Poster #236: Tue 6:30pm @ Pacific Ballroom

A Framework for Bayesian Optimization in Embedded Subspaces

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Bayesian Global Optimization of Expensive Functions



Applications of high-dim. BO are ubiquitous

- Policy search in Reinforcement Learning
- Aerospace design
- Network architecture search
- Calibration of simulations to observed data
- Control of chemical processes
- Drug design







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Theorem: <u>Active subspace</u> embedding accurately preserves GP-prior (with constant probability)

- For a <u>variety of popular kernels</u>: linear, polynomial, (squared) exponential, Matérn.
- The embedding can be combined with many GP-based BO algorithms, e.g., Knowledge Gradient (KG), BLOSSOM, Expected Improvement (EI).

Experiments demonstrate

- Efficient and easy to code using hash functions.
- <u>Robustness</u> to ambient dimension **D**.
- <u>Outperforms</u> state-of-the-art: REMBO, BOCK, EBO, additive BO.

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Great performance even if subspace assumption not met, e.g., for

100-dim. Styblinski-Tang Function Neural Network Parameter Search (Oh, Gavves, and Welling '18)



Visit <u>https://github.com/aminnayebi/HesBO</u> for HeSBO for KG, BLOSSOM, and EI.

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