Abstract

Multi-Task Learning (MTL) is a well-established paradigm for training deep neural network models for multiple correlated tasks. Often the task objectives conflict, requiring trade-offs between them during model building. In such cases, MTL models can use gradient-based multi-objective optimization (MOO) to find one or more Pareto optimal solutions. A common requirement in MTL applications is to find an Exact Pareto optimal (EPO) solution, which satisfies user preferences with respect to task-specific objective functions. Further, to improve model generalization, various constraints on the weights may need to be enforced during training. Addressing these requirements is challenging because it requires a search direction that allows descent not only towards the Pareto front but also towards the input preference, within the constraints imposed and in a manner that scales to high-dimensional gradients. We design and theoretically analyze such search directions and develop the first scalable algorithm, with theoretical guarantees of convergence, to find an EPO solution, including when box and equality constraints are imposed. Our unique method combines multiple gradient descent with carefully controlled ascent to traverse the Pareto front in a principled manner, making it robust to initialization. This also facilitates systematic exploration of the Pareto front, that we utilize to approximate the Pareto front for multi-criteria decision-making. Empirical results show that our algorithm outperforms competing methods on benchmark MTL datasets and MOO problems.

1 Introduction

Multi-Task Learning (MTL) is a paradigm where data for multiple related tasks is used to learn models for all the tasks simultaneously. It aims to improve over learning each task independently by utilizing the shared signal in the data through an inductive transfer mechanism (Caruana 1997). State-of-the-art models use deep neural network architectures based on MTL in many areas such as computer vision, e.g., Ding et al. (2020), Liu et al. (2019a), natural language processing, e.g., Kendall et al. (2018), Majumder et al. (2019), Liu et al. (2019b), speech recognition, e.g., Tao and Busso (2020), Kapil and Ekbal (2020), multimodal learning, e.g., Al-Rawi and Valveny (2019), Lu et al. (2020), Yang et al. (2020), recommendations, e.g., Ma et al. (2018), Wang et al. (2018) and biomedicine, e.g., Lin et al. (2017), Zhou et al. (2018), Wang et al. (2020).

A common approach to train MTL models is by minimizing the weighted sum of the empirical losses for each task, also known as the linear scalarization approach (figure 1(a)). However, this formulation cannot model conflicting tasks that arise in many real-world applications, e.g., during drug design we may want to jointly increase drug effectiveness and decrease development cost. It may not be possible to optimize all the objectives simultaneously and trade-offs between tasks may

Preprint. Under review.
Exact Pareto Optimal (EPO) Search remains linear in the gradient dimensions (similar to the method of Sener and Koltun (2018)). They extended the Multiple Gradient Descent Algorithm (MGDA) of Desideri (2012) to handle high-dimensional gradients, thereby making it suitable for deep MTL models. However, their method finds a single arbitrary Pareto optimal solution (figure 1(b)) and cannot be used by MTL designers to explore solutions with different trade-offs. Lin et al. (2019) partly address this problem by decomposing the MTL problem and solving multiple subproblems with different trade-offs to yield solutions distributed over the Pareto front (see figure 1(c) and §3.3). In many MTL applications, the designer may want to explore solutions with specific trade-offs in the form of preferences or priorities among the tasks. For instance, in their multi-task recommender system, Milojkovic et al. (2020) optimize semantic relevance, content quality and revenue. In different applications, we may want models with varying priorities for relevance, quality and revenue. Similar requirements arise in, e.g., emotion recognition (Zhang et al. 2017) and the autonomous driving self-localization problem (Wang et al. 2018b). In other words, a Pareto optimal solution (in terms of network weights) is required such that for the $i^{th}$ and $j^{th}$ tasks, if preferences $r_i \geq r_j$, then the corresponding objective functions, i.e., training losses follow $l_i \leq l_j$. We call such a solution a preference-specific Pareto optimal solution. A preference vector determines a direction given by $r^{-1} := (1/r_1, \ldots, 1/r_m)$ and hence a point on the Pareto front intersecting the vector (figure 1(d)). This defines an Exact Pareto Optimal (EPO) solution as a preference-specific solution where $r_1 l_1 = \cdots = r_j l_j = \cdots = r_m l_m$ for all $m$ objectives (formal definitions are in §3.1). To the best of our knowledge, finding preference-specific or exact Pareto optimal solutions cannot be solved by existing multi-objective MTL methods. Deep MTL models typically have non-convex losses and in such cases scalarization or direction-based MOO methods do not guarantee a preference-specific solution. The main problem lies in finding an appropriate search direction in each iteration of gradient descent such that the search ‘balances’ the dual goals of moving towards the Pareto front as well as towards the preference vector. Further, a stopping strategy is required that does not halt the algorithm at any Pareto optimal solution, but only at an EPO solution. To achieve this, we make fundamental theoretical advances in gradient-based MOO through the design and analysis of such balancing search directions. Our techniques for finding a balancing search direction equip us to combine gradient descent with carefully controlled ascent in our algorithm EPO Search to find an EPO solution for any input preference. Further, most deep MTL models require constraints on the weights that provide various forms of regularization to prevent over-fitting and improve model generalization. No previous MOO-based MTL method allows such constraints in their formulation. EPO Search is designed to handle both the unconstrained case and cases of equality, inequality and box constraints. These advantages in EPO Search are achieved without compromising on its efficiency – the per-iteration complexity of EPO Search remains linear in the gradient dimensions (similar to the method of Sener and Koltun).
(2018) that neither uses input preferences nor handles constraints). Thus, EPO Search offers a more flexible approach to efficiently train large-scale deep MTL models.

