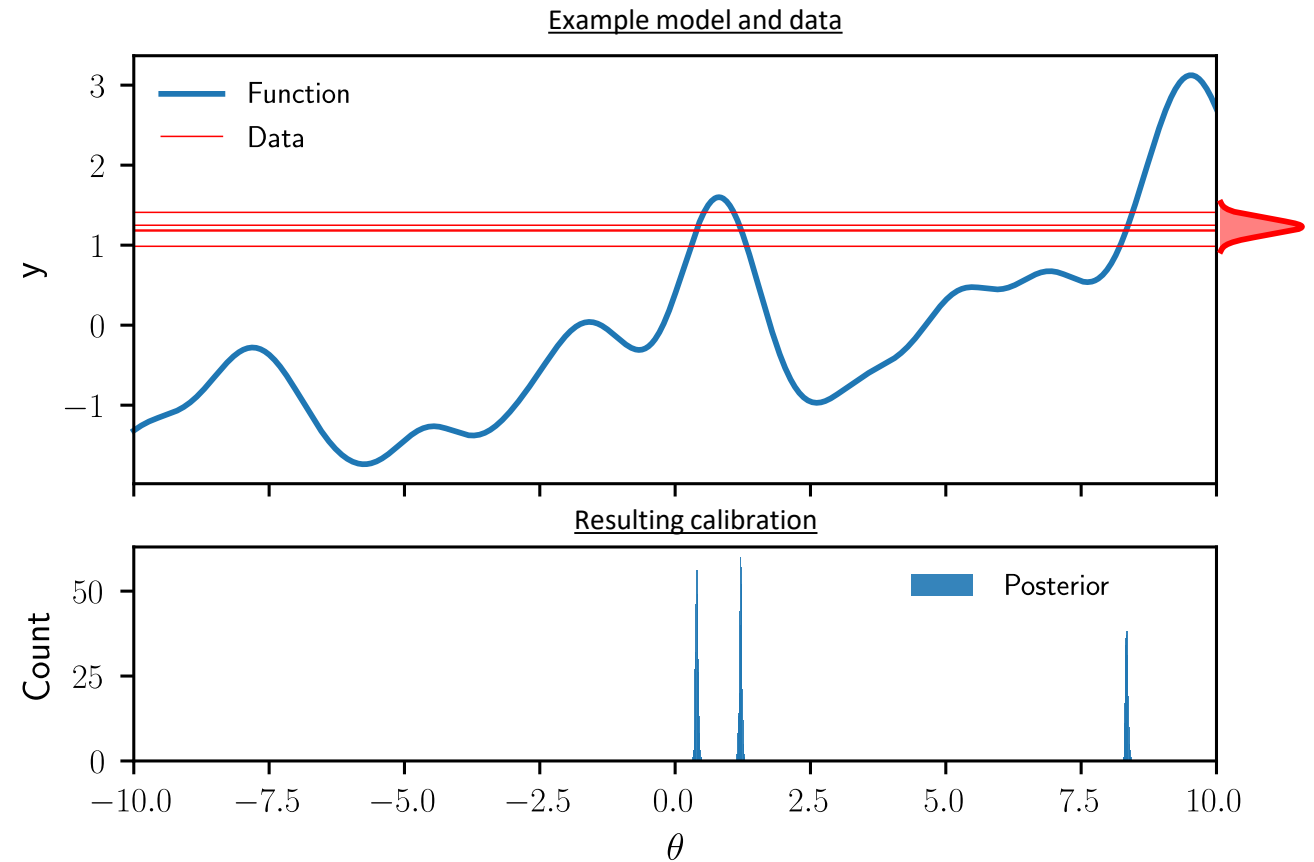


Probabilistic Calibration of Expensive Models using Efficiently Trained Surrogates

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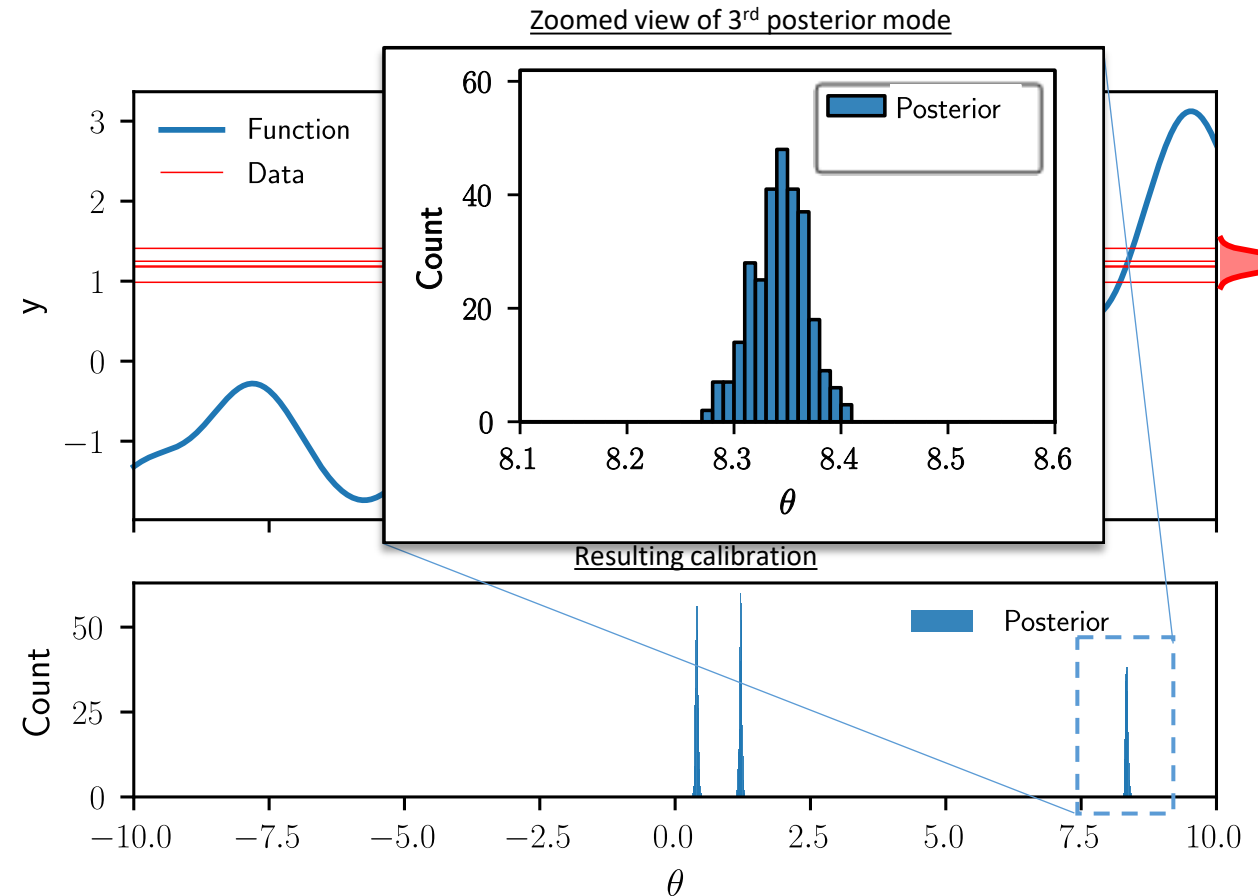
Motivation

- Calibrating models to noisy observations
 - Well-established approach: Bayesian inference + sampling methods



