

SMOG: Scalable Meta-Learning for Multi-Objective Bayesian Optimization

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Abstract

Multi-objective optimization aims to solve problems with competing objectives, often with only black-box access to a problem and a limited budget of measurements. In many applications, historical data from related optimization tasks is available, creating an opportunity for meta-learning to accelerate the optimization. Bayesian optimization, as a promising technique for black-box optimization, has been extended to meta-learning and multi-objective optimization independently, but methods that simultaneously address both settings—meta-learned priors for multi-objective Bayesian optimization—remain largely unexplored. We propose SMOG, a scalable and modular meta-learning model based on a multi-output Gaussian process that explicitly learns correlations between objectives. SMOG builds a structured joint Gaussian process prior across meta- and target tasks and, after conditioning on metadata, yields a closed-form target-task prior augmented by a flexible residual multi-output kernel. This construction propagates metadata uncertainty into the target surrogate in a principled way. SMOG supports hierarchical, parallel training: meta-task Gaussian processes are fit once and then cached, achieving linear scaling with the number of meta-tasks. The resulting surrogate integrates seamlessly with standard multi-objective Bayesian optimization acquisition functions.

1. Introduction

Many high-impact optimization problems are intrinsically *multi-objective*: engineers and machine-learning practitioners rarely optimize a single scalar, but rather trade off competing goals such as performance vs. cost, quality vs. speed, or accuracy vs. latency/energy. At the same time, these

objectives are often *expensive* and *noisy* to evaluate, which naturally puts us in the low-data regime where Bayesian optimization (BO)/multi-objective Bayesian optimization (MOBO) is particularly effective (Snoek et al., 2012; Zhang et al., 2020; Shahriari et al., 2016; Daulton et al., 2020; 2021). Crucially, such optimizations are rarely one-off: organizations accumulate logs of past runs on related products, machines, datasets, workloads, or environments. This makes *meta-learning for expensive multi-objective optimization* a natural setting: rather than starting each new optimization from scratch, we would like to leverage prior tasks to achieve good Pareto-optimal trade-offs with far fewer evaluations. Examples span industrial process tuning and calibration (where competing quality metrics must be balanced), scientific design (e.g., materials discovery and advanced manufacturing with multiple competing properties), and machine-learning system design (e.g., multi-objective hyperparameter and architecture tuning trading off accuracy, latency, and resource use) (Gopakumar et al., 2018; Myung et al., 2025; Pfisterer et al., 2022; Eggensperger et al., 2021; Marco et al., 2017; Herbol et al., 2018).

Despite its promise, meta-learning for multi-objective optimization is technically subtle in the low-data regime. First, in multi-objective settings, “what to transfer” is not a single optimum but information about a *Pareto set/front*, and decision making typically depends on uncertainty-aware criteria (e.g., hypervolume-based utilities) (Knowles, 2006; Daulton et al., 2020; 2021). Second, historical data are often scarce and heterogeneous across tasks; transfer must therefore account for *meta-task uncertainty* to avoid over-confident bias from weak or mismatched prior tasks (Dai et al., 2022; Volpp et al., 2020; Feurer et al., 2022; Tighineanu et al., 2024). Third, multi-objective problems add another layer: objectives can be correlated, so efficiently using evidence often requires non-trivial *probabilistic multi-output surrogates*. Treating objectives independently can waste information precisely when evaluations are precious.

These challenges leave a key gap: we need meta-learning methods that are (i) Bayesian uncertainty-aware, (ii) scalable across many meta-tasks, and (iii) able to exploit cross-objective correlations. Fully joint multi-task multi-output GP models are principled but quickly become infeasible at meta-learning scale (Rasmussen & Williams, 2006; Álvarez et al., 2012), while most scalable alternatives are developed

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for single-objective transfer and treat objectives independently when adapted to MOBO.

Contribution. We introduce SMOG (Scalable Meta-Learning and Multi-Objective GP), a probabilistic framework that closes this gap by *meta-learning a correlated multi-objective Gaussian process (GP) surrogate* while retaining principled Bayesian uncertainty propagation from historical tasks. Building on the modular GP meta-learning perspective of Tighineanu et al. (2024), SMOG constructs a structured multi-output prior that (i) remains *fully Bayesian* over all task data, (ii) *learns correlations between objectives* through vector-valued GP structure, and (iii) is *scalable in the number of meta-tasks* via a modular decomposition that enables parallel training and caching of meta-task posteriors. This yields a target-task surrogate that can be dropped into standard MOBO pipelines (e.g., hypervolume-based acquisition optimization) (Daulton et al., 2020; 2021; Knowles, 2006), with coherent propagation of meta-data uncertainty to the target task.

2. Related Work

Most work on meta-learning for BO focuses on learning a better surrogate for a single-objective target task. A principled approach is to build a *joint* Bayesian model across tasks (e.g., a multi-task GP), which yields coherent uncertainty estimates but is computationally prohibitive—scaling cubically in the total number of observations and, at best, quadratically in the task-correlation hyperparameters (Bonilla et al., 2007; Cao et al., 2010; Álvarez et al., 2012; Swersky et al., 2013; Yogatama & Mann, 2014; Joy et al., 2016; Poloczek et al., 2017; Shilton et al., 2017; Tighineanu et al., 2022). To improve scalability, a number of methods rely either on heuristic combinations of per-task surrogates (e.g., GP ensembles) (Feurer et al., 2022; Wistuba et al., 2018; Dai et al., 2022) or on building a parametric GP prior on the metadata (Perrone et al., 2018a; Salinas et al., 2020; Wistuba & Grabocka, 2021; Wang et al., 2021). These scale better with the number of meta-tasks but sacrifice a joint Bayesian treatment and thus principled uncertainty propagation across tasks. A recent work addresses this tension by introducing assumptions that lead to a modular GP model: conditioning on meta-data exposes a modular decomposition into M independent meta-task GP posteriors and a target-task GP prior, enabling scalable and fully Bayesian transfer (Tighineanu et al., 2024).

In contrast to the rich single-objective literature, meta-learning methods that directly target multi-objective optimization remain scarce. A notable exception is the task-similarity extension of MO-TPE by Watanabe et al. (2023), which transfers knowledge by reweighting the acquisition based on task similarity. While effective and scalable, it

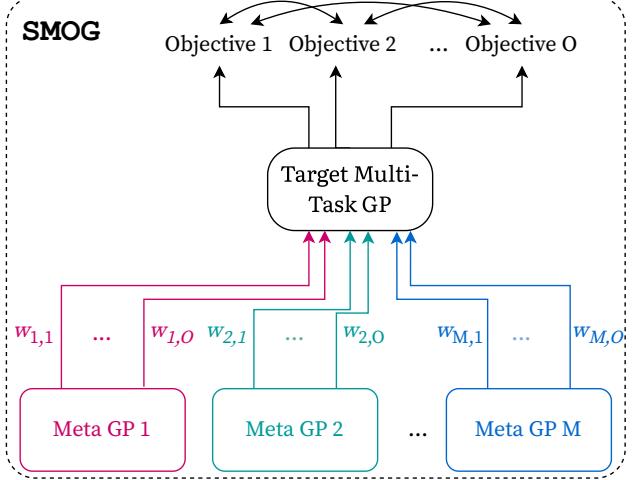


Figure 1. High-level view of SMOG: Meta tasks are modeled independently of the target GP. The target GP models correlations between objectives and uses the weighted means and covariances of the meta GPs to learn an informative target-task prior.

operates at the level of density models/acquisition rather than a unified probabilistic multi-output surrogate. Recent few-shot surrogate-assisted evolutionary methods for expensive multi-objective optimization meta-learn surrogates (Yu, 2025). However, both approaches typically do not learn a correlated multi-output posterior and thus cannot exploit cross-objective dependencies or propagate meta-task uncertainty to the target surrogate in a principled way. Our work targets this underexplored regime by combining scalable GP meta-learning with a multi-output surrogate that models cross-objective dependencies.

3. Method

We aim to find the Pareto set of a *target* black-box function $f_t : \mathcal{X} \rightarrow \mathbb{R}^O$, where $\mathcal{X} \subset \mathbb{R}^D$ is the search space of dimensionality D and O is the number of objectives. Observations $\mathbf{y}_n = (y_{n,o})_{o \in \mathcal{O}}$ of f_t may be corrupted by independent zero-mean Gaussian noise, $\mathbf{y}_n = f_t(\mathbf{x}_n) + \boldsymbol{\varepsilon}_n$ with $\boldsymbol{\varepsilon}_n \sim \mathcal{N}(\mathbf{0}, \text{diag}(\sigma_1^2, \dots, \sigma_O^2))$. We use the target data $\mathcal{D}_t = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^{N_t}$ to build a probabilistic model. Specifically, we model f_t with a multi-output GP prior with mean $m_o(\cdot)$ and kernel $k_{oo'}(\cdot, \cdot)$ for $o, o' \in \mathcal{O} = \{1, \dots, O\}$. Conditioned on \mathcal{D}_t , the posterior is again a GP with mean and covariance (Williams & Rasmussen, 2006)

$$\begin{aligned} \hat{m}_{t,o}(\mathbf{x}) &= m_o(\mathbf{x}) + \mathbf{k}((\mathbf{x}, o), \mathbf{X}_t) \\ &\quad [\mathbf{K}(\mathbf{X}_t, \mathbf{X}_t) + \boldsymbol{\Sigma}_\varepsilon]^{-1} (\mathbf{Y}_t - \mathbf{m}(\mathbf{X}_t)), \\ \hat{k}_{t,oo'}(\mathbf{x}, \mathbf{x}') &= \mathbf{k}((\mathbf{x}, o), (\mathbf{x}', o')) - \mathbf{k}((\mathbf{x}, o), \mathbf{X}_t) \\ &\quad [\mathbf{K}(\mathbf{X}_t, \mathbf{X}_t) + \boldsymbol{\Sigma}_\varepsilon]^{-1} \mathbf{k}(\mathbf{X}_t, (\mathbf{x}', o')), \end{aligned} \quad (1)$$

where $\mathbf{X}_t = ((\mathbf{x}_n, o))_{n=1, \dots, N_t, o \in \mathcal{O}}$ stacks the objective-augmented inputs and $\mathbf{Y}_t = (y_{n,o})_{n,o}$ the corresponding observations. We assume per-objective Gaussian noise $\Sigma_\varepsilon = \text{diag}(\sigma_1^2 \mathbf{I}_{N_t}, \dots, \sigma_O^2 \mathbf{I}_{N_t})$.

