THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 18: Decisions and Bandits

Instructor: Sergei V. Kalinin

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

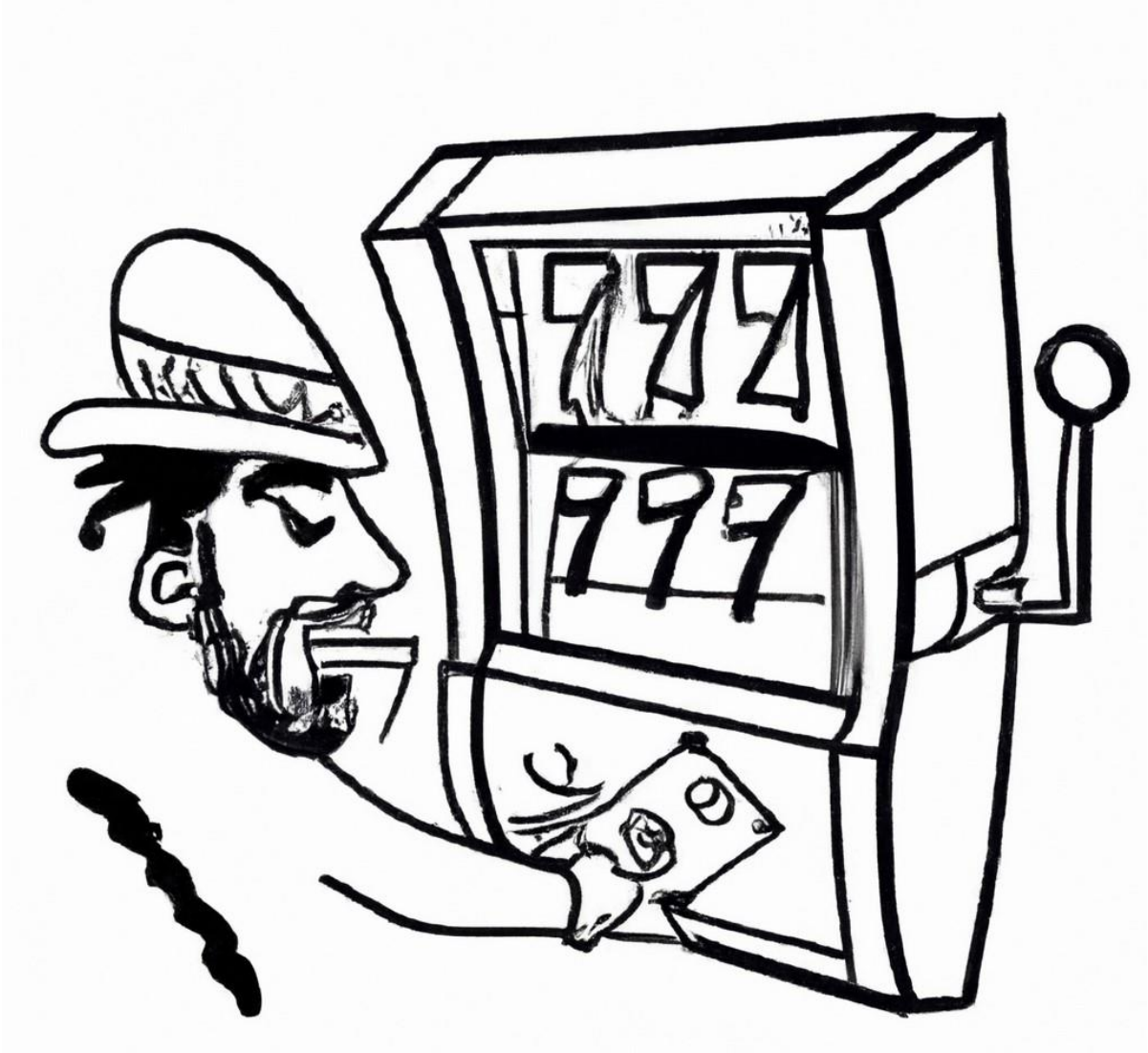
- **Value:** expected reward. Difference between reward and value is a feedback signal for multiple types of active learning

- **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

Bandit problem



- Imagine that we have a number of slot machines with different probabilities of win…
- Or different web-sites to places ads on…
- Or groups of patients for specific medical protocol….
- Or team members to synthesize certain material…
- Or reaction pathways to choose

How do we optimize this problem and maximize our reward?

Bandits

- **Objective:** get rich!
- **Reward:** pay-off from specific hand/click-rate of ad/effectiveness of drug
- **Value:** expected reward
- **Action:** playing a hand/placing ad/administering drug
- **State:** no state
- **Policy:** gameplan given the values of specific actions

A/B Testing

- The most common exploration strategy is **A/B testing**, a method to determine which one of the two alternatives (of online products, pages, ads etc.) performs better.
- The users are randomly split into two groups to try different alternatives. At the end of the testing period, the results are compared to choose the best alternative, which is then used in production for the rest of the problem horizon.
- This approach can be applied for more then two alternatives - **A/B/n testing**.

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

Definitions: reward and value

$$Q_n \triangleq \frac{R_1 + R_2 + \cdots + R_{n-1}}{n-1}$$

- First, we denote the reward (i.e. 1 for click, 0 for no click) received after selecting the action a for the n^{th} time by R_i.

- Q_n estimates the expected value of the reward that this action yields, R, after n-1 observations.

- Q_n is also called the action value of a. Here, Q_n estimates of the action value after selecting this action n - 1 times.

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

Updating value

$$Q_{n+1} = \frac{R_1 + R_2 + \cdots + R_n}{n} = Q_n + \frac{1}{n} \cdot (R_n - Q_n)$$

- Q_n is the estimate for the action value of a before we take it for the n^{th} time.
- When we observe the reward R_n, it gives us another signal for the action value.
- We adjust our current estimate, Q_n, in the direction of the **error** that we calculate based on the latest observed reward, R_n, with a **step size** $1/n$ and obtain a new estimate Q_{n+1}
- For convenience, $Q_0 = 0$ (But - Human heuristics!)

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

Updating value: generalization

$$Q_{n+1}(a) = Q_n(a) + \alpha(R_n(\alpha) - Q_n(a))$$

- The rate at which we adjust our estimate will get smaller as we make more observations
- The step size must be smaller than 1 for the estimate to converge (and larger than 0 for a proper update).
- Using a fixed α will make the weights of the older observations to decrease exponentially as we take action a more and more.

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

Limitations of A/B testing

- **A/B/n testing is inefficient as it does not modify the experiment dynamically by learning from the observations.** It fails to benefit from the early observations in the test by writing off/promoting an alternative even if it is obviously under- or outperforming the others.

- **It is unable to correct a decision once it's made.** There is no way to correct the decision for the rest of the deployment horizon.

- **It is unable to adapt to the changes in a dynamic environment.** If the underlying reward distributions change over time, plain A/B/n testing has no way of detecting such changes after the selection is fixed.

- **The length of the test period is a hyperparameter to tune, affecting the efficiency of the test.** If this period is chosen to be shorter than needed, an incorrect alternative could be declared the best because of the noise in the observations. If the test period is chosen to be too long, too much money gets wasted in exploration.

- **A/B/n testing is simple.** Despite all these shortcomings, it is intuitive and easy to implement, therefore widely used in practice