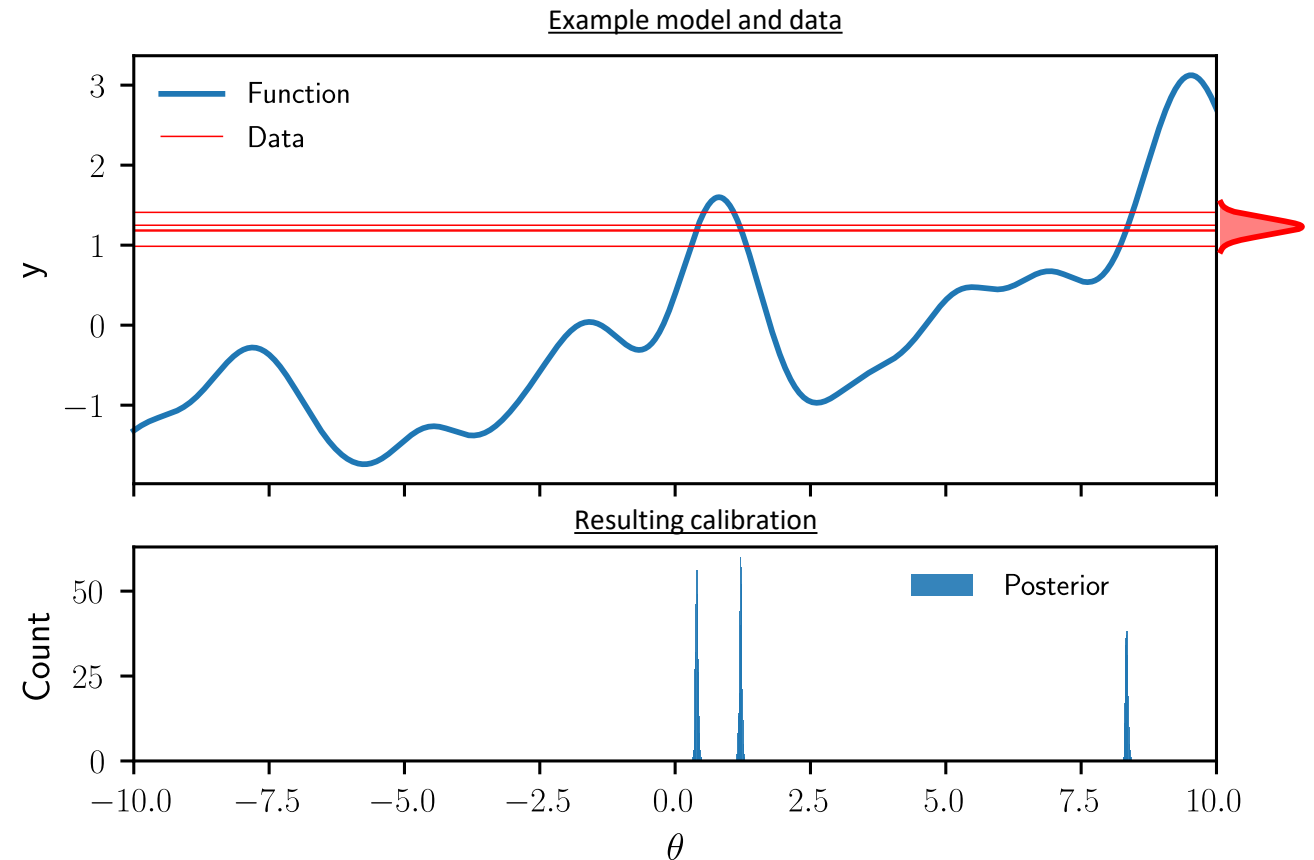
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Motivation

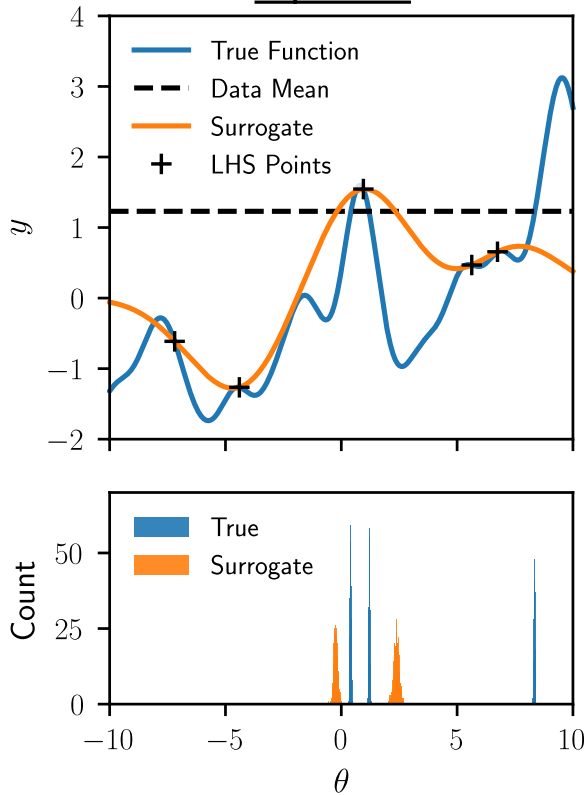
- Calibrating models to noisy observations
 - Well-established approach: Bayesian inference + sampling methods
 - Works if the model is inexpensive
- For expensive models:
 - Data-driven surrogate models (fast)
 - But generating training data can be prohibitive if, for example:
 - Multiple calibrations required
 - Parameter space is much broader than posterior support
 - Model is *very* expensive
- **Goal:** efficiently train a surrogate for the purpose of model calibration



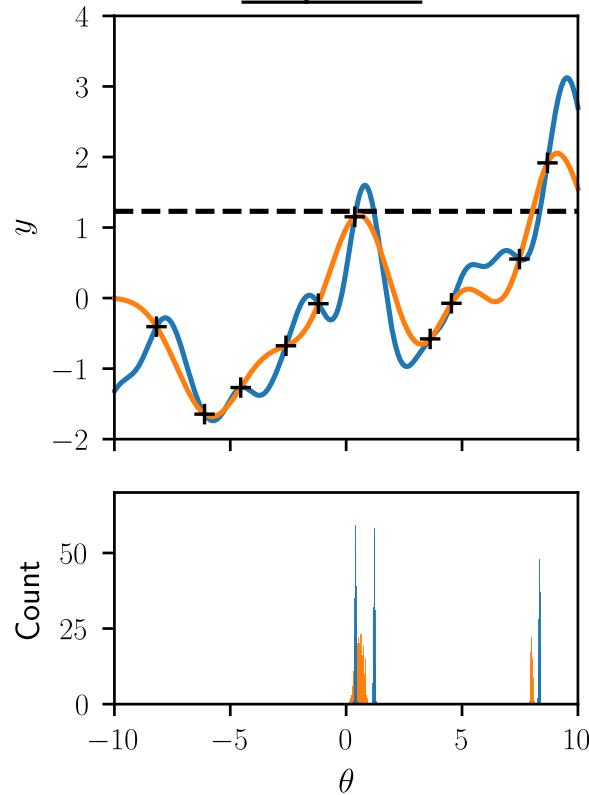
Space-filling Designs

(e.g., Latin Hypercube Sampling (LHS))

