objective is to learn θ_a for all actions based on the data.

$\Rightarrow$ At each time step t, given context x_t, LinUCB selects the action a_t that has the maximum UCB:

$$a_t = \arg\max_{a\in A}\left(x_t^T\theta_a + \alpha\sqrt{x_t^T A_a^{-1} x_t}\right)$$

A_a is a matrix that keeps track of the features seen so far for action a,
α is a parameter controlling the trade-off between exploration and exploitation,
the second term is the UCB, which is proportional to the standard deviation of the estimated reward.

Linear UCB Update

Chosen action:

$$a_t = \arg\max_{a \in A} \left(x_t^T \theta_a + \alpha \sqrt{x_t^T A_a^{-1} x_t} \right)$$

Model updates:

$$A_a = A_a + x_t x_t^T$$

$$b_a = b_a + r_t x_t$$

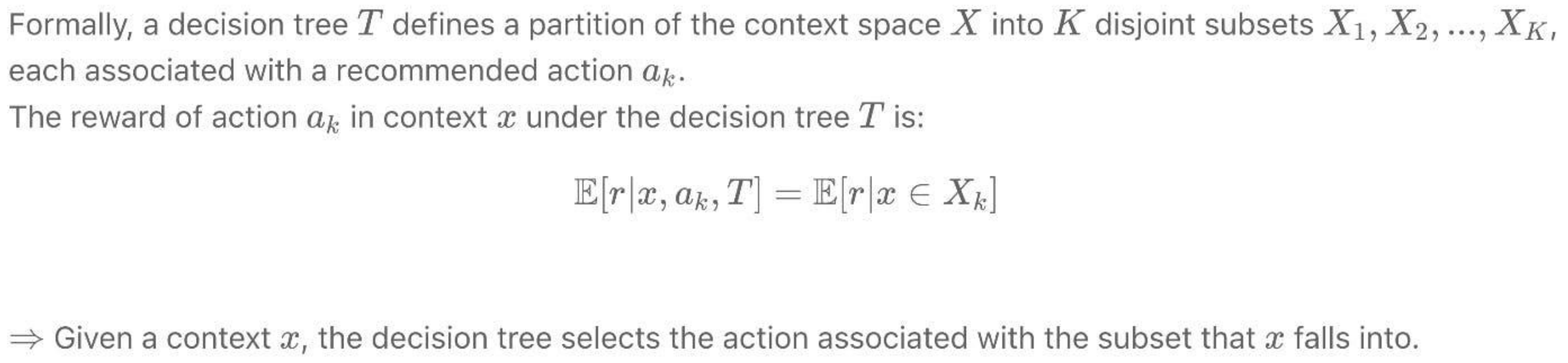
$$\theta_a = A_a^{-1} b_a$$

- LinUCB algorithm is a contextual bandit algorithm that models the expected reward of an action given a context as a linear function

- LinUCB it selects actions based on the Upper Confidence Bound (UCB) principle to balance exploration and exploitation.

- It exploits the best option available according to the linear, but it also explores options that could potentially provide higher rewards, considering the uncertainty in the model's estimates.

Decision Tree cMAB



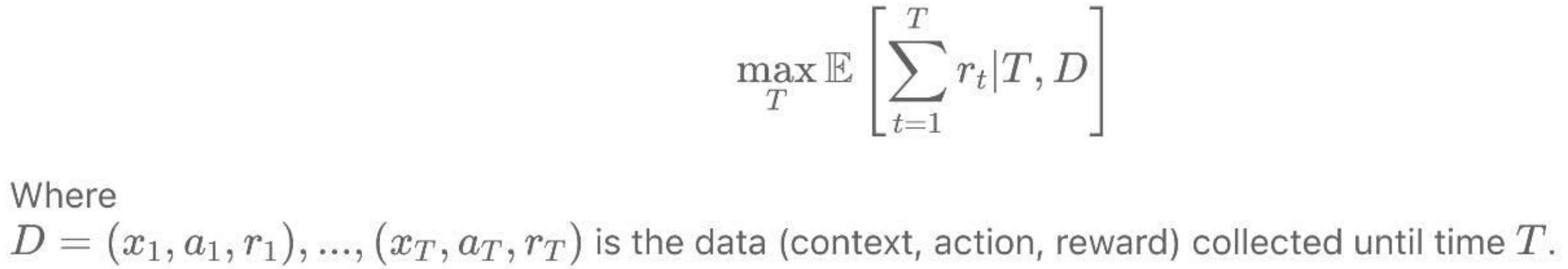
Formally, a decision tree T defines a partition of the context space X into K disjoint subsets $X_1, X_2, ..., X_K$, each associated with a recommended action a_k.

