Multi-Fidelity Bayesian Optimization with Unreliable Information Sources

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Aalto University

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Bayesian Optimization 101

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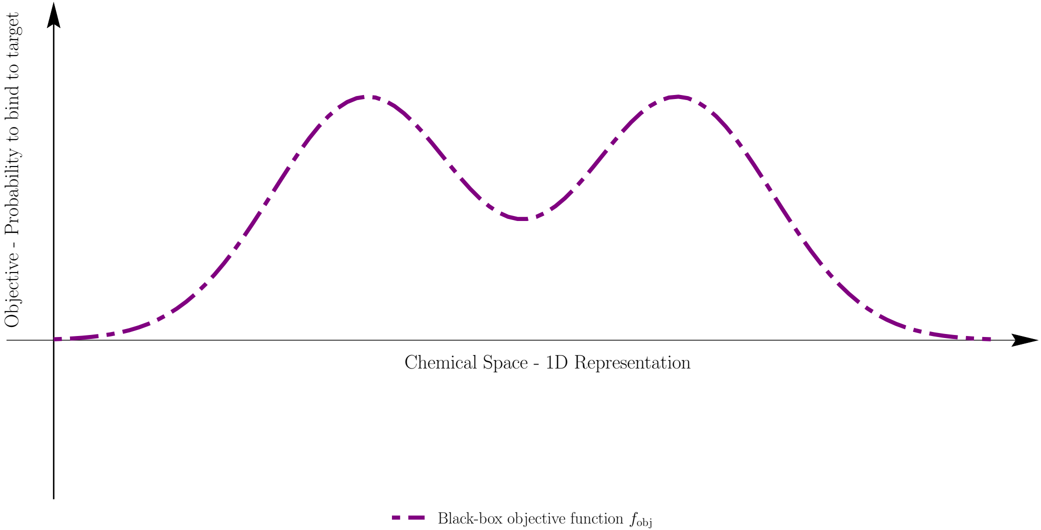

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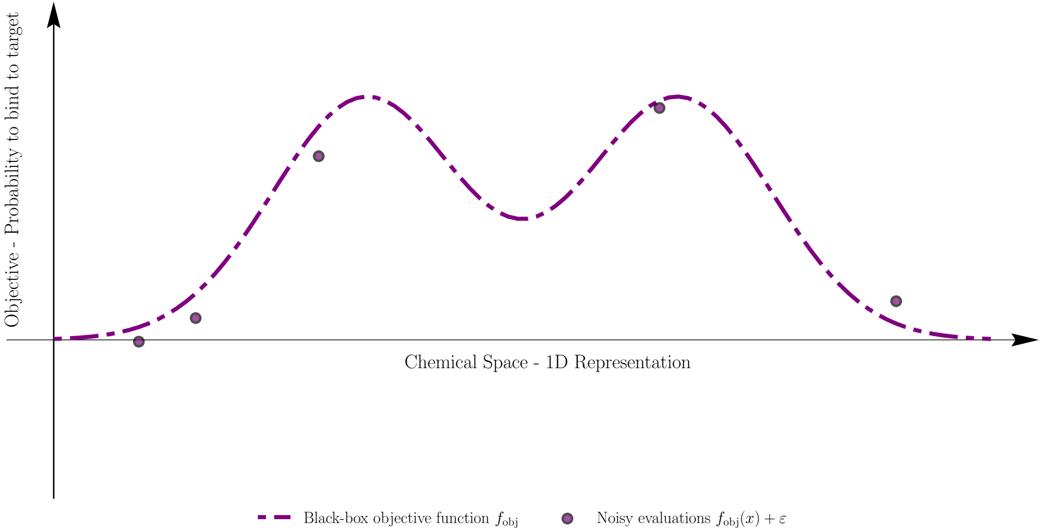

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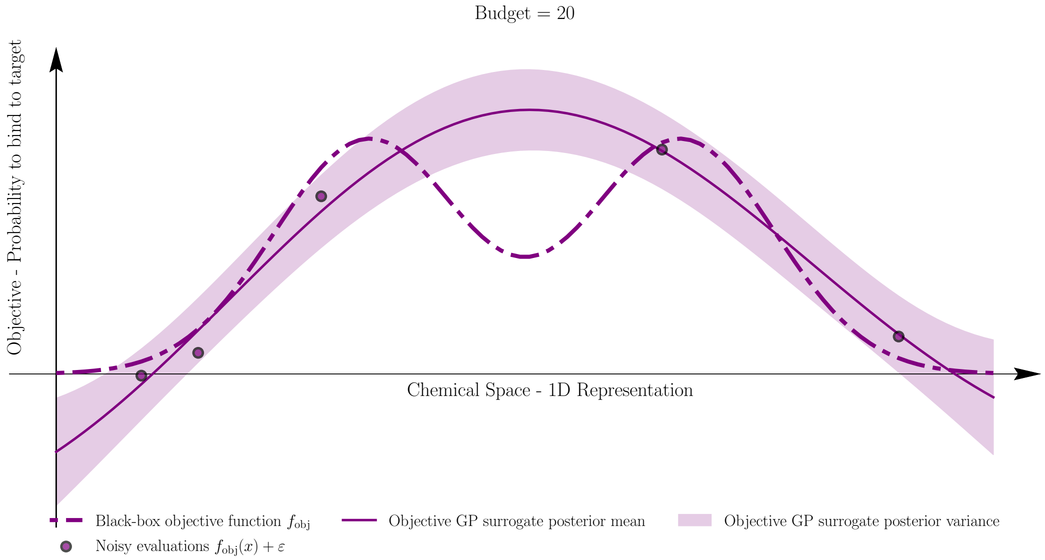

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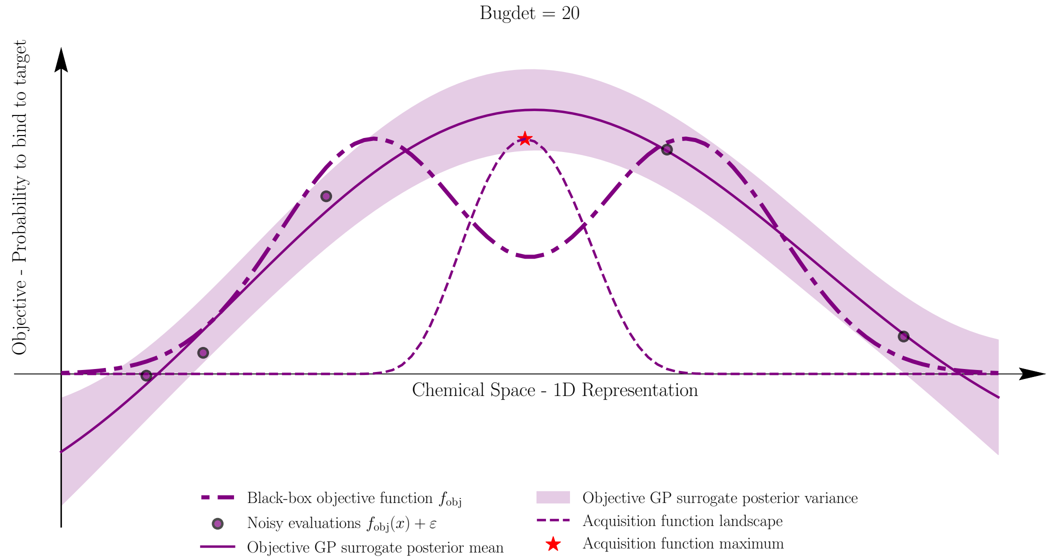

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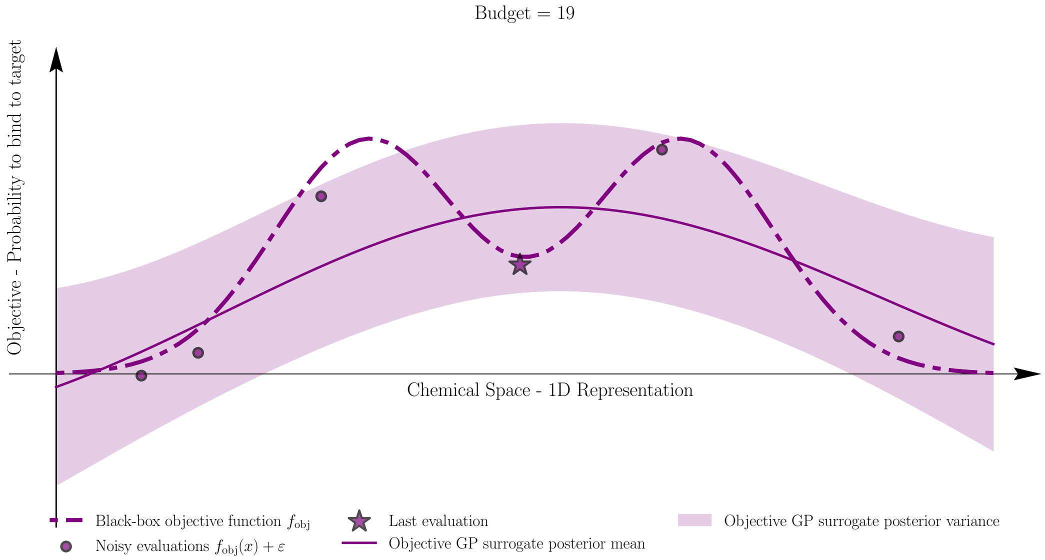

