Constrained Multi-objective Bayesian Optimization through Optimistic Constraints Estimation

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Motivating Applications

Drug discovery must balance therapeutic effectiveness with safety standards [Mellinghoff and Cloughesy, 2022], and hyper-parameter optimization must avoid overfitting or violating constraints [Karl et al., 2023].

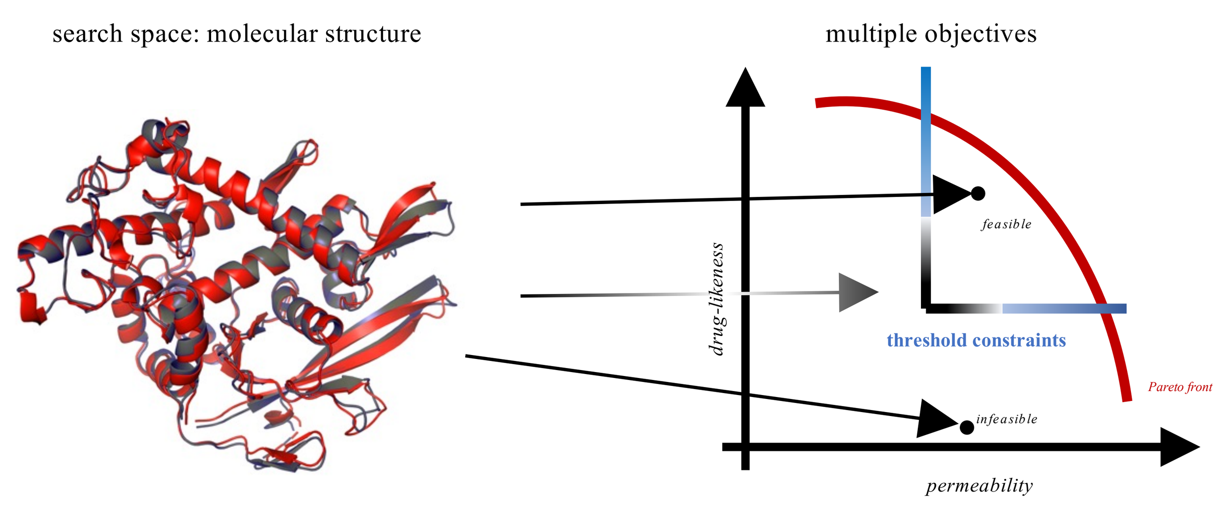


Figure 1: Constrained multi-objective optimization in drug-discovery. Left illustration: DEEPMIND.

Problem Formulation

Consider the following constrained multi-objective optimization problem:

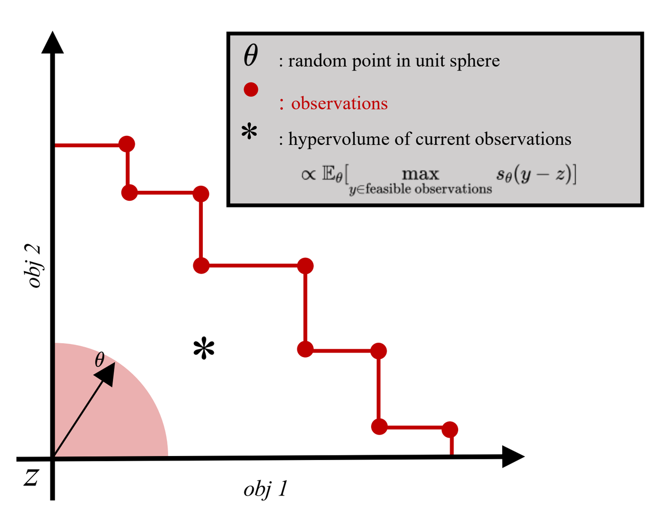
$$\arg\max_{\mathbf{x}\in\mathcal{X}} \quad F(\mathbf{x}) = [f_1(\mathbf{x}), ..., f_m(\mathbf{x})], \tag{1}$$

$$\text{s.t.} \quad G(\mathbf{x}) = [g_1(\mathbf{x}), ..., g_c(\mathbf{x})] \geq 0. \tag{2}$$

where $F = [f_1, ..., f_m] : \mathcal{X} \to \mathbb{R}^m$ is a multi-objective function with m objective functions. Let $G = [g_1, ..., g_c] : \mathcal{X} \to \mathbb{R}^c$ be the multi-objective function with c constraint functions. Here $f_i, \forall i \in [m], g_j, \forall j \in [c]$ are black-box functions.

- Goal: Explore the solution set to CMO prolems, the *Pareto front*, within the feasible region induced by (2).
- We use *Gaussian Process* (GP) to model each component of F and G.
- We use *hypervolume regret* to assess Pareto front exploration and *simple violation* to measure constraint violations. The *constraint regret* is defined as the weighted sum of these two metrics to evaluate the method's mixed performance.

