Sample-efficient Bayesian optimisation using known invariances

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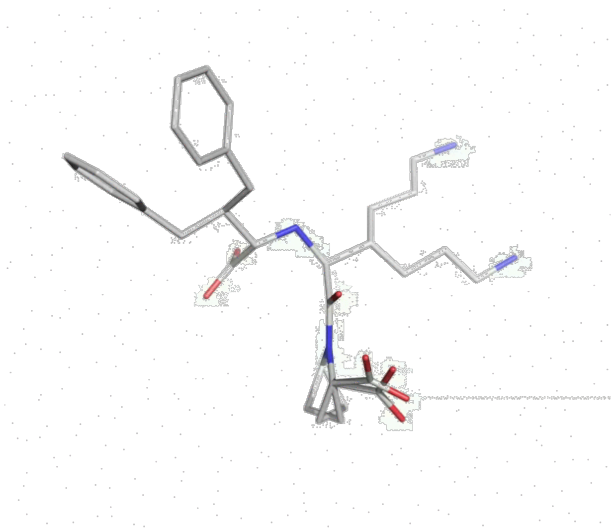
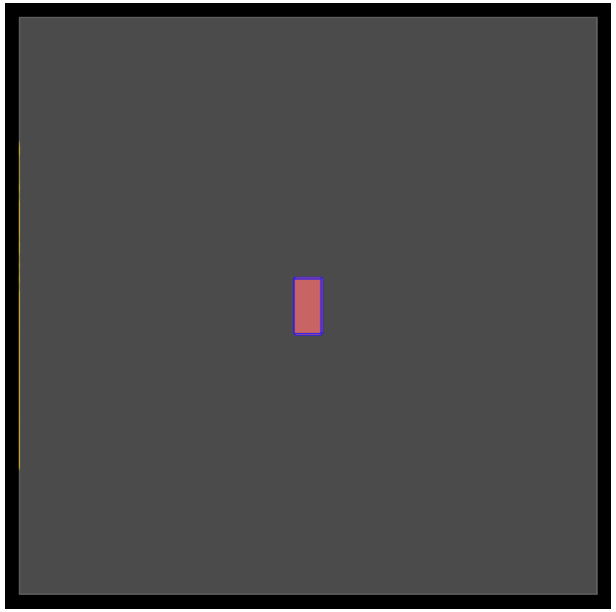
Bayesian optimisation

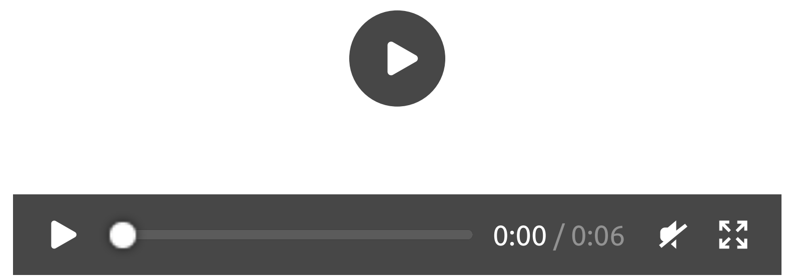
Wide range of applications



Drug discovery [C4XD]



Chip design [NVIDIA]