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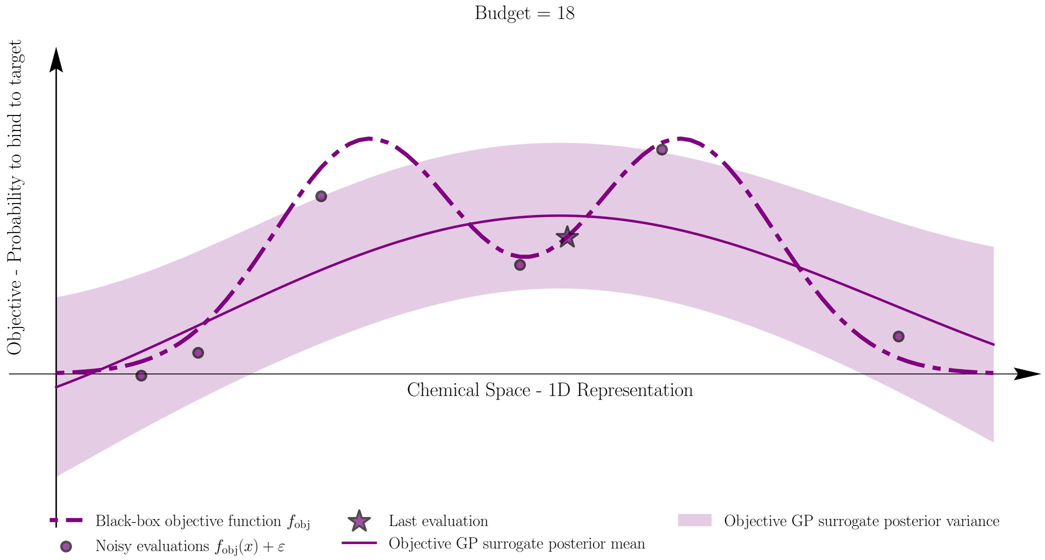

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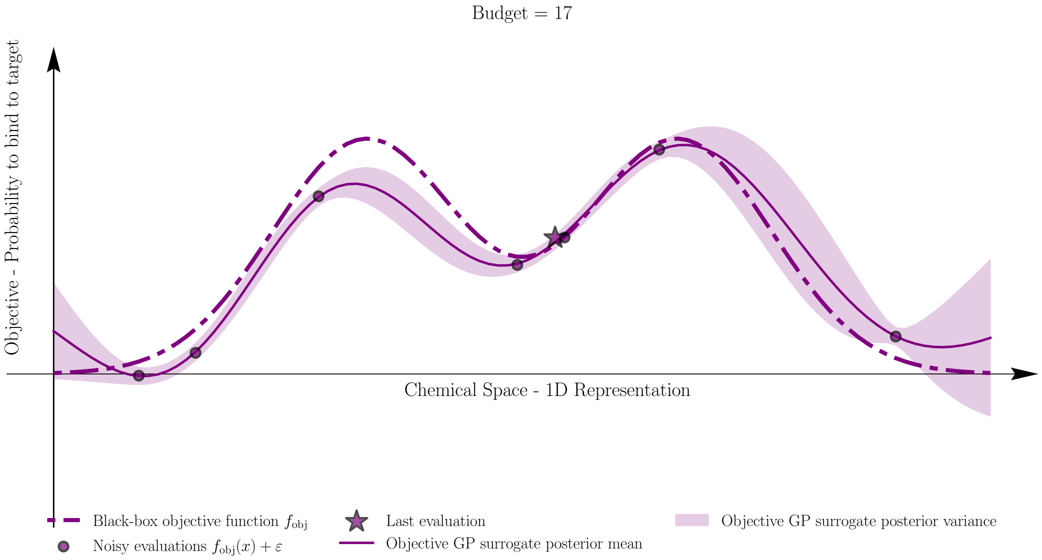

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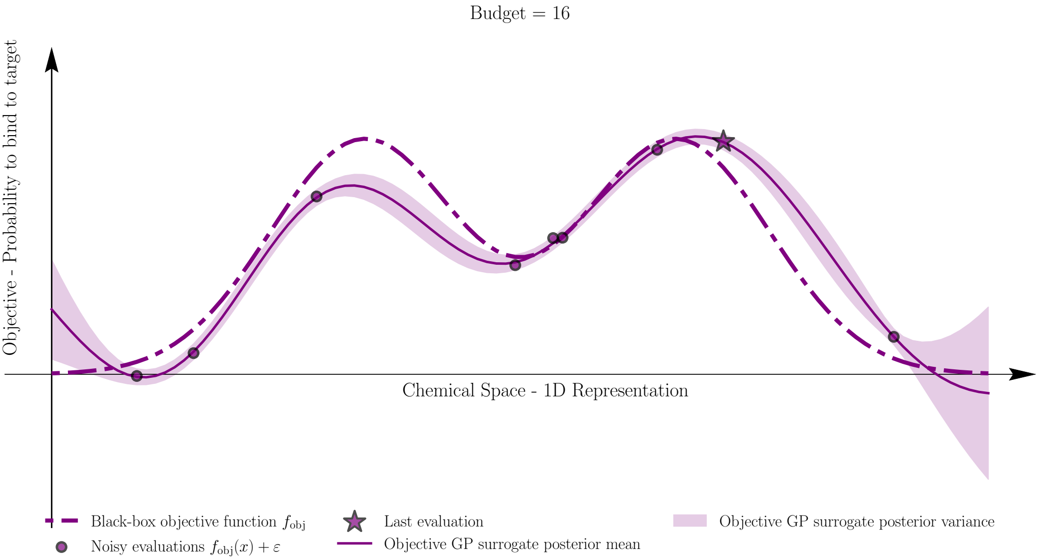

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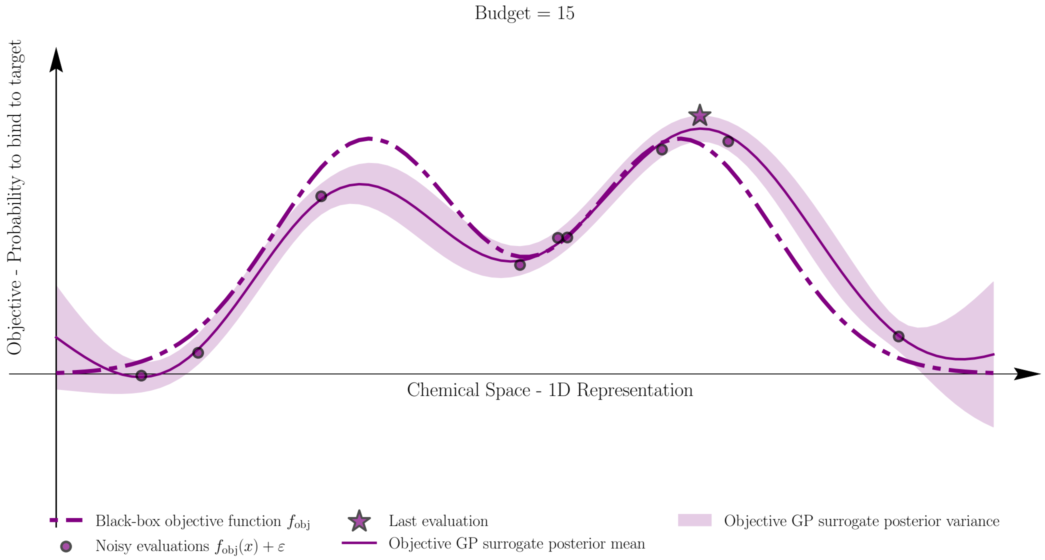

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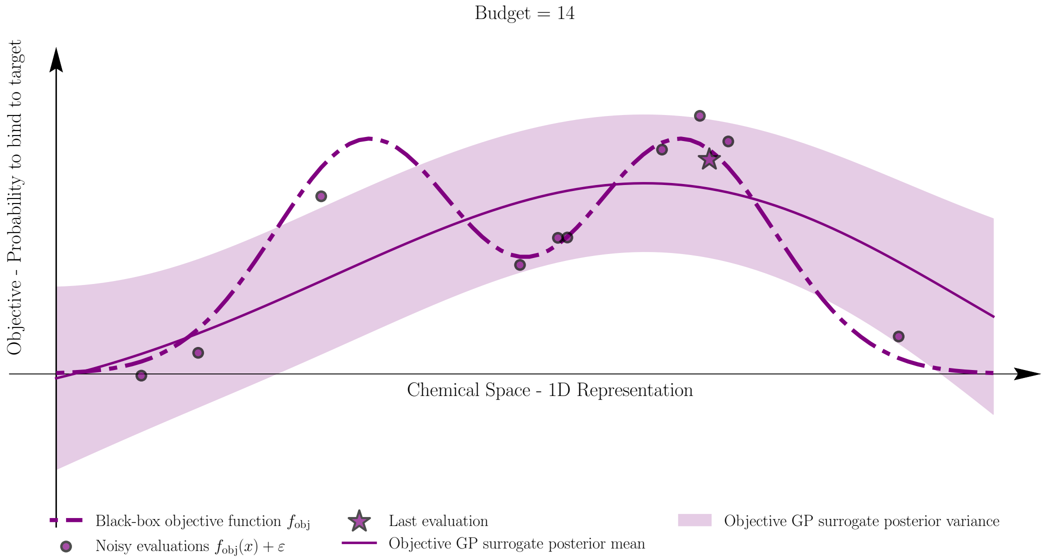

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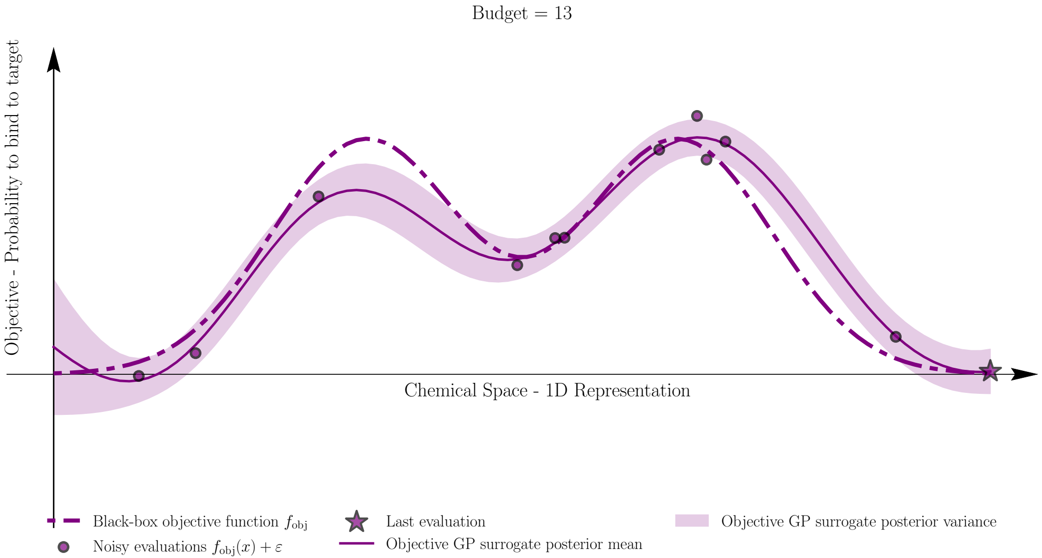

