Max-value Entropy Search for Multi-Objective Bayesian Optimization with Constraints

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Abstract

We consider the problem of constrained multi-objective blackbox optimization using expensive function evaluations, where the goal is to approximate the true Pareto set of solutions satisfying a set of constraints while minimizing the number of function evaluations. For example, in aviation power system design applications, we need to find the designs that trade-off total energy and the mass while satisfying specific thresholds for motor temperature and voltage of cells. This optimization requires performing expensive computational simulations to evaluate designs. In this paper, we propose a new approach referred as Max-value Entropy Search for Multi-objective Optimization with Constraints (MESMOC) to solve this problem. MESMOC employs an output-space entropy based acquisition function to efficiently select the sequence of inputs for evaluation to uncover high-quality pareto-set solutions while satisfying constraints. We apply MESMOC to two real-world engineering design applications to demonstrate its effectiveness over state-of-the-art algorithms.

1. Introduction

Many engineering and scientific applications involve making design choices to optimize multiple objective. Some examples include tuning the knobs of a compiler to optimize performance and efficiency of a set of software programs; and designing new materials to optimize strength, elasticity, and durability. There are three common challenges in solving this kind of multi-objective optimization (MO) problems: 1) The objective functions are unknown and we need to perform expensive experiments to evaluate each candidate design choice. For example, performing computational simulations and physical lab experiments for compiler optimization and material design applications respectively. 2) The objectives are conflicting in nature and all of them cannot be optimized simultaneously. 3) The problem involves several black-box constraints that need to be satisfied. Therefore, we need to find the Pareto optimal set of solutions satisfying the constraints. A solution is called Pareto optimal if it cannot be improved in any of the objectives without compromising some other objective. The overall goal is to approximate the true Pareto set satisfying the constraints while minimizing the number of function evaluations.

Bayesian Optimization (BO) (Shahriari et al. (2016)) is an effective framework to solve blackbox optimization problems with expensive function evaluations. The key idea behind BO is to build a cheap surrogate model (e.g., Gaussian Process (Williams and Rasmussen (2006))) using the real experimental evaluations; and employ it to intelligently select the
sequence of function evaluations using an acquisition function, e.g., expected improvement (EI). There is a large body of literature on single-objective BO algorithms (Shahriari et al. (2016); Baptista and Poloczek (2018); Deshwal et al. (2020a,b)) and their applications including hyper-parameter tuning of machine learning methods (Snoek et al. (2012); Kotthoff et al. (2017)). However, there is relatively less work on the more challenging problem of BO for multiple objectives (Knowles (2006); Emmerich and Klinkenberg (2008); Hernández-Lobato et al. (2016); Belakaria et al. (2019, 2020a)) and very limited prior work to address constrained MO problems (Garrido-Merchán and Hernández-Lobato (2019); Feliot et al. (2017)). PESMOC (Garrido-Merchán and Hernández-Lobato (2019)) is the current state-of-the-art method in this problem setting. PESMOC is an information-theoretic approach that relies on the principle of input space entropy search. However, it is computationally expensive to optimize the acquisition function behind PESMOC. A series of approximations are performed to improve the efficiency potentially at the expense of accuracy.

In this paper, we propose a new and principled approach referred as Max-value Entropy Search for Multi-objective Optimization with Constraints (MESMOC). MESMOC employs an output space entropy based acquisition function to select the candidate inputs for evaluation. The key idea is to evaluate the input that maximizes the information gain about the optimal Pareto front in each iteration while satisfying the constraints. Output space entropy search has many advantages over algorithms based on input space entropy search (Belakaria et al. (2019)); a) allows tighter approximation; b) significantly cheaper to compute; and c) naturally lends itself to robust optimization. MESMOC is an extension of the MESMO algorithm Belakaria et al. (2019) based on output space information gain, which was shown to be efficient and robust, to the challenging constrained MO setting.