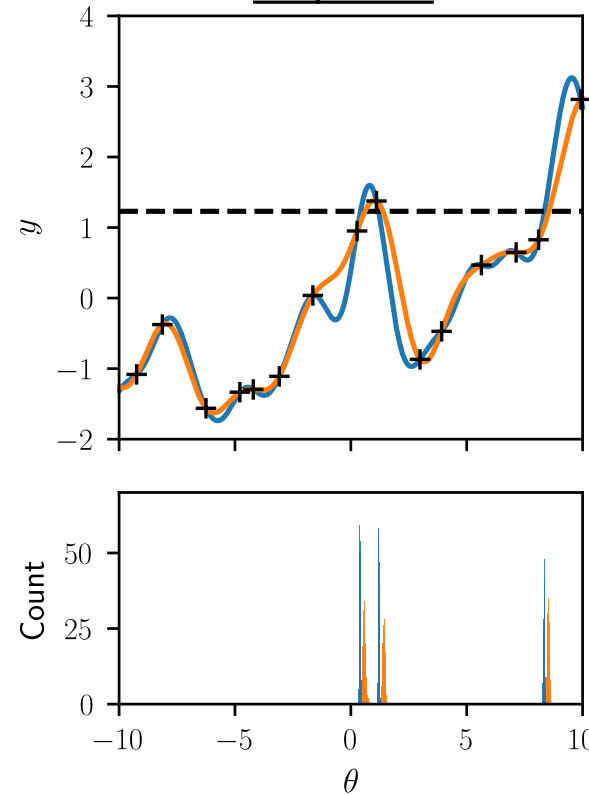
5 points



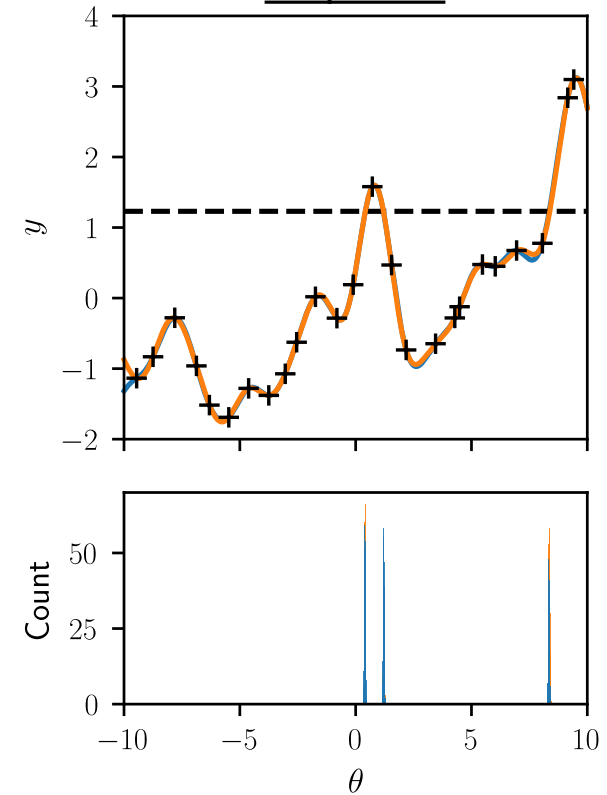
10 points



15 points



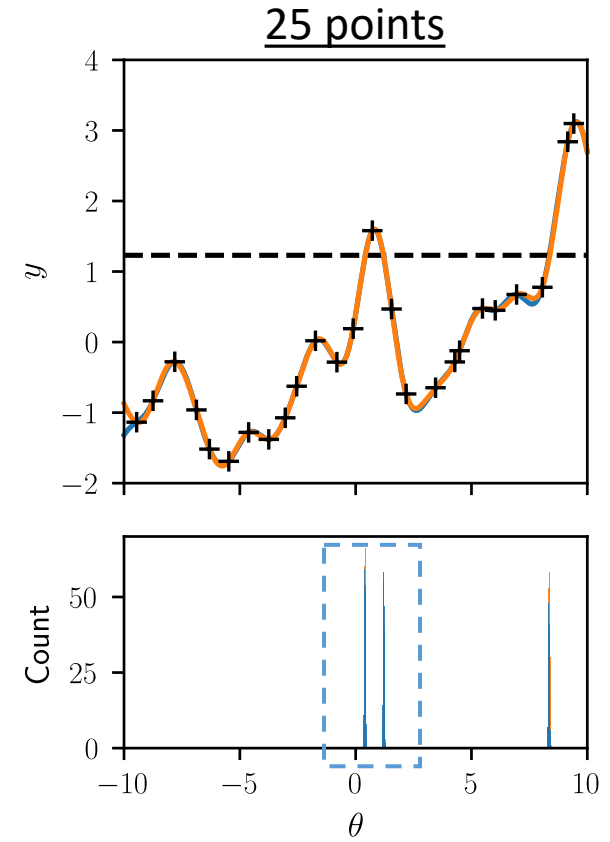
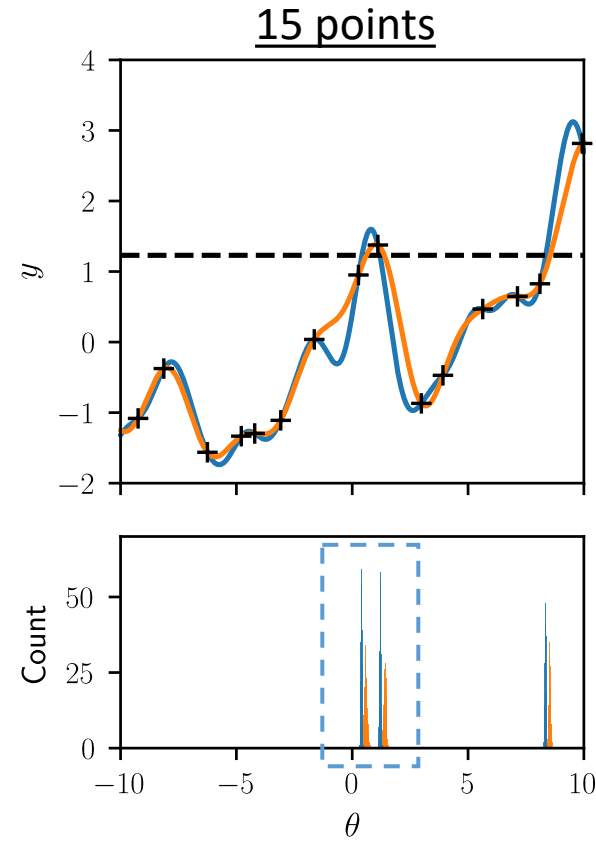
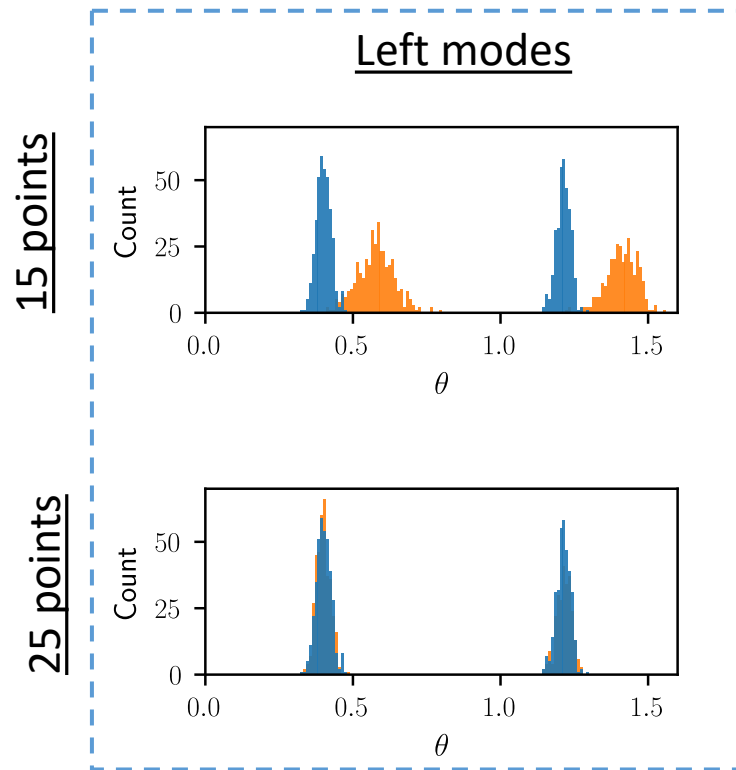
25 points



➤ Convergence of the surrogate in regions of non-zero posterior probability is slow.

