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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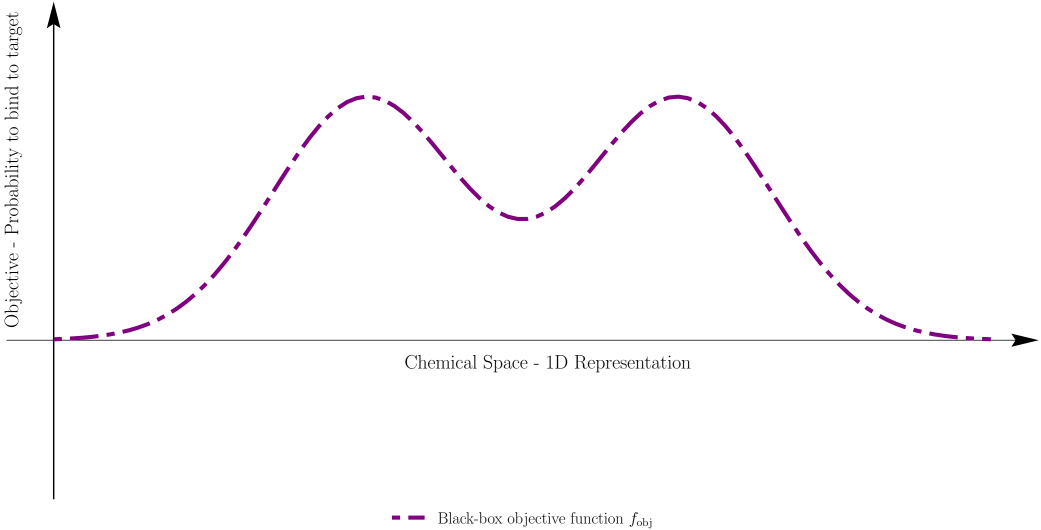

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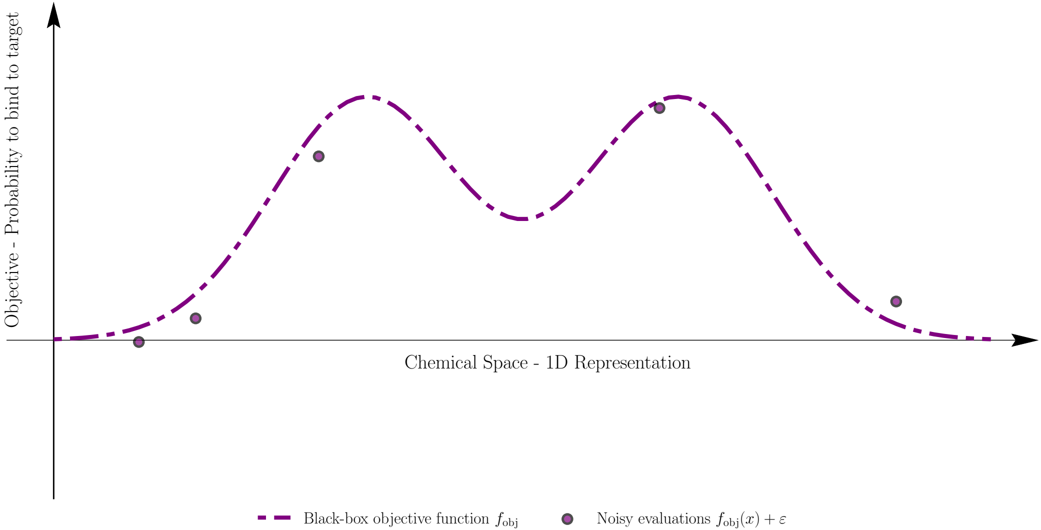

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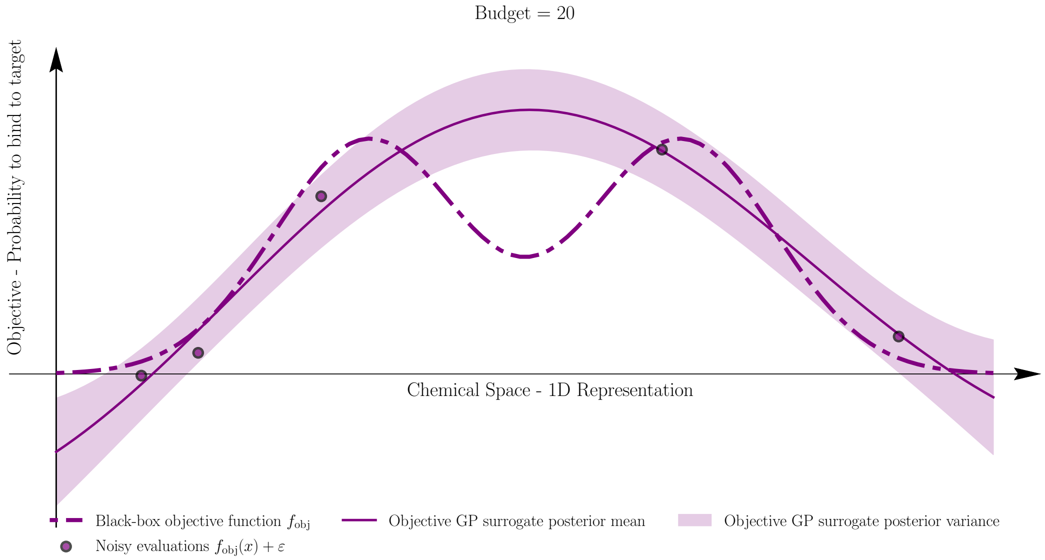

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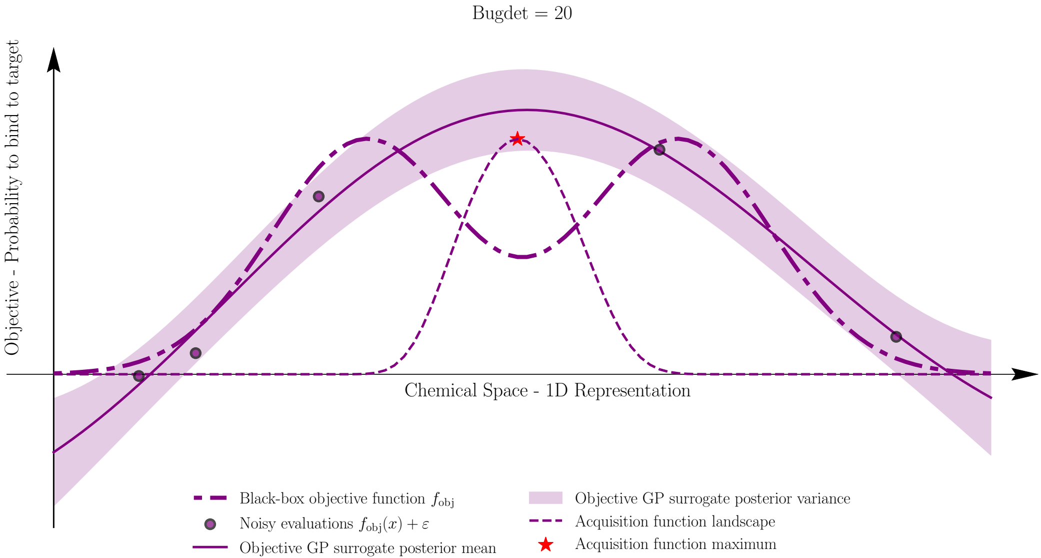

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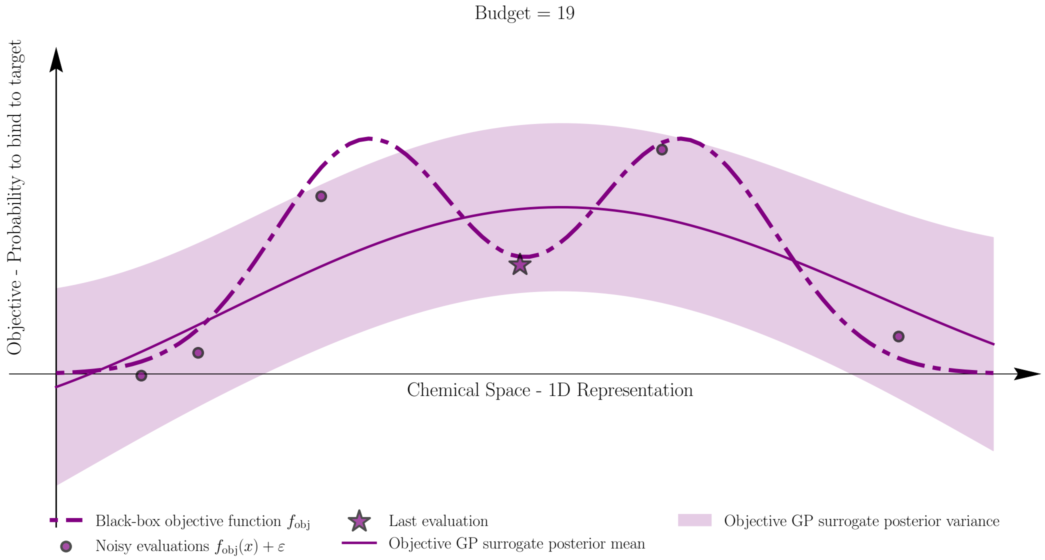

