THE UNIVERSITY of TENNESSEE KNOXVILLE

# Hypothesis Learning and GPax beyond 1D

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# What have we learned from Lecture 1 and 2

**Lecture 1:**

- Gaussian Process
- Kernel, Kernel Priors, and Noise Priors
- Posteriors
- Bayesian Optimization
- Bayesian Optimization based on Gaussian Process
- Acquisition Functions

**Lecture 2:**

- Bayesian Inference
- Prior and posterior Distribution
- Least Square Fit
- WAIC
- Structured Gaussian Process
- Prior Distributions (kernel, parameters, noise)
- Posterior Distributions (kernel, parameters, noise)
- sGP based BO

# GP Augmented with Structural model

Define a probabilistic model:

$$\mathbf{y} \sim MVNormal(\mathbf{m}, \mathbf{K})$$

$$K_{ij} = \sigma^2 \exp(0.5(x_i - x_j)^2 / l^2$$

$$\sigma \sim LogNormal(0, s_1)$$

$$l \sim LogNormal(0, s_2)$$

- We substitute a constant GP prior mean function **m** with a structured probabilistic model of the expected system's behavior.
- This probabilistic model reflects our prior knowledge about the system, but it does not have to be precise.
- The model parameters are inferred together with the kernel parameters via the Hamiltonian Monte Carlo.
- The fully Bayesian treatment of the model allows additional control over the optimization via the selection of priors for the model parameters.

Prediction on new data $X_*$:

$$\mathbf{f}_*^i \sim MVNormal\left(\mu_{\boldsymbol{\theta}^i}^{\text{post}}, \Sigma_{\boldsymbol{\theta}^i}^{\text{post}}\right)$$

replaced with

$$\mu_{\boldsymbol{\theta}^i}^{\text{post}} = \mathbf{m}(X_*) + \mathbf{K}(X_*, X|\boldsymbol{\theta}^i)\mathbf{K}\left(X, X|\boldsymbol{\theta}^i\right)^{-1}(\mathbf{y} - \mathbf{m}(X)) \rightarrow \mu_{\boldsymbol{\Omega}^i}^{\text{post}} = \mathbf{m}\left(X_*|\phi^i\right) + \mathbf{K}(X_*, X|\boldsymbol{\theta}^i)\mathbf{K}\left(X, X\middle|\boldsymbol{\theta}^i\right)^{-1}(\mathbf{y} - \mathbf{m}(X|\phi^i))$$

$$\Sigma_{\boldsymbol{\theta}^i}^{\text{post}} = \mathbf{K}\left(X_*, X_*|\boldsymbol{\theta}^i\right) - \mathbf{K}(X_*, X|\boldsymbol{\theta}^i)\mathbf{K}\left(X, X|\boldsymbol{\theta}^i\right)^{-1}\mathbf{K}(X, X_*|\boldsymbol{\theta}^i)$$

$\boldsymbol{\Omega}^i = \{\phi^i, \boldsymbol{\theta}^i\}$ is a single HMC posterior sample with the kernel and prob model parameters

# GP Augmented with Structural model

## Probabilistic model

$$m = y_0 - \sum_{n=1}^{N} L_n \quad (N{=}2)$$

$$y_0 \sim Uniform(-10, 10)$$

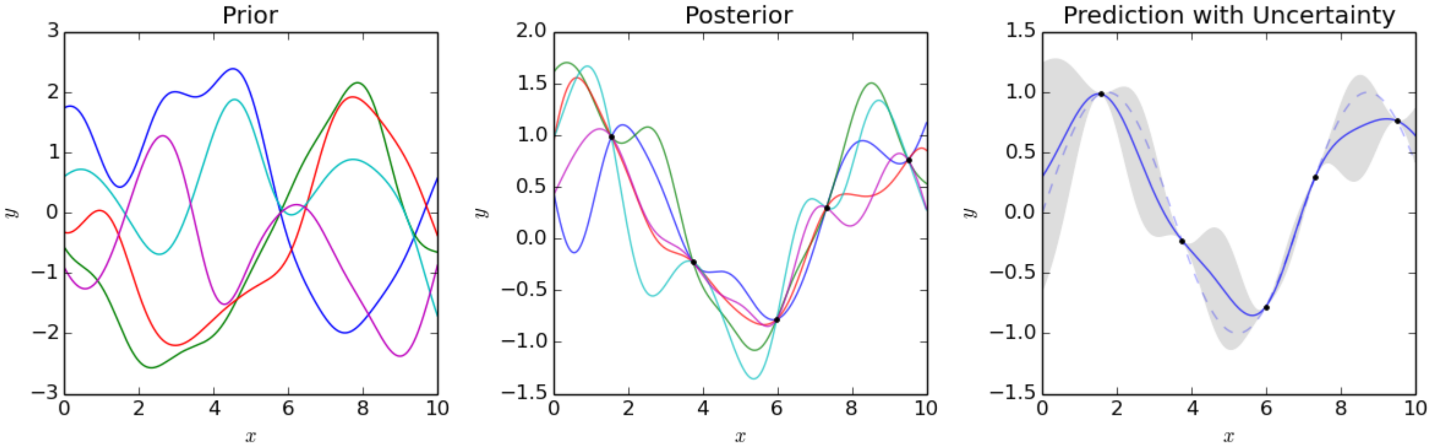
$$L_n \sim \frac{A_n}{\sqrt{(x - x_n^0)^2 + w_n^2}}$$