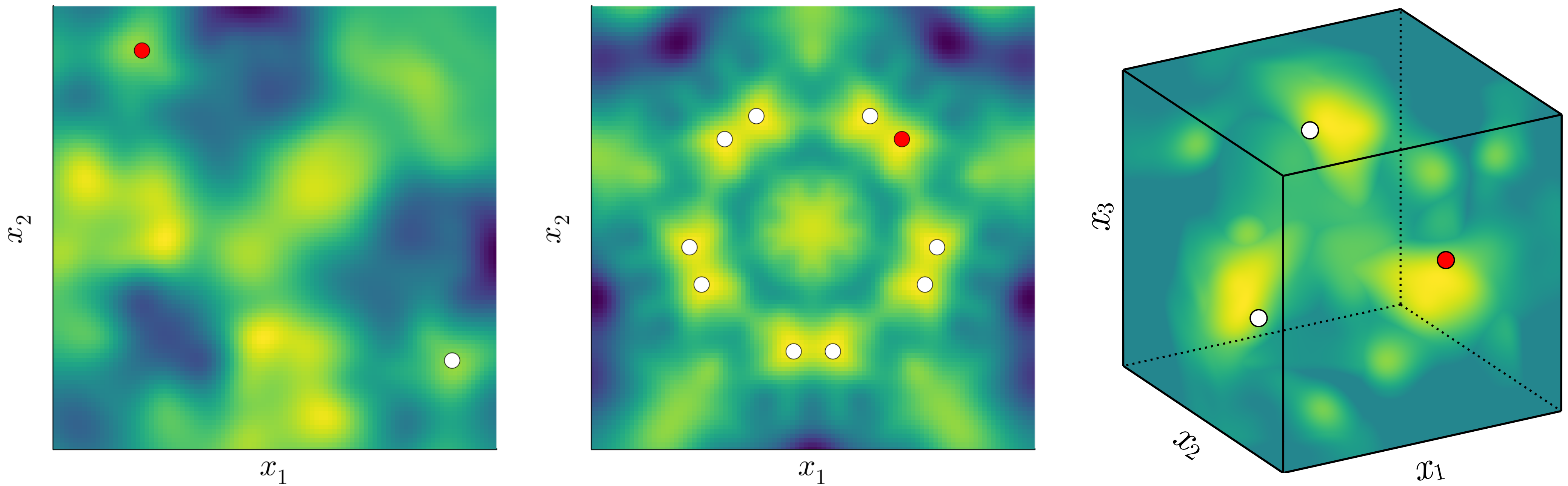
Nuclear fusion reactors [Proxima Fusion]

Goal: sample efficiency

Symmetry and invariance

How can we exploit symmetry in BO?

- Objective function is known to be symmetric
- Key insight: **making one observation gives additional information**
- In the noiseless case, this is perfect information



Invariant Gaussian processes

Naive method: data augmentation

- Key insight: making one observation gives additional information
- Data augmentation: add transformed data to dataset

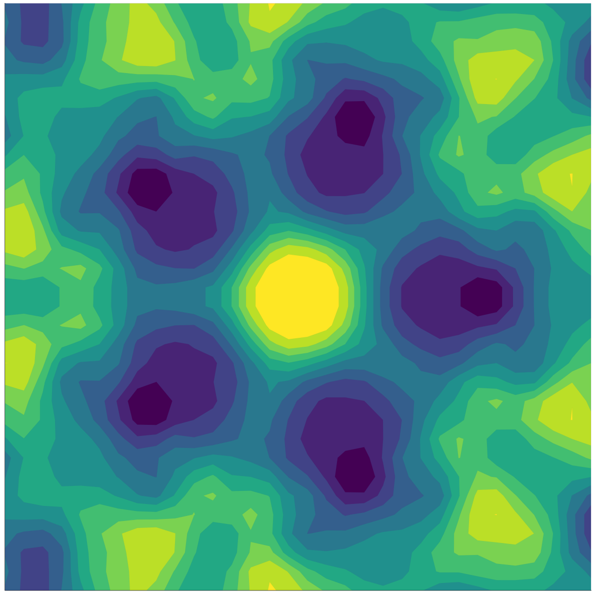
$$\mathcal{D} \leftarrow \mathcal{D} \cup \{(\sigma(x), f(x)) \quad \forall \sigma \in G, x \in \mathcal{D}\}$$

- **Problem:** computational cost of GP scales with $\mathcal{O}(|G|^3 n^3)$

Can we do better?

Invariant Gaussian processes

Our method: invariant kernel



- Construct an invariant kernel:

$$k_G(x, x') = \frac{1}{|G|} \sum_{\sigma \in G} k(x, \sigma(x'))$$

- GPs with this kernel are distributions over **invariant functions**!