Although motivated by requirements for MTL, our new algorithmic techniques also contribute significantly to multi-criteria decision making (Greco et al. 2016) where the need for diverse Pareto optimal solutions arises. In its pursuit of an EPO solution, EPO Search traces the Pareto front without stopping at Pareto optimal solutions that are not exact. Leveraging this ability, and using multiple input preferences, we demonstrate that the Pareto front can be efficiently approximated to find diverse solutions.

To summarize, our contributions are the following.

1. **EPO Search: theory and algorithms.** We design and analyze the properties of a ‘balancing’ search directions. We use these balancing directions to develop EPO Search, the first gradient-based MOO algorithm to efficiently find EPO solutions, including those with box and equality constraints to enable regularization during model training. Under mild assumptions, we prove convergence from any random initialization to the EPO solution. Thus, EPO Search offers an efficient and flexible approach to train large-scale deep MTL models. On synthetic data and real benchmark MTL datasets for classification and regression tasks, we find that EPO Search outperforms state-of-the-art MOO-based MTL methods in per-task accuracy, proximity to input preference vectors as well as scalability with respect to the number of objectives.

2. **Pareto front tracing.** We show how EPO Search can trace the Pareto front from an arbitrary Pareto optimal solution to an EPO solution and prove its convergence. We use this ability to design a method to approximate the Pareto front, i.e., generate a diverse set of optimal solutions, by tracing towards the EPO solutions for different input preference vectors. On benchmark MOO problems we find that, in most cases, Pareto front approximations obtained through EPO Search are better and found faster than those from competing approaches.

The rest of the paper is organized as follows. We survey related work on MTL and MOO in §2. In §3 we give a formal description of the problem setting and relevant background. This is followed by the design and analysis of techniques to find balancing search directions (§4). Variants and extensions of EPO Search along with convergence results are in §5. Experimental results follow in §6 and our concluding remarks are in §7. Proofs and additional results are in the Appendices.

## 2 Related Work

### 2.1 Multi-Task Learning

Multi-Task Learning (MTL) has been studied extensively in Machine Learning. Zhang and Yang (2021) provide a general survey and Ruder (2017) gives an overview of neural MTL models. Learning multiple tasks together leads to inductive bias towards hypotheses that can explain (or internal representations that are predictive of) more than one task and has been found to improve model generalization. Recent successful neural MTL models use hard parameter sharing, where a subset of network weights are shared across tasks and remaining are task-specific. The general architecture is that of one shared encoder and multiple decoders catering to multiple tasks. These models are trained using gradient-based optimization and typically involve linear scalarization or its variants, e.g., with adaptive weights (Qiu et al. 2018, Chen et al. 2018, Kendall et al. 2018, Heydari et al. 2019). However, these methods cannot model competing tasks and the trade-offs between them.

Gradient-based MOO algorithms, such as MGDA (described in §2.2), are a natural choice for MOO-based MTL: task-specific gradients are used to update the neural network weights during training in both the method of Sener and Koltun (2018) and PML (Lin et al. 2019). PMTL could be considered to take preferences into account but cannot scale to many objectives. Since this work is closest to ours, we give a detailed technical description in §3.3 Navon et al. (2021) solve the related problem of learning the entire Pareto front for multiple preference vectors. Their approach is based on a hypernetwork (Ha et al. 2017), which, for an input preference vector, gives a deep neural network tuned for that objective preference. However, there are no theoretical guarantees of compliance with the preference.

Thus, current MOO-based MTL methods to find Pareto optimal solutions either do not use preferences or cannot find Exact Pareto Optimal solutions based on the input preferences in a scalable manner.
Recent solutions to approximate the Pareto front for MTL do not provide theoretical guarantees. Moreover, none of these methods can model constraints in the underlying MOO.

2.2 Multi-Objective Optimization (MOO)

Simultaneously optimizing multiple, possibly conflicting criteria in multi-objective optimization problems (MOOP) has been studied extensively. Excellent surveys can be found in Marler and Arora (2004), Gandibleux (2002), Deb (2014), and Evtushenko and Posypkin (2014). Gradient-free approaches are commonly used in MOO solvers (e.g., evolutionary algorithms (Deb 2001, Coello 2006), continuation methods (Schütze et al. 2005, Ringkamp et al. 2012) and deterministic approaches (Ehrgott 2005, Evtushenko and Posypkin 2014)). Various kinds of preferences, such as objective weights, goal specification and desirability thresholds, can be incorporated in a MOOP, as surveyed in Rachmawati and Srinivasan (2006), Bechikh et al. (2015). Reference point or weight vector based methods that can model priorities between criteria, e.g., (Deb and Sundar 2006, Cheng et al. 2016), typically find regions in the Pareto front close to the given references. The most closely related works to ours, that use scalarization or gradients, are reviewed in the following.

Scalarization and Direction-based Methods.

Scalarization converts the original MOOP to a single objective optimization problem (SOOP). The simplest way is linear scalarization, where the weighted sum of the objectives is optimized. These weights specify different preferences over the objectives. Its limitation is well known: it cannot obtain Pareto optimal solutions for all preferences when the objectives are non-convex (Boyd and Vandenberghe 2004). Another way is the weighted Tchebycheff method (Steuer 1989) and its variants (see Wieck et al. 2016 for a survey). Although preference-specific solution can be found for certain weights, these methods cannot explore the Pareto Front for all trade-off combinations (Miettinen 1998).