$$A_n \sim LogNormal(0, 1)$$

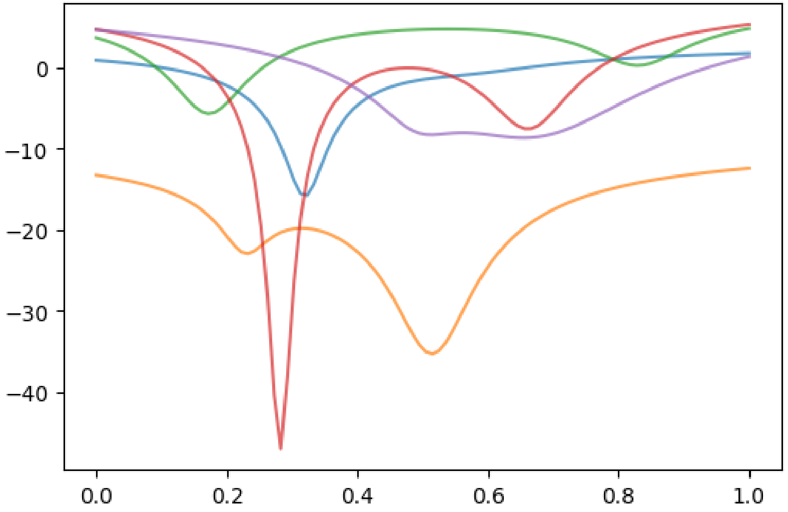
$$w_n \sim HalfNormal(.1)$$

$$x_n^0 \sim Uniform(0, 1)$$

## Prior predictive distribution: GP

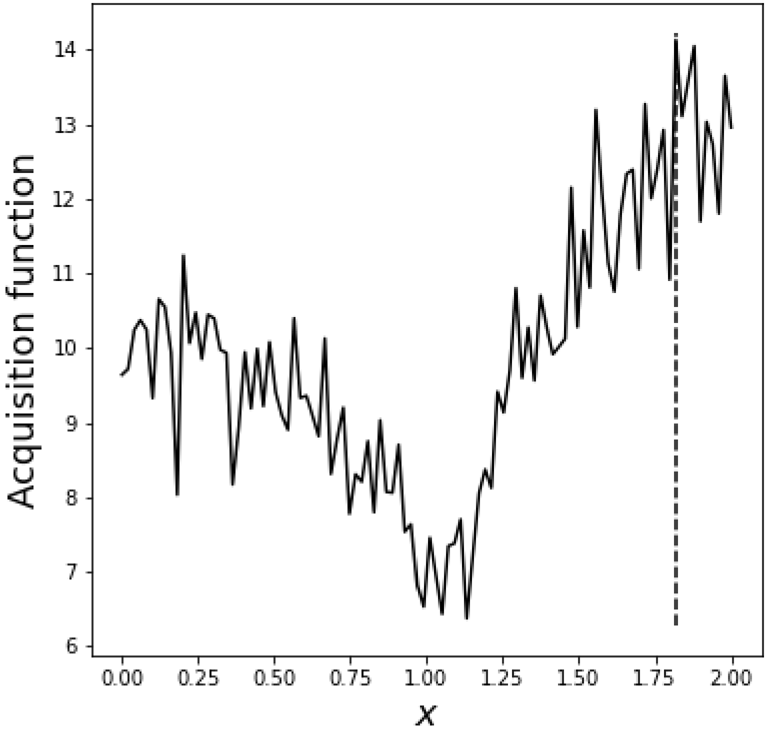


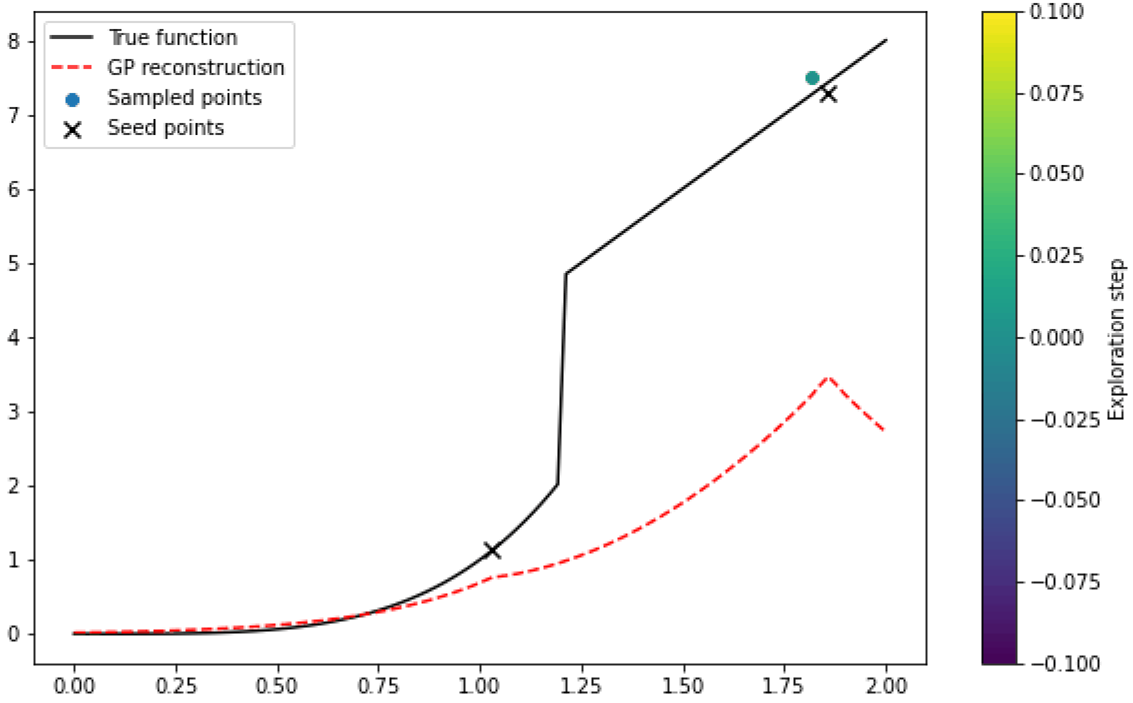

## Prior predictive distribution: sGP




This model simply tells us that there are two minima in our data but does not assume to have any prior knowledge about their relative depth, width, or distance