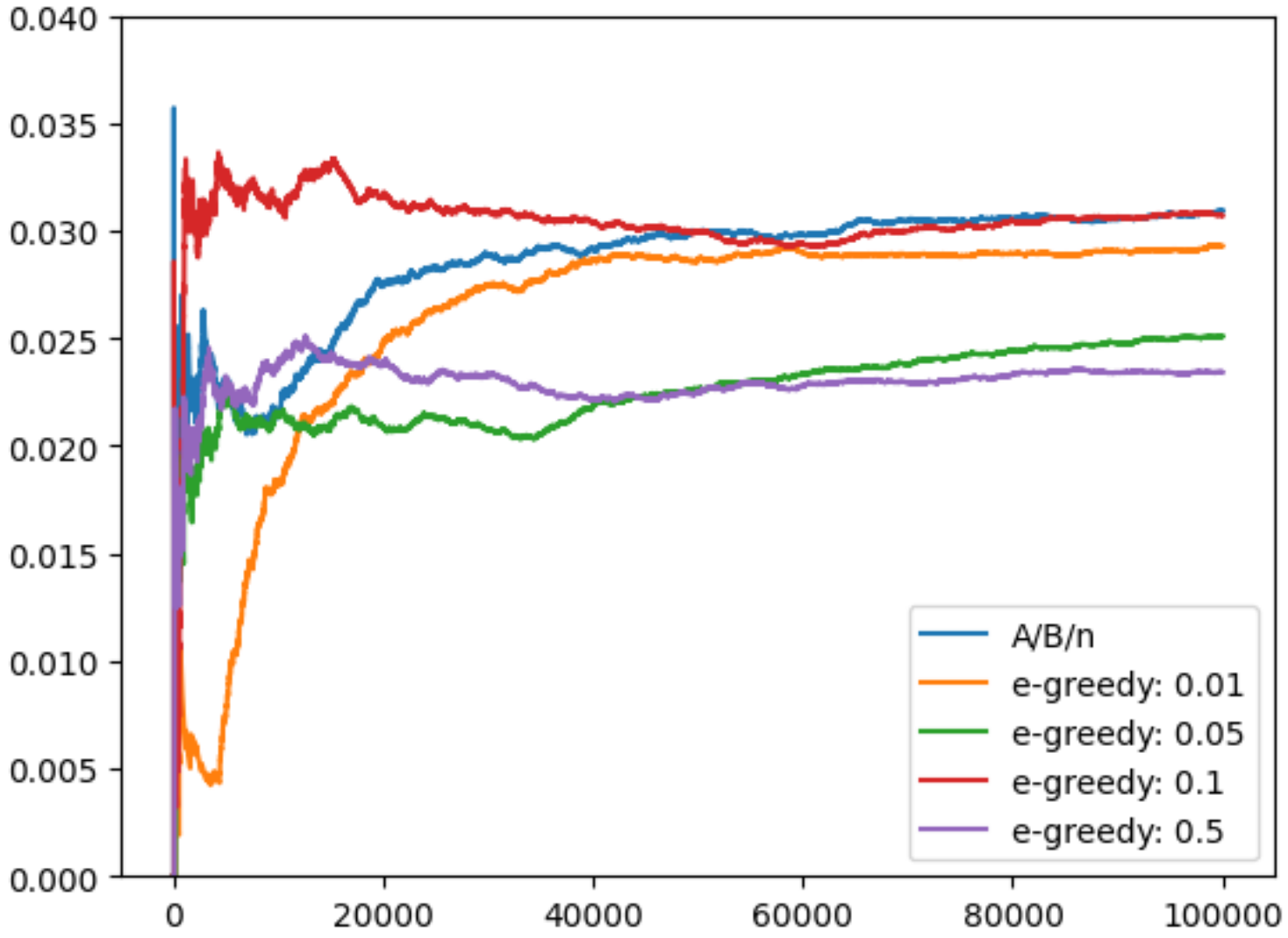
From Enes Bilgin, Mastering Reinforcement Learning with Python, Packt 2020

ε-greedy policies

- Most of the time, greedily taking the action that is the best according to the rewards observed that far in the experiment (i.e. with 1-ε probability)
- Once in a while (i.e. with ε probability) take a random action regardless of the action performances.
- Here ε is a number between 0 and 1, usually closer to zero (e.g. 0.1) to "exploit" in most decisions.
- Obviously, the number of alternatives has to be fairly small
- Parameter ε can change during the experiment

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

ε-greedy policies



A/B vs. ε-greedy policies

- ε-greedy actions and A/B/n tests are similarly inefficient and static in allocating the exploration budget. The ε-greedy approach, too, fails to write off actions that are clearly bad and continues to allocate the same exploration budget to each alternative. Similarly, if a particular action is under-explored/over-explored at any point, the exploration budget is not adjusted accordingly.

- With ε-greedy actions, exploration is continuous, unlike in A/B/n testing. This means if the environment is not stationary, the ε-greedy approach has the potential to pick up the changes and modify its selection of the best alternative.

- The ε-greedy actions approach could be made more efficient by dynamically changing the ε. For example, one could start with a high ε to explore more at the beginning and gradually decrease it to exploit more later. This way, there is still continuous exploration, but not as much as at the beginning when there was no knowledge of the environment.

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

A/B vs. ε-greedy policies

The ε-greedy actions approach could be made more dynamic by increasing the importance of the more recent observations:

$$Q_{n+1}(a) = Q_n(a) + \alpha(R_n(a) - Q_n(a))$$

- **Modifying the ε-greedy actions approach introduces new hyperparameters, which need to be tuned.**
- Both gradually diminishing ε and using exponential smoothing for *Q*, come with additional hyperparameters, and it may not be obvious what values to set these to.
- Incorrect selection of these hyperparameters may lead to worse results than what the standard version would yield.

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

Upper Confidence Bound (UCB)

$$A_t \triangleq \arg\max_a \left[Q_t(a) + c\sqrt{\frac{\ln t}{N_t(a)}} \right]$$

- At each step, we select the action that has the highest potential for reward.
- The potential of the action is calculated as the sum of the action value estimate and a measure of the uncertainty of this estimate. This sum is what we call the upper confidence bound.
- **Overall:** the action is selected either because our estimate for the action value is high, or the action has not been explored enough (i.e. as many times as the other ones) and there is high uncertainty about its value, or both.

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

Digging deeper: UCB

$$A_t \triangleq \arg\max_a \left[Q_t(a) + c\sqrt{\frac{\ln t}{N_t(a)}} \right]$$

- $Q_t(a)$ and $N_t(a)$ have the same meanings as before. This formula looks at the variable values, which may have been updated a while ago, at the time of decision making a, whereas the earlier formula described how to update them.
- In this equation, the square root term is a measure of the uncertainty for the estimate of the action value of a.
- The more we select a, the less we are uncertain about its value, and so is the $N_t(a)$ term in the denominator.
- As the time passes, however, the uncertainty grows due to the $\ln t$ term (which makes sense especially if the environment is not stationary), and more exploration is encouraged.
- The emphasis on uncertainty during decision making is controlled by a hyperparameter, c. This obviously requires tuning and a bad selection could diminish the value in the method.

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

Advantages and disadvantages of UCB

• **UCB is a set-and-forget approach.** It systematically and dynamically allocates the budget to alternatives that need exploration. If there are changes in the environment, for example, if the reward structure changes because one of the ads gets more popular for some reason, the method will adapt its selection of the actions accordingly.

• **UCB can be further optimized for dynamic environments, potentially at the expense of introducing additional hyperparameters.** The formula we provided for UCB is a common one, but it can be improved, for example, by using exponential smoothing. There are also more effective estimations of the uncertainty component in literature. These modifications, though, could potentially make the method more complicated.

• **UCB could be hard to tune.** It is somewhat easier make the call and say "I want to explore 10% of the time, and exploit for the rest" for the ε-greedy approach than saying "I want my uncertainty to be 0.729" for the UCB approach, especially if you are trying these methods on a brand-new problem. When not tuned, an UCB implementation could give unexpectedly bad results.

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

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

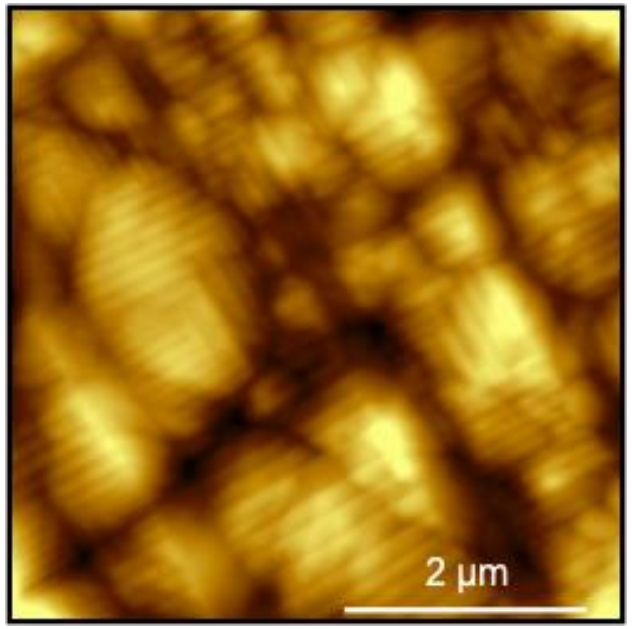
- **Value:** expected reward. Difference between reward and value is a feedback signal for multiple types of active learning

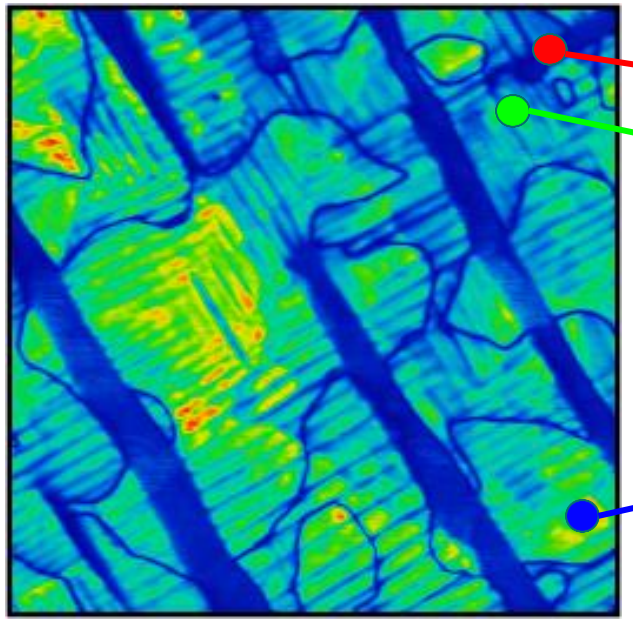
- **Action:** how can ML agent interact with the system

