Summary and Open Challenges in BO

Outline of the Tutorial

- Background on GPs and Single-Objective BO
- Bayesian Optimization over Combinatorial Spaces
- Bayesian Optimization over Hybrid Spaces

Break

- Multi-Fidelity Bayesian Optimization
- Constrained Bayesian Optimization
- Multi-Objective Bayesian Optimization
- Summary and Outstanding Challenges in BO

Open Challenges in BO

- **High-dimensional BO**
  - Need more effective approaches for high-dimensional spaces
- **BO over Combinatorial Structures**
  - How to combine domain knowledge, kernels, and (geometric) deep learning to build effective surrogate models?
  - Effective methods to select large and diverse batches?
- **BO over Hybrid Spaces**
  - Methods to sample functions from GP posterior?
  - Effective latent space BO methods?

Open Challenges in BO

- **Constrained BO**
  - Need more effective approaches for input spaces, where no. of invalid inputs >> no. of valid inputs
- **BO over Nested Function Pipelines**
  - Relatively less explored problem
- **BO with Resource Constraints**
  - Real-world experiments need resources and setup time
  - Critical for BO deployment in science and engineering labs

Acknowledgements: Collaborators

- Nano-porous materials

- Hardware design





- Microbial fuel cells

- Electric transportation systems

- Catalysis


- Agriculture





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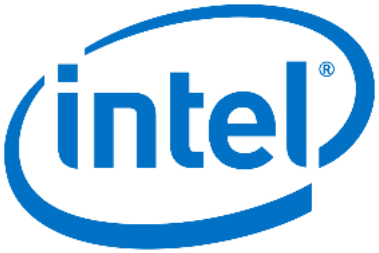
Primary source



Questions ?