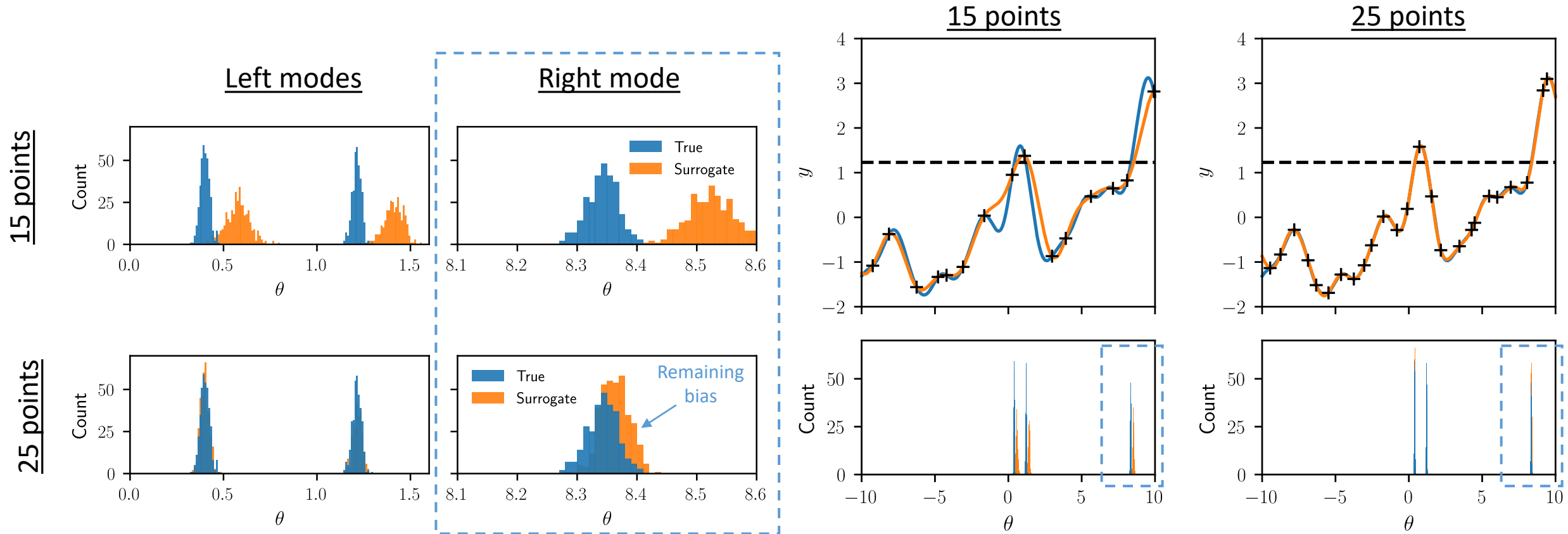
Space-filling Designs

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Space-filling Designs

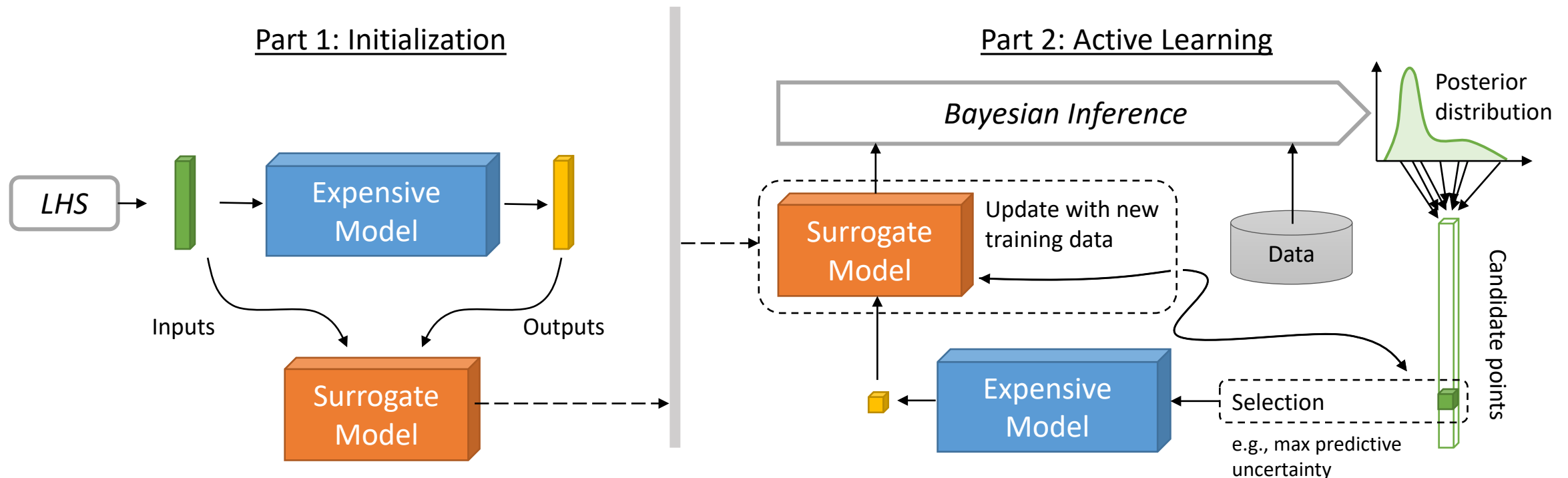
(e.g., Latin Hypercube Sampling (LHS))



