Bayesian Optimization over Hybrid Spaces

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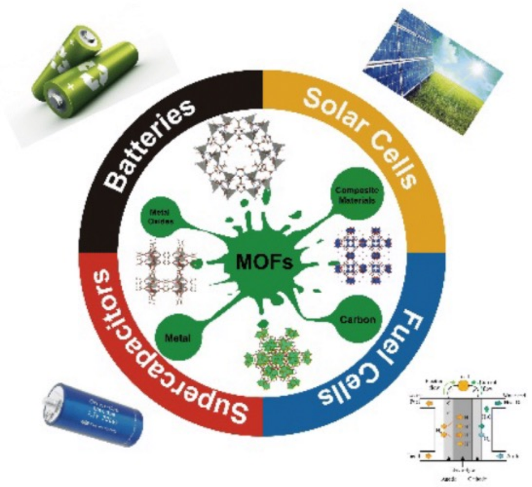
(Joint work w/ Syrine Belakaria and Jana Doppa)

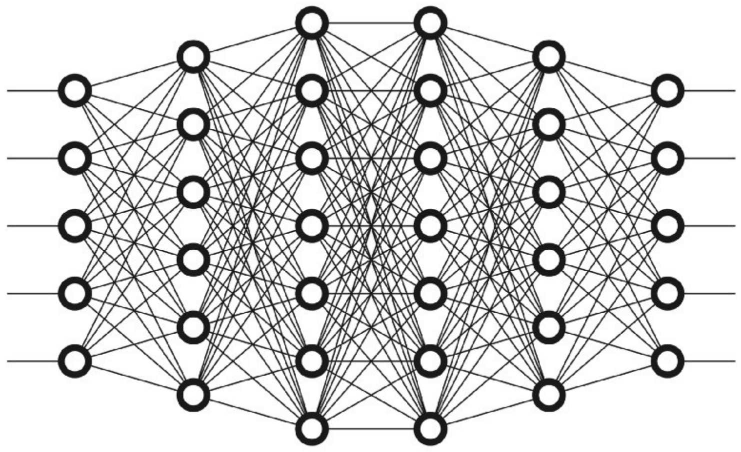
Motivation

- **Goal:** find optimized hybrid structures via expensive experiments
  - x = mixture of x_d (discrete variables) and x_c (continuous variables)