2. Background and Problem Setup

Bayesian Optimization (BO) Framework. BO is a very efficient framework to solve global optimization problems using black-box evaluations of expensive objective functions. Let \( \mathcal{X} \subseteq \mathbb{R}^d \) be an input space. In single-objective BO formulation, we are given an unknown real-valued objective function \( f : \mathcal{X} \mapsto \mathbb{R} \), which can evaluate each input \( x \in \mathcal{X} \) to produce an evaluation \( y = f(x) \). Each evaluation \( f(x) \) is expensive in terms of the consumed resources. The main goal is to find an input \( x^* \in \mathcal{X} \) that approximately optimizes \( f \) by performing a limited number of function evaluations. BO algorithms learn a cheap surrogate model from training data obtained from past function evaluations. They intelligently select the next input for evaluation by trading-off exploration and exploitation to quickly direct the search towards optimal inputs. The three key elements of BO framework are:

1) **Statistical Model** of the true function \( f(x) \). Gaussian Process (GP) Williams and Rasmussen (2006) is the most commonly used model. A GP over a space \( \mathcal{X} \) is a random process from \( \mathcal{X} \) to \( \mathbb{R} \). It is characterized by a mean function \( \mu : \mathcal{X} \mapsto \mathbb{R} \) and a covariance or kernel function \( \kappa : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R} \). If a function \( f \) is sampled from \( \text{GP}(\mu, \kappa) \), then \( f(x) \) is distributed normally \( N(\mu(x), \kappa(x, x)) \) for a finite set of inputs from \( x \in \mathcal{X} \).

2) **Acquisition Function** \( \alpha \) to score the utility of evaluating a candidate input \( x \in \mathcal{X} \) based on the statistical model. Some popular acquisition functions in the single-objective literature include expected improvement (EI), upper confidence bound (UCB),
predictive entropy search (PES) Hernández-Lobato et al. (2014), and max-value entropy search (MES) Wang and Jegelka (2017).

3) Optimization Procedure to select the best scoring candidate input according to \( \alpha \) depending on statistical model. DIRECT Jones et al. (1993) is a very popular approach for acquisition function optimization.

Multi-Objective Optimization (MOO) Problem. Without loss of generality, our goal is to minimize real-valued objective functions \( f_1(x), f_2(x), \ldots, f_K(x) \), with \( K \geq 2 \), while satisfying \( L \) black-box constraints of the form \( C_1(x) \geq 0, C_2(x) \geq 0, \ldots, C_L(x) \geq 0 \) over continuous space \( X \subseteq \mathbb{R}^d \). Each evaluation of an input \( x \in X \) produces a vector of objective values and constraint values \( y = (y^{f_1}, y^{f_2}, \ldots, y^{f_K}, y^{c_1}, \ldots, y^{c_L}) \) where \( y^{f_j} = f_j(x) \) for all \( j \in \{1, 2, \ldots, K\} \) and \( y^{c_i} = C_i(x) \) for all \( i \in \{1, 2, \ldots, L\} \). We say that a valid point \( x \) (satisfies all constraints) Pareto-dominates another point \( x' \) if \( f_j(x) \leq f_j(x') \forall j \) and there exists some \( j \in \{1, 2, \ldots, K\} \) such that \( f_j(x) < f_j(x') \). The optimal solution of MOO problem with constraints is a set of points \( X^* \subseteq X \) such that no point \( x' \in X \setminus X^* \) Pareto-dominates a point \( x \in X^* \) and all points in \( X^* \) satisfies the problem constraints. The solution set \( X^* \) is called the optimal Pareto set and the corresponding set of function values \( Y^* \) is called the optimal Pareto front. Our goal is to approximate \( X^* \) by minimizing the number of function evaluations.

3. MESMOC for Multi-Objective Optimization with Constraints

In this section, we explain the technical details of our proposed MESMOC algorithm. We first mathematically describe the output space entropy based acquisition function and provide an algorithmic approach to efficiently compute it.

Surrogate models. Gaussian processes (GPs) are shown to be effective surrogate models in prior work on single and multi-objective BO Hernández-Lobato et al. (2014); Wang et al. (2016); Wang and Jegelka (2017); Srinivas et al. (2009); Hernández-Lobato et al. (2016). Similar to prior work Hernández-Lobato et al. (2016), we model the objective functions and blackbox constraints by independent GP models \( \mathcal{M}_{f_1}, \mathcal{M}_{f_2}, \ldots, \mathcal{M}_{f_K} \) and \( \mathcal{M}_{c_1}, \mathcal{M}_{c_2}, \ldots, \mathcal{M}_{c_L} \) with zero mean and i.i.d. observation noise. Let \( D = \{(x_i, y_i)\}_{i=1}^{t-1} \) be the training data from past \( t-1 \) function evaluations, where \( x_i \in X \) is an input and \( y_i = (y_i^{f_1}, \ldots, y_i^{f_K}, y_i^{c_1}, \ldots, y_i^{c_L}) \) is the output vector resulting from evaluating the objective functions and constraints at \( x_i \). We learn surrogate models from \( D \).