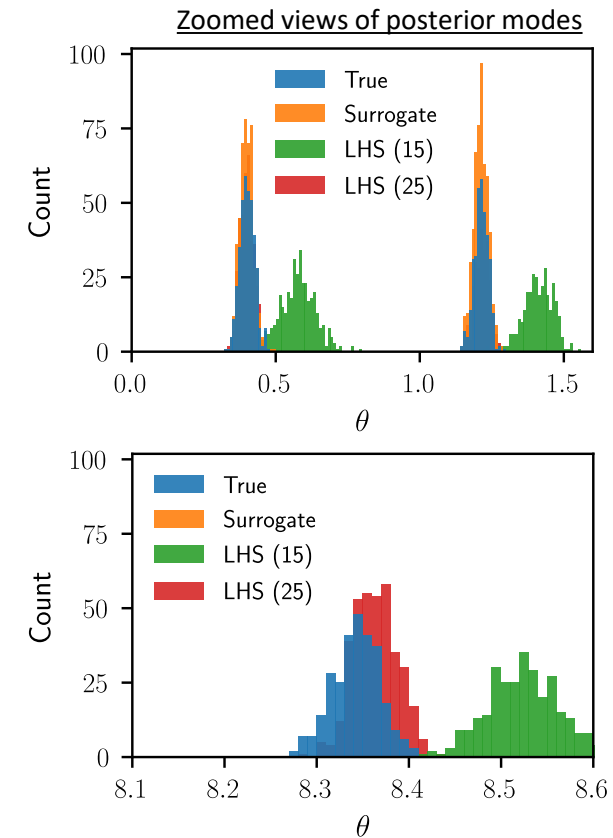
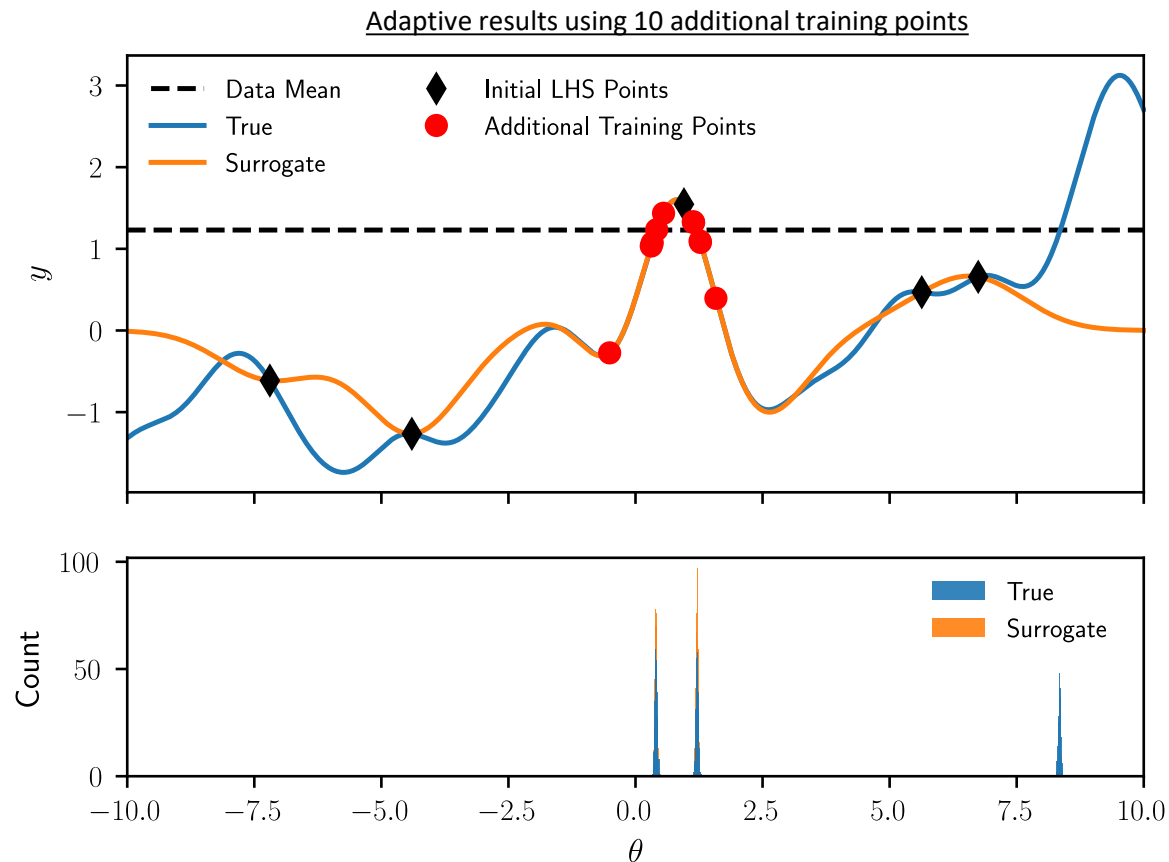
➤ After qualitative *global* convergence, relatively large bias due to remaining *local* error

Method

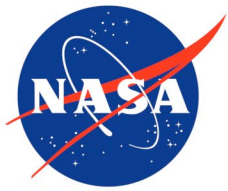
- Adopt an active learning training approach
- Target training points that are within/near the support of the posterior (i.e., where accuracy matters for calibration)



Basic Implementation

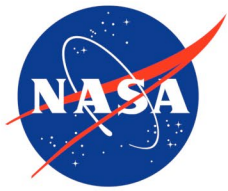


➤ Using only samples from the posterior (*exploitation*) can reduce bias but also miss modes



Sequential Monte Carlo (SMC)

- Candidate point generation via SMC has a number of advantages
 1. Allows for parallel computations and is generally faster than alternatives



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- Candidate point generation via SMC has a number of advantages
 1. Allows for parallel computations and is generally faster than alternatives
 2. Tunable exploitation vs. exploration

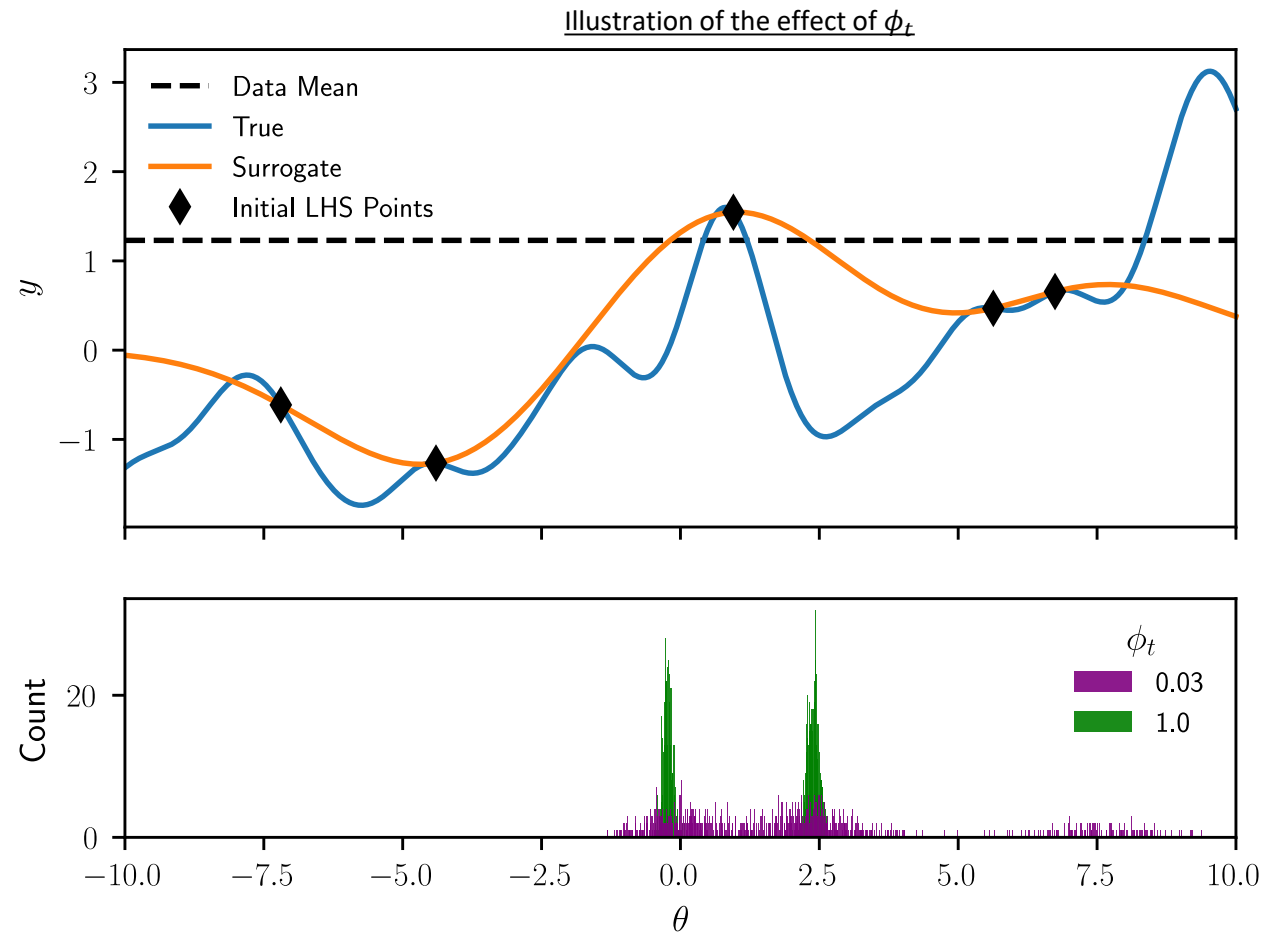
$$t^{th} \text{ Target} \propto (\text{Likelihood})^{\phi_t} \times \text{Prior}$$

where $\Phi = [0, \dots, \phi_t, \dots, 1]$ and $\phi_t > \phi_{t-1}$

↑
Targets the
prior
(exploration)

