Adapting Multi-Objective Bayesian Optimization for Online Particle Accelerator Tuning

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SLAC NATIONAL ACCELERATOR LABORATORY

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Abstract

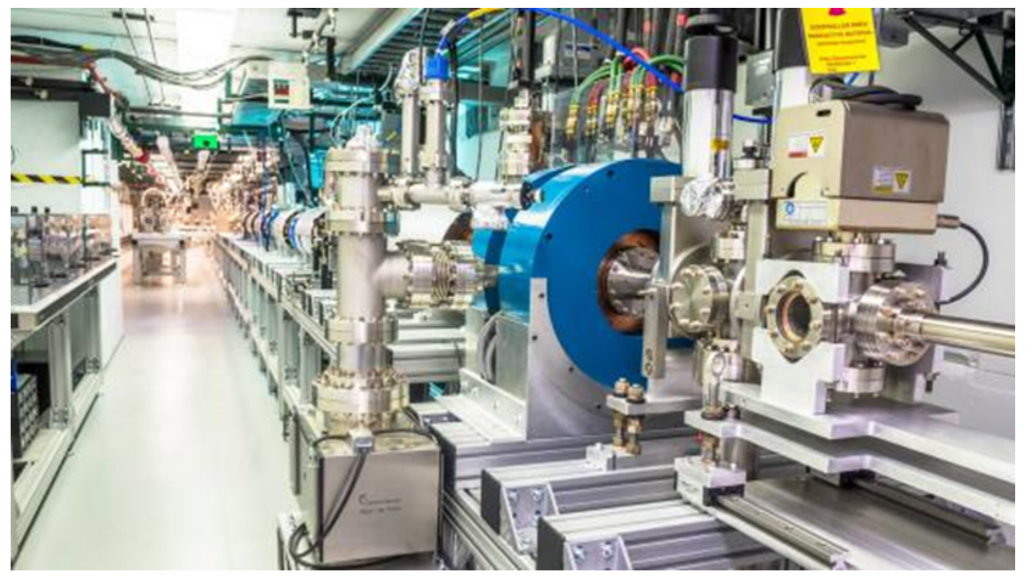
Particle accelerators require constant tuning during operation to meet goals for beam quality, total charge and particle energy for use in a wide variety of physics, chemistry and biology experiments. Maximizing the performance of an accelerator facility often necessitates multi-objective optimization, where operators must balance trade-offs between objectives, often using limited, real-time, temporally expensive beam observations. Unfortunately parallelized methods typically used to solve multi-objective problems don't have sufficient sample efficiency to be used practically during accelerator operation. This is due, in part, because fitness evaluation of a given input must be done serially. Here, we introduce modifications to a multi-objective Bayesian optimization scheme for use in practical particle accelerator control algorithms, by including optimization constraints, objective preferences and localized parameter tuning.

Online Particle Accelerator Optimization

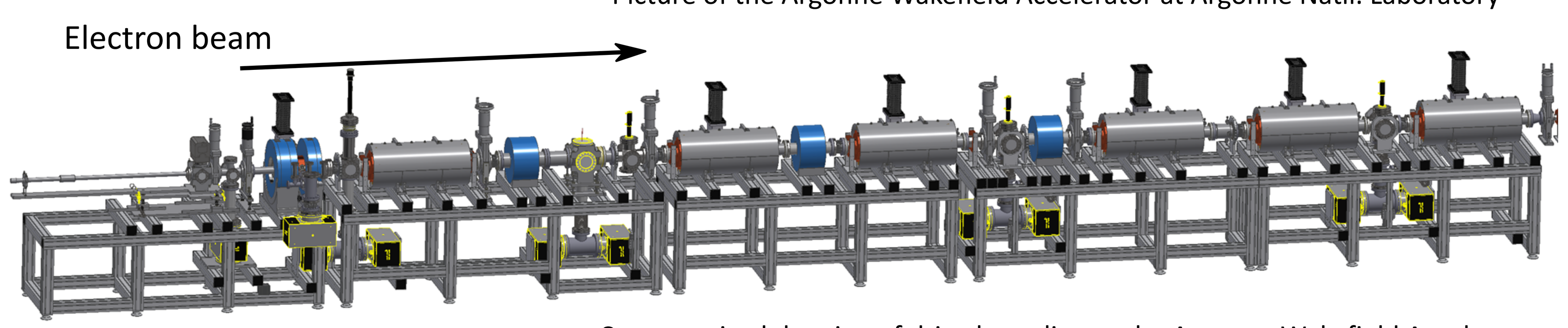
Particle accelerators require constant tuning that require:

- Optimization of **multiple objective goals** simultaneously
- Must be done **serially**
- **Expensive** (time consuming) to make function observations
- Must satisfy hard/soft **constraints** and/or **preferences**

Argonne NATIONAL LABORATORY



Picture of the Argonne Wakefield Accelerator at Argonne Natl. Laboratory



Computerized drawing of drive beamline at the Argonne Wakefield Accelerator

Multi-Objective Bayesian Optimization (MOBO)

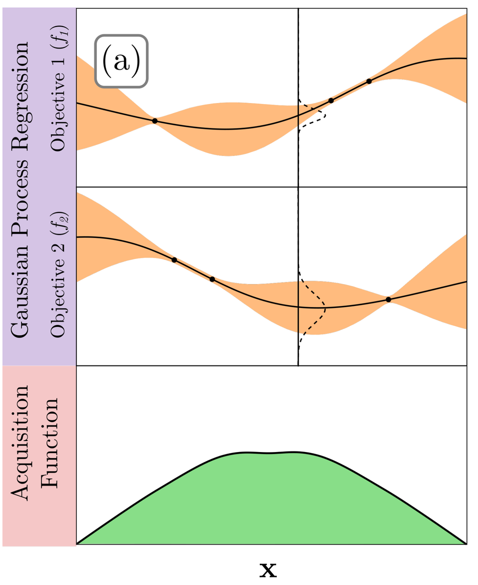
Goal: Find the **Pareto front (PF)** - A set of **non-dominated points in objective space** that represents the **ideal trade-off between competing objectives.**

- Use multi-objective Bayesian optimization (MOBO) [1] to reduce number of function evaluations needed to reach convergence
- Model each objective as an independent Gaussian process (GP) model
- Combine with an acquisition function which characterizes the predicted hyper-volume improvement

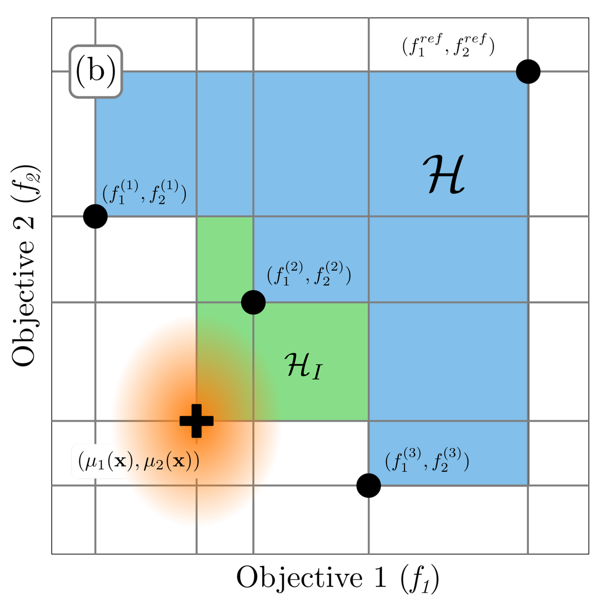
$\mathcal{H} :=$ Pareto front hypervolume

$\mathcal{H}_I :=$ Hypervolume improvement

Gaussian Process Models

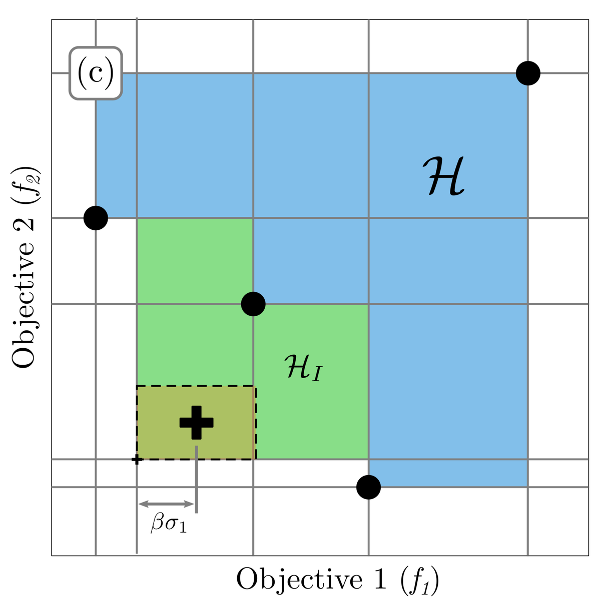


Expected Hyper-volume Improvement (EHVI)