Output space entropy based acquisition function. Input space entropy based methods such as PESMO Hernández-Lobato et al. (2016) selects the next candidate input \( x_t \) (for ease of notation, we drop the subscript in below discussion) by maximizing the information gain about the optimal Pareto set \( X^* \). The acquisition function based on input space entropy is given as follows:

\[
\alpha(x) = I(\{x, y\}, X^* \mid D) \tag{1}
\]

\[
= H(X^* \mid D) - \mathbb{E}_y[H(X^* \mid D \cup \{x, y\})] \tag{2}
\]

\[
= H(y \mid D, x) - \mathbb{E}_{X^*}[H(y \mid D, x, X^*)] \tag{3}
\]

Information gain is defined as the expected reduction in entropy \( H(\cdot) \) of the posterior distribution \( P(X^* \mid D) \) over the optimal Pareto set \( X^* \) as given in Equations 2 and 3.
(resulting from symmetric property of information gain). This mathematical formulation relies on a very expensive and high-dimensional \((m \cdot d)\) dimensions distribution \(P(X^* | D)\), where \(m\) is size of the optimal Pareto set \(X^*\). Furthermore, optimizing the second term in r.h.s poses significant challenges: a) requires a series of approximations Hernández-Lobato et al. (2016) which can be potentially sub-optimal; and b) optimization, even after approximations, is expensive c) performance is strongly dependent on the number of Monte-Carlo samples.

To overcome the above challenges of computing input space entropy based acquisition function, Belakaria et al. (2019) proposed to maximize the information gain about the optimal Pareto front \(Y^*\). However, MESMO did not address the challenge of constrained Pareto front. We propose an extension of MESMO’s acquisition function to maximize the information gain between the next candidate input for evaluation \(x\) and constrained Pareto front \(Y^*_c\) given as:

\[
\alpha(x) = I\{\{x, y\}, Y^* | D\} = H(Y^* | D) - E_{y}[H(Y^* | D \cup \{x, y\})] = H(y | D, x) - E_{Y^*}[H(y | D, x, Y^*)]
\]

In this case, the output vector \(y\) is \(K + L\)-dimensional: \(y = (y_f^1, y_f^2, \ldots, y_f^K, y_c^1, \ldots, y_c^L)\) where \(y_f^j = f_j(x)\) for all \(j \in \{1, 2, \ldots, K\}\) and \(y_c^i = C_i(x)\) for all \(i \in \{1, 2, \ldots, L\}\). Consequently, the first term in the r.h.s of equation 6, entropy of a factorizable \((K + L)\)-dimensional Gaussian distribution \(P(y | D, x)\), can be computed in closed form as shown below:

\[
H(y | D, x) = \frac{(K + C)(1 + \ln(2\pi))}{2} + \sum_{j=1}^{K} \ln(\sigma_{f_j}(x)) + \sum_{i=1}^{L} \ln(\sigma_{c_i}(x))
\]

where \(\sigma_{f_j}^2(x)\) and \(\sigma_{c_i}^2(x)\) are the predictive variances of \(j^{th}\) function and \(i^{th}\) constraint GPs respectively at input \(x\). The second term in the r.h.s of equation 6 is an expectation over the Pareto front \(Y^*\). We can approximately compute this term via Monte-Carlo sampling as shown below:

\[
E_{Y^*}[H(y | D, x, Y^*)] \approx \frac{1}{S} \sum_{s=1}^{S} [H(y | D, x, Y^*_s)]
\]

where \(S\) is the number of samples and \(Y^*_s\) denote a sample Pareto front. The main advantages of our acquisition function are: computational efficiency and robustness to the number of samples (Belakaria et al. (2019)).

There are two key algorithmic steps to compute Equation 8: 1) How to compute Pareto front samples \(Y^*_s\)?; and 2) How to compute the entropy with respect to a given Pareto front sample \(Y^*_s\)? We provide solutions for these two questions below.

