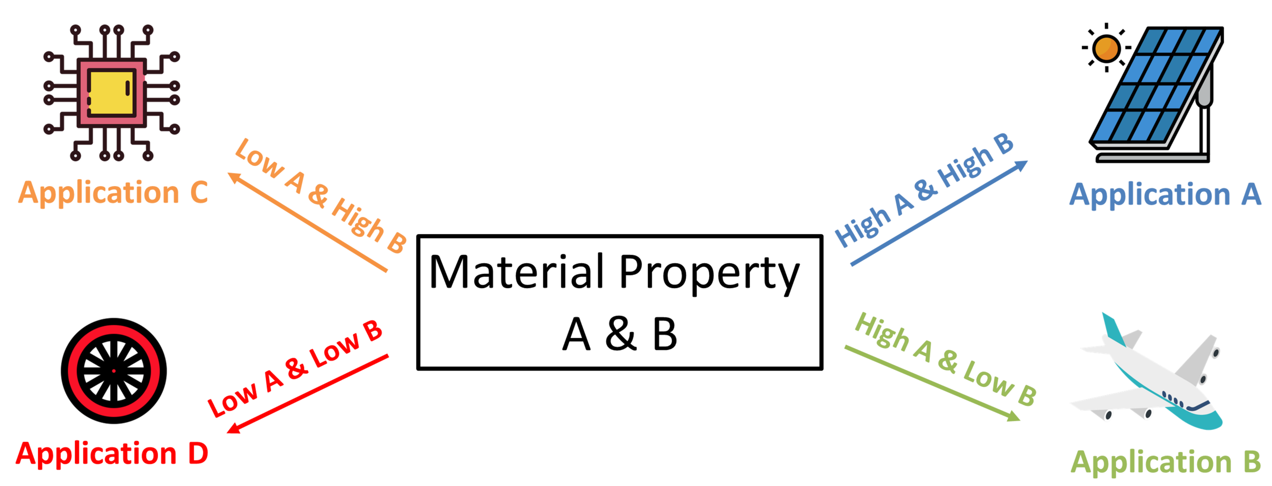
BEACON: A Bayesian Novelty Search Algorithm for Efficient Material Property Discovery

Wei-Ting (Jonathan) Tang, Ankush Chakrabarty & Joel A. Paulson

Motivation

- Optimal choice of objective is not always obvious in material exploration problem, especially when multiple properties need to be considered simultaneously

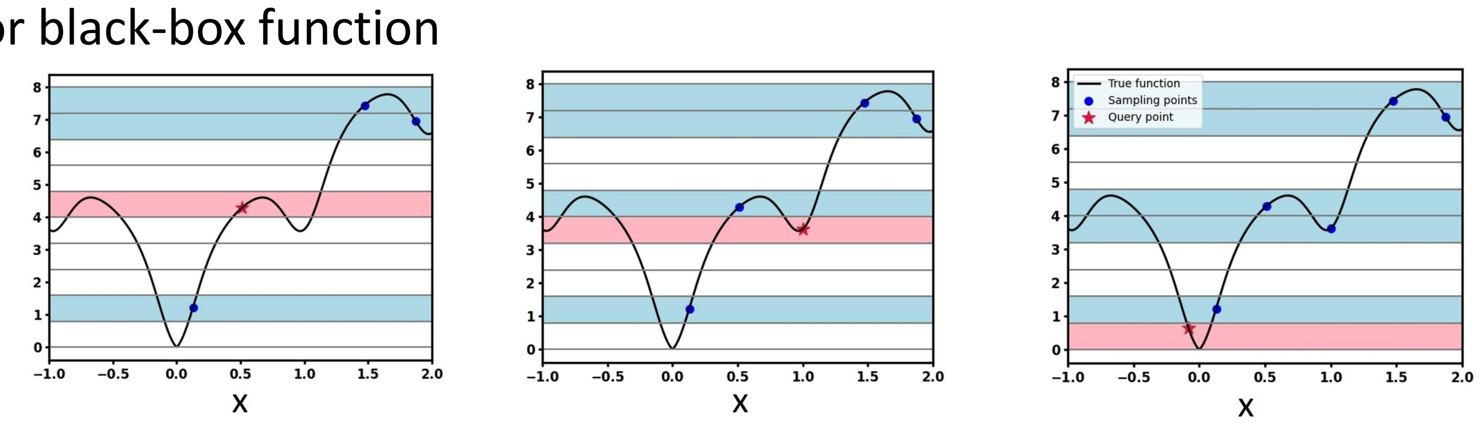


- Novelty search is an objective-free strategy designed to explore multi-dimensional properties for black-box system
- Vanilla novelty search is based on evolutionary algorithm and suffers from sample inefficiency

