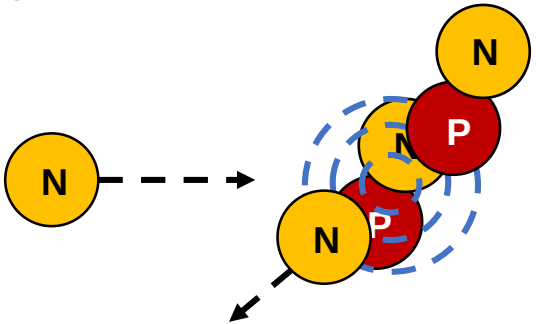
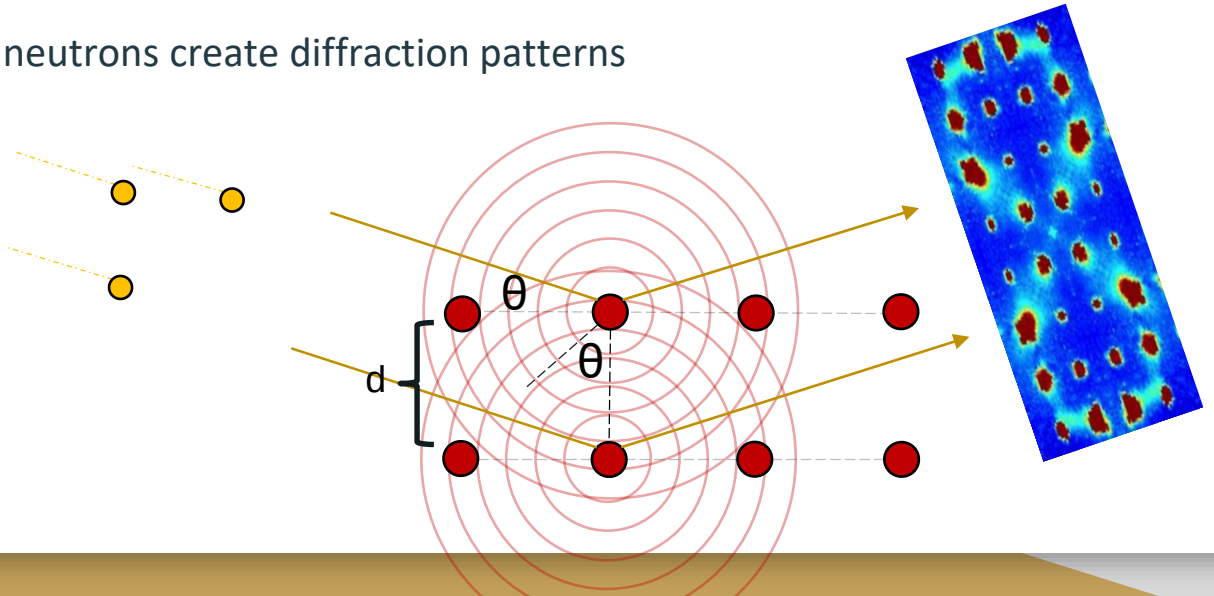
The Applications of Reinforcement Learning to Neutron Diffraction

Joseph Rath, William Ratcliff, Paul Kienzle

What is Neutron Diffraction?

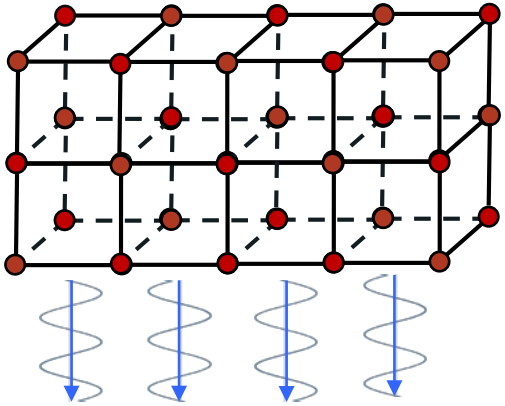
- Materials scatter neutrons
  - Due to interactions with nuclei
  - Via strong force
- Scattered neutrons create diffraction patterns

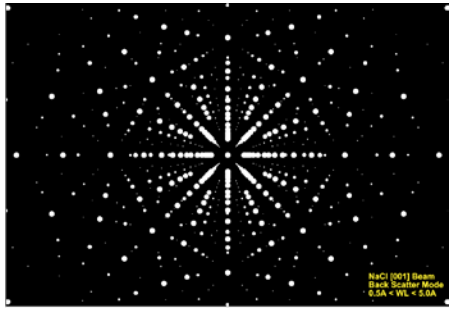




Why is it useful?

