Bayesian Algorithm Execution for Tuning Particle Accelerator Emittance with Partial Measurements

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...and others!

OUTLINE

1. **Motivation** Multi-Point Queries and Emittance Optimization
2. **Method**
   a. Optimization with Multi-Point Queries
   b. Info-Based BAX Overview
   c. Info-Based BAX for Emittance in LCLS and FACET-II
3. **Results**
   a. Noisy LCLS Simulation
   b. LCLS and FACET-II Live Optimization
4. **Next Steps**

Emittance is a critical parameter for X-ray FELs

- Determines the X-ray beam brightness
- Crucial for LCLS-II-HE
- *Quadrupole scan* method used at LCLS, LCLS-II, FACET-II

Emittance tuning is VERY slow:

- Each iteration requires a "secondary scan" along quadrupole domain
- Each scan step is slow (beam size measurement via wires/screens)
- Information from the individual quad scans is lost

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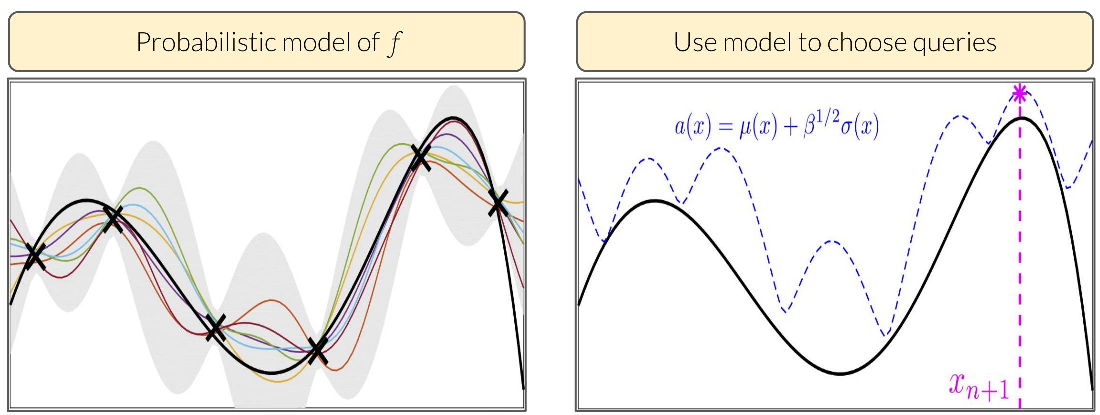
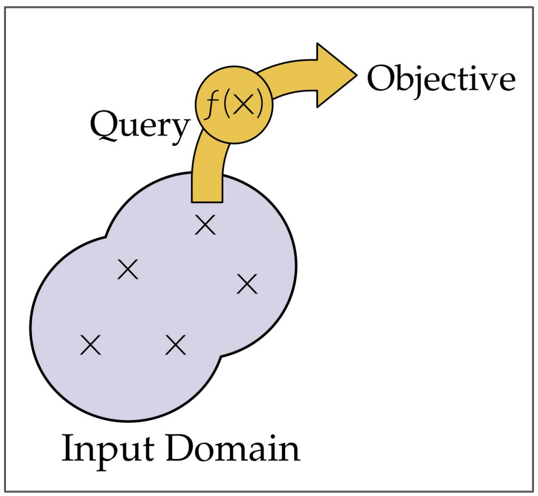
One solution: deploy a black-box optimization algorithm, such as **Bayesian optimization**.



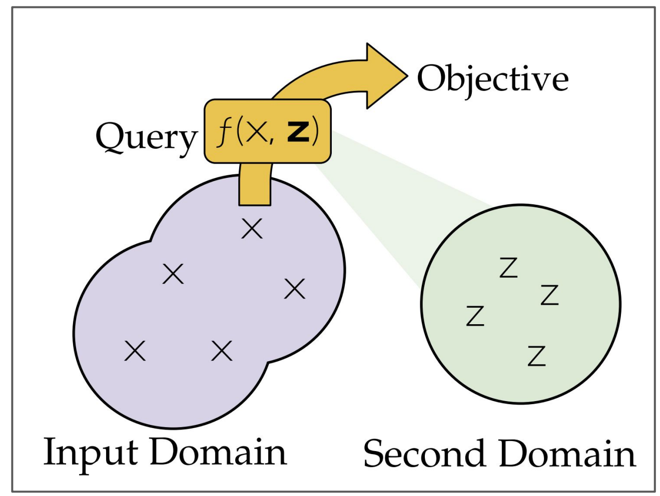
MULTI-POINT QUERIES & EMITTANCE OPTIMIZATION

Emittance measurements are what we call “multi-point queries”

Standard black-box query



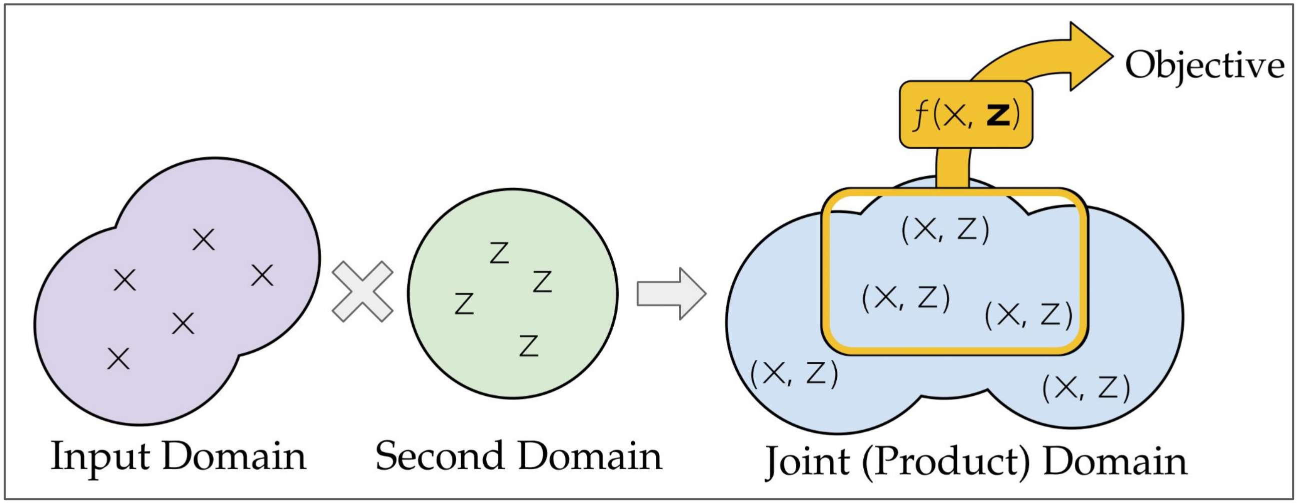
Multi-point query



Given this additional known structure, can we perform more-efficient black-box optimization?

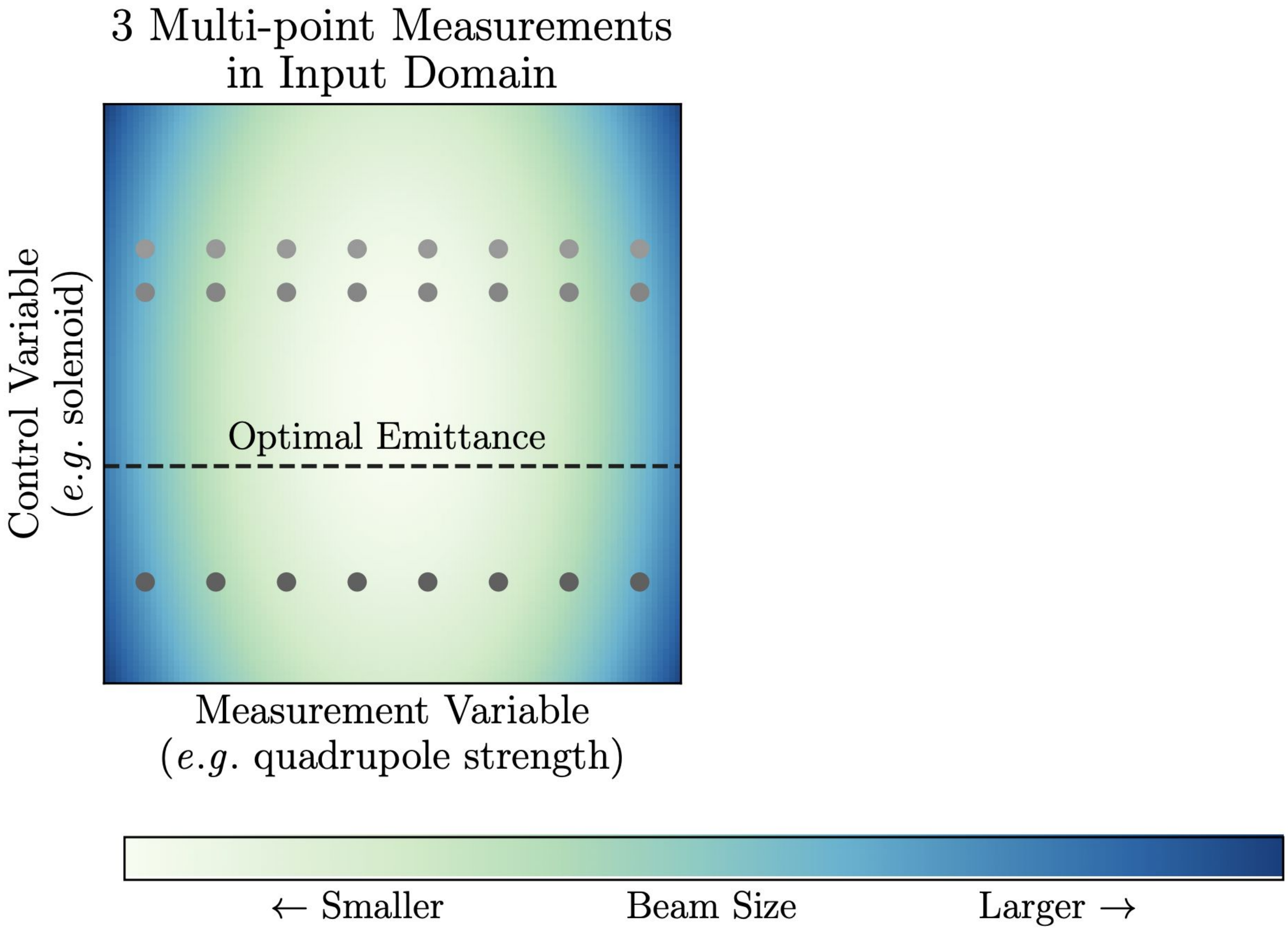
Our strategy: make "partial measurements" in "joint" domain