1) Computing Pareto front samples via cheap multi-objective optimization. To compute a Pareto front sample \(Y^*_s\), we first sample functions and constraints from the posterior GP models via random fourier features (Hernández-Lobato et al. (2014); Rahimi
and Recht (2008)) and then solve a cheap multi-objective optimization over the \(K\) sampled functions and \(L\) sampled constraints.

Cheap MO solver. We sample \(\tilde{f}_i\) from GP model \(\mathcal{M}_{f_j}\) for each of the \(K\) functions and \(C_i\) from GP model \(\mathcal{M}_{c_i}\) for each of the \(L\) constraints. A cheap constrained multi-objective optimization problem over the \(K\) sampled functions \(\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_K\) and the \(L\) sampled constraints \(\tilde{C}_1, \tilde{C}_2, \ldots, \tilde{C}_L\) is solved to compute the sample Pareto front \(\mathcal{Y}_s^*\). This cheap multi-objective optimization also allows us to capture the interactions between different objectives while satisfying the constraints. We employ the popular constrained NSGA-II algorithm (Deb et al. (2002a b)) to solve the constrained MO problem with cheap objective functions noting that any other algorithm can be used to similar effect.

2) Entropy computation with a sample Pareto front. Let \(\mathcal{Y}_s^* = \{z_1, \ldots, z_m\}\) be the sample Pareto front, where \(m\) is the size of the Pareto front and each \(z_i\) is a \((K + L)\)-vector evaluated at the \(K\) sampled functions and \(L\) sampled constraints \(z_i = \{z_{f_1}^i, \ldots, z_{f_K}^i, z_{c_1}^i, \ldots, z_{c_L}^i\}\). The following inequality holds for each component \(y^j\) of the \((K + L)\)-vector \(y = \{y_{f_1}, \ldots, y_{f_K}, y_{c_1}, \ldots, y_{c_L}\}\) in the entropy term \(H(y | D, x, \mathcal{Y}_s^*)\):

\[
y^j \leq \max\{z_{1}^j, \ldots, z_{m}^j\} \quad \forall j \in \{f_1, \ldots, f_K, c_1, \ldots, c_L\}\]

(9)

The inequality essentially says that the \(j^{th}\) component of \(y\) (i.e., \(y^j\)) is upper-bounded by a value obtained by taking the maximum of \(j^{th}\) components of all \(m\) \((K + L)\)-vectors in the Pareto front \(\mathcal{Y}_s^*\). This inequality had been proven by a contradiction in (Belakaria et al. (2019)) for \(j \in \{f_1, \ldots, f_K\}\). We assume the same for \(j \in \{c_1, \ldots, c_L\}\).

By combining the inequality 9 and the fact that each function is modeled as an independent GP, we can model each component \(y^j\) as a truncated Gaussian distribution since the distribution of \(y^j\) needs to satisfy \(y^j \leq \max\{z_{1}^j, \ldots, z_{m}^j\}\). Furthermore, a common property of entropy measure allows us to decompose the entropy of a set of independent variables into a sum over entropies of individual variables Cover and Thomas (2012):

\[
H(y | D, x, \mathcal{Y}_s^*) \simeq \sum_{j=1}^{K} H(y_{f_j} | D, x, \max\{z_{1}^{f_j}, \ldots, z_{m}^{f_j}\}) + \sum_{i=1}^{C} H(y_{c_i} | D, x, \max\{z_{1}^{c_i}, \ldots, z_{m}^{c_i}\})
\]

(10)

The r.h.s is a summation over entropies of \((K + L)\)-variables \(y = \{y_{f_1}, \ldots, y_{f_K}, y_{c_1}, \ldots, y_{c_L}\}\). The differential entropy for each \(y^j\) is the entropy of a truncated Gaussian distribution (Michalowicz et al. (2013)) and given by the following equations:

\[
H(y_{f_j} | D, x, y_s^{f_j*}) \simeq \left[\frac{1 + \ln(2\pi)}{2} + \ln(\sigma_{f_j}(x)) + \ln \Phi(\gamma_{s}^{f_j}(x)) - \frac{\gamma_{s}^{f_j}(x)\phi(\gamma_{s}^{f_j}(x))}{2\Phi(\gamma_{s}^{f_j}(x))}\right]
\]

