Are Random Decompositions all we need in High-Dimensional Bayesian Optimisation?

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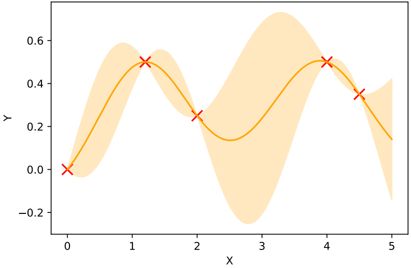
Bayesian Optimisation

- Bayesian Optimisation (BO) [Srinivas et al, 2010] aims to optimise a black-box function by using a surrogate Gaussian Process (GP) model



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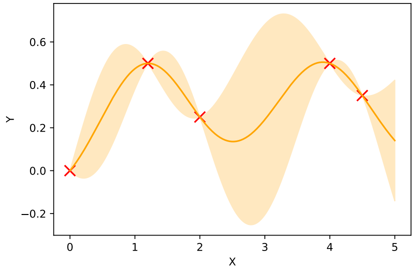

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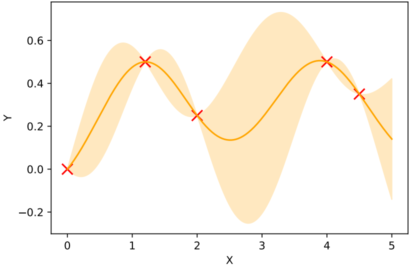

- Based on the GP model, we optimise **acqusition function** to find most promising point to query next
- This works great with a small number of dimensions; struggles in high-dimensional spaces

Bayesian Optimisation with Additive Functions

- One solution: Assume the additive function ([Kandasamy et al, 2015], [Rolland et al, 2018], [Han et al, 2021])

$$f(\boldsymbol{x}) = \sum_{c \in g} f_c(\boldsymbol{x}_{[c]})$$

for each group of dimensions c in decomposition g, for example if $g = \{(1,4),(2),(3)\}$:

$$f(x_1, x_2, x_3, x_4) = f_{1,4}(x_1, x_4) + f_2(x_2) + f_3(x_3)$$

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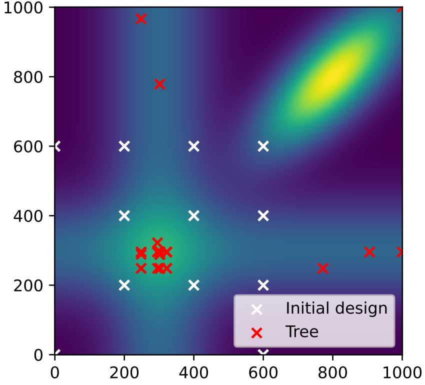
- Problem: If the function is black-box, we do not know g
- Existing methods learn g by maximum likelihood by selecting g that produces model with highest marginal likelihood $p(\mathcal{D}|g)$

Misleading decomposition learners



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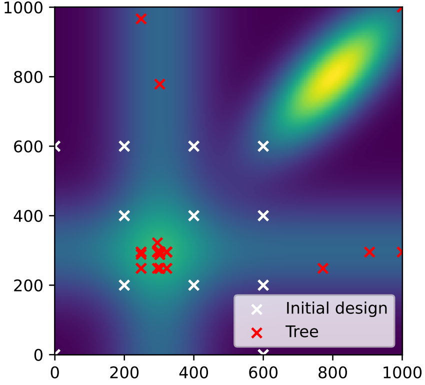

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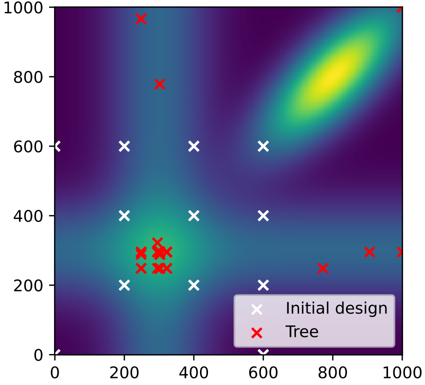

- State-of-art Tree algorithm [Han et al, 2021] gets stuck in a sub-optimal mode
- This is because, in BO we have limited, local data
  $\rightarrow$ hard to extrapolate, easy to overfit

Analysing decomposition rules

- Instead of relying on limited, local data, let us consider data-independent pre-defined schemes for choosing decompositions

Theorem (Corollary 4.2 in the paper)