For each query from the domain, *measure a single point in 2nd domain*:
Cost- and information-efficient



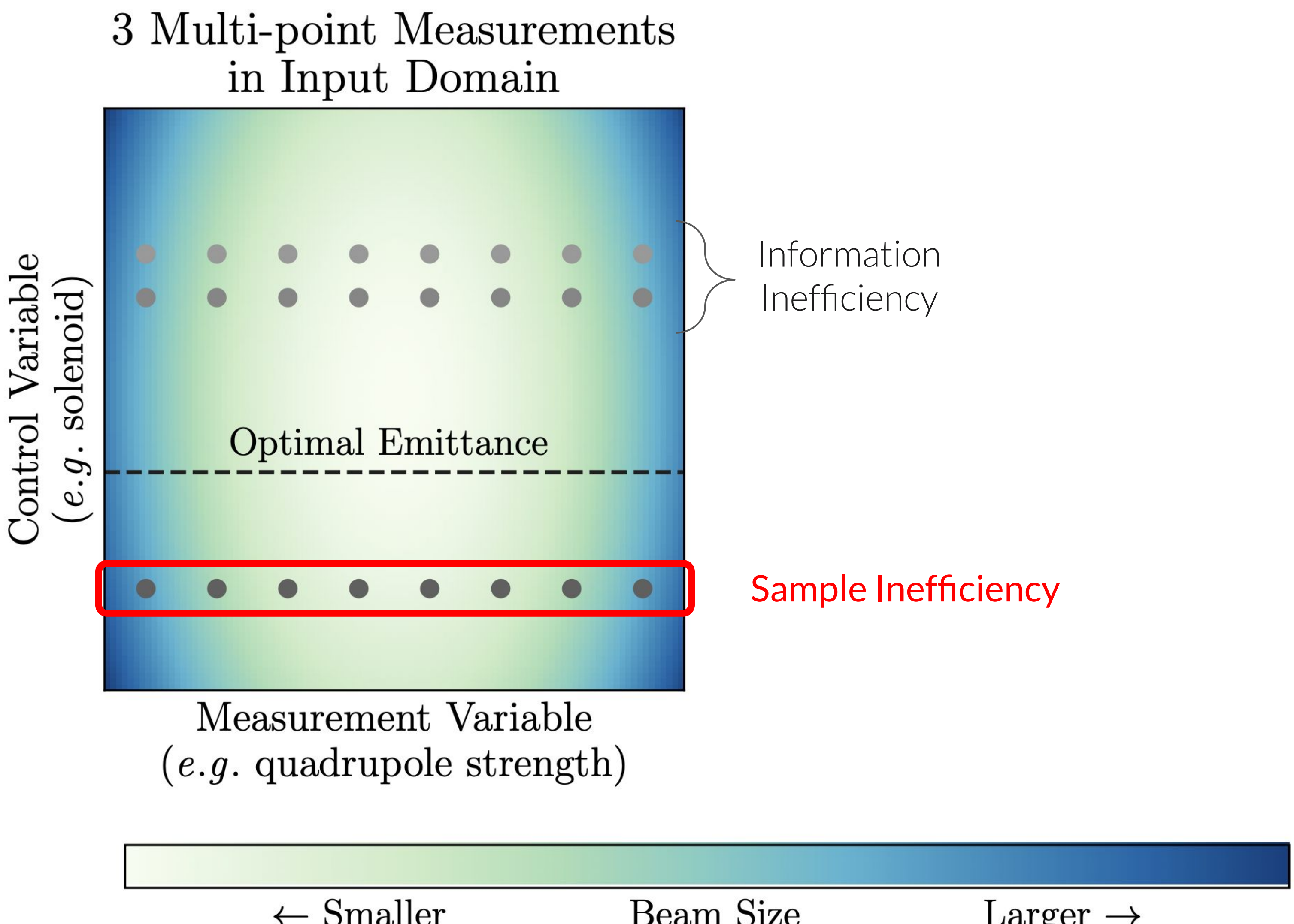
Still *same* optimization problem, i.e. find a point in our original domain that optimizes the function.

EMITTANCE OPTIMIZATION IN JOINT SPACE

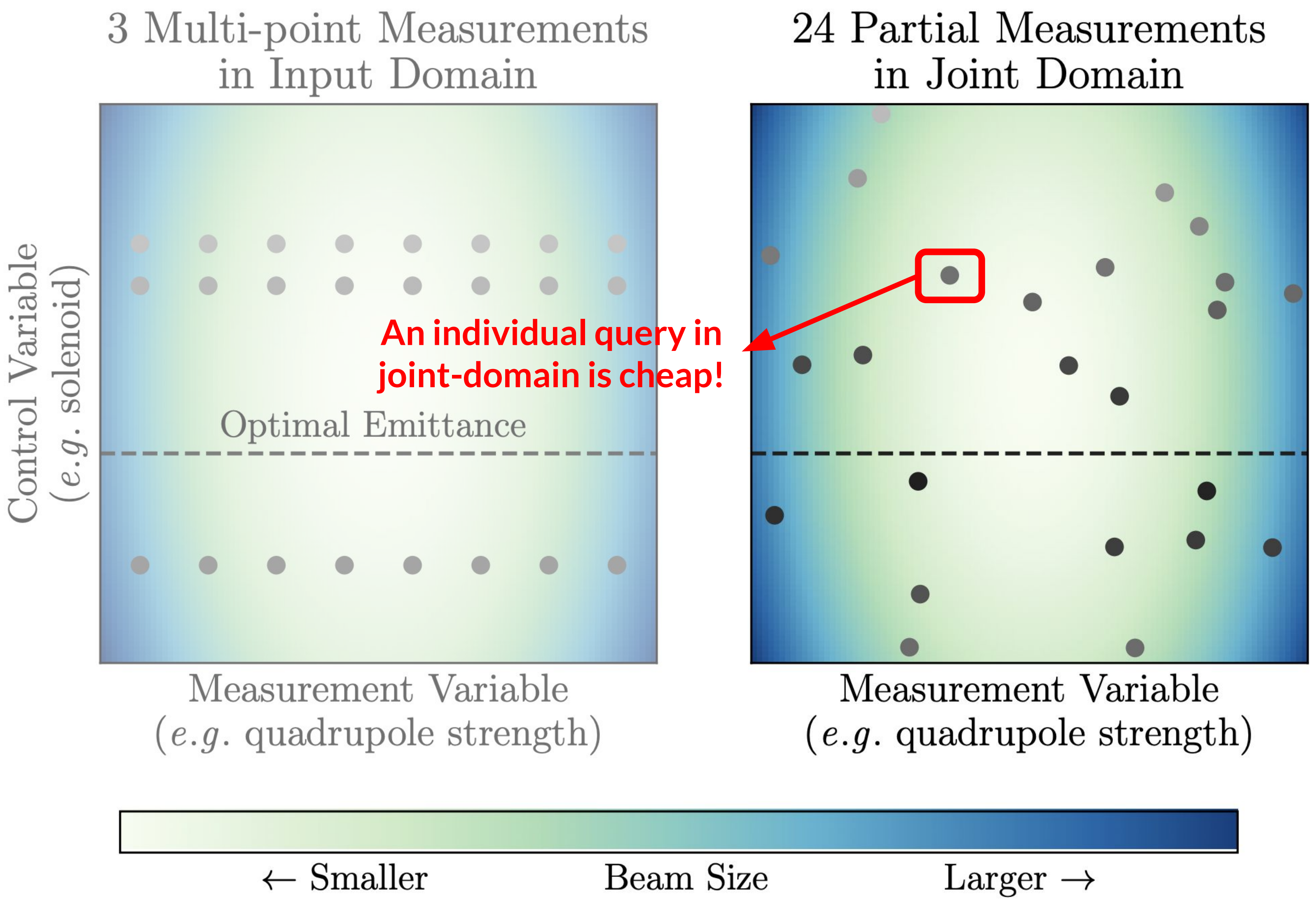


EMITTANCE OPTIMIZATION IN JOINT SPACE

Traditional method: Need **full scans** with no shared information.
Slow and inefficient! (A subset might have sufficient info.)