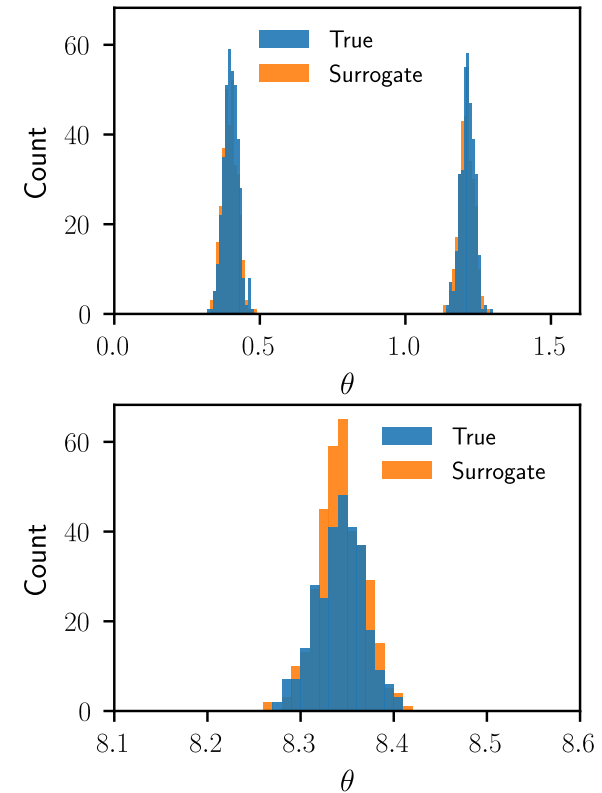
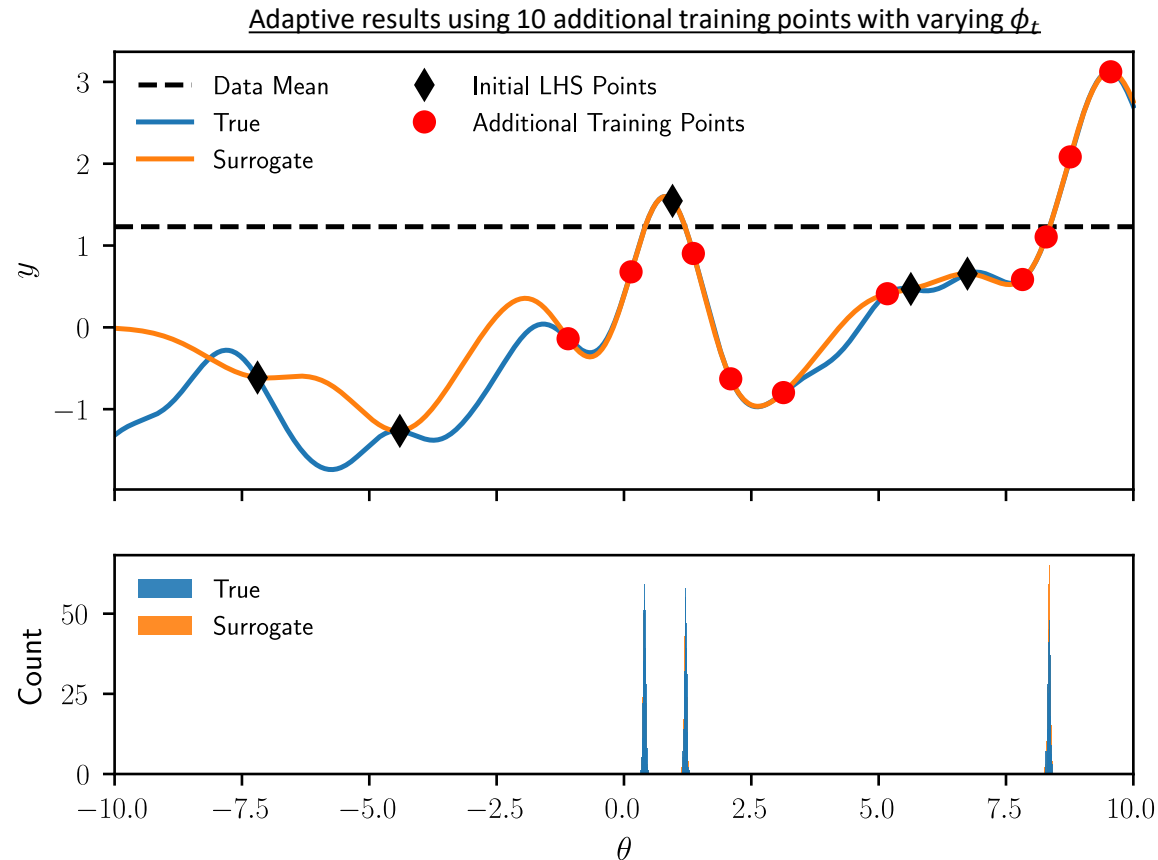
↑
Targets the
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Exploitation vs. Exploration

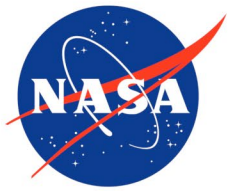


➤ If $\text{supp}(\text{Posterior}) \subseteq \text{supp}(\text{Prior})$, ϕ_t can be used to tune the degree of exploration

Exploitation vs. Exploration



- Balanced exploitation & exploration eliminates bias and discovers the additional mode (using same number of surrogate updates as before)



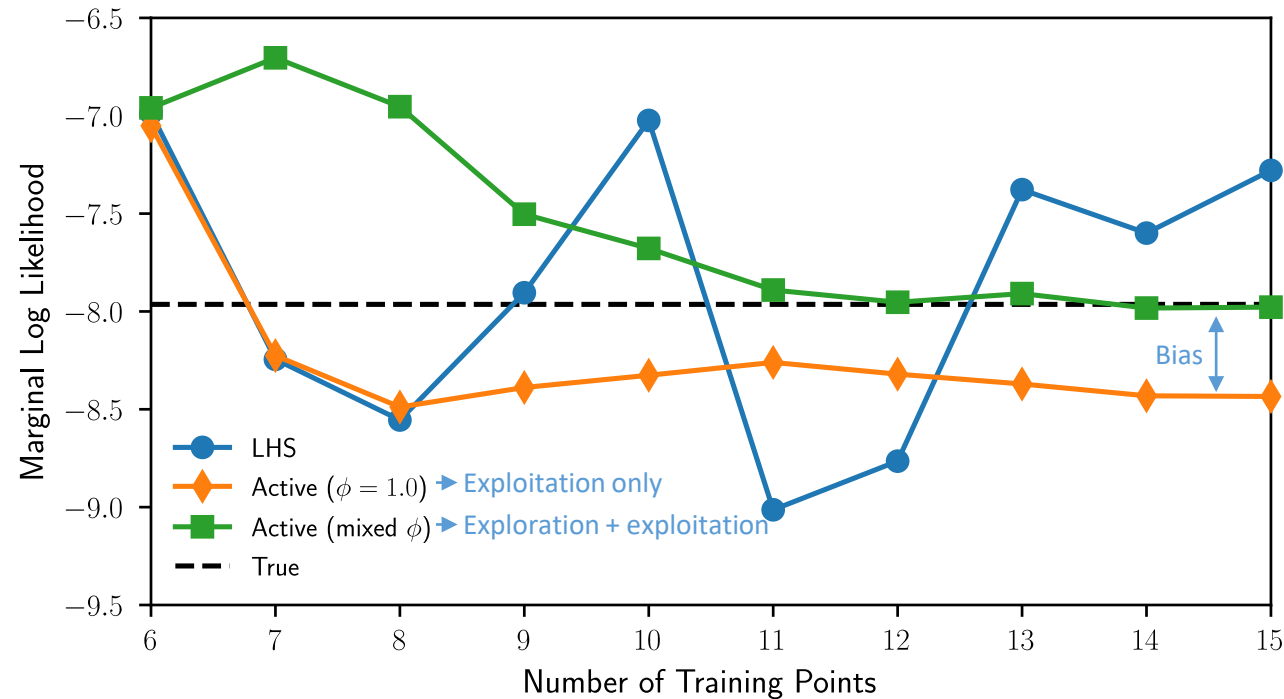
Sequential Monte Carlo (SMC)

- Candidate point generation via SMC has a number of advantages
 1. Allows for parallel computations and is generally faster than alternatives
 2. Tunable exploitation vs. exploration
 3. Provides an estimate of marginal likelihood, which can be used for convergence monitoring

$$Posterior = \frac{Likelihood \times Prior}{\text{Normalizing Constant}}$$

The denominator, "Normalizing Constant", is enclosed in a dashed blue box and underlined in blue.