Materials have some ordered arrangement: **Crystal Structure**
Smallest repeating pattern in structure: **Unit Cell**
Atom positions and symmetries in unit cell reveal: **Physical Properties**





Diffraction patterns are dependent on a material's:

- Crystal structure/symmetry
- Elemental composition

Analysis of them patterns:

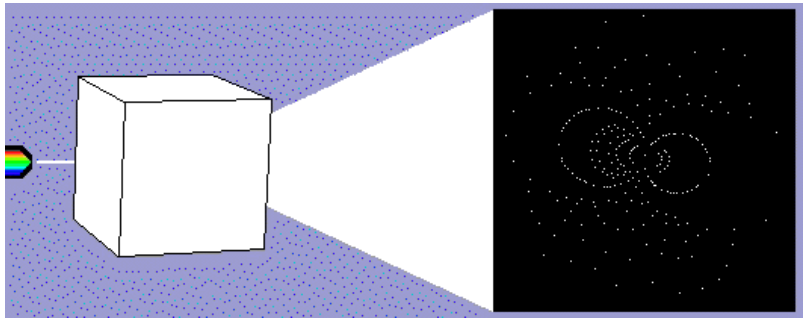
- Intensities -> Elemental composition
- Patterns -> Crystal symmetries
- Further -> Atomic positions / Properties

$$I(h,k,l) \propto \left|F(h,k,l)\right|^2$$

$$F(h,k,l) = \sum_j f_j e^{2\pi i(hx_j+ky_j+lz_j)-\phi(h,k,l)}$$

Problems Arise...

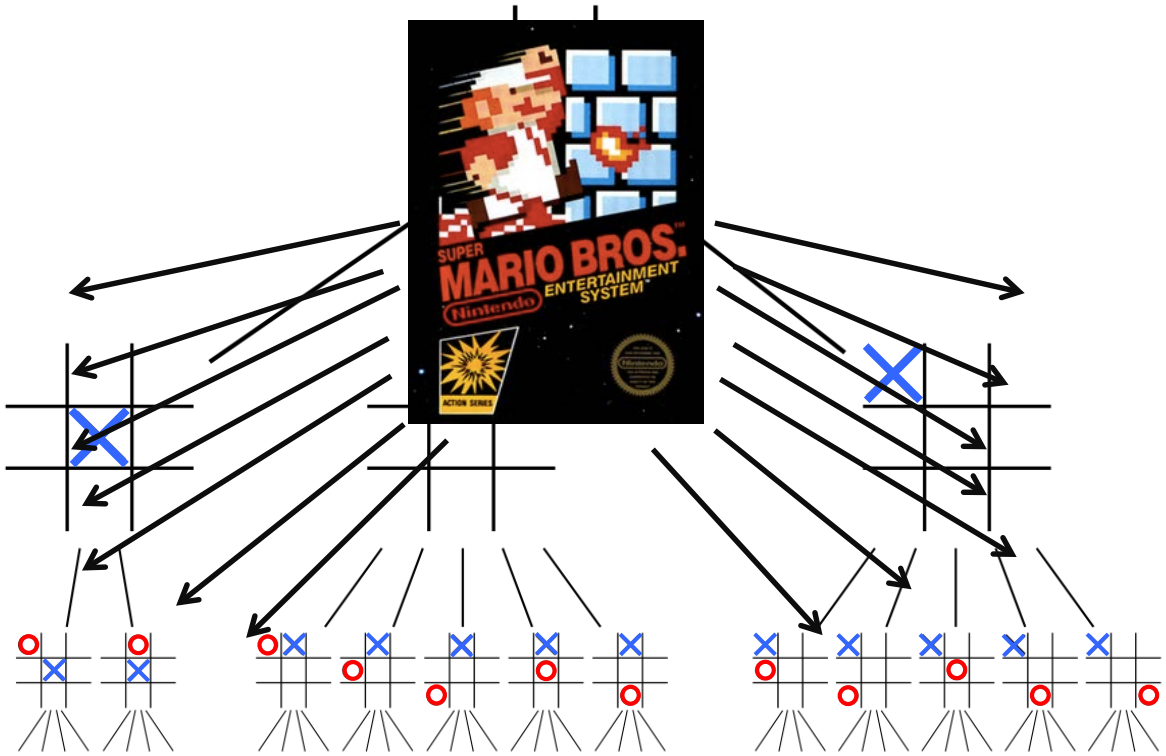
- Diffraction analysis takes time!
  - Lots of interaction/calculation
  - Small # of facilities
  - Beam-time limited/precious