Compute cost reduced from $\mathcal{O}(|G|^3 n^3)$ to $\mathcal{O}(|G| n^3)$

Sample complexity for invariant kernel BO

Number of samples T for precision ϵ

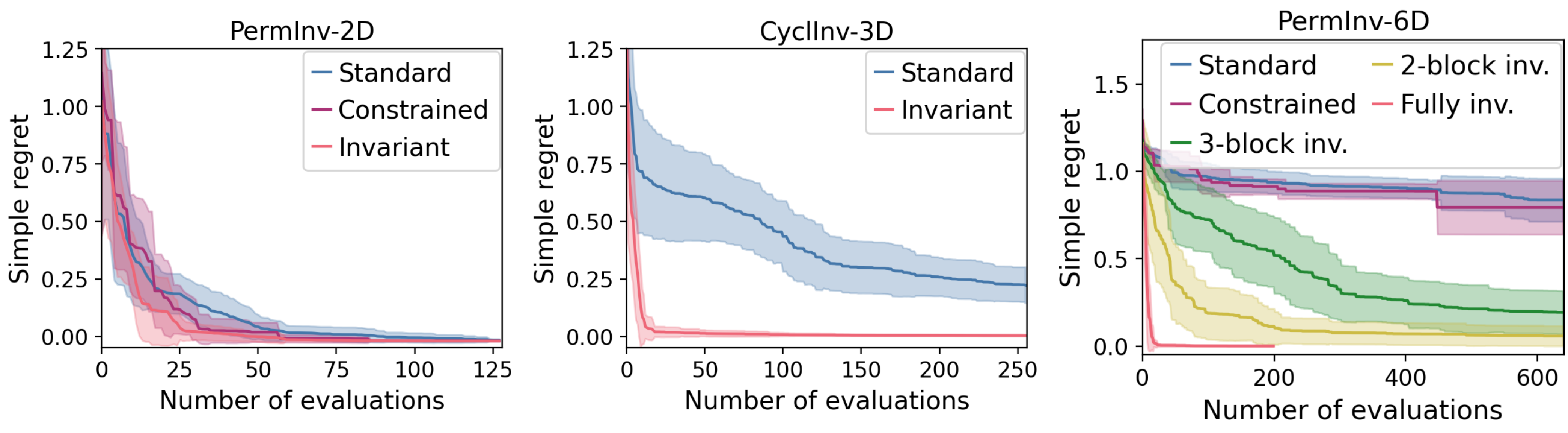
- Our upper bound:

$$T = \tilde{\mathcal{O}}\left(\left(\frac{1}{|G|}\right)^{\frac{2\nu+d-1}{2\nu}} \epsilon^{-\frac{2\nu+d-1}{\nu}}\right)$$

- Large $|G| \rightarrow$ large reduction in number of samples
- Lower bound in our paper

Synthetic experiments

Invariant GP-MVR



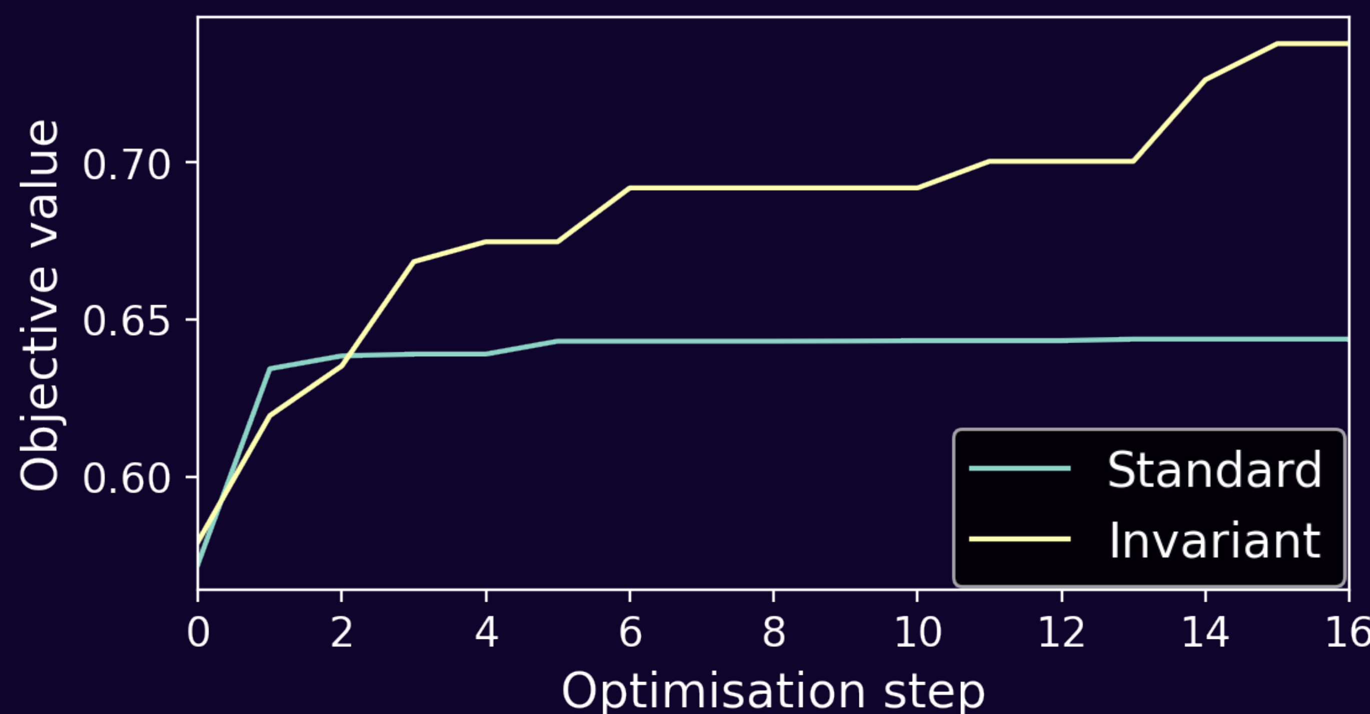
- Invariant beats standard
- Invariant beats constrained
- Use **subgroups** for low-cost approximation (2- and 3- block invariance)