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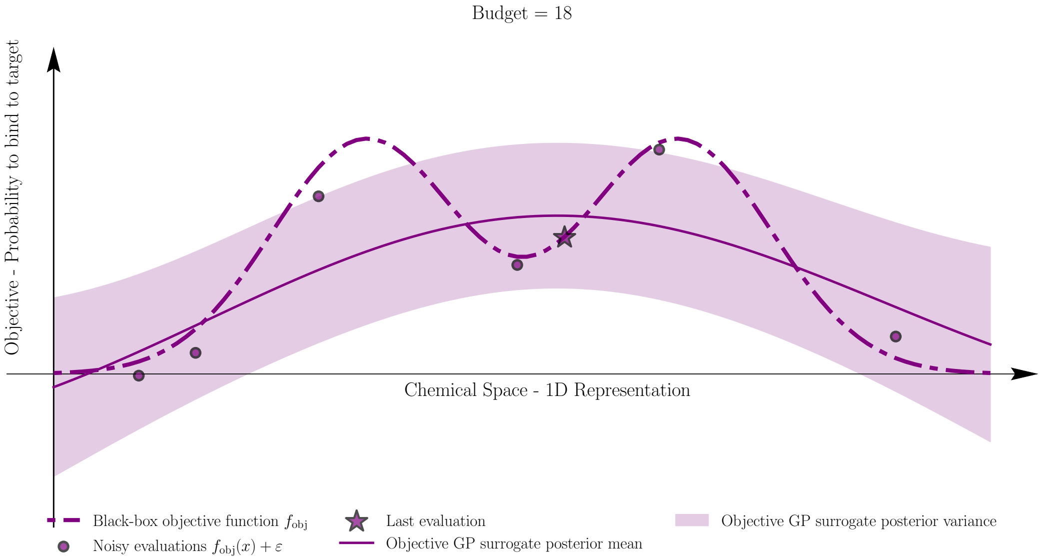

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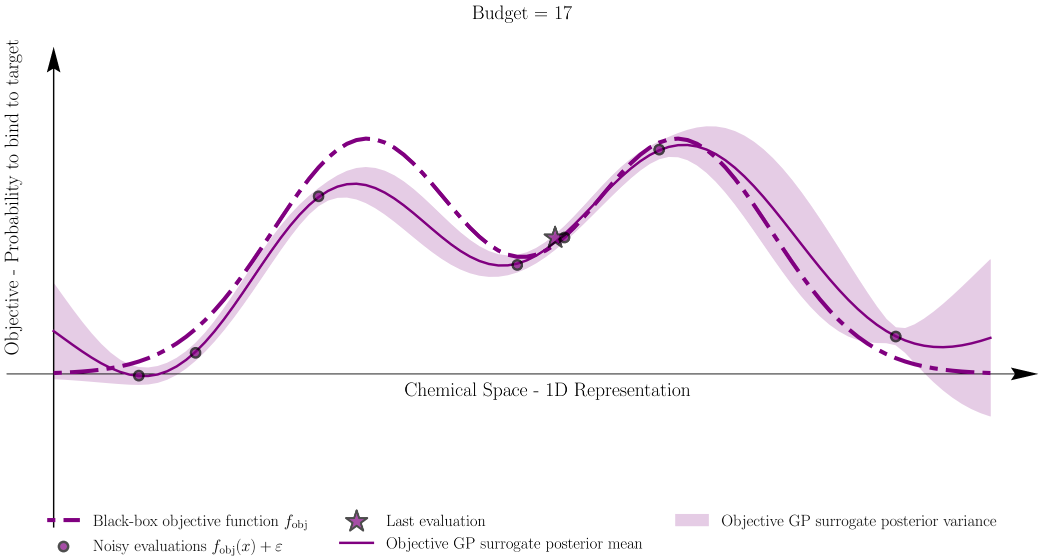

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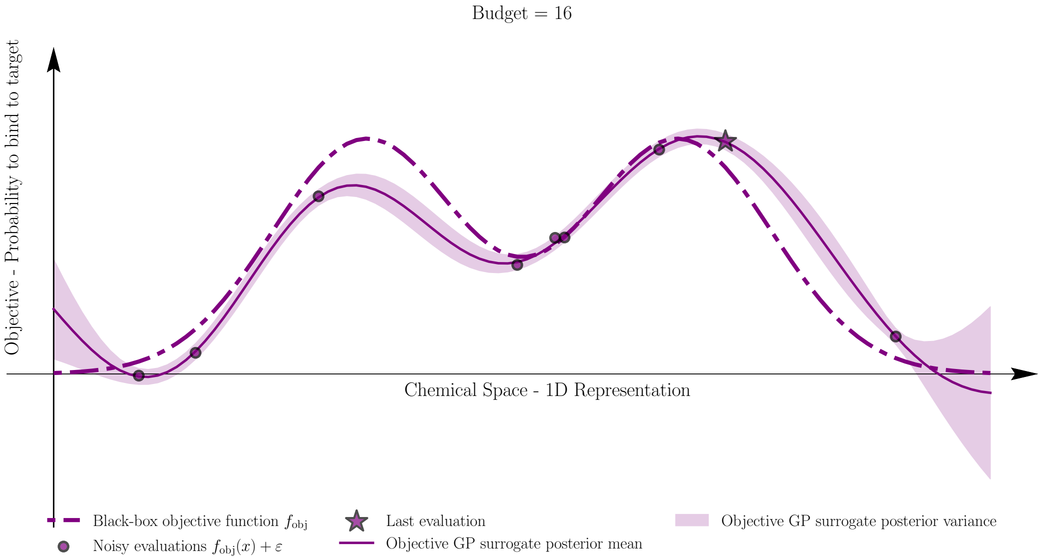

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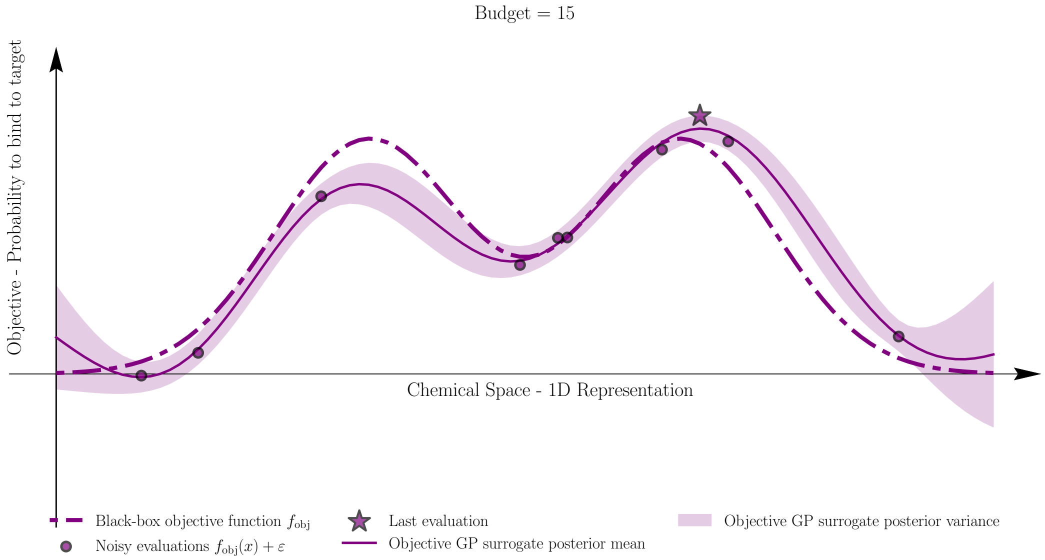

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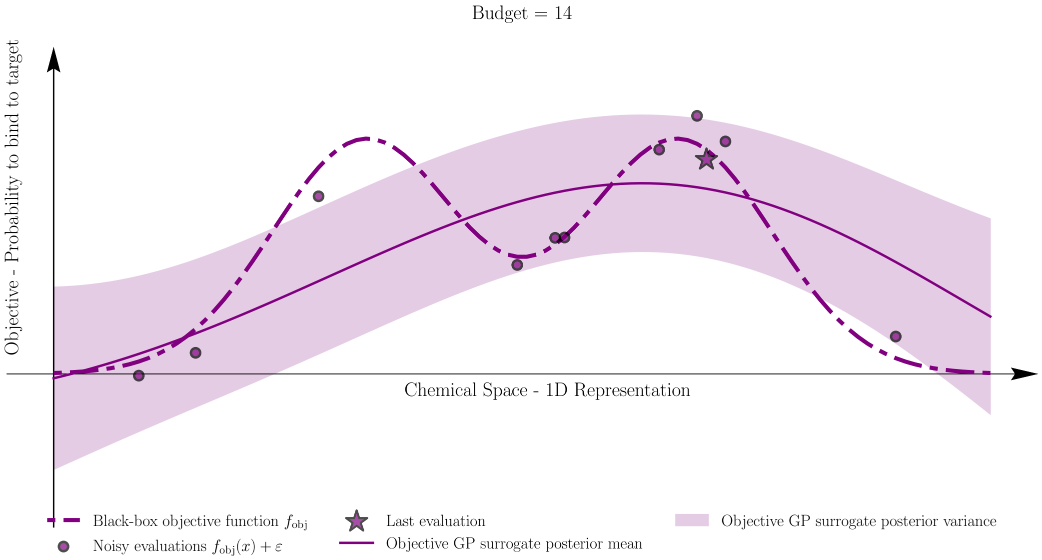