The reward of action a_k in context x under the decision tree T is:

$$\mathbb{E}[r|x, a_k, T] = \mathbb{E}[r|x \in X_k]$$

⇒ Given a context x, the decision tree selects the action associated with the subset that x falls into.

The objective is to learn the best decision tree that maximizes the expected cumulative reward:



$$\max_T \mathbb{E}\left[\sum_{t=1}^{T} r_t | T, D\right]$$

Where

$D = (x_1, a_1, r_1), ..., (x_T, a_T, r_T)$ is the data (context, action, reward) collected until time T.

Decision Tree Bandit models the reward function as a decision tree, where each leaf node corresponds to an action and each path from the root to a leaf node represents a decision rule based on the context. It performs exploration and exploitation through a statistical framework, making splits and merges in the decision tree based on statistical significance tests.

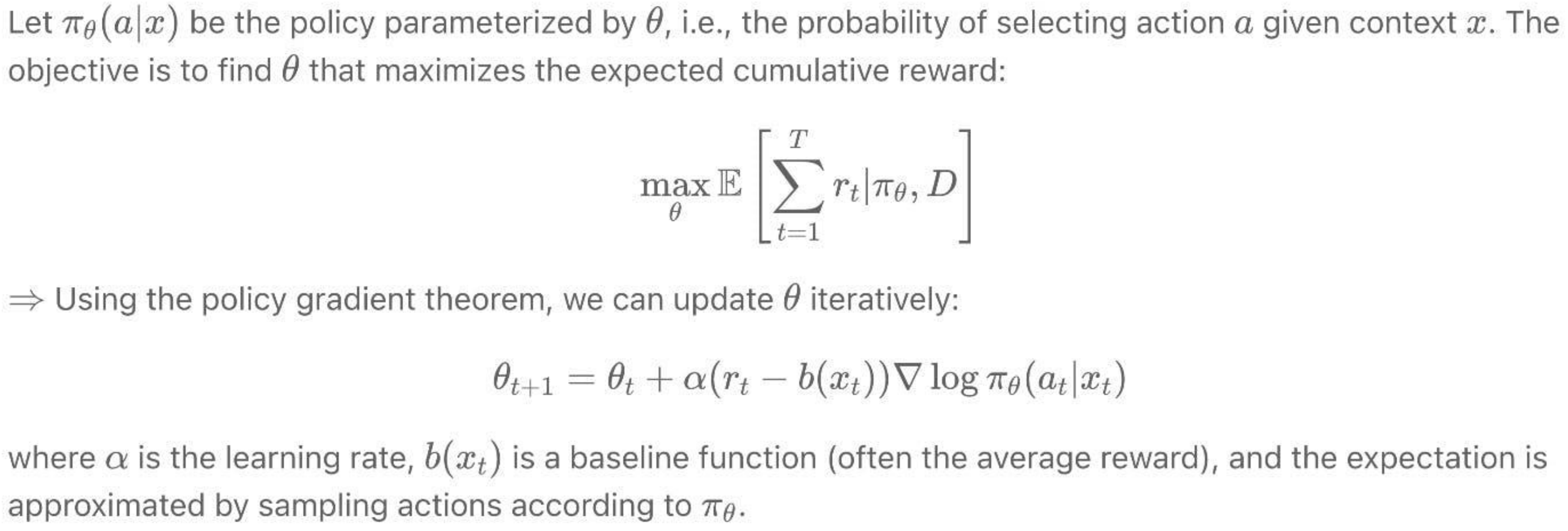
Neural Network cMAB

- Deep learning models can be used to approximate the reward function in high-dimensional or non-linear cases. The policy is typically a neural network that takes the context and available actions as input and outputs the probabilities of taking each action.

- A popular deep learning approach is to use an actor-critic architecture, where one network (the actor) decides which action to take, and the other network (the critic) evaluates the action taken by the actor.

- For more complex scenarios where the relationship between the context and the reward is not linear, we can use a neural network to model the reward function. One popular method is to use a policy gradient method, such as REINFORCE or actor-critic.

Neural Network cMAB



Let $\pi_\theta(a|x)$ be the policy parameterized by θ, i.e., the probability of selecting action a given context x. The objective is to find θ that maximizes the expected cumulative reward:

$$\max_\theta \mathbb{E}\left[\sum_{t=1}^{T} r_t | \pi_\theta, D\right]$$

$\Rightarrow$ Using the policy gradient theorem, we can update θ iteratively:

$$\theta_{t+1} = \theta_t + \alpha(r_t - b(x_t))\nabla \log \pi_\theta(a_t|x_t)$$

where α is the learning rate, $b(x_t)$ is a baseline function (often the average reward), and the expectation is approximated by sampling actions according to π_θ.