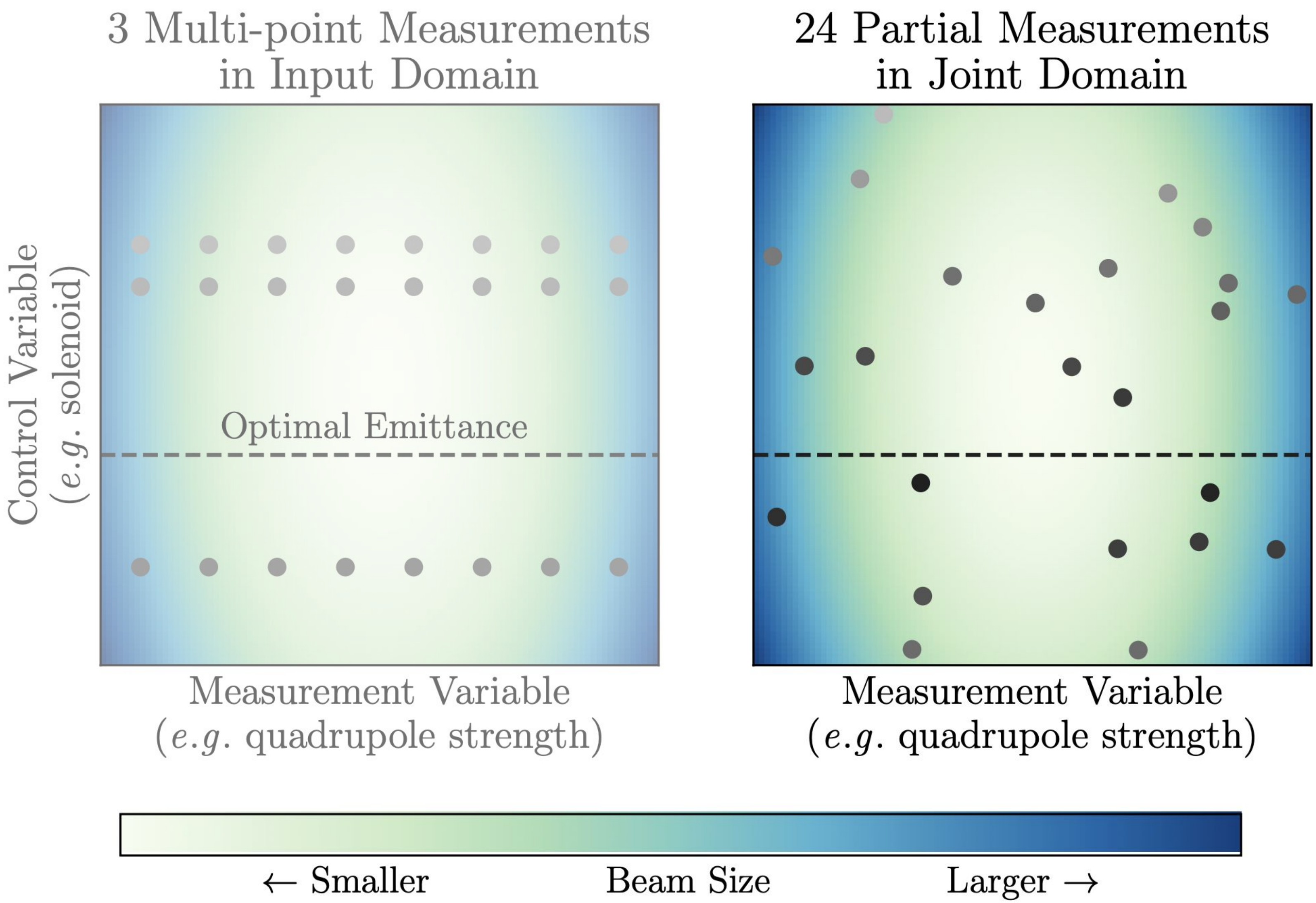


To maximize information gain of each measurement



EMITTANCE OPTIMIZATION IN JOINT SPACE

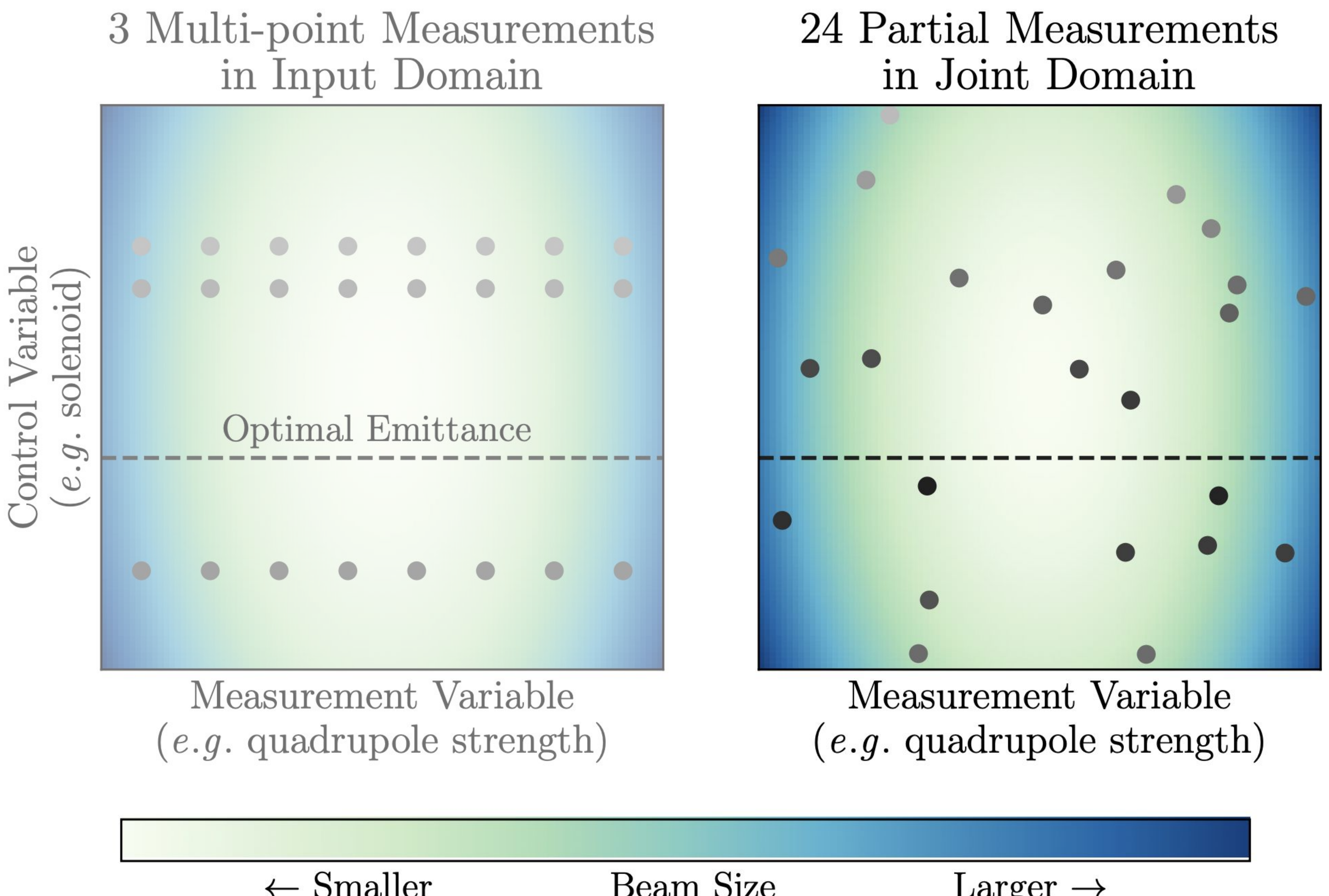
But, how do we optimize for emittance while also trying to learn a beam size model?



EMITTANCE OPTIMIZATION IN JOINT SPACE

But, how do we optimize for emittance while also trying to learn a beam size model?

⇒ Solution is "BAX: Bayesian Algorithm Execution"



BAX one-sentence summary:

Extending Bayesian optimization from estimating **global optima** to estimating **other function properties** defined by the output of **algorithms**.

For more info, see the website:
https://willieneis.github.io/bax-website/

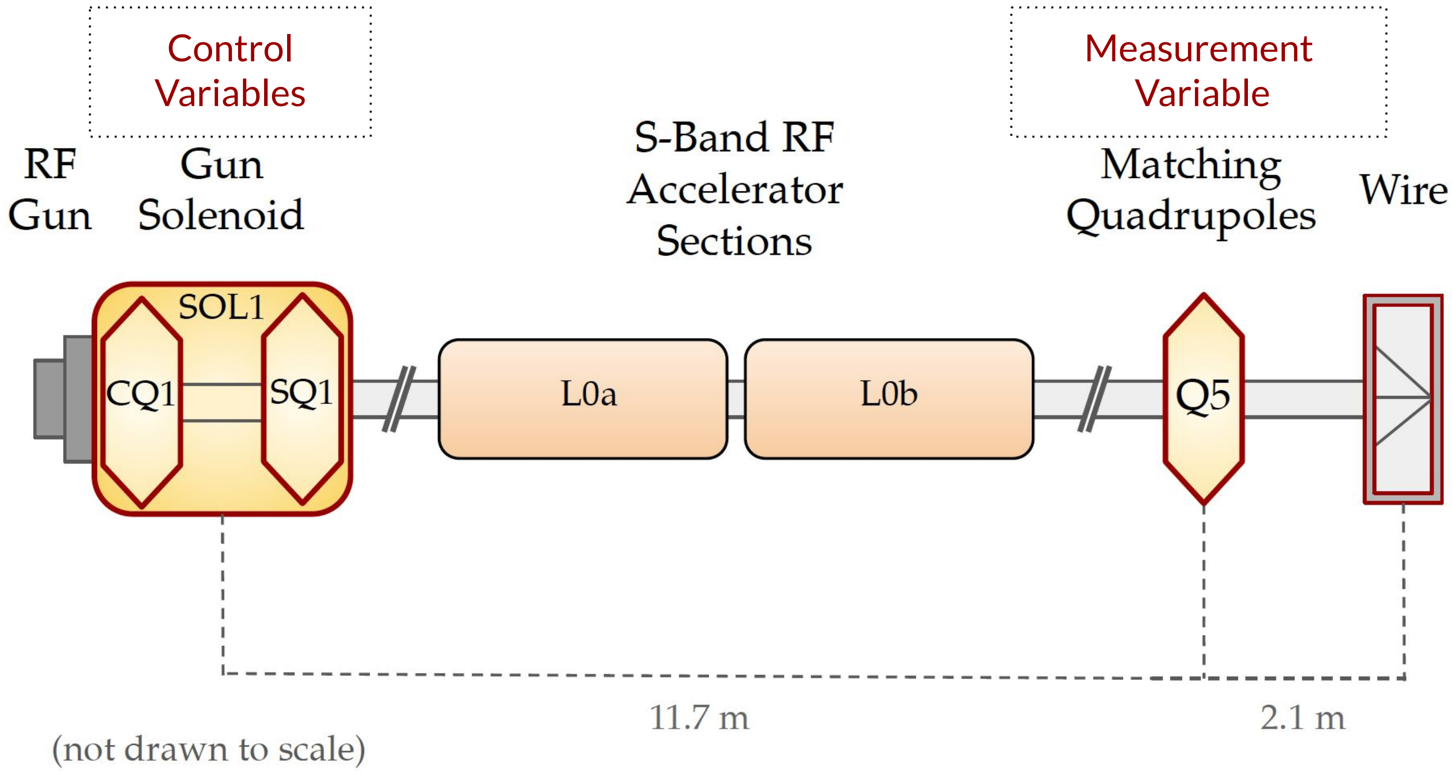
BAX one-sentence summary *for emittance tuning*:

We want to **estimate the emittance** *(a function property)* computed by quadrupole scans *(the algorithm)* **using a model of the beam size** as a function of accelerator parameters.