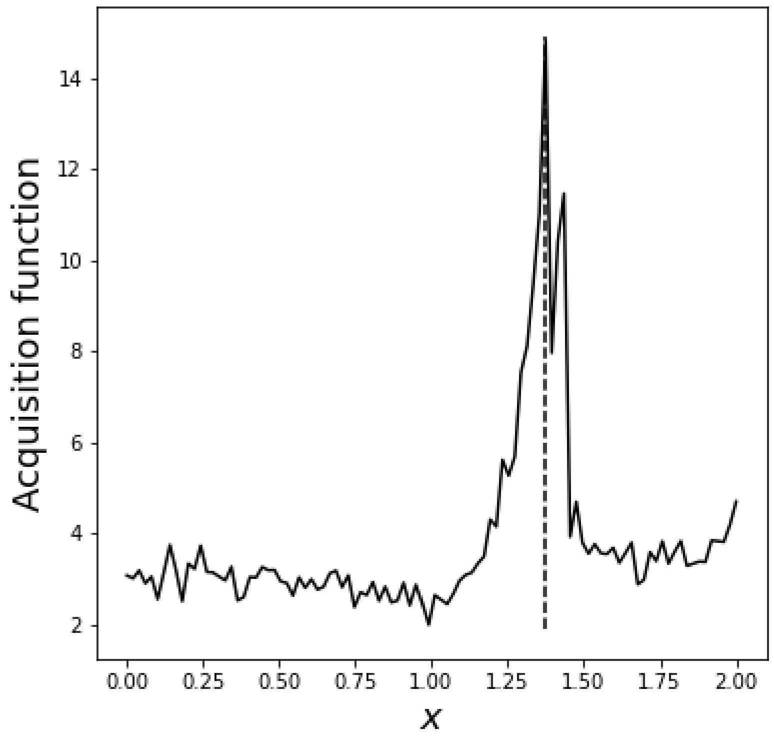
# Simple GP search

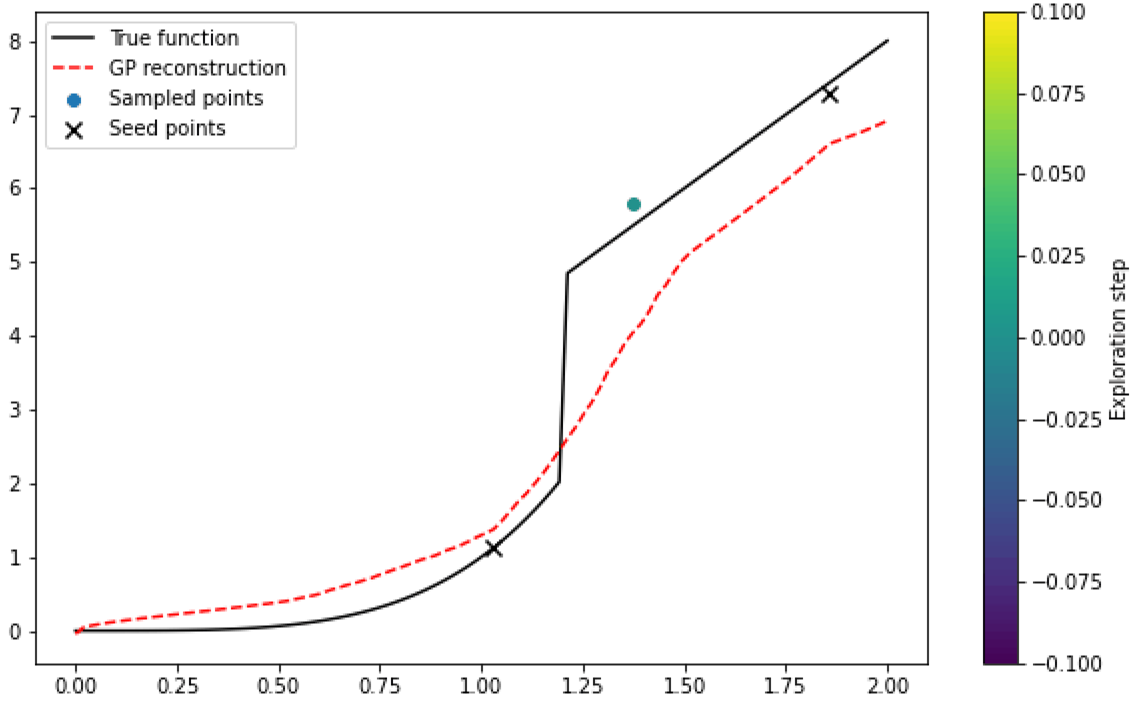


# Structured GP search





# Application to Ising model

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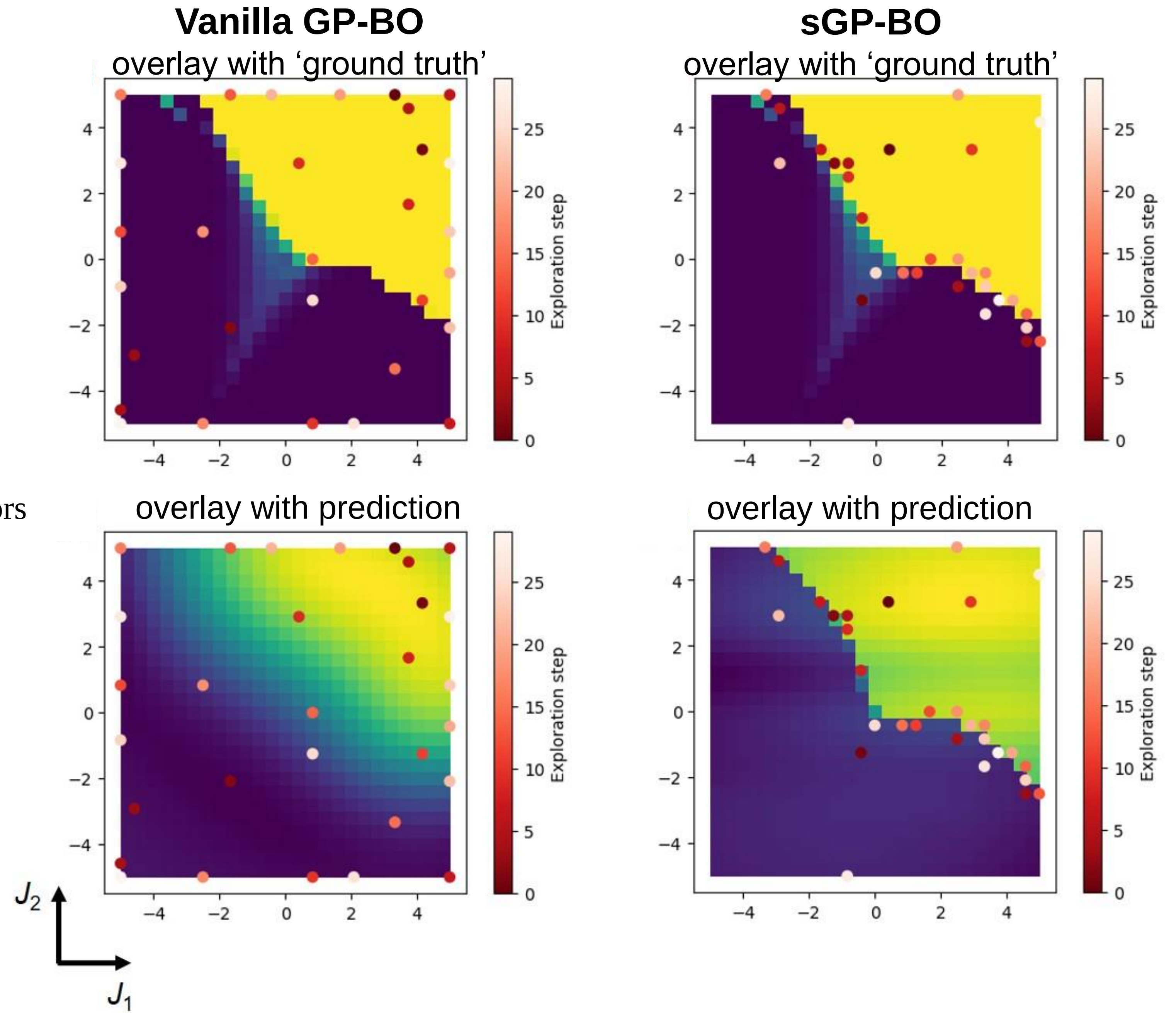
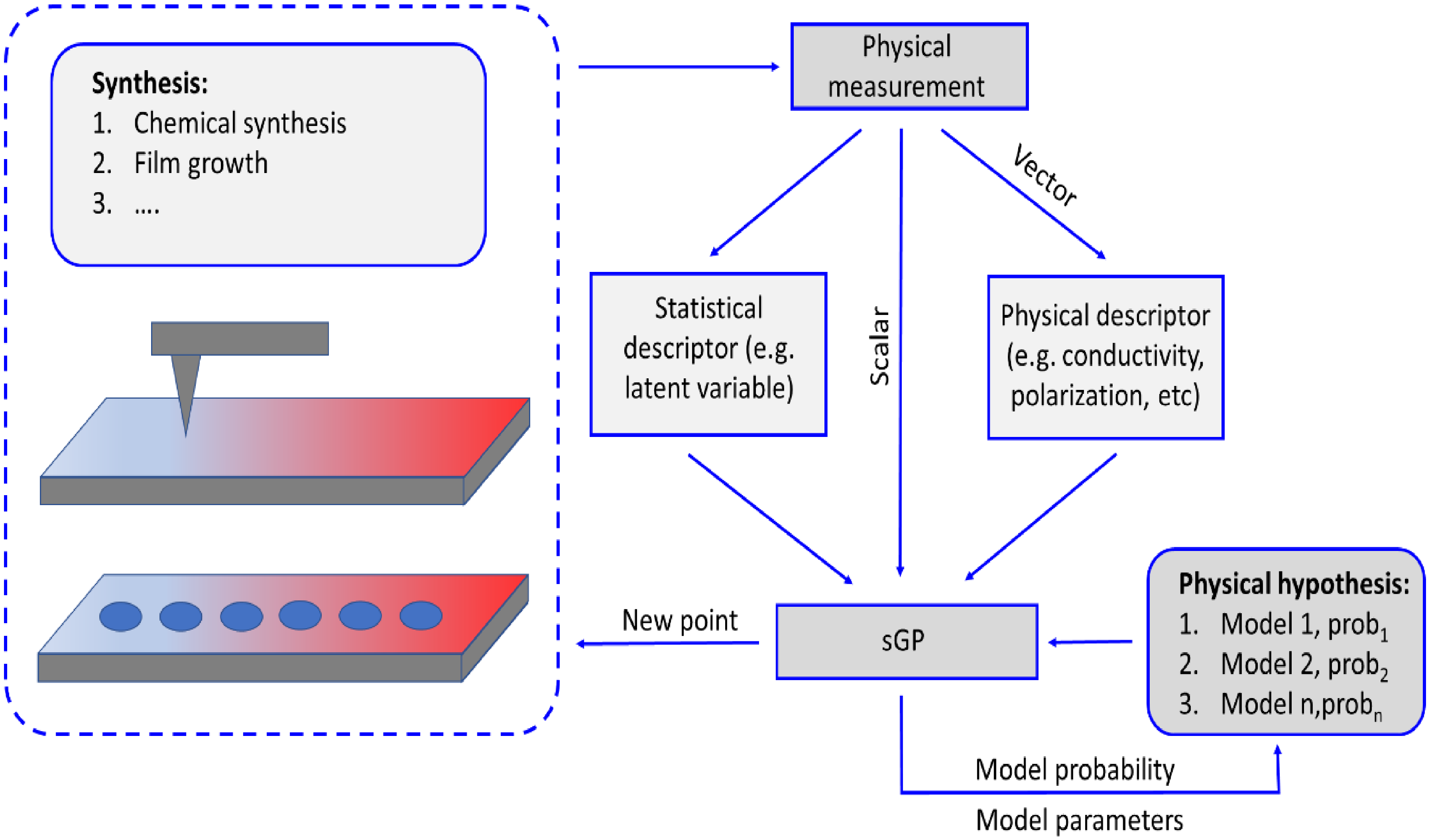



Probabilistic model

$A/\tanh(\frac{f(J_1)+f(J_2)}{w})$

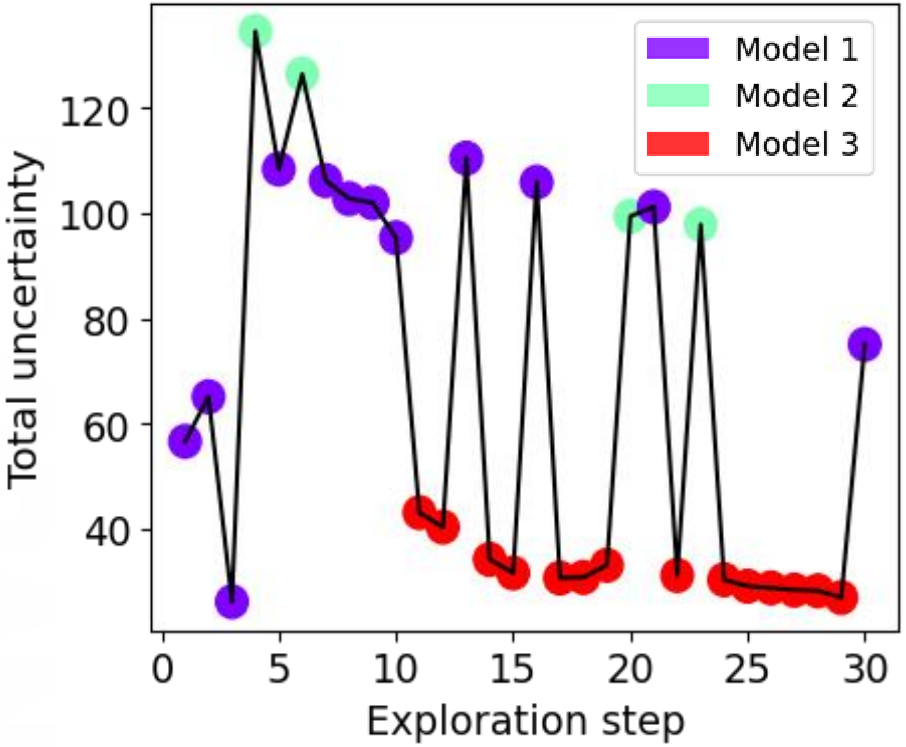
where $f(J)$ is a third-degree polynomial with normal priors on its parameters