Preference weights are associated with a direction in the objective space and a Pareto optimal solution. This characteristic of a preference vector is leveraged in direction-based MOO solvers. For instance, Roy (1971), Gembicki and Haimes (1975), and Korhonen and Wallenius (1988) consider a preference direction in the objective space along which the search is performed, and a scalar objective measuring the progress along that direction is minimized. Other direction-based solvers developed by Das and Dennis (1998), Ismail-Yahaya and Messac (2002) approximate the whole Pareto front. They find Pareto optimal solutions along many directions normal to the convex hull of the individual minima of the objective functions.

In summary, scalarization and direction-based methods formulate the MOOP problem as a SOOP by taking a preference vector into account. But they don’t provide theoretical guarantees that a random initialization for a non-convex problem can reach the preferred Pareto optimal solution.

Gradient-based MOO.

Steepest descent methods, originally proposed by Fliege and Svaiter (2000), ensure that in every iteration all the objective values are decreased. This is achieved by solving an optimization problem in each iteration to find the steepest descent direction. This method enjoys the theoretical guarantee of reaching a Pareto optimal solution, proved by Bento et al. (2012) using Armijo’s rule, and by Vieira et al. (2012) with the golden section method for an unconstrained MOOP. To solve the inner optimization problem of finding the steepest descent direction Fliege et al. (2009) used Newton’s method and Drummond and Iusem (2004), Fukuda and Drummond (2011) used the projected gradient method. Both these methods were extended for constrained MOOP in Fliege and Vaz (2010) and Fukuda and Graña Drummond (2013) respectively.

Désideri (2012) formulated the steepest descent as a convex combination of the objective gradients and developed the multiple gradient descent algorithm (MGDA). This reduced the dimension of the inner optimization problem from that of solution space to objective space, which is particularly useful for steepest descent in training deep MTL models where the dimension of objective space (number of loss functions) is typically less than that of the solution space (number of network weights). We provide a technical description in §3.2. To summarize, descent based methods provide theoretical guarantee of convergence to a Pareto optimal solution. However, except for those discussed earlier
for MTL, these methods do not take user preferences into account, and therefore cannot reach a preference-specific solution.

3 Preliminaries

For the Multi-objective Optimization Problem (MOOP), we consider \( m \) non-negative objective functions, \( f_j : \mathbb{X} \rightarrow \mathbb{R}_+ \), \( j \in [m] \). The constrained domain or Solution Set is defined as

\[
\mathbb{X} := \left\{ \mathbf{x} \in \mathbb{R}^n \mid \begin{array}{l}
 b_j' \leq x_i \leq b_n' \\
 g_k(\mathbf{x}) \leq 0 \\
 h_k(\mathbf{x}) = 0
\end{array} \forall i \in [n], \forall k \in [p] \right\},
\]

(1)

where \( b' \) & \( b'' \) are domain boundaries for each variable, \( g : \mathbb{R}^n \rightarrow \mathbb{R}^p \) are \( p \) inequality constraints, and \( h : \mathbb{R}^n \rightarrow \mathbb{R}^q \) are \( q \) equality constraints. This formulation is fairly general, since problems with different specifications can be converted to this form. For instance, if an objective \( f_j \) is negative at its minimizer, i.e., \( \min_{\mathbf{x} \in \mathbb{X}} f_j(\mathbf{x}) = f_j^* \leq 0 \), then one can reformulate it as \( f_j(\mathbf{x}) := f_j(\mathbf{x}) - f_j^* \) to make it non-negative. Appendix A has a list of symbols for reference.

We use \( f \) to denote both the vector valued loss function and a point in Objective Space \( \mathbb{R}^m \), which should be unambiguous from the context. The range of \( f \) is denoted by \( \mathcal{O} \). It is a subset of the positive cone defined as:

\[
\mathbb{R}^m_+ := \{ \mathbf{f} \in \mathbb{R}^m \mid f_j \geq 0 \ \forall j \in [m] \}.
\]

(2)

The partial ordering for any two points \( \mathbf{f}^1, \mathbf{f}^2 \in \mathbb{R}^m \), denoted by \( \mathbf{f}^1 \geq \mathbf{f}^2 \), is defined by \( \mathbf{f}^1 - \mathbf{f}^2 \in \mathbb{R}^m_+ \), which implies \( f_j^1 \geq f_j^2 \) for every \( j \in [m] \) and strict inequality \( \mathbf{f}^1 > \mathbf{f}^2 \) occurs when there is at least one \( j \) for which \( f_j^1 > f_j^2 \). Geometrically, \( \mathbf{f}^1 > \mathbf{f}^2 \) means that \( \mathbf{f}^1 \) lies in the positive cone pivoted at \( \mathbf{f}^2 \), i.e., \( \mathbf{f}^1 \in \{ \mathbf{f}^2 \} + \mathbb{R}^m_+ := \{ \mathbf{f}^2 + \mathbf{f} \mid \mathbf{f} \in \mathbb{R}^m_+ \} \), and \( \mathbf{f}^1 \neq \mathbf{f}^2 \).