(11)

\[
H(y_{c_i} | D, x, y_s^{c_i*}) \simeq \left[\frac{1 + \ln(2\pi)}{2} + \ln(\sigma_{c_i}(x)) + \ln \Phi(\gamma_{s}^{c_i}(x)) - \frac{\gamma_{s}^{c_i}(x)\phi(\gamma_{s}^{c_i}(x))}{2\Phi(\gamma_{s}^{c_i}(x))}\right]
\]

(12)
Consequently we have:

\[
H(y \mid D, x, Y^*_{s}) \simeq \sum_{j=1}^{K} \left[ \frac{1 + \ln(2\pi)}{2} + \ln(\sigma_{fj}(x)) + \ln(\Phi(\gamma_{fs}^j(x))) - \frac{\gamma_{fs}^j(x)\phi(\gamma_{fs}^j(x))}{2\Phi(\gamma_{fs}^j(x))} \right] \\
+ \sum_{i=1}^{L} \left[ \frac{1 + \ln(2\pi)}{2} + \ln(\sigma_{ci}(x)) + \ln(\Phi(\gamma_{cs}^i(x))) - \frac{\gamma_{cs}^i(x)\phi(\gamma_{cs}^i(x))}{2\Phi(\gamma_{cs}^i(x))} \right]
\]

(13)

where \(\gamma_{cs}^i(x) = \frac{y_{ci}^*-\mu_{ci}(x)}{\sigma_{ci}(x)}\), \(\gamma_{fs}^j(x) = \frac{y_{fj}^*-\mu_{fj}(x)}{\sigma_{fj}(x)}\), \(y_{ci}^*\) and \(y_{fj}^*\) are the maximum values of constraint \(\tilde{c}_i\) and function \(\tilde{f}_j\) reached after the cheap multi-objective optimization over sampled functions and constraints. \(\phi\) and \(\Phi\) are the p.d.f and c.d.f of a standard normal distribution respectively. By combining equations 7 and 13 with Equation 6, we get the final form of our acquisition function as shown below:

\[
\alpha(x) \simeq \frac{1}{S} \sum_{s=1}^{S} \left[ \sum_{j=1}^{K} \frac{\gamma_{fs}^j(x)\phi(\gamma_{fs}^j(x))}{2\Phi(\gamma_{fs}^j(x))} - \ln(\Phi(\gamma_{fs}^j(x))) + \sum_{j=1}^{L} \frac{\gamma_{cs}^i(x)\phi(\gamma_{cs}^i(x))}{2\Phi(\gamma_{cs}^i(x))} - \ln(\Phi(\gamma_{cs}^i(x))) \right]
\]

(14)

A complete description of the MESMOC algorithm is given in Algorithm 1. The blue colored steps correspond to computation of our output space entropy based acquisition function via sampling.

4. Experiments and Results

In this section, we describe our experimental evaluation of MESMOC on two real-world engineering applications, namely, electrified aviation power system design and analog circuit design optimization tasks.

4.1 Experimental Setup

We compare MESMOC with PESMOC (Garrido-Merchán and Hernández-Lobato (2019)). Due to lack of BO approaches for constrained MO, we compare to known genetic algorithms (NSGA-II and MOEAD). However, they require large number of function evaluations to converge which is not practical for optimization of expensive functions. We use a GP based statistical model with squared exponential (SE) kernel in all our experiments. The hyper-parameters are estimated after every 5 function evaluations. We initialize the GP models for all functions by sampling initial points at random. The code is available in (github.com/belakaria/MESMOC)

**Electrified aviation power system design.** We consider optimizing the design of electrified aviation power system of unmanned aerial vehicle (UAV) via a time-based static simulation. The UAV system architecture consists of a central Li-ion battery pack, hex-bridge DC-AC inverters, PMSM motors, and necessary wiring (Belakaria et al. (2020b)). Each candidate input consists of a set of 5 \((d=5)\) variable design parameters such as the battery pack configuration (battery cells in series, battery cells in parallel) and motor size...
The remaining input variables are four output voltage references $V_{\text{ref}}$, four resistances $R_i$, variables are the width, length, and unit of the eight capacitors of the circuit $W_i, L_i, M_i \forall i \in 1 \cdots 8$. The remaining input variables are four output voltage references $V_{\text{ref}}$, four resistances $R_i$, and a switching frequency $f$. We optimize nine objectives:

(number of motors, motor stator winding length, motor stator winding turns). We minimize two objective functions: mass and total energy. This problem has 5 black-box constraints:

$$C_0 : \text{Maximum final depth of discharge} \leq 75\%$$
$$C_1 : \text{Minimum cell voltage} \geq 3V$$
$$C_2 : \text{Maximum motor temperature} \leq 125^\circ C$$
$$C_3 : \text{Maximum inverter temperature} \leq 120^\circ C$$
$$C_5 : \text{Maximum modulation index} \leq 1.3$$

For a design to be valid, the simulated UAV must be capable of completing the specified mission without violating any of the constraints. The overall design space has a total of 250,000 possible candidate designs. Out of the entire design space, only 9% of the designs are valid (i.e., satisfy all the constraints), which makes it a very challenging task. Additionally, only five points are in the optimal Pareto front.

**Analog circuit optimization domain.** We consider optimizing the design of a multi-output switched-capacitor voltage regulator via Cadence circuit simulator that imitates the real hardware Belakaria et al. (2020c). This circuit relies on a dynamic frequency switching clock. Each candidate circuit design is defined by 33 input variables ($d=33$). The first 24 variables are the width, length, and unit of the eight capacitors of the circuit $W_i, L_i, M_i \forall i \in 1 \cdots 8$. The remaining input variables are four output voltage references $V_{\text{ref}}$, four resistances $R_i$, and a switching frequency $f$.

**Algorithm 1** MESMOC Algorithm

| Input: input space $X$; $K$ blackbox functions $f_1(x), f_2(x), \cdots, f_K(x)$; $L$ blackbox constraints $C_1(x), C_2(x), \cdots, C_L(x)$; and maximum no. of iterations $T_{\text{max}}$ |
|---|
| 1: Initialize Gaussian process models $M_{f_1}, M_{f_2}, \cdots, M_{f_K}$ and $M_{c_1}, M_{c_2}, \cdots, M_{c_L}$ by evaluating at $N_0$ initial points |
| 2: for each iteration $t = N_0 + 1$ to $T_{\text{max}}$ do |
| 3: Select $x_t \leftarrow \text{arg max}_{x \in X} \alpha_t(x)$ s.t $(\mu_{c_1} \geq 0, \cdots, \mu_{c_L} \geq 0)$ |
| 4: $\alpha_t(.)$ is computed as: |
| 5: for each sample $s \in 1, \cdots, S$: |
| 6: Sample $\tilde{f}_j \sim M_{f_j}, \ \forall j \in \{1, \cdots, K\}$ |
| 7: Sample $\tilde{C}_i \sim M_{c_i}, \ \forall i \in \{1, \cdots, L\}$ |
| 8: $\tilde{Y}_s \leftarrow \text{arg max}_{x \in X}(\tilde{f}_1, \cdots, \tilde{f}_K)$ s.t $(\tilde{C}_1 \geq 0, \cdots, \tilde{C}_L \geq 0)$ |
| 9: Compute $\alpha_t(.)$ based on the $S$ samples of $\tilde{Y}_s$ as given in Equation 14 |
| 10: Evaluate $x_t$; $y_t \leftarrow (f_1(x_t), \cdots, f_K(x_t), C_1(x_t), \cdots, C_L(x_t))$ |
| 11: Aggregate data: $D \leftarrow D \cup \{(x_t, y_t)\}$ |
| 12: Update models $M_{f_1}, M_{f_2}, \cdots, M_{f_K}$ and $M_{c_1}, M_{c_2}, \cdots, M_{c_L}$ |
| 13: $t \leftarrow t + 1$ |
| end for |
| return Pareto front of $f_1(x), f_2(x), \cdots, f_K(x)$ based on $D$ |
maximize efficiency $Eff$, maximize four output voltages $V_{o1} \cdots V_{o4}$, and minimize four output ripples $OR_{1} \cdots OR_{4}$. Our problem has a total of nine constraints. Since some of the constraints have upper bounds and lower bounds, they are defined in the problem by 15 different constraints:

$$C_0 : \text{Cp}_{\text{total}} \simeq 20nF \text{ with } \text{Cp}_{\text{total}} = \sum_{i=1}^{8}(1.955W_iL_i + 0.54(W_i + L_i))M_i$$

$$C_1 \text{ to } C_4 : V_{o_i} \geq V_{\text{ref}_i} \forall i \in 1 \cdots 4$$

$$C_5 \text{ to } C_8 : OR_{lb} \leq OR_i \leq OR_{ub} \forall i \in 1 \cdots 4$$

$$C_9 : Eff \leq 100\%$$

where $OR_{lb}$ and $OR_{ub}$ are the predefined lower-bound and upper-bound of $OR_i$ respectively. $C_{p\text{total}}$ is the total capacitance of the circuit.