Microbiome design



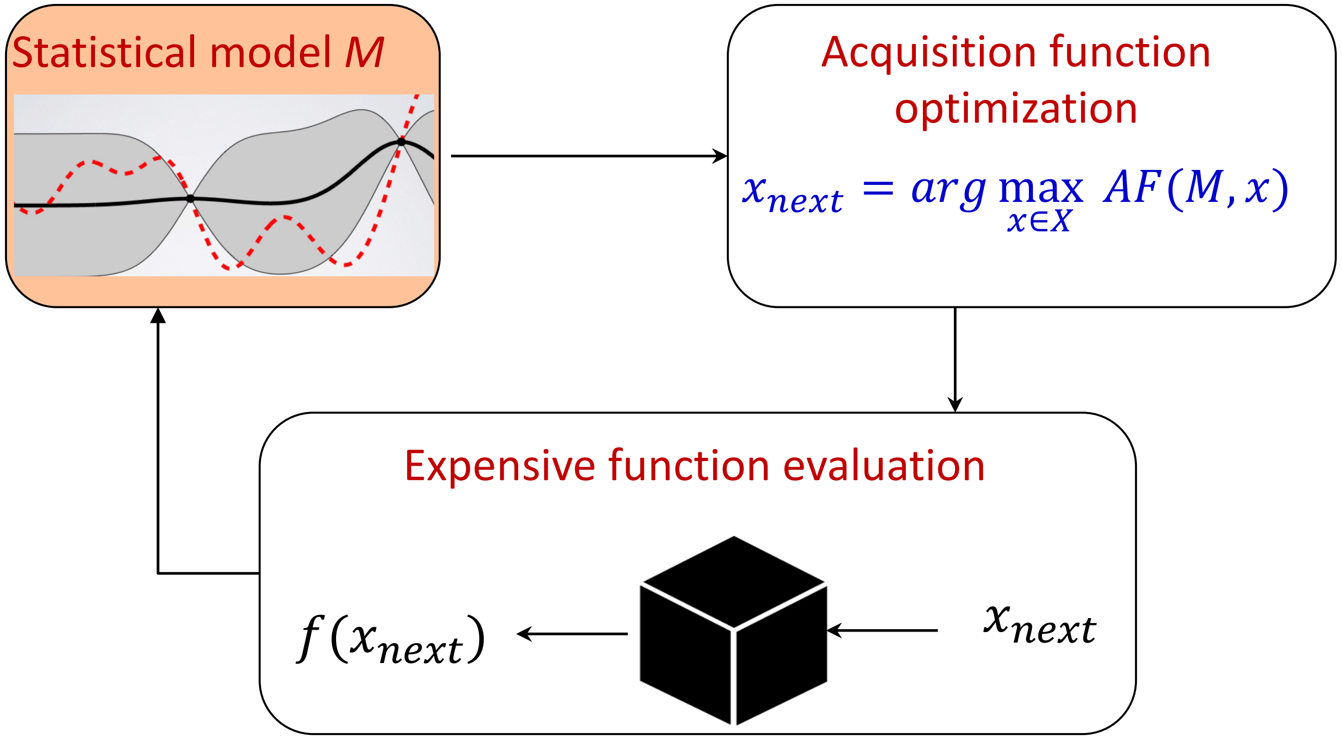
Material design



Hyper-parameter tuning / Auto ML

- Many other science and engineering applications

The Key Challenge



- How to accurately model the complex interactions among discrete and continuous variables?

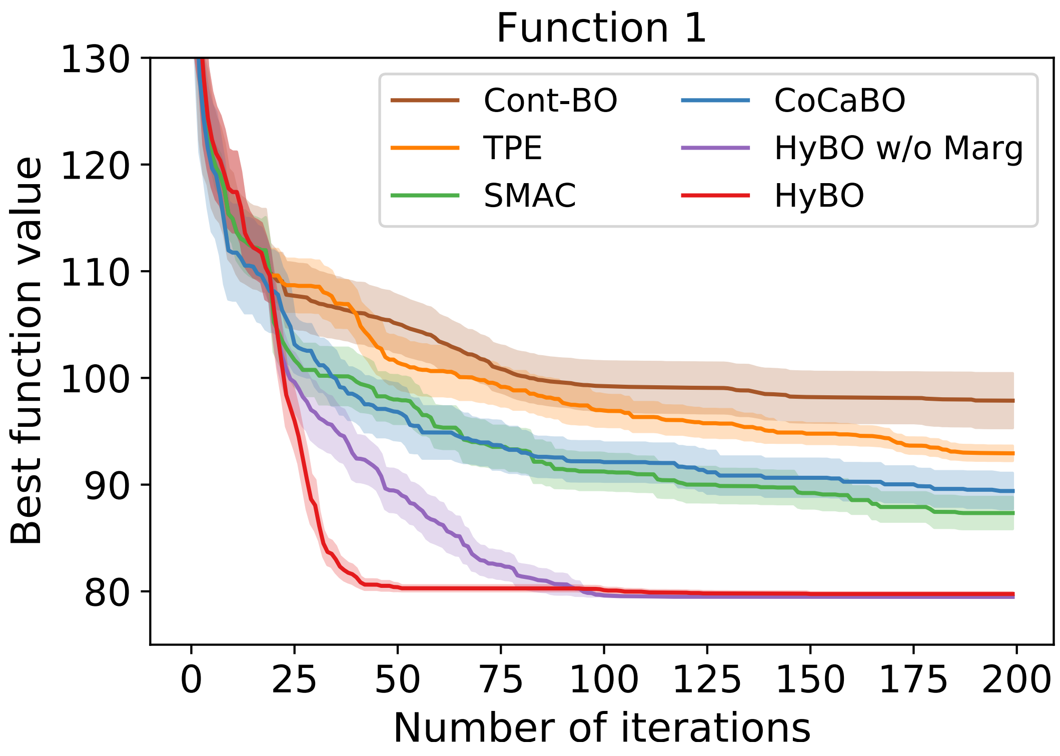
HyBO: Gaussian Process Statistical Model