In the context of minimization, a solution \( \mathbf{x}^1 \in \mathbb{X} \) is dominated by another solution \( \mathbf{x}^2 \in \mathbb{X} \) iff \( f(\mathbf{x}^1) \geq f(\mathbf{x}^2) \). Note that \( f(\mathbf{x}^1) \not\supseteq f(\mathbf{x}^2) \) if \( \mathbf{x}^1 \) is not dominated by \( \mathbf{x}^2 \), i.e., \( f(\mathbf{x}^1) \not\supseteq f(\mathbf{x}^2) \) + \( \mathbb{R}^m_+ \). A solution \( \mathbf{x}^* \) is Pareto optimal if it is not dominated by any other solution. The set of all global Pareto optimal solutions is given by:

\[
\mathcal{P}_{\text{glo}} := \{ \mathbf{x}^* \in \mathbb{X} \mid \forall \mathbf{x} \in \mathbb{X} - \{ \mathbf{x}^* \}, \ f(\mathbf{x}^*) \not\supseteq f(\mathbf{x}) \}.
\]

(3)

We are interested in the set of local Pareto optimal solutions given by:

\[
\mathcal{P} := \{ \mathbf{x}^* \in \mathbb{X} \mid \exists \mathcal{N}(\mathbf{x}^*) \subset \mathbb{X}, \ s.t. \forall \mathbf{x} \in \mathcal{N}(\mathbf{x}^*) - \{ \mathbf{x}^* \}, \ f(\mathbf{x}^*) \not\supseteq f(\mathbf{x}) \}
\]

(4)

where \( \mathcal{N}(\mathbf{x}^*) \) is an open neighbourhood of \( \mathbf{x}^* \) in \( \mathbb{X} \). Note that \( \mathcal{P}_{\text{glo}} \subset \mathcal{P} \). The set of multi-objective values of the Pareto optimal solutions, \( f(\mathcal{P}) \subset \mathcal{O} \), is called the Pareto front.

3.1 Preference-Specific and Exact Pareto Optimal Solutions

Given a preference vector \( \mathbf{r} \in \mathbb{R}_+^m \), a Preference-specific Pareto optimal solution belongs to the set:

\[
\mathcal{P}_{ps} = \{ \mathbf{x}^* \in \mathcal{P} \mid \text{if } r_j \geq r_j', \text{ then } f_j(\mathbf{x}^*_j) \leq f_j'(\mathbf{x}^*_j) \ \forall j, j' \in [m] \}. \]

An Exact Pareto optimal (EPO) solution with respect to a preference vector \( \mathbf{r} \in \mathbb{R}_+^m \) belongs to the set:

\[
\mathcal{P}_r = \{ \mathbf{x}^* \in \mathcal{P} \mid r_1 f_1^* = \cdots = r_j f_j^* = \cdots = r_m f_m^* \},
\]

(5)

where \( f_j^* = f_j(\mathbf{x}^*) \). Note that for any EPO solution \( \mathbf{x}^*_r, \ f^*_r = f(\mathbf{x}^*_r) \) is a point on the Pareto front intersecting the ray towards \( \mathbf{r}^{-1} := (1/r_1, \ldots, 1/r_m) \) (see figure [IV]). In other words, \( f^*_r \) is perfectly proportional to the \( \mathbf{r}^{-1} \) ray. An EPO solution is a preference-specific Pareto optimal solution, i.e., \( \mathcal{P}_r \subset \mathcal{P}_{ps} \).

3.2 Gradient-based Multi-Objective Optimization

Gradient-based MOO solvers find a Pareto optimal solution by starting from an arbitrary initialization \( \mathbf{x}^0 \in \mathbb{R}^n \) and iteratively obtaining the next solution \( \mathbf{x}^{i+1} \) that dominates the previous one \( \mathbf{x}^i \) (i.e.,
we name such a direction \( \mathbf{d} \), by moving against a direction \( \mathbf{d} \) with step size \( \eta \), i.e. \( \mathbf{x}^{t+1} = \mathbf{x}^t - \eta \mathbf{d} \), such that descent happens in every objective, \( f_j^{t+1} \leq f_j^t \). This can happen only if \( \mathbf{d} \) has positive angles with the gradients of every objective function at \( \mathbf{x}^t \):

\[
\mathbf{d}^T \nabla f_j^t \geq 0, \quad \text{for all } j \in [m];
\]

we name such a direction \( \mathbf{d} \) as a descent direction.

Desideri (2012) showed that descent directions can be found in the Convex Hull of the gradients, defined by \( \mathcal{CH}_x := \left\{ \sum_{j=1}^{m} \nabla f_j \beta_j \mid \beta \in S^m \right\} \), where

\[
S^m := \left\{ \beta \in \mathbb{R}^m_+ \left\vert \sum_{j=1}^{m} \beta_j = 1, \text{ and } \beta_j \geq 0 \quad \forall j \in [m] \right\}.
\]

is the \((m-1)\)-dimensional simplex. Their Multiple Gradient Descent Algorithm (MGDA) converges to a local Pareto optimal by iteratively using the descent direction:

\[
\mathbf{d}^* = \arg \min_{\mathbf{d} \in \mathcal{CH}_x} \| \mathbf{d} \|_2^2.
\]

### 3.3 Limitations of previous methods

First, we note that the popular approach of linear scalarization of the MOP with a preference vector \( \mathbf{r} \in \mathbb{R}_+^m \) finds

\[
\mathbf{x}^*(\mathbf{r}) = \arg \min_{\mathbf{x} \in \mathcal{X}} \langle \mathbf{r}, \mathbf{f}(\mathbf{x}) \rangle = \mathbf{r}^T \mathbf{f}(\mathbf{x}).
\]

If the range of vector valued objective \( \mathbf{f} \), i.e. \( \mathcal{O} \), is convex then for every \( \mathbf{x}^* \in \mathcal{P} \) there exists a \( \mathbf{r} \) such that \( \mathbf{x}^* = \mathbf{x}^*(\mathbf{r}) \). However, if \( \mathcal{O} \) is non-convex then it may not be possible to reach every optimal point in \( \mathcal{P} \) using linear scalarization (see Boyd and Vandenberghe (2004) Ch 4.7).