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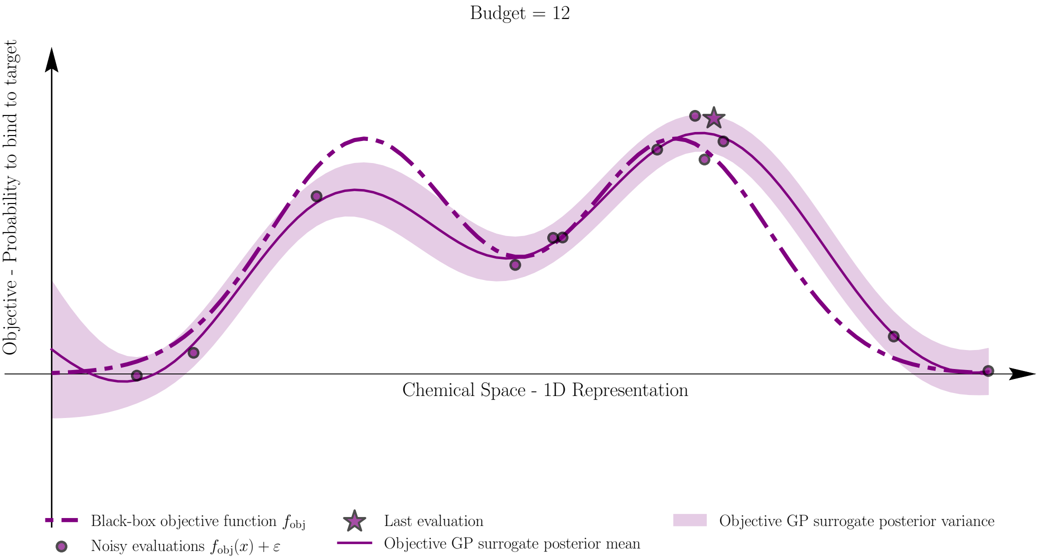

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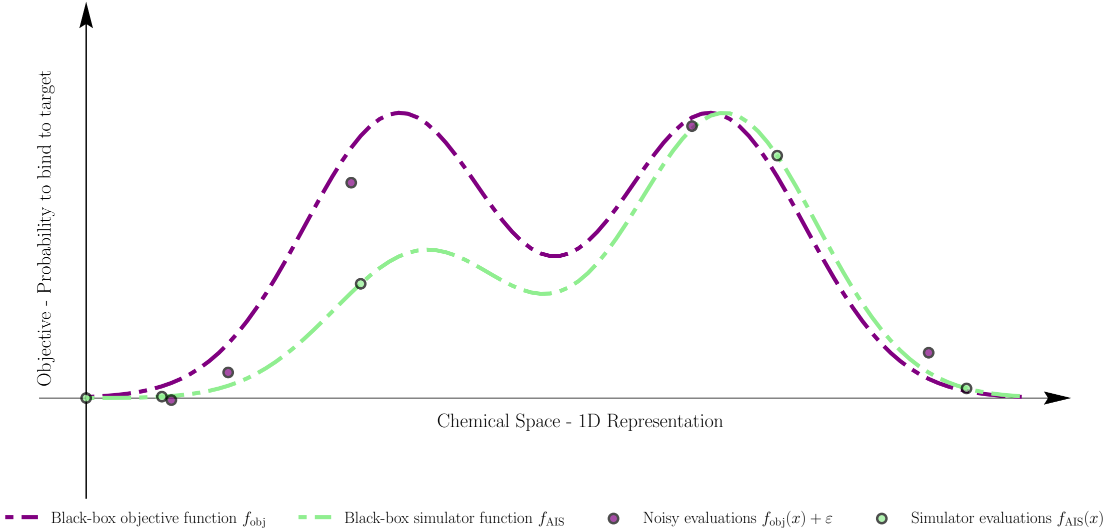

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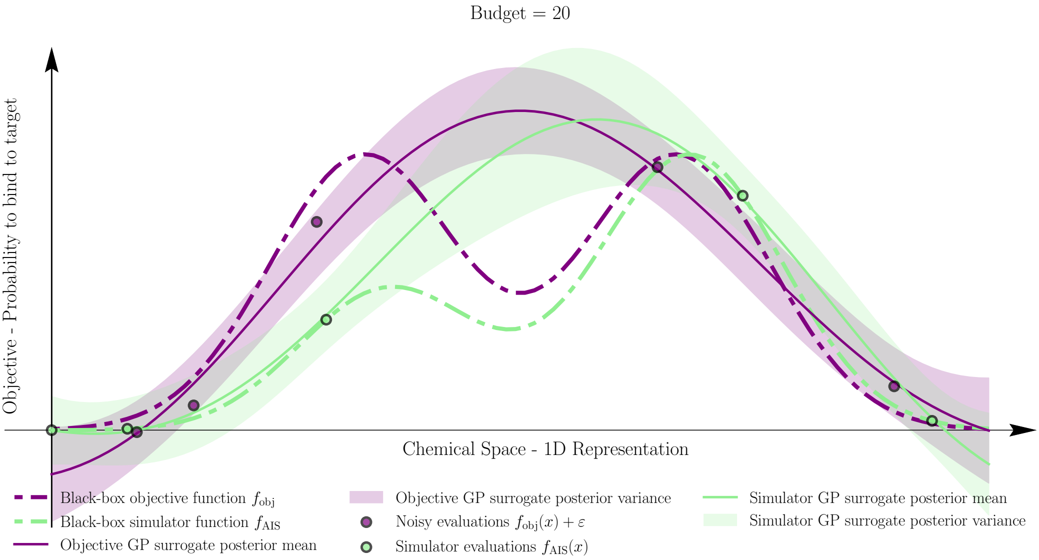

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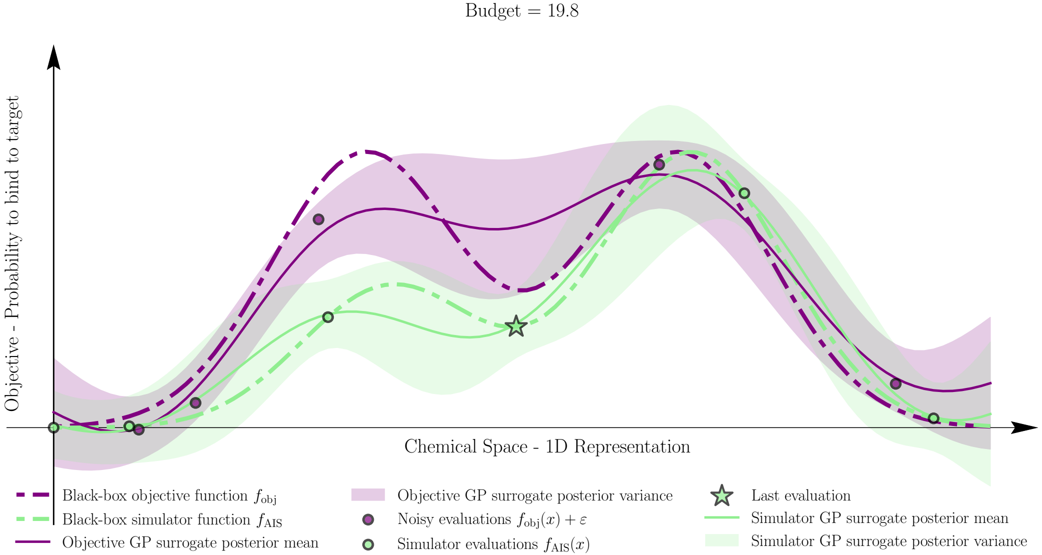

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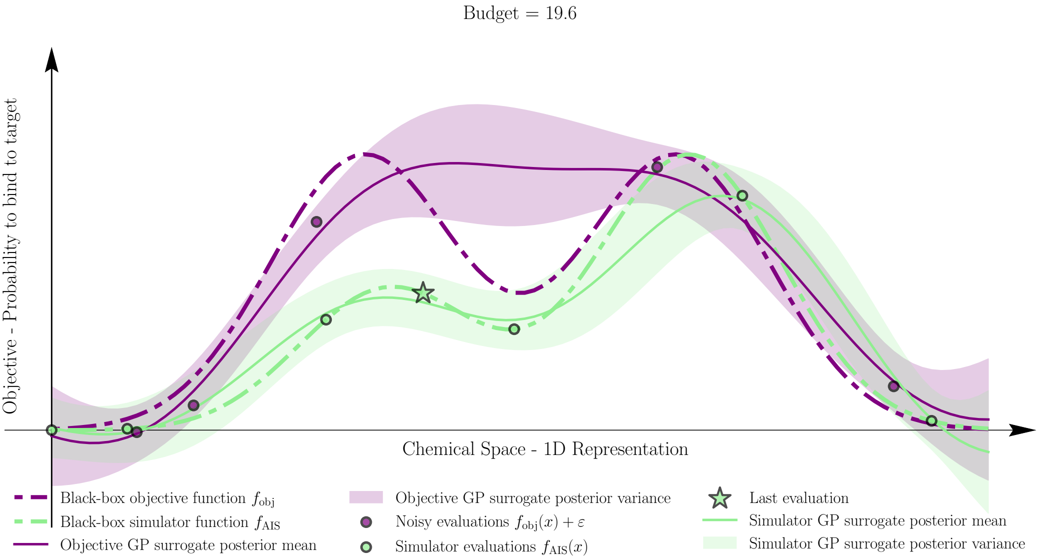