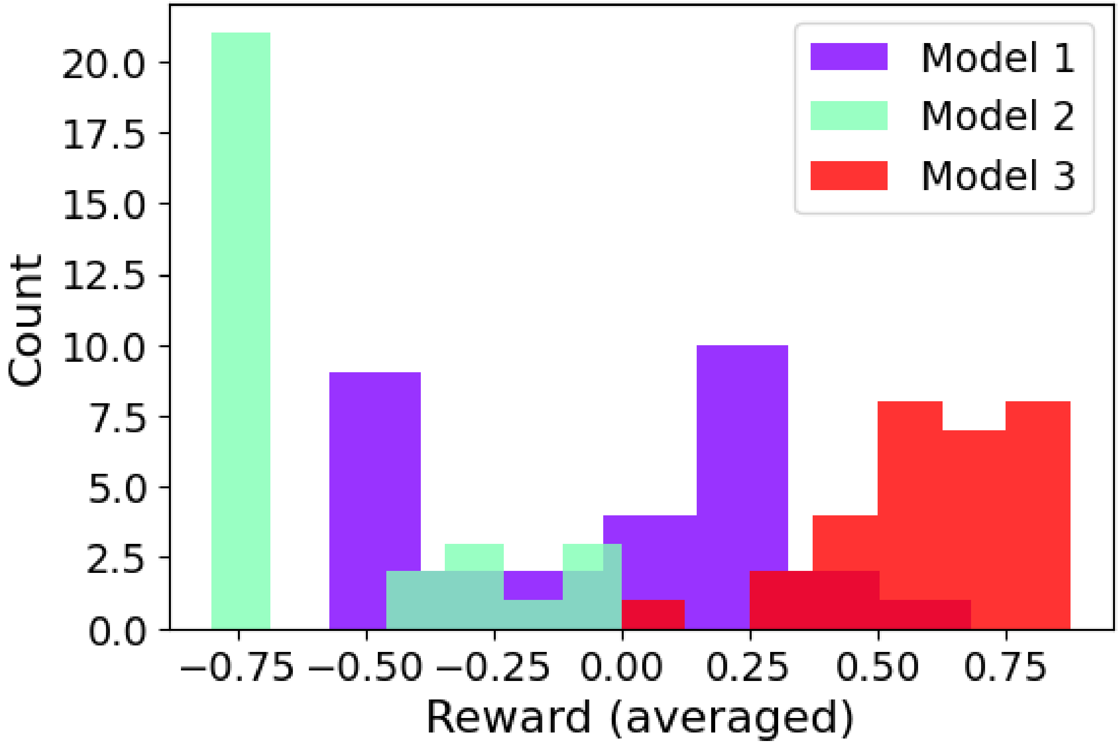
# Hypothesis active learning: hypoAL



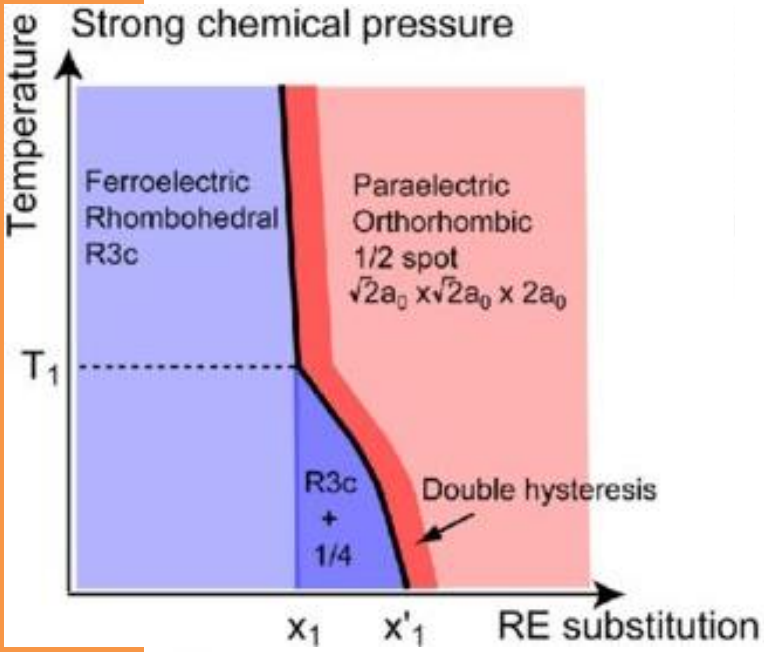
# Next step: active model selection





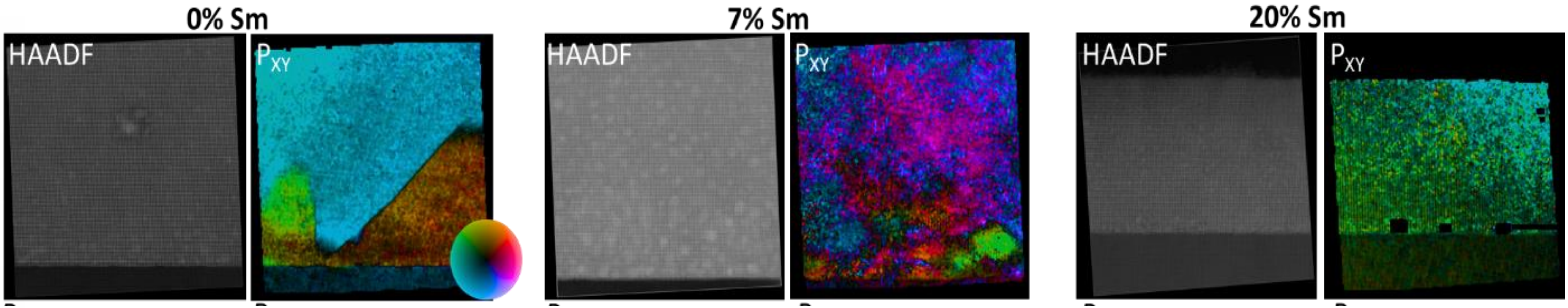



# Combinatorial Synthesis




Sample by I. Takeuchi, UMD
Phase diagram by N. Valanoor et al.

