NEURAL INFORMATION PROCESSING SYSTEMS

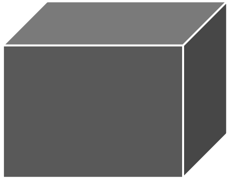
Risk-averse Heteroscedastic Bayesian Optimization

Anastasia Makarova, Ilnura Usmanova, Ilija Bogunovic, Andreas Krause

ETH zürich

Black-box optimization arises in high-stakes applications

Black Box

x →  → $y = f(x) + \xi$

$f(x)$

Drug discovery

→ Compound efficiency

Tuning accelerators

Beam positions → → Pulse energy

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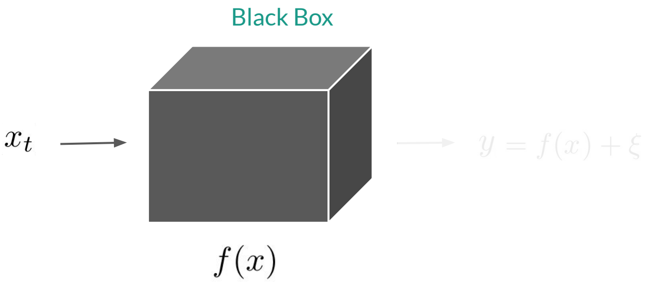

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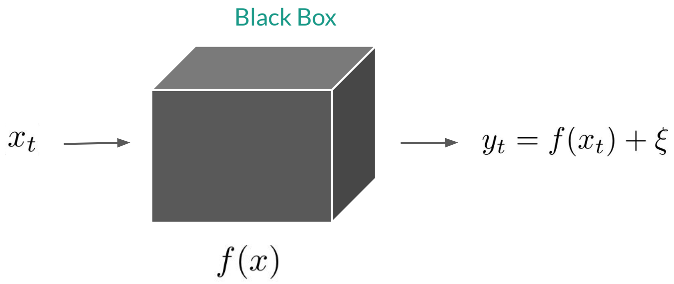

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Black-box optimization arises in high-stakes applications

where one needs to trade off attaining high utility vs minimizing risk

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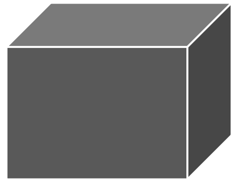
x_t →  → $y_t = f(x_t) + \xi$

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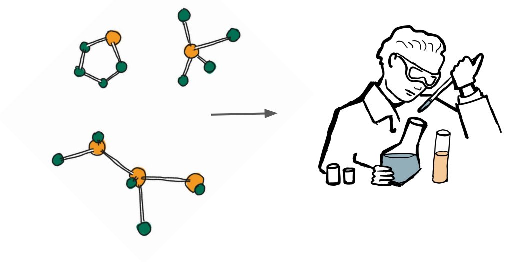 → Compound efficiency

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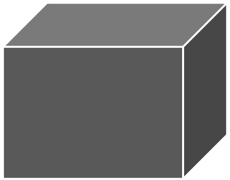

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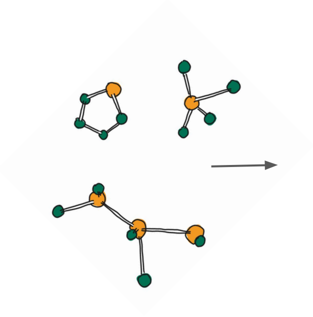

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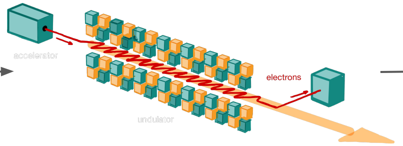

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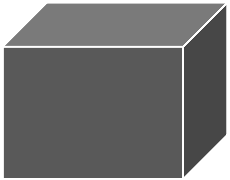

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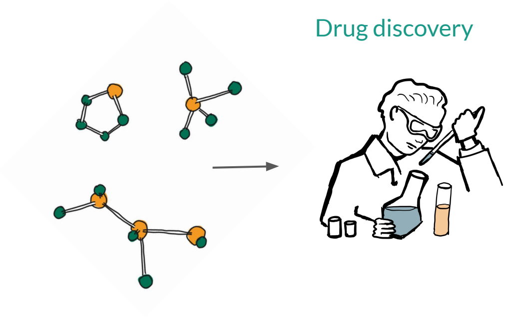

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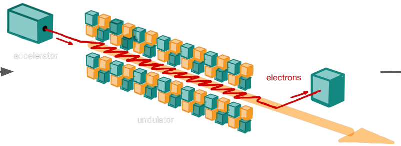

Pulse energy

In these applications, one needs to trade off attaining high utility vs minimizing risk

Bayesian optimization is a powerful framework for black-box functions

trading off exploration & exploitation

objective $f(x)$

$$x^* \in \arg\max_{x \in \mathcal{X}} f(x)$$

regret $R_T = \sum_{t=1}^{T} \left[f(x^*) - f(x_t) \right]$

Noise-perturbed evaluations

$$y_t = f(x_t) + \xi(x_t)$$

ρ -sub-Gaussian noise

Optimism under uncertainty via GP Upper Confidence bound

$$x_t \in \arg\max_{x \in \mathcal{X}} \underbrace{\mu_{t-1}(x) + \beta_t \sigma_{t-1}(x)}_{=:\mathrm{ucb}_t^f(x)}$$

GP posterior mean and variance

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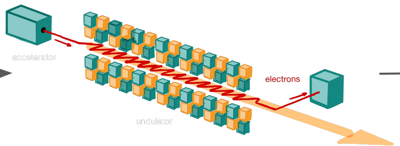