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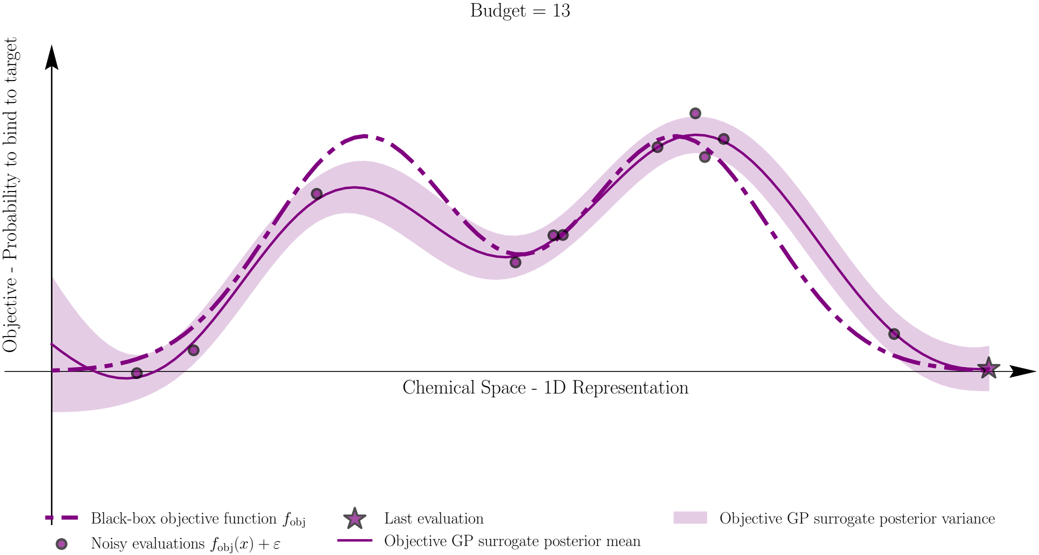

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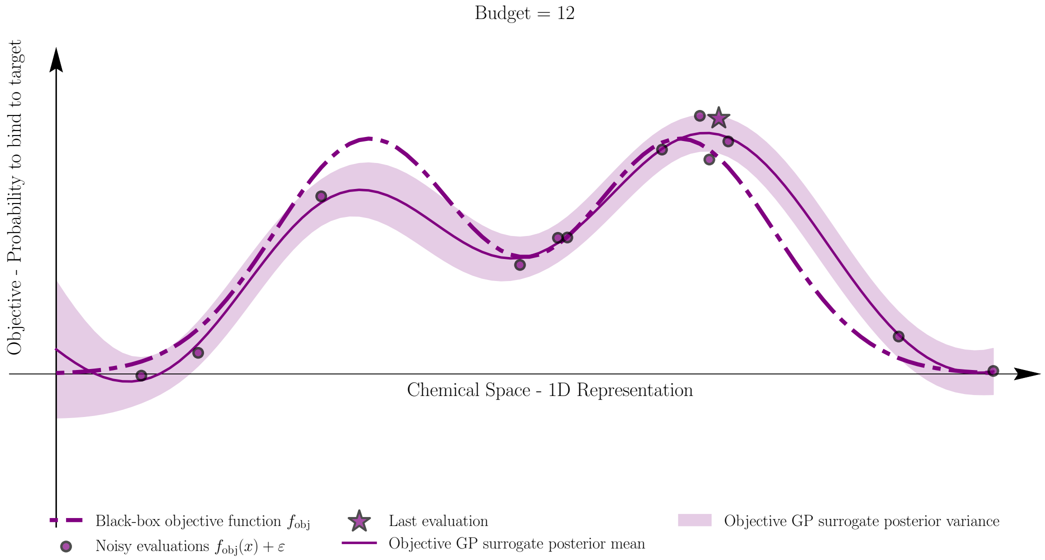
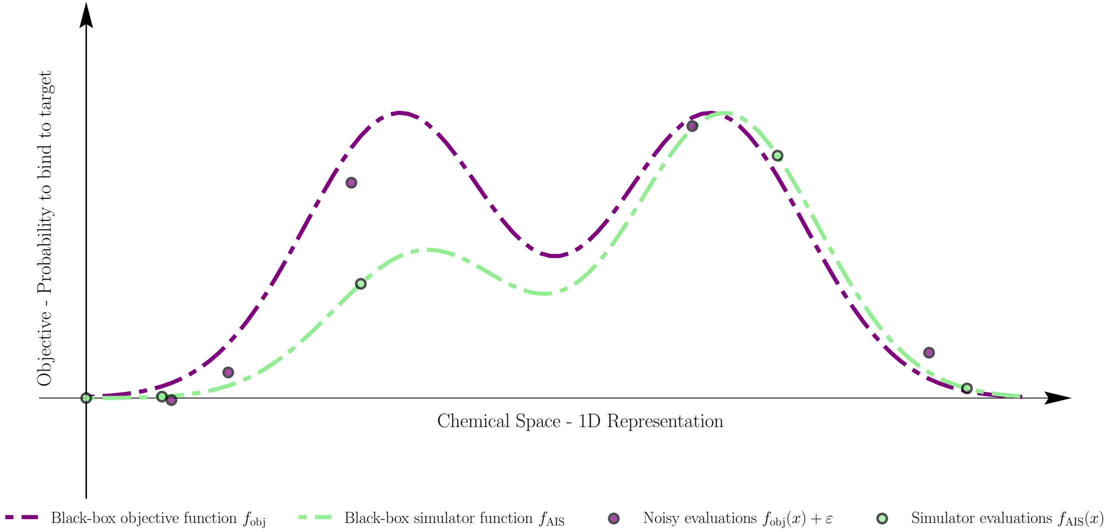


Multi Fidelity Bayesian Optimization 101



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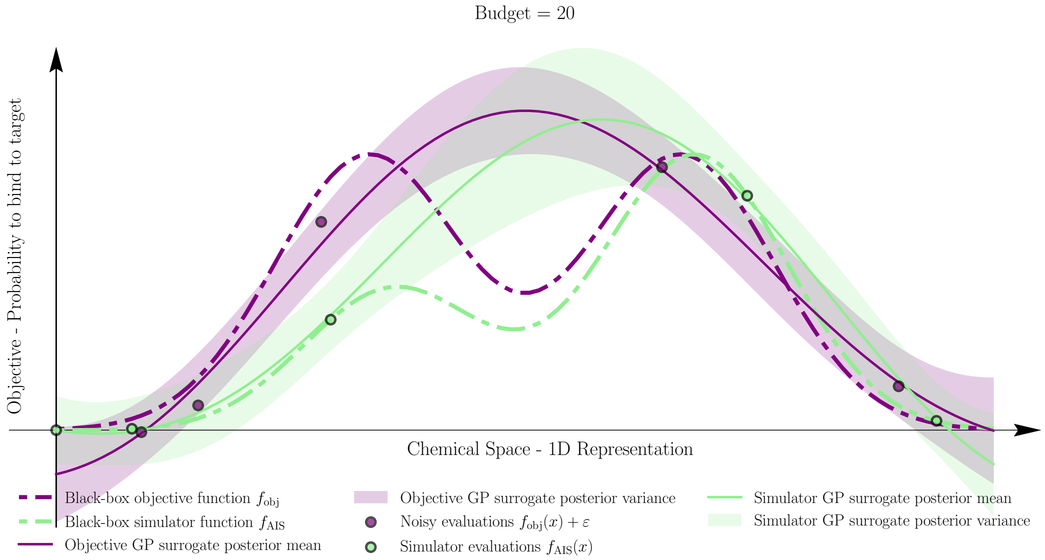

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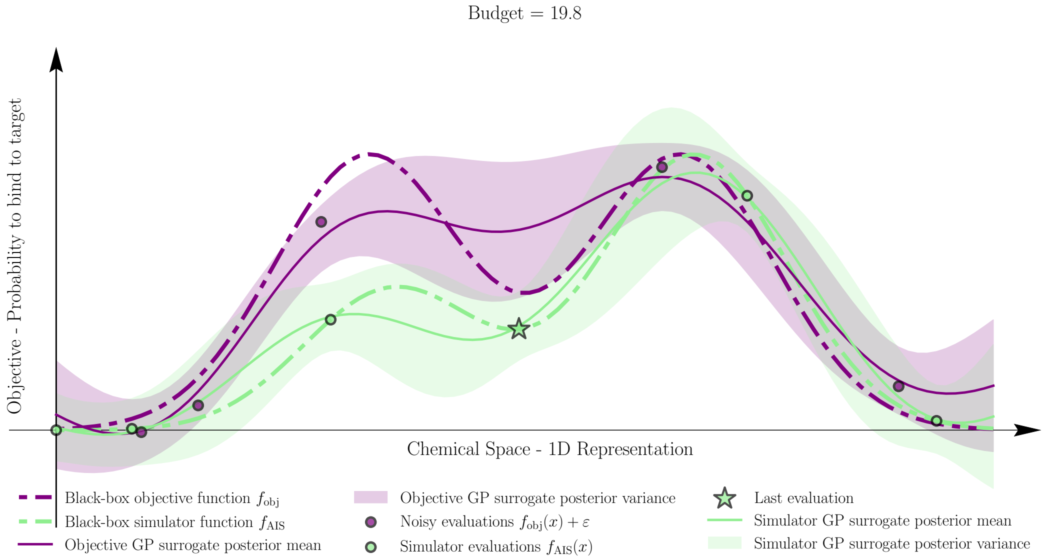

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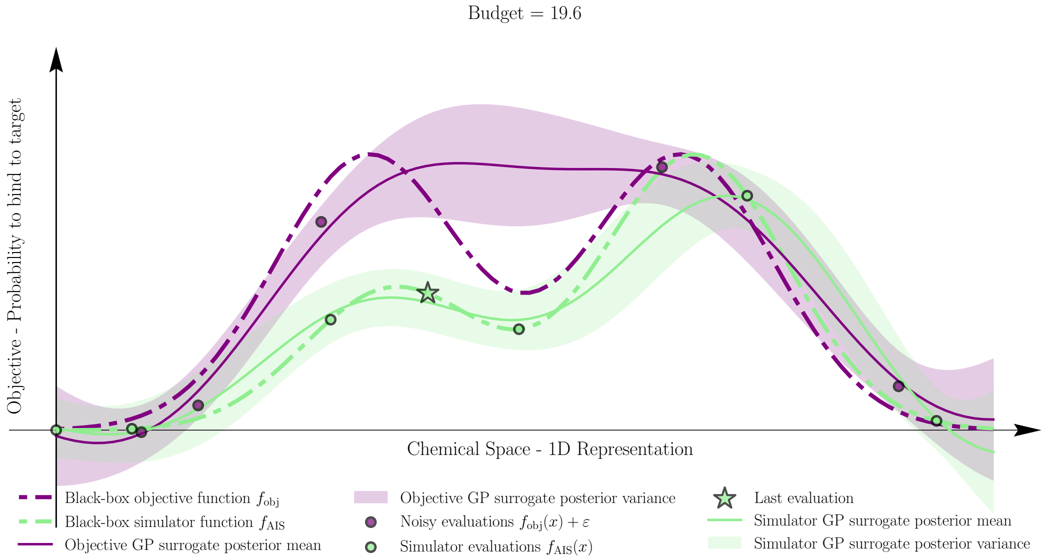