Introduction

Novelty Search

- Novelty search is a sequential strategy for discovering novel outcome for black-box function



- Novelty search defines the fitness function (F) of Evolutionary Algorithm as the sum of the k-nearest distance from a given function value $f(x)$
  - ➢ $F(x) = \frac{1}{k}\sum_{i=1}^{k} \text{dist}(f(x), y_i^*)$
  - ➢ Where $f(x)$ is the sampled function value
  - ➢ y_i^* is the k-nearest neighbor of $f(x)$

Bayesian Optimization

- Bayesian optimization (BO) is a sequential strategy for global optimization of black-box function

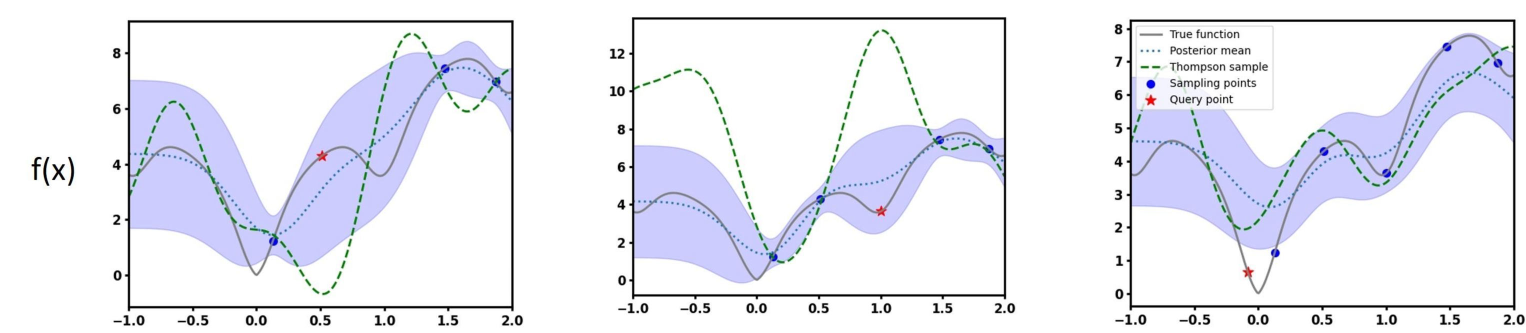
While {budget not exhausted}
1. Fit a Bayesian machine learning model (usually **Gaussian process regression**) to observations (x, f(x))
2. Find x that maximizes **acquisition(x, posterior)**
3. Sample x & then observe f(x)

end

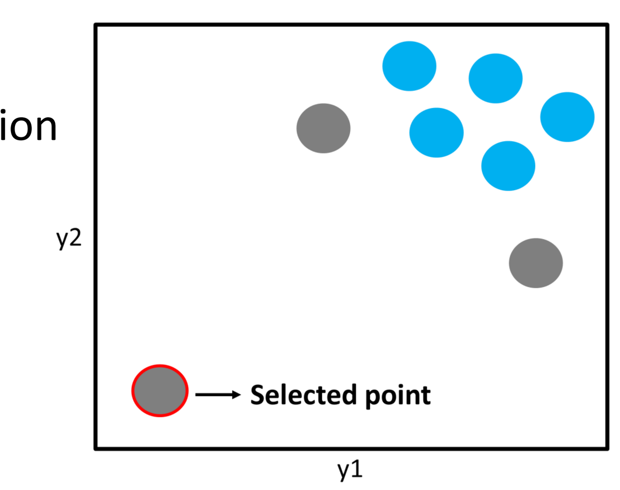
BEACON

- BEACON (**B**ayesian **E**xploration **A**lgorithm for out**CO**me **N**ovelty) is a combination strategy between Novelty Search and Bayesian Optimization
- BEACON iteratively executing the following two steps:

1. Build Gaussian process (GP) surrogate with sampled data points

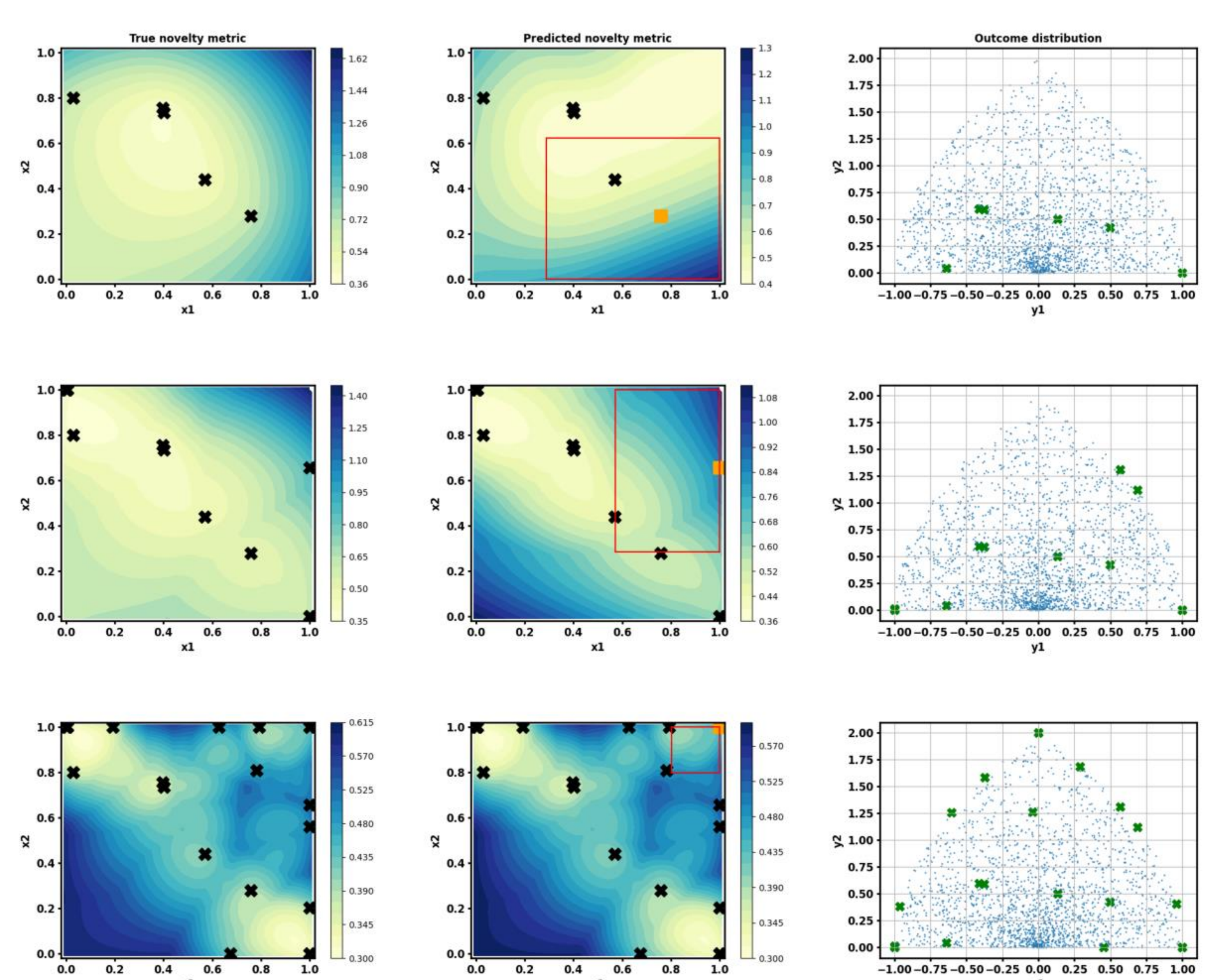


2. Query new data point by maximizing the following acquisition function:
   - ➢ $\alpha(x|D) = \frac{1}{k}\sum_{i=1}^{k} \text{dist}(\boldsymbol{GP}(\boldsymbol{x}), y_i^*)$
   - ➢ Where $GP(x)$ is a GP posterior prediction
   - ➢ y_i^* is the k-nearest neighbor of $\text{GP}(x)$



TR-BEACON

- Trust region-based BEACON (TR-BEACON) is designed to tackle problems with high-dimensional feature space
- The trust region expands when a novel outcome is discovered (indicated by an increase in the variance of sampled outcomes) and shrinks after failing to discover a novel outcome for N consecutive attempts.