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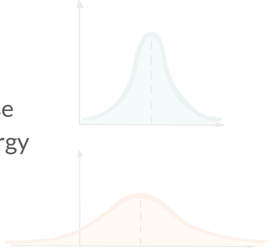

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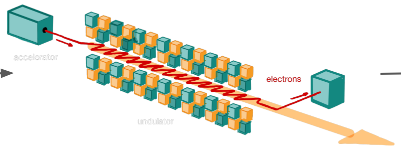

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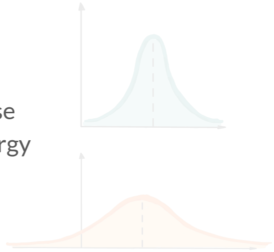

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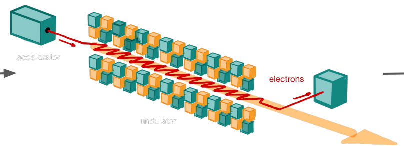

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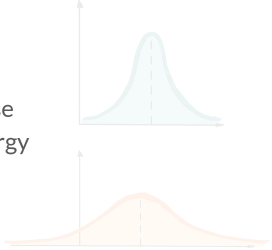

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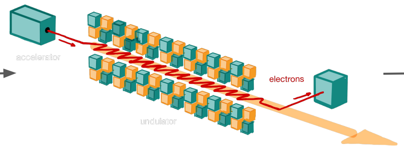

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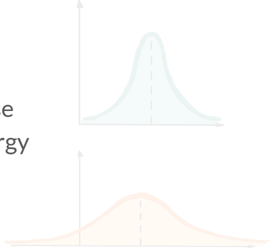

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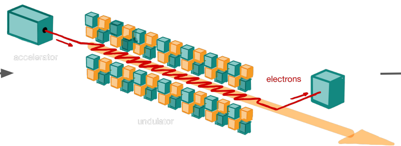

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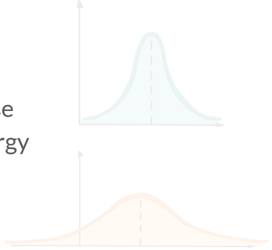

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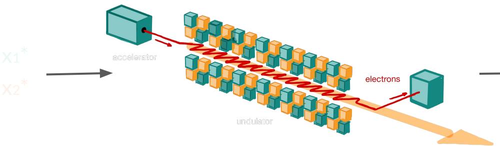

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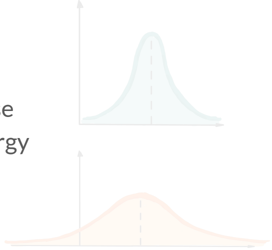

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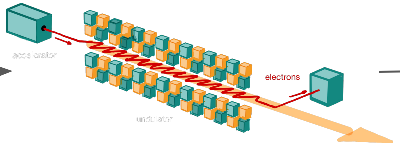

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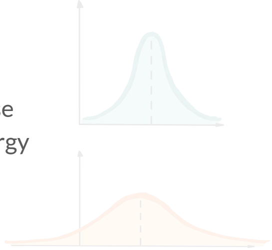

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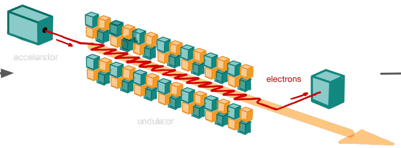

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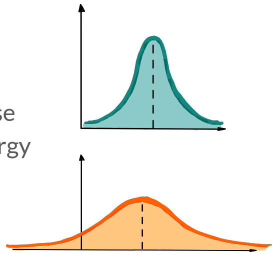

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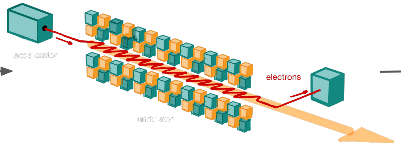

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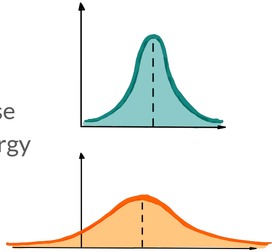

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Heteroscedastic Bayesian optimization is a powerful framework for black-box functions trading off exploration & exploitation **& risk**

Mean-Variance objective

$$\mathrm{MV}(x) = f(x) - \alpha\rho^2(x)$$

$$x^* \in \arg\max_{x \in \mathcal{X}} \mathrm{MV}(x)$$

Risk-averse regret

$$R_T = \sum_{t=1}^{T}\left[\mathrm{MV}(x^*) - \mathrm{MV}(x_t)\right]$$

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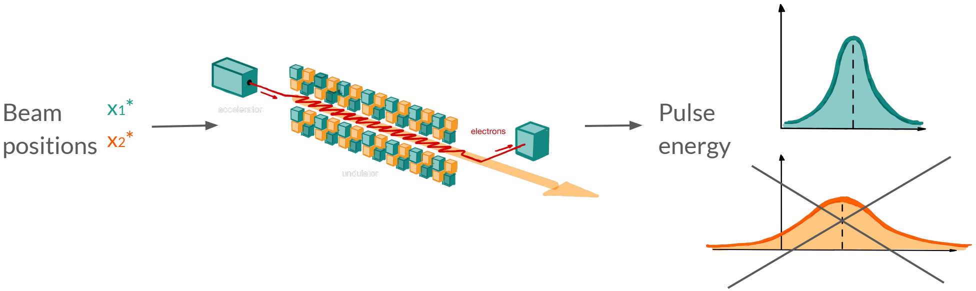
Optimism under uncertainty via RAHBO:

$$x_t \in \arg\max_{x \in \mathcal{X}} \ \mathrm{ucb}^f_{t-1}(x) - \alpha\, \mathrm{lcb}^{\rho^2}_{t-1}(x)$$

Tuning accelerators



RAHBO idea: Generalize Bayesian optimization to **trade mean and input-dependent variance** of the objective, despite both of them being unknown a priori.