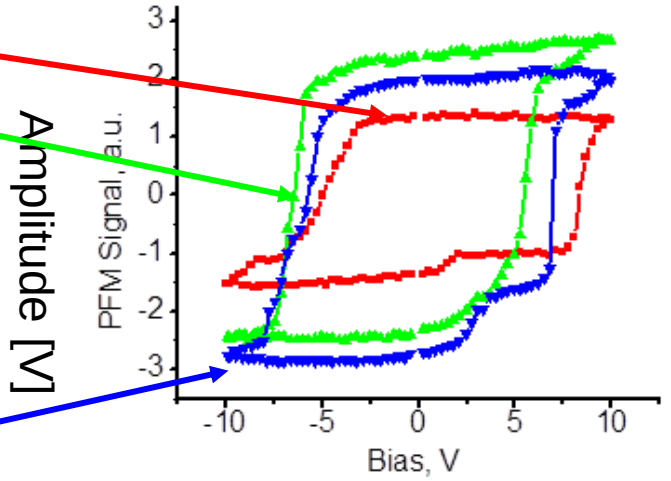
- **State:** information about the system available to ML agent

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

Rewards and policies in microscopy world

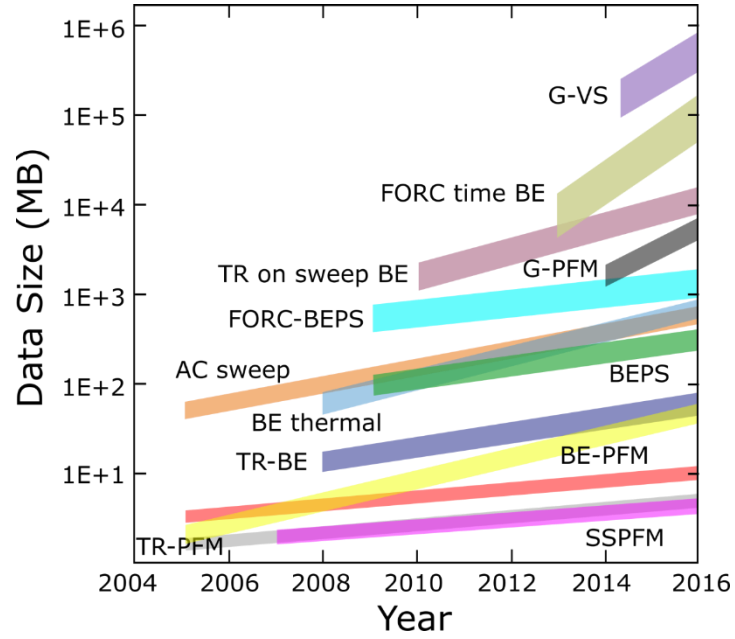






- Interesting functionalities are expected at the certain elements of domain structure
- We can guess some; we have to discover others

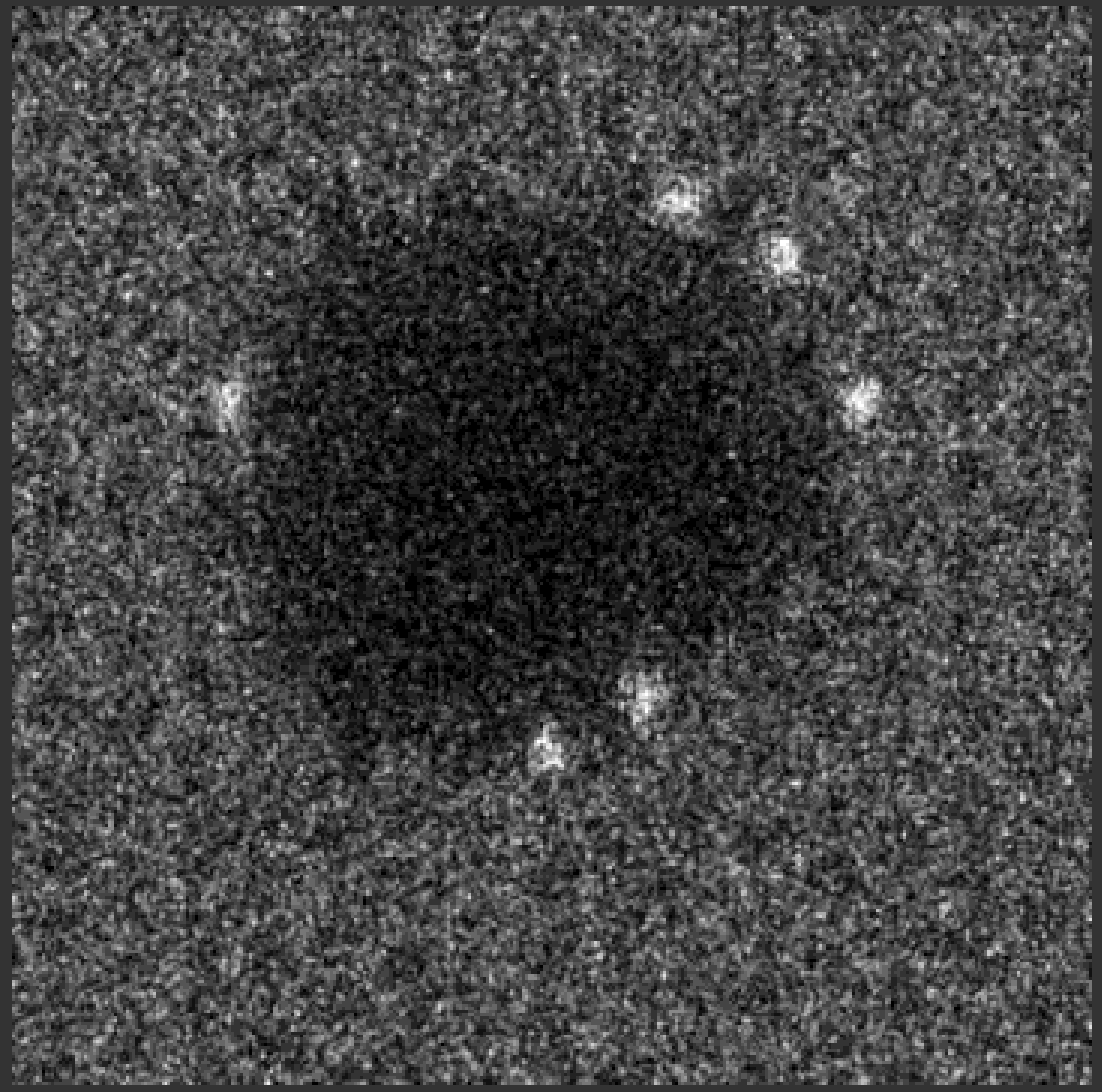
- **Experimental objectives → ML Rewards**
  - Microscope optimization
  - Properties of a priori known regions of interest
  - Discovery of regions with interesting properties
  - Physical theory falsification