Monitoring Convergence



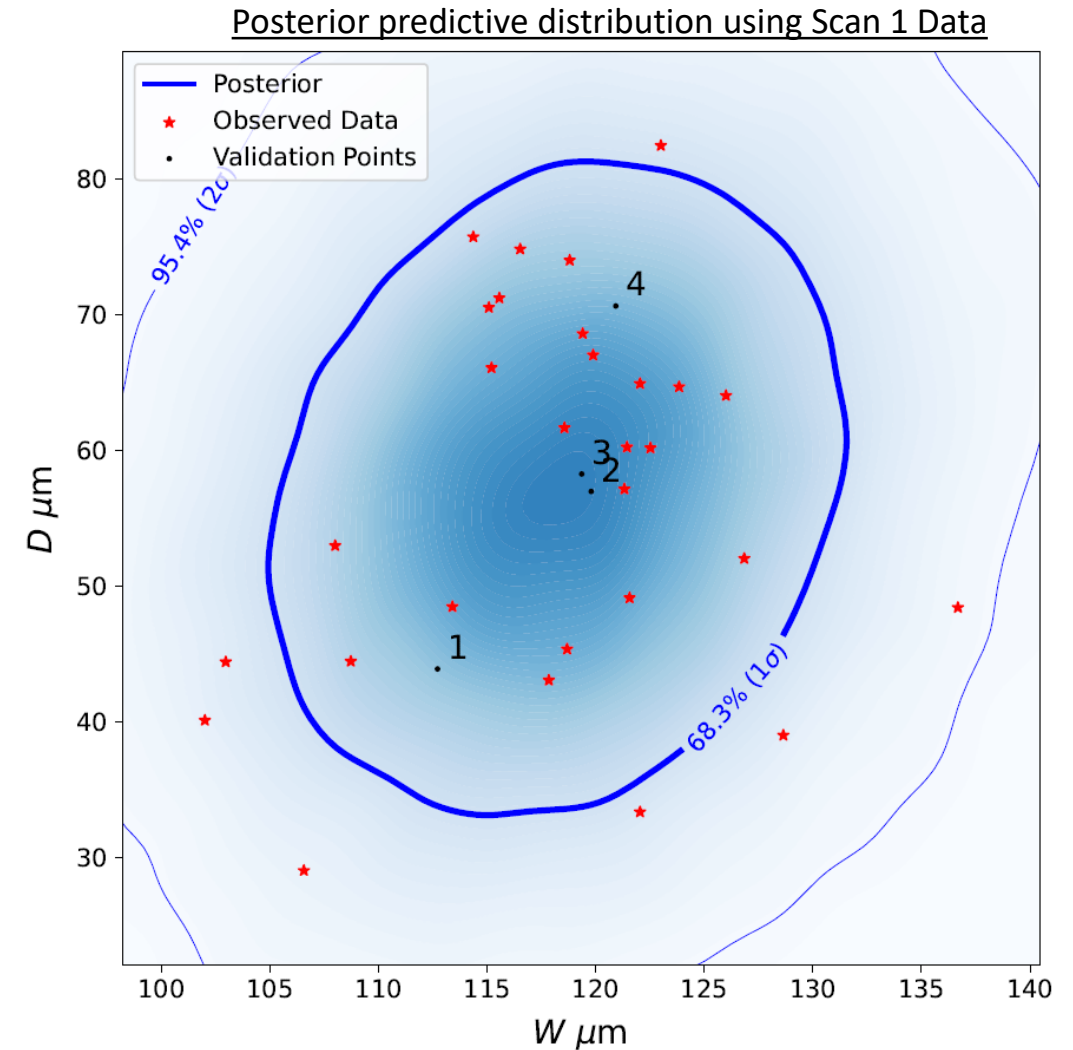
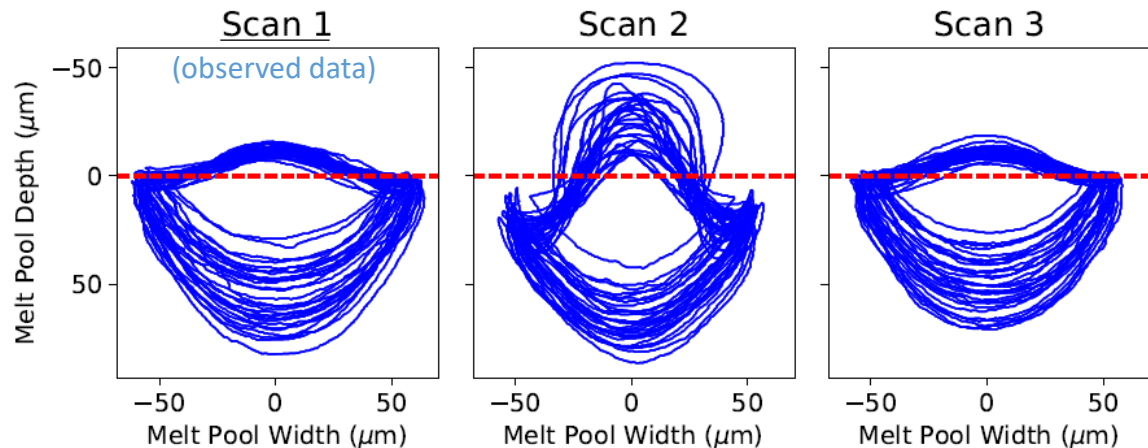
- Convergence observed for both active learning cases, but exploration required to remove bias due to missing mode.