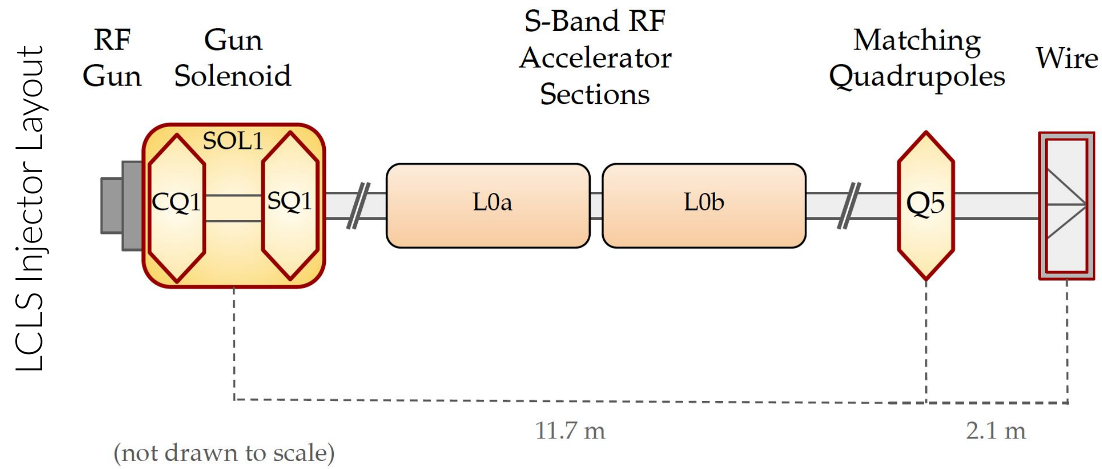
Note that:

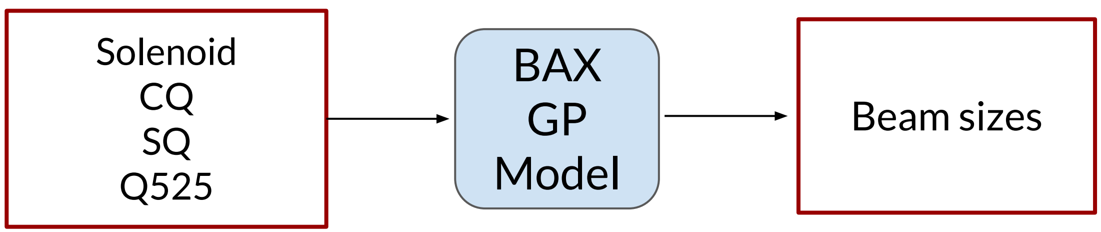
- **Only ever measure beam size** as a function of scanning quad + accelerator parms
- Emittance quad scan **only done on BAX learned model of beam size**

INFO-BASED BAX FOR LCLS EMITTANCE TUNING



LCLS Injector Layout



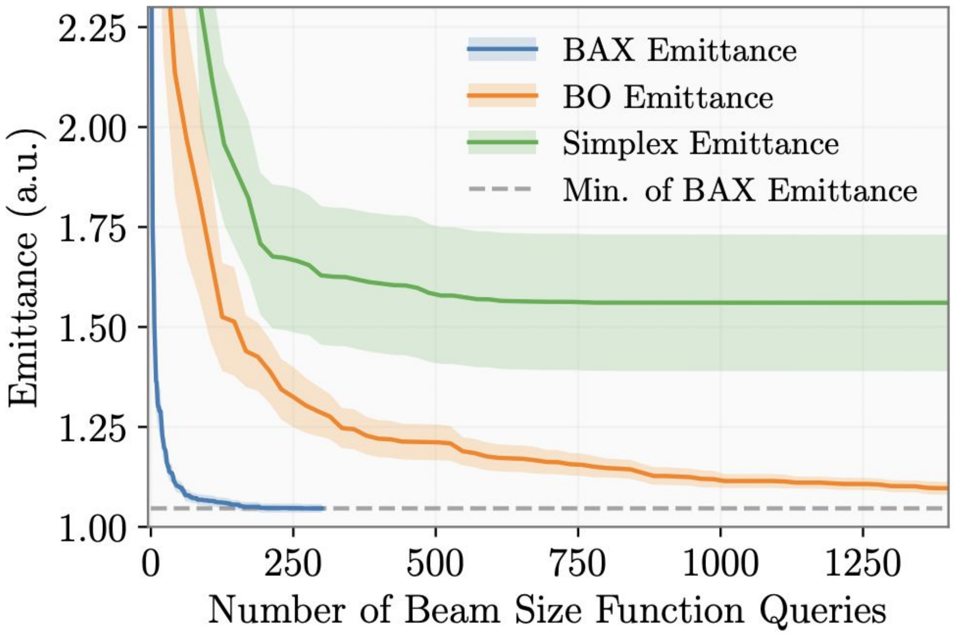


BAX learns a **virtual beam size model**

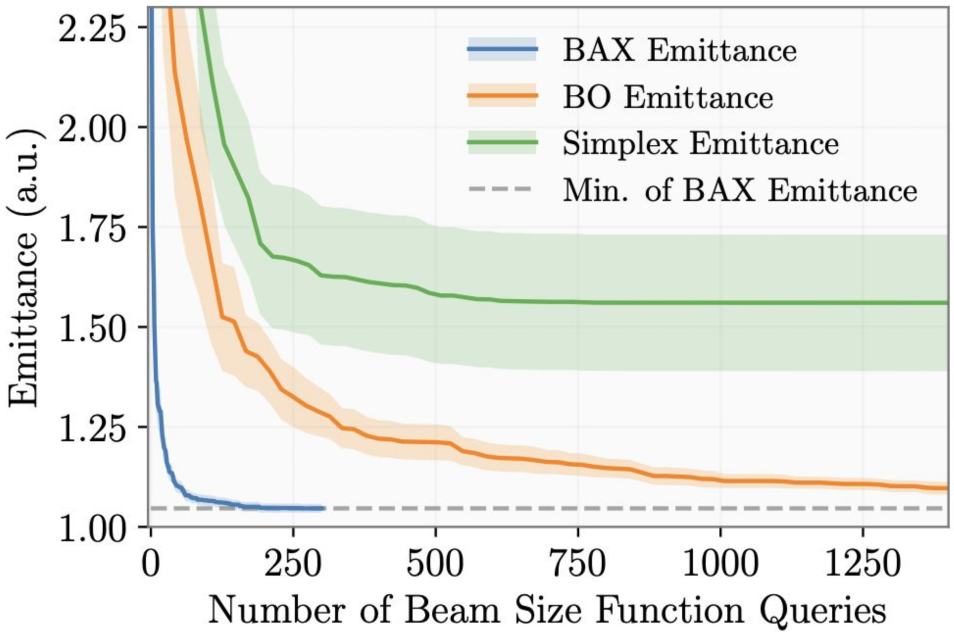
→ Via emittance scans on **posterior samples of the GP**, chooses queries that **maximizes the information gain** about the ***SOL, CQ, SQ that lead to minimal emittance***

RESULTS: NOISY LCLS SIMULATION

Normalized by the minimum of the ground truth emittance



BAX shows a 20x increase in efficiency compared to standard BO!

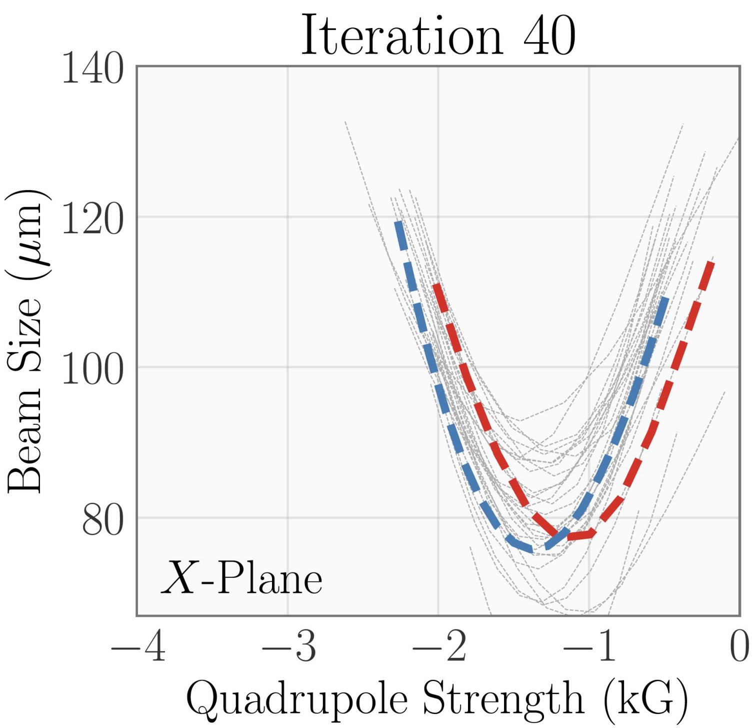


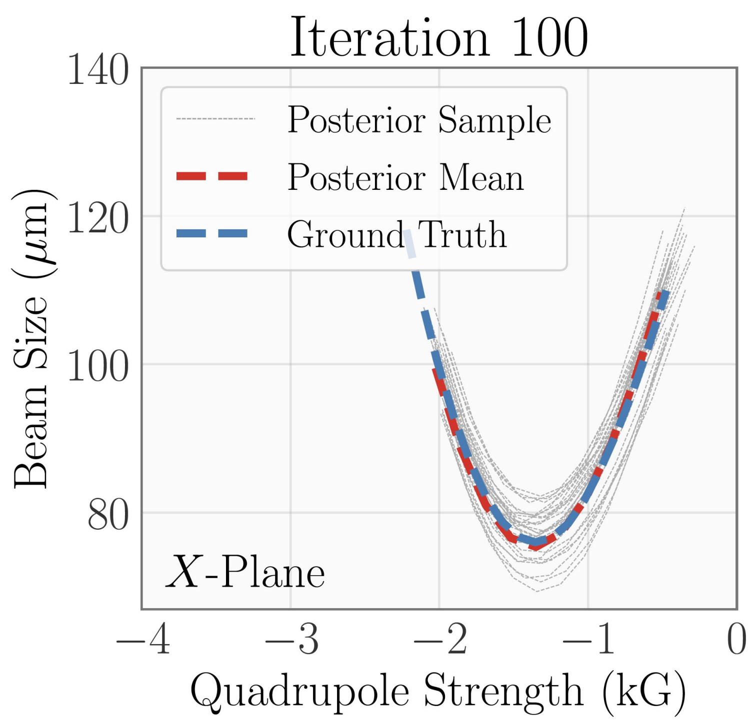
Normalized by the minimum of the ground truth emittance

BAX shows a 20x increase in efficiency compared to standard BO!