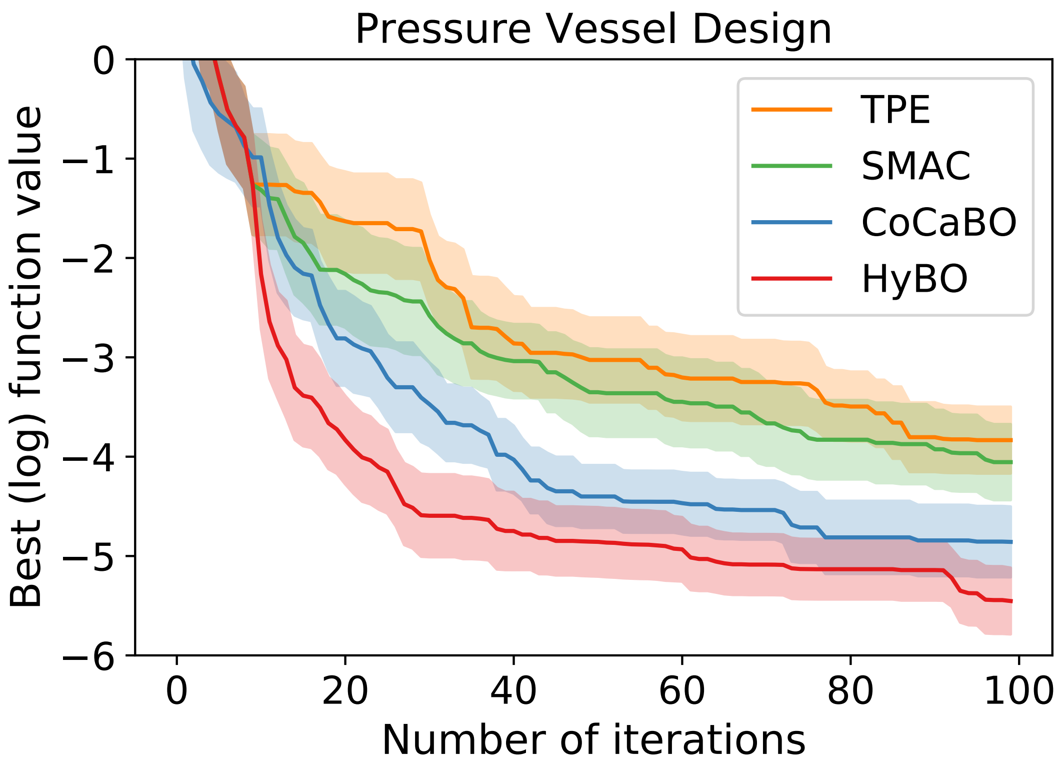
- Contribution #1: Construction of additive hybrid diffusion kernel
  - Exploits the general recipe of additive kernels [Duvenaud et al., 2011]
  - Instantiation w/ discrete & continuous diffusion kernels [Kondor & Vert, 2004]
  - Bayesian treatment of the hyper-parameters

$$\mathcal{K}_{HYB} = \boxed{\sum_{p=1}^{m+n} \left(\boxed{\theta_p^2} \sum_{i_1,\cdots,i_p} \prod_{d=1}^{p} \boxed{k_{i_d}(x_{i_d}, x'_{i_d})} \right)}$$