**Multi-objective BO algorithms.** We compare MESMOC with the existing constrained MO method PESMOC. Due to lack of BO approaches for constrained MO setting, we compare to known genetic algorithms (NSGA-II and MOEAD). However, they require large number of function evaluations to converge which is not practical for the optimization of expensive functions.

### 4.2 Results and Discussion

We evaluate the performance of our algorithm and the baselines using the Pareto hypervolume (PHV) metric. PHV is a commonly employed metric to measure the quality of a given Pareto front Zitzler (1999). Figure 1 shows that MESMOC outperforms existing baselines. It recovers a better Pareto front with a significant gain in the number of function evaluations. Both of these experiments are motivated by real-world engineering applications where further analysis of the designs in the Pareto front is crucial.

**Electrified aviation power system design.** In this setting, the input space is discrete with 250,000 combinations of design parameters. Out of the entire design space, only 9% of design combinations passed all the constraints and only five points are in the optimal Pareto front. From a domain expert perspective, satisfying all the constraints is critical. Hence, the results reported for the hypervolume include only points that satisfy all the constraints. Despite the hardness of the problem, 50% of the designs selected by MESMOC satisfy all the constraints while for PESMOC, MOEAD, and NSGA-II, this was 1.5%, 9.5%, and 7.5% respectively. MESMOC was not able to recover all the five points of the optimal Pareto front. However, it was able to reach closely approximate the true Pareto front and recover better designs than the baselines.

**Analog circuit design optimization.** In this setting, the input space is continuous, consequently there is an infinite number of candidate designs. From a domain expert perspective, satisfying all the constraints is not critical and is impossible to achieve. The main goal is to satisfy most of the constraints (and getting close to satisfying the threshold for violated constraints) while reaching the best possible objective values. Therefore, the results reported for the hypervolume include all the evaluated points. In this experiment, the efficiency of circuit is the most important objective function. The table in Figure 2 shows the optimized circuit parameters from different algorithms.
Figure 1: Results of different constrained multi-objective algorithms including MESMOC. The hypervolume metric is shown as a function of the number function evaluations.

| SPECS | NSGA-II | PESMOC | MESMOC |
|-------|---------|--------|--------|
| $V_{ref}(V)$ | 0.6 | 0.5 | 0.52 | 0.53 | 0.63 | 0.52 |
| $V_{ref}(V)$ | 0.55 | 0.62 | 0.55 | 0.61 | 0.51 | 0.53 |
| $V_{ref}(V)$ | 1.06 | 1.06 | 1.07 | 1.12 | 1.05 | 1.13 |
| $V_{ref}(V)$ | 1.07 | 1.09 | 1.09 | 1.06 | 1.05 | 1.06 |
| $V_{in}(mV)$ | 699.6 | 713.1 | 677.10 | 760.60 | 678.40 | 551.62 |
| $V_{out}(mV)$ | 700.4 | 712.2 | 690.70 | 725.70 | 520.61 | 632.80 |
| $V_{out}(V)$ | 1.10 | 1.06 | 1.08 | 1.15 | 1.12 | 1.16 |
| $V_{out}(V)$ | 1.09 | 1.09 | 1.08 | 0.99 | 1.14 | 1.08 |
| Eff(%) | 73.26 | 71.85 | 76.20 | 74.82 | 88.81 | 88.53 |

Figure 2: Comparison table of optimized circuit parameters obtained different algorithms (designs are selected from the Pareto set prioritized by efficiency)

All algorithms can generate design parameters for the circuit that meets the voltage reference requirements. The optimized circuit using MESMOC can achieve the highest conversion efficiency of 88.81% (12.61% improvement when compared with PESMOC with fixed frequency optimization and 17.86% improvement when compared with NSGA-II) with similar output ripples. The circuit with optimized parameters can generate the target output voltages within the range of 0.52V to 0.76V (1/3x ratio) and 0.99V to 1.17V (2/3x ratio) under the loads varying from 14 Ohms to 1697 Ohms.
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