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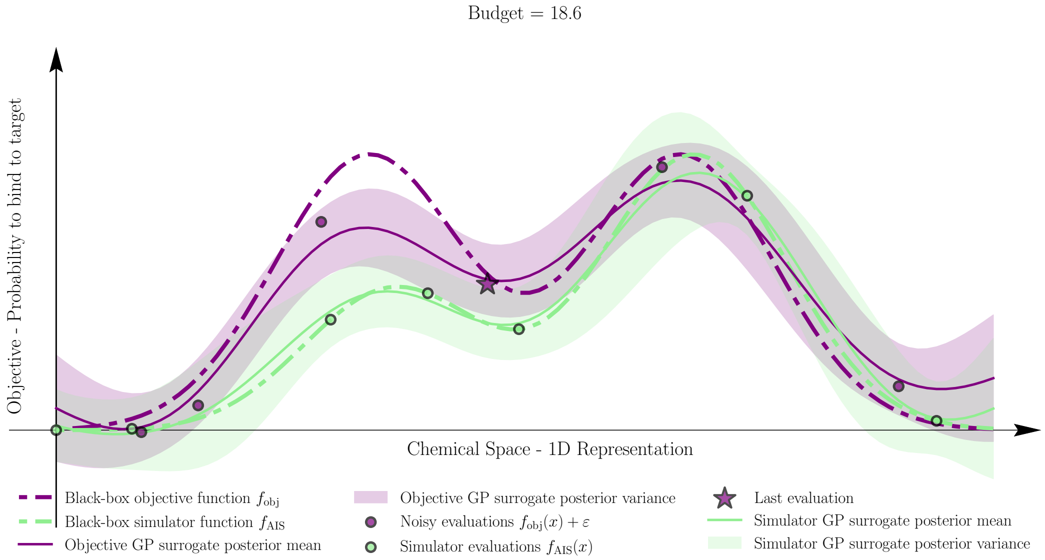

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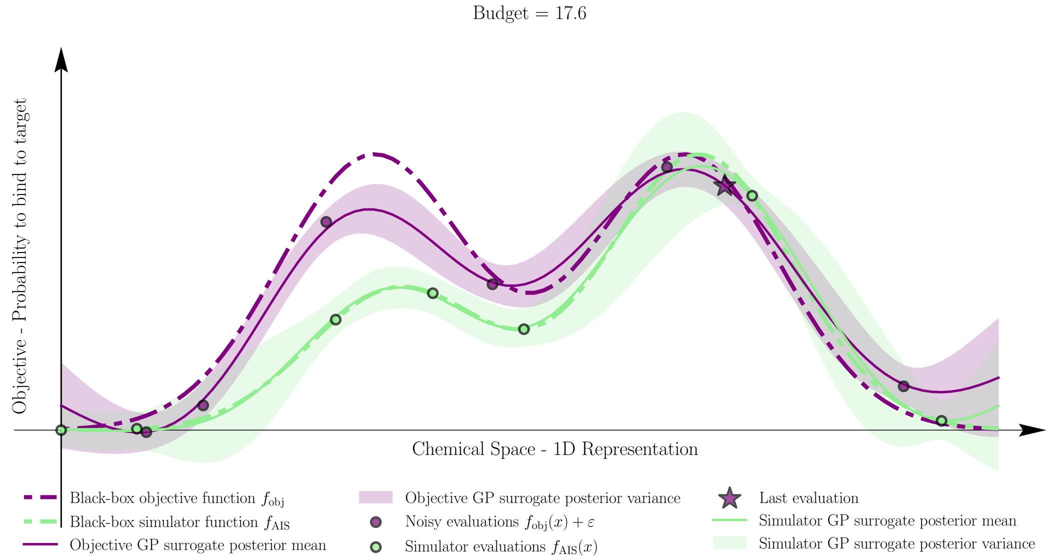

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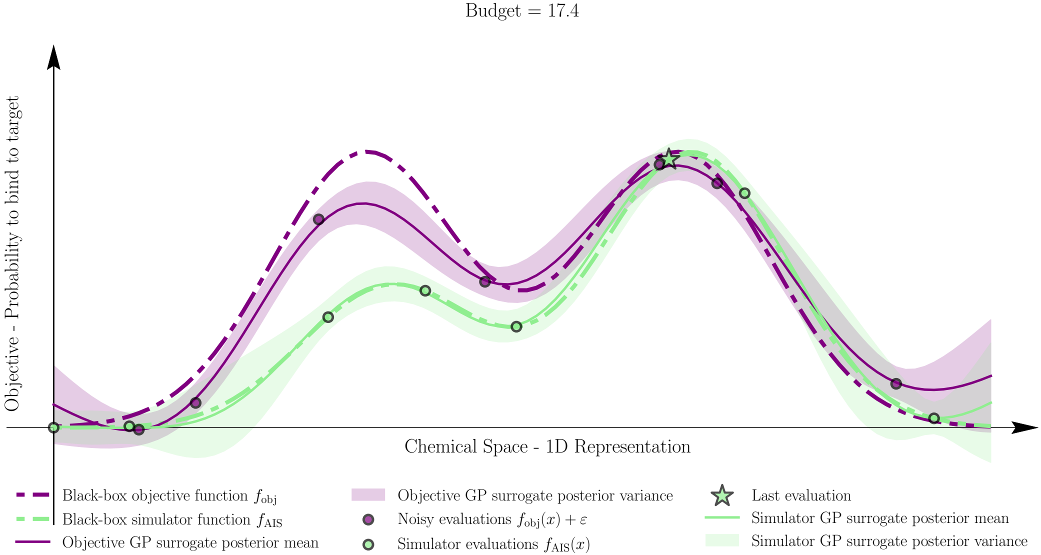

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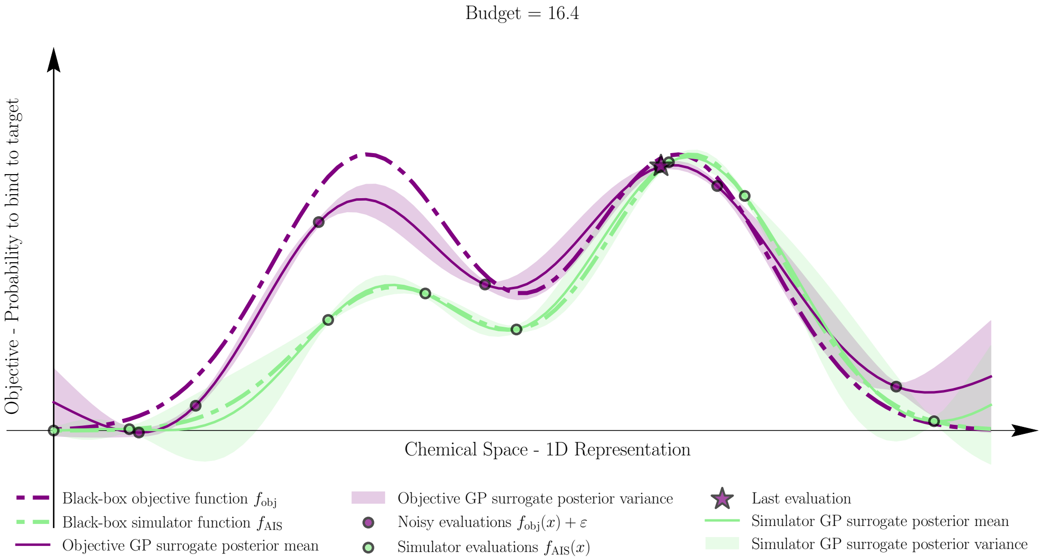

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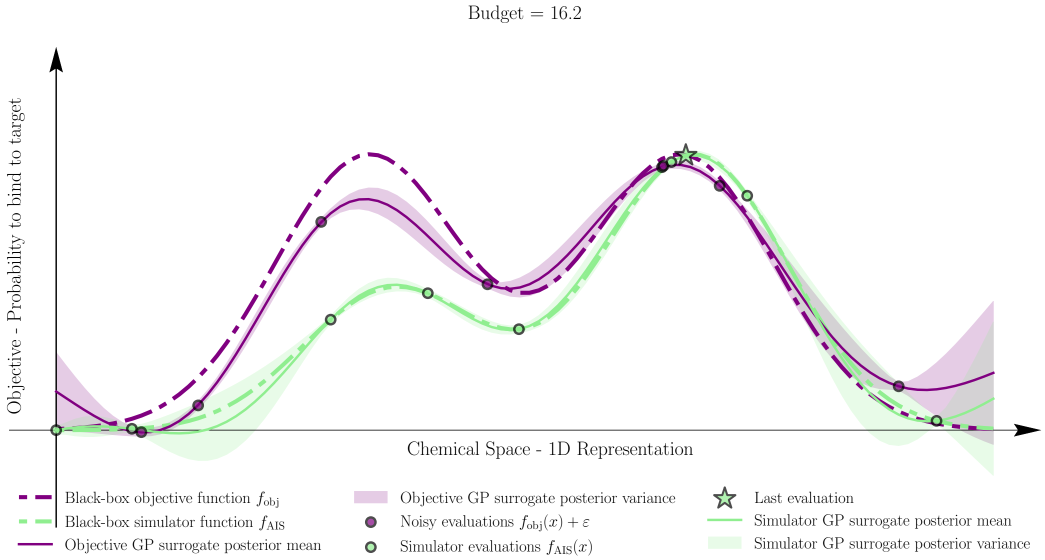

