Bayesian optimization

Wednesday, May 15, 2024 12:59 AM

https://arxiv.org/pdf/1012.2599v1
A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning

Step-by-Step Guide to Bayesian Optimization: A Python-based Approach | by Okan Yenigün | Medium

[2204.13753] High Dimensional Bayesian Optimization with Kernel Principal Component Analysis (arxiv.org)

4e5046fc8d6a97d18a5f54beaed54dea-Paper.pdf (neurips.cc)

Sampling_Multitask_GPs(1) (nips.cc)
Bayesian Optimization with High-Dimensional Outputs

Freethraw, top 3

40C, top 3

Sugar_Salt_label

Uncertainty more important

Additive_label no level
Sugar_Salt_label no level, add one more category

pH

Different level of solution

40C,
Relative order under different conditions

From Zhiyuan: Find optimal conditions for each buffer type, and then vary the pH from the optimal condition (+/- 1)

Buffer Type label correspondence with actual types
0: Ace (Acetate), Triangle
1: His (Histidine), Circle
2: Cit (Citrate), Star
3: Phos (Phosphate), Square

Sugar_Salt label correspondence
0: 4% Sorbitol, red
1: 0.1M NaCl, green

0% Sorbital
0 NaCL

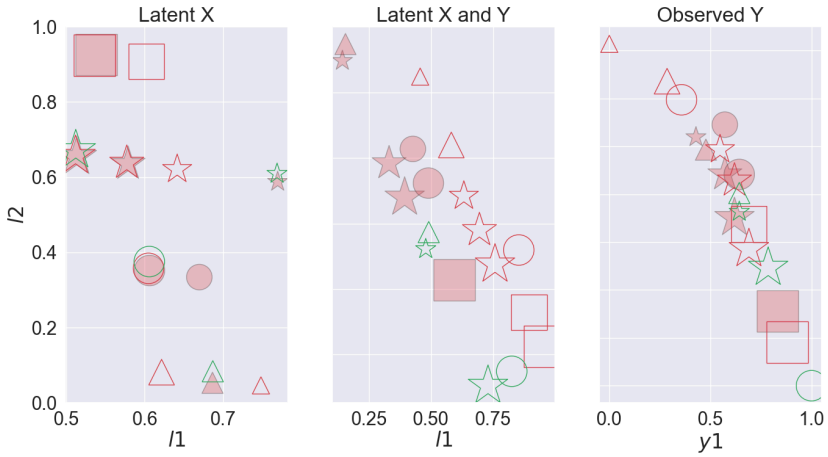
Additive_label Correspondence
0: Arginine, solid shape
1: Glycine, hollow shape

No Arginine
No Glycine

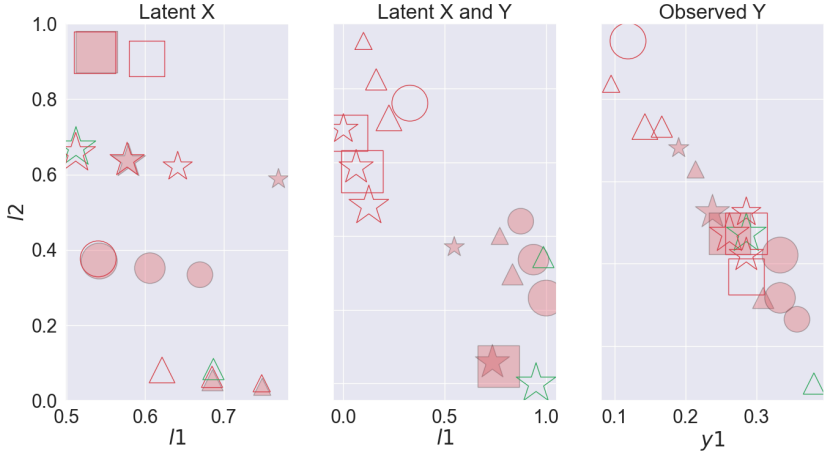
Best formulations

```
Buffer_Type_label    0.0
Sugar_Salt_label     0.0
Additive_label       1.0
pH                   4.5
task_ind             2.0

Buffer_Type_label    1.0
Sugar_Salt_label     0.0
Additive_label       1.0
pH                   6.5
task_ind             1.0

Buffer_Type_label    0.0
Sugar_Salt_label     0.0
Additive_label       1.0
pH                   4.5
task_ind             0.0
```

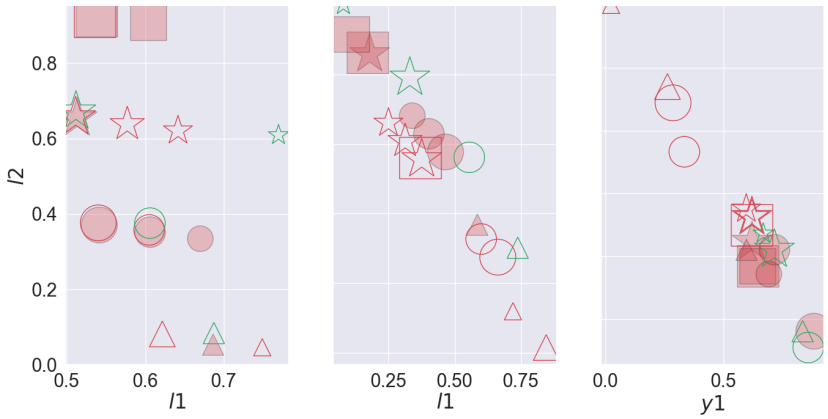
Task 2



Task 1



Task 0



Ti-chiun: Legend
Part of perspective