Development of an Efficient Batch Multi-Objective Bayesian Optimization Method for Engineering Design
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**Background**

**Bayesian optimization:**
Bayesian optimization (BO) is commonly used in engineering design to evaluate blackbox functions that are expensive to evaluate.

In BO, a surrogate model is created from known evaluations to provide a predicted model of the function. The next points to be evaluated are determined by an acquisition function that is minimized to suggest the next point. The figure to the right depicts the point selection process.

**Gaussian Process Surrogate Model:**
Gaussian process surrogate model suggests a new set of parameters by calculating the mean and standard deviation of the points.

**Sequential and Batch Optimization:**
Batch optimization makes real-time computation significantly lower compared to sequential methods.

**Objective**
To develop an efficient batch multi-objective bayesian optimization code for engineering design applications.

**Results**

**Ensemble Creation:**
- Creation of a BO Python Object Oriented Programming (OOP) package
- Sequential and batch BO
- Single and multi-objective

**Acquisition functions:**
- Exploration: Prioritizes choosing points farther away from known points
- Exploitation: Prioritizes finding absolute maximum/minimum in known area

**Penalty Functions:**
Penalty functions are used to encourage exploration by negatively weighting areas with local minima.

*The figure above depicts a penalty function (in blue) being applied to an acquisition function (in green). The black star shows the next highest point to penalize [1].*

**Expected Improvement (EI)**
\[ a_{EI}(x) = (\mu_x - \tau_x)\text{norm.cdf}\left(\frac{\mu_x - \tau_x}{\sigma_x}\right) + \sigma_x\text{norm.pdf}\left(\frac{\mu_x - \tau_x}{\sigma_x}\right) \]

**Upper/Lower Confidence Bound (UCB/LCB)**
\[ a_{UCB/LCB}(x) = \mu_x \pm \beta\sigma_x \]

**Probability Improvement (PI)**
\[ a_{PI}(x) = \text{norm.cdf}\left(\frac{\mu_x - \tau_x}{\sigma_x}\right) \]

**Results (cont.)**

**Future Work**
Utilize the code's generated cones to serve as penalizers for batch point selection during multi-objective optimization. Also, make the penalty function more customizable so the user can decide if they wish to prioritize exploration or exploitation, when it should do each, and how intense the preference should be.

Expand from 1D sequential optimization and simple multi-objective optimization into the nth-dimension, allowing for the input of many input variables and the optimization of problems with several objectives.

Utilize the codebase to analyze and optimize real-world engineering design problems, such as those found when designing trusses or electrical circuits.

**References**