Hypervolume Scalarization



- Proposed by Deng and Zhang (2019); Golovin and Zhang (2020), s_θ, the *hypervolume scalarization* is a scalarization function that converts a set of observed m-dimensional objective values to a scalar related to the true hypervolume of the observations.
- θ is a point uniformly sampled from the positive quadrant of a m-dimensional unit sphere.
- The expectation with respect to θ of the maximum among the scalarized objectives is proportional to the hypervolume, which allows us conducting *Monte Carlo estimation of the hypervolume*.

'UCB' for constrained HV

Upper confidence bound (UCB) was applied as an acquisition functions in pervious works of single-objective BO, also representing an *optimistic view to the unknown objectives*. Let $U_t(\mathbf{x}) \in \mathbb{R}^m$ denote the UCB vector associated with m objectives $f_1, f_2, \ldots, f_m$, evaluated at the point $\mathbf{x}$ at time step t. We define the acquisition function $\alpha_t(\mathbf{x})$ as the scalarized value of $U_t(\mathbf{x})$ under the hypervolume scalarization function s_θ, i.e.,

$$U_t(\mathbf{x}) = (u_{f_1,t}(\mathbf{x}) - z_1, ..., u_{f_m,t}(\mathbf{x}) - z_m)$$
$$\alpha_t(\mathbf{x}) = s_\theta(U_t(\mathbf{x}))$$

where $z = (z_1, ..., z_m)$ is a chosen sub-optimal value.

Optimistic Constraint Learning

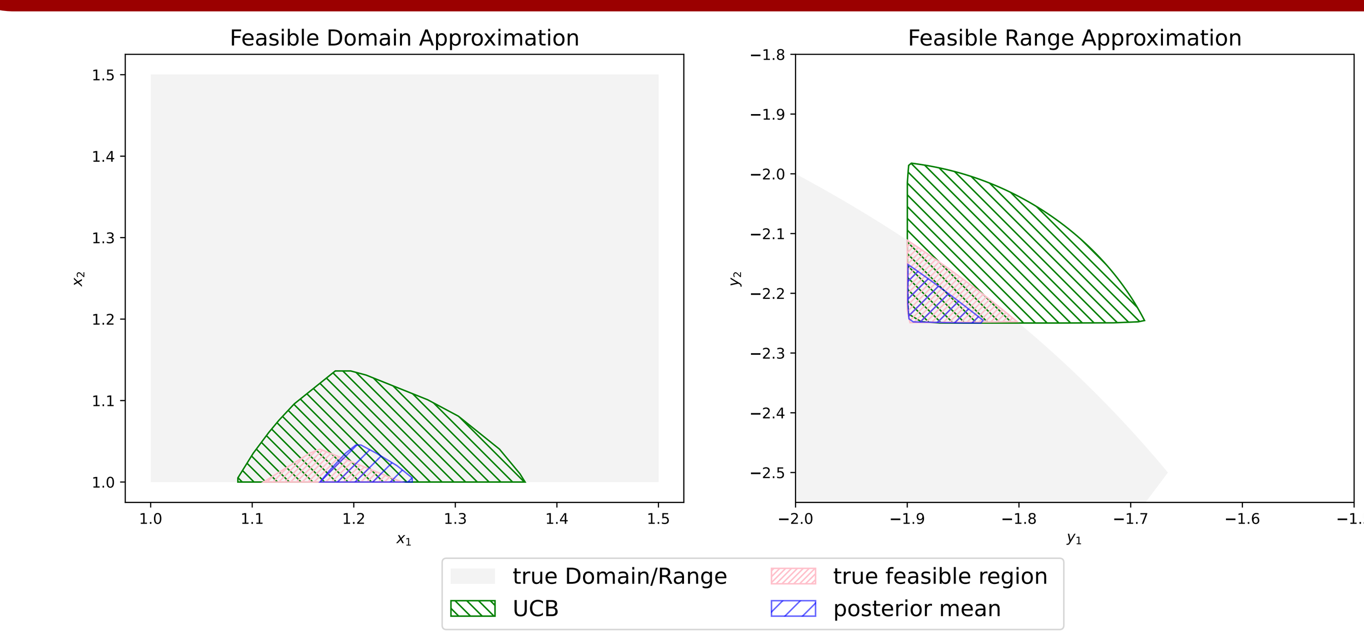
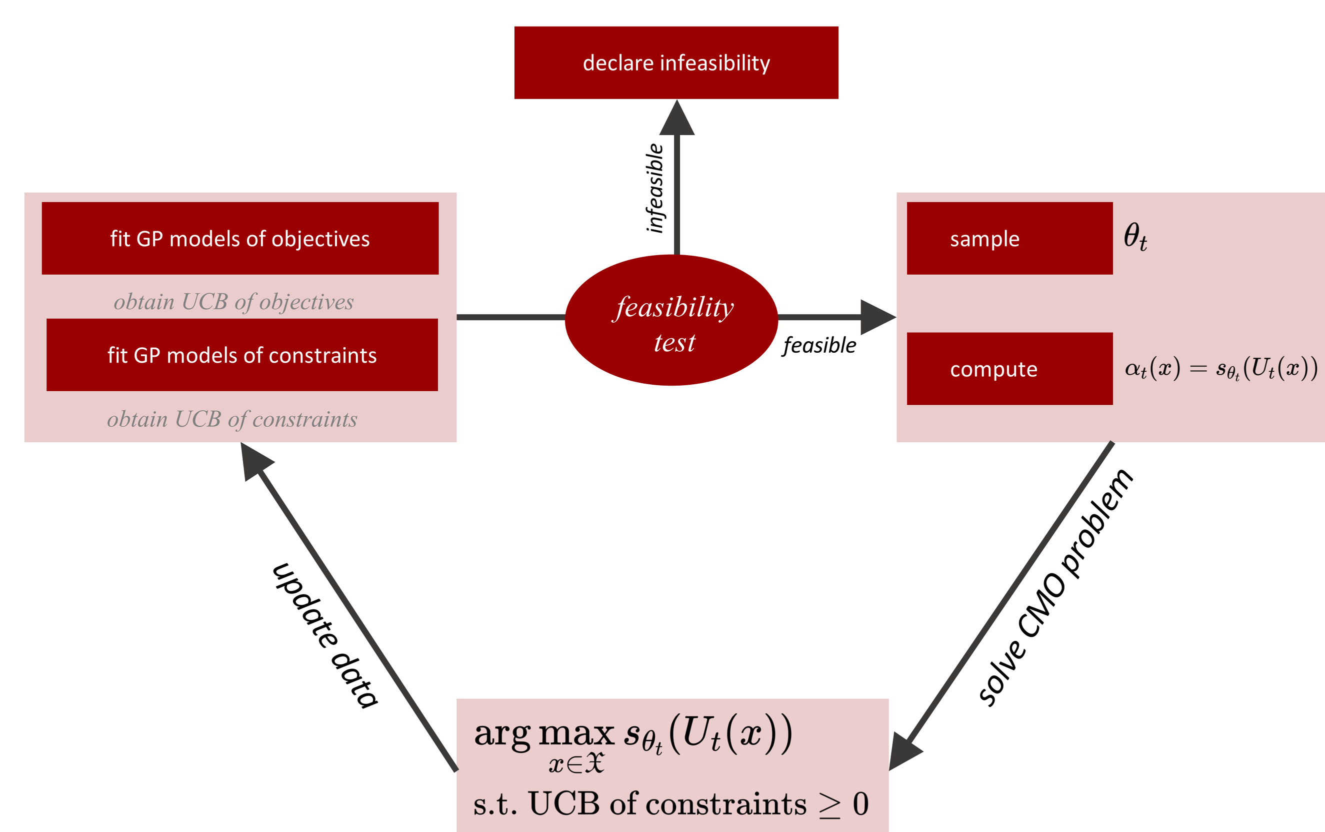