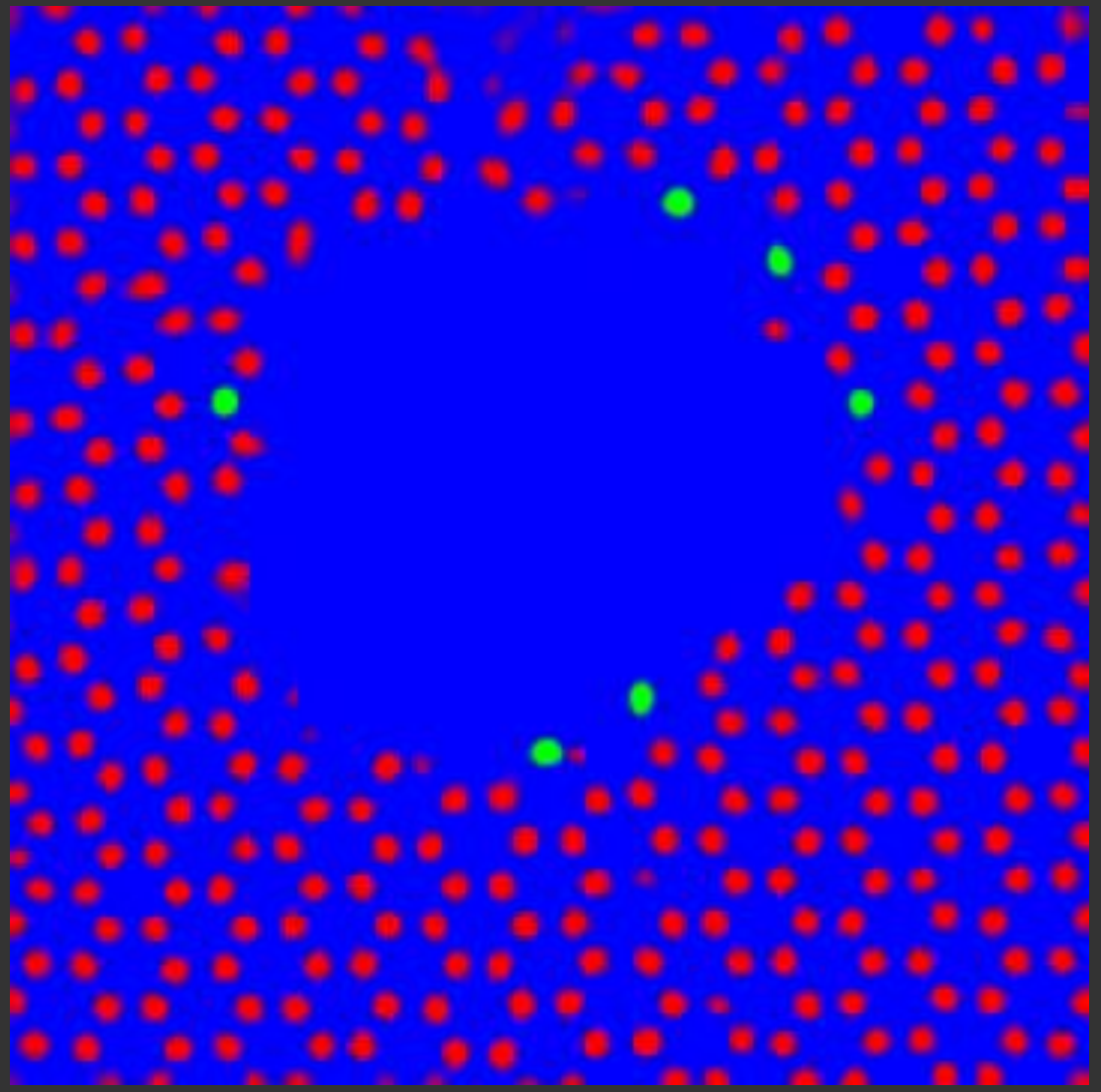


Fixed policy experiments

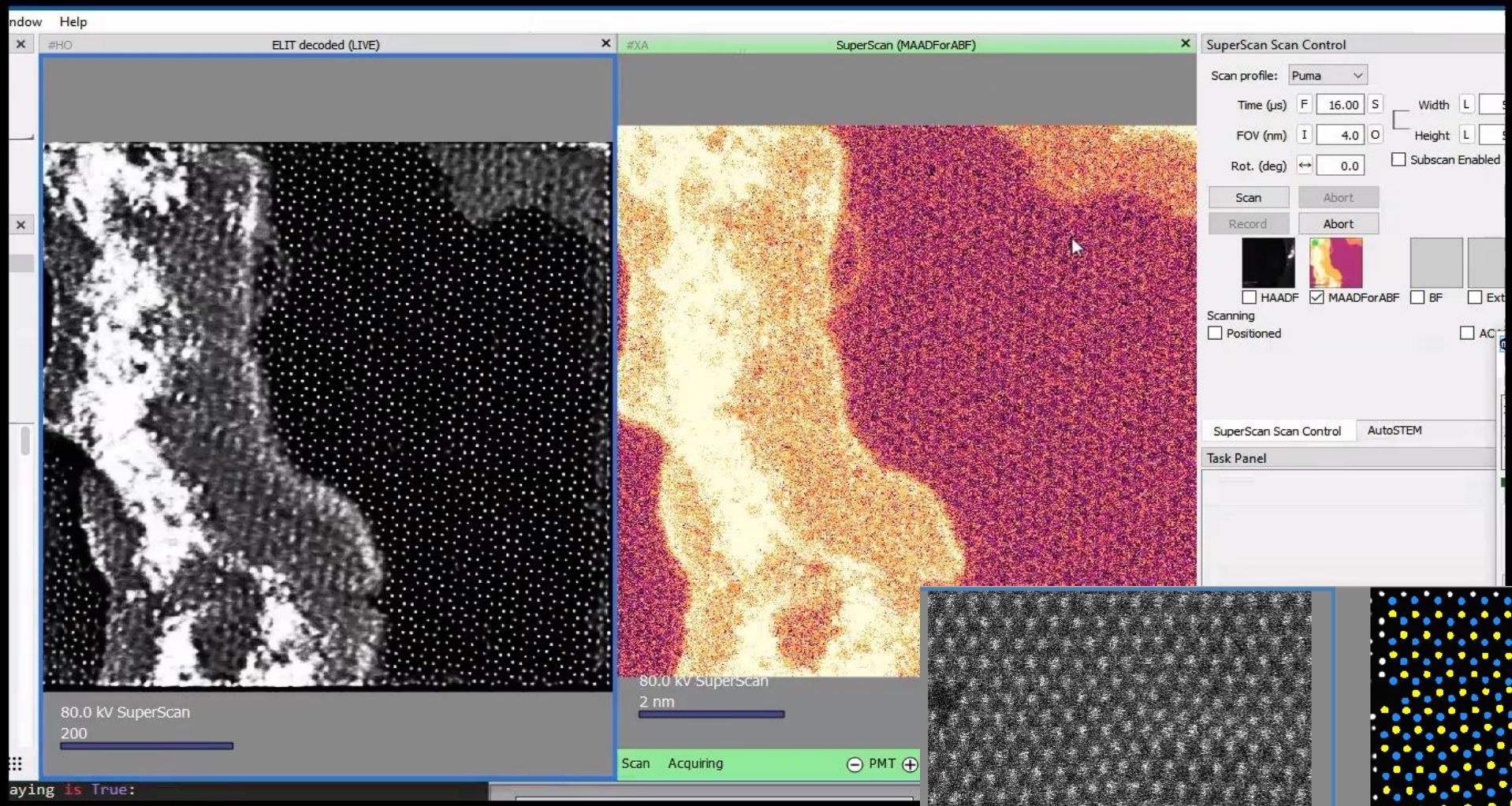
Deep learning works like a charm for:

- Drift correction
- Denoising
- Data processing/dimensionality reduction
- Feature finding (physics is in the training set)





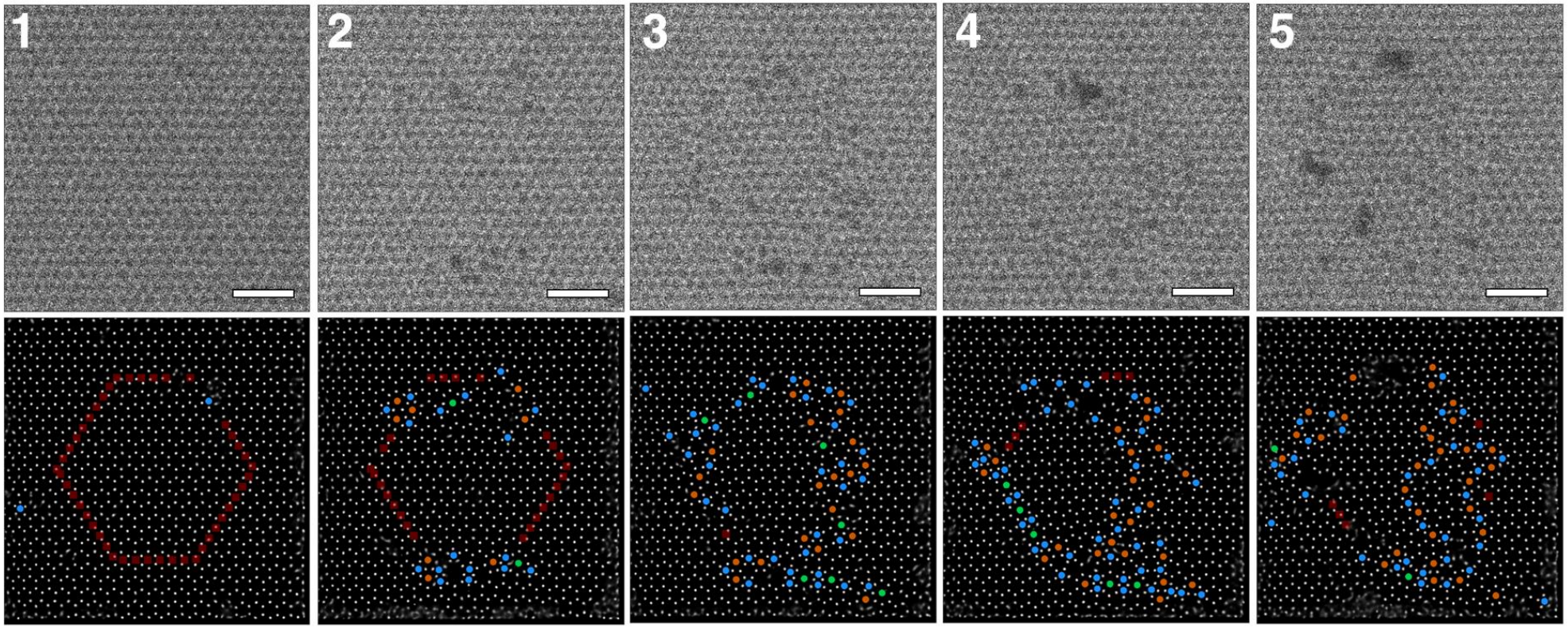
AE with Fixed Policies



Implementation: Kevin Roccapriore, Ayana Ghosh, Sergei V. Kalinin & Maxim Ziatdinov, 2021