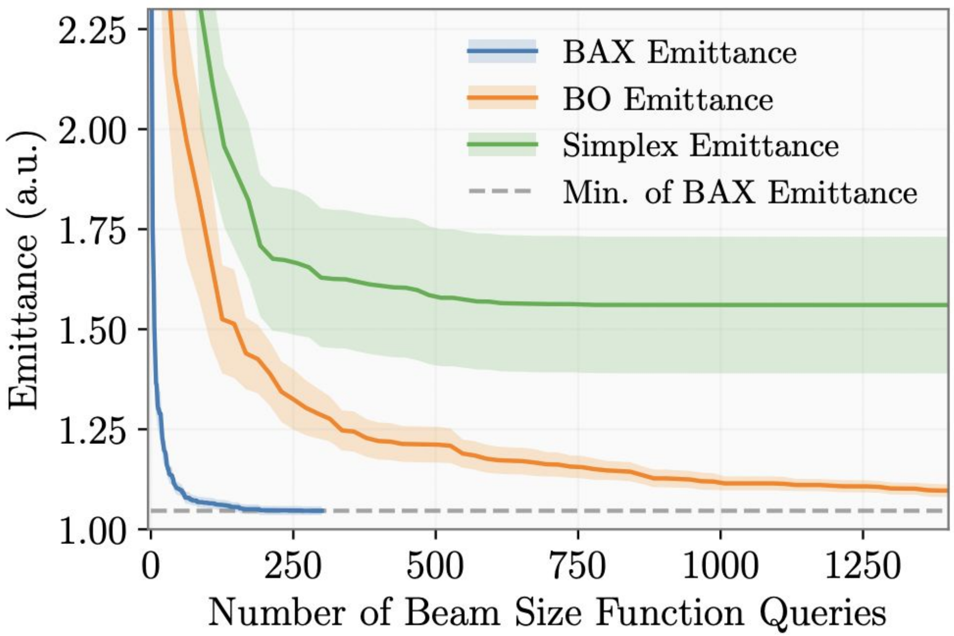
But BAX never does full scans... **how do we know when it's converged?**

BAX GP predictions compared to the true beam sizes at optimal (fixed) accelerator injector variables

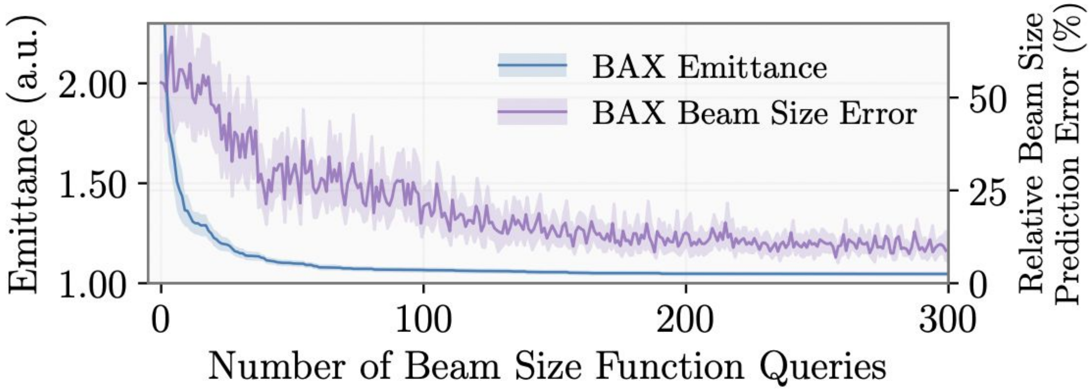




→ Looking at error between the model and beam sizes shows convergence



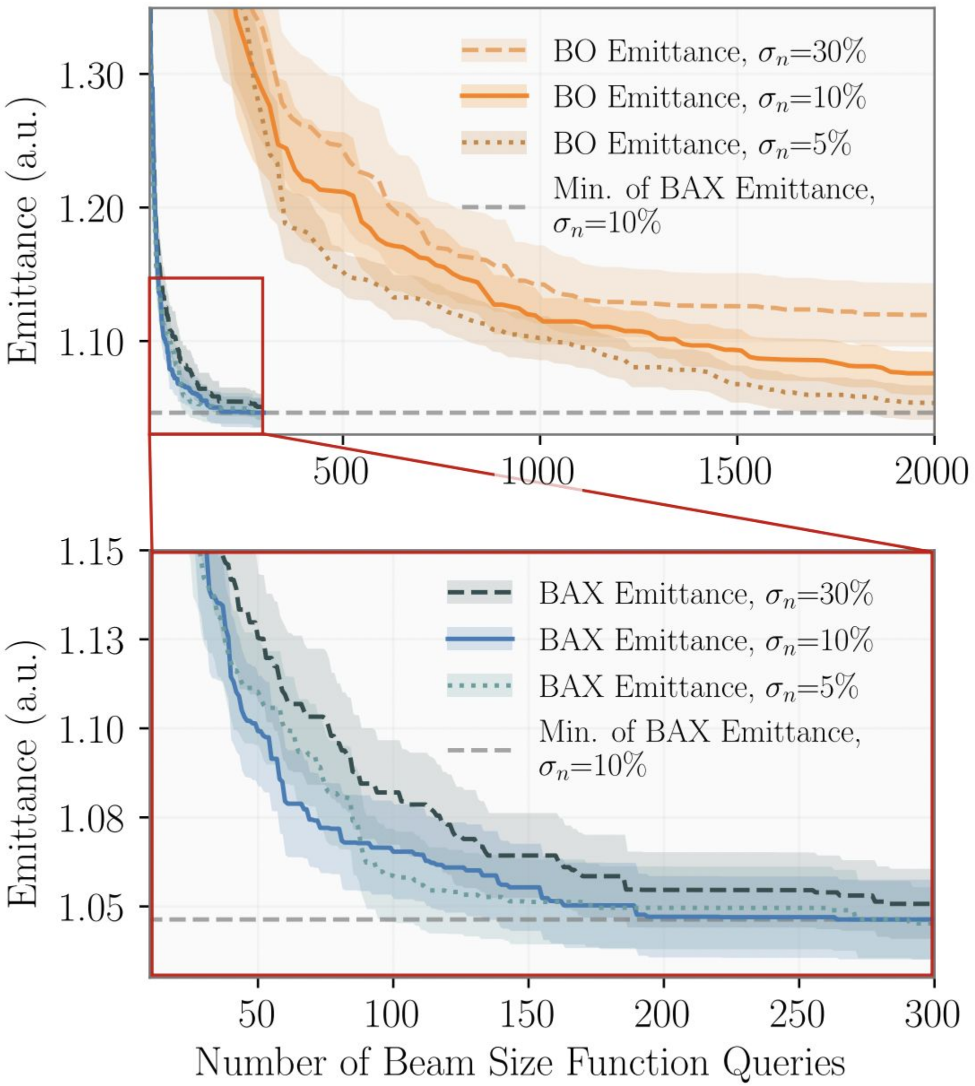
Normalized by the minimum of the ground truth emittance



Proxy for convergence

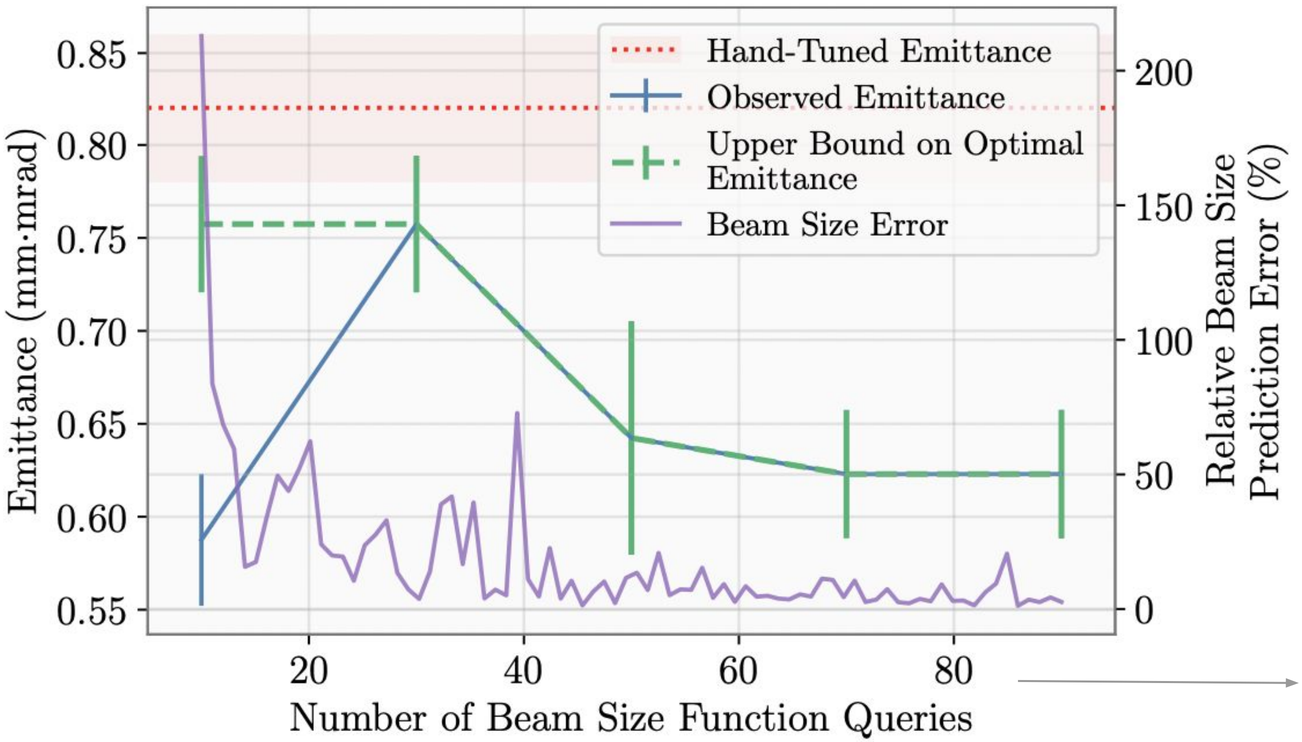
Hypothesis: Sharing of information makes BAX more robust to noise

BO only sees final emittance result from scans, doesn't know when the individual measurements are bad (garbage in = garbage out)