To leverage related tasks, we assume access to $M \geq 1$ meta-tasks with datasets $\mathcal{D}_{1:M} = \bigcup_{m \in \mathcal{M}} \mathcal{D}_m$, where $\mathcal{M} = [M]$. Each meta-task m provides $\mathcal{D}_m = \{(\mathbf{x}_{m,n}, y_{m,n})\}_{n=1}^{N_m}$ with $y_{m,n} \in \mathbb{R}^O$ and per-objective Gaussian noise $y_{m,n} = f_m(\mathbf{x}_{m,n}) + \varepsilon_{m,n}$, $\varepsilon_{m,n} \sim \mathcal{N}(\mathbf{0}, \text{diag}(\sigma_{m,1}^2, \dots, \sigma_{m,O}^2))$. For notational convenience, we collect all observations of meta-task m by stacking the objective-augmented inputs and corresponding outputs as $\mathbf{X}_m = ((\mathbf{x}_{m,n}, o))_{n=1, \dots, N_m, o \in \mathcal{O}}$ and $\mathbf{Y}_m = (y_{m,n,o})_{n=1, \dots, N_m, o \in \mathcal{O}}$.

3.1. Method Description

SMOG combines meta-learning and multi-objective optimizations. Our derivation starts by assuming that the metadata and target data are described jointly by a multi-task kernel over all tasks and objectives

$$k[(\mathbf{x}, \nu, o), (\mathbf{x}', \nu', o')] = \sum_{v \in \mathcal{M}^*} \sum_{\theta \in \mathcal{O}} [c_{v\theta}]_{\nu o, \nu' o'} k_{v\theta}(\mathbf{x}, \mathbf{x}'), \quad (2)$$

where $\mathcal{M}^* = \mathcal{M} \cup \{t\}$ is the set of all tasks, t denotes the target index, $\nu, \nu' \in \mathcal{M}^*$ are task indices, $o, o' \in \mathcal{O}$ are indices of the objective, $k_{v\theta}$ are arbitrary kernel functions, and $C_{v\theta}$ positive semi-definite (PSD) matrices called *coregionalization matrices*, since their entries $[c_{v\theta}]_{\nu o, \nu' o'}$ model the covariances between two objectives (ν, o) and (ν', o') (Álvarez et al., 2012). We derive SMOG by imposing two assumptions on the multi-task GP in Equation (2) that focus learning on the most informative covariance terms, yielding a scalable, modular posterior with efficient evaluation.

Assumption 1. We neglect correlations between meta-task models and model each meta-task with its own kernel: $\text{Cov}(f_{mo}, f_{m'o'}) = \delta_{m=m'} k_m[(\mathbf{x}, o), (\mathbf{x}', o')]$ for all $m, m' \in \mathcal{M}$ and $o, o' \in \mathcal{O}$ (Tighineanu et al., 2024).

Assumption 1 is motivated by the fact that meta-tasks typically come from *complete* optimizations and thus contain far more data than the target task. Thus, modeling correlations between different meta-tasks is usually of limited value: the metadata is typically sufficient to learn each meta-task in isolation. Importantly, this independence is only assumed in the prior—conditioning on meta- and target data induces posterior correlations between meta-task functions via an explaining-away effect. This prior independence allows SMOG to scale to large numbers of meta tasks. With the second assumption, we model the target objectives $f_{t,o}$ as an additive combination of functions that are perfectly (anti-)correlated with the meta-task priors.

Assumption 2. The target-task model is given by a sum

of scaled meta-task functions, $\sum_{m \in \mathcal{M}} \tilde{f}_{mo}$, and a residual function, \tilde{f}_{to} . Explicitly, $f_{to} = \tilde{f}_{to} + \sum_{m \in \mathcal{M}} \tilde{f}_{mo}$, with $|\text{Corr}(\tilde{f}_{mo}, f_{mo})| = 1$, $\text{Cov}(\tilde{f}_{to}, f_{mo}) = 0$, and $\text{Cov}(\tilde{f}_{to}, \tilde{f}_{to'}) = k_t[(\mathbf{x}, o), (\mathbf{x}', o')], m \in \mathcal{M}, o, o' \in \mathcal{O}$.

Together, these two assumptions make SMOG learn efficiently for a large number of meta-tasks, M . By constraining the target-task components \tilde{f}_{mo} to be perfectly correlated with the corresponding meta-task models f_{mo} , we capture the idea that transferable structure from the meta-tasks should re-appear in the target task. This transfer is encoded by one free parameter $w_{mo} \in \mathbb{R}$ that must be learned. The residual function \tilde{f}_{to} captures aspects of the target task that the meta-task models cannot explain. Meta-learning is therefore effective if this residual can be learned faster than the target function from scratch. Assumptions 1 and 2 impose sparse structure on the coregionalization matrices $C_{m\theta}$ in Equation (2), which are parametrized by unconstrained scalar parameters $w_m \in \mathbb{R}^O$ for each meta-task $m \in \mathcal{M}$.

Lemma 1. Applying Assumptions 1 and 2 to Equation (2) yields a sparse structure with the following non-zero entries of the coregionalization matrices

$$\begin{aligned} [c_{t\theta}]_{to, to'} &= [c_{t\theta}]_{to', to} \equiv [h_{t\theta}]_{oo'}, \\ [c_{m\theta}]_{mo, mo'} &= [c_{m\theta}]_{mo', mo} = [h_{m\theta}]_{oo'}, \\ [c_{m\theta}]_{mo, to'} &= [c_{mo}]_{to', mo} = w_{mo'} [h_{m\theta}]_{oo'}, \\ [c_{m\theta}]_{to, to'} &= [c_{m\theta}]_{to', to} = w_{mo} w_{mo'} [h_{m\theta}]_{oo'}, \end{aligned} \quad (3)$$

where $[h_{v\theta}]_{oo'}$ are PSD in the basis (o, o') .

See Section A.1 for a proof. This sparse structure decreases the number of parameters in the kernel from $\mathcal{O}[M^3 O^3]$ in Equation (2) to $\mathcal{O}[MO^3]$ in Equation (3), which is linear in M . In other words, the coregionalization matrices are now populated by $O \times O$ blocks of $[h_{v\theta}]_{oo'}$.

Example for two meta-tasks and objectives. In the case of two meta-tasks and two objectives, we have the following coregionalization matrices in the basis $(m = 1, o = 1), (m = 1, o = 2), (m = 2, o = 1), (m = 2, o = 2), (t, o = 1), (t, o = 2)$:

$$\begin{aligned} C_{1\theta} &= \begin{pmatrix} \mathbf{H}_{1\theta} & \mathbf{0}_{2 \times 2} & W_1 \odot \mathbf{H}_{1\theta} \\ \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} \\ W_1^\top \odot \mathbf{H}_{1\theta} & \mathbf{0}_{2 \times 2} & W_1^\times \odot \mathbf{H}_{1\theta} \end{pmatrix} \\ C_{2\theta} &= \begin{pmatrix} \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} \\ \mathbf{0}_{2 \times 2} & \mathbf{H}_{2\theta} & W_2 \odot \mathbf{H}_{2\theta} \\ \mathbf{0}_{2 \times 2} & W_i^\top \odot \mathbf{H}_{2\theta} & W_2^\times \odot \mathbf{H}_{2\theta} \end{pmatrix} \\ C_{t\theta} &= \begin{pmatrix} \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} \\ \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} \\ \mathbf{0}_{2 \times 2} & \mathbf{0}_{2 \times 2} & \mathbf{H}_{t\theta} \end{pmatrix}, \\ W_i &= \begin{pmatrix} w_{i1} & w_{i2} \\ w_{i1} & w_{i2} \end{pmatrix}, \quad W_i^\times = \begin{pmatrix} w_{i1}^2 & w_{i1}w_{i2} \\ w_{i1}w_{i2} & w_{i2}^2 \end{pmatrix}, \end{aligned} \quad (4)$$

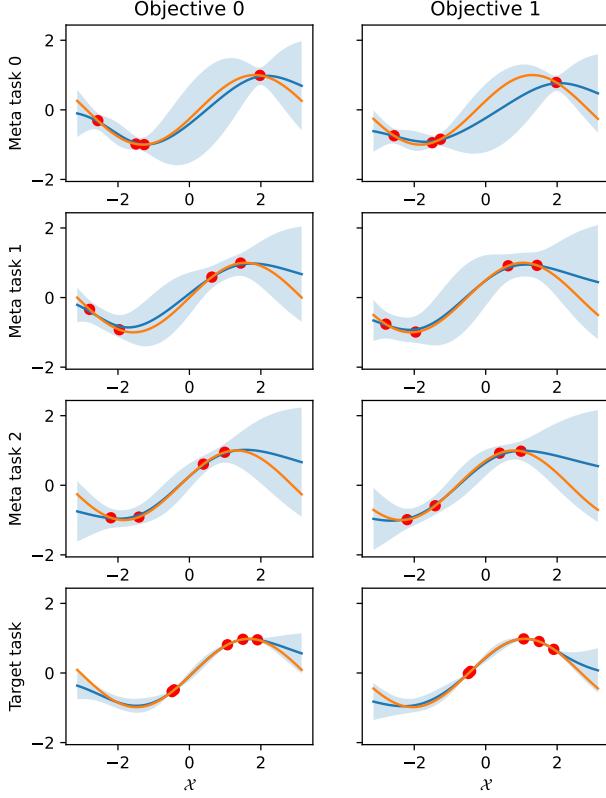


Figure 2. Example of a Sinusoidal function with two outputs (columns), three source tasks (rows 1–3), and one target task (row 4). SMOG learns a strong target-task posterior by leveraging meta tasks to learn an informative target-task prior, which is further refined by conditioning on the target data. See Section 4.2 for details on the benchmark.

where \odot is the elementwise (Hadamard) product. Here, $H_{v\theta}$ is matrix notation for $[h_{v\theta}]_{oo'}$ and describes cross-objective correlations.

Lemma 2. *Assumptions 1 and 2 with $w_{mo} \in \mathbb{R}$ for $m \in \mathbb{R}$ and $o \in \mathcal{O}$ yield a valid multi-task kernel given by*

$$k_{SMOG}[(\mathbf{x}, \nu, o), (\mathbf{x}', \nu', o')] = \sum_{v \in \mathcal{M}^*} g_v(\nu, o) g_v(\nu', o') k_v[(\mathbf{x}, o), (\mathbf{x}', o')], \quad (5)$$

where $g_v(\nu, o)$ is one if $v = \nu$, w_{mo} if $(v = m) \wedge (\nu = t)$, and zero otherwise.

See Section A.2 for a proof. According to Lemma 2, we have a valid joint kernel that defines the prior distribution over all meta- and target functions *before* observing data. The parameters of our kernel are successfully constrained to only scale linearly in M . The modular and computationally scalable nature of SMOG is revealed when conditioning Equation (5) on the metadata, yielding a valid GP as we show next.