Defect patterning in graphene

- Locate atomic coordinates (and defects)
- Direct beam in predetermined path to generate defects (vacancies) – unclear if they form / remain in place
- Repeat scan path, but avoid formed defects
- **Hexagon pattern**



What were we doing?

- **Objective(s):**
  - Understanding electronic and vibrational properties of defects
  - Building structures on the atomic level for biological sequencing and quantum sensing
  - … and so on. We will find out later!

- **Reward:**
  - The number of discovered defects (not used as feedback)
  - Atom moved in desired location

- **Value:** expected reward

- **Action:** position electron beam at given location, take EELS spectrum

- **State:** image

- **Policy:** fixed action table (if detect defect, take EELS)

File Edit View Insert Cell Kernel Widgets Help

Trusted gpuenv

Run Code

```
27
28
29
30 move_(-volt*2-(offsetvx), 0, 0-offsetvy, 0, move_speed)
```

scanning line #56

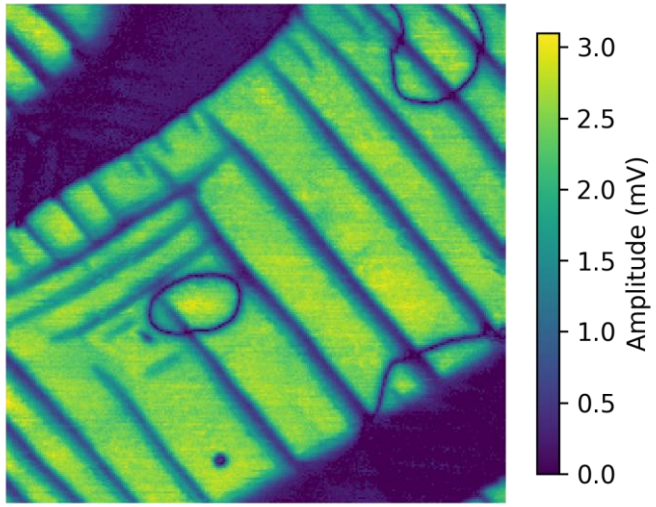
In [ ]:

```
1
```

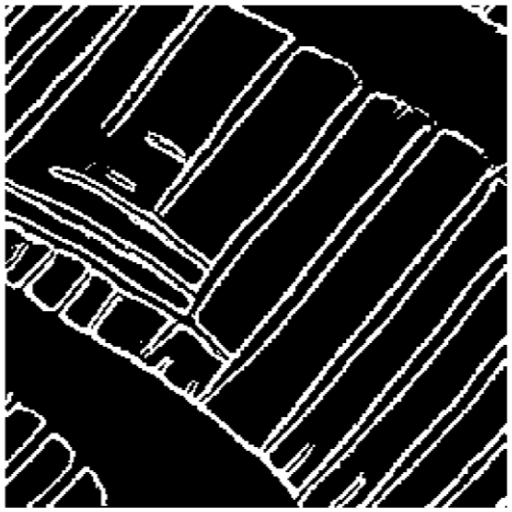
In [ ]:

```
1
```

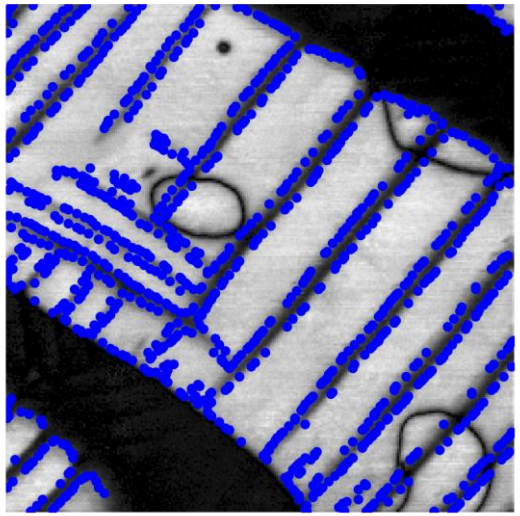
Mapping Activity of Domain Walls



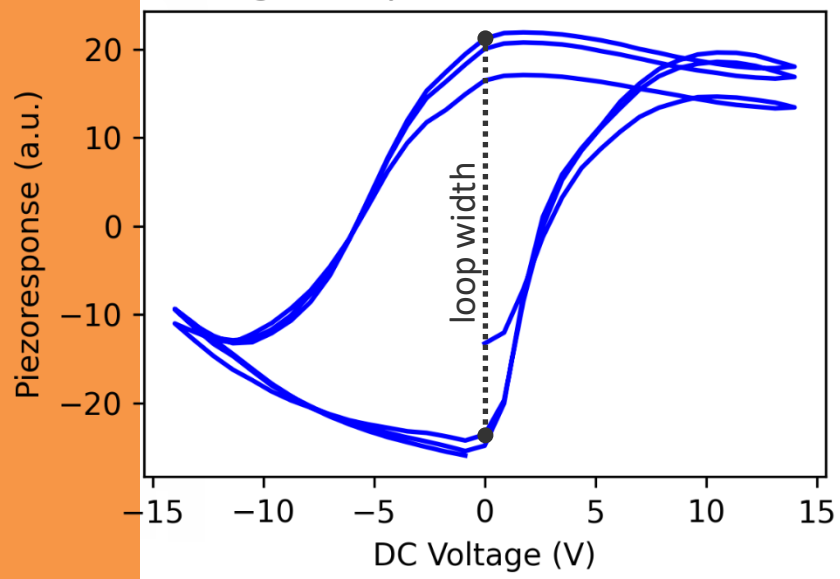
ResHedNet Prediction



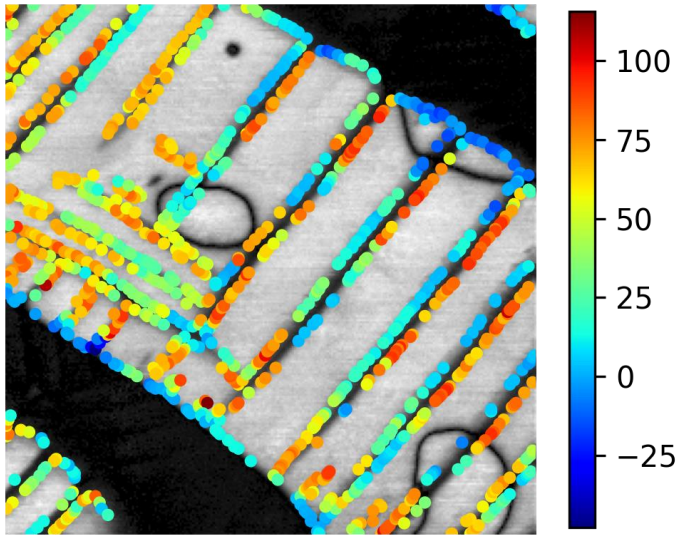
BEPS Measurement Points

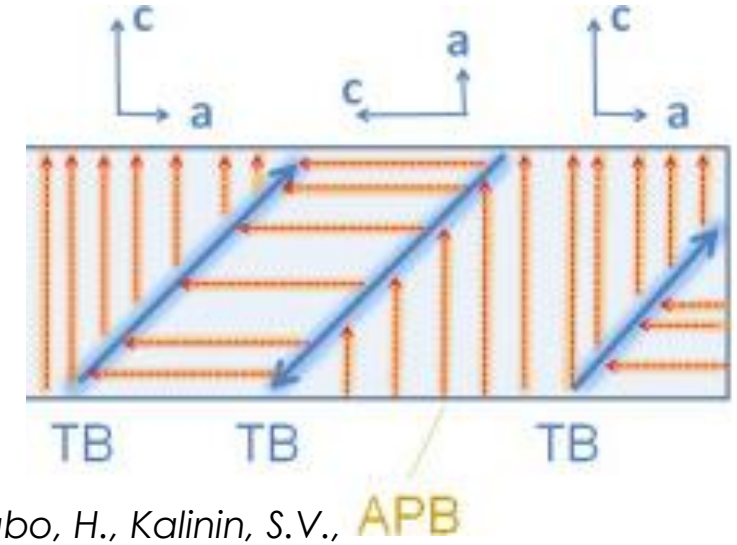


Averaged loop over ferroelastic walls



Loop height at ferroelastic walls





Liu, Y., Kelley, K.P., Funakubo, H., Kalinin, S.V., Ziatdinov, M., Arxiv, submitted

What were we doing?