- Contribution #2: Theoretical proof for universality of this kernel

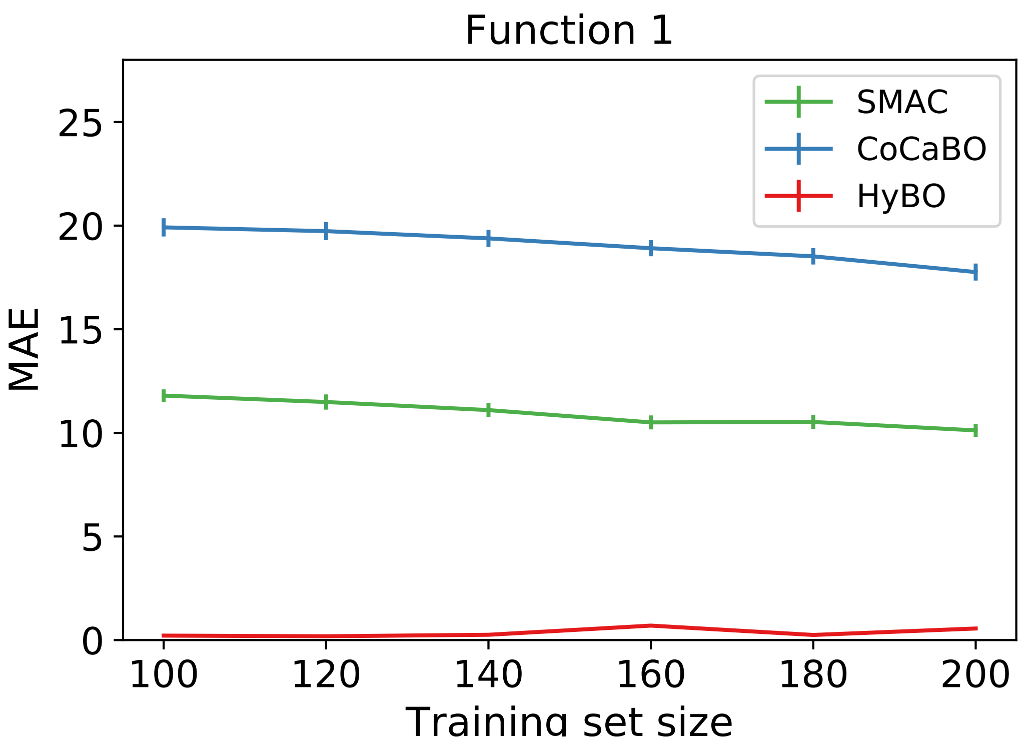
Experimental Results #1

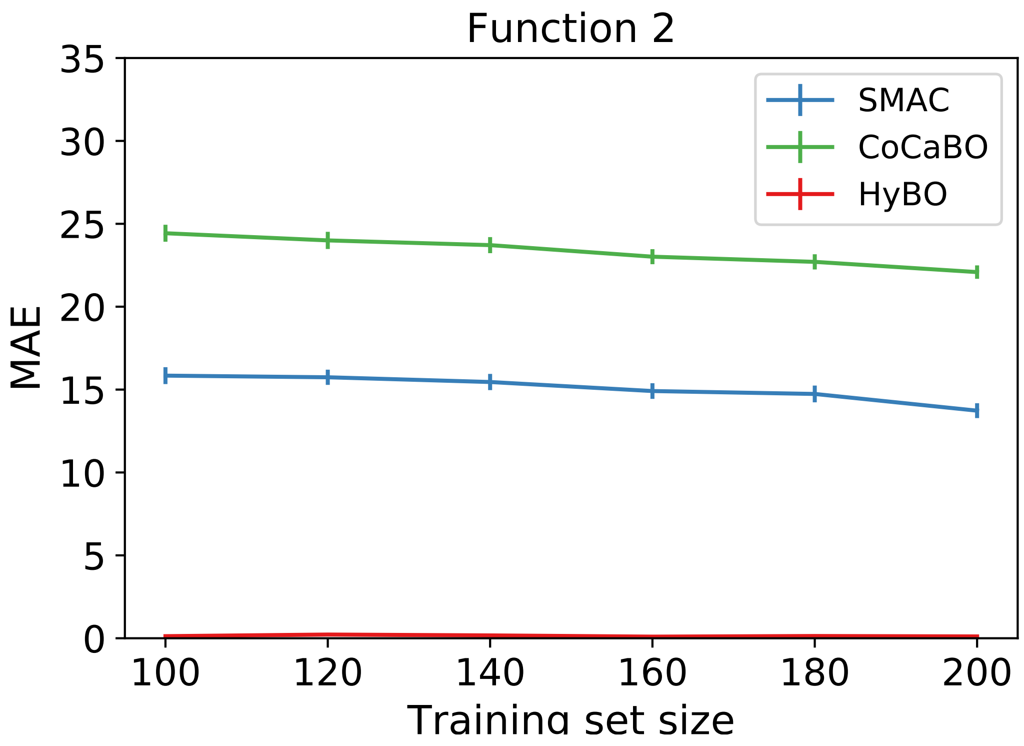




- HyBO performs significantly better than prior methods

Experimental Results #2





- HyBO's better BO performance is due to better surrogate model

Thank you!

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