In MGDA and MGDA-based algorithms (e.g., Sener and Koltun (2018), starting from a random initialization, iterating along descent directions can lead to a Pareto optimal solution, but it may not be a preference-specific optimal. This is illustrated in figure 2.

Figure 2: (Color Online) Illustration of how a descent-only search cannot find the preferred optimal \( \mathbf{f}^*_p \) starting from a random initialization \( \mathbf{x}^0 \), where \( \mathbf{f}^0 = \mathbf{f}(\mathbf{x}^0) \). Any descent direction \( \mathbf{d} \) will keep the objective vector \( \mathbf{f}^{t+1} \) of next iterate \( \mathbf{x}^{t+1} = \mathbf{x}^t - \eta \mathbf{d} \) in the blue shaded region.

The Pareto MTL (PMTL) algorithm by Lin et al. (2019) finds multiple solutions on the Pareto front by using a decomposition strategy. They use several reference vectors \( \mathbf{u}^k, k = 1, \ldots, K \) to partition the solution space into \( K \) sub-regions \( \Omega_k := \left\{ \mathbf{x} \in \mathbb{R}^n \mid \langle \mathbf{u}^k, \mathbf{f}(\mathbf{x}) \rangle \geq \langle \mathbf{u}^{k'}, \mathbf{f}(\mathbf{x}) \rangle, \forall k' \neq k \right\} \). With this decomposition, if \( \mathbf{u}^k = \mathbf{r} \), then the EPO solution \( \mathbf{x}^*_p \in \Omega_k \). There are two phases in their algorithm. In the first phase, starting from a random initialization, they find a point \( \mathbf{x}^0 \in \Omega_k \), such that the corresponding \( \mathbf{u}^k = \mathbf{r} \). In the second phase, they iterate using descent-only directions to reach a Pareto optimal \( \mathbf{x}^* \in \mathcal{P} \). However, their method does not guarantee that the outcome of second phase \( \mathbf{x}^* \) also lies in \( \Omega_k \). Moreover, to reach a desired preference, they have to increase the number of reference vectors \( \mathbf{u}^k \) exponentially with increase in number of objectives \( m \), making it practically infeasible. Thus, although their reference vectors can be based on user preferences, their method, by design, does not reach the exact preference but only in the sub-regions of the Pareto front between the references (see figure 1 and Appendix B.2).
4 Gauge of Proportionality and Direction of Improvement

To find the EPO solution by an iterative procedure, it is not sufficient to advance only along the descent directions \( \hat{\mathbf{d}} \) because it leads to an arbitrary solution in the Pareto front. Moreover, even if \( f^{t+1} < f^t \) for every \( t \), the solution may not lie on the \( r^{-1} \) ray (figure 2), and hence will not satisfy the condition in [5]. Therefore, we need to consider a direction \( \mathbf{d} \in \mathbb{R}^m \) (tangent plane of \( \mathcal{X} \)) that moves the objective vector \( \mathbf{f}^t \) closer to the \( r^{-1} \) ray.

To find such a direction, we first construct an anchoring direction \( \mathbf{a} \in \mathbb{R}^m \) (tangent plane of \( \mathcal{O} \)) according to the desired change in the consecutive objective vectors: \( f^{t+1} \) should be more proportional to the \( r^{-1} \) ray than \( f^t \) in addition to \( f^{t+1} \neq f^t \). We define and analyze three specific ways of quantifying the proportionality in §4.2, §4.3 and §4.4. Before that, in §4.1 we describe the properties required from such a measure to gauge proportionality that allow us to characterize the search direction in terms of the anchor direction.

4.1 A Balancing Search Direction

Let \( \mu : \mathbb{R}_+^m \times \mathbb{R}_+^m \rightarrow \mathbb{R}_+ \) be a function that measures the degree of proportionality between two vectors, such that, for any given \( \mathbf{f} \in \mathbb{R}_+^m \) and \( \mathbf{r} \in \mathbb{R}_+^m \):

1. \( \mu(\mathbf{f}, r^{-1}) = 0 \) only when \( \mathbf{f} \) is a positive scalar multiple of \( r^{-1} \), and
2. \( \mu(\cdot, \mathbf{r}) \) is differentiable w.r.t \( \mathbf{f} \) and increases monotonically along \( (1-\lambda)r^{-1} + \lambda \mathbf{f} \), for \( \lambda \geq 0 \).

For a given preference vector \( \mathbf{r} \) and a point \( \mathbf{f} \), the anchoring direction in \( \mathbb{R}^m \) is defined as \( \mathbf{a}(\mathbf{f}, \mathbf{r}) := \nabla_\mathbf{f} \mu(\cdot, \mathbf{r}) \). We use this anchoring direction to characterize a search direction \( \mathbf{d} \in \mathbb{R}^m \) that can move the objective vector \( \mathbf{f}(\mathbf{x}) \) closer to the \( r^{-1} \) ray.