Live Optimization at LCLS

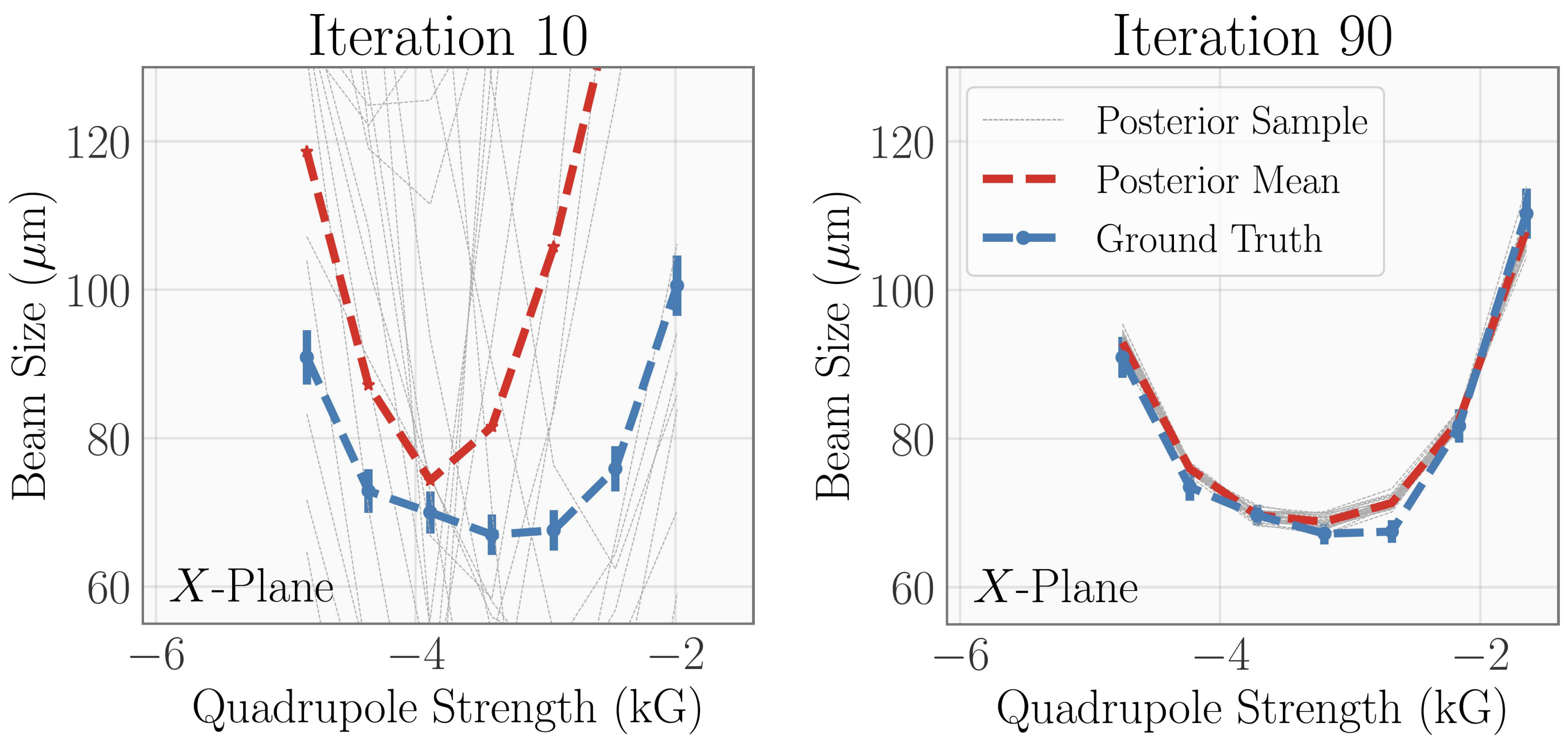
(250 pC)



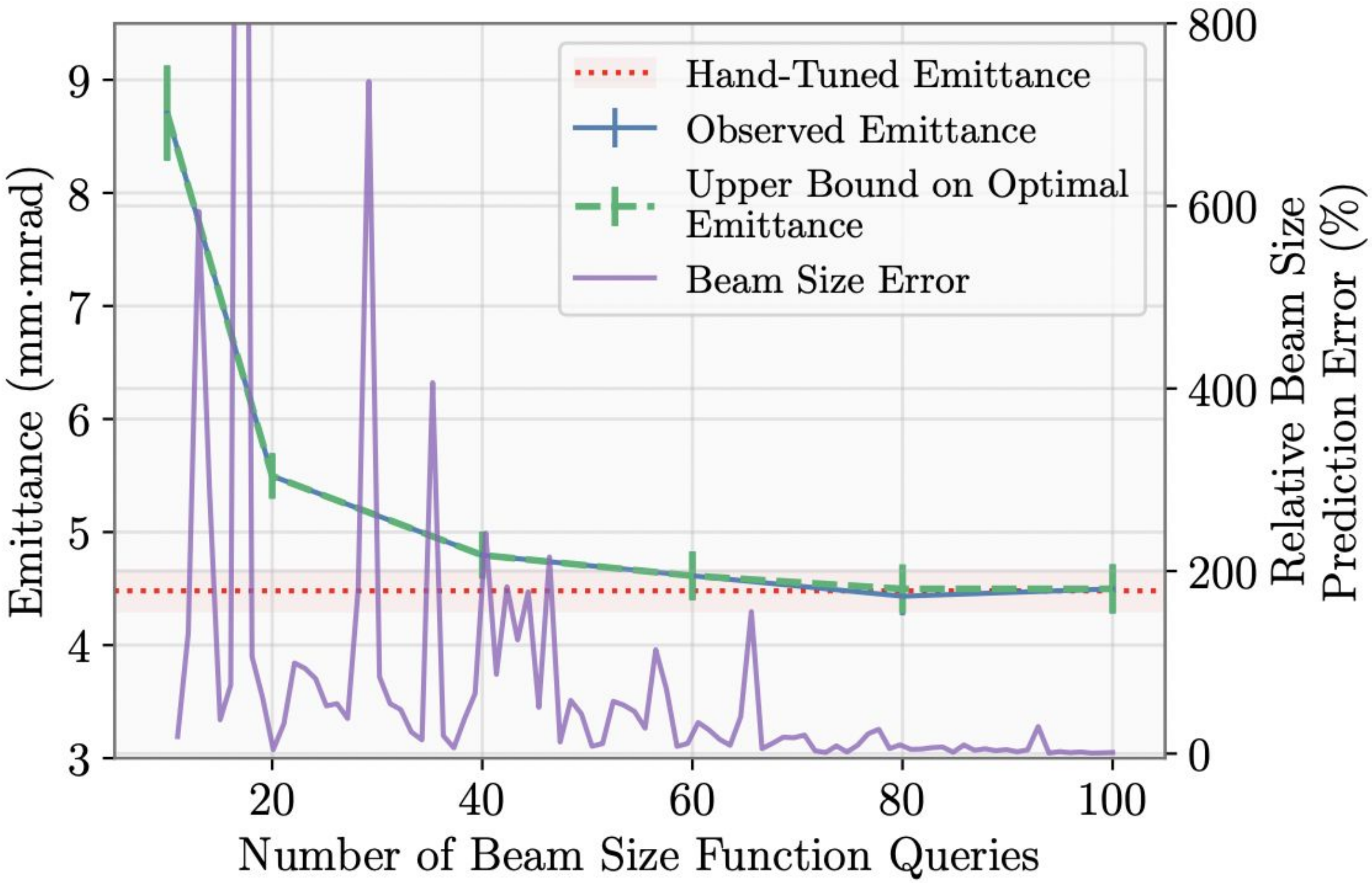
24 min of beam time (wires)

Optimal emittance 24% lower than that obtained by hand-tuning.

BAX GP predictions compared to the true beam sizes from the live LCLS optimization



Live Optimization at FACET-II
(2 nC)



- Rather than directly optimizing complex properties, we learn a model of the system on-the-fly
→ **“virtual measurement” on the fast-executing model**

- **Paradigm shift**: replacing expensive indirect beam measurements with **computation on easy-to-acquire samples from surrogate models**

- **We see 20x increase in efficiency in sim, 24% lower emittance live on LCLS, and comparable emittace live on FACET-II**

Ongoing Work and Next Steps

- Expanding to higher dimensions in deployment-ready code
- Targeting more complex objectives
- Physics-informed kernel
- Increase computational efficiency (GPU parallelization)
- Live comparisons to BO on LCLS and FACET-II
- Optimization during LCLS-II commissioning