Risk-averse Heteroscedastic Bayesian optimization (RAHBO) is a framework for black-box functions trading off exploration & exploitation **& risk**

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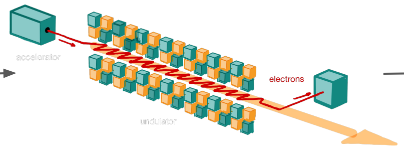

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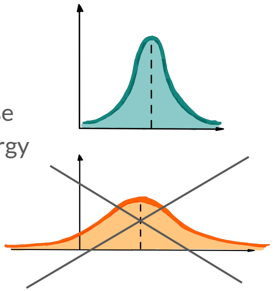

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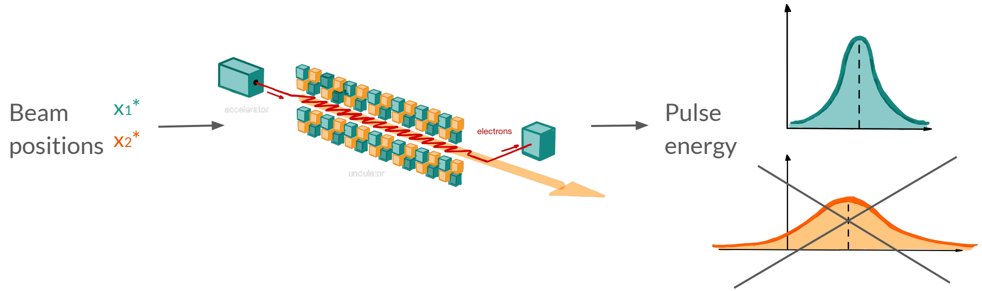

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coefficient of absolute risk tolerance

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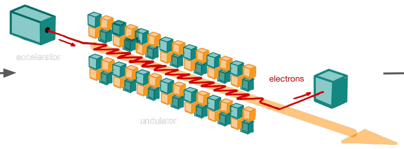

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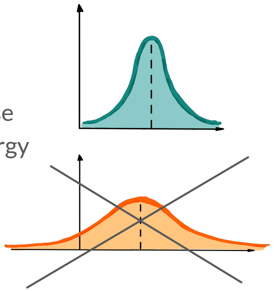

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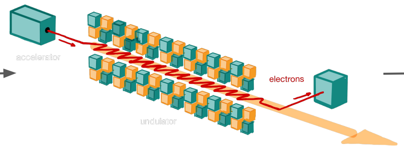

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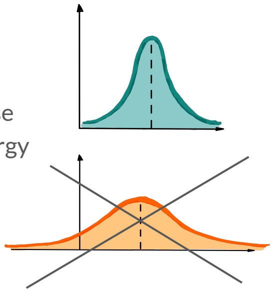

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$$R_T = \sum_{t=1}^{T} \Big[\mathbf{MV}(x^*) - \mathbf{MV}(x_t)\Big]$$

Noise-perturbed evaluations

$$y_t = f(x_t) + \xi(x_t)$$

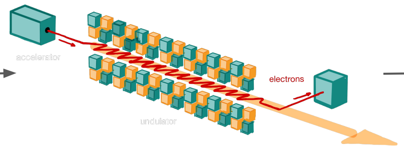
$\rho(x)$-sub-Gaussian noise

Optimism under uncertainty via RAHBO:

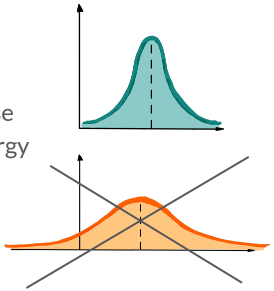
$$x_t \in \arg\max_{x \in \mathcal{X}} \ \mathrm{ucb}^f_{t-1}(x) - \alpha\, \mathrm{lcb}^{\rho^2}_{t-1}(x)$$

Tuning accelerators

Beam positions x_1^* x_2^*



Pulse energy

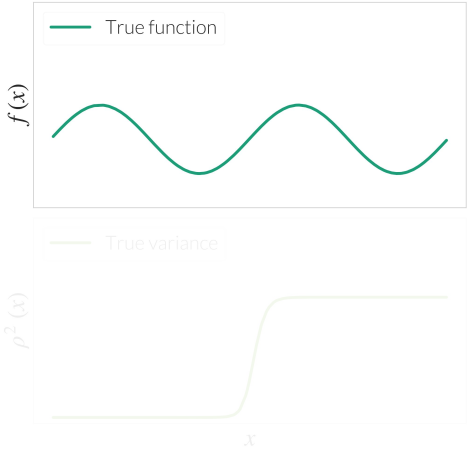


RAHBO idea: Generalize Bayesian optimization to **trade mean and input-dependent variance** of the objective, despite both of them being unknown a priori.