**Lemma 1.** If all the objective functions are differentiable, then for any direction \( \mathbf{d} \in \mathbb{R}^n \) satisfying \( \mathbf{a}^T \mathbf{F} \mathbf{d} \geq 0 \), where \( \mathbf{F} \) is the Jacobian of \( \mathbf{f} \), and \( \max_j \{ \mathbf{d}^T \nabla f_j \} > 0 \), there exists a step size \( \eta_0 > 0 \) such that

\[
\mu(\mathbf{f}(\mathbf{x} - \eta \mathbf{d}), \mathbf{r}^{-1}) \leq \mu(\mathbf{f}(\mathbf{x}), \mathbf{r}^{-1}), \text{ and } \mathbf{f}(\mathbf{x} - \eta \mathbf{d}) \geq \mathbf{f}(\mathbf{x}) \text{ for all } \eta \in [0, \eta_0].
\]

A move against the search direction \( \mathbf{d} \) of lemma 1 reduces the variations in relative objective values \( f_j / r_j \) to make them equal: brings “balance” among the values of \( \mathbf{f} \circ \mathbf{r} = [f_1 r_1, \cdots, f_m r_m] \). Therefore, we call this \( \mathbf{d} \) a **Balancing Search** direction, and \( \mathbf{a} \) a **Balancing Anchor** direction. We qualify the \( \mu \) function by enforcing scale in-variance in the anchor direction.

**Lemma 2.** If \( \mu \) is such that the anchor direction is scale invariant to the preference vector, i.e. \( \overline{\mathbf{a}}(\mathbf{f}, s \mathbf{r}) = \overline{\mathbf{a}}(\mathbf{f}, \mathbf{r}) \) for all \( s > 0 \), where \( \overline{\mathbf{a}} = \frac{\mathbf{a}}{||\mathbf{a}||} \) then

\[
\sum_{j=1}^m f_j a_j = \langle \mathbf{f}, \mathbf{a} \rangle \geq 0 \geq \langle \mathbf{r}^{-1}, \mathbf{a} \rangle = \sum_{j=1}^m \frac{a_j}{r_j}.
\]

Using lemma 1 and 2, we narrow down the characteristics of a balancing search direction.

**Theorem 1.** If the anchor direction is scale invariant to preference vector \( \mathbf{r} \), and all the objective functions are differentiable at \( \mathbf{x}^t \), then moving against a direction \( \mathbf{d} \in \mathbb{R}^m \) with \( \mathbf{F} \mathbf{d} = s \mathbf{a} \), for some \( s > 0 \), yields a non-dominated solution \( \mathbf{x}^{t+1} \) whose objective vector \( \mathbf{f}^{t+1} \) is closer to the \( r^{-1} \) ray than that of \( \mathbf{f}^t \).

Note that, for a small step size \( \eta \), the difference between the consecutive objective vectors can be approximated as \( \Delta \mathbf{f} = f^{t+1} - f^t \approx -\eta \mathbf{F} \mathbf{d} \) from the first order Taylor series expansion. So the search direction in theorem 1 moves the objective vector against the anchoring direction \( \mathbf{a} \) in the objective space. In the following, we propose three different functions – using KL divergence, Cauchy–Schwarz inequality and Lagrange’s identity – for gauging the proportionality between two vectors and analyze them based on their respective balancing anchor directions.
4.2 Gauge of Proportionality: from KL Divergence

In Mahapatra and Rajan (2020), the authors formulated a proportionality measuring function from the KL divergence between the normalized vectors of \( \mathbf{f} \odot \mathbf{r} \) and \( \mathbf{1} = [1, \ldots, 1] \):

\[
\mu(\mathbf{f}, \mathbf{r}^{-1}) = \sum_{j=1}^{m} \frac{f_j r_j}{\|\mathbf{f} \odot \mathbf{r}\|_1} \log \left( \frac{m f_j r_j}{\|\mathbf{f} \odot \mathbf{r}\|_1} \right) = \text{KL}(\mathbf{f} \odot \mathbf{r} \| \mathbf{1}) ,
\]

where \( \mathbf{b} \) is the \( \ell_1 \)-normalized vector of \( \mathbf{b} \). It can be verified that this \( \mu \) satisfies both conditions 1 and 2 of a proportionality measuring function. Figure 3a shows the corresponding \( \mu_r \) in case of 3 objectives and a particular preference vector.

We can obtain the anchoring direction of this \( \mu \) by computing its gradient w.r.t \( \mathbf{f} \). However, it is sufficient to analyze a simplified \( \mathbf{a} \) that is aligned with, but has a different magnitude compared to, \( \nabla_{\mathbf{f}} \mu_r \). In fact, the anchor direction proposed in Mahapatra and Rajan (2020), given by

\[
a_j = r_j \log \left( \frac{f_j r_j}{\|\mathbf{f} \odot \mathbf{r}\|_1} \right) - \mu(\mathbf{f}, \mathbf{r}^{-1}) , \quad j \in [m],
\]

is such that \( \mathbf{a} = \|\mathbf{f} \odot \mathbf{r}\|_1 \nabla_{\mathbf{f}} \mu_r \).

Notice that, unless all \( f_j r_j \) are equal, the anchor elements \( a_j \) are non-negative for some objectives and negative for the rest. As a result, if we move against the search direction \( \mathbf{d} \) in theorem 1, we will be descending for the objectives with \( a_j \) and negative for the rest. As a result, if we move against the search direction \( \mathbf{f} \) and the anchor direction \( \mathbf{a} \) in (13), as shown in the figure 3a and 3e. The trajectory of objectives and a particular preference vector.

Claim 1 (Mahapatra and Rajan (2020)). The objective vector \( \mathbf{f} \) and the anchor direction \( \mathbf{a} \) in (13) are always orthogonal: \( \mathbf{a}^T \mathbf{f} = 0 \).