Figure 2: Left: Estimated feasible domain in the input space $\mathcal{X} \subset \mathbb{R}^2$ (d=2, m=2), comparing UCB-based and posterior mean-based constraint estimations. Right: Area below feasible Pareto fronts (UCBs, posterior means, and true values), highlighting UCBs' advantage in preserving the global maximum.

- In each iteration, we optimize α_t subject to the constraints defined by the UCBs of the constraint functions, representing an *optimistic perspective on the constraints*, which has empirically demonstrated good performance in minimizing violations during the sampling process.

Constrained Multi-objective Bayesian Optimization



Algorithm 1 **Co**nstrained **M**ulti-Objective **B**ayesian **O**ptimization through **O**ptimistic Constraints Estimation (**COMBOO**)

for $t \in [T]$ **do**
  if $\max_{\mathbf{x}\in\mathcal{X}}\{\min_{j\in[c]} u_{g_j,t}(\mathbf{x})\} < 0$ **then**
    Declare infeasibility.
  end if
  Sample θ_t uniformly from $\mathcal{S}^+_{k-1}$
  Find $\mathbf{x}_t \in \arg\max_{\mathbf{x}\in\mathcal{X}} \alpha_t(\mathbf{x})$
    s.t. $u_{g_j,t} \geq 0, \forall j \in [c]$
  Evaluate F, G at $\mathbf{x}_t$.
  Update GP posteriors with new evaluations.
end for

- For an infeasible problem, the feasibility test allows users to terminate the algorithm loop early, preventing unnecessary costs associated with constraint evaluations. This is achieved by assessing the feasibility of the UCBs of the constraints.
- The scalarization function enables the integration of multiple single-objective acquisition functions into a unified acquisition function, establishing a meaningful relationship with the hypervolume.

Key Theoretical Results

We provide a set of probabilistic regret bounds similar to that in the single-objective BO. Until T iterations, we have the following results:

- **Hypervolume regret bound**: $\mathcal{R}_T \leq O(m^2[\gamma_T T \ln(T)]^{1/2})$
- **Cumulative constraint violation bound**: $\mathcal{V}_{j,T} \leq O((\gamma_T T \ln T)^{1/2}), \forall j \in [c]$

with high probability. Here, γ_T represents the Maximum Information Gain (MIG).

Experiment Results