- **Objective(s):**
  - Understanding the role of domain walls on polarization switching
  - Discover what makes these materials good piezoelectrics
  - … and so on. For fundamental research, vey often impact is clear later!

- **Reward:**
  - The number of explored domain walls (not used as feedback)

- **Value:** expected reward

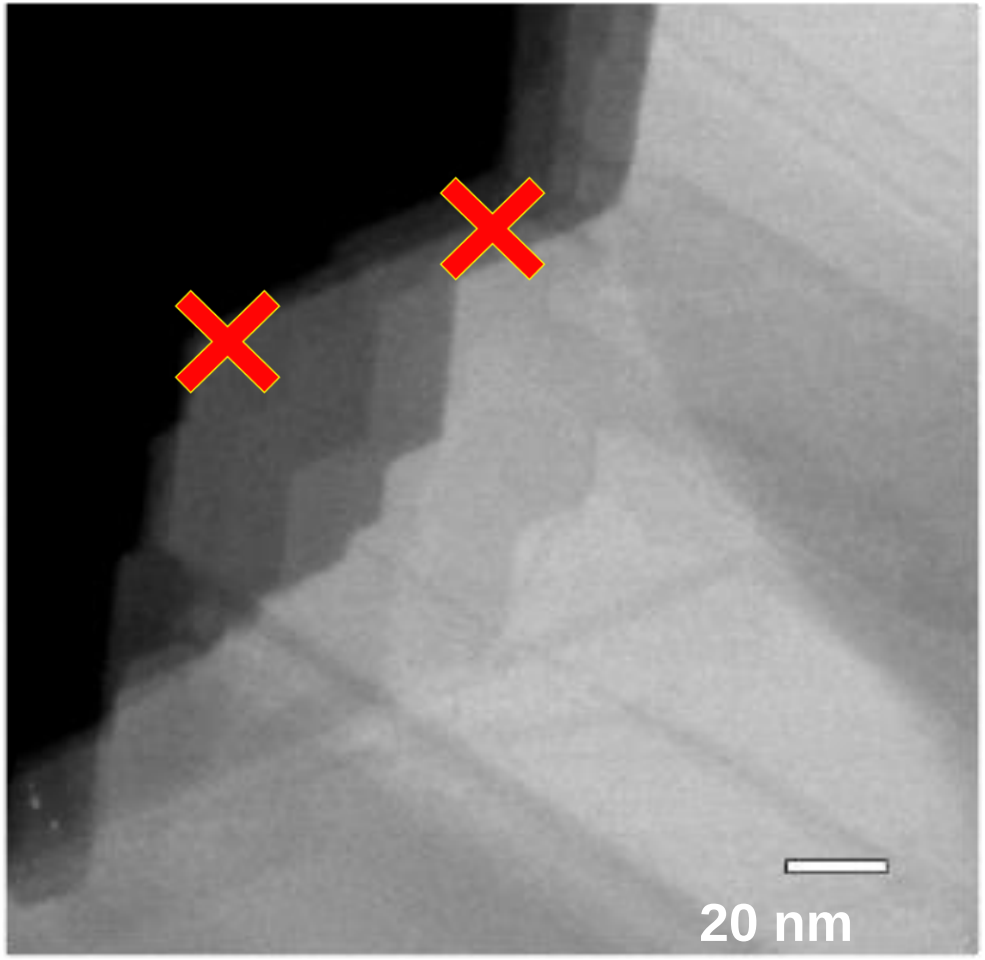
- **Action:** position SPM probe at a given location, take PFM spectrum

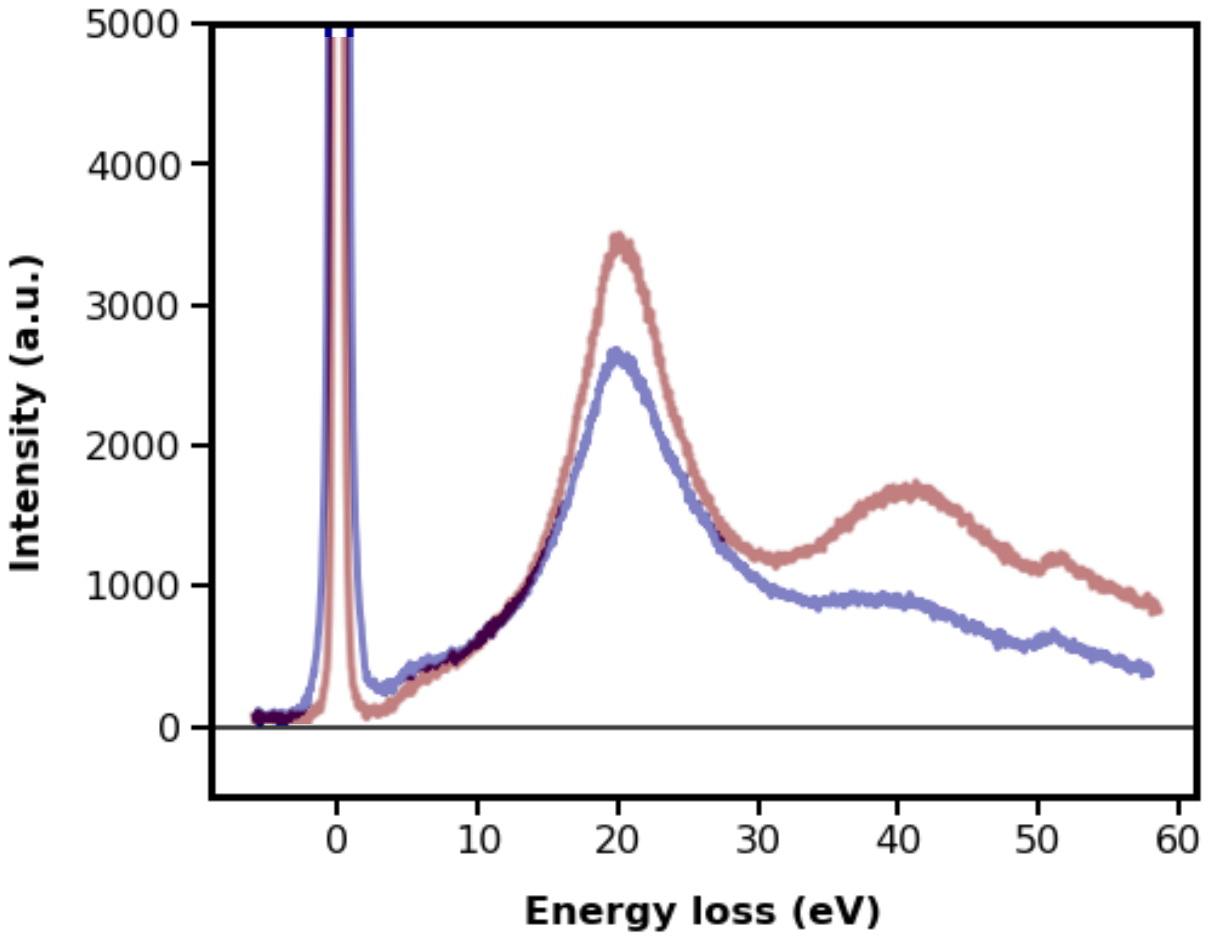
- **State:** image

- **Policy:** fixed action table (if detect wall, take spectrum)

Myopic policy experiments (basically, bandits)