Failure of GP-UCB

In the risk-averse setting the maximizers for mean-variance (RAHBO) and for mean (GP-UCB) might not coincide

Unknown objective (sine) with two global optimizers
-- but one has much higher noise variance



RAHBO: exploration & exploitation **& risk** tradeoff

GP-UCB: exploration & exploitation tradeoff

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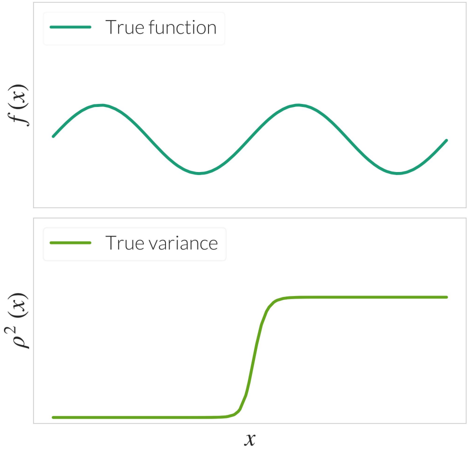

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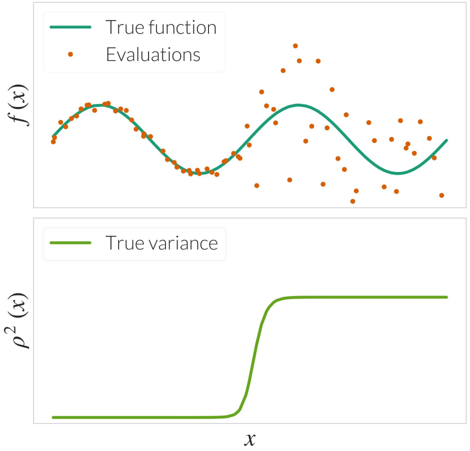

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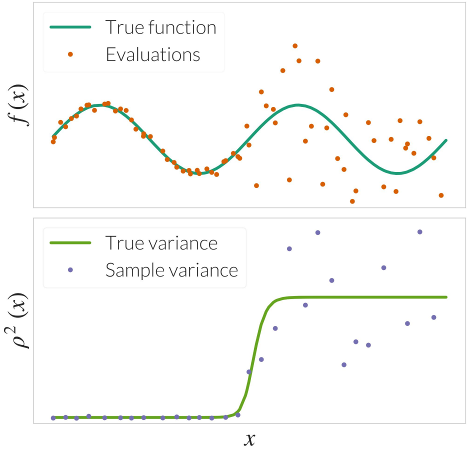

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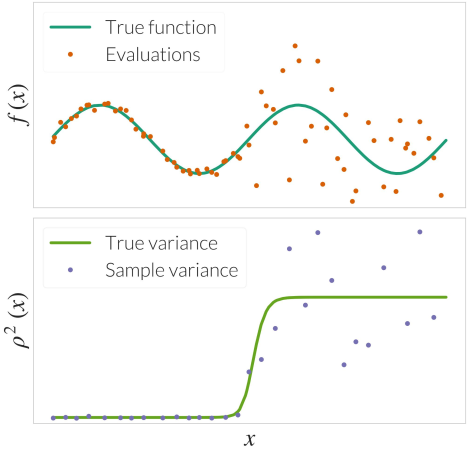

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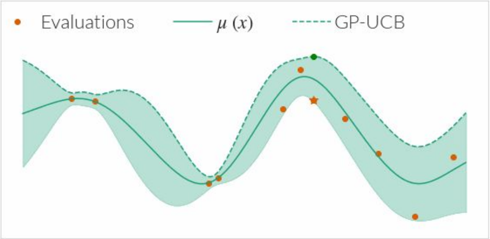

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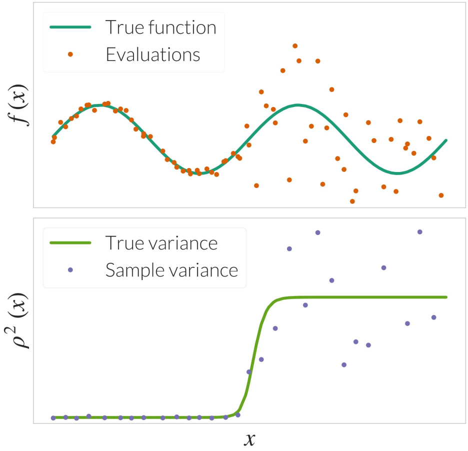

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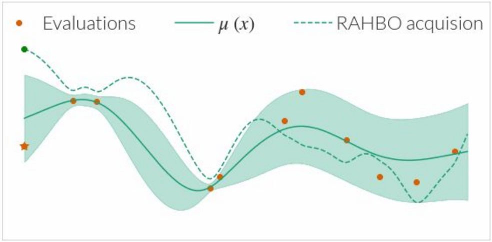

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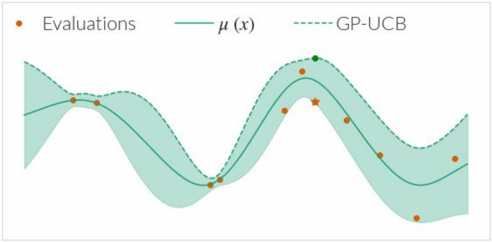

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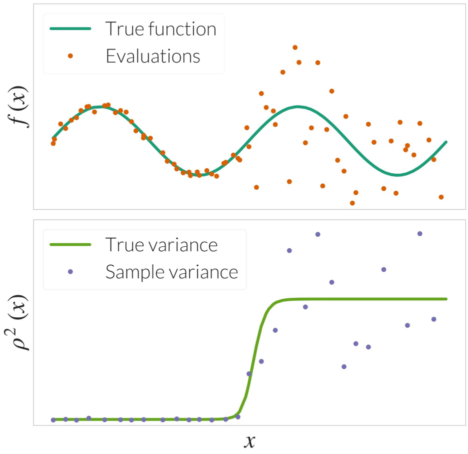