$$\alpha_{EHVI}(\mu,\sigma,\mathcal{P},\mathbf{r})$$
$$:= \int_{\mathbb{R}^P} \mathcal{H}_I(\mathcal{P},\mathbf{y},\mathbf{r})\mathrm{PDF}_{\mu,\sigma}(\mathbf{y})d\mathbf{y}$$

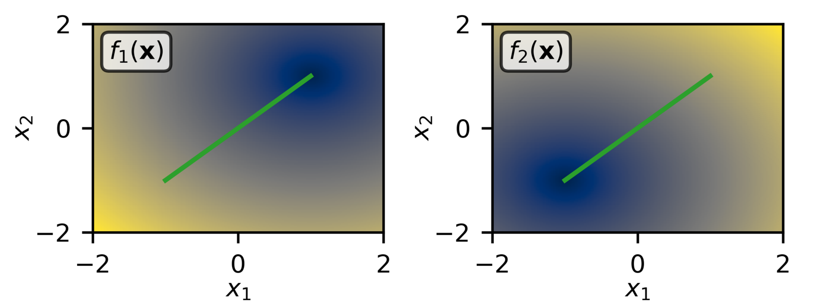
Upper Confidence Bound Hyper-volume Improvement (UCB-HVI)



$$\alpha_{UCB-HVI}(\mu,\sigma,\mathcal{P},\mathbf{r},\beta)$$
$$:= \mathcal{H}_I(\mathcal{P},\mu-\sqrt{\beta}\sigma,\mathbf{r}).$$

Two Objective MOBO Test Problem

$$\text{minimize } \{f_1(\mathbf{x}), f_2(\mathbf{x})\}$$
$$f_1(\mathbf{x}) = ||\mathbf{x}-\mathbf{1}||$$
$$f_2(\mathbf{x}) = ||\mathbf{x}+\mathbf{1}||$$
$$x_n = [-2,2],\ n=1,2.$$



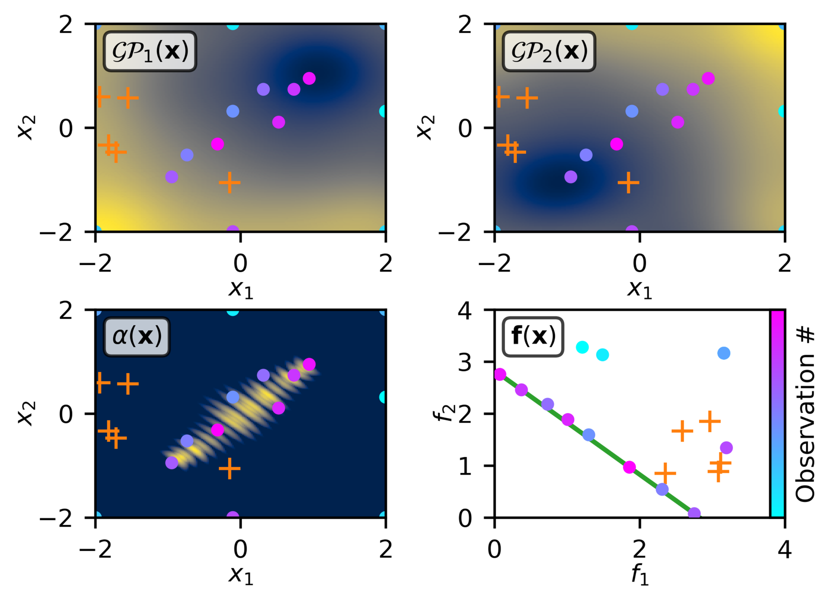
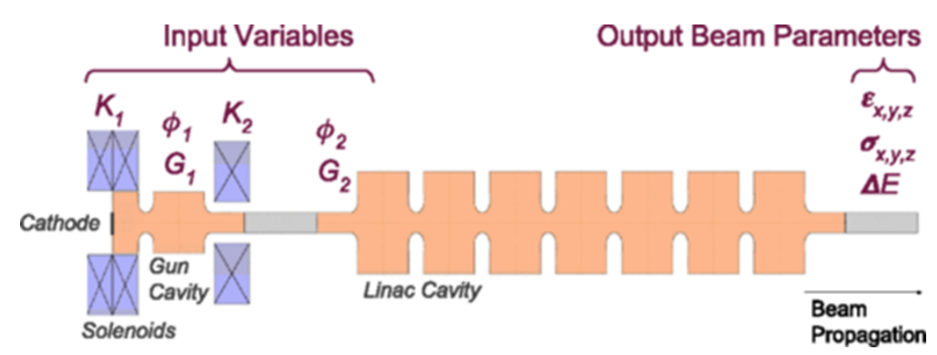