From Static to Active Learning

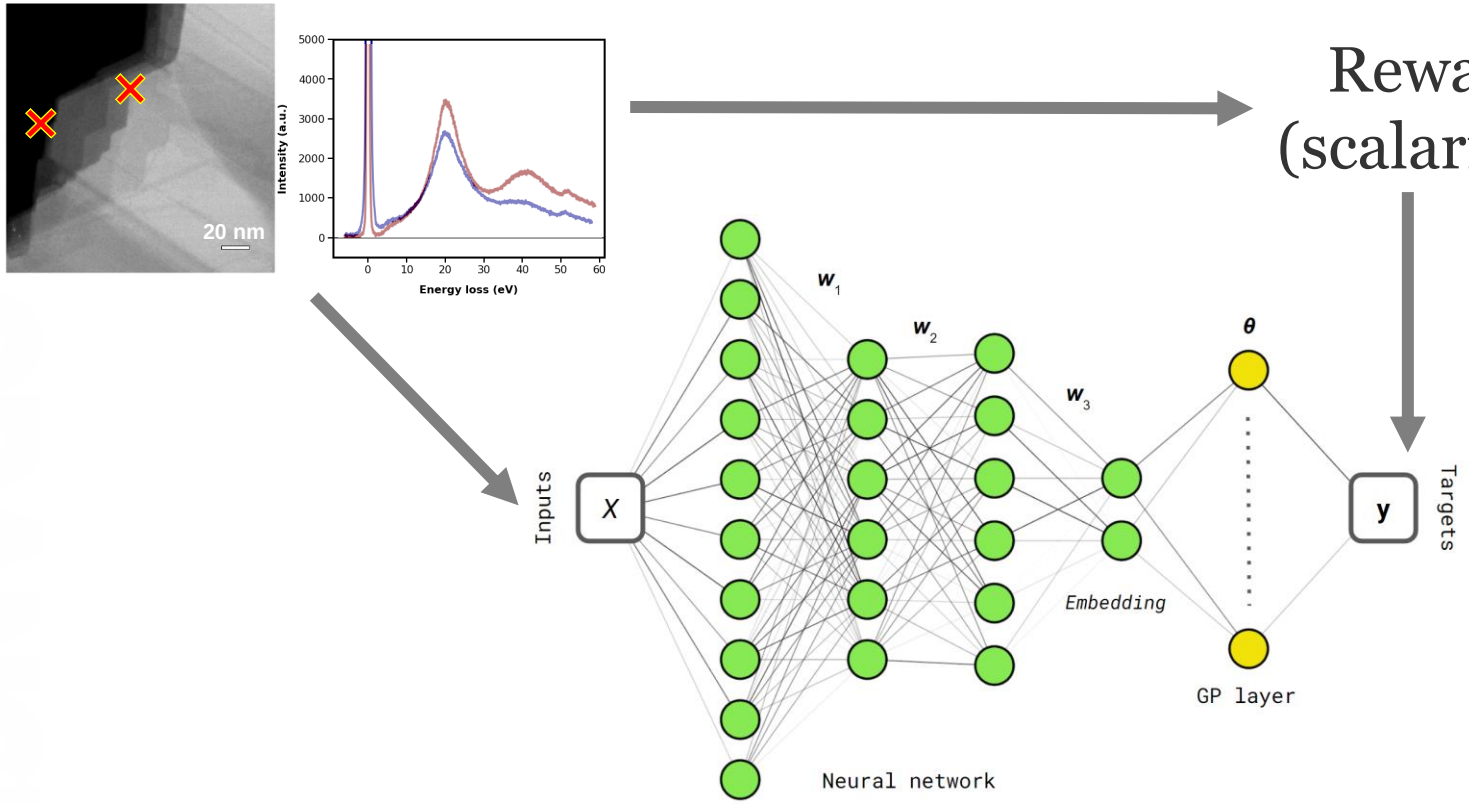




1. What if we have full access to structural information
2. And want to choose locations for (EELS, 4D STEM, CL, EDX) measurements
3. So as to **learn** relationship between structure and spectrum fastest
4. Or **discover** which microstructural elements give rise to specific **desired** spectral features?

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



Specify physics criteria

Acquire **structural data**

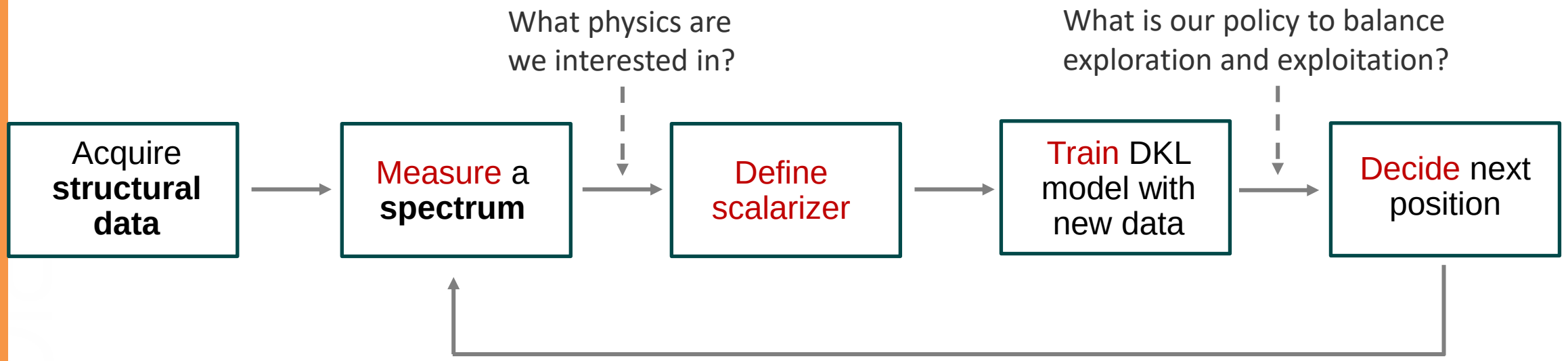
Measure a **spectrum**

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



Key concepts:

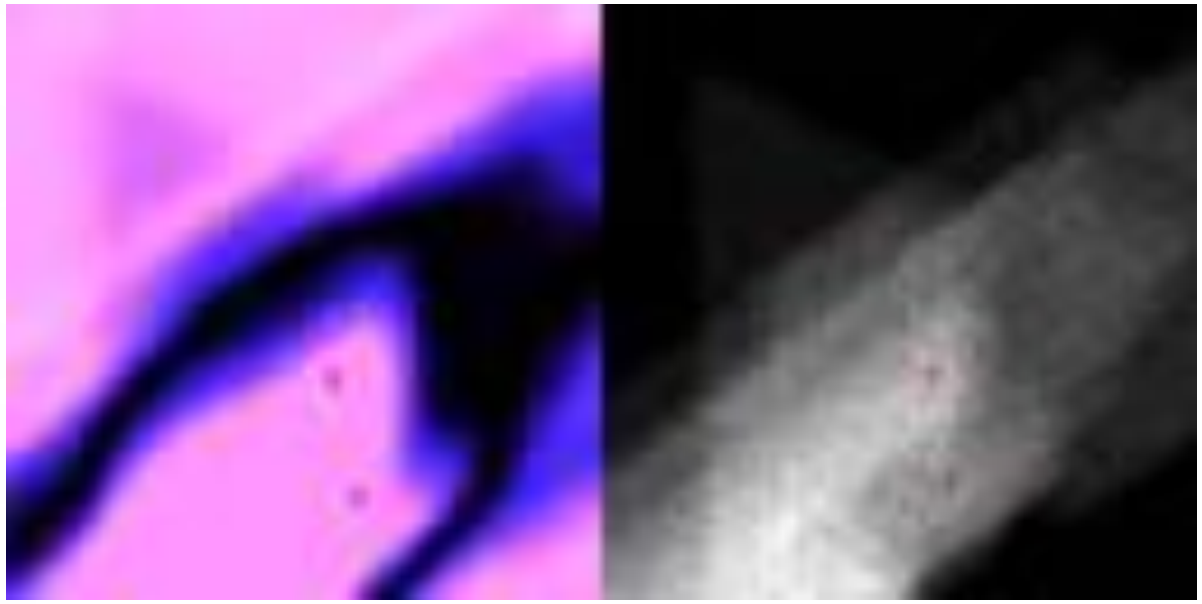
- **Scalarizer:** (any) function that transforms spectrum into measure of interest. Can be integration over interval, parameters of a peak fit, ration of peaks, or more complex analysis
- **Experimental trace:** collection of image patches and associated spectra acquired during experiment. Note that 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