Theorem 1. *Under a zero-mean GP prior with the multi-task kernel given by Equation (5), the distribution of the target-task objectives conditioned on the metadata is*

$$f_{to} | \mathcal{D}_{1:M}, \mathbf{x} \sim \mathcal{GP}(m_{t,SMOG}(\mathbf{x}, o), k_{t,SMOG}[(\mathbf{x}, o), (\mathbf{x}', o')]), \quad (6)$$

with

$$\begin{aligned} m_{t,SMOG}(\mathbf{x}, o) &= \sum_{m \in \mathcal{M}} w_{mo} \hat{m}_{mo}(\mathbf{x}) \\ k_{t,SMOG}[(\mathbf{x}, o), (\mathbf{x}', o')] &= k_t[(\mathbf{x}, o), (\mathbf{x}', o')] \\ &\quad + \sum_{m \in \mathcal{M}} w_{mo} w_{mo'} \hat{k}_{mo'}(\mathbf{x}, \mathbf{x}'), \end{aligned} \quad (7)$$

where $\hat{m}_{mo}(\mathbf{x})$ and $\hat{k}_{mo'}(\mathbf{x}, \mathbf{x}')$ are the posterior mean and covariance functions of the individual meta-task GPs conditioned only on their corresponding data, \mathcal{D}_m .

See Section B for a proof. According to Theorem 1, we can model each meta-task with an individual GP with a zero-mean prior and a multi-objective kernel $k_{mo'}$. The prior distribution of the target-task is also a GP, given by the weighted sum of the meta-task posteriors, as in Equation (7). This prior has striking similarity with the single-objective ScaML-GP, with an identical weighting of the meta-task posterior mean functions, while the posterior covariances differ: ScaML-GP scales them by a scalar w_m^2 , whereas SMOG uses products $w_{mo} w_{mo'}$ that weight and couple the full objective-objective covariance blocks. If the objectives are independent, SMOG reduces to describing each objective with a ScaML-GP model.

Equation (7) captures the key mechanism by which SMOG enables meta-learning. SMOG *learns* how to combine the predictions of meta-task models by tuning the weights w_{mo} during marginal likelihood optimization. Meta-tasks that align with the target receive large weights, while unrelated ones are effectively downweighted to zero. SMOG can therefore quickly meta-learn in the presence of even a few similar meta-tasks. At the core of SMOG’s meta-learning process lies a principled flow of uncertainty from the meta-task models to the target-task. This flow is fully Bayesian and is modulated by how well the posterior distribution of meta-task model m explains the target-task data. Figure 1 sketches the core ideas of SMOG. The linear sum in Equation (7) implies that SMOG reduces the complexity of the multi-task Gaussian process (MTGP) in Equation (2) from cubic in the number of points to *linear* in the number of tasks. We achieve this only via Assumptions 1 and 2 and without numerical approximations. The prior in Equation (7) is conditioned on \mathcal{D}_t via Equation (1) to obtain the target posterior

$$p(f_{to} | \mathbf{x}, \mathcal{D}_m, \mathcal{D}_t) = \mathcal{N}(\mu_{to}(\mathbf{x}), \Sigma_{too'}(\mathbf{x}, \mathbf{x}')). \quad (8)$$

Figure 2 shows how SMOG learns a strong target-task posterior with only four observations of the target task by leveraging observations on related meta-tasks.

Likelihood optimization In the following, we present an efficient implementation of SMOG, following the strategy by Tighineanu et al. (2024). We assume that the parameters of each meta-task model, θ_m , depend only on that meta-task’s data and are independent of the target data.

Assumption 3. For all meta-tasks $m \in \mathcal{M}$, we have $p(\theta_m | \mathcal{D}_m, \mathcal{D}_t) = p(\theta_m | \mathcal{D}_m)$.

The justification for this assumption is that meta-tasks typically have significantly more data than the target task, so we expect the meta-task model parameters to depend only weakly on the target data. Since the full marginal likelihood can be decomposed into a target-task and a meta-task term

$$\begin{aligned} p(\mathbf{Y}_t, \mathbf{Y}_{1:M} | \mathbf{X}_t, \mathbf{X}_{1:M}, \boldsymbol{\theta}_t, \boldsymbol{\theta}_{1:M}) &= \\ p(\mathbf{Y}_t | \mathcal{D}_{1:M}, \mathbf{X}_t, \boldsymbol{\theta}_t, \boldsymbol{\theta}_{1:M}) \prod_{m \in \mathcal{M}} p(\mathbf{Y}_m | \mathbf{X}_m, \boldsymbol{\theta}_m), \end{aligned} \quad (9)$$

this allows for modularizing the training procedure and inferring the meta-task hyperparameters (HPs) $\boldsymbol{\theta}_m$, containing the HPs of the meta-task GPs, independently of $\boldsymbol{\theta}_t$, containing the HPs of the target-task kernel k_t and the weights w_{mo} . In light of Assumption 1, we can train the meta-task GPs in parallel based only on their individual data, $\boldsymbol{\theta}_m^* = \arg \max_{\boldsymbol{\theta}_m} \log(p(\mathbf{Y}_m | \mathbf{X}_m, \boldsymbol{\theta}_m))$. Afterwards we compute the meta-task GP’s posterior mean, $\hat{\mathbf{m}}_{mo}(\mathbf{X}_t)$, and covariance matrix, $\hat{\mathbf{K}}_{mo'}(\mathbf{X}_t, \mathbf{X}_t)$, and cache them. This allows us to evaluate the target-task prior in Equation (7) and optimize the target-task log-likelihood via

$$\boldsymbol{\theta}_t^* = \arg \max_{\boldsymbol{\theta}_t} \log p(\mathbf{Y}_t | \mathcal{D}_{1:M}, \mathbf{X}_t, \boldsymbol{\theta}_t, \boldsymbol{\theta}_m^*), \quad (10)$$

which is cheap to evaluate. Since the meta-task GPs are independent of the target task, they can be computed once and reused during the entire optimization of the target task. We summarize SMOG in Algorithm 1.

Complexity Analysis A key feature of SMOG is that its computational complexity scales linearly in M . To see this, consider the cost incurred by the different steps of Algorithm 1. Step 2 involves the inversion of the data of each meta-task with an overhead $\mathcal{O}(O^3 \sum_{m \in \mathcal{M}} N_m^3)$. This happens only once during pre-training—those inverted matrices are cached. To construct the prior in step 3, we evaluate each meta-task posterior mean and covariance at \mathbf{X}_t with an overhead $\mathcal{O}(O^3 N_t^2 \sum_{m \in \mathcal{M}} N_m + O^3 N_t \sum_{m \in \mathcal{M}} N_m^2)$. Finally, step 4 involves inverting the target-task kernel matrix, which takes $\mathcal{O}(O^3 N_t^3)$. All these terms scale linearly in M and are cheap to evaluate in the practically relevant regime of small N_t and O , and moderate data per meta-task, given our assumption to be in the low-data regime.

Algorithm 1 SMOG

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- 1: **Input:** metadata $\mathcal{D}_{1:M} = \cup_{m \in \mathcal{M}} \mathcal{D}_m$
 - 2: Train individual GPs per meta-task and optimize $\boldsymbol{\theta}_m$
 - 3: Construct the target-task prior as in Equation (7), and cache $\hat{\mathbf{m}}_{mo}(\mathbf{X}_t)$ and $\hat{\mathbf{K}}_{mo'}(\mathbf{X}_t, \mathbf{X}_t)$
 - 4: Optimize the target-task HPs $\boldsymbol{\theta}_t$ as in Equation (10)
 - 5: Condition the prior on \mathcal{D}_t to obtain the posterior distribution for f_t as in Equation (1)
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4. Experimental Setup

We study the performance of SMOG relative to a wide range of competing optimization algorithms on benchmarks that reflect synthetic and real-world scenarios. We initialize each optimizer with only one uniformly randomly selected configuration, reflecting the data scarcity prevalent in meta-learning scenarios, and run each optimizer 50 times with different random seeds. For each run and at each iteration, we observe the difference of a configuration’s hypervolume to the best-observed hypervolume across models, repetitions, and iterations. We plot the mean difference (averaged across repetitions) and its standard error.

For every iteration following the initial random sample, each optimizer chooses the point of maximum LogNoisyExpectedHypervolumeImprovement (Ament et al., 2023), which depends on a reference point. We set this reference point using BoTorch’s infer_reference_point¹ applied to normalized Pareto-optimal objective values. The reference point is chosen slightly worse than the Pareto nadir point by moving it back by a fixed fraction (we use BoTorch’s default 0.1, proposed by Ishibuchi et al. (2011)) of the observed objective range in each dimension. To improve numerical stability, we standardize the objective values to have zero mean and unit variance before computing reference point and expected hypervolume.

4.1. Equicorrelated Multitask Kernel

For SMOG, we propose a lightweight parameterization of the task covariance in multi-output Gaussian processes. Assuming a separable (Kronecker) structure

$$\text{Cov}[f_i(x), f_j(x')] = k_X(x, x') K_T[i, j],$$

we restrict the task kernel $K_T \in \mathbb{R}^{m \times m}$ to have *equicorrelation*: all pairs of distinct tasks share a single correlation parameter ρ , while each task retains its own marginal scale

¹https://botorch.readthedocs.io/en/v0.16.1/_modules/botorch/utils/multi_objective/hypervolume.html, accessed on 01/26/2026

$\sigma_i > 0$:

$$K_T[i, j] = \begin{cases} \sigma_i^2, & i = j, \\ \rho \sigma_i \sigma_j, & i \neq j, \end{cases} \quad \rho \in (0, 1).$$

This can be written as a diagonal plus rank-1 decomposition,

$$K_T = (1 - \rho) \text{diag}(\sigma^2) + \rho \sigma \sigma^\top,$$

which is positive semidefinite by construction and computationally convenient. The decomposition also shows that our kernel is a constrained rank-1 multitask model: compared to the generic form $K_T = BB^\top + \text{diag}(v)$, our method ties $B = \sqrt{\rho} \boldsymbol{\sigma}$ and $v = (1 - \rho)\boldsymbol{\sigma}^2$, reducing the number of free parameters from $O(m)$ per component to $m + 1$ total. $\text{Corr}(i, j) = \rho$ for all $i \neq j$.

We impose at Beta(2, 2) hyperprior on ρ , i.e., we only model *positive* correlations, which is motivated by the fact that SMOG only models the difference between the output of the objective function and the target-task prior.