Photo-injector Optimization Problem

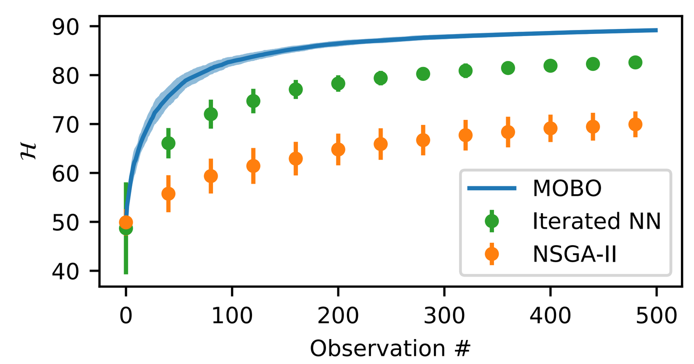


Optimization variables:

- Solenoid focusing strengths (K_1, K_2)
- Radio-frequency field amplitude (G_1, G_2)
- Radio-frequency field phases (φ_1, φ_2)

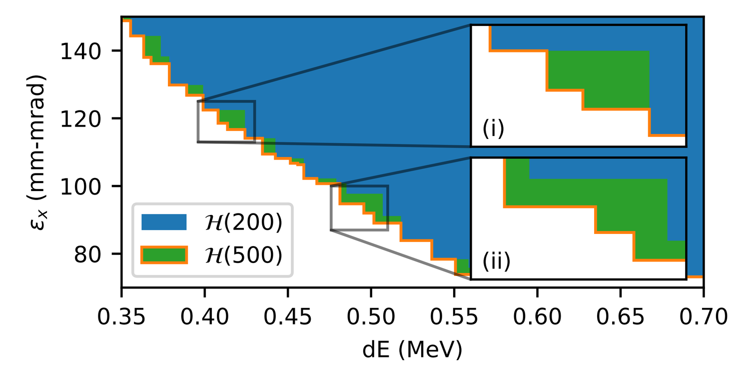
Optimization objectives:

- Beam size (x, y, z directions)
- Beam phase space volume (x, y, z directions)
- Energy spread



Pareto front hyper-volume increases much faster using MOBO vs. NSGA-II and iterated Neural Network [2]

- **Convergence speed acceptable for practical online use**



Due to high D objective space, MOBO increases the hyper-volume by:

(i) increasing the resolution of the PF

(ii) observing new non-dominated points

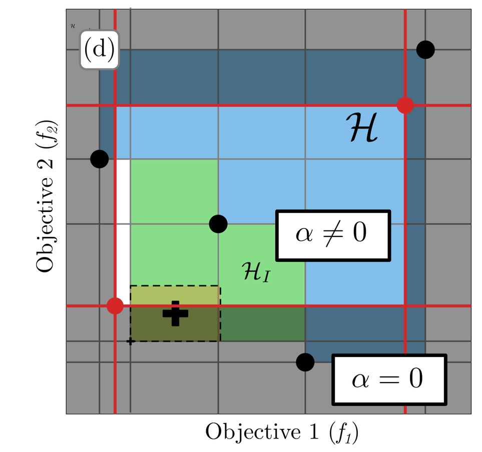
Adapting MOBO to Accelerator Optimization

Adding Preferences/Constraints to Multi-Objective Bayesian Optimization

Prioritize optimizing specific objectives over others by **restricting objective space**