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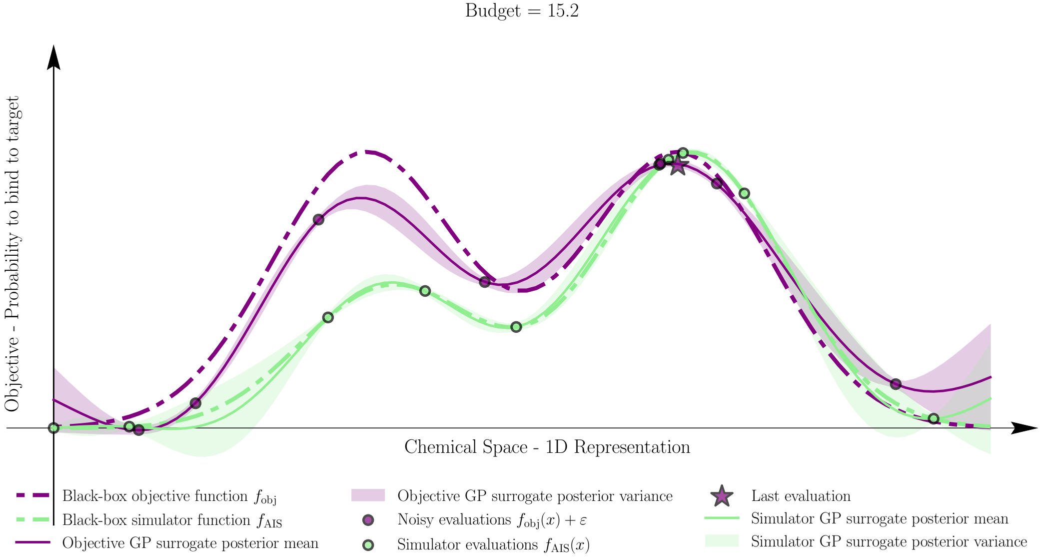
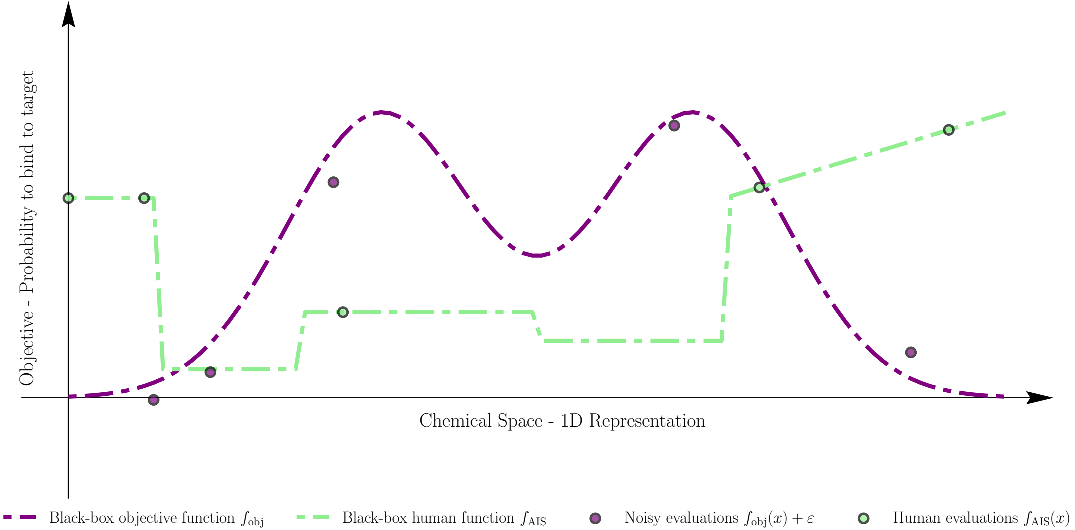


Multi Fidelity Bayesian Optimization with Unreliable Sources



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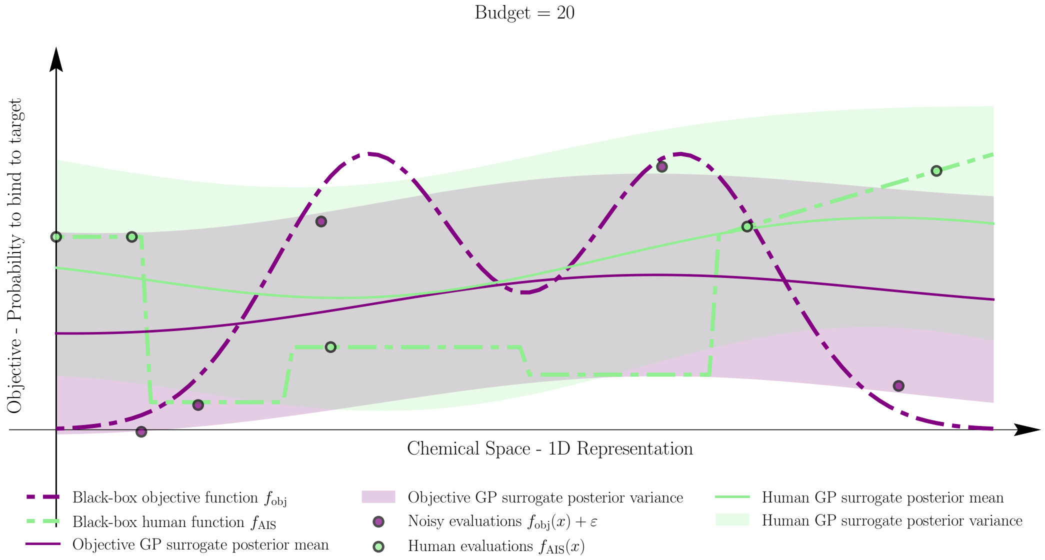

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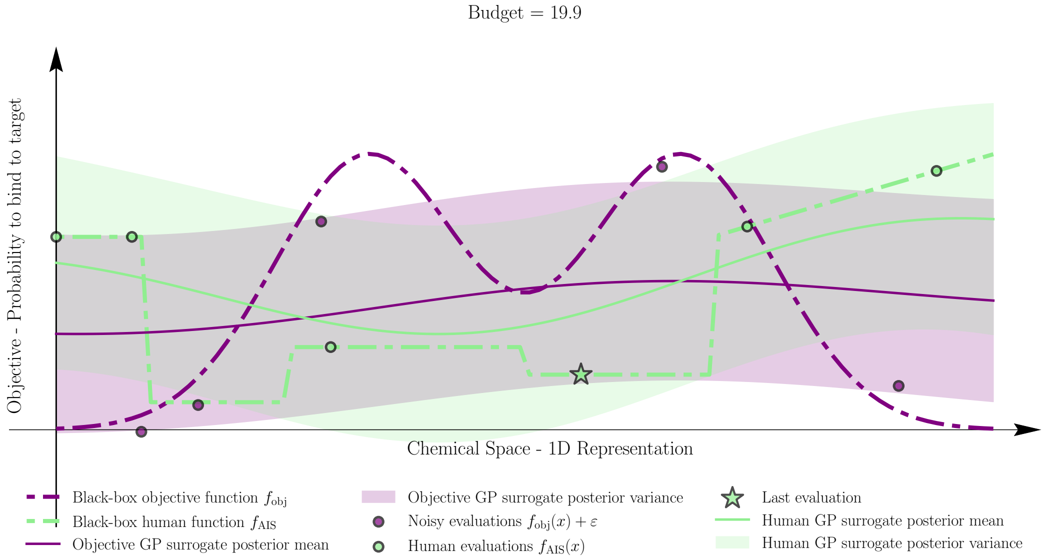

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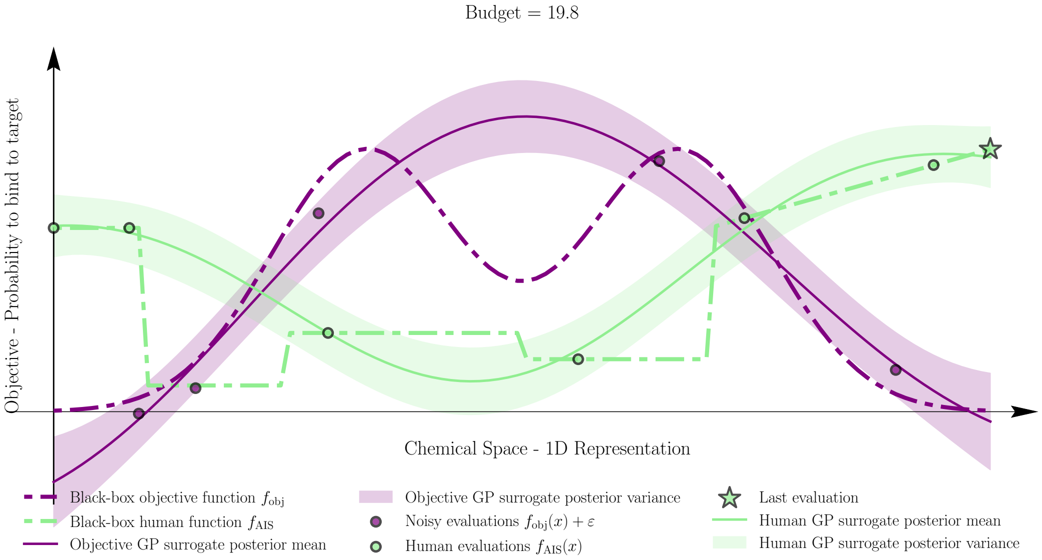