4.2. Benchmarks

We evaluate the performance of SMOG in controlled synthetic and real-world settings.

Sinusoidal Benchmark. To test whether SMOG behaves as expected, we define a simple one-dimensional benchmark function

$$\begin{aligned} f_{1,1}(x) &= \sin(x - \delta), & f_{2,1}(x) &= \sin(x) \\ f_{3,1}(x) &= \sin(x + \delta), & f_{m,2}(x) &= f_{m,1}(x + \phi) \end{aligned}$$

where $\delta = \frac{\pi}{12}$ and $\phi = \frac{\pi}{6}$. The target task is a weighted sum of the source tasks $f_{t,o}(x) = \mathbf{f}_o(x)^\top \mathbf{w}_o$, where $\mathbf{f}_o(x) = (f_{1,o}(x), \dots, f_{3,o}(x))$, $\mathbf{w}_1 = (0.5, 0.35, 0.15)$, and $\mathbf{w}_2 = (0.4, 0.4, 0.2)$. We do not run extensive experiments on this problem, but it is instructive to visualize the intermediate posterior of SMOG (see Figure 2).

Adapted Hartmann6 Benchmark. We define an adapted variant of the popular Hartmann6² benchmark problem. The Hartmann6 problem is defined as

$$f(\mathbf{x}) = -\sum_{i=1}^4 \alpha_i \exp \left(-\sum_{j=1}^6 A_{ij}(x_j - P_{ij})^2 \right),$$

where α is a vector of length 4 and A and P are known 4×6 matrices. We adapt this benchmark as follows to allow for meaningful multi-task, multi-objective optimization. First, we sample a separate coefficient vector, α_m , for each task. Second, we define an offset vector ε_o per objective and, for

²<https://www.sfu.ca/~ssurjano/hart6.html>, accessed on: 10/23/2025

each combination of task and objective $(m, o) \in \mathcal{M}^* \times \mathcal{O}$, aim to minimize

$$f_{m,o}(\mathbf{x}) = -\sum_{i=1}^4 \alpha_{m,i} \exp \left(-\sum_{j=1}^6 A_{ij}(x_j - P_{ij} - \varepsilon_{o,k}) \right).$$

See Appendix C.2 for additional details.

The 6-dimensional Hartmann benchmark can be configured to have varying numbers of objectives and meta-tasks. We set the number of meta tasks to 8 and observe 64 points per meta task, sampled uniformly at random. We additionally study the behavior of SMOG for different numbers of meta tasks and observations per meta task in Appendix D.

Tabular HPO Benchmarks To evaluate how SMOG performs in real-world settings, we investigate its performance on HPOBench benchmarks (Klein & Hutter, 2019). The goal in HPOBench is to jointly optimize a neural network architecture and its hyperparameters. The performance of a configuration can be observed on four different datasets: *Slice Localization*, *Protein Structure*, *Naval Propulsion*, and *Parkinson’s Telemonitoring*. The benchmark has two objectives: validation MSE and runtime. HPOBench can be run in a multi-fidelity setting by reducing the number of epochs. We always run for the maximum (100 epochs) and use one dataset as the target task and the remaining datasets as meta tasks.

Terrain Benchmark In this benchmark, we study unmanned aerial vehicle (UAV) trajectory optimization problems (Shehadeh & Kudela, 2025). The goal is to find a trajectory of 20 three-dimensional waypoints through one of 56 predefined landscapes that minimizes four target metrics: path length cost, obstacle avoidance cost, altitude cost, and smoothness cost. The performance in other landscapes is used as metadata for SMOG. We use the first three landscapes as target tasks and sample meta tasks uniformly at random from the remaining landscapes. See Appendix C.2 for additional details.

4.3. Models

We compare SMOG to the following set of optimization algorithms:

- MO-GP: A multi-task GP with Kronecker structure (Bonilla et al., 2007)
- Ind.-GP: A GP model without meta-learning and independent outputs
- Ind.-ScaML-GP: A ScaML-GP model with independent outputs (Tighineanu et al., 2024)
- MO-TPE: A tree-structured Parzen estimator (TPE)-based model that naturally handles multiple objectives and meta-learning (Watanabe et al., 2023)

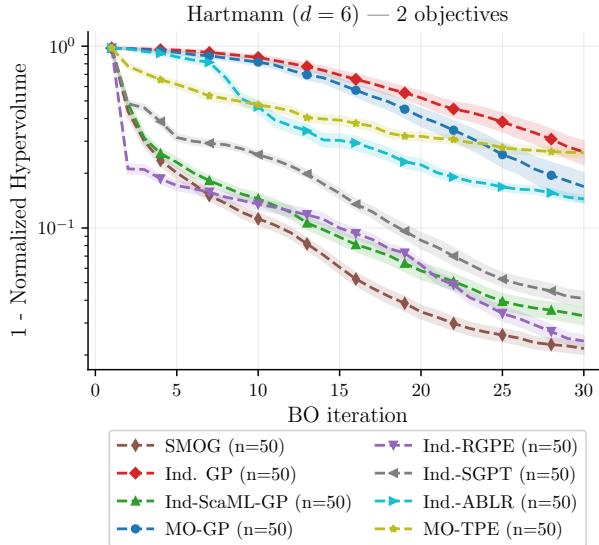


Figure 3. Performance of SMOG and competitors on the 6-dimensional two-objective Hartmann benchmark with 8 meta tasks and 64 observations per meta task.

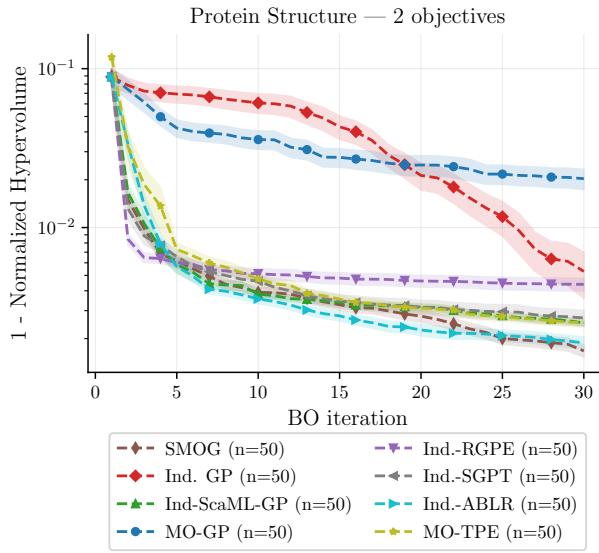


Figure 4. Performance of SMOG and competitors on the Protein Structure Problem. SMOG and Ind.-ABLR show the best performance, with SMOG having a slight advantage at the end of the optimization loop.

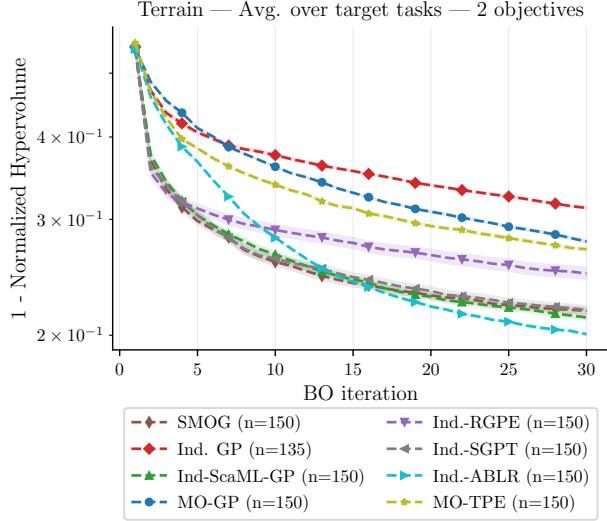


Figure 5. Performance of SMOG and competitors on the two-objective Terrain benchmark. The results are averaged over different target tasks. SMOG shows competitive aggregated performance.

- Ind.-RGPE: The RGPE model by Feurer et al. (2018) with independent outputs
- Ind.-ABLR: Adaptive Bayesian linear regression with independently-modeled outputs (Perrone et al., 2018b)
- Ind.-SGPT: The Scalable Gaussian Process Transfer framework by Wistuba et al. (2018) with independently-modeled outputs

5. Experimental Results

We empirically study the performance of SMOG and the methods defined in Section 4.3 on the synthetic and real-world benchmarks. We either plot the hypervolume (HV) of the Pareto front built from all solutions found up to a given BO iteration, or the gap to the best-observed HV across all optimization runs in a single plot.

5.1. Hartmann Benchmark

We first study the 6-dimensional Hartmann benchmark. Figure 3 shows the performance of SMOG and competitors on the variant with two objectives. As expected, the methods that do not leverage metadata (Ind.-GP and MO-GP) initially struggle to find good observations. MO-GP, which can model correlations across tasks, has an edge over Ind.-GP, arguably due to the more sample-efficient surrogate model. Next, we turn our attention to Ind.-ScaML-GP. Compared to Ind.-GP and MO-GP, this method achieves a considerable initial speedup by leveraging metadata. Similarly, Ind.-RGPE and Ind.-SGPT find good solutions early on, while Ind.-ABLR initially outperforms both Ind.-GP and MO-GP but later loses its ability to find sig-

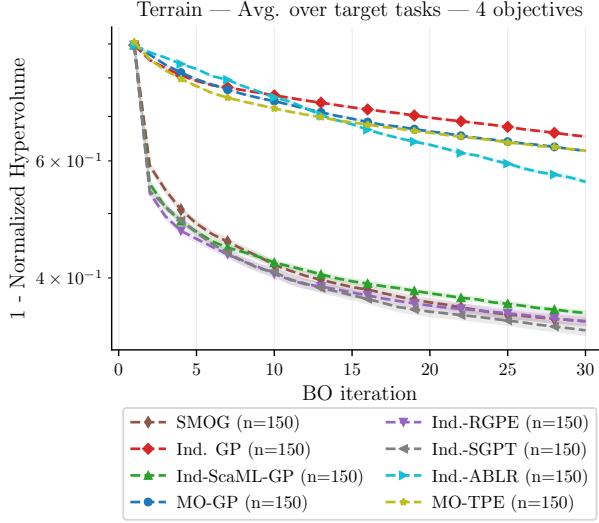


Figure 6. Performance of SMOG and competitors on the four-objective Terrain benchmark. The results are averaged over different target tasks. SMOG shows competitive aggregated performance.

nificantly better solutions.

Since SMOG not only leverages metadata but also models task correlations, it achieves a significant initial speedup and outperforms Ind.-ScaML-GP, which is most similar to SMOG but lacks the ability to model task correlations. In Section E.2, we study the solutions found by the different optimizers on these benchmarks in more detail.