- set the hyper-volume improvement to **zero** outside a given region

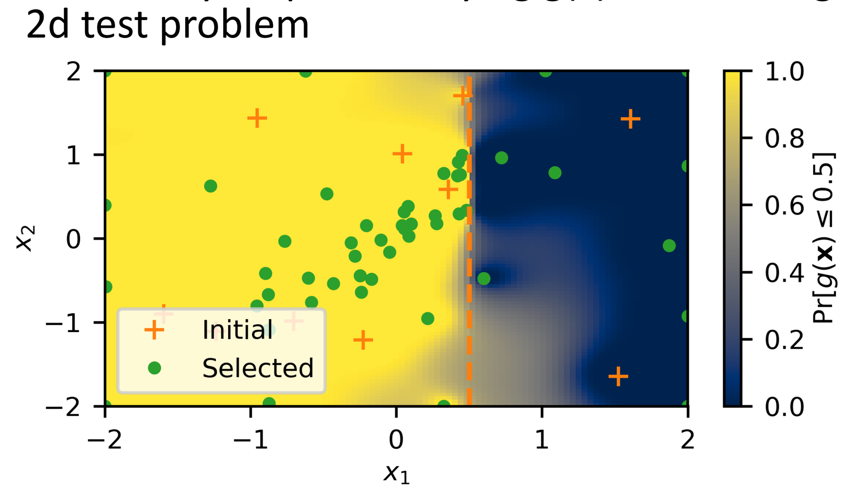
$$\alpha_{TUCB-HVI}(\mu,\sigma,\mathcal{P},\beta,\mathbf{A},\mathbf{B}) :=$$
$$\begin{cases} \mathcal{H}_I(\mathcal{P},\mathbf{y},\mathbf{B}) & \mathbf{y}\in\mathcal{T} \\ 0 & \text{otherwise} \end{cases}$$



Specify **inequality constraint** and multiply acquisition function by **satisfaction probability via separate GP prediction** [3]

$$P_g(\mathbf{x}) := Pr[g(\mathbf{x}) \leq h] = \int_{-\infty}^{h} p(g(\mathbf{x})|\mathcal{D}_g)dg(\mathbf{x})$$
$$\hat{\alpha}(\mathbf{x}) = \alpha(\mathbf{x})P_g(\mathbf{x})$$

Probability map of satisfying g(x) < 0.5 during 2d test problem



Smoothing Input Parameter Space Exploration

Some accelerator parameters are **difficult to change**, where the cost to change a parameter is **proportional to the magnitude of the change**. Want to explore input space **smoothly**!