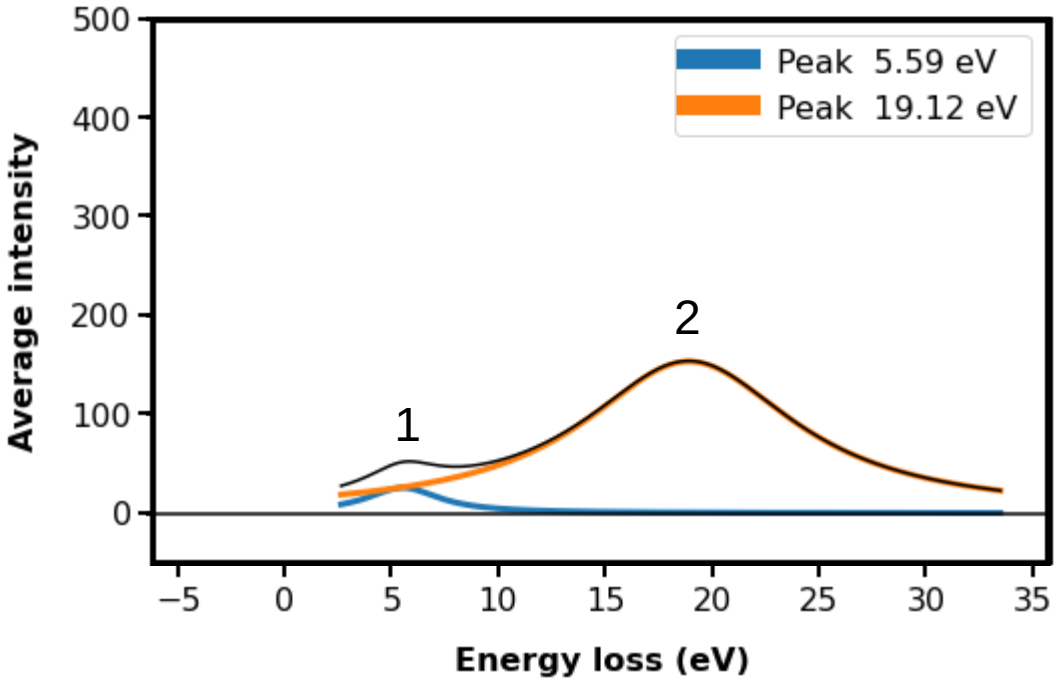
"Acquisition function"

HAADF-STEM



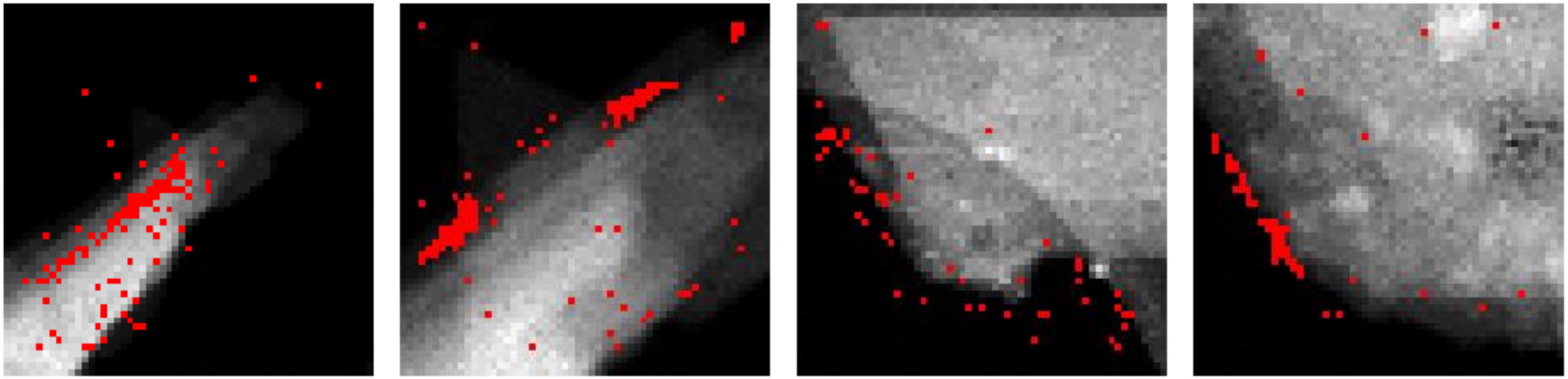
Physics search criteria:

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



More Examples of Physics Discovery

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



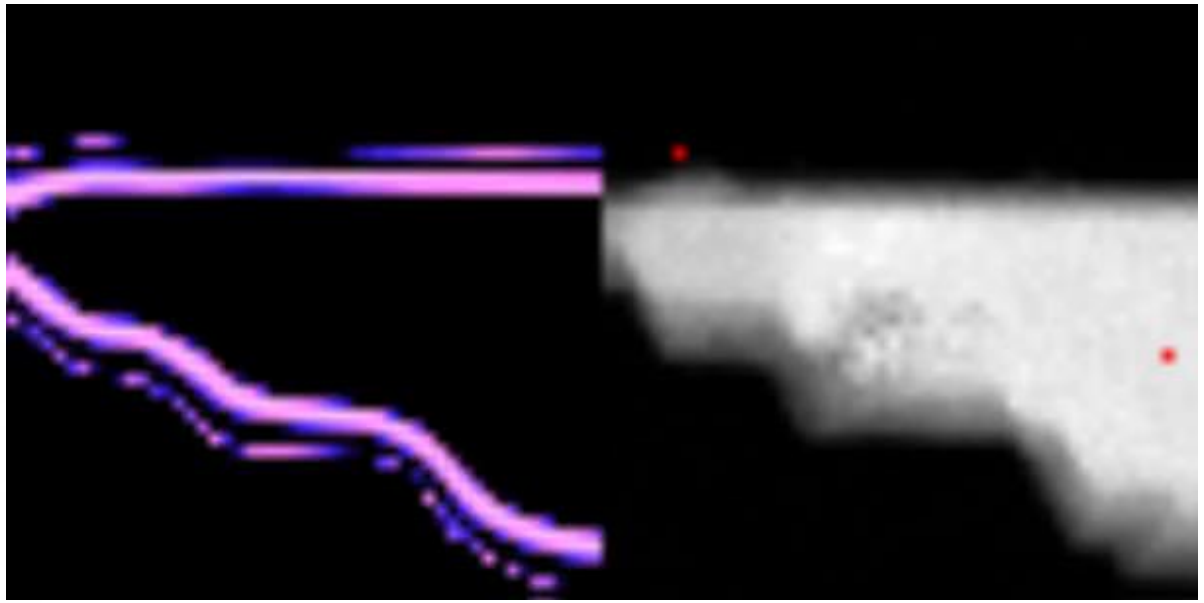
Discovery pathway depends on the reward structure (scalarizer that defines signature of physics we want to discover)!

Changing the scalarizer

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

"Acquisition function"

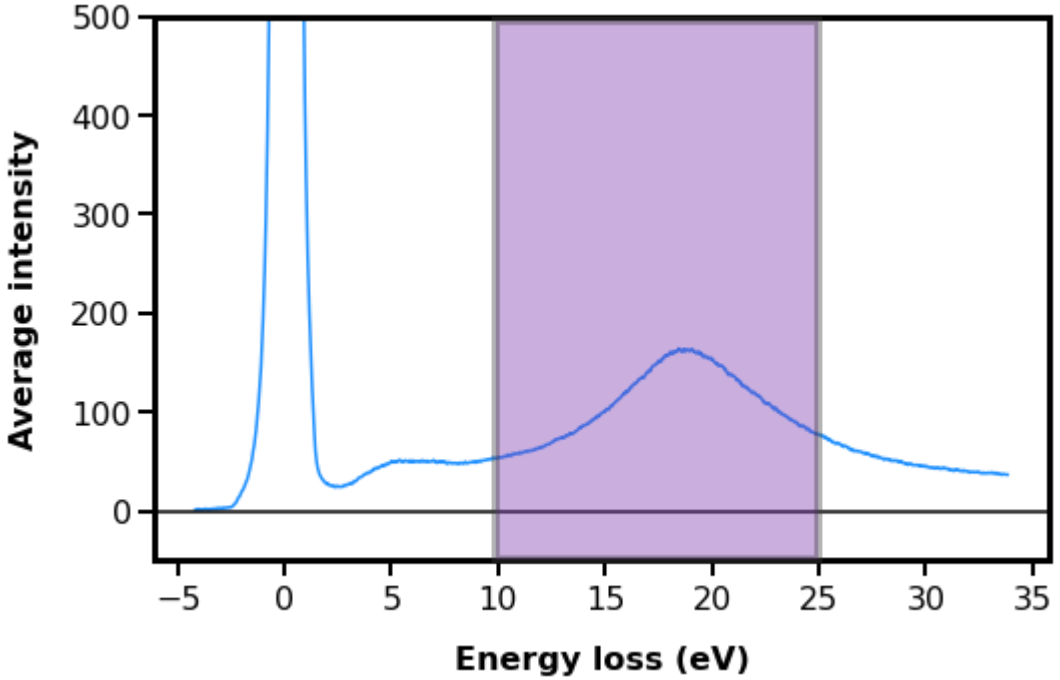
HAADF-STEM
+ points visited



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