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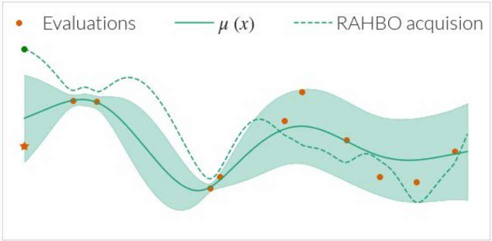

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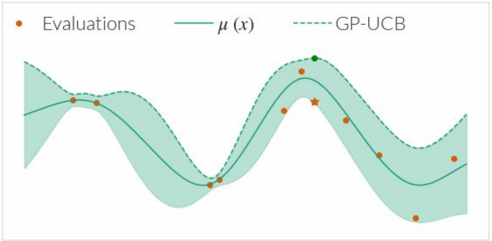
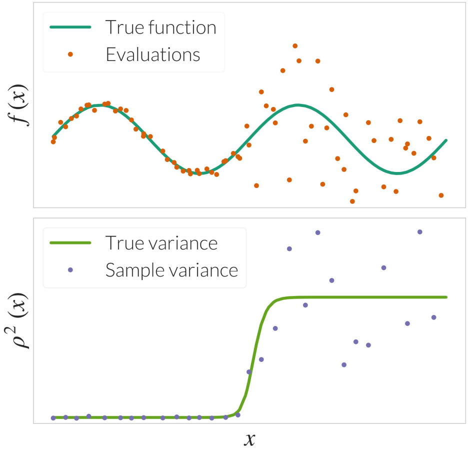


The Risk-averse Heteroscedastic Bayesian Optimization (RAHBO) Algorithm

RAHBO attaints sublinear regret $R_T = \mathcal{O}(\sqrt{T})$



Model for $f(x)$

Model for $\rho^2(x)$

$$x_t \in \arg\max_{x \in \mathcal{X}} \ \mathrm{ucb}^{f}_{t-1}(x) - \alpha \ \mathrm{lcb}^{\rho^2}_{t-1}(x)$$

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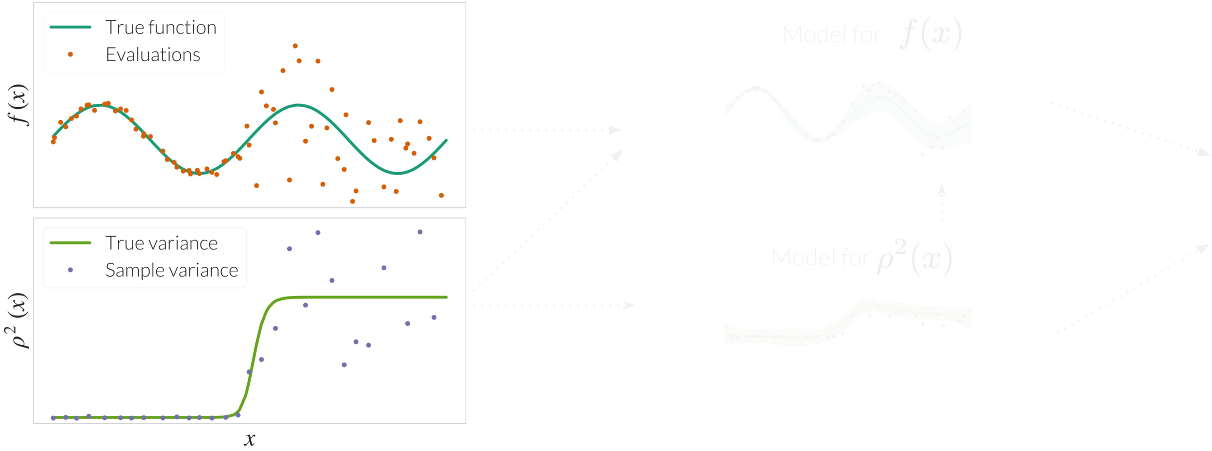

Optimism under uncertainty

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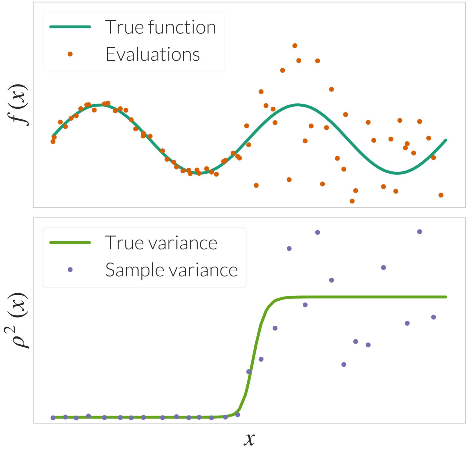