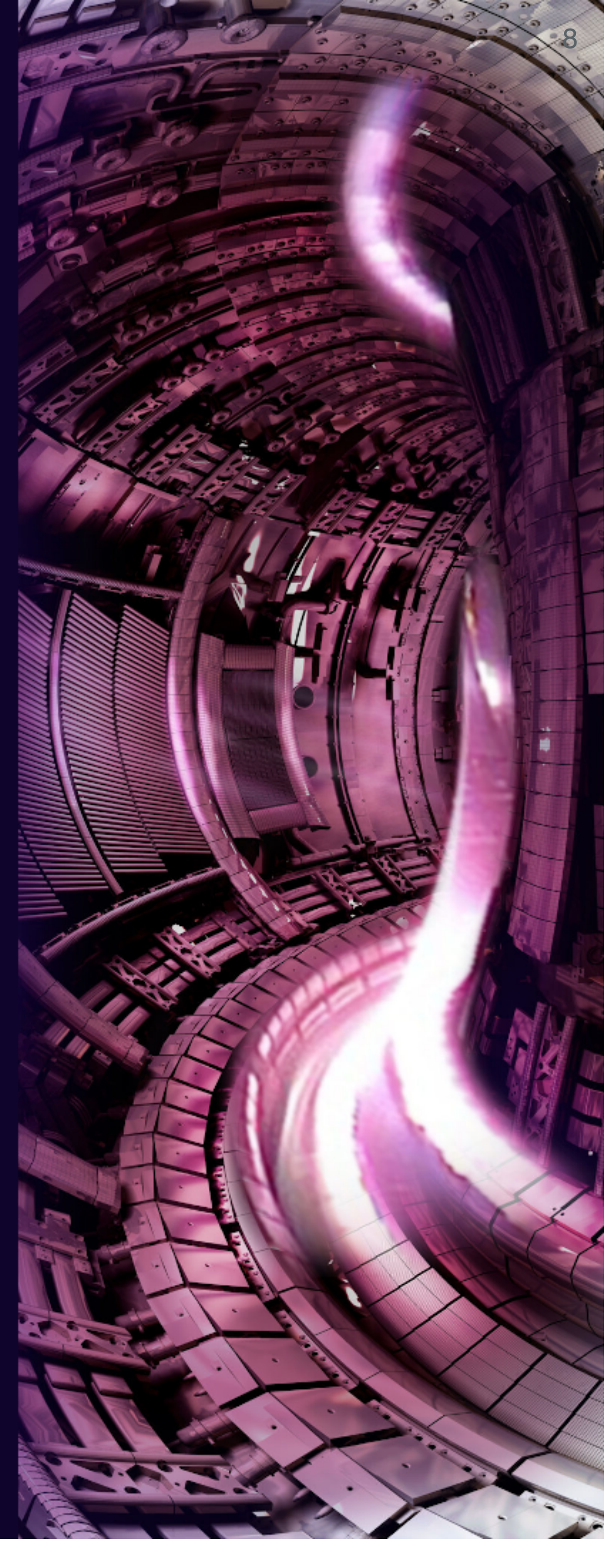
Application: fusion reactor design

High-temperature plasma → zero-carbon, low-waste energy

- **Task:** find an operating point with high stability
- Actuators are **permutation invariant**

- Using an invariant kernel achieves better results!





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🪧 Check out our poster

📝 Read the paper on arXiv

🌐 See our blog for more info

✉️ Reach out to theo.brown@ukaea.uk