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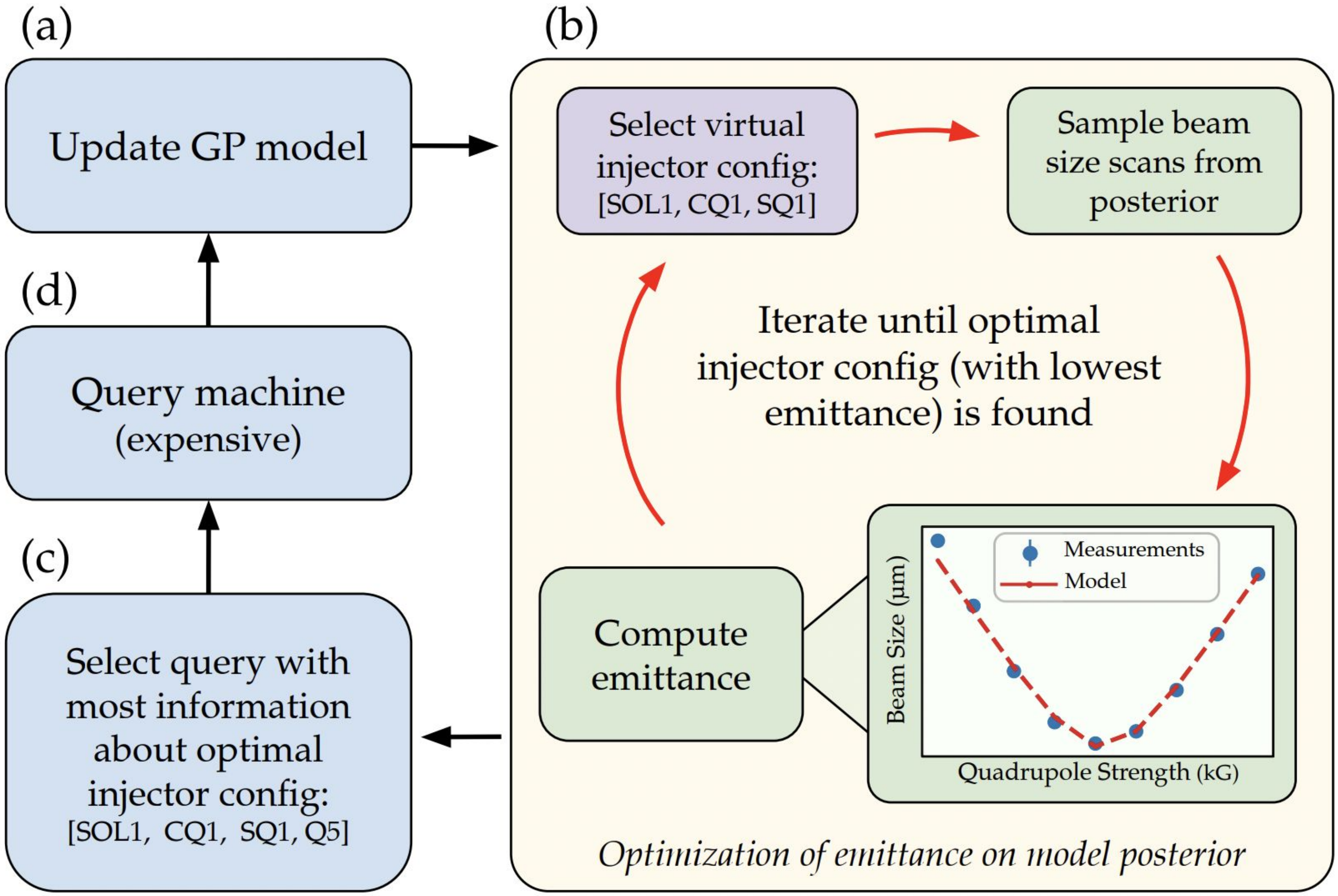
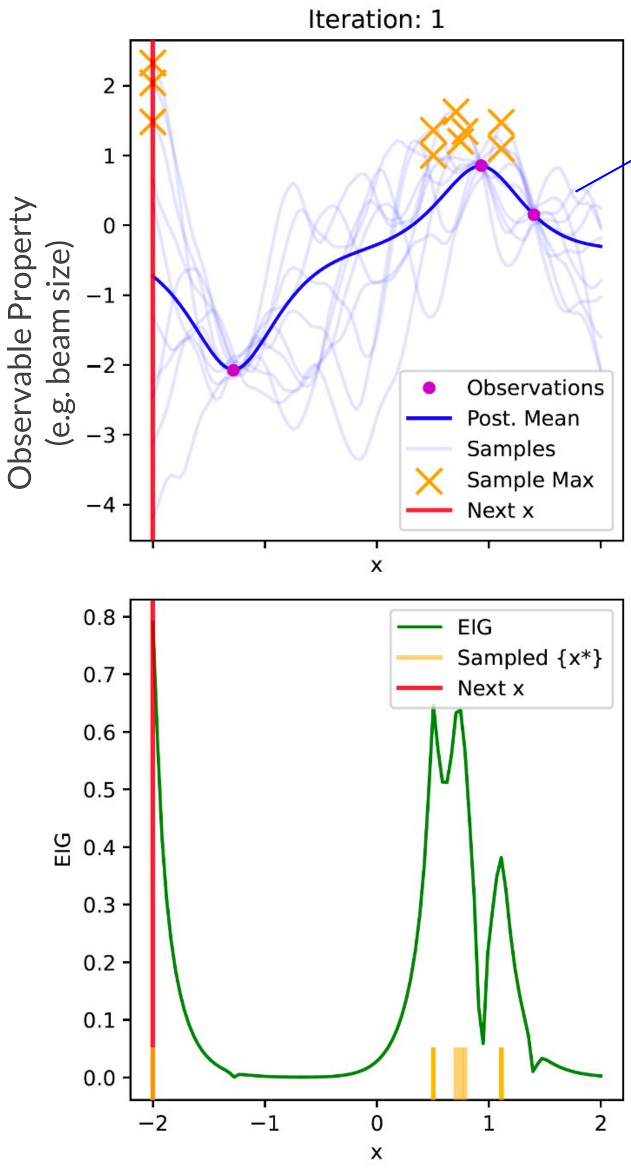
Preprint on arXiv:
https://arxiv.org/abs/2209.04587

BAX website:
https://willieneis.github.io/bax-website/



BAX Procedure for Emittance Optimization in LCLS

INFO-BASED BAX: 1-D EXAMPLE



1. Run complex measurement on samples from GP posterior

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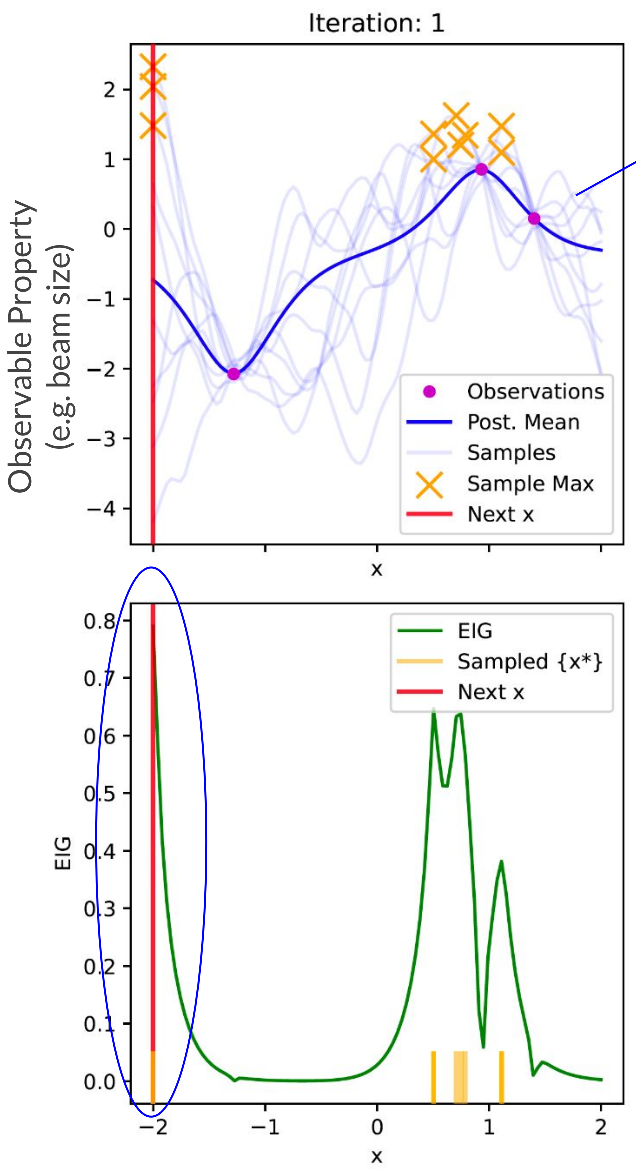
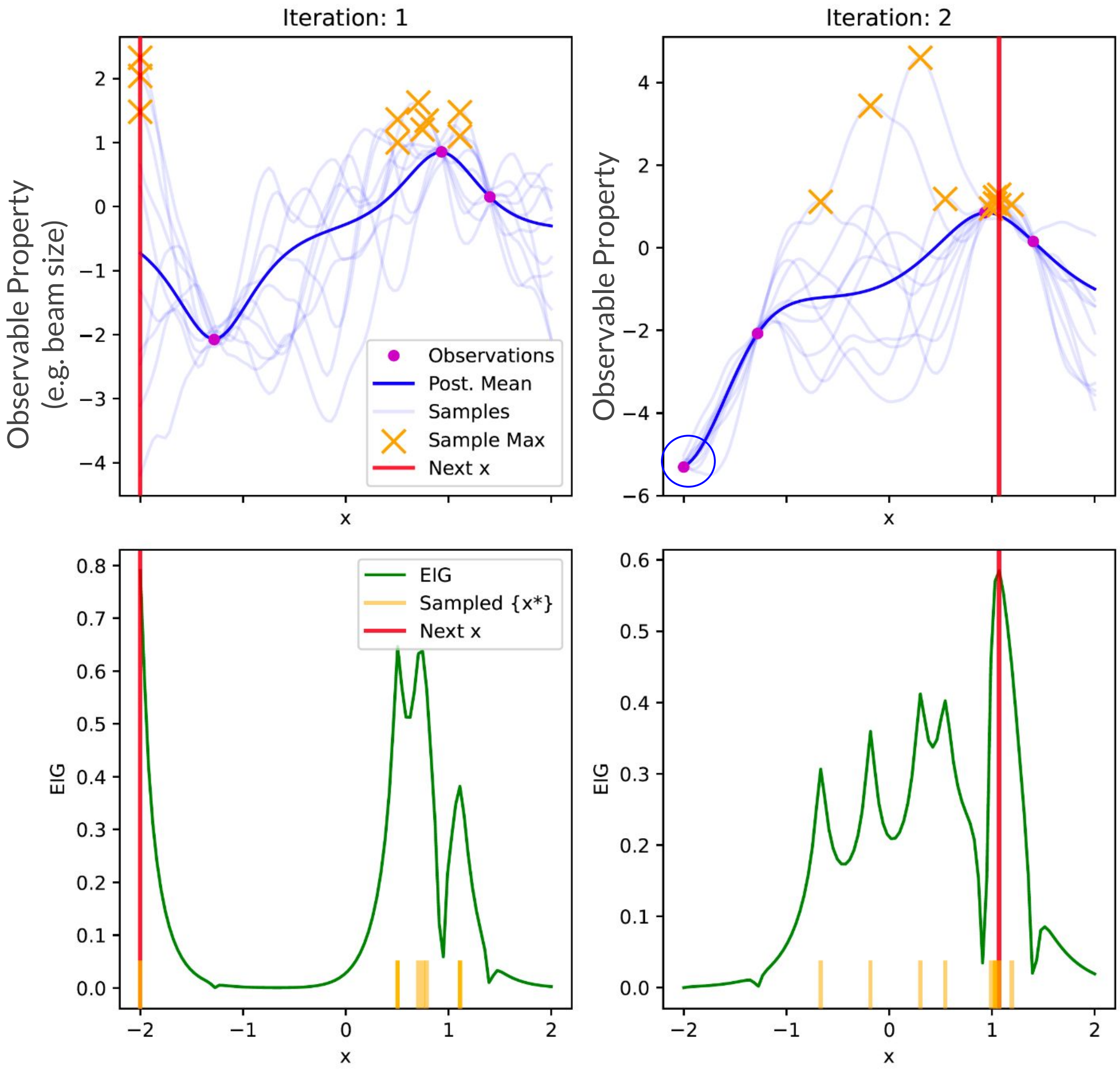