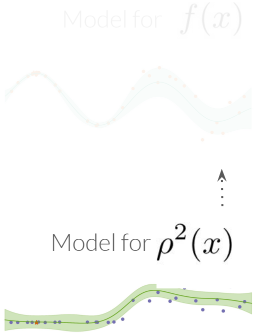

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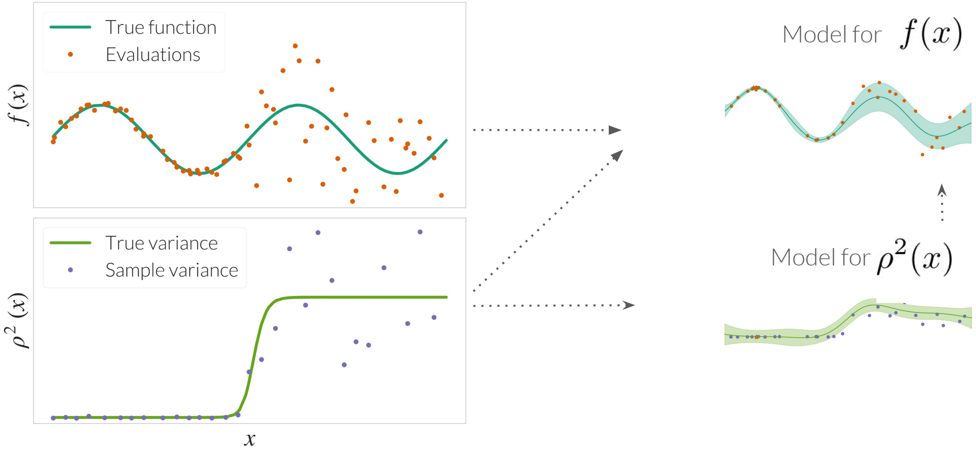

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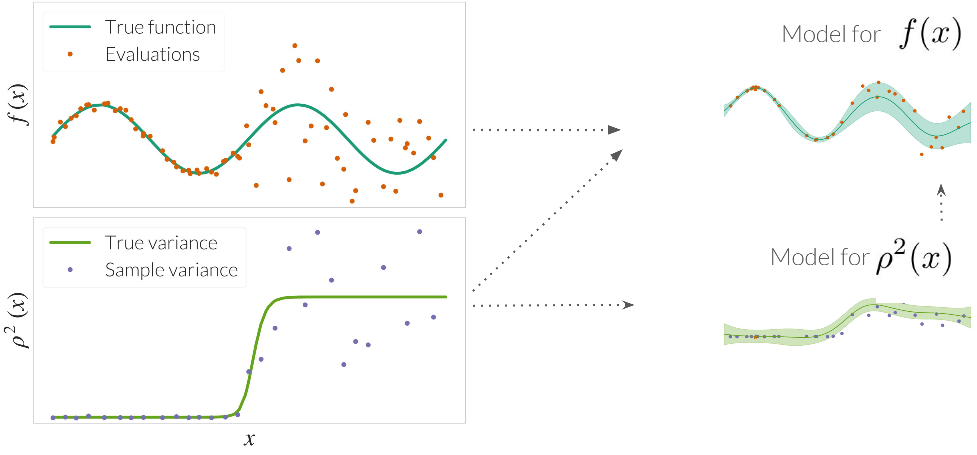

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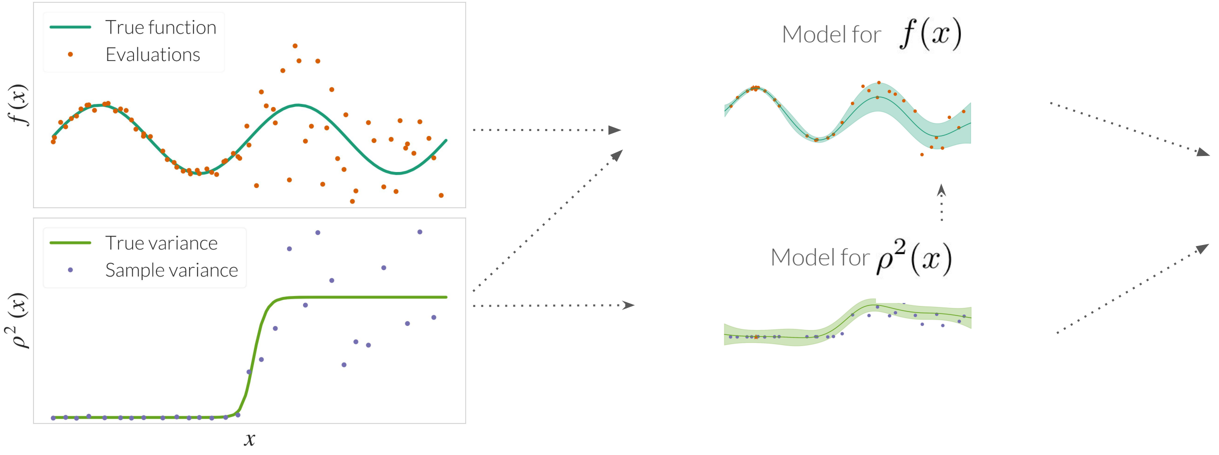
The Risk-averse Heteroscedastic Bayesian Optimization (RAHBO) Algorithm

Convergence guarantees (informal):
Under certain assumptions (see the paper for details),
RAHBO attains sublinear regret.



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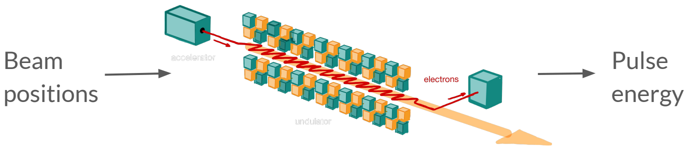
RAHBO results for SwissFEL

Tuning Swiss Free Electron Laser



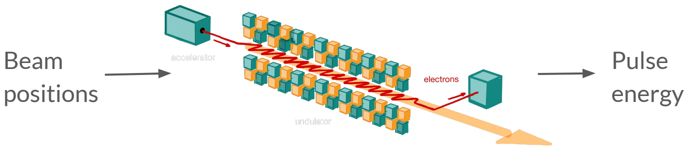
Empirical distribution of true values at acquired points