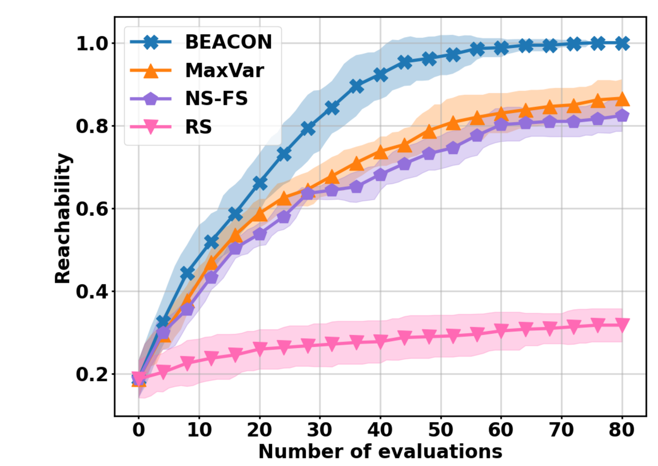


Results

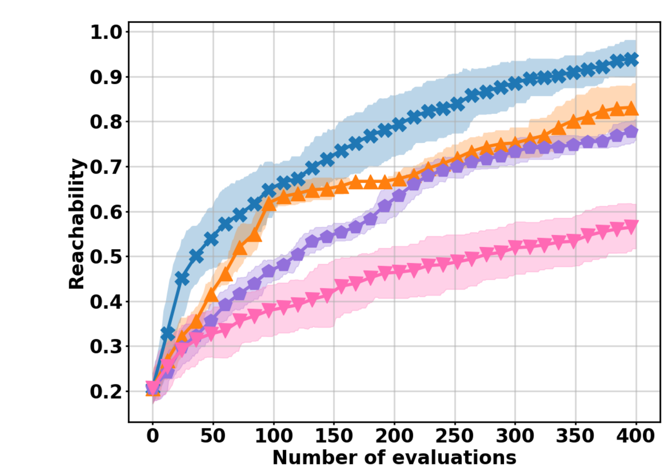
Material Exploration Tasks

- We compare BEACON with several state-of-the-art algorithms on several material exploration tasks
- The goal is to discover as many property value as possible within given budget

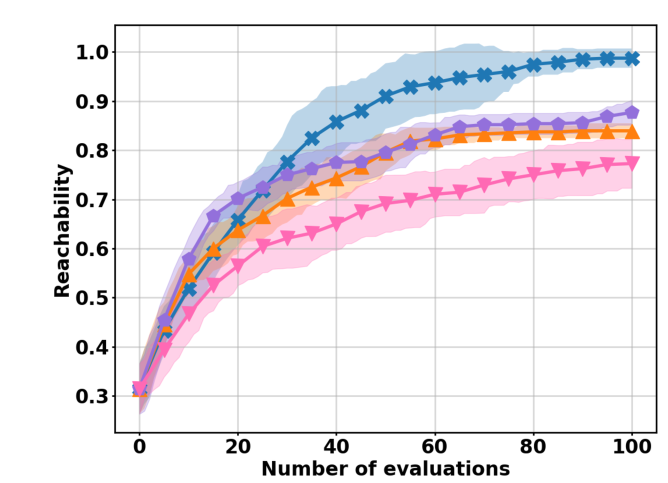
- **Hydrogen uptake capacity for MOFs**



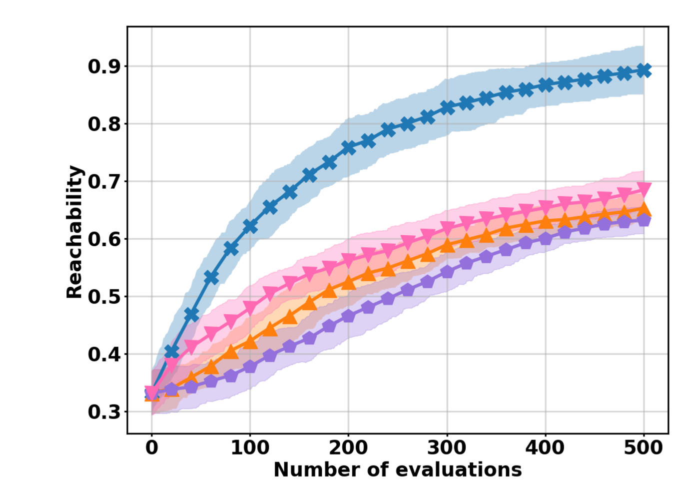
- **Nitrogen uptake capacity for MOFs**



- **Water solubility for molecules**



- **CH4/CO2 joint uptake capacity for MOFs**



Maze Navigation Task

- The goal for the maze navigation problem is to find the optimal control policy to navigate the green ball to the red ball within given time steps
- Control policy is defined as a bias-free single layer feedforward neural network with 24 weight parameters

- Reward = $\frac{\text{initial distance from target - final distance from target}}{\text{initial distance from target}}$