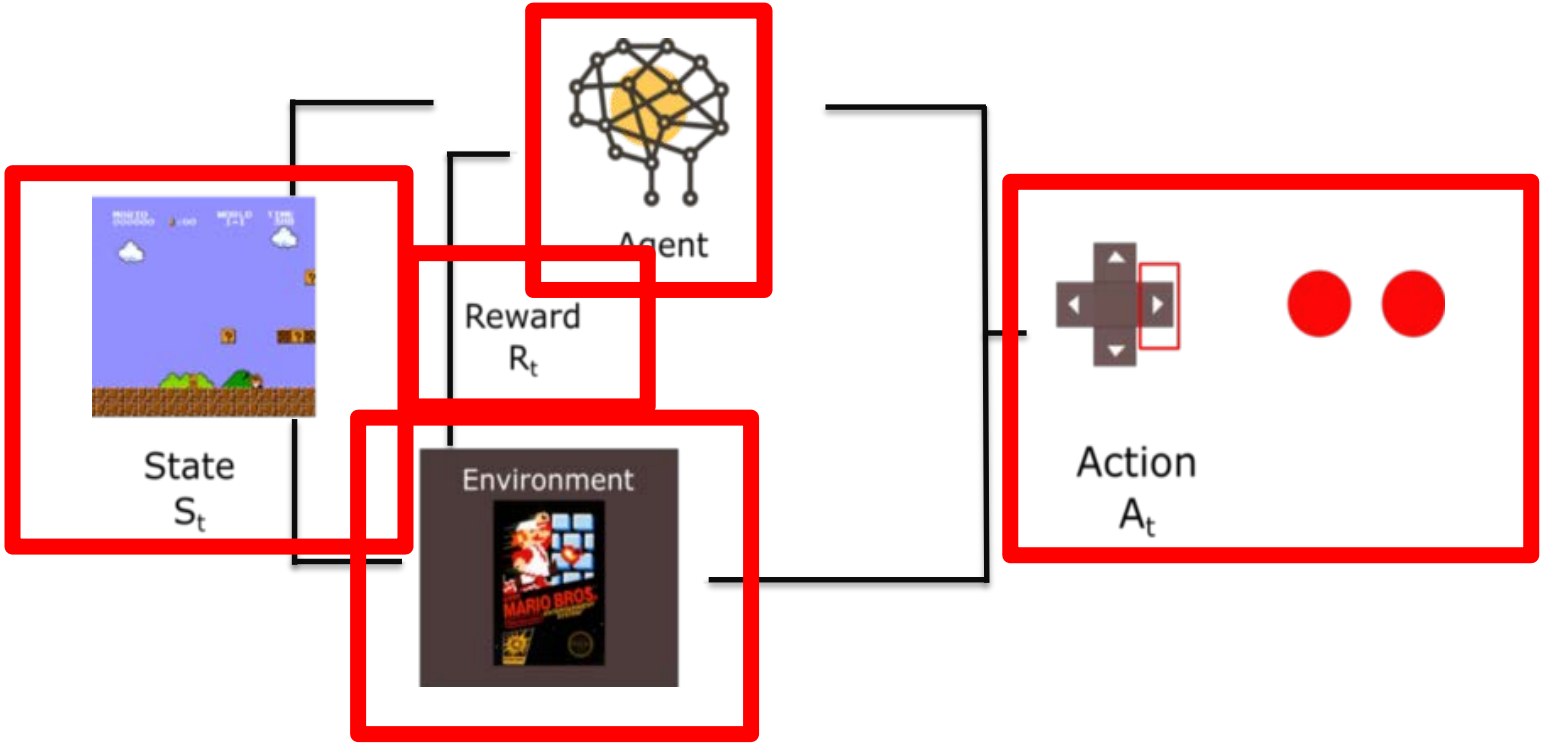
- Solution:
  - Machine Learning → Efficient beam-time?
  - What kind of algorithm is best?

Reinforcement Learning

Reward Hypothesis: An algorithm reaches some goal by maximizing cumulative reward