Let the black-box function f be selected by an adversary from an RKHS $\mathcal{H}^g$ of kernel k^g, defined over some decomposition g that is also selected by an adversary. After T rounds, a UCB-style BO algorithm with an $S(t) : \mathbb{Z}^+ \to \mathcal{G}$ decomposition rule, incurs with a probability of at least $1 - \delta_a - \delta_B$ the following total cumulative regret R_T:

$$R_T = \mathcal{O}\left(\sqrt{T \underbrace{\gamma_T}_{\text{Kernel Complexity}}}\left(B + \sqrt{\ln \frac{1}{\delta_A} + \underbrace{\gamma_T}_{\text{Kernel Complexity}}} + \frac{1}{\delta_B} \underbrace{\mathbb{E}_S\left[\sum_{t=1}^{T} \epsilon_t\right]}_{\text{Expected mismatch}}\right)\right),$$

where $B = \max_{t \in T} \|\hat{f}_t\|_t$ and $\|\cdot\|_t$ denotes the norm in $\mathcal{H}_t$.

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- **Our algorithm should select tree decompositions randomly!**

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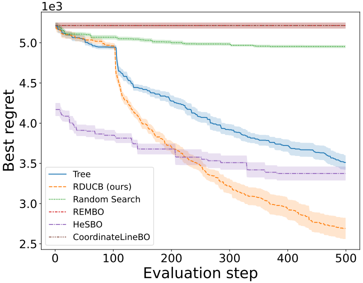
Practical Algorithm

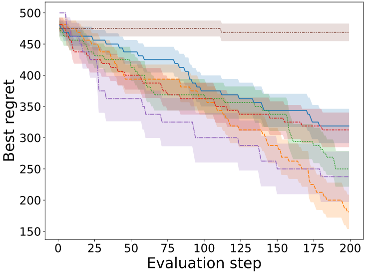
Algorithm RDUCB

Inputs: Black-box function f, evaluation budget N, initial budget N_{init}, exploration bonuses $\{\beta_t\}_{t=1}^{N}$
Evaluate N_{init} random inputs in f & populate $\mathcal{D}_{N_{\text{init}}}$
for $t = N_{\text{init}} + 1$ **to** N **do**
    Sample tree decomposition g
    Fit a GP using $\mathcal{D}_{t-1}$ with the kernel $k_g(\cdot)$
    Maximise $\alpha_t^{(\text{add-UCB})}(\boldsymbol{x}|\mathcal{D}_{t-1})$ with message passing
    Evaluate f on the suggested query & add to $\mathcal{D}_{t-1}$
end for

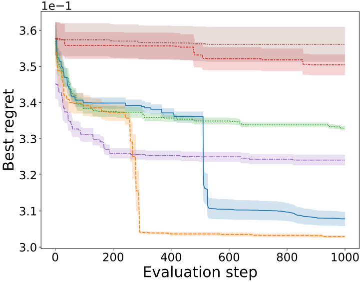
Selected Empirical Results



(a) 250-d Stybtang Function



(b) 74-d `misc05inf` MIP Task



(c) 180-d DNA LassoBench Dataset

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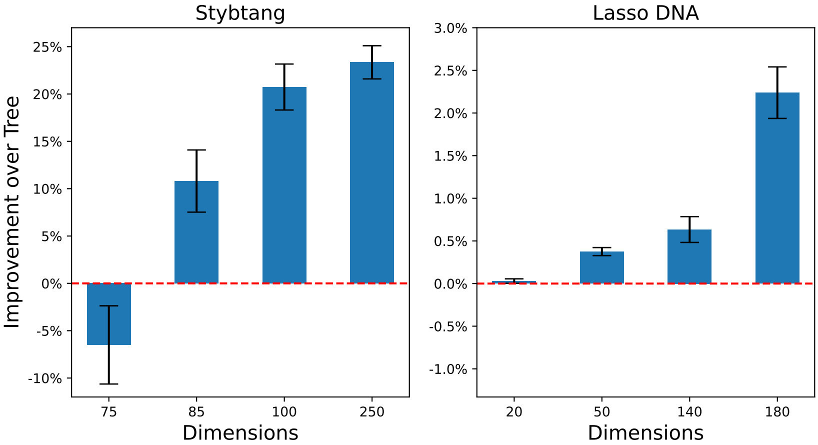
Performance as dimensionality increases



Plug&Play for HEBO [Cowen-Rivers et al, 2022]

HEBO = Multi-acquisition + Input warping + Evolution + BO

RDHEBO = Random Decompositions + HEBO

Problem	**HEBO**	**RDHEBO**
MLP-Adam	92.68 ± 0.22	$\mathbf{93.67 \pm 0.30}$
MLP-SGD	90.66 ± 0.81	$\mathbf{91.65 \pm 0.10}$
DT	79.42 ± 0.45	$\mathbf{80.79 \pm 0.15}$
RF	84.97 ± 0.32	$\mathbf{87.64 \pm 2.00}$
Average	86.93 ± 0.45	$\mathbf{88.44 \pm 0.64}$

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