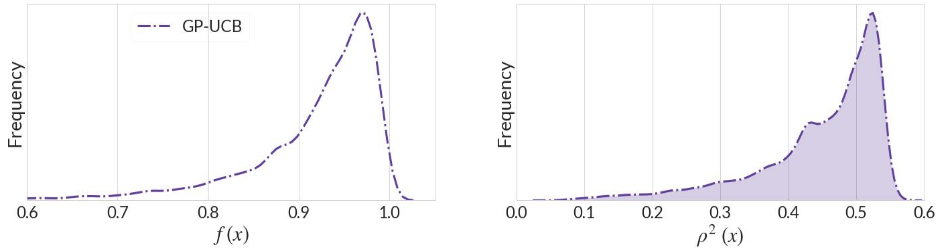
(b) Mean-variance tradeoff (FEL) (c) Cum. regret ($\alpha = 0.5$) (d) Cum. regret ($\alpha = 1$)

GP-UCB tends to query points with higher noise, while RAHBO achieves substantially reduced variance and minimal reduction in mean performance.

RAHBO results for SwissFEL

Tuning Swiss Free Electron Laser





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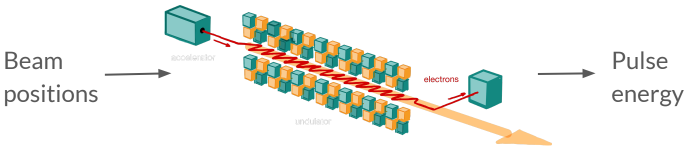

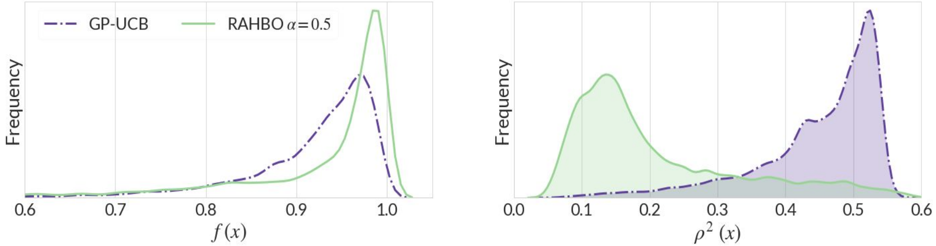

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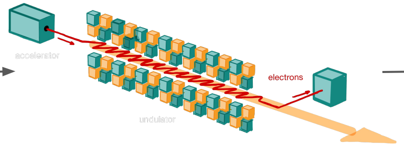
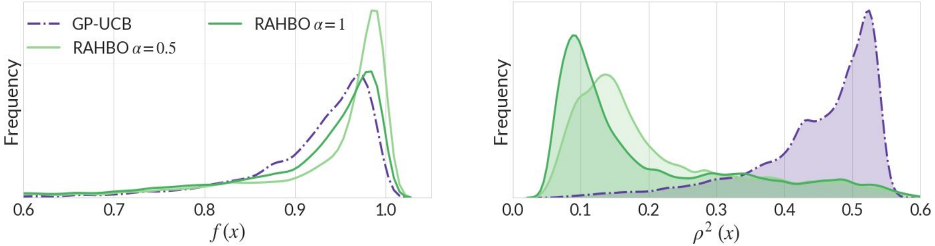
Tuning Swiss Free Electron Laser

Beam positions



Pulse energy



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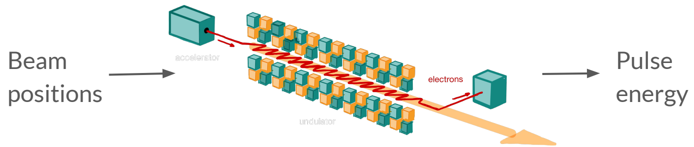
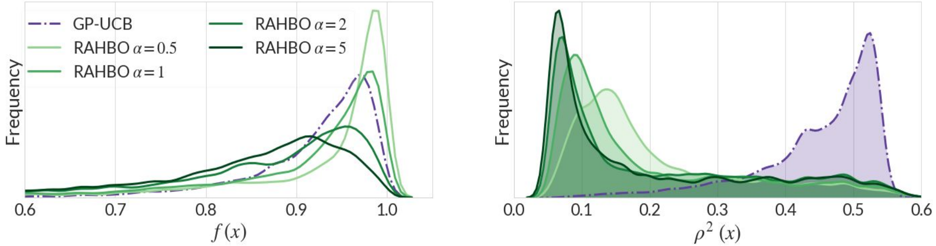
Tuning Swiss Free Electron Laser





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Tuning Swiss Free Electron Laser

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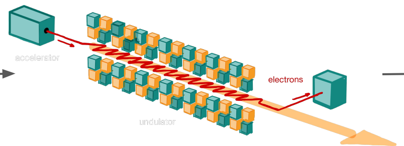

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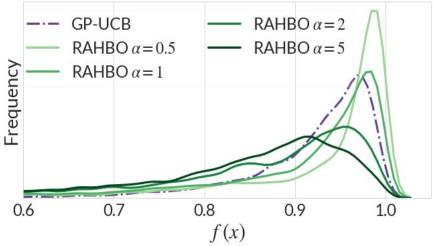