- Neural Bandit uses neural networks to model the reward function, taking into account the uncertainty in the parameters of the neural network.
- It further introduces exploration through policy gradients where it updates the policy in the direction of higher rewards.
- This form of exploration is more directed, which can be beneficial in large action spaces.

LinUCB: The Linear Upper Confidence Bound (LinUCB) model uses linear regression to estimate the expected reward for each action given a context. It also keeps track of the uncertainty of these estimates and uses it to encourage exploration.

Advantages:

- It is simple and computationally efficient.
- It provides theoretical guarantees for its regret bound.

Disadvantages:

- It assumes the reward function is a linear function of the context and action, which may not hold for more complex problems.

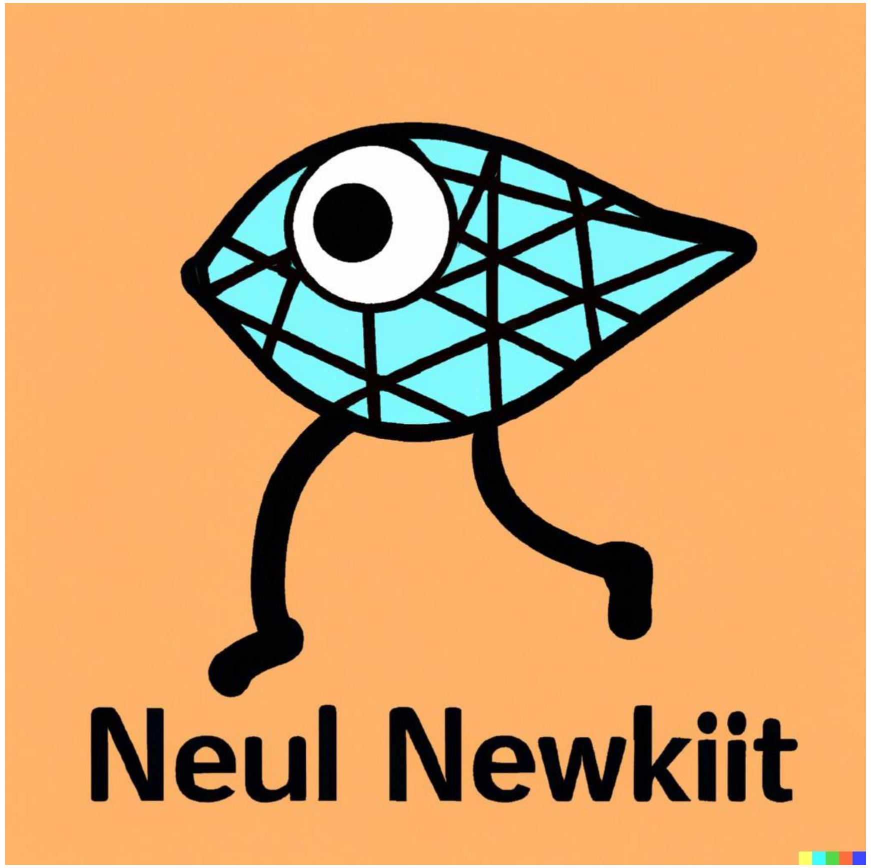
Decision Tree Bandit: The Decision Tree Bandit model represents the reward function as a decision tree. Each leaf node corresponds to an action, and each path from the root to a leaf node represents a decision rule based on the context.

Advantages:

- It provides interpretable decision rules.
- It can handle complex reward functions.

Disadvantages:

- It may suffer from overfitting, especially for large trees.
- It requires tuning hyperparameters such as the maximum depth of the tree.



Neural Bandit: The Neural Bandit model uses a neural network to estimate the expected reward for each action given a context. It uses policy gradient methods to encourage exploration.

Advantages:

- It can handle complex, non-linear reward functions.
- It can perform directed exploration, which is beneficial in large action spaces.

Disadvantages:

- It requires tuning hyperparameters such as the architecture and learning rate of the neural network.
- It may be computationally expensive, especially for large networks and large action spaces.

Multistage decisions

There is no computation without representation!

- Learn algorithms: from simple to complex ones
- Learn new concepts that emerge as a part of ML, e.g. VAE, decision making, etc.
- Learn how to represent the system in the ML setting
- Learn how to formulate the reward functions