1. Run complex measurement on samples from GP posterior

2. Estimate info-based acquisition and select point at max info gain

INFO-BASED BAX: 1-D EXAMPLE



3. Query **single point** from real system

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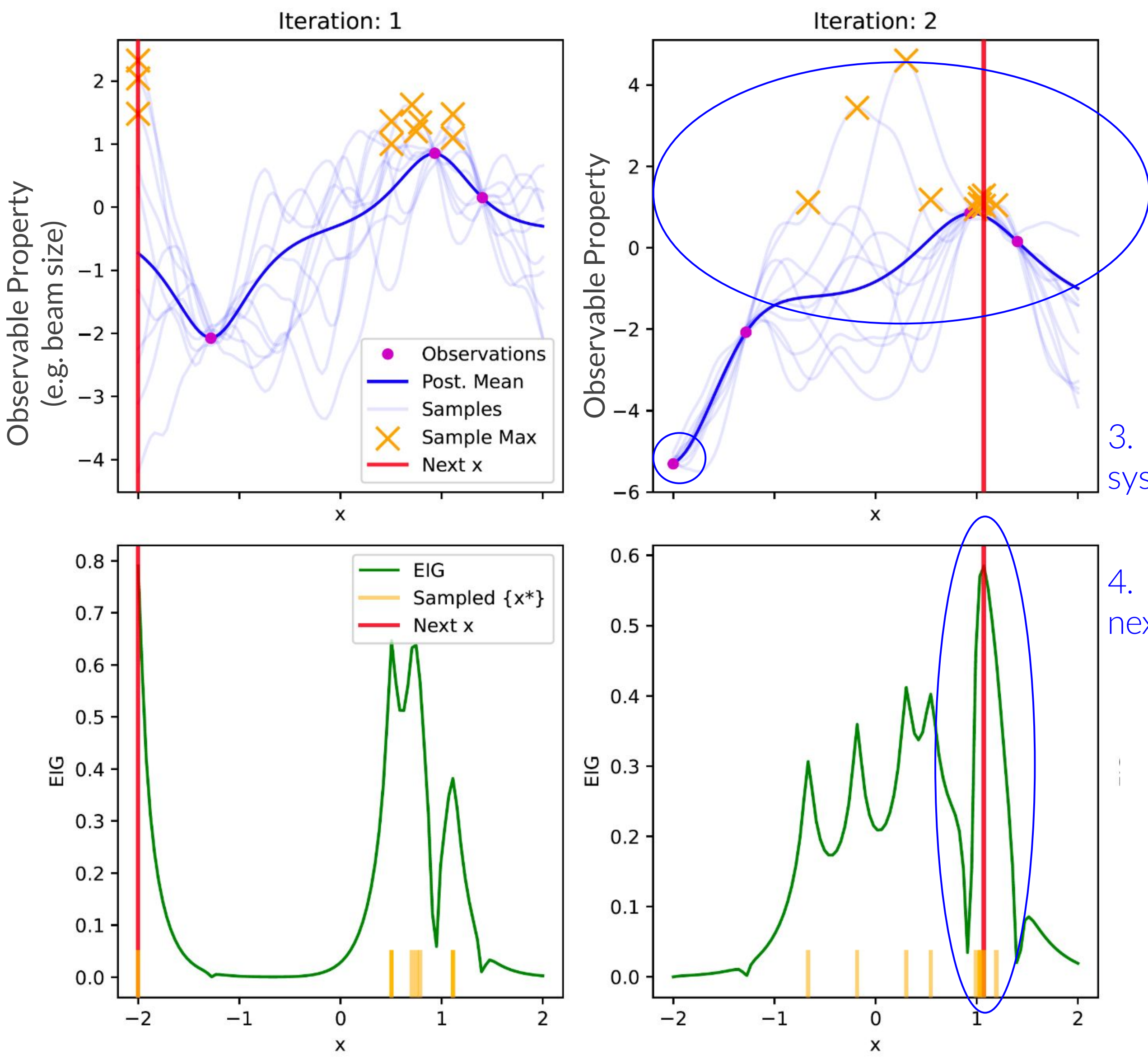
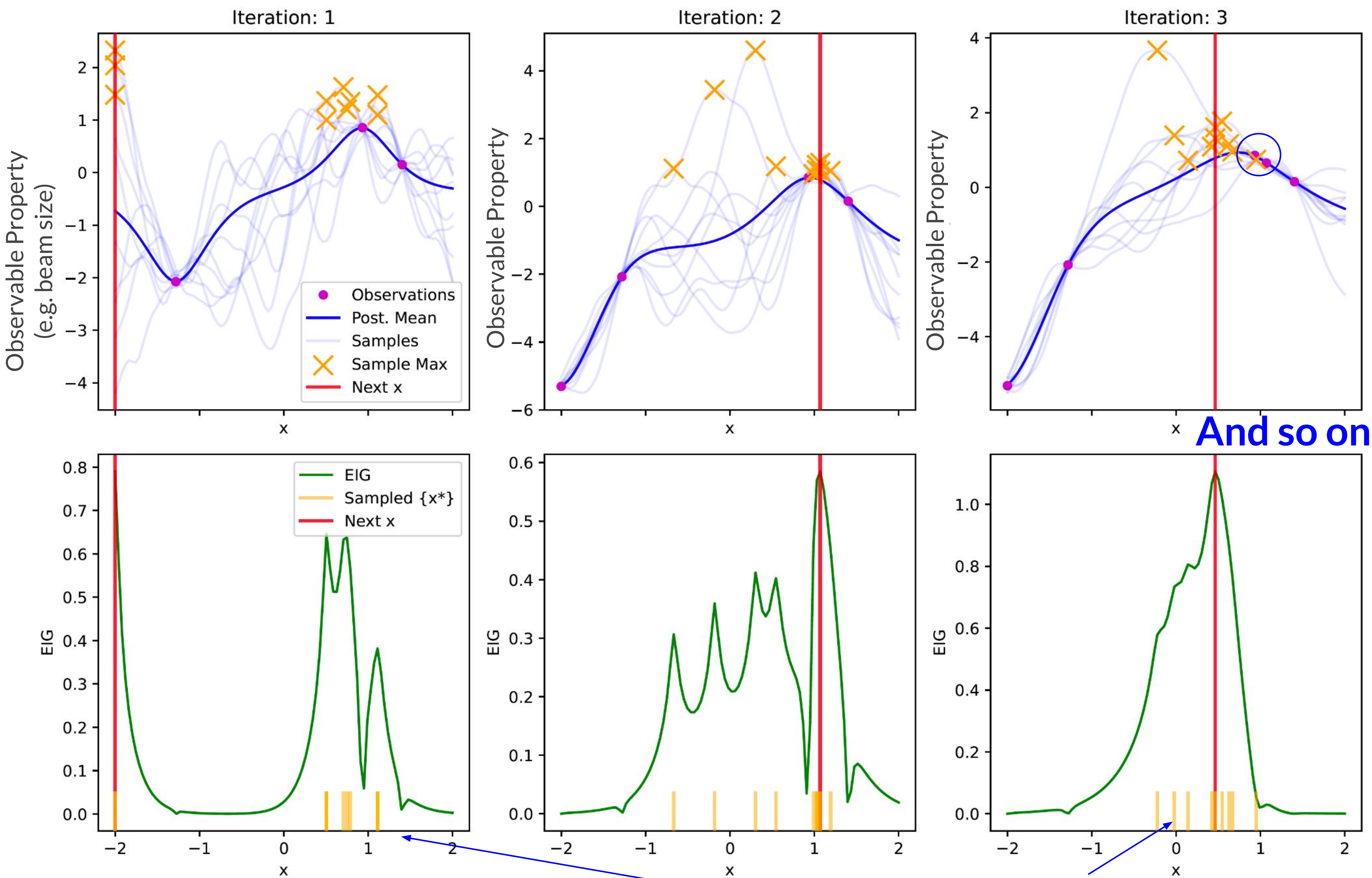


3. Query **single point** from real system

4. Repeat steps 1 and 2 to select next point based on EIG max

INFO-BASED BAX: 1-D EXAMPLE



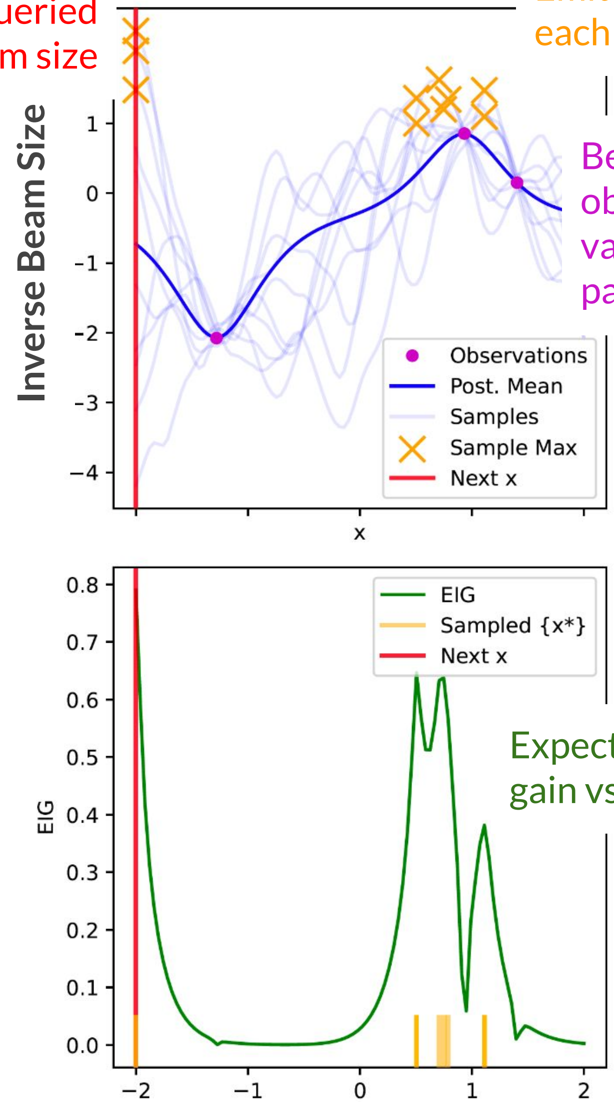
And so on...

Note sample optimals are converging

INFO-BASED BAX: 1-D EXAMPLE APPLIED TO EMITTANCE

Only time machine is queried for one beam size

Emittance values from each GP sample



Beam size observation for one value of tuning parameter

Expected information gain vs. control variable

Injector Tuning Parameter (e.g. solenoid)