Since the change in consecutive objective vectors \( \delta \mathbf{f} = \mathbf{f}^{t+1} - \mathbf{f}^t \) is approximately aligned to \( -\mathbf{a}^T \mathbf{f} \), claim 1 suggests that \( \delta \mathbf{f}^T \mathbf{f}^t \approx 0 \). In other words, since \( \mathbf{f} \) is an all positive vector, changes in some objectives \( \delta f_j \) are positive and others are negative. The advantage of an orthogonal anchoring direction lies in its ability to simultaneously ascend and descend which helps in escaping a local Pareto optimal solution that is not an EPO solution (formalized in theorem 3).

However, iterating based on the anchoring direction in (13) has a limitation. It does not move the objective vectors to the \( \mathbf{r}^{-1} \) ray in the shortest possible path. The shortest path between \( \mathbf{f}^t \) and the \( \mathbf{r}^{-1} \) ray should lie on the hyperplane containing both these vectors. So, in order for \( \mathbf{f}^{t+1} \approx \mathbf{f}^t - \eta \mathbf{a} \) to be on the shortest path, a necessary condition is \( \mathbf{a} \) should lie in the span of \( \mathbf{f}^t \) and \( \mathbf{r}^{-1} \). This is violated in case of anchoring direction of (13), as shown in the figure 3a and 3e. The trajectory of objective vectors deviates from the span of \( \{\mathbf{r}^{-1}, \mathbf{f}^0\} \) and follows a curved path. Therefore it does not reach as close to the \( \mathbf{r}^{-1} \) ray as the other alternatives (discussed in the following sections) in the same number of iterations (steps in numerical integration).

4.3 Gauge of Proportionality: from Cauchy–Schwarz Inequality

The Cauchy-Schwarz inequality pertaining to our non-zero vectors \( \mathbf{f}, \mathbf{r}^{-1} \in \mathbb{R}_+^m \),

\[
\langle \mathbf{f}, \mathbf{r}^{-1} \rangle^2 = \left( \sum_{j=1}^{m} f_j r_j^{-1} \right)^2 \leq \left( \sum_{j=1}^{m} f_j^2 \right) \left( \sum_{j=1}^{m} r_j^{-2} \right) = \|\mathbf{f}\|^2 \|\mathbf{r}^{-1}\|^2 , \quad (14)
\]

is tight, i.e. equality is attained, when both the vectors are proportional to each other. Rearranging the terms to one side, we get the following

\[
\mu(\mathbf{f}, \mathbf{r}^{-1}) = 1 - \frac{\langle \mathbf{f}, \mathbf{r}^{-1} \rangle^2}{\|\mathbf{f}\|^2 \|\mathbf{r}^{-1}\|^2} , \quad (15)
\]

which satisfies both conditions 1 and 2 of the required proportionality measuring function.

The simplified form of its anchoring direction, up to a constant factor of \( \nabla_{\mathbf{f}} \mu_r \), is given by

\[
a = \frac{\langle \mathbf{f}, \mathbf{r}^{-1} \rangle}{\|\mathbf{f}\| \|\mathbf{r}^{-1}\|} \mathbf{f} - \frac{\|\mathbf{f}\|}{\|\mathbf{r}^{-1}\|} \mathbf{r}^{-1} . \quad (16)
\]

Much like the previous anchoring direction we can state the relation between \( \mathbf{a} \) and \( \mathbf{f} \):
Claim 2. The objective vector \( f \) and the anchor direction \( a \) in (16) are always orthogonal: \( a^T f = 0 \).

Therefore this anchoring direction can also escape local non-EPO solutions. Since \( a \) is a linear combination of \( f \) and \( r^{-1} \), the trajectory of the objective vectors lies in the span of \( \{ r^{-1}, f^0 \} \).

However, it still does not result in the shortest trajectory to reach \( r^{-1} \) ray (see figure 3d). The shortest path between a point \( f^0 \) and the \( r^{-1} \) ray is the line segment from \( f^0 \) that is orthogonal to the \( r^{-1} \) ray. So every change \( \delta f \), and hence every anchoring direction \( a \), should be orthogonal to the \( r^{-1} \) ray.

4.4 Gauge of Proportionality: from Lagrange’s Identity

Instead of using the ratio between the RHS and LHS in (14), we can also take the difference between them to quantify the proportionality between \( f \) and \( r^{-1} \). The residue, RHS - LHS, is given by the Lagrange’s identity:

\[
\mu(f, r^{-1}) = ||f||^2 ||r^{-1}||^2 - \langle f, r^{-1} \rangle^2 = \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{m} (f_j r_j^{-1} - f_k r_k^{-1})^2,
\]

which satisfies both conditions 1 and 2 of a proportionality measuring function. The simplified form of its anchoring direction, up to a constant factor of \( \nabla f \mu r \), is given by

\[
a = f - \frac{\langle f, r^{-1} \rangle}{||r^{-1}||^2} r^{-1}.
\]

This anchor direction can yield the trajectory of shortest path (figure 3d) due the following relation:
Claim 3. The $r^{-1}$ ray and anchor direction $a$ in (18) are always orthogonal: $a^T r^{-1} = 0$.

However, since $a^T f > 0$ when $f$ and $r^{-1}$ are not proportional, ascent in some of the objectives cannot be guaranteed. Therefore, using this anchoring direction may not escape local non-EPO solutions.

4.5 Anchor Direction Selection

Among the three anchor directions discussed above, when the initialisation is random, the anchor direction from Lagrange’s identity, given by equation (18), should be used since it can yield the trajectory of shortest path. However, if the initialisation $x^0$ is itself a local Pareto optimal solution and $f^0$ lies on the Pareto front then $a$ from Cauchy-Schwarz inequality, given by equation (16), should be used to escape local non-EPO solutions which the Lagrange anchor may not.