The 4-objective Hartmann benchmark shows a similar picture as the 2-objective variant. For space reasons, we defer it to Figure 10 in the Appendix. Again, the methods leveraging metadata are mostly outperforming the metadata-free Ind.-GP and MO-GP. Interestingly, MO-TPE—the only other method naturally combining meta-learning and multi-objective optimization—outperforms the meta-learning-free Ind.-GP and MO-GP at early stages, but is otherwise not competitive with the other methods we studied.

5.2. HPOBench Benchmarks

Figure 4 shows the performance of SMOG and competitors on *Protein Structure* task of HPOBench. For space reasons, we defer the results on the datasets to Figure 13 in the Appendix. As observed in Figure 3, MO-GP initially finds better solutions than Ind.-GP. Later on, however, Ind.-GP outperforms MO-GP, which could be due to the simpler model. All other methods leverage metadata and outperform Ind.-GP and MO-GP by a wide margin. Notably, SMOG and also Ind.-ABLR, which is not competitive on the Hartmann benchmark, show the strongest performance on this benchmark.

5.3. Terrain Benchmark

Next, we study the optimizers’ performances on the Terrain benchmark. Figure 5 shows the HVs of the different optimizers for the two-objective variant of the Terrain benchmark, averaged over three target tasks and 50 random restarts per target task. Figure 6 studies the four-objective variant.

Interestingly, Ind.-ABLR, which achieves the best performance on the two-objective variants, fails to find a competitive solution on the four-objective problem. Again, the two methods that do not leverage metadata (MO-GP and Ind.-GP) are not competitive, indicating that observations from other terrains can help find a good solution for the target task. SMOG shows robust performance and is competitive with the best-performing methods on both problems.

6. Discussion

Many impactful applications require optimizing competing objectives: In aerospace engineering, one seeks a lightweight structure with the highest possible strength, while in machine learning, one aims to find accurate yet small models. In many cases, practitioners have access to data from related tasks or earlier experiments that they can use to quickly find a good solution for a new task.

In this paper, we introduce SMOG—a scalable meta-learning algorithm for multi-objective black-box optimization problems. SMOG leverages observations from related tasks and models inter-task correlations to construct an informative target-task posterior, improving sample efficiency in the initial BO iterations. SMOG is principled, with a clear theoretical motivation, and performs robustly when studied in practice: even though not the incumbent on every benchmark, it is competitive on every benchmark while every other method struggles on at least one problem. With its robust performance and principled approach, SMOG fills a gap for a ready-to-use algorithm that combines meta-learning and multi-objective optimization.

Impact. This paper presents work whose goal is to advance the field of machine learning. There are many potential societal consequences of our work, none of which we feel must be specifically highlighted here.

Acknowledgments. Calculations (or parts of them) for this publication were performed on the HPC cluster PALMA II of the University of Münster, subsidised by the DFG (INST 211/667-1). The authors gratefully acknowledge the computing time granted by the Resource Allocation Board and provided on the supercomputer Emmy/Grete at NHR-Nord@Göttingen as part of the NHR infrastructure. The calculations for this research were conducted with computing resources under the project nhr_nw_test. The authors grate-

fully acknowledge the computing time provided to them at the NHR Center NHR4CES at RWTH Aachen University (project number p0026398). This is funded by the Federal Ministry of Education and Research, and the state governments participating on the basis of the resolutions of the GWK for national high performance computing at universities (www.nhr-verein.de/unsere-partner).

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A. Kernel Properties

Here we prove the key properties of SMOG's kernel encoded in Lemmas 1 and 2.

A.1. Coregionalization Matrices

Here we prove Lemma 1, which we restate below.

Lemma 1. *Applying Assumptions 1 and 2 to Equation (2) yields a sparse structure with the following non-zero entries of the coregionalization matrices*

$$\begin{aligned} [c_{t\theta}]_{to,to'} &= [c_{t\theta}]_{to',to} \equiv [h_{t\theta}]_{oo'}, \\ [c_{m\theta}]_{mo,mo'} &= [c_{m\theta}]_{mo',mo} = [h_{m\theta}]_{oo'}, \\ [c_{m\theta}]_{mo,to'} &= [c_{mo}]_{to',mo} = w_{mo'} [h_{m\theta}]_{oo'}, \\ [c_{m\theta}]_{to,to'} &= [c_{m\theta}]_{to',to} = w_{mo} w_{mo'} [h_{m\theta}]_{oo'}, \end{aligned} \quad (3)$$

where $[h_{v\theta}]_{oo'}$ are PSD in the basis (o, o') .

Proof. We begin by showing that the coregionalization matrices in Equation (3) are uniquely defined by Assumptions 1 and 2. We collect all terms in Equation (2):

$$k[(\mathbf{x}, m, o), (\mathbf{x}', m, o')] = \text{Cov}[f_{mo}(\mathbf{x}), f_{mo'}(\mathbf{x}')] = k_m[(\mathbf{x}, o), (\mathbf{x}', o')] \quad (\text{Assumption 1}) \quad (11)$$

$$k[(\mathbf{x}, m, o), (\mathbf{x}', m' \neq m, o')] = 0 \quad (\text{Assumption 1}) \quad (12)$$

$$\begin{aligned} k[(\mathbf{x}, t, o), (\mathbf{x}', m, o')] &= \text{Cov}[f_{to}(\mathbf{x}), f_{mo'}(\mathbf{x}')] = \text{Cov}\left[\tilde{f}_{to} + \sum_{m' \in \mathcal{M}} \tilde{f}_{m'o}, f_{mo'}\right] \quad (\text{Assumption 2}) \\ &= \sum_{m' \in \mathcal{M}} w_{m'o} \text{Cov}[f_{m'o}, f_{mo'}] \quad (\text{Assumption 2}) \\ &= w_{mo} k_m[(\mathbf{x}, o), (\mathbf{x}', o')] \quad (\text{Assumption 1}), \end{aligned} \quad (13)$$

where we have made use of the fact that the covariance is a bilinear function, and that the perfect (anti-)correlation $\text{Corr}[f_{mo}(\mathbf{x}), \tilde{f}_{mo}(\mathbf{x}')] = \pm 1$ in Assumption 2 implies that $\tilde{f}_{mo}(\mathbf{x}) = w_{mo} f_{mo} + c$ with $w_{mo}, c \in \mathbb{R}$. Finally, we have

$$\begin{aligned} k[(\mathbf{x}, t, o), (\mathbf{x}', t, o')] &= \text{Cov}[f_{to}(\mathbf{x}), f_{to'}(\mathbf{x}')] \\ &= \text{Cov}\left[\tilde{f}_{to}(\mathbf{x}), \tilde{f}_{to'}(\mathbf{x}')\right] + \sum_{m, m' \in \mathcal{M}} w_{mo} w_{m'o'} \text{Cov}[f_{mo}(\mathbf{x}), f_{m'o'}(\mathbf{x}')] \quad (\text{Assumption 2}) \quad (14) \\ &= k_t[(\mathbf{x}, o), (\mathbf{x}', o')] + \sum_{m \in \mathcal{M}} w_{mo} w_{mo'} k_m[(\mathbf{x}, o), (\mathbf{x}', o')] \quad (\text{Assumptions 1 and 2}) \end{aligned}$$

By collecting the coefficients corresponding to k_m and k_t , we obtain the coregionalization matrices of SMOG in Equations (3) and (4).

These coregionalization matrices are elements of the original MTGP, implying that they are PSD by definition. To see this, consider the expression for the meta-task block of the MTGP kernel in Equation (2) (excluding the target task and all meta-task-to-target-task couplings):

$$k[(\mathbf{x}, m, o), (\mathbf{x}', m', o')] = \delta_{m=m'} \sum_{\theta \in \mathcal{O}} [h_{m\theta}]_{oo'} k_{m\theta}(\mathbf{x}, \mathbf{x}') \equiv \delta_{m=m'} k_m[(\mathbf{x}, o), (\mathbf{x}', o')], \quad (15)$$

where $[h_{m\theta}]_{oo'} = [c_{m\theta}]_{mo,mo'}$. This formulation does not make any additional assumptions about the kernel across objectives, $k_m[(\mathbf{x}, o), (\mathbf{x}', o')] = \sum_{\theta \in \mathcal{O}} [h_{m\theta}]_{oo'} k_{m\theta}(\mathbf{x}, \mathbf{x}')$. The elements $[h_{m\theta}]_{oo'}$ appear directly in Equation (3) and are by definition PSD. Similar reasoning can be applied to the other elements, implying that all entries of SMOG's coregionalization matrices in Equation (3) are PSD. \square

A.2. SMOG Kernel

Next, we prove Lemma 2, which we restate below.

Lemma 2. *Assumptions 1 and 2 with $w_{mo} \in \mathbb{R}$ for $m \in \mathbb{R}$ and $o \in \mathcal{O}$ yield a valid multi-task kernel given by*

$$k_{\text{SMOG}}[(\mathbf{x}, \nu, o), (\mathbf{x}', \nu', o')] = \sum_{v \in \mathcal{M}^*} g_v(\nu, o) g_v(\nu', o') k_v[(\mathbf{x}, o), (\mathbf{x}', o')], \quad (5)$$

where $g_v(\nu, o)$ is one if $v = \nu$, w_{mo} if $(v = m) \wedge (\nu = t)$, and zero otherwise.