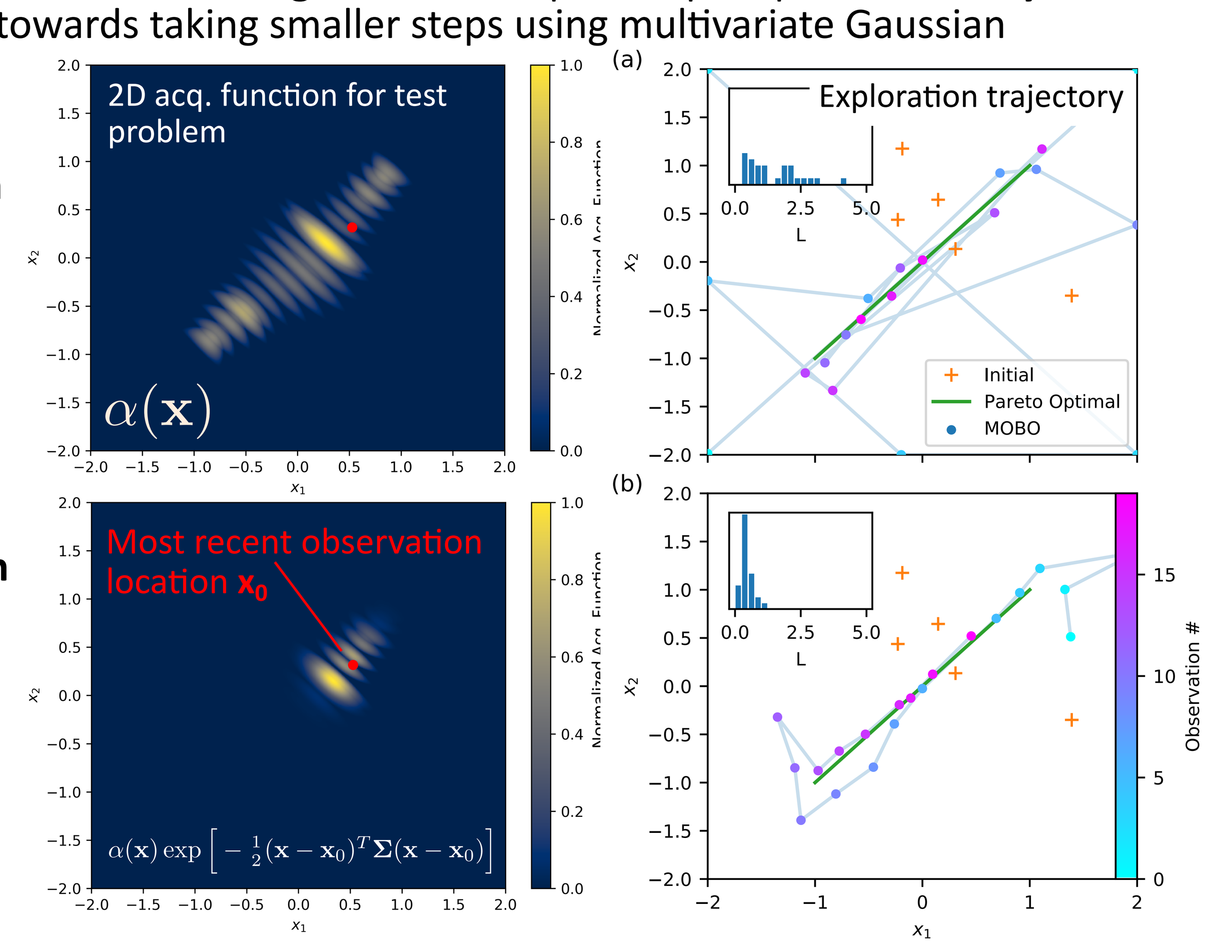
- Bias acquisition function towards taking smaller steps using multivariate Gaussian

Normal acquisition function

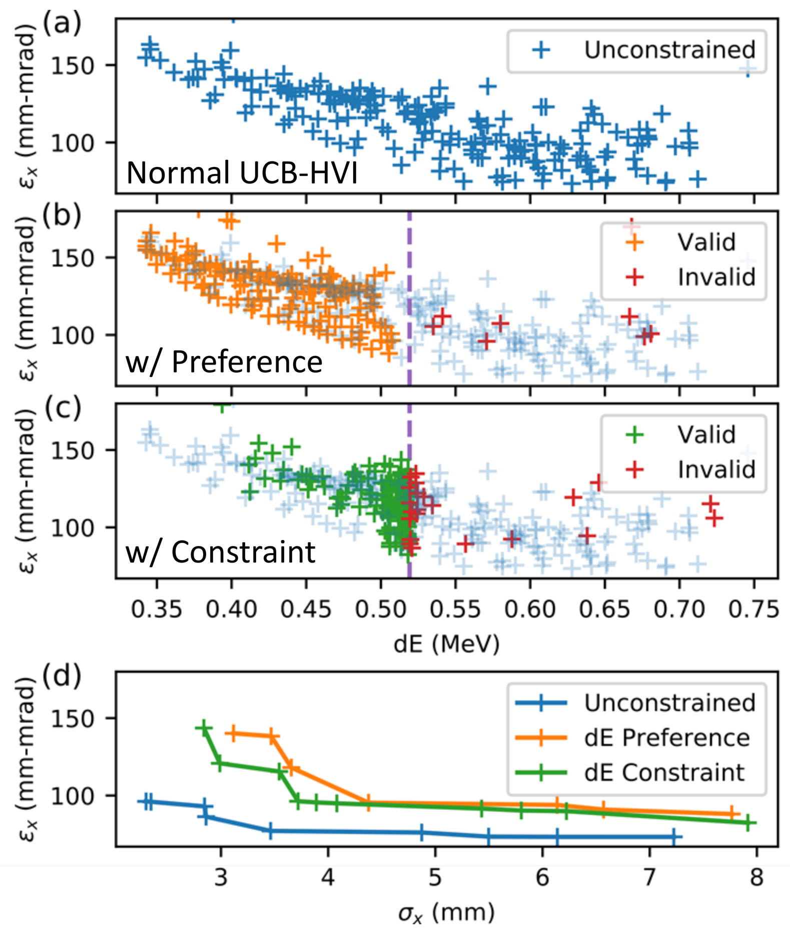
- semi-randomly explores input space
- frequent large jumps