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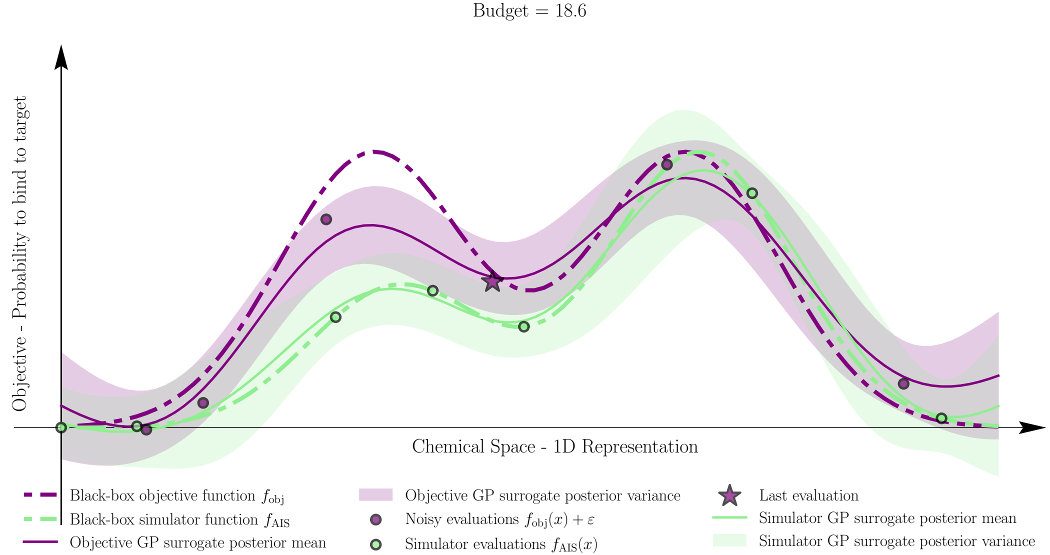

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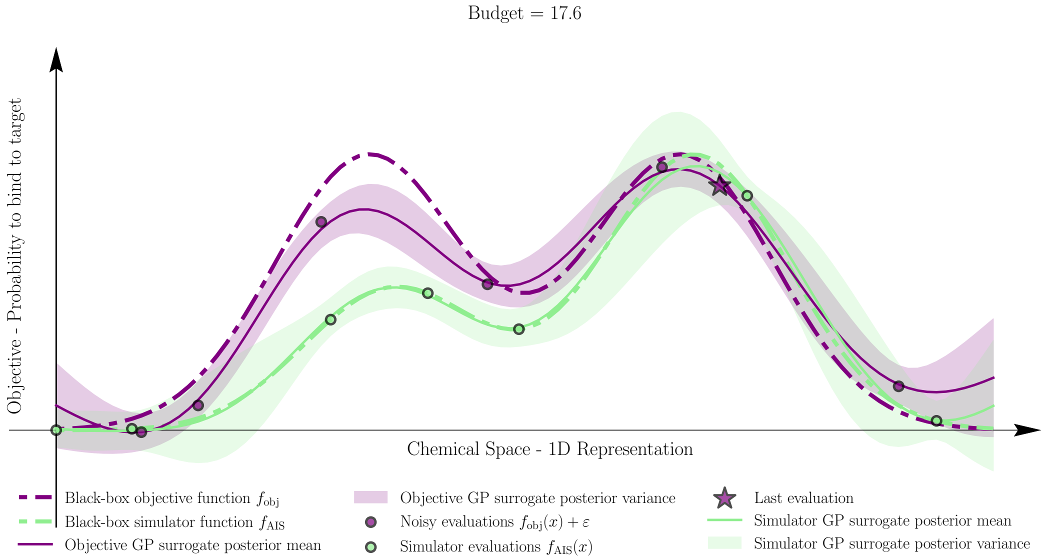

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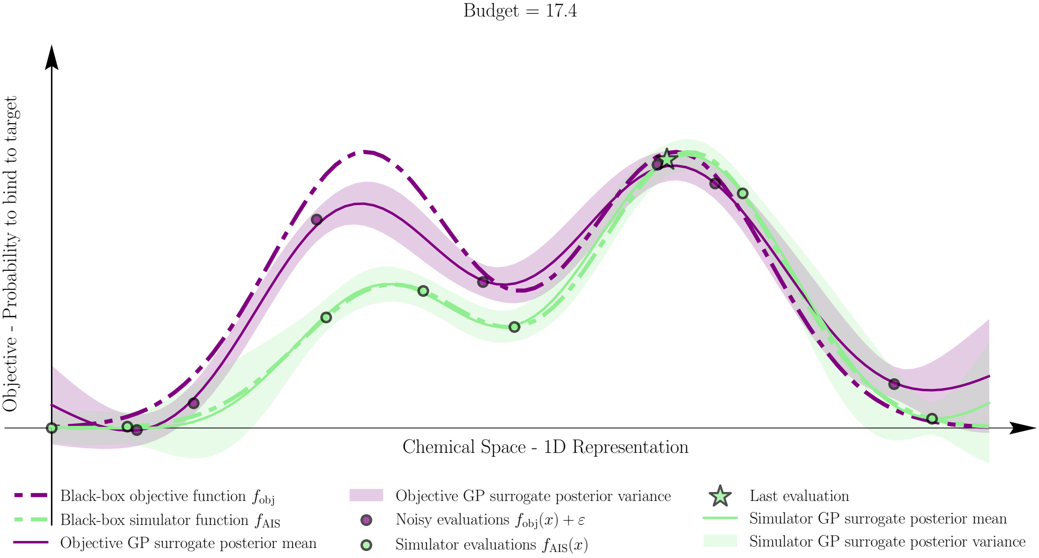

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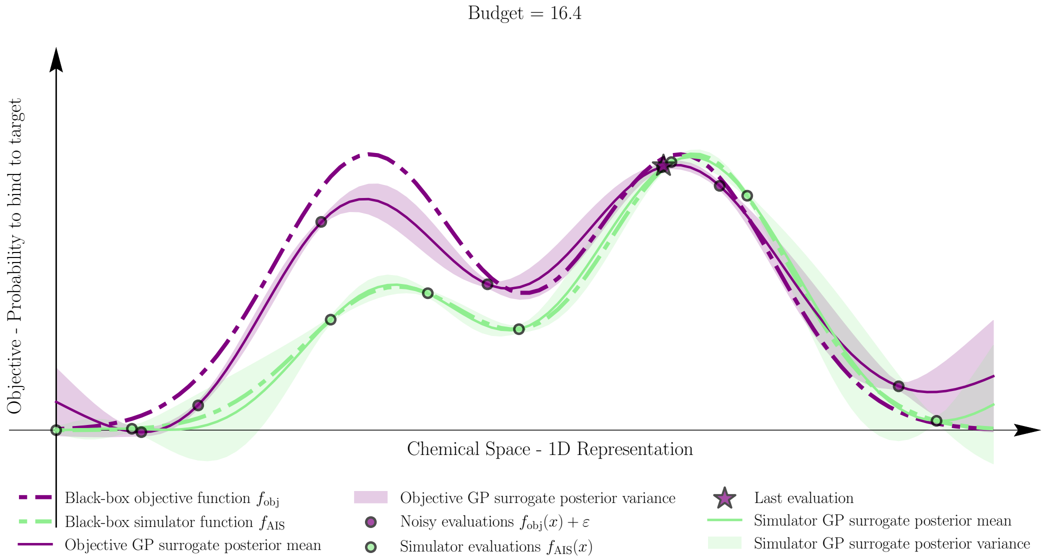

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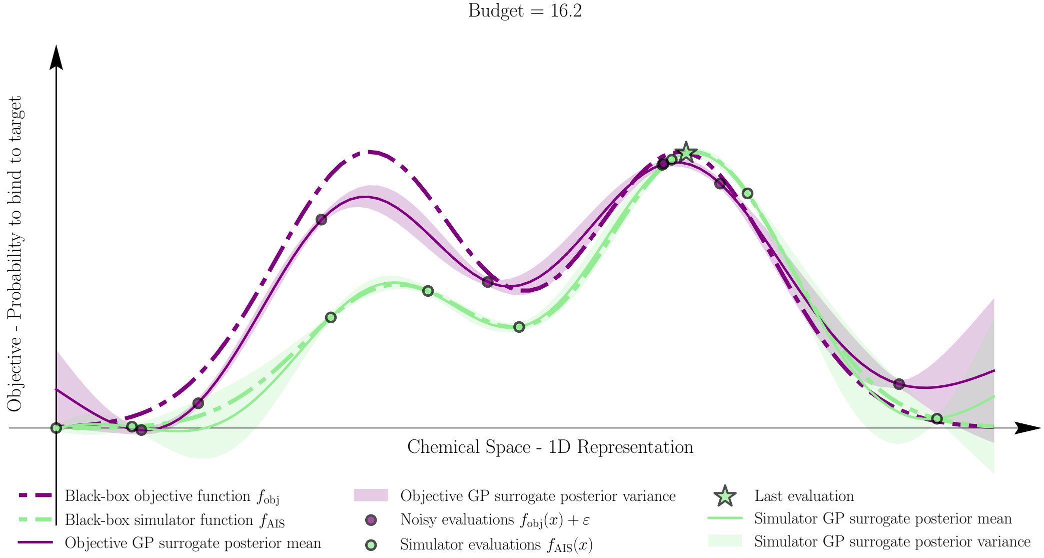