When the iterate $f^t$ is on or close to the $r^{-1}$ ray, i.e. $\mu p f^t, r^{-1} q \epsilon$ for small $\epsilon > 0$, to reach the EPO solution, we require descent for every objective. The anchor directions proposed earlier do not guarantee descent in every objective. A simple and effective strategy is to consider $a^f$.

5 Exact Pareto Optimal Search Algorithms

We now develop iterative methods to find the EPO solution w.r.t a preference vector $r$. In each iteration, we solve a Quadratic Programming (QP) problem to obtain a search direction $d$ at $x^t \in X$, the tangent plane (or cone, if $X$ is constrained) at $x^t \in X$, such that it corresponds to an anchor direction $a$ at $f(x^t) \in O$. We describe the main ingredients of the QP problem in §5.1 and then use it to develop two algorithms. Algorithm 1 detailed in §5.2 finds the EPO solution for any random initializaiton $x^0 \in X$ that is not a Pareto optimal solution. Algorithm 2 described in §5.3 finds the EPO solution when the intialization is a Pareto optimal solution $x^0 \in P$ but not exact w.r.t $r$. Algorithm 3 traces the Pareto front from $x^0$ to $x^r$, a capability that we use to approximate the Pareto front, described in §5.3.

5.1 Quadratic Program for Search Direction

We model the search direction as a linear combination of the objective gradients

$$d = \sum_{j=1}^{m} \beta_j \nabla_x f_j = F^T \beta, \quad \beta \in [-1, 1]^m$$

where $F$ is the Jacobian of objective vector. Note that, unlike Désidéri (2012), we do not restrict $d$ to the convex hull of the gradients, which was used to find a descent–only direction. As a result, we facilitate gradient ascent for some of the objectives whenever necessary. We obtain the search direction by solving a QP problem to align $Fd$ to the anchor direction as much as possible; we minimize the following quadratic cost for the coefficients $\beta \in [-1, 1]^m$.

$$|Fd - a|^2 = \| FF^T \beta - a \|^2$$

5.1.1 Modes of Operation.

Depending on the choice of anchor direction in (21), there could be two modes of operation:

1. Balance Mode: where any of the balancing anchor directions, Cauchy-Schwarz anchor (16) or Lagrange anchor (18), is used to improve the proportionality between $f$ and $r^{-1}$.

2. Descent Mode: where descending anchor direction (19) is used to decrease all objective values.
5.1.2 Incorporating Constraints.

We check for the infeasibility of boundary, equality and inequality constraints in each iteration. If \( x^t \) violates any of the boundary constraints, we simply project element-wise to \( \pi(\mathbf{x}^t) \), to constrain them to remain within the bounds, where

\[
\pi(x^i) = \begin{cases} 
  b_i^l, & \text{if } x^i < b_i^l, \\
  x^i, & \text{if } x^i \in [b_i^l, b_i^u], \\
  b_i^u, & \text{if } x^i > b_i^u 
\end{cases} \quad \text{for all } i \in [n],
\]

(22)

Let the number of active inequality constraints be \( p_a \), making \( p_a + q \) total active constraints, since the equality constraints are always active. Let the active inequality constraints be \( h_k \) for \( k = 1, \ldots, p_a \) without loss of generality. Then the cone of first order feasible directions at \( \mathbf{x}^t \) against which we can move to obtain \( \mathbf{x}^{t+1} \in \mathcal{X} \) is given by

\[
\mathcal{F}_{\mathbf{x}^t}\mathcal{X} = \left\{ \mathbf{d} \in \mathbb{R}^n \mid \mathbf{d}^T \nabla_{\mathbf{x}} g_k^l \geq 0 \ \forall \ k \in [p_a], \ \text{and} \ \mathbf{d}^T \nabla_{\mathbf{x}} h_k^l = 0 \ \forall \ k \in [q] \right\},
\]

(23)

where \( g_k^l = g_k(\mathbf{x}^t) \) and \( h_k^l = h_k(\mathbf{x}^t) \). When there is no active constraint it is the same as the tangent plane: \( \mathcal{F}_{\mathbf{x}^t}\mathcal{X} = \mathcal{T}_{\mathbf{x}^t}\mathcal{X} = \mathbb{R}^n \). But when there are active constraints, this doesn’t hold in general. The tangent cone \( \mathcal{T}_{\mathbf{x}^t}\mathcal{X} \) of the constrained set is unique and depends on the geometrical property of \( \mathcal{X} \) at \( \mathbf{x}^t \). But the \( \mathcal{F}_{\mathbf{x}^t}\mathcal{X} \) cone is not unique and depends on the algebraic specification of the constraints (see Nocedal and Wright [2006] (Ch 12.2)). Therefore to make \( \mathcal{F}_{\mathbf{x}^t}\mathcal{X} \) same as the tangent cone \( \mathcal{T}_{\mathbf{x}^t}\mathcal{X} \), and render the conditions in (23) useful, we assume the Linear Independence Constraint Qualification (LICQ) to be satisfied at \( \mathbf{x}^t \). In other words, we assume that the gradients of active constraints are linearly independent. Finally, with \( \mathbf{d} = F^T \beta \) and the LICQ assumption, we constrain the coefficients \( \beta \) in the quadratic cost (21) with \( \beta^T F \nabla g_k \geq 0 \) for all \( k \in [p_a] \) and \( \beta^T F \nabla h_k = 0 \) for all \( k \in [q] \) to obtain the search direction.

5.2 EPO Search for Random Initialization

When the goal is to find the EPO solution for a given preference \( r \) starting from a random initialization \( \mathbf{x