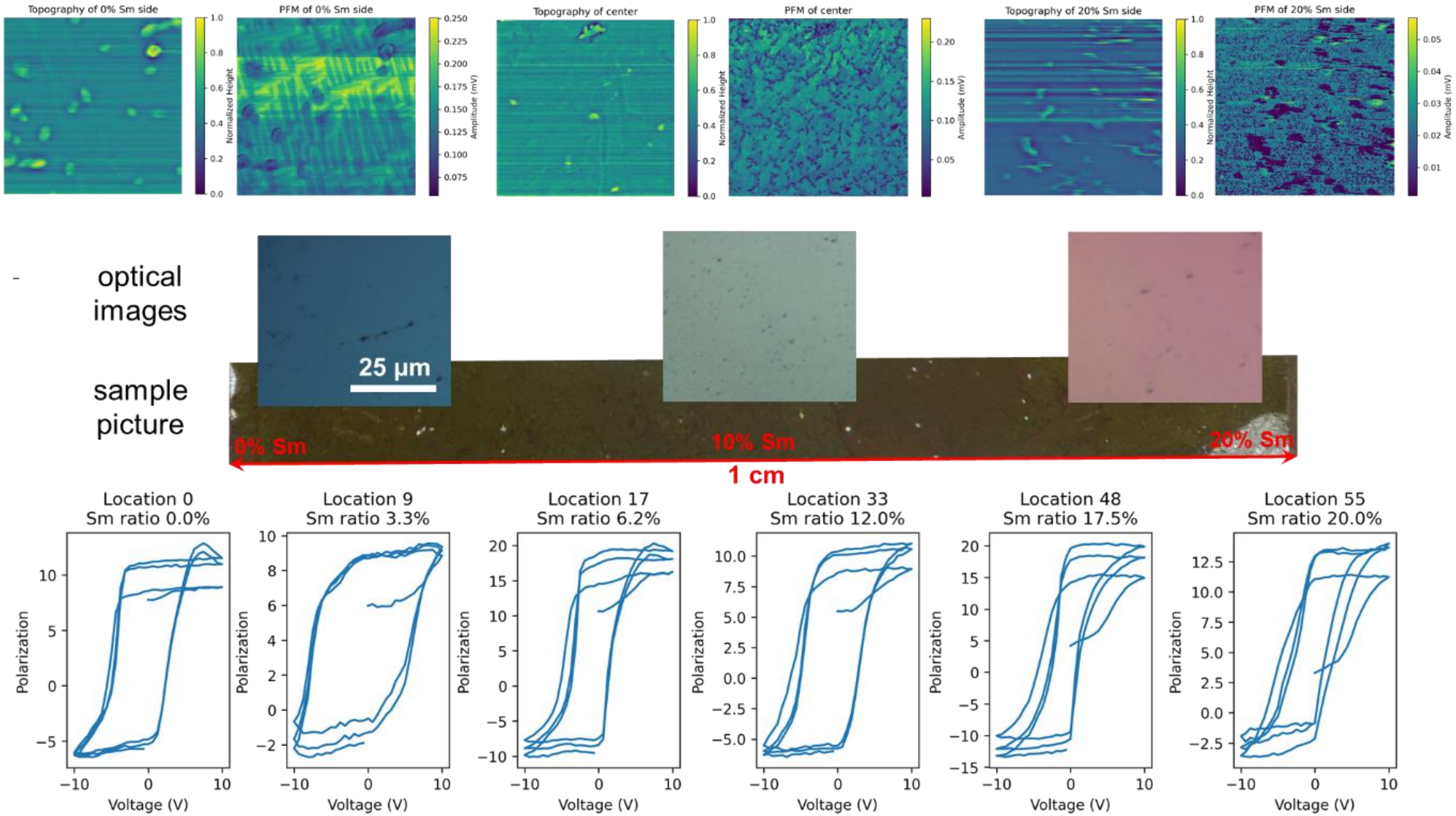
$BiFeO_3$ Linear est. 7%Sm $BiFeO_3$ 20%Sm $BiFeO_3$




arXiv:2004.11817

# Combinatorial libraries:





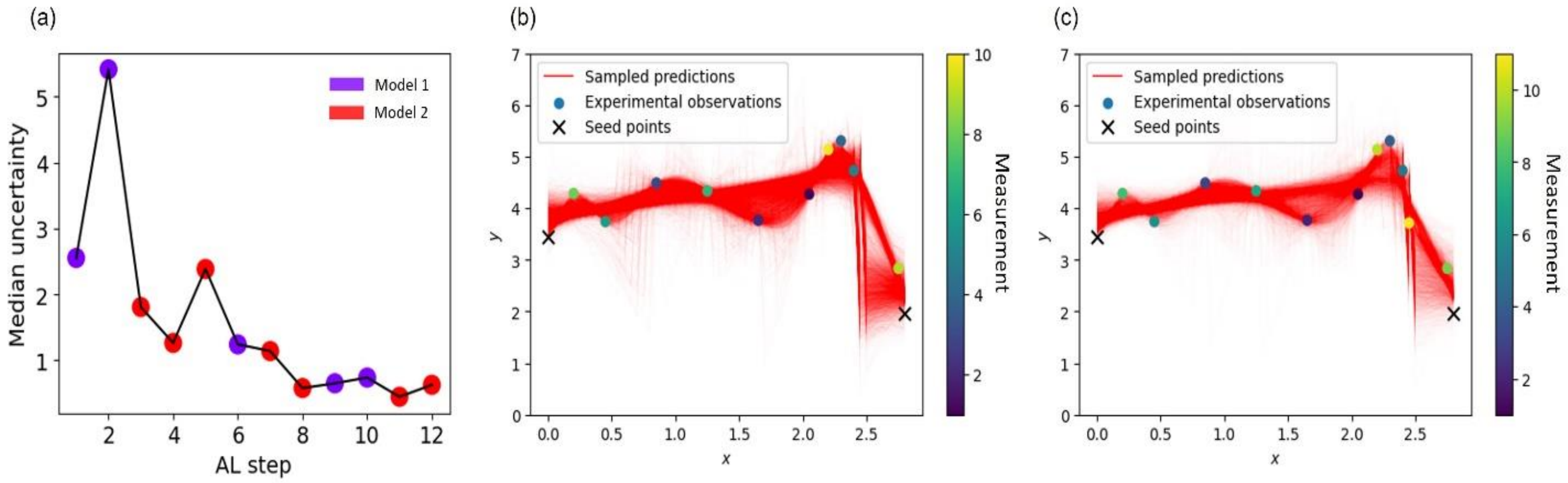
# Hypothesis selection for ferroelectric response

Model 1 (second order phase transition):

$$S = \begin{cases} S_0\left(1 - \dfrac{x}{x_0}\right)^2 + C, & x \le x_c, \\ C, & x > x_c \end{cases}$$

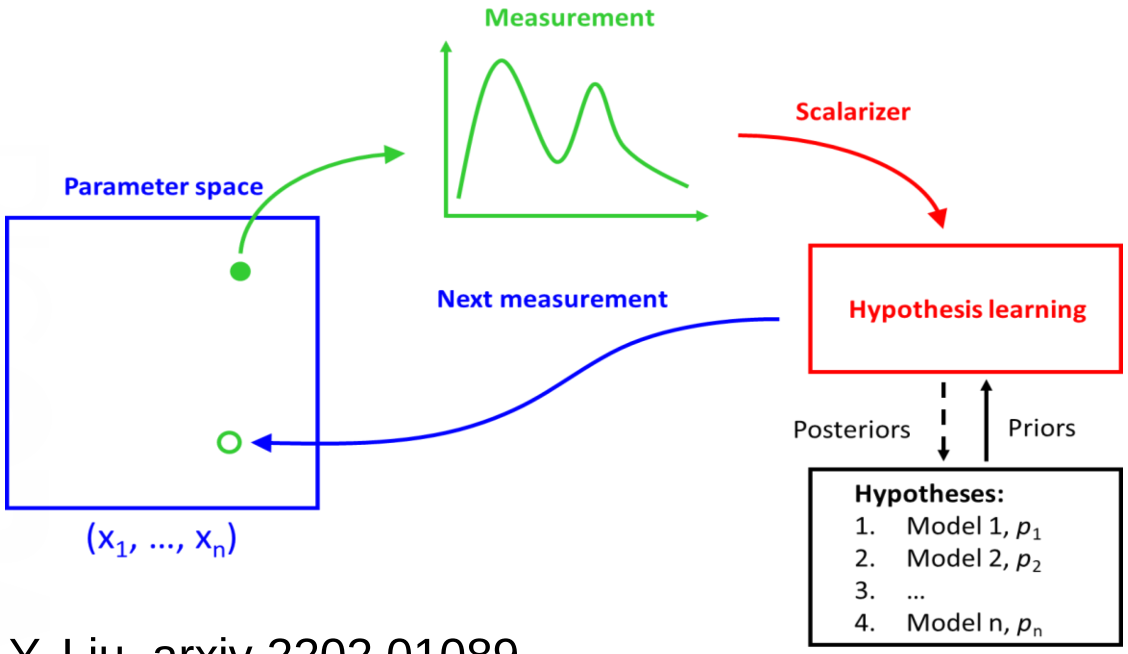
Model 2 (first order phase transition):