Smooth acquisition function

- follows a smooth path through input space
- large jumps only occur when jumping over previously explored input space

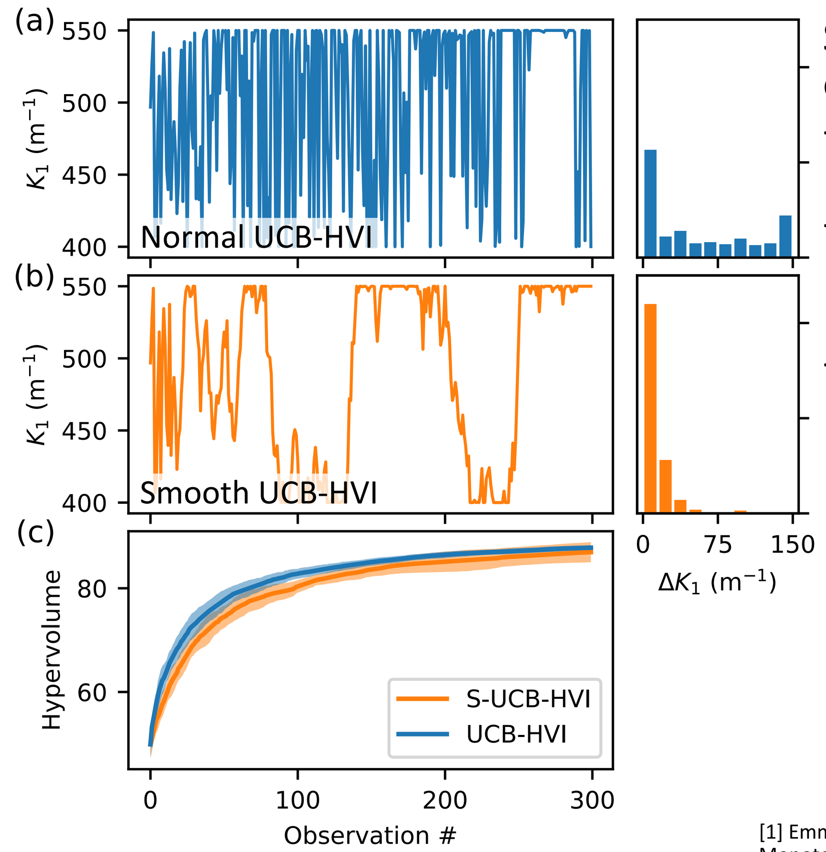


Photoinjector Optimization Results



Observed PF after 300 iterations

- projected into energy spread (dE) vs. beam phase space in horizontal direction (ε_x)
- adding a preference for dE < 0.52 MeV leads to a **higher resolution PF in subdomain**
- adding a constraint for dE < 0.52 MeV leads to a higher density of points near the constraint boundary
- PF in other objective spaces (for example beam size (σ_x) vs. beam phase space in horizontal direction (ε_x)) **improves with constraint relative to preference case**



Solenoid strength (K_1) during optimization

- Normal UCB-HVI leads to **frequent, large jumps** in parameter value (a)
- Using smooth UCB-HVI (S-UCB-HVI) the frequency and magnitude of jumps is **significantly reduced** (b)
- Tolerable decrease in hyper-volume convergence speed (c)

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References

[1] Emmerich, Michael T. M., André H. Deutz, and Jan Willem Klinkenberg. “Hypervolume-Based Expected Improvement: Monotonicity Properties and Exact Computation.” In 2011 IEEE Congress of Evolutionary Computation (CEC), 2147–54, 2011. https://doi.org/10.1109/CEC.2011.5949880.

[2] Edelen, Auralee., et. al.“Machine Learning for Orders of Magnitude Speedup in Multiobjective Optimization of Particle Accelerator Systems.” PRAB https://doi.org/10.1103/PhysRevAccelBeams.23.044601.

[3] Gardner, Jacob R, Matt J Kusner, Zhixiang Eddie Xu, Kilian Q Weinberger, and John P Cunningham. “Bayesian Optimization with Inequality Constraints.” In ICML, 2014:937–945, 2014.