Proof. We start off by using the results of Lemma 1, Equation (4). The first notational simplification for the coregionalization matrices can be done by pulling the common $\mathbf{H}_{v\theta}$ term outside the big matrix. To do this, we introduce a custom matrix product \boxtimes between matrices \mathbf{A} of size $(\alpha + \beta) \times (\alpha + \beta)$ and \mathbf{B} of size $\beta \times \beta$. Each $\beta \times \beta$ block of matrix \mathbf{A} is Hadamard-multiplied with matrix \mathbf{B} :

$$(\mathbf{A} \boxtimes \mathbf{B})_{\beta \times \beta} = \mathbf{A}_{\beta \times \beta} \odot \mathbf{B} \quad (16)$$

Applying this to Equation (4) yields coregionalization matrices that are described by a \boxtimes -product between a $(M + 1)O \times (M + 1)O$ matrix containing only weights, \mathbf{W}_v , and a $O \times O$ matrix $\mathbf{H}_{v\theta}$ describing task-specific correlations across its objectives:

$$\mathbf{C}_{v\theta} = \mathbf{W}_v \boxtimes \mathbf{H}_{v\theta} \quad (17)$$

Careful inspection of \mathbf{W}_v reveals that it can be written as an outer product, $\mathbf{w}_v \mathbf{w}_v^T$, where $\mathbf{w}_v = (\mathbf{w}_m^T, \mathbf{w}_t^T)^T$ and

$$\begin{aligned} \mathbf{w}_m &= (\dots, \mathbf{0}_{1 \times O}, \underbrace{\mathbf{1}_{1 \times O}}_{\text{m-th entry}}, \mathbf{0}_{1 \times O}, \dots, \mathbf{0}_{1 \times O}, w_{m1}, w_{m2}, \dots, w_{mO})^T \\ \mathbf{w}_t &= (\dots, \mathbf{0}_{1 \times O}, \mathbf{1}_{1 \times O})^T, \end{aligned} \quad (18)$$

implying that \mathbf{W}_v is PSD for all $w_{mo} \in \mathbb{R}$. Inserting this into Equation (2) yields the final expression for our kernel, which we write in matrix form of size $(M + 1)O \times (M + 1)O$ for convenience:

$$\begin{aligned} \mathbf{K}_{\text{SMOG}}(\mathbf{x}, \mathbf{x}') &= \sum_{v \in \mathcal{M} \cup \{t\}} \mathbf{w}_v \mathbf{w}_v^T \boxtimes \mathbf{K}_v(\mathbf{x}, \mathbf{x}'), \\ \mathbf{K}_v(\mathbf{x}, \mathbf{x}') &= \sum_{\theta \in \mathcal{O}} \mathbf{H}_{v\theta} k_{v\theta}(\mathbf{x}, \mathbf{x}'), \end{aligned} \quad (19)$$

where $\mathbf{K}_v(\mathbf{x}, \mathbf{x}')$ is a kernel of size $O \times O$ that acts on the objectives of task v . Since $\mathbf{K}_v(\mathbf{x}, \mathbf{x}')$ and \mathbf{W}_v are both PSD, the kernel in Equation (19) is also PSD and is therefore a valid kernel. Expressing the kernel in Equation (19) in index notation concludes the proof of Lemma 2. \square

B. SMOG Target-Task Prior

In the following we prove Theorem 1, which we restate below.

Theorem 1. *Under a zero-mean GP prior with the multi-task kernel given by Equation (5), the distribution of the target-task objectives conditioned on the metadata is*

$$f_{to} \mid \mathcal{D}_{1:M}, \mathbf{x} \sim \mathcal{GP}(m_{t,\text{SMOG}}(\mathbf{x}, o), k_{t,\text{SMOG}}[(\mathbf{x}, o), (\mathbf{x}', o')]) \quad (6)$$

with

$$\begin{aligned} m_{t,\text{SMOG}}(\mathbf{x}, o) &= \sum_{m \in \mathcal{M}} w_{mo} \hat{m}_{mo}(\mathbf{x}) \\ k_{t,\text{SMOG}}[(\mathbf{x}, o), (\mathbf{x}', o')] &= k_t[(\mathbf{x}, o), (\mathbf{x}', o')] \\ &\quad + \sum_{m \in \mathcal{M}} w_{mo} w_{mo'} \hat{k}_{mo o'}(\mathbf{x}, \mathbf{x}'), \end{aligned} \quad (7)$$

where $\hat{m}_{mo}(\mathbf{x})$ and $\hat{k}_{mo' mo'}(\mathbf{x}, \mathbf{x}')$ are the posterior mean and covariance functions of the individual meta-task GPs conditioned only on their corresponding data, \mathcal{D}_m .

Proof. According to Equation (5), the joint prior model for the meta-observations $\mathbf{Y}_{\text{meta}} = (\mathbf{Y}_1, \dots, \mathbf{Y}_M)$ and the test-task function value at a query point (\mathbf{x}, o) given by

$$\begin{bmatrix} \mathbf{Y}_{\text{meta}} \\ f_{to}(\mathbf{x}) \end{bmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{bmatrix} \mathbf{K}_{\text{meta}} & \mathbf{k}_{\text{meta},o} \\ \mathbf{k}_{\text{meta},o}^T & k_{t,oo} \end{bmatrix} \right) \quad (20)$$

where \mathbf{K}_{meta} is of size $N_{\text{meta}} \times N_{\text{meta}}$, \mathbf{k}_{meta} of size $N_{\text{meta}} \times 1$, and k_t a scalar, and are given by

$$\begin{aligned} \mathbf{K}_{\text{meta}} &= \text{diag}(k_1[(\mathbf{X}_1, \mathbf{o}_1), (\mathbf{X}_1, \mathbf{o}_1)] + \text{diag}(\sigma_{11}^2, \dots, \sigma_{1O}^2) \otimes \mathbf{I}_{\mathbf{X}_1}, \dots), \\ \mathbf{k}_{\text{meta},o} &= (w_{1o}k_1[(\mathbf{X}_1, \mathbf{o}_1), (\mathbf{x}, o)], \dots, w_{Mo}k_M[(\mathbf{X}_M, \mathbf{o}_M), (\mathbf{x}, o)]), \\ k_{t,oo} &= \left(k_t[(\mathbf{x}, o), (\mathbf{x}, o')] + \sum_{m \in \mathcal{M}} w_{mo}w_{mo'}k_m[(\mathbf{x}, o), (\mathbf{x}, o')] \right) \delta_{oo'} \equiv k_{t,oo'}\delta_{oo'} \end{aligned}$$

Conditioning on the metadata $\mathcal{D}_{1:M}$ yields

$$p(f_{to} \mid \mathcal{D}_{1:M}, \mathbf{x}) = \mathcal{N}(m_{t,\text{SMOG}}(\mathbf{x}, o), k_{t,\text{SMOG}}[(\mathbf{x}, o), (\mathbf{x}, o')]), \quad (21)$$

where the test-task prior mean $m_{t,\text{SMOG}}$ and covariance $k_{t,\text{SMOG}}$ are given by the standard Gaussian conditioning rules

$$\begin{aligned} m_{t,\text{SMOG}}(\mathbf{x}, o) &= \mathbf{k}_{\text{meta},o}^T \mathbf{K}_{\text{meta}}^{-1} \mathbf{y}_{\text{meta}}, \\ k_{t,\text{SMOG}}[(\mathbf{x}, o), (\mathbf{x}, o')] &= k_{t,oo'} - \mathbf{k}_{\text{meta},o}^T \mathbf{K}_{\text{meta}}^{-1} \mathbf{k}_{\text{meta},o'}. \end{aligned}$$

Now since \mathbf{K}_{meta} is block-diagonal in m , we have

$$\mathbf{K}_{\text{meta}}^{-1} = \text{diag}((k_1[(\mathbf{X}_1, \mathbf{o}_1), (\mathbf{X}_1, \mathbf{o}_1)] + \text{diag}(\sigma_1^2, \dots, \sigma_O^2) \otimes \mathbf{I}_{\mathbf{X}_1})^{-1}, \dots),$$

so that

$$\begin{aligned} m_{t,\text{SMOG}}(\mathbf{x}, o) &= \sum_m w_{mo}k_m[(\mathbf{x}, o), (\mathbf{X}_m, \mathbf{o}_m)] (k_m[(\mathbf{X}_m, \mathbf{o}_m), (\mathbf{X}_m, \mathbf{o}_m)] + \text{diag}(\sigma_{m1}^2, \dots, \sigma_{mO}^2) \otimes \mathbf{I}_{\mathbf{X}_m})^{-1} \mathbf{y}_m, \\ &= \sum_m w_{mo}\hat{m}_{mo}(\mathbf{x}), \end{aligned}$$

where $\hat{m}_m(\mathbf{x}, o)$ is the per meta-task posterior mean after conditioning on the corresponding data \mathcal{D}_m . Similarly, for the covariance we have

$$\begin{aligned} k_{t,\text{SMOG}}[(\mathbf{x}, o), (\mathbf{x}', o')] &= k_{t,oo'} - \mathbf{k}_{\text{meta},o}^T \mathbf{K}_{\text{meta}}^{-1} \mathbf{k}_{\text{meta},o'}, \\ &= k_t[(\mathbf{x}, o), (\mathbf{x}', o')] + \sum_m w_{mo}w_{mo'}k_m[(\mathbf{x}, o), (\mathbf{x}', o')] - \sum_m w_{mo}k_m[(\mathbf{x}, o), (\mathbf{X}_m, \mathbf{o}_m)] \\ &\quad \times (k_m[(\mathbf{X}_m, \mathbf{o}_m), (\mathbf{X}_m, \mathbf{o}_m)] + \text{diag}(\sigma_{m1}^2, \dots, \sigma_{mO}^2) \otimes \mathbf{I}_{\mathbf{X}_m})^{-1} w_{mo'}k_m[(\mathbf{X}_m, \mathbf{o}_m), (\mathbf{x}', o')], \\ &= k_t[(\mathbf{x}, o), (\mathbf{x}', o')] + \sum_m w_{mo}w_{mo'}(k_m[(\mathbf{x}, o), (\mathbf{x}', o')] - k_m[(\mathbf{x}, o), (\mathbf{X}_m, \mathbf{o}_m)] \\ &\quad \times (k_m[(\mathbf{X}_m, \mathbf{o}_m), (\mathbf{X}_m, \mathbf{o}_m)] + \text{diag}(\sigma_{m1}^2, \dots, \sigma_{mO}^2) \otimes \mathbf{I}_{\mathbf{X}_m})^{-1} k_m[(\mathbf{X}_m, \mathbf{o}_m), (\mathbf{x}', o')]), \\ &= k_t[(\mathbf{x}, o), (\mathbf{x}', o')] + \sum_m w_{mo}w_{mo'}\hat{k}_m[(\mathbf{x}, o), (\mathbf{x}', o')], \end{aligned}$$

where \hat{k}_m is the corresponding per meta-task posterior covariance. \square

C. Implementation Details

C.1. Mixed Space Acquisition Function Optimization

We employ an interleaving scheme to optimize the acquisition function, similar to that used by Wan et al. (2021) or Papenmeier et al. (2023). In particular, we optimize over the discrete variables by selecting the point with the maximum acquisition value from 2^{14} candidates uniformly sampled from the set of all possible discrete combinations. We then fix the discrete variables and optimize over the remaining variables using gradient-based acquisition function maximization with two random restarts and 512 initial samples to select the two starting points. We repeat this interleaving scheme 5 times, starting with the discrete optimization and a uniformly random initialization of the continuous variables.

For categorical variables, we use one-hot encoding, representing n categories as n distinct problem dimensions. We exclude invalid configurations (e.g., two categories being set to “1”) from the set of candidates of the acquisition function (AF) maximizer.