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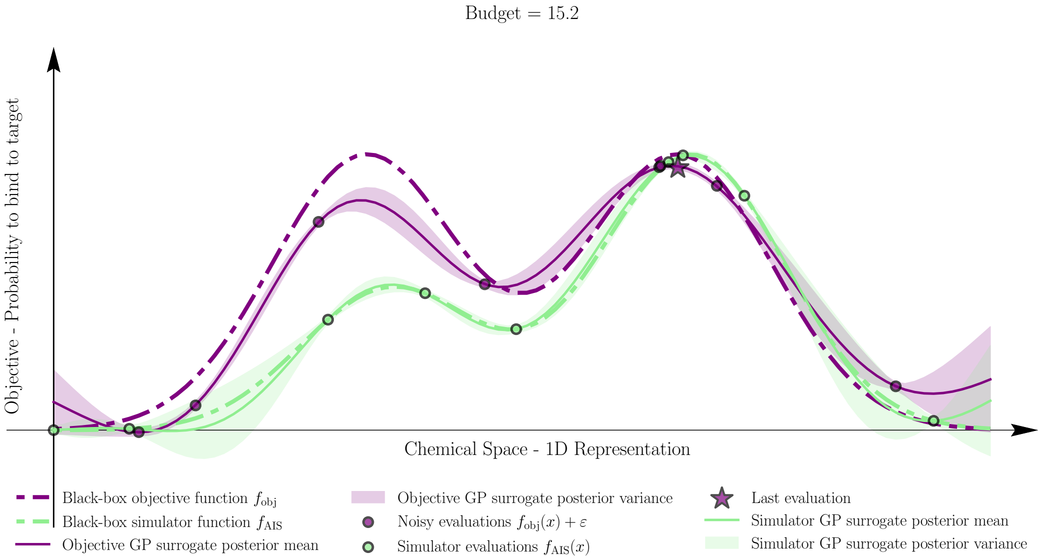
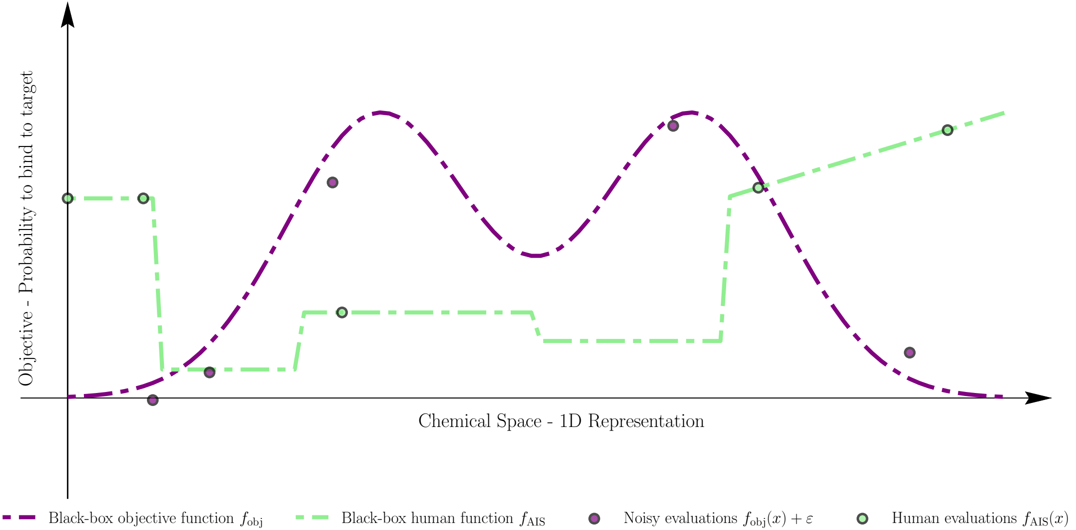


Multi Fidelity Bayesian Optimization with Unreliable Sources



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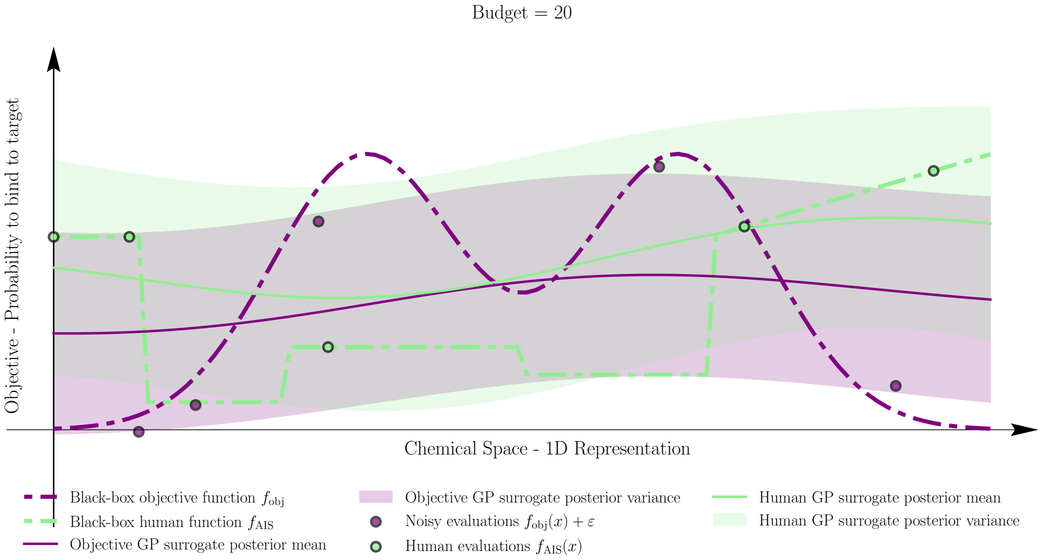

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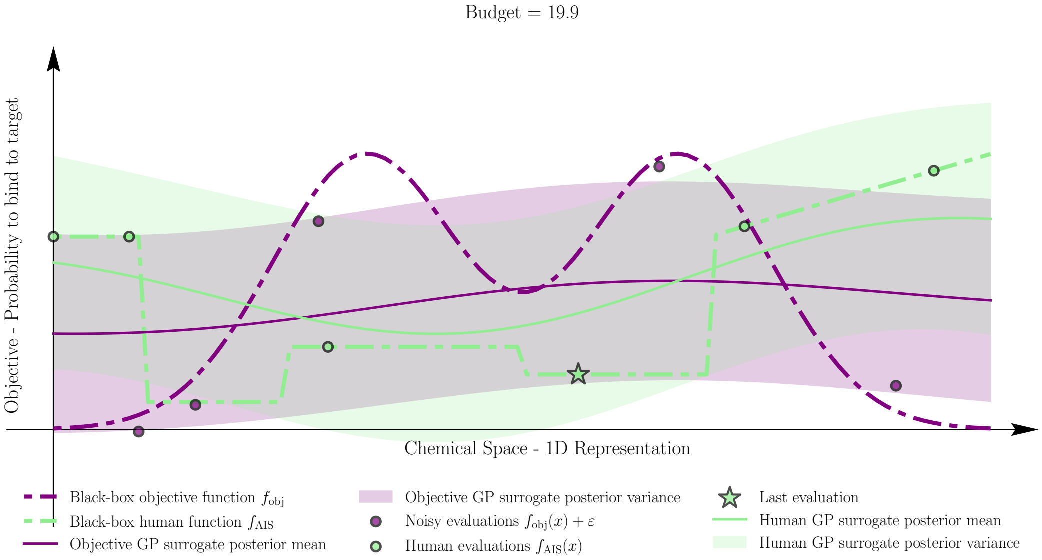

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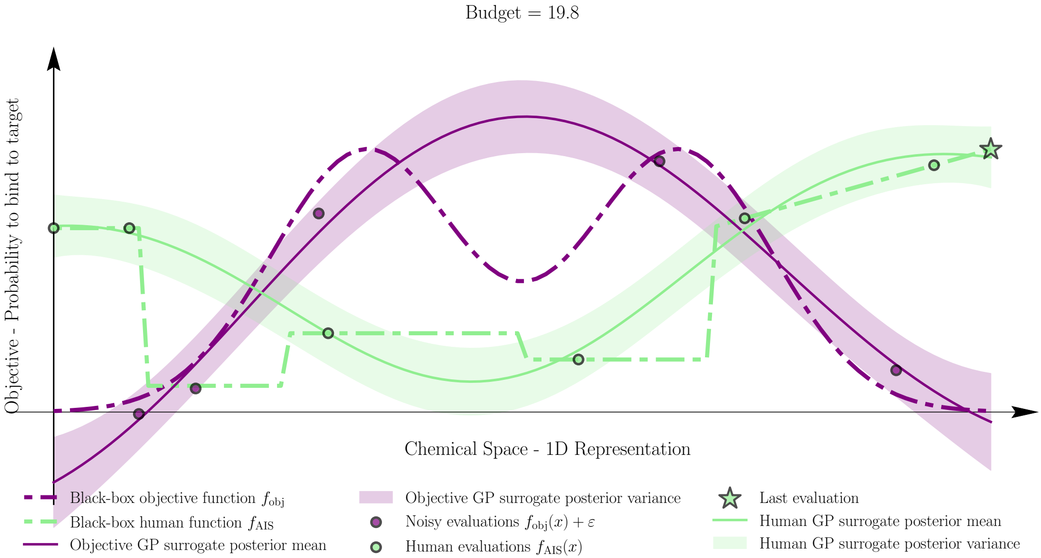

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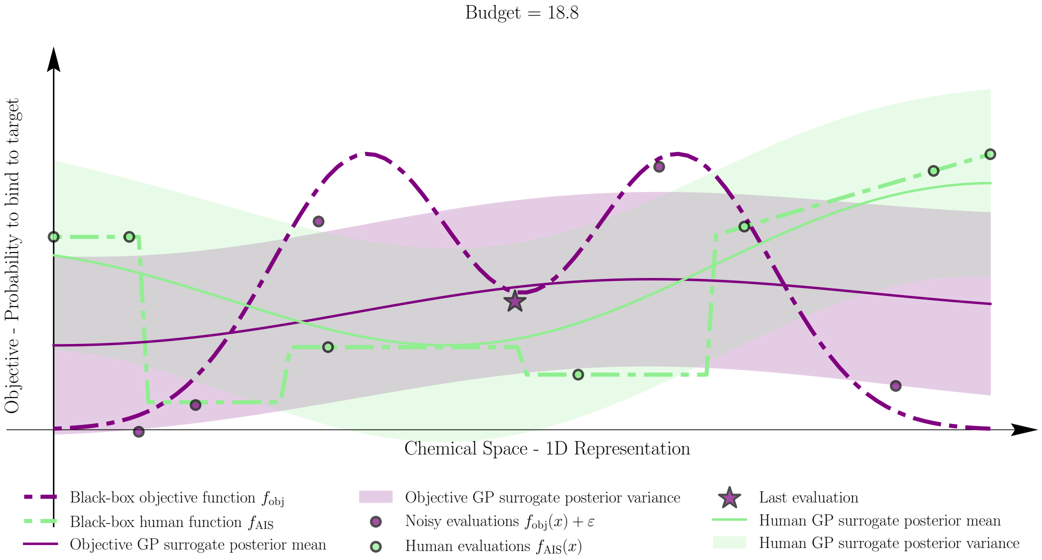