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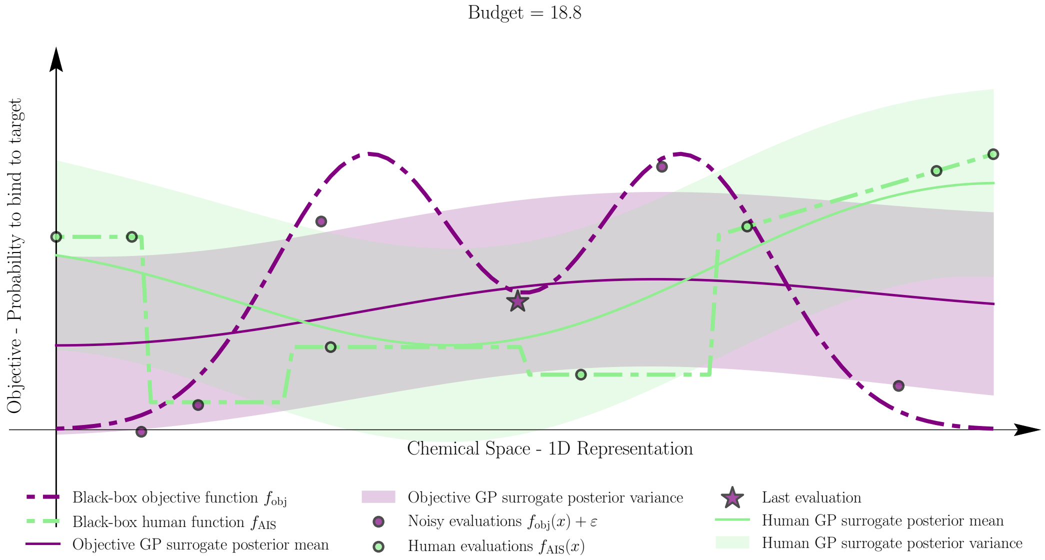

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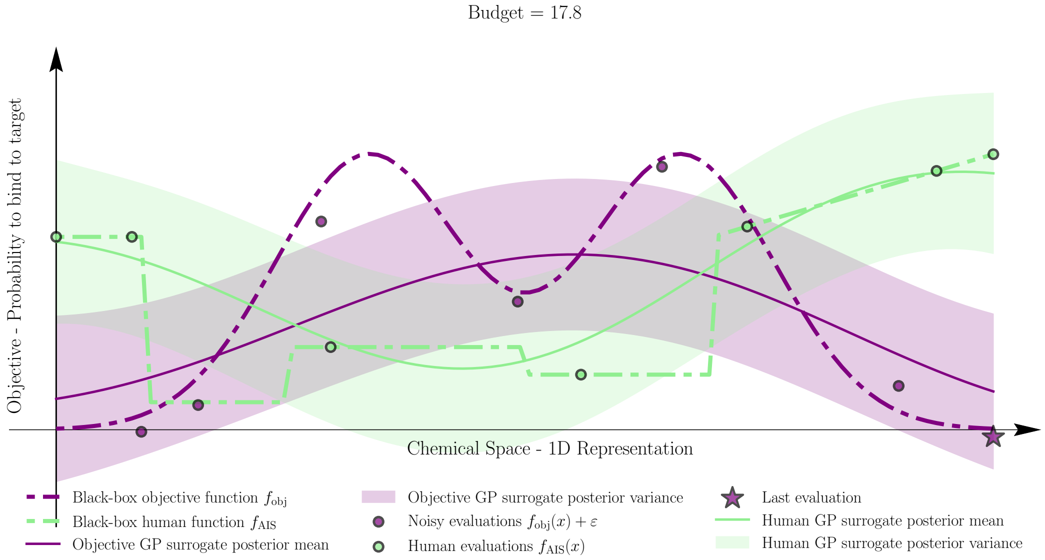

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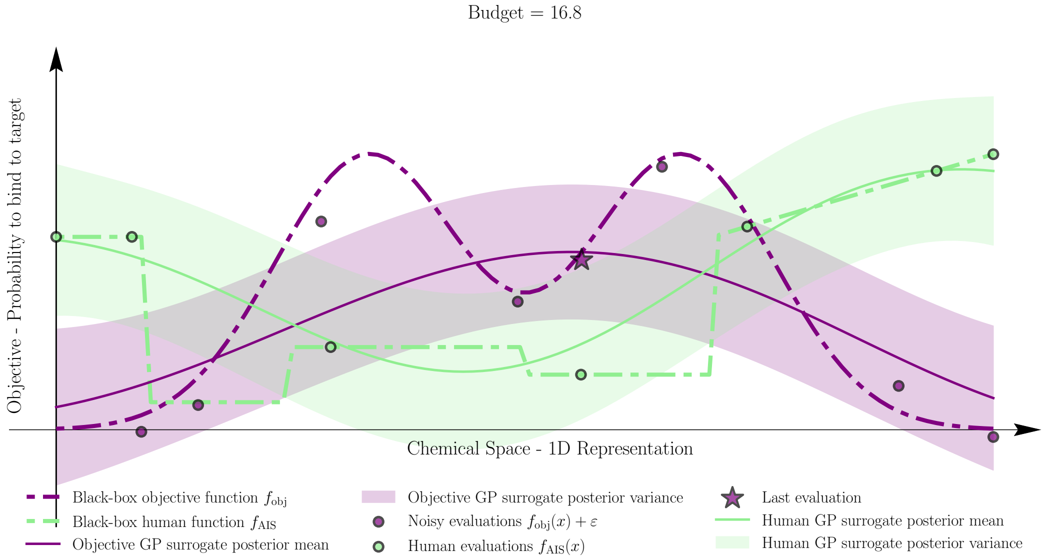

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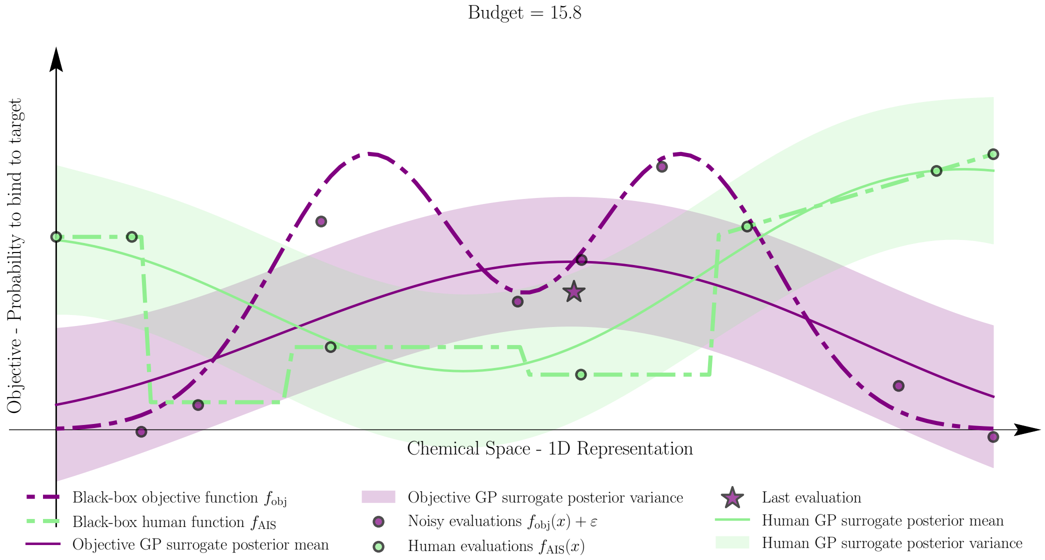

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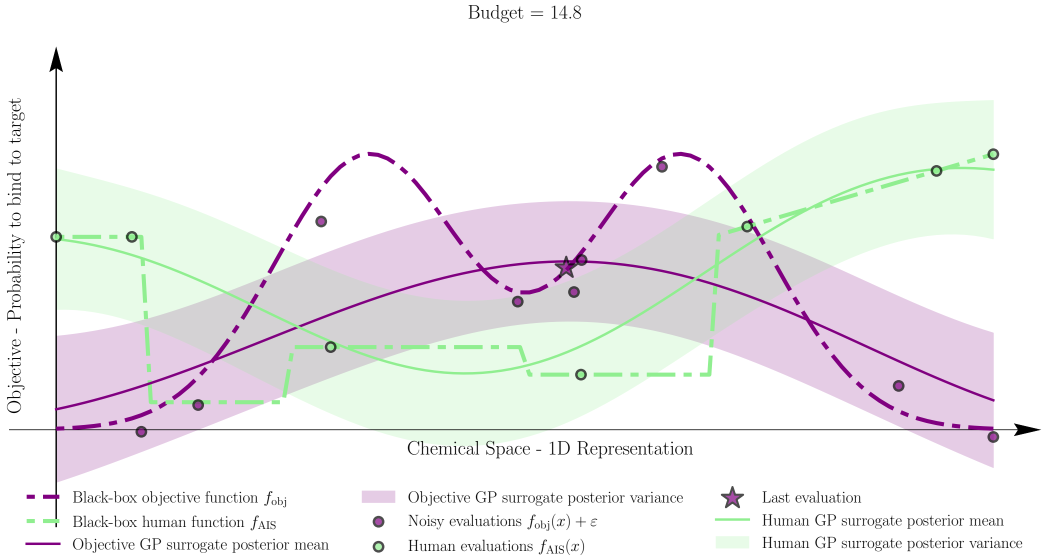