C.2. Benchmark Details

The Adapted Hartmann6 Benchmark. The \mathbf{A} and \mathbf{P} matrices are defined as follows:

$$\mathbf{A} = \begin{pmatrix} 10 & 3 & 17 & 3.5 & 1.7 & 8 \\ 0.05 & 10 & 17 & 0.1 & 8 & 14 \\ 3 & 3.5 & 1.7 & 10 & 17 & 8 \\ 17 & 8 & 0.05 & 10 & 0.1 & 14 \end{pmatrix} \quad (22)$$

$$\mathbf{P} = \frac{1}{1000} \begin{pmatrix} 1312 & 1696 & 5569 & 124 & 8283 & 5886 \\ 2329 & 4135 & 8307 & 3736 & 1004 & 9991 \\ 2348 & 1451 & 3522 & 2883 & 3047 & 6650 \\ 4047 & 8828 & 8732 & 5743 & 1091 & 381 \end{pmatrix} \quad (23)$$

We sample α_m and ε_o as follows:

$$\alpha_{m,1} \sim \mathcal{U}(1.0, 1.02) \quad (24)$$

$$\alpha_{m,2} \sim \mathcal{U}(1.18, 1.2) \quad (25)$$

$$\alpha_{m,3} \sim \mathcal{U}(2.0, 3.0) \quad (26)$$

$$\alpha_{m,4} \sim \mathcal{U}(3.2, 3.4) \quad (27)$$

$$\varepsilon_{o,j} \sim \mathcal{U}(0, 0.15) \quad (28)$$

$$(29)$$

The distribution for $\varepsilon_{o,j}$ is chosen such that the Gaussian blobs still overlap. The minimum full width at half maximum of any Gaussian blob is given by $2\sqrt{\frac{\ln 2}{17}} \approx 0.4$, where 17 is the smallest element in \mathbf{A} . Hence, a maximum offset of 0.15 is sufficient to ensure correlation and a non-trivial Pareto front between the objectives.

The Terrain Benchmark. We rely on the MetaBox implementation by Ma et al. (2025), which implements the Terrain benchmark defined in Shehadeh & Kudela (2025). While MetaBox provides an additional path-clearance cost, we use only the four defined in Shehadeh & Kudela (2025) (path-length cost, obstacle-avoidance cost, altitude cost, and smoothness cost). Furthermore, we define a variant with two objectives, optimizing both path length cost and obstacle avoidance cost.

We choose target and “meta” terrains uniformly at random with a fixed seed

C.3. Model Details

In this section, we detail the implementations of the different models used in our experiments. For GP-based methods, we use a Matérn- $\frac{5}{2}$ kernel with automated relevance determination (ARD) and a Gamma(1.5, 1) lengthscales hyperprior, a Gaussian likelihood with a LogNormal(-4, 1) prior with a lower bound of 10^{-6} on the noise term. For SMOG and Ind.-ScaML-GP, which train meta-GPs and only model the difference between the intermediate prior and the function output, we use Matérn- $\frac{5}{2}$ kernels with a LogNormal(0.5, 1.5) kernel. The models using multi-task kernels (SMOG and

MO-GP) learn a global noise term, again with a LogNormal($-4, 1$) hyperprior and can model the function variance as part of their multi-task kernel. To allow for the same level of flexibility, Ind.-ScaML-GP and Ind.-GP feature a function variance term with a LogNormal($-2, 3$) kernel.

Models starting with “Ind.” (Ind.-GP, Ind.-ABLR, Ind.-RGPE, Ind.-ScaML-GP, Ind.-SGPT) are implemented as independent models, i.e., the parameters of the model of output 1 are independent of the parameters of the model of output 2.

D. Ablation Studies

We conduct ablation studies to study the sensitivity of SMOG and the other optimizers to different benchmark properties. We set the default to 2 objectives, 8 meta tasks, and 64 observations per task, and vary one of these parameters per experiment.

In Figure 7, we vary the number of meta tasks and study how this affects the behavior of the different optimizers. Generally, increasing the number meta tasks improves performance, particularly in early iterations. The only exception to this is Ind.-SGPT, which is only minimally sensitive to the number of meta tasks. Comparing the different optimizers, SMOG shows the best performance regardless of the number meta tasks.

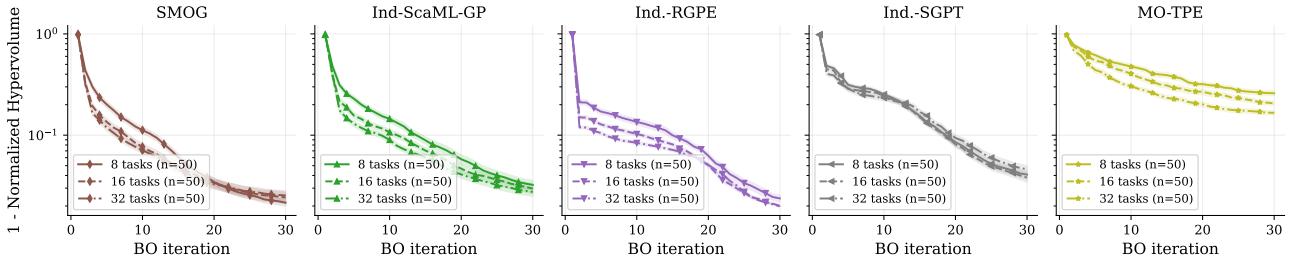


Figure 7. Ablation over the number of meta tasks.

Next, we study how varying the number of objectives affects optimization performance (see Figure 8). Interestingly, varying the number of objectives has only a small impact on relative performance: relative to the other optimizers, MO-TPE seems to perform worse with more objectives.

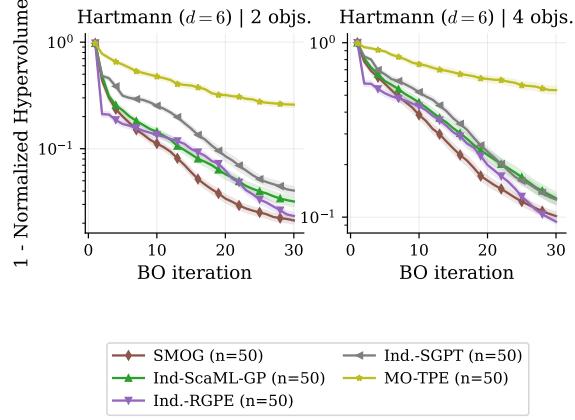


Figure 8. Ablation over the number of objectives.

Finally, we study how varying the number of observations per meta task affects the optimizer’s performance in Figure 9. As expected, a higher number of observations per task improves optimization performance for all optimizers. Ind.-SGPT shows little difference between 64 and 128 observations per task, but gains a significant improvement from 64 vs 16 observations per meta task. All other methods show a clear benefit from 128 vs 64 observations, with SMOG being the top-performing method.

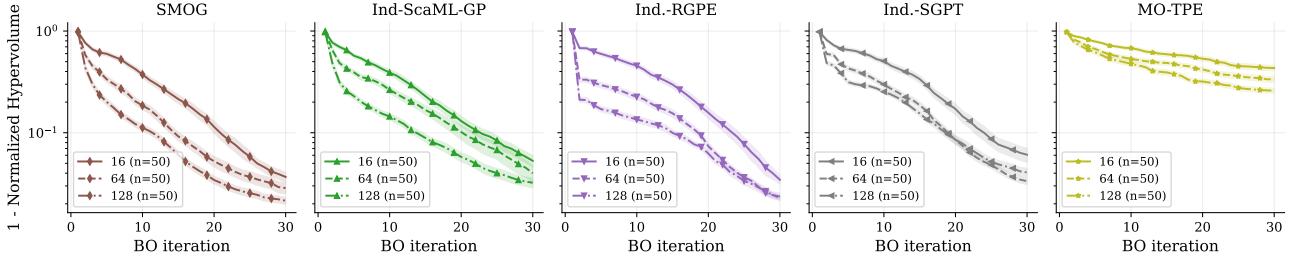


Figure 9. Ablation over the number of observations per meta task.

E. Additional Plots

E.1. Hartmann Benchmark

In this section, we present the result on the 4-objective variant of the Hartmann benchmark (see Figure 10). Again, SMOG shows strong optimization performance whereas the metadata-free methods (MO-GP and Ind.-GP) only slowly find good solutions.

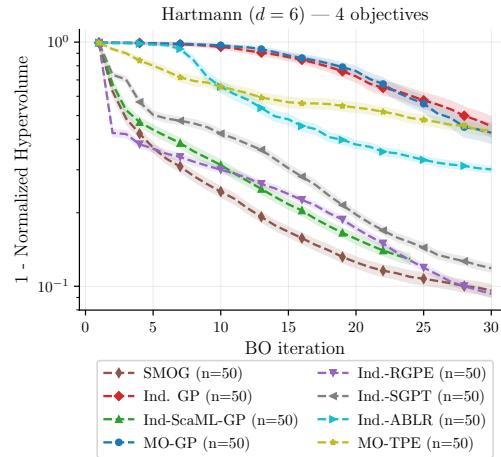


Figure 10. Performance of SMOG and competitors on the 6-dimensional four-objective Hartmann benchmark with 8 meta tasks and 64 observations per meta task.

E.2. Exemplary Hartmann Pareto front

In this section, we highlight how SMOG learns well-behaved Pareto fronts on the two-dimensional Hartmann6 benchmark. For each optimizer, we study the first 15 observations of the run of median HV at iteration 15. Based on these 15 observations, we plot the Pareto front and show the results in Figure 11. Additionally, we estimate a “true” Pareto front by observing 10^7 points sampled uniformly at random from the search space \mathcal{X} . Even though Ind.-SGPT and Ind.-RGPE can find well-performing solutions, SMOG finds more Pareto-optimal solutions, with a larger spread. Furthermore, the solutions found by SMOG are close to the “true” Pareto front with only 15 observations on the target task. The metadata-free optimizers MO-GP and Ind.-GP perform considerably but still outperform MO-TPE by a wide margin.

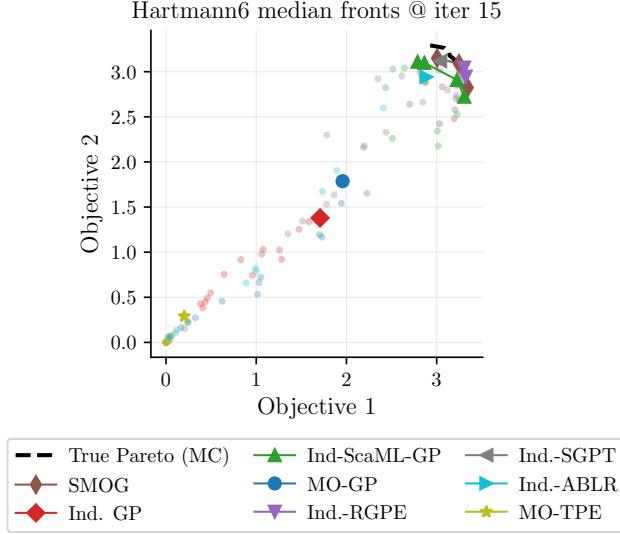


Figure 11. Pareto fronts of the first 15 observations of SMOG and competitors on the 6-dimensional four-objective Hartmann benchmark for the run of median HV at iteration 15. SMOG learns a Pareto front close to the true Pareto front within 15 iterations.