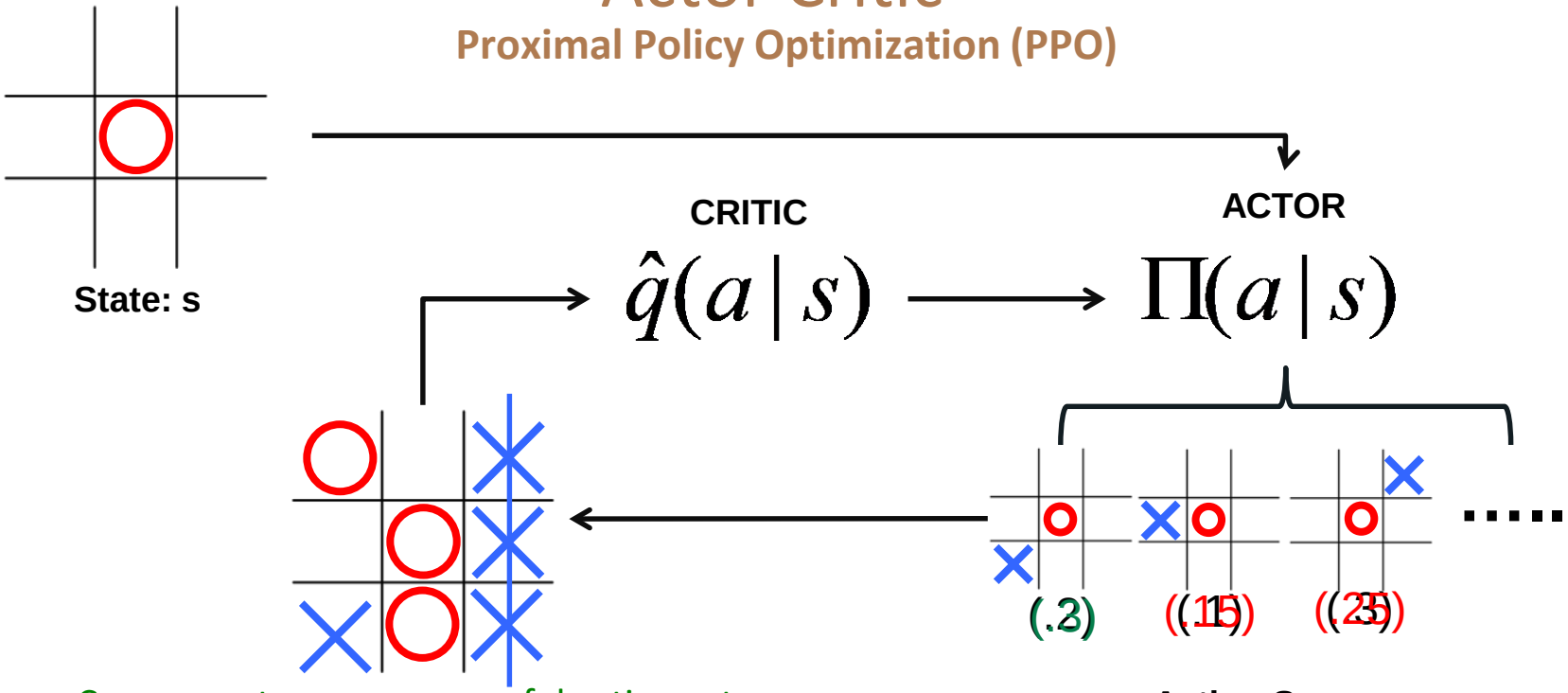


Reinforcement Learning



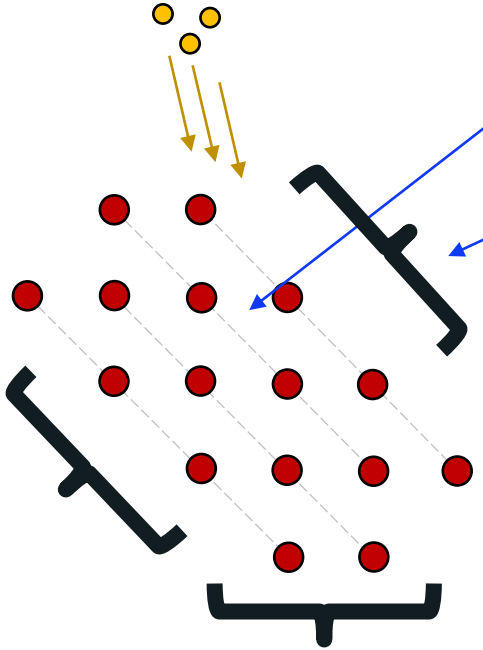
Actor Critic

Proximal Policy Optimization (PPO)



- Converges to some successful action set
- Handles larges action spaces
- Faster learning

Crystallographic Environment



Sample: Pr2NiO4

Goal: Find Pr Z-position

Agent: Neutron Detector

Actions: 198 Possible Reflections

Reward: Chi^2 Fit, Uncertainty, #Actions

h	k	l	I
2	6	0	558.9791
4	6	0	59.4729
1	1	1	56.7652
3	1	1	41.7464
5	1	1	26.7419
7	1	1	25.2044
9	1	1	19.6393
1	3	1	42.1271
3	3	1	33.1617
5	3	1	32.8350
7	3	1	22.1332
1	5	1	27.3004
3	5	1	31.9012
5	5	1	23.9531
1	7	1	26.2984

	Atom	X-pos	Y-pos	Z-pos		
ATOM Pr	PR	0.50000	0.50000	0.35973	0.00000	1.00000
ATOM Ni	NI	0.00000	0.00000	0.00000	0.00000	0.50000
ATOM O1	O	0.25000	0.25000	0.00000	0.00000	0.50000
ATOM O2	O	0.00000	0.00000	0.17385	0.00000	0.50000
ATOM Oi	O	0.25000	0.25000	0.25000	0.00000	0.10000
ATOM Od	O	0.07347	0.07347	0.17349	2.31435	0.58500