Additive Manufacturing Example

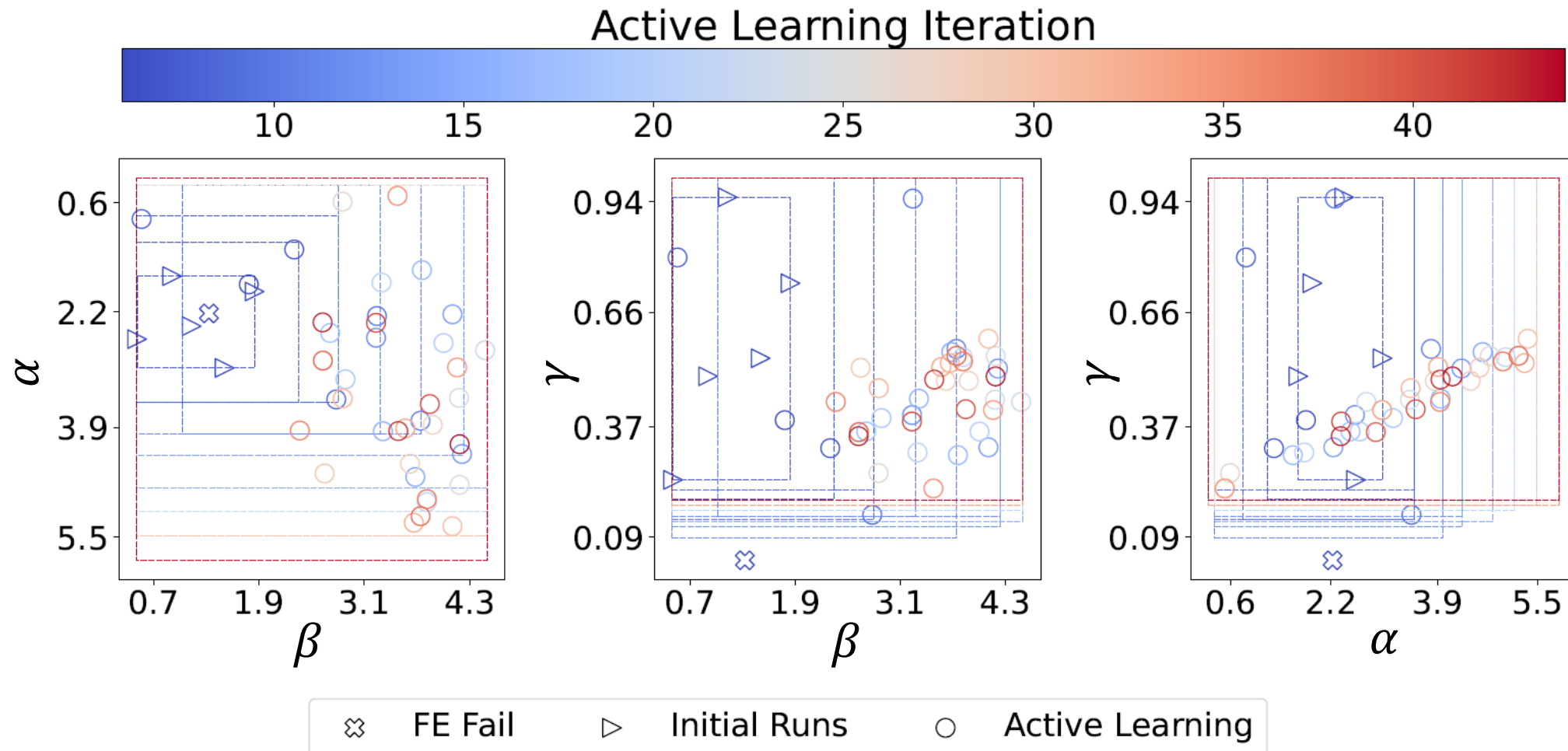
- **Goal:** efficiently calibrate parameters of laser powder bed fusion process model
- **Data:** melt pool widths and depths measured from cross sectioning laser scan tracks and using optical microscopy and computer vision¹

1. J. M. Fody et al. "A semantic segmentation algorithm for automated rapid melt pool identification from cross-sectional micrographs," Materials Characterization, (2024).

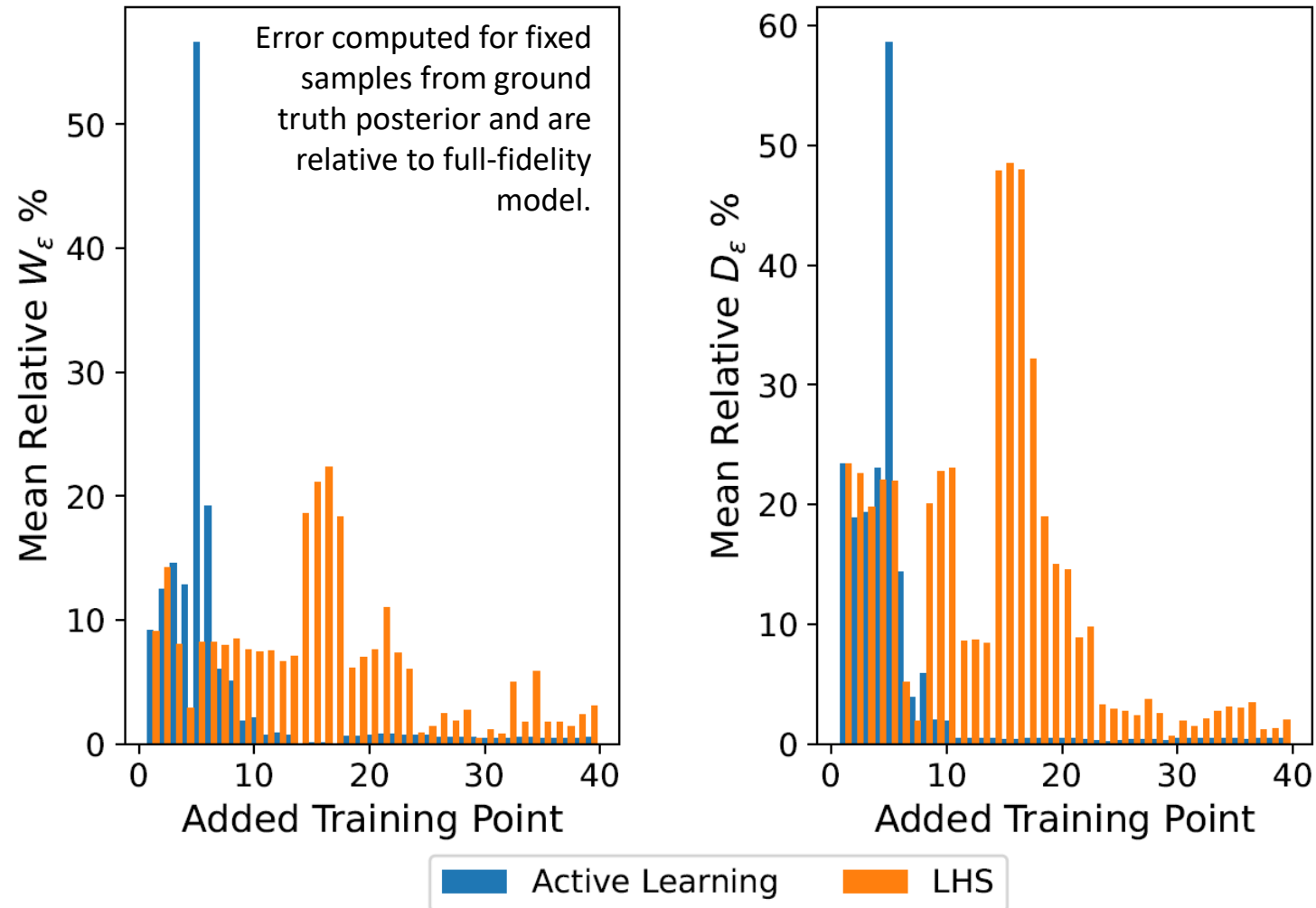
- **Model:** $[W, D] = f(\alpha, \beta, \gamma, \dots)$
Calibrated Parameters

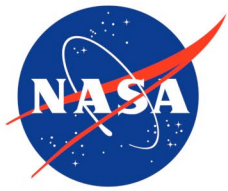


Generating Training Data



Comparison to LHS





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Conclusion

- Probabilistic calibration of expensive models can be intractable
- Training a surrogate model can still present computational challenges
- Relative to space-filling, the proposed active learning approach was shown to:
 - Improve accuracy of surrogate-based posterior estimates under a fixed budget
 - Reduce the amount of training data required for convergence to a given accuracy
 - Enable identification of unknown/multiple posterior modes
- More details provided in [1] and code necessary to implement a similar training algorithm can be found at [2]

1. Leser, Patrick E., and Joshua M. Fody. "Efficient Calibration of Expensive Computational Models." NASA/TM–20230006753 (2023).
2. SMCPy open-source Python package: <https://github.com/nasa/SMCPy>