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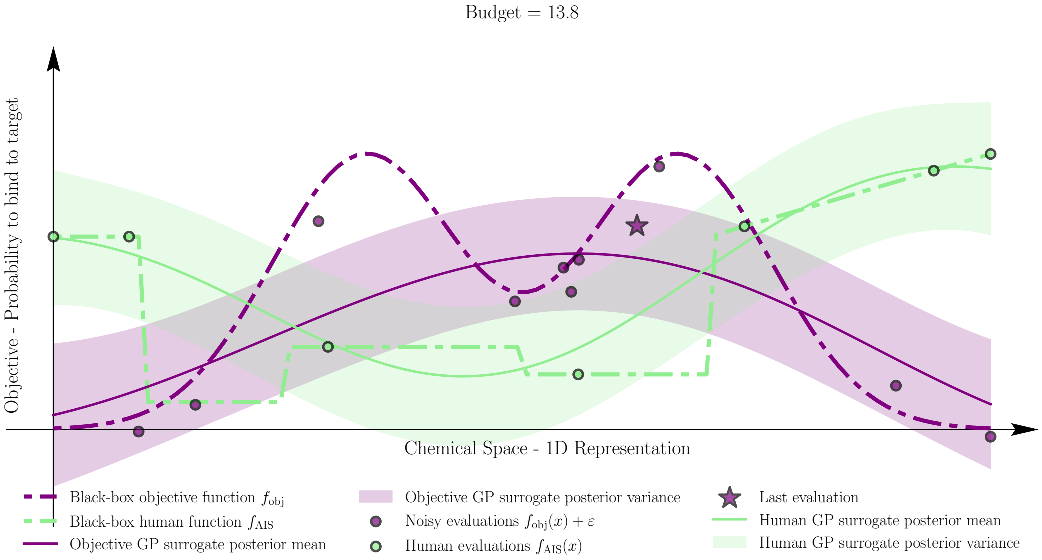

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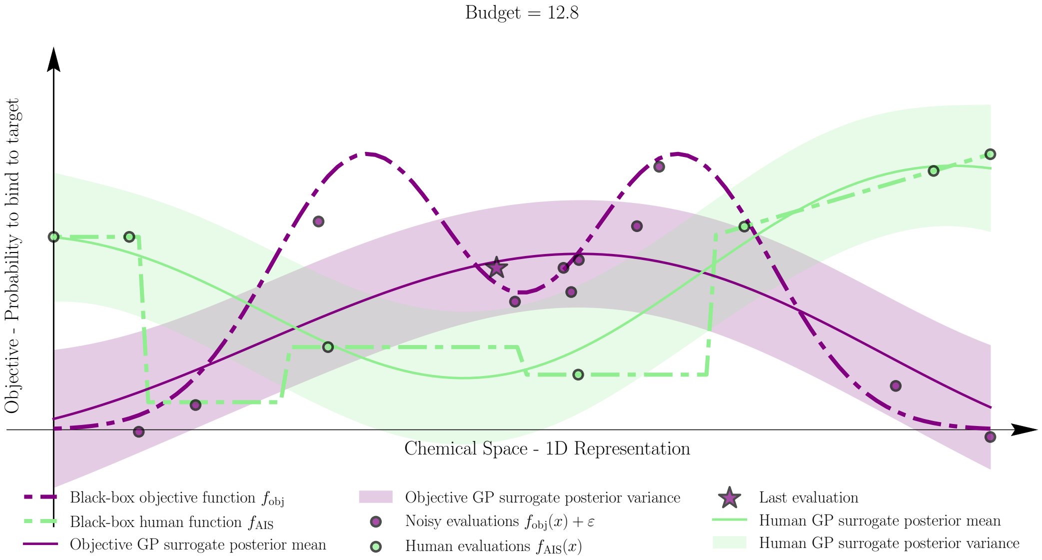

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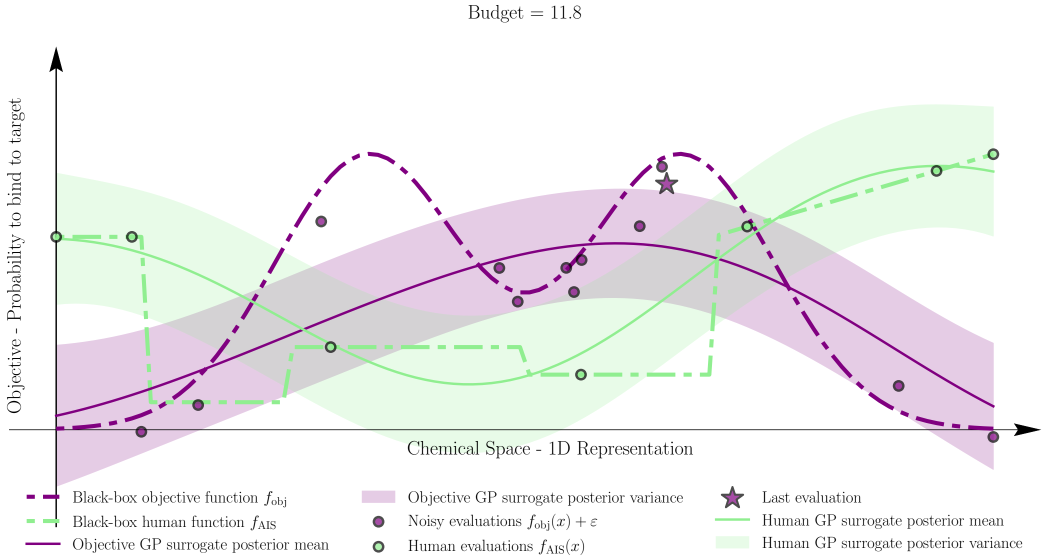

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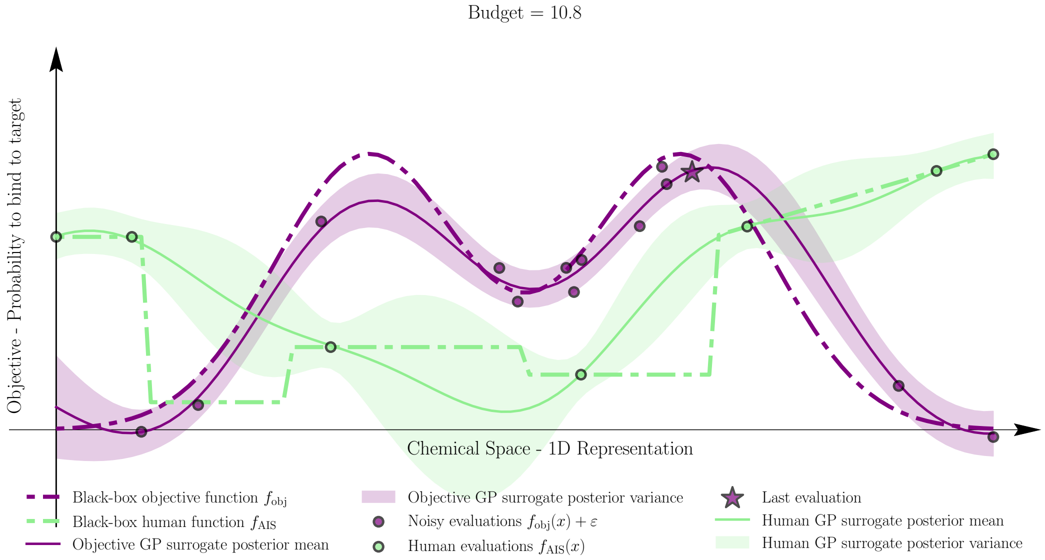
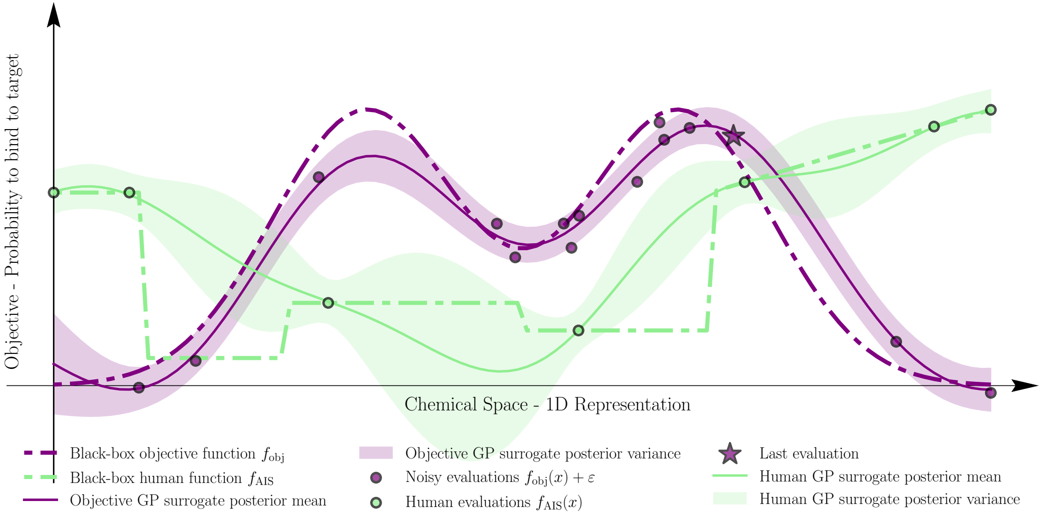
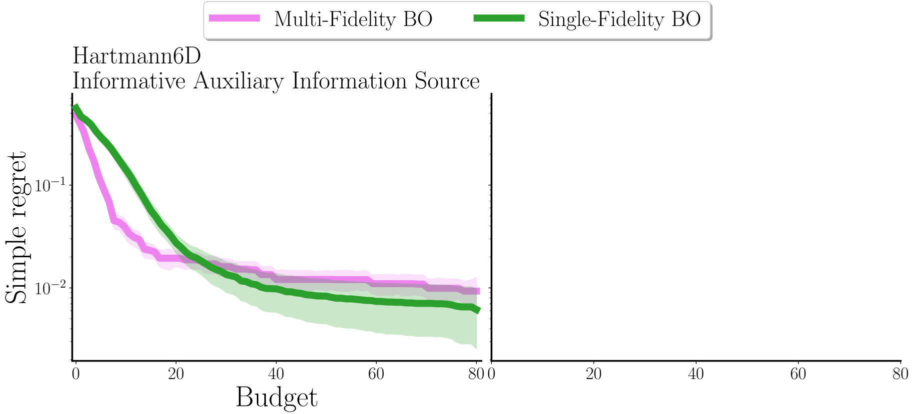