SPACEG F m m m

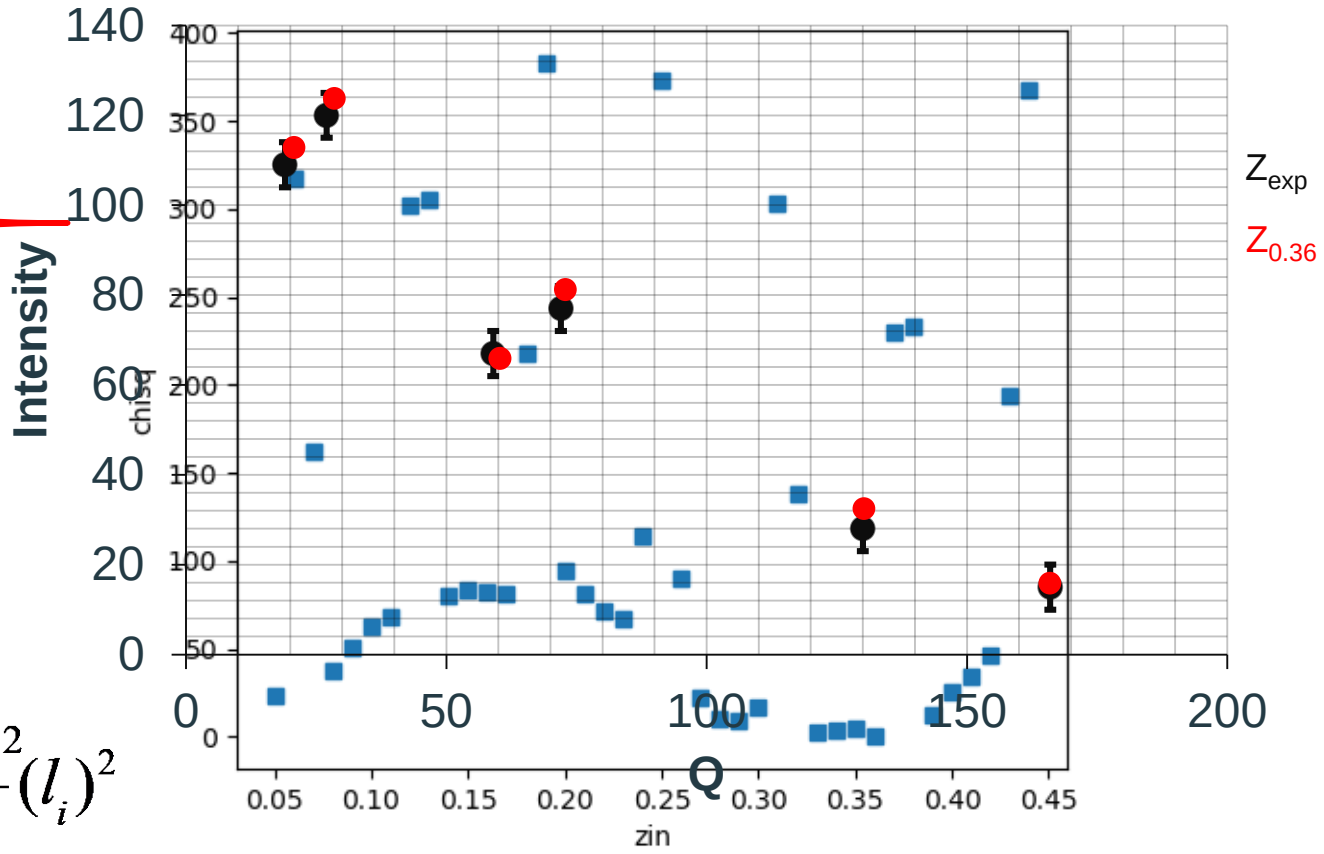
CELL 5.417799 5.414600 12.483399 90.0000 90.0000 90.0000

!box -0.26 1.26 -0.26 1.26 -0.26 1.26

Results

Generated Reflections

h	k	l
[7	1	3]
[0	2	16]
[5	1	1]
[0	0	20]
[3	1	1]
[4	4	4]
[5	5	3]
[3	1	3]
[1	5	9]
⋮	⋮	⋮



Cubic Lattice:

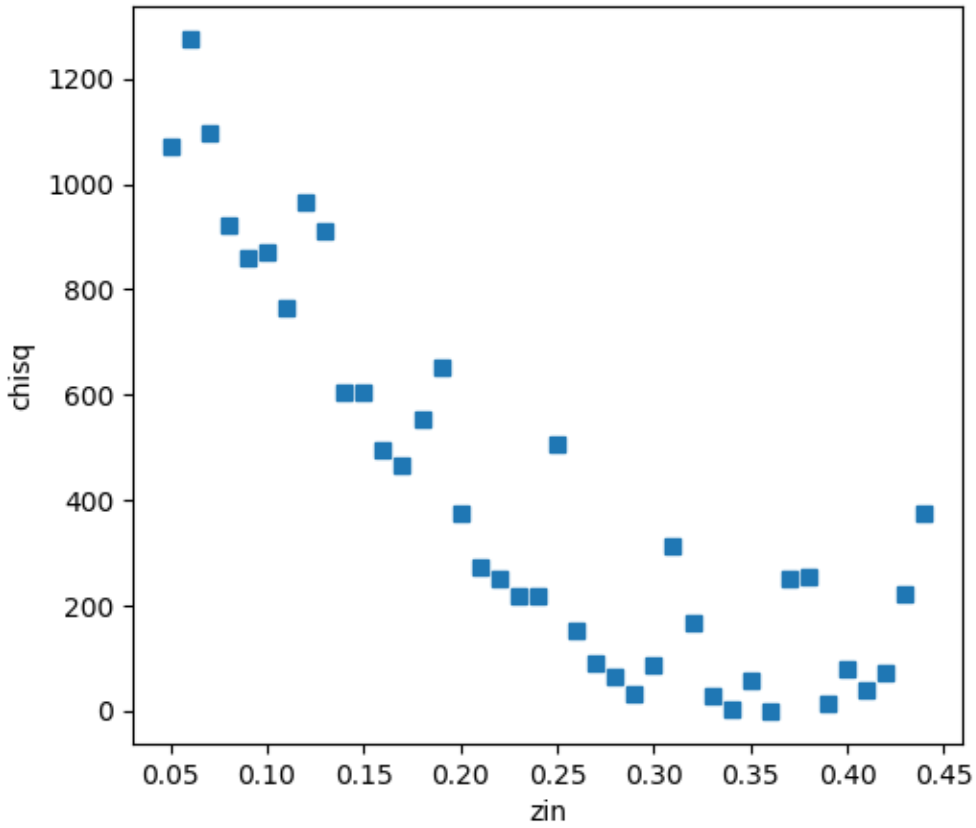
$$Q_i^2 = \left|\frac{1}{d_{calc}}\right|^2 = \frac{(h_i)^2}{a^2} + \frac{(k_i)^2}{b^2} + \frac{(l_i)^2}{c^2}$$

Results

Generated Reflections

h	k	l
[7	1	3]
[0	2	16]
[5	1	1]
[0	0	20]
[3	1	1]
[4	4	4]
[5	5	3]
[3	1	3]
[1	5	9]

$$\chi^2 = \left| I_{ex} - I_{calc} \right|^2$$

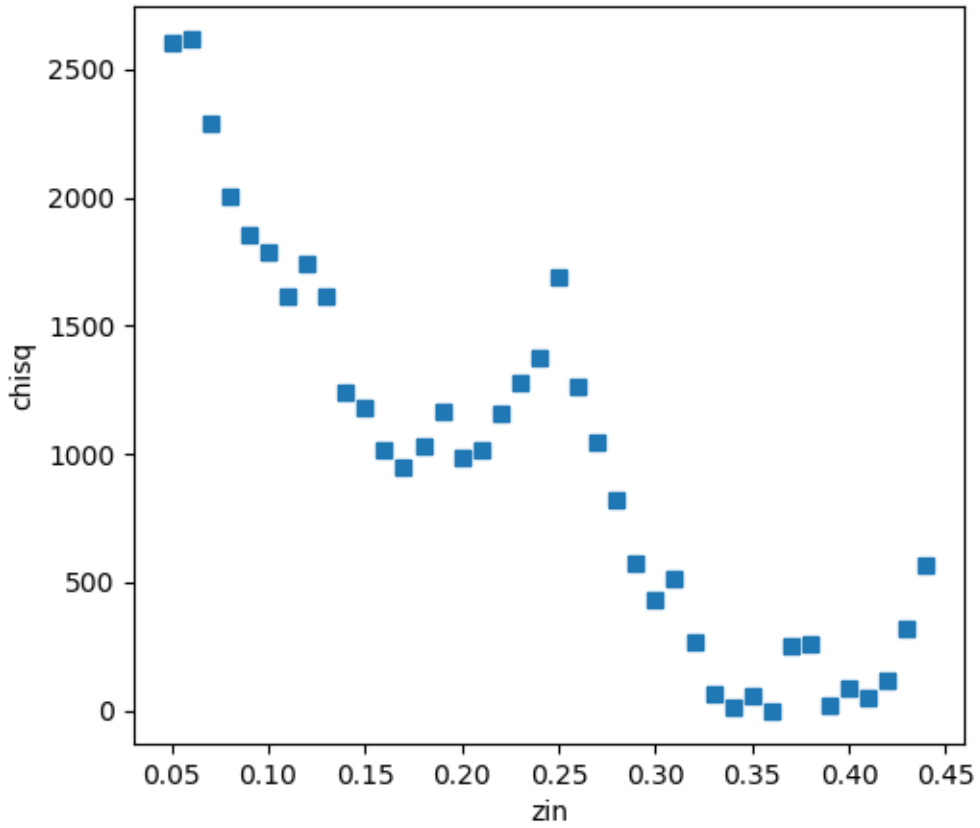


Results

Generated Reflections

h	k	l
[7	1	3]
[0	2	16]
[5	1	1]
[0	0	20]
[3	1	1]
[4	4	4]
[5	5	3]
[3	1	3]
[1	5	9]