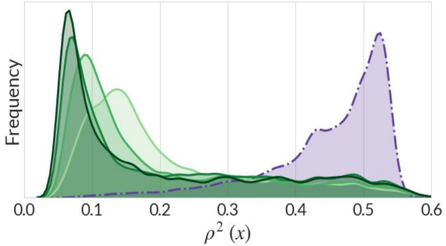

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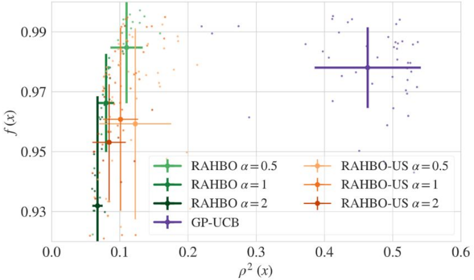

Mean-variance trade off

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Tuning Swiss Free Electron Laser

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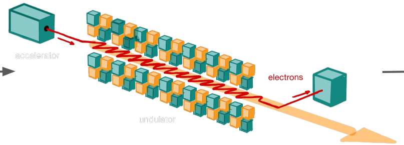

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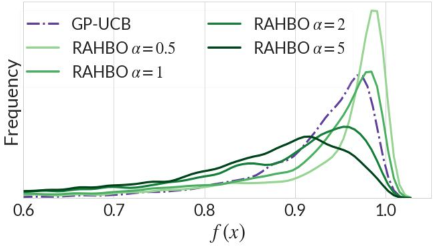

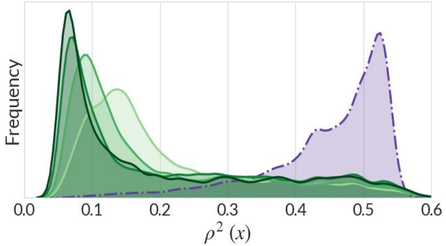

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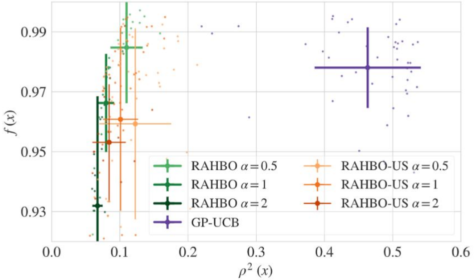

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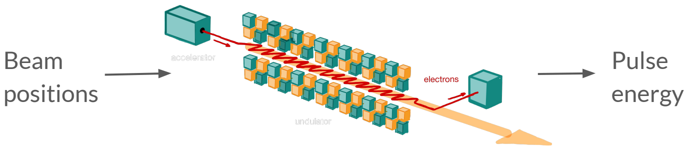
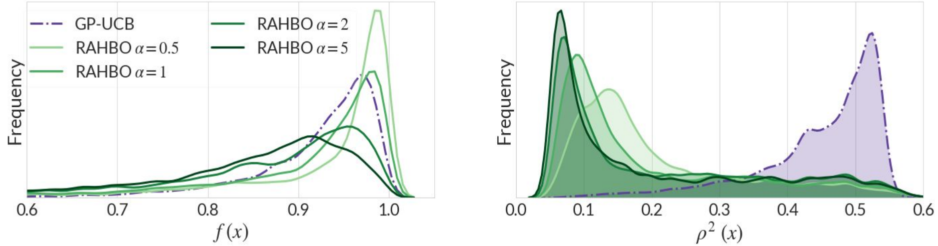
RAHBO results for Swiss FEL

Tuning Swiss Free Electron Laser





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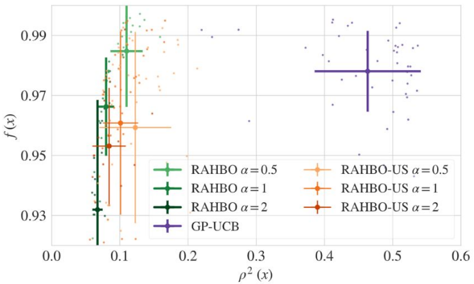

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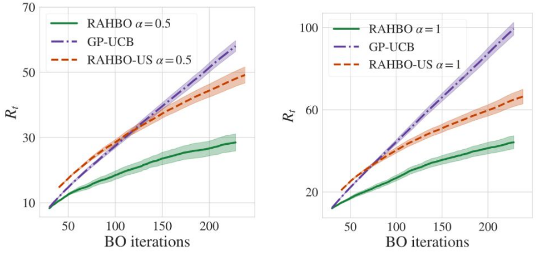

Cumulative regret

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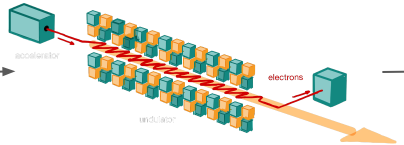
Summary

Tuning Swiss Free Electron Laser

Beam positions



Pulse energy

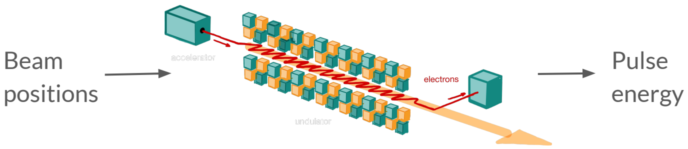
Goal:

- Incorporate risk into exploration-exploitation trade-off

Our contributions:

- Mean-variance approach for Bayesian optimization
- Practical algorithm based on optimism under the face of uncertainty
- Theoretical regret bounds
- Empirical results on SwissFEL simulator and ML model tuning

Tuning Swiss Free Electron Laser



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Summary

Tuning Swiss Free Electron Laser

Beam positions

Pulse energy

Goal:

- Avoid cost of failure due to noisy realizations in high-stakes applications
- Incorporate risk into exploration-exploitation trade-off

Drop by our poster for more details :)

Our contributions:

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Paper ID 26309