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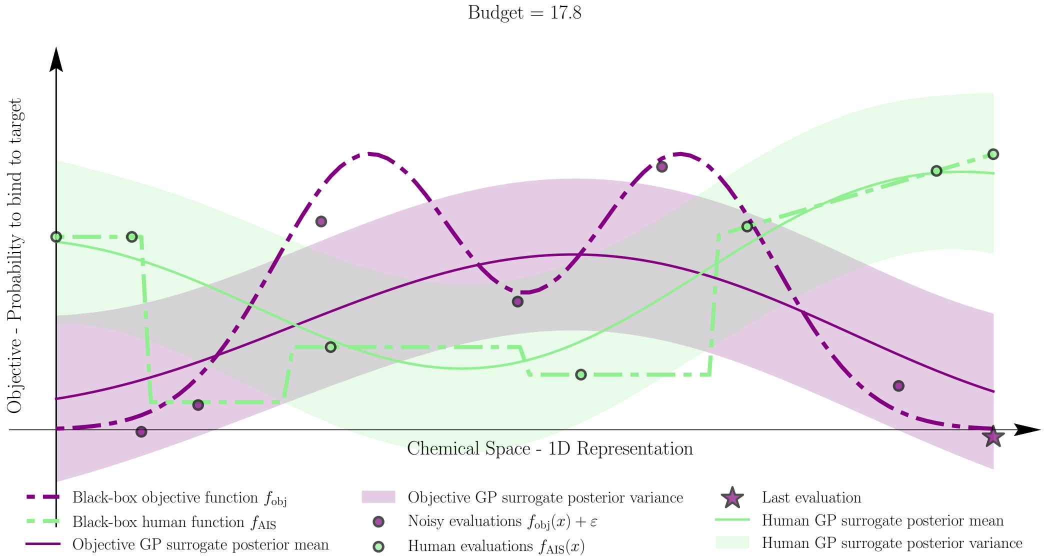

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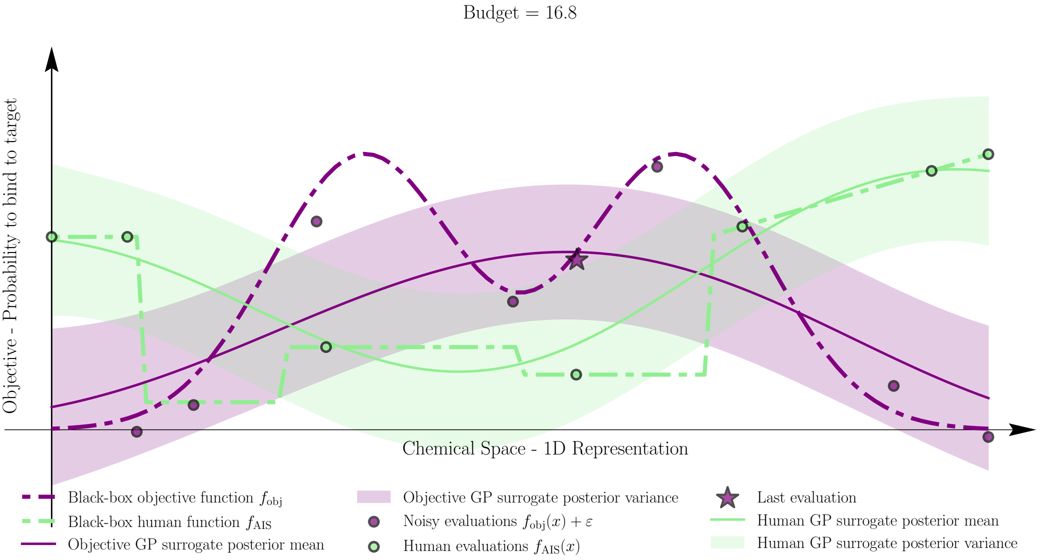

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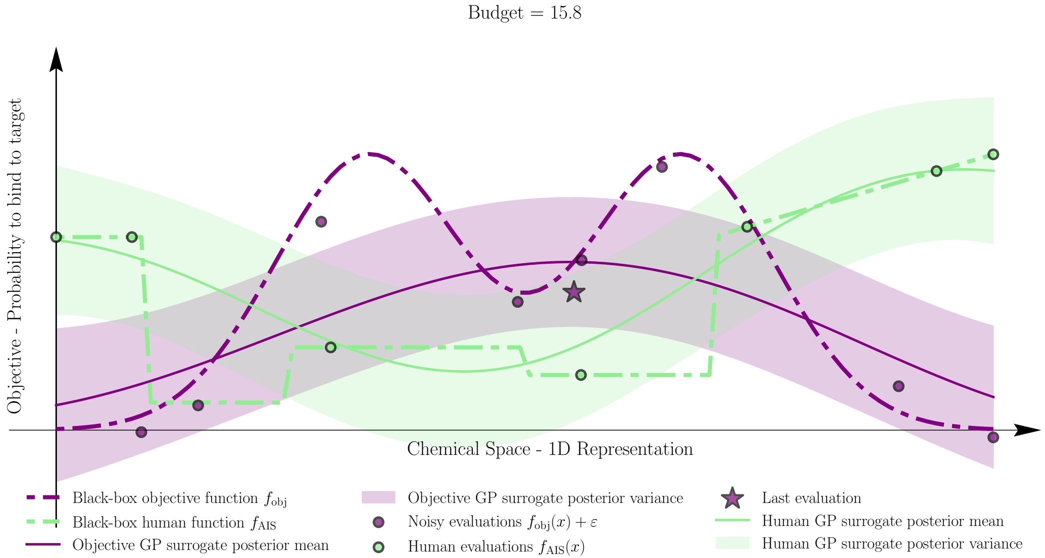

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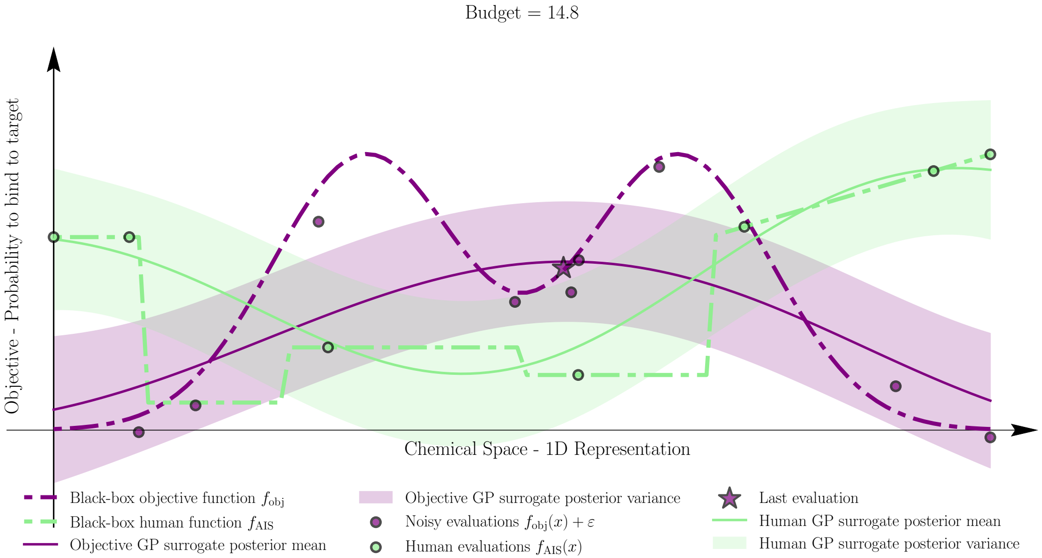

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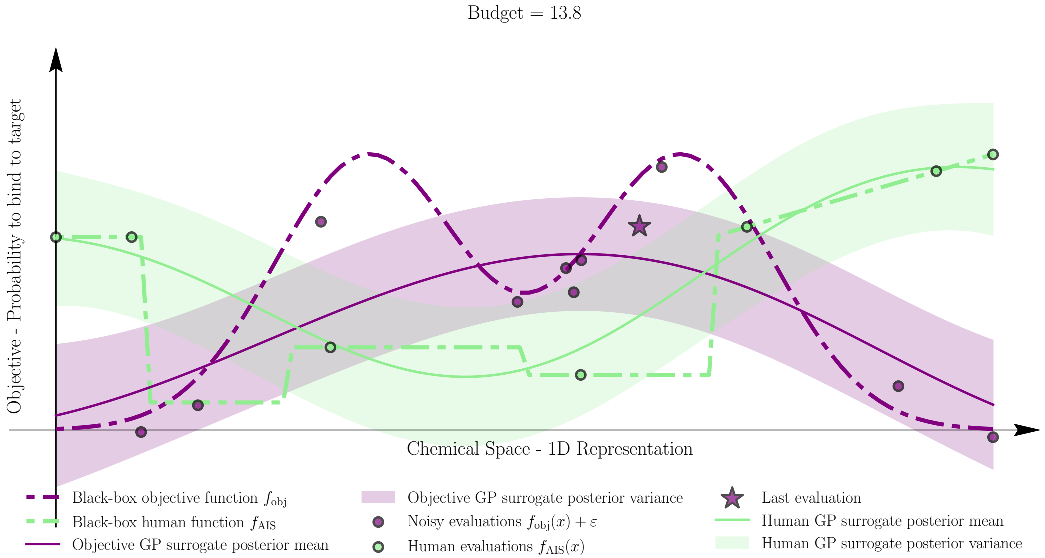