$$\chi^2 = \left| I_{ex} - I_{calc} \right|^2$$

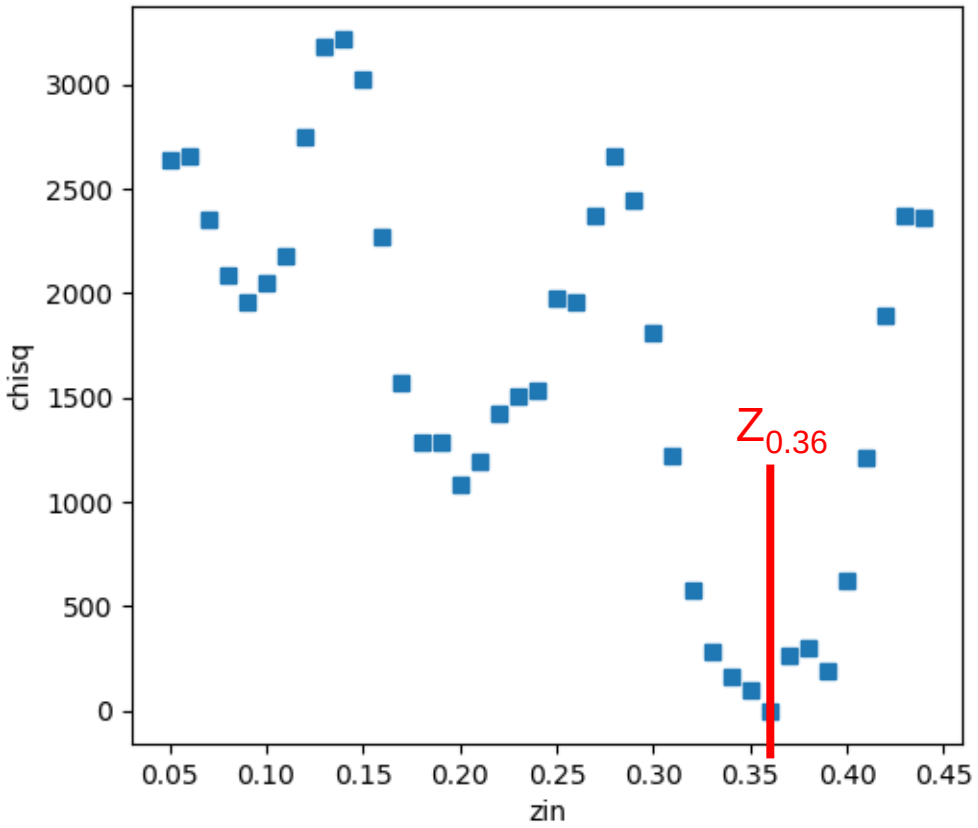


Results

Generated Reflections

h	k	l
[7	1	3]
[0	2	16]
[5	1	1]
[0	0	20]
[3	1	1]
[4	4	4]
[5	5	3]
[3	1	3]
[1	5	9]