Multi Fidelity Bayesian Optimization with Unreliable Sources

Budget = 9.8



Multi-Fidelity BO is not robust to unreliable Information Sources



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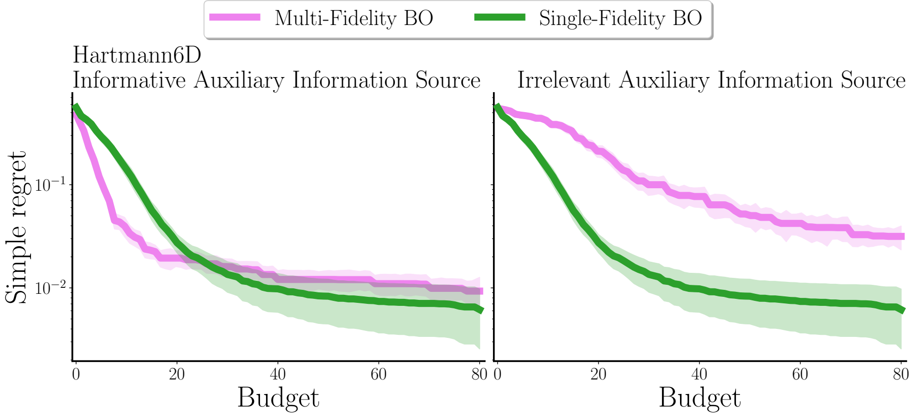

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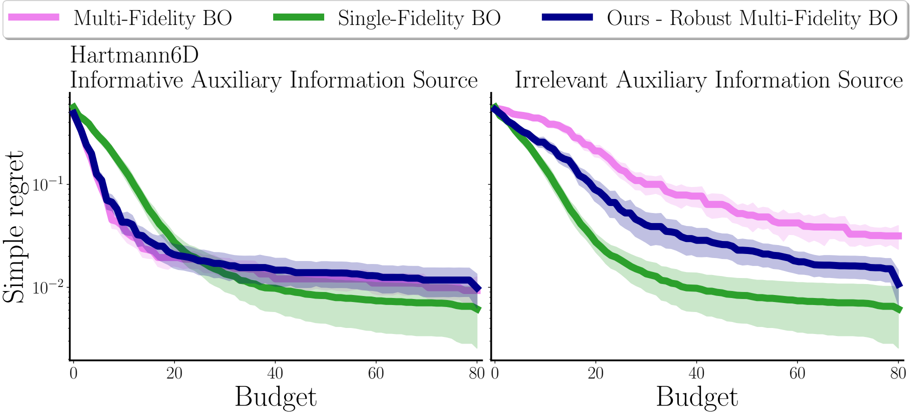

Not far from a well-known problem in transfer learning: **negative transfer**

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

Introducing robust MFBO (rMFBO)

- In a nutshell, carry MFBO ... **BUT** ...
- ...Keep track of what would have looked like the acquisition trajectory without AIS using a single-output GP $\Longrightarrow$ **HOW?**

At iteration t, choose between two queries:

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

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

If $\sigma_{\mathsf{MF}}(\mathrm{x}_t^{\mathsf{pSF}}, \mathsf{obj}) \leq c_1 \Longrightarrow$ joint model reliable at $\mathrm{x}_t^{\mathsf{pSF}}$, i.e. $\mu_{\mathsf{MF}}^{\mathsf{obj}}\left(\mathrm{x}_t^{\mathsf{pSF}}\right) \approx f^{\mathsf{obj}}\left(\mathrm{x}_t^{\mathsf{pSF}}\right)$

Therefore $\mathscr{D}^{\mathsf{pSF}} \leftarrow \left(\mathrm{x}_t^{\mathsf{pSF}}, \mu_{\mathsf{MF}}^{\mathsf{obj}}\left(\mathrm{x}_t^{\mathsf{pSF}}\right)\right)$: creating a *pseudo* single fidelity track

Summary

$$\sigma_{\mathsf{MF}}(\mathsf{x}_t^{\mathsf{pSF}}, \mathsf{obj}) \leq c_1 \implies \begin{cases} \text{pick } (\mathsf{x}_t^{\mathsf{MF}}, \ell_t) \\ \mathscr{D}^{\mathsf{MF}} \leftarrow (\mathsf{x}_t^{\mathsf{MF}}, f^{(\ell_t)}(\mathsf{x}_t^{\mathsf{MF}})) \\ \mathscr{D}^{\mathsf{pSF}} \leftarrow (\mathsf{x}_t^{\mathsf{pSF}}, \mu_{\mathsf{MF}}^{\mathsf{obj}}(\mathsf{x}_t^{\mathsf{pSF}})) \end{cases}$$

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because $\mathrm{x}_t^{\mathsf{pSF}}$ only brings little information

Summary

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Ensures pseudo-queries added to SFBO are trustworthy: **unreliable case**

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Summary

$\sigma_{\mathrm{MF}}(\mathrm{x}_t^{\mathrm{pSF}}, \mathrm{obj}) \leq c_1 \implies \begin{cases} \text{pick } (\mathrm{x}_t^{\mathrm{MF}}, \ell_t) \\ \mathscr{D}^{\mathrm{MF}} \leftarrow (\mathrm{x}_t^{\mathrm{MF}}, f^{(\ell_t)}(\mathrm{x}_t^{\mathrm{MF}})) \\ \mathscr{D}^{\mathrm{pSF}} \leftarrow (\mathrm{x}_t^{\mathrm{pSF}}, \mu_{\mathrm{MF}}^{\mathrm{obj}}(\mathrm{x}_t^{\mathrm{pSF}})) \end{cases}$

Ensures pseudo-queries added to SFBO are trustworthy: **unreliable case**

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If not satisfied:

1. Pick $(\mathrm{x}_t^{\mathrm{pSF}}, \mathrm{obj})$
2. $\mathscr{D}^{\mathrm{MF}} \leftarrow \left(\mathrm{x}_t^{\mathrm{pSF}}, f^{\mathrm{obj}}\left(\mathrm{x}_t^{\mathrm{pSF}}\right)\right)$
3. $\mathscr{D}^{\mathrm{pSF}} \leftarrow \left(\mathrm{x}_t^{\mathrm{pSF}}, f^{\mathrm{obj}}\left(\mathrm{x}_t^{\mathrm{pSF}}\right)\right)$

$\mathscr{D}^{\mathrm{pSF}}$ and $\mathscr{D}^{\mathrm{SF}}$ only differ at the points where we inputted $\mu_{\mathrm{MF}}^{\mathrm{obj}}(\mathrm{x}_t^{\mathrm{pSF}})$!

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 twice differentiable
- $\mathbb{P}\left(\sup_{\mathrm{x} \in \mathcal{X}} \left| \frac{\partial f^{\text{obj}}}{\partial x_j} \right| > L \right) \leq a e^{-(L/b_j)^2} \quad \forall\ j \in \{1, \dots, d\}$, for $a, b_j > 0$

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Theorem:

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

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No assumption on the amount of information that f^{AIS} can provide about f^{obj}!

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

$c_1(\varepsilon, q) = \frac{\varepsilon}{\sqrt{-2\log(1-q)}}.$

Interested? Have a look at the paper ¯_(ツ)_/¯

Petrus Mikkola, **Julien Martinelli**, Louis Filstroff, Samuel Kaski
Multi-Fidelity Bayesian Optimization with Unreliable Sources. AISTATS 2023.

Some stuff (continued) ¯_(ツ)_/¯

$$k_{\mathsf{MISO}}((\mathrm{x},\ell),(\mathrm{x}',\ell')) = \begin{cases} k_{\mathsf{input}}(\mathrm{x},\mathrm{x}') + k_{\ell}(\mathrm{x},\mathrm{x}') & \ell = \ell' \neq 1 \\ k_{\mathsf{input}}(\mathrm{x},\mathrm{x}') & \text{otherwise} \end{cases}$$

$$k_{\mathsf{LT}}((\mathrm{x},\ell),(\mathrm{x}',\ell')) = \begin{cases} k_{\mathsf{input}}(\mathrm{x},\mathrm{x}') + (1-\ell)(1-\ell')k_{\mathsf{IS}}(\mathrm{x},\mathrm{x}') & \ell \neq 1,\ \ell' \neq 1 \\ k_{\mathsf{input}}(\mathrm{x},\mathrm{x}') & \text{otherwise} \end{cases}$$

$$k_{\mathsf{DS}}((\mathrm{x},\ell),(\mathrm{x}',\ell')) = \begin{cases} ck_{\mathsf{input}}(\mathrm{x},\mathrm{x}') + (1-\ell)(1-\ell')k_{\mathsf{input}}(\mathrm{x},\mathrm{x}') & \ell \neq 1,\ \ell' \neq 1 \\ ck_{\mathsf{input}}(\mathrm{x},\mathrm{x}') & \text{otherwise} \end{cases}$$