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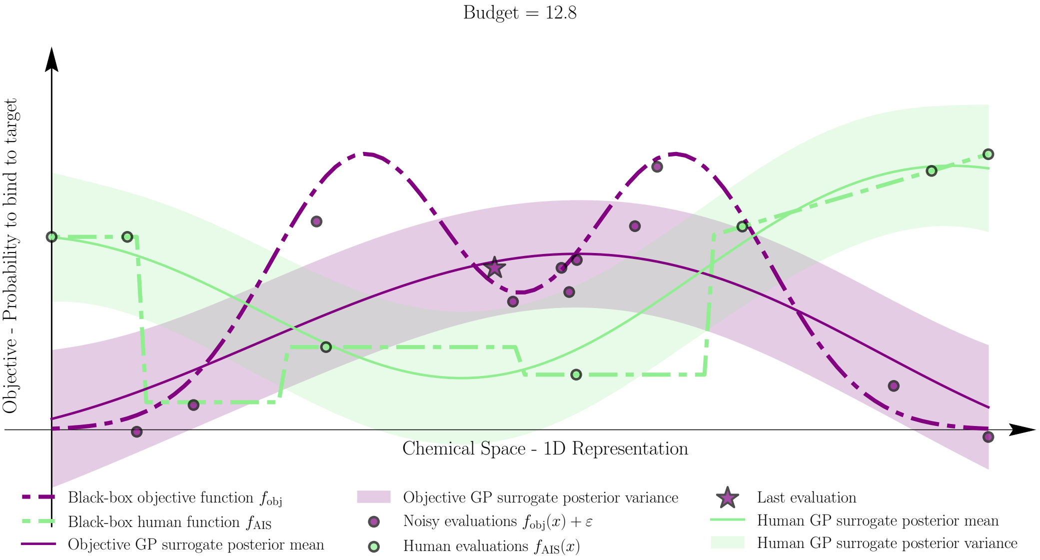

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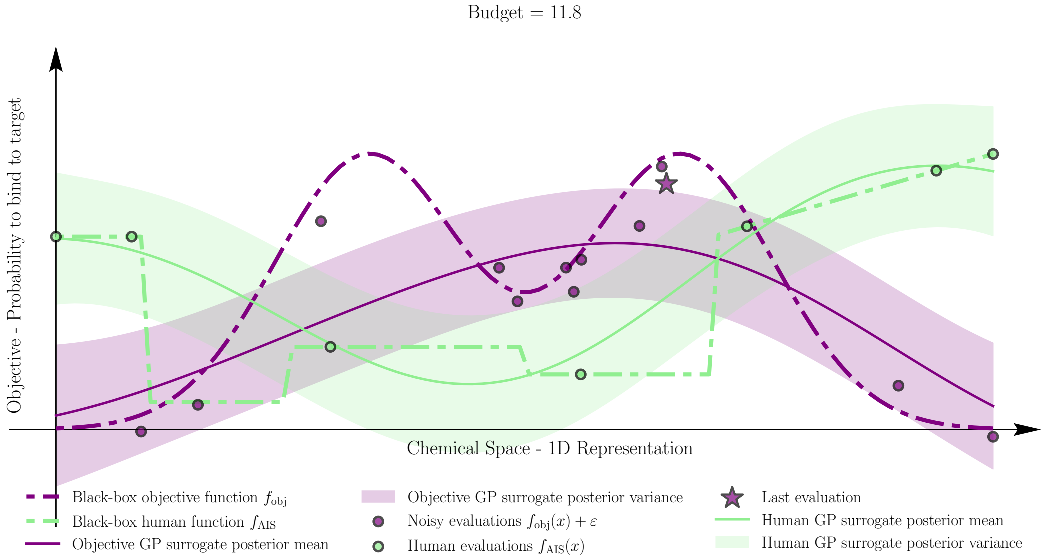

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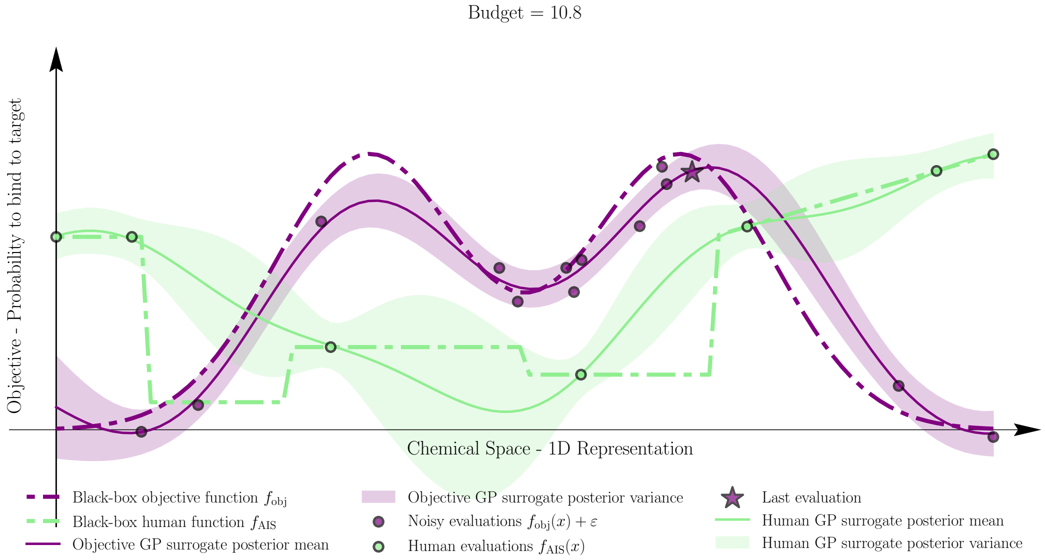

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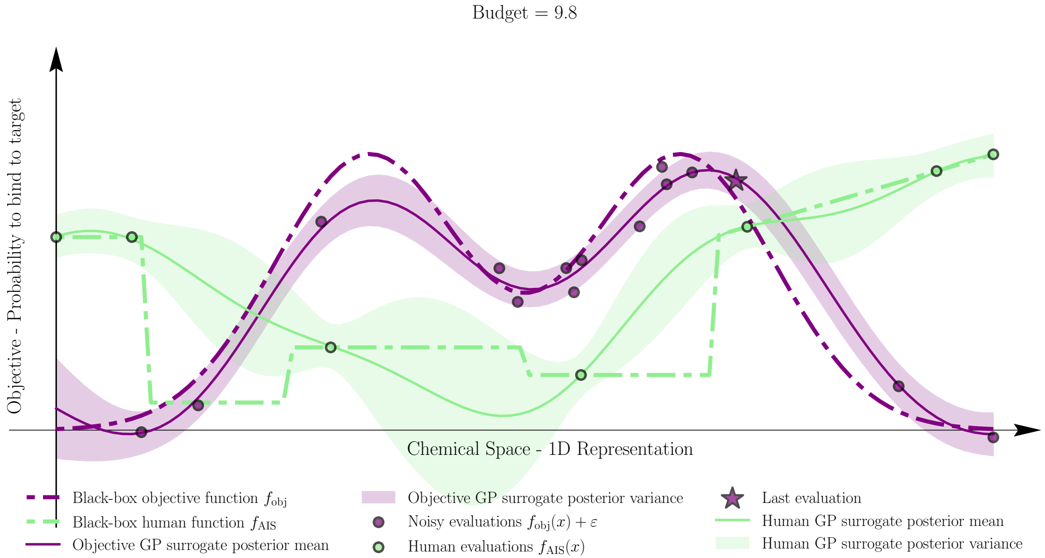


A 6D case: the Hartmann problem

For $A, P \in \mathscr{M}_{4,6}(\mathbb{R})$ two matrices, $\mathrm{x} \in [0,1]^6$ $\ell \in [0,1]$, we define

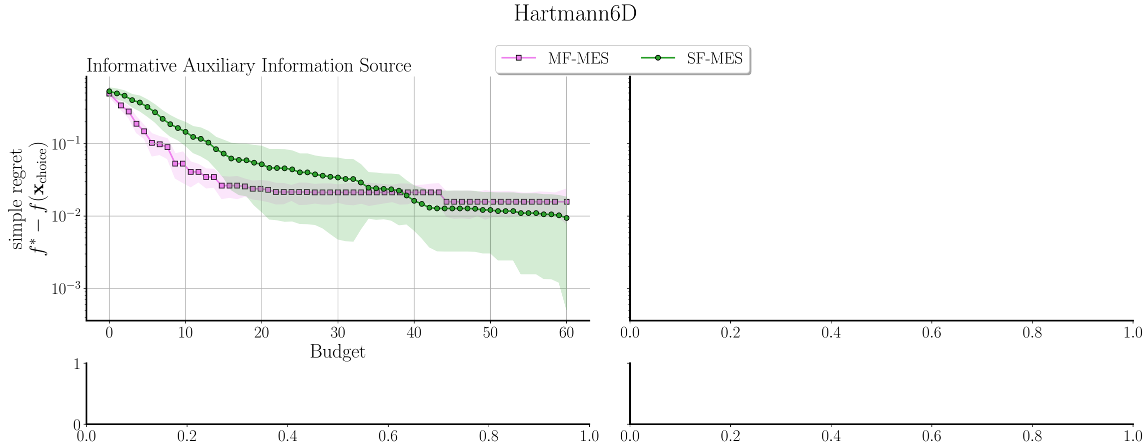
$$f^{(\ell)}(\mathrm{x}) = -\sum_{i=1}^{4} \alpha_i \exp\left(-\sum_{j=1}^{6} A_{ij}(x_j - P_{ij})\right)$$

$$\alpha = (1.0 - 0.1(1-\ell), 1.2, 3.0, 3.2)^T$$

The objective is $f^{(1)}$, with query cost $\lambda_{\text{obj}} = 1$. BO is performed in 3 scenarios, using:

- Only $f^{(1)}$ (Single-Fidelity BO)
- $f^{(1)}$ and an **informative** AIS: $f^{(0.2)}$, $\lambda_{\text{AIS}} = 0.2$ (Multi-Fidelity BO)
- $f^{(1)}$ and an **irrelevant** AIS: $f(\mathrm{x}) = \sum_{i=1}^{5}\left(100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2\right)$, $\lambda_{\text{AIS}} = 0.2$

Multi-Fidelity BO is not robust to unreliable Information Sources



- SF-MES: Single-Fidelity BO w/ Maximum Entropy Search Acquisition Function
- MF-MES: Multi-Fidelity BO w/ Maximum Entropy Search Acquisition Function