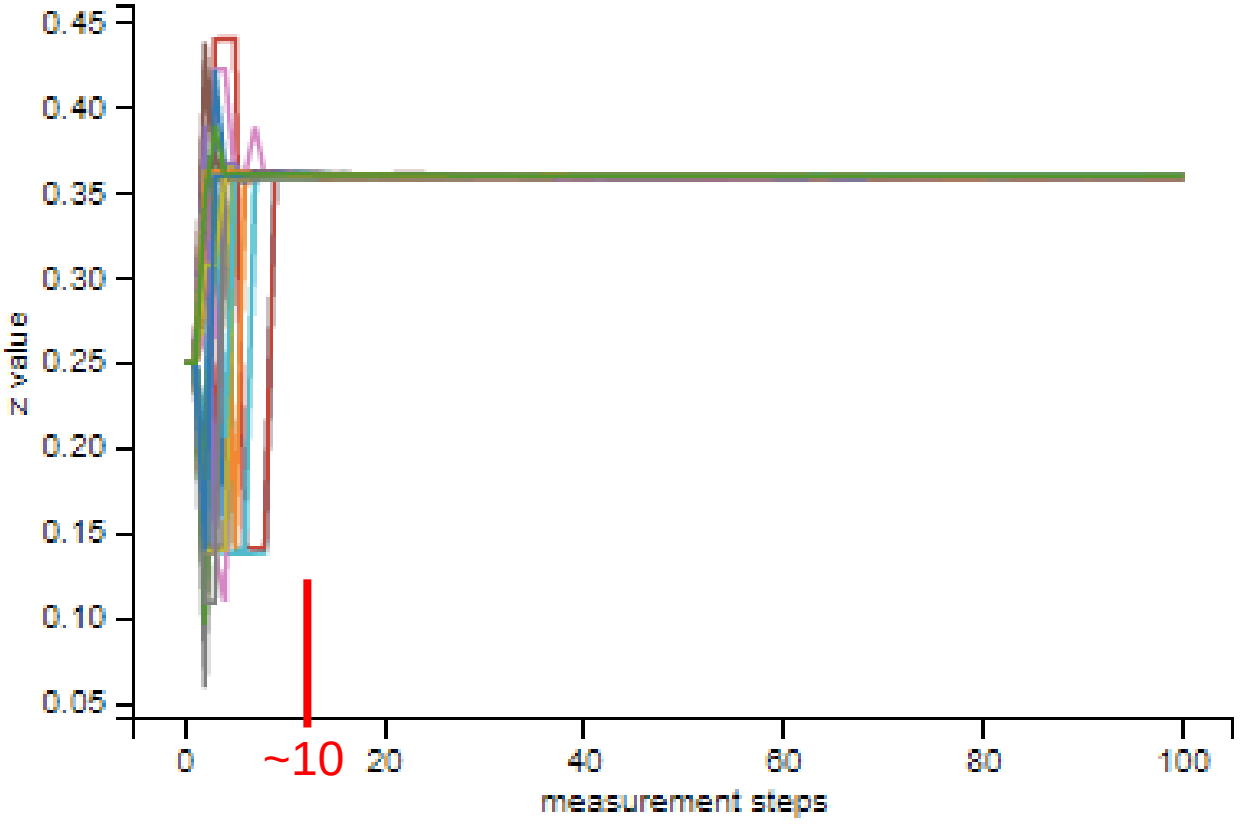
$$\chi^2 = \left| I_{ex} - I_{calc} \right|^2$$



Results

Generated Reflections

h	k	l
[7	1	3]
[0	2	16]
[5	1	1]
[0	0	20]
[3	1	1]
[4	4	4]
[5	5	3]
[3	1	3]
[1	5	9]
⋮	⋮	⋮



Discussion

Algorithm:

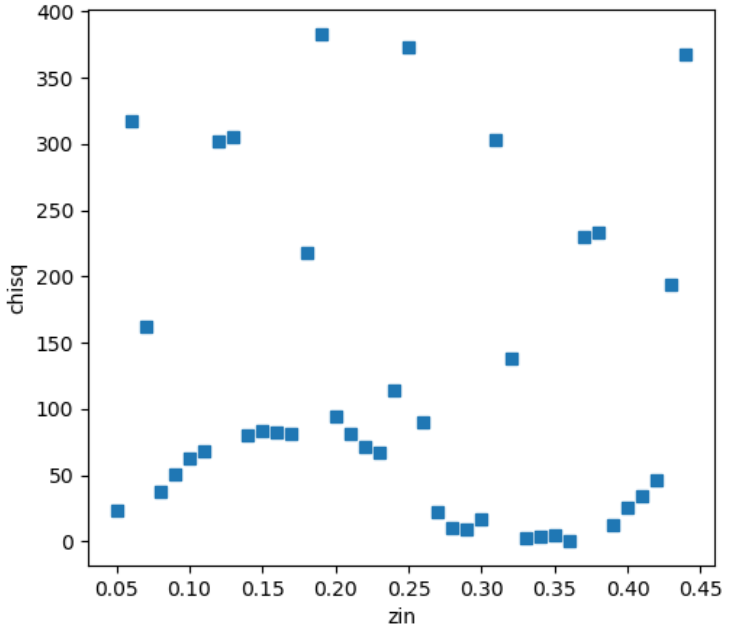
- Z-coordinate found!
- Fast convergence / low deviation

BUT

- Reward Function
- For a simple system
- Realistically could be very slow

Future:

- More parameters
- Better RL algorithms



References

- https://www.ill.eu/users/instruments/instruments-list/orientexpress/how-it-works/principle-of-neutron-laue-diffraction/
- https://towardsdatascience.com/policy-gradients-in-a-nutshell-8b72f9743c5d
- https://www.freecodecamp.org/news/an-introduction-to-policy-gradients-with-cartpole-and-doom-495b5ef2207f/
- https://www.ncnr.nist.gov/programs/crystallography/
- http://www.crystal0studio.com/news.php

Acknowledgements

- Dr. William Ratcliff
- Dr. Paul Kienzle
- SURF Directors: Julie Borchers & Joe Dura
- SHIP students: Jess & Kate
- Other NCNR SURFers

CHRNS
CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING
NSF
NIST

NIST Center for Neutron Research

OpenAI