E.3. HPOBench Pareto Fronts

To assess the quality of solutions produced by the different optimizers, we plot the Pareto fronts based on observations across 50 repetitions (see Figure 12). Since HPOBench is a tabular benchmark, one can enumerate all possible solutions and compute a “true” Pareto front. However, since the HPOBench dataset provides four observations per configuration and we observe only once, we plot an estimated true Pareto front, which explains why some observations are better than the “true” Pareto front.

Importantly, the solutions found by the optimizers are close to the “true” Pareto front, showing that the solutions actually are of good quality – a fact that is not evident from only studying the normalized HV.

Furthermore, methods that do not leverage metadata (Ind.-GP and MO-GP) tend to perform worse, confirming the intuition that metadata access improves solution quality.

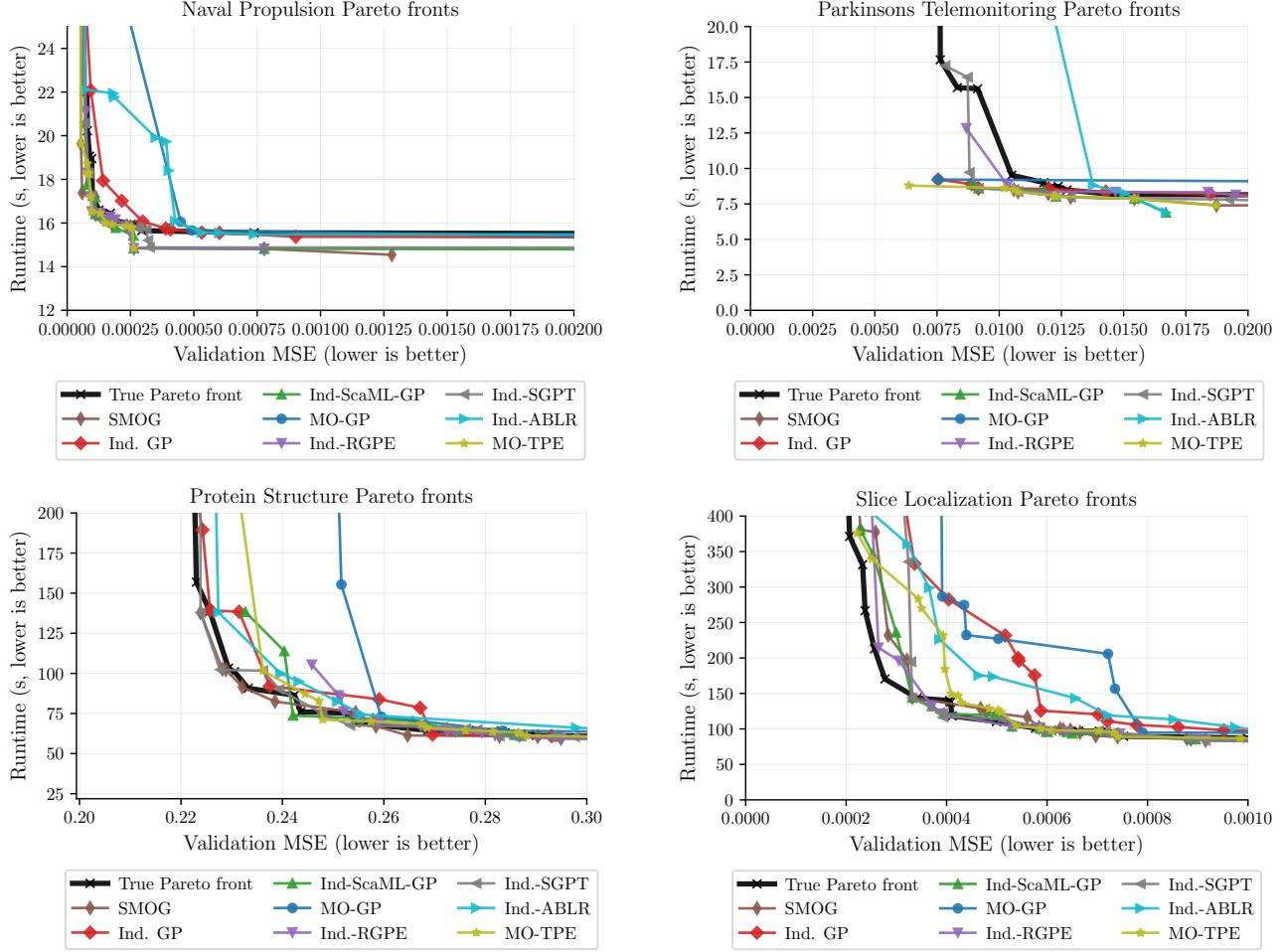


Figure 12. Pareto fronts of the HPOBench benchmark, pooled across the 50 repetitions. The black line shows an estimated true Pareto front.

E.4. HPOBench Benchmarks

In this section, we show the performances on the other datasets of the HPOBench benchmark.

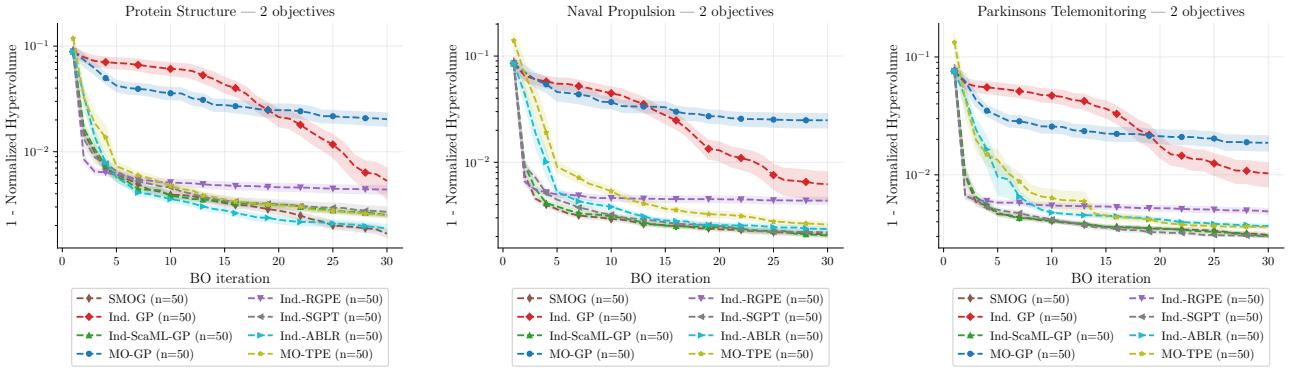


Figure 13. Additional Results on the HPOBench Benchmark

E.5. Terrain Benchmarks

In this section, we show the per-target-task performances on the Terrain benchmarks.

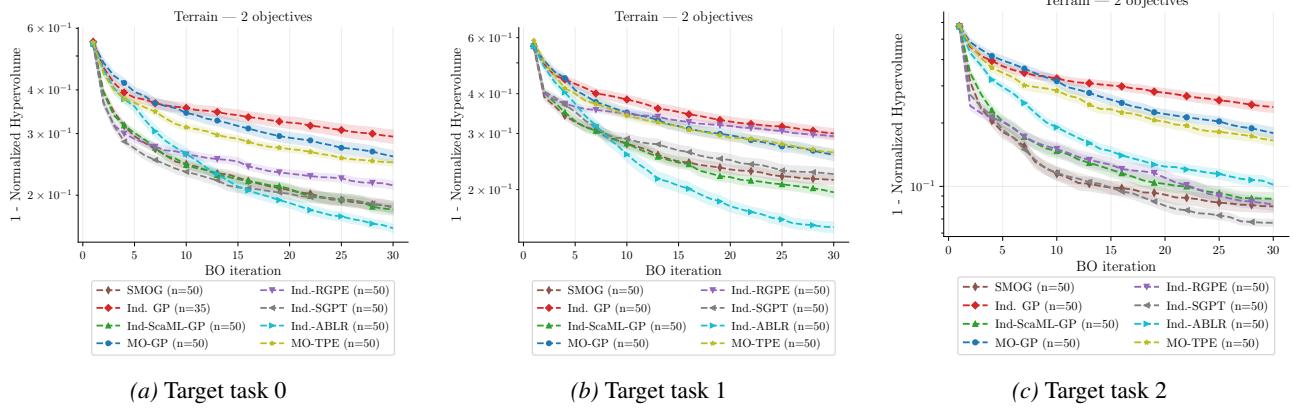


Figure 14. Terrain Benchmark (2 objectives)

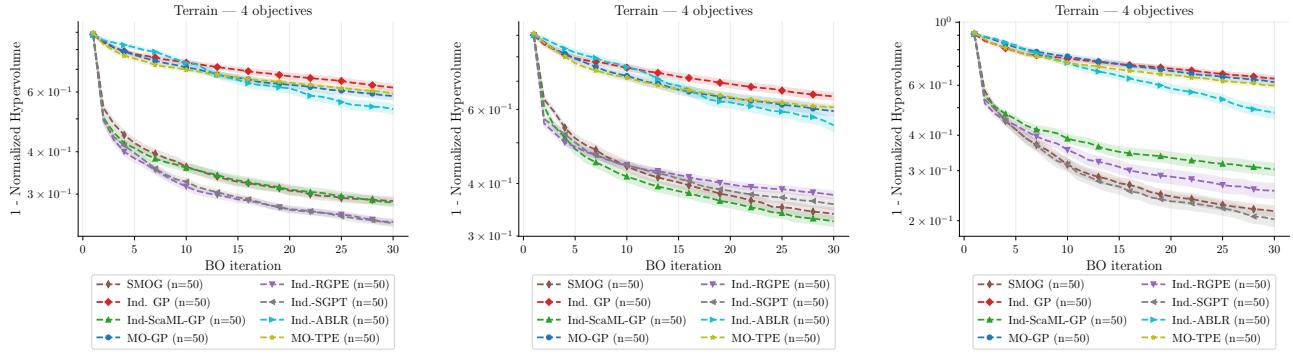


Figure 15. Terrain Benchmark (4 objectives)