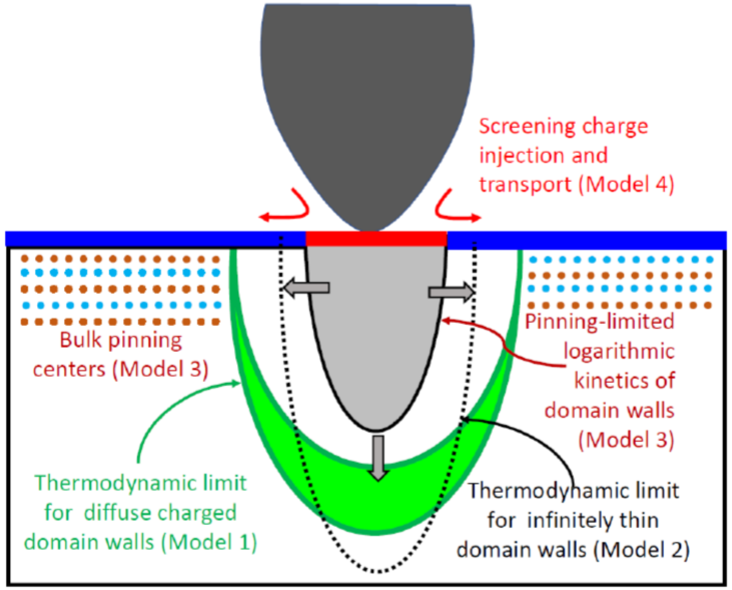
$$S = \begin{cases} S_0\left(1 - \dfrac{x}{x_0}\right)^{\frac{5}{4}} + C_0, & x \le x_c, \\ C_1, & x > x_c \end{cases}$$



# Hypothesis learning for domain growth laws

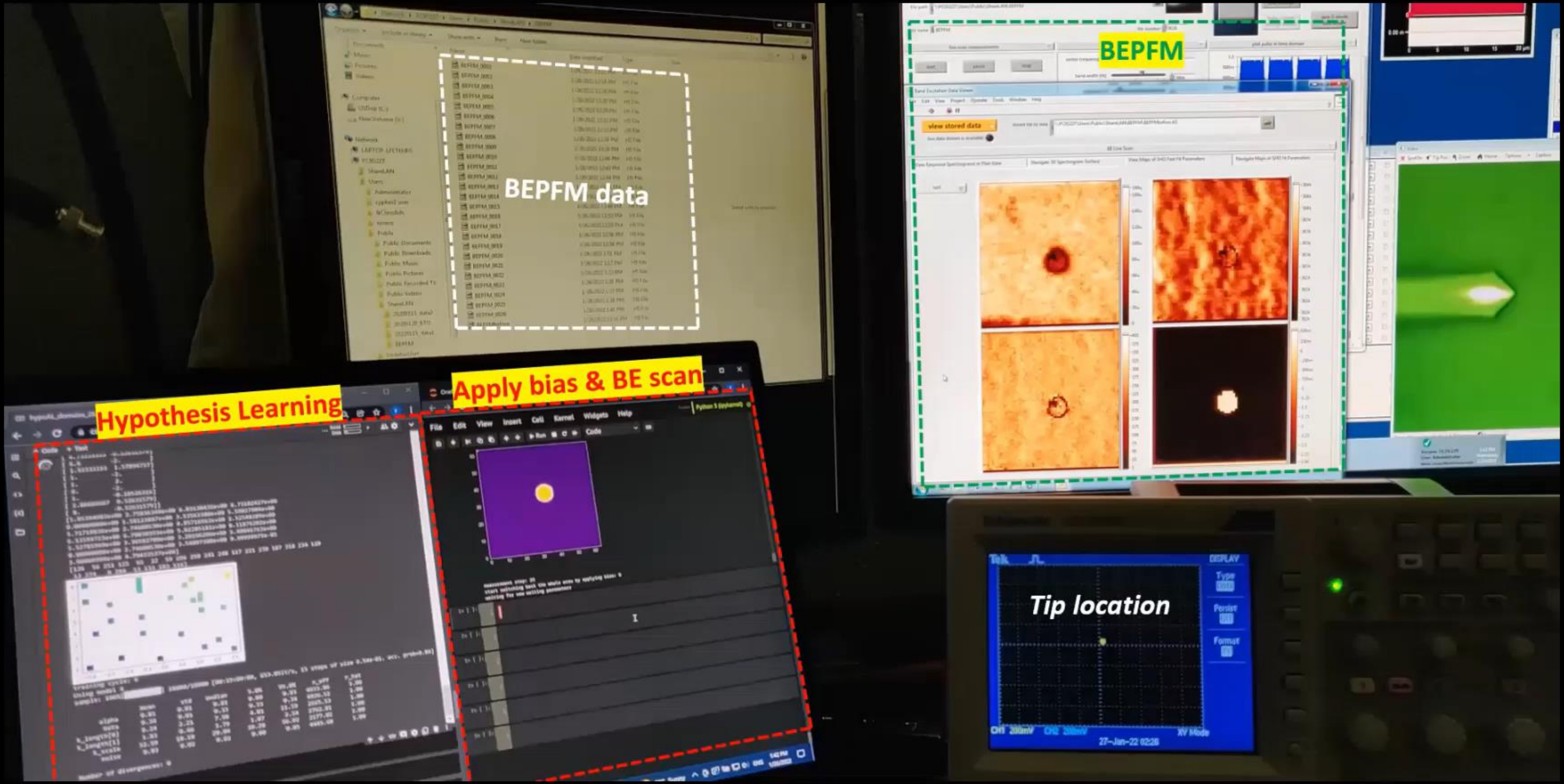
- Can ML algorithm think like a scientist?
- Yes – automated experiment can pursue hypothesis-driven science!



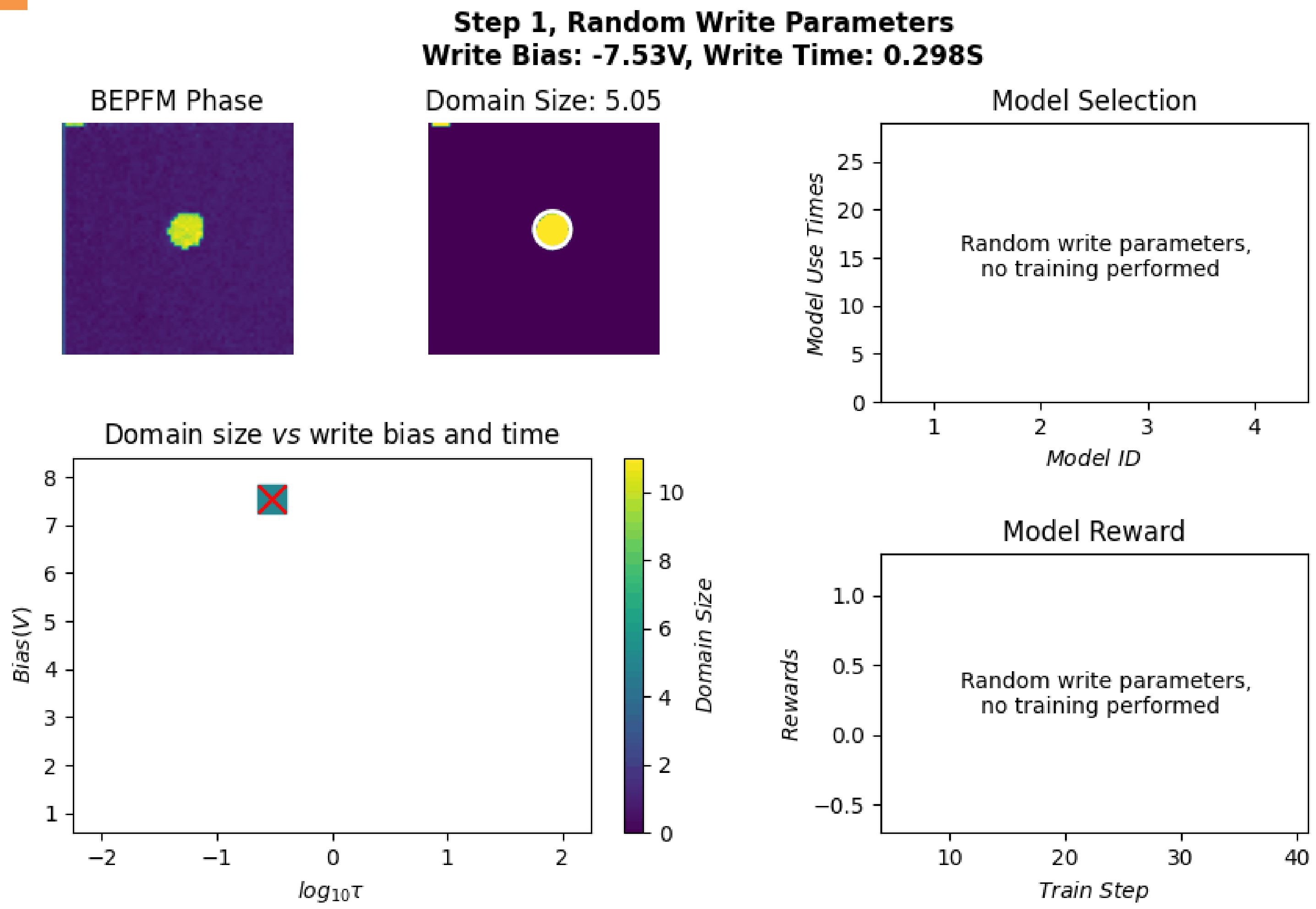




| | Model | Equation |
|---|---|---|
| Thermodynamic 1 | Model I | $r(V) = r_{cr} + r_0\sqrt{\left(\frac{V}{V_c}\right)^{2/3} - 1}$ |
| Thermodynamic 2 | Model II | $r(V) = r_{cr} + r_0\sqrt[3]{\left(\frac{V}{V_c}\right)^{2} - 1}$ |
| Wall pinning | Model III | $r(V,t) = V^{\alpha}\log\tau$ |
| Charge injection | Model IV | $r(V,t) = V^{\alpha}\tau^{\beta}$ |

