Fitting Order Parameters through Reinforcement Learning

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Goals and Impact

- Beam time is valuable – limited access
- Want more efficient measurements as not all are required
- Software to be implemented on multiple instruments (BT4, BT7, etc.) using NICE
Order Parameters You’re Familiar With

- Liquid-gas transitions use density (calculated using M, P, and T) as order parameter
- Distinguishes phases (difference in properties)
- Other parameters are useful for other materials
Magnetic Order Parameter

- Magnets use “orientation”
- The magnitude of magnetic (dipole) fields in the “normal” direction
- Phases are magnetic and nonmagnetic
Magnetic Order Parameter

- Scattering intensity is proportional to magnetism
- Temperature where intensity becomes 0 is also where the material becomes weakly magnetic
The Measurement

- In **most** basic form, a curve fitting problem
- Solved by classical fitters (bumps)
- Goal is picking most informative point on curve given what has been measured so far, using constant increases in temperature
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Reinforcement Learning

Defined:
Teaching a computer to make optimal decisions using rewards

How does it work?
1. The agent is in an environment
2. The environment returns a state
3. Agent makes action based on state
4. Agent is rewarded after action
5. Algorithm learns how to best make actions based on rewards
Reinforcement Learning

EPISODE: 1

Reward:

EPISODE: 2

Reward:

EPISODE: 3

Reward:
Applying Reinforcement Learning

- Action: positive change in temperature
- State: last measured temperature
- Reward: low chi squared
- Ends episode with low chi squared, too many steps, or temperature too high
Other Parameters to Fit

- **Jt**: Magnetic moment
- **Nf**: Number of magnetic ions/volume (number density)
- **Bk**: Background intensity
Results: Stage One

Algorithm improves with more episodes, takes less steps to fit the transition temperature

Model successfully finds transition temperatures (yellow) when experiment parameters are similar to training values
Results: Stage Two (failure)

- Fitting on new set of four random variables each episode
- Better reflects application
- Worsening convergence, mediocre rewards
Results: Stage Two (failure)

- Limit random variables to three
- Mildly better in trends, but bad preliminary results
- 30, 25 measurements is not ideal
(bimodality?)

- Distinct groups in reward and convergence graphs
- Represent successful fits and failed fits where algorithm went over max temperature
- Distinction between the two may be low transition temperature
On Fitting

Fit is much better before measuring past the transition temperature
Results: Stage Two (failure)

- Two variables!
- Does well consistently with fast convergence
- However, no improvement - success from fitter
Future Steps

- Improve convergence and reward trends through reward function, fitter usage
- Replace simulated data with real-world data
- Implement model in application software to work with NICE
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Questions