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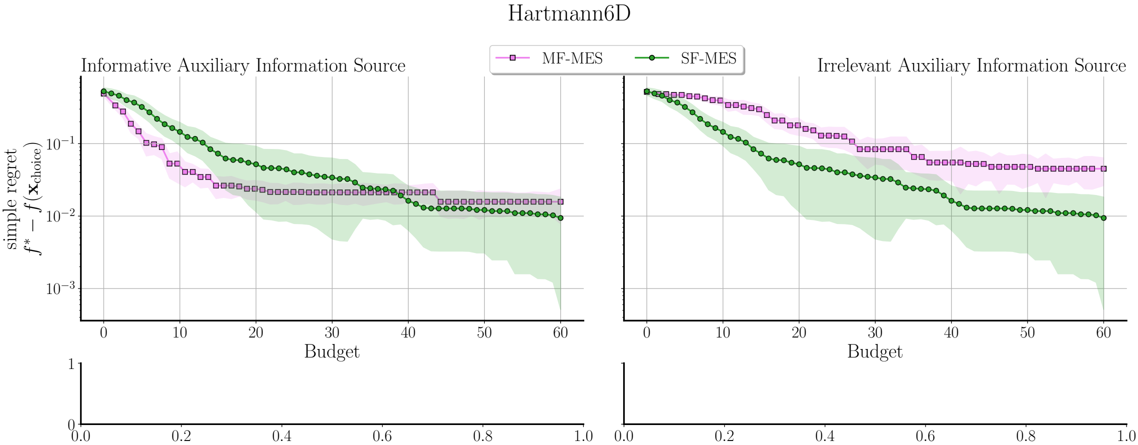

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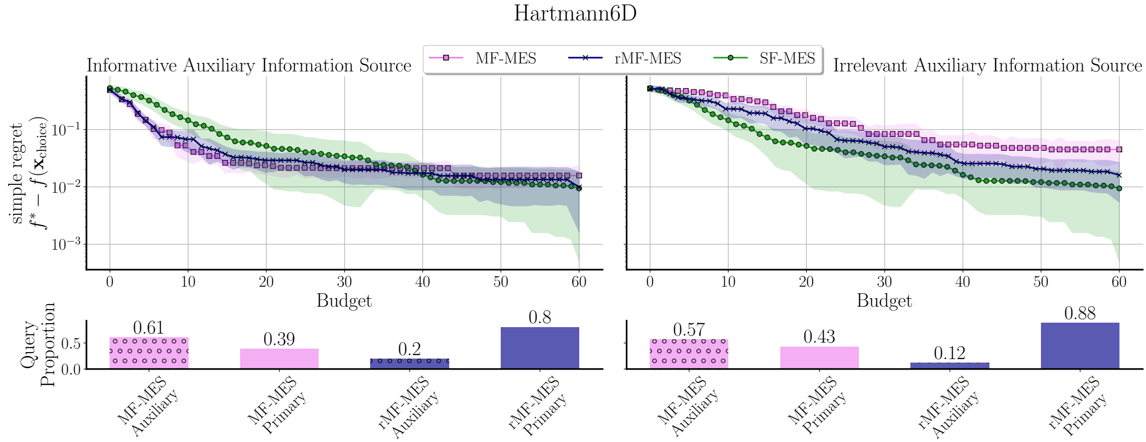

- Main aim of our contribution: **robustness** to irrelevant AIS...
- ...While still accelerating convergence for relevant AIS

Introducing robust MFBO (rMFBO)

We modify the BO loop with a **building block added on top of any** MFBO method

- Two separate GPs: $\mu_{\mathsf{SF}}, \sigma_{\mathsf{SF}}$ using objective queries only $\mathscr{D}^{\mathsf{pSF}}$, and a MOGP $\mu_{\mathsf{MF}}, \sigma_{\mathsf{MF}}$ using $\mathscr{D}^{\mathsf{MF}}$

$$(\mathrm{x}_t^{\mathsf{MF}}, \ell_t) = \underset{\mathrm{x}\in\mathscr{X}, \ell\in\{\mathsf{obj}, \mathsf{AIS}\}}{\operatorname{argmax}} \alpha(\mathrm{x}, \ell | \mu_{\mathsf{MF}}, \sigma_{\mathsf{MF}}, \mathscr{D}^{\mathsf{MF}})$$

$$(\mathrm{x}_t^{\mathsf{pSF}}, \mathsf{obj}) = \underset{\mathrm{x}\in\mathscr{X}}{\operatorname{argmax}}\, \alpha(\mathrm{x} | \mu_{\mathsf{SF}}, \sigma_{\mathsf{SF}}, \mathscr{D}^{\mathsf{pSF}})$$

- $\sigma_{\mathsf{MF}}(\mathrm{x}_t^{\mathsf{pSF}}, \mathsf{obj}) \leq c_1$ $\longrightarrow$ do I trust my joint model at the objective?
- $s(\mathrm{x}_t^{\mathsf{MF}}, \ell_t) \geq c_2$ $\longrightarrow$ is my joint model suggestion informative enough?

- Upon satisfaction: query $(\mathrm{x}_t^{\mathsf{MF}}, \ell_t)$ and add *pseudo-observation* of objective: $\mathscr{D}^{\mathsf{pSF}} \leftarrow (\mathrm{x}_t^{\mathsf{pSF}}, \mu_{\mathsf{MF}}(\mathrm{x}_t^{\mathsf{pSF}}, \mathsf{obj}))$ $\longrightarrow$ what if we had queried the objective?
- Otherwise, query $(\mathrm{x}_t^{\mathsf{pSF}}, \mathsf{obj})$

Theorem: rMFBO regret can be tied to that of SFBO

Assumptions:

- f_{obj} is drawn from a GP with zero-mean and covariance function $\kappa(\mathrm{x}, \mathrm{x}')$
- κ is known and at least twice differentiable
- $\mathbb{P}\left(\sup_{\mathrm{x} \in \mathscr{X}} \left|\frac{\partial f_{\text{obj}}}{\partial x_j}\right| > L\right) \leq a e^{-(L/b_j)^2}, \quad \forall\ j \in [\![d]\!]$ for $a, b_j > 0$ (satisfied for RBF kernel)
- The acquisition function is twice differentiable

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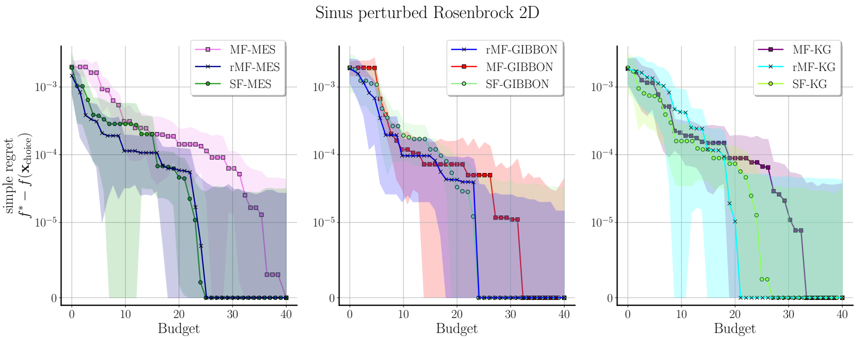
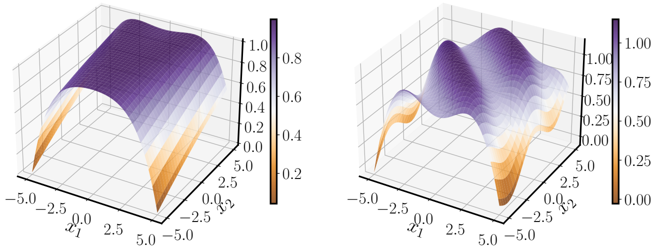
Theorem: $R(\Lambda, \mathrm{x}_T^{\text{rMF}}) \leq R(\Lambda, \mathrm{x}_T^{\text{SF}}) + \varepsilon \max\left\{T \hat{M}_T d^{T+1}, 2\right\}$ w/ prob $\geq q\left(1 - da \exp(-\frac{1}{b^2})\right)$

$c_1(\varepsilon, q) = \frac{\varepsilon}{\sqrt{-2\log(1-q)}}$. Theorem does not depend on c_2.

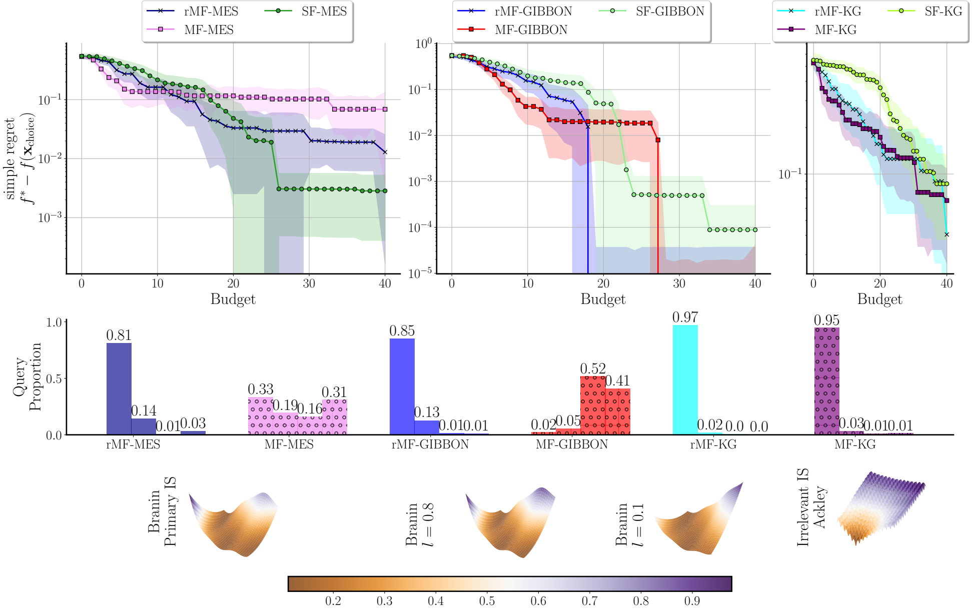
For any AIS, the difference in regrets achieved by SFBO and rMFBO can be bounded.

Results on 2D case





Multiple Information Sources of varying relevance - 2D case



Perspectives

For the method itself:

- Theoretical insights on how to set hyperparameter c_2
- Try against more joint models

From an applied point of view:

- Carry user studies
- Concrete application with human experts