Y. Liu, arxiv 2202.01089
Y. Liu, arxiv 2112.06649


BEPFM data
BEPFM
Hypothesis Learning
Apply bias & BE scan
Tip location

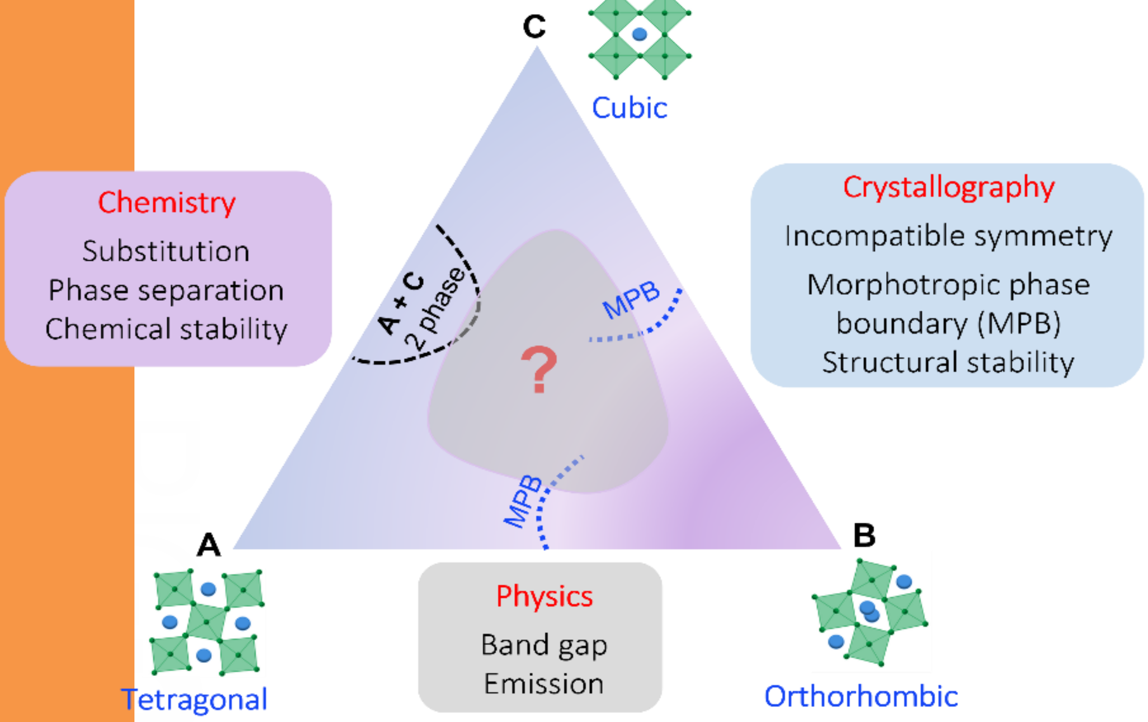
# Hypothesis learning in action




- ML algorithm has 4 competing hypothesis on domain switching mechanisms
- These hypothesis represent full set of possibilities for this system
- The microscope chooses experimental parameters in such a way as to establish which hypothesis is correct fastest
- Important: the same approach can be implemented in synthesis and electrical characterization
- Machine learning meets hypothesis-driven scientific discovery!

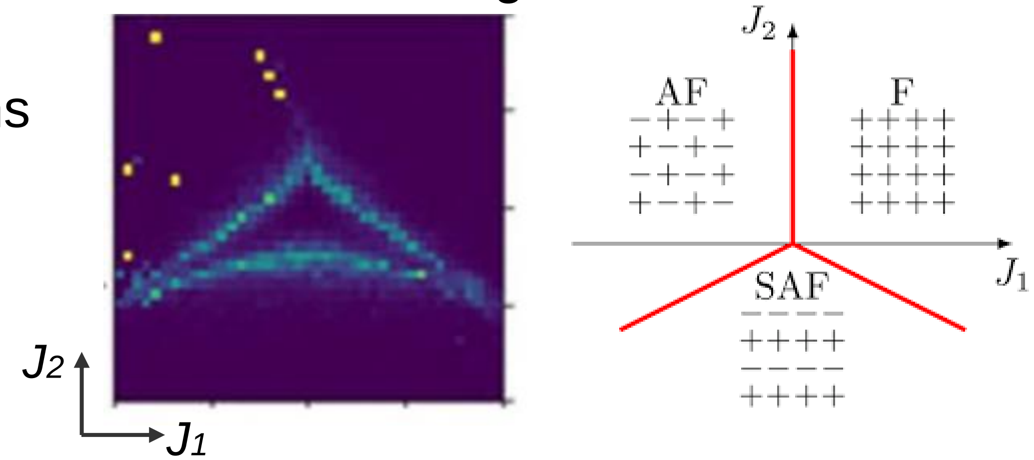

Y. Liu, arxiv 2202.01089
Y. Liu, arxiv 2112.06649

# Why synthesis (or theory)?





**Ising model**




- Automated synthesis in its simplest form requires some way to navigate phase diagrams
- In more complex form, processing space.
- Ideally, incorporate physical knowledge

- Similar problem - theory

# The World is Bayesian

**Hypothesis driven science:**
What we want to learn

**Forward model:** Theory

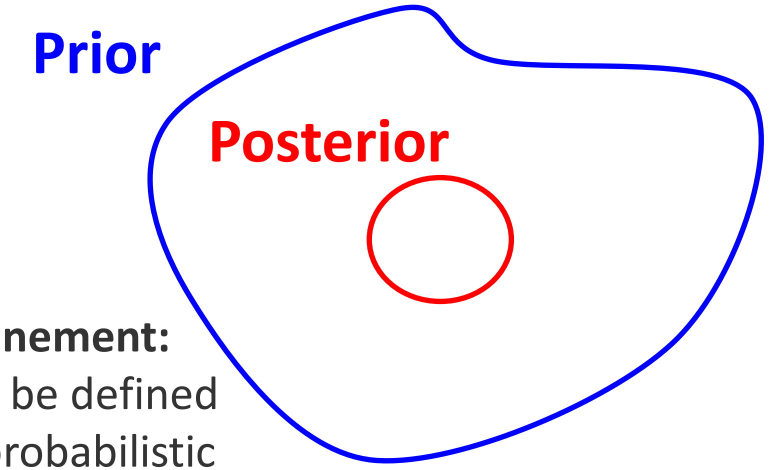
**Domain expertise:**

$$P(Theory|Data) = \frac{P(Data|Theory)P(Theory)}{P(Data)}$$

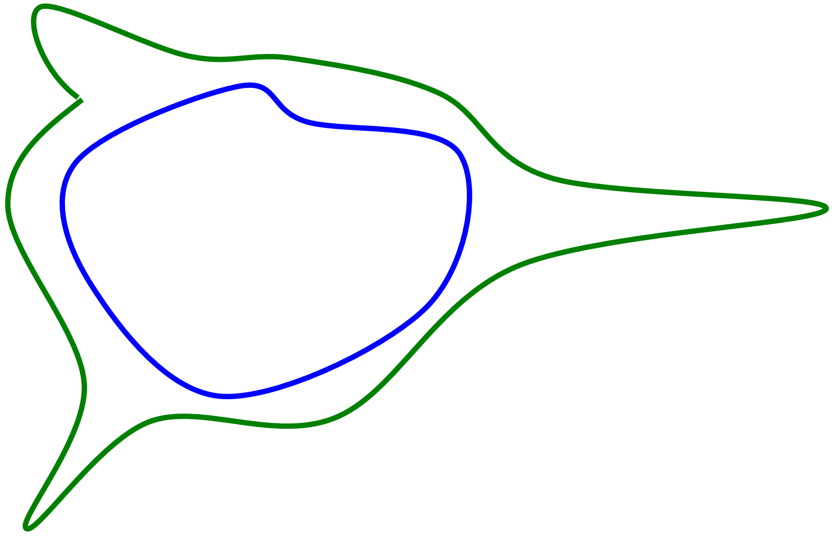
**High Performance Computing**

Experimentalists know the priors. Albeit they do not know that they know it, or how to convert them to algorithmic form

**However, how do we make guesses about the unknown?**



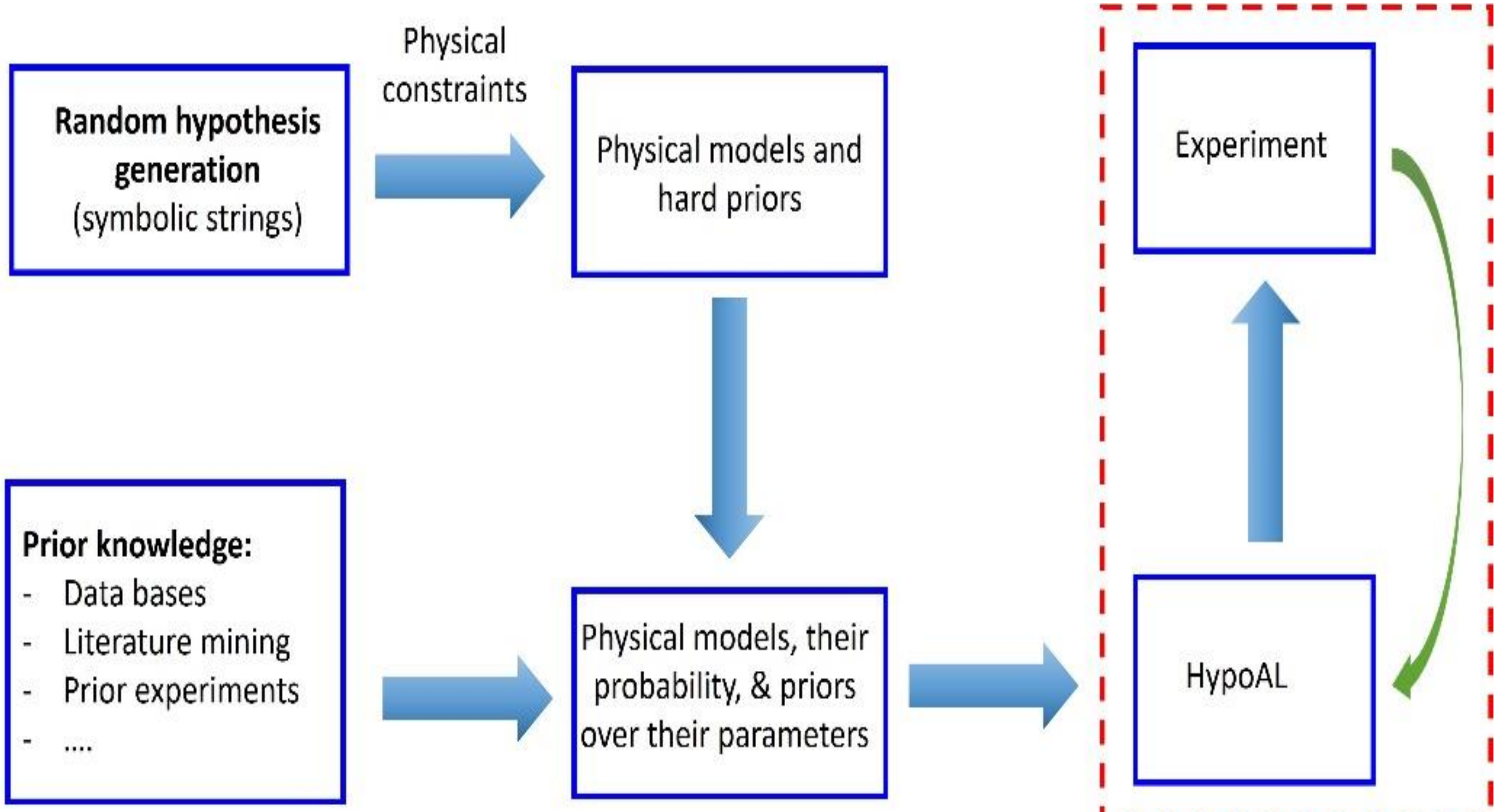

**Refinement:**
Can be defined as probabilistic model



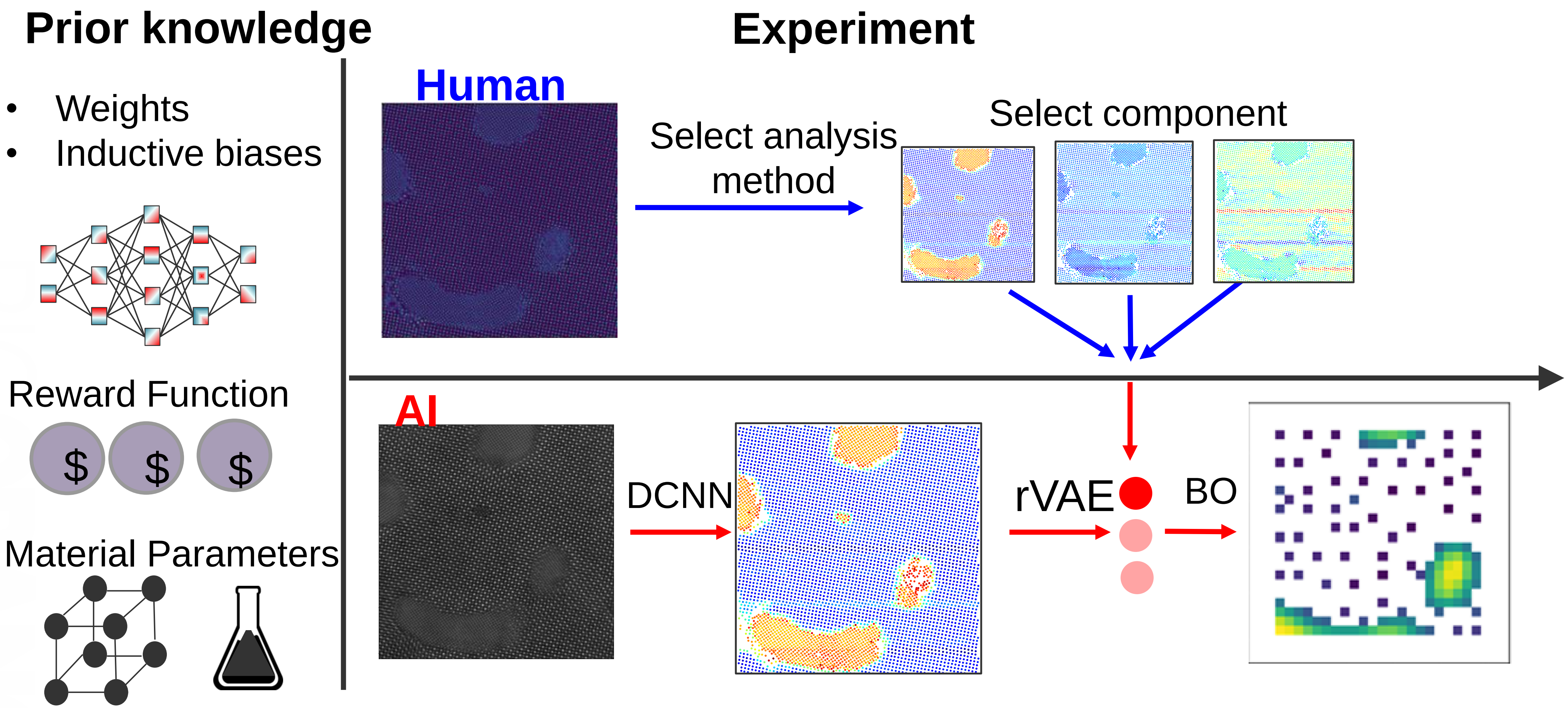
**Hypothesis formation:**
How can we do it?

# Towards hypothesis learning

- Data already exists: Eureka, SISSO, SinDY, etc.
- What if we make hypothesis learning a part of active experiment?
- Need policies for hypothesis generation



# Human in the Loop: Hypothesis injection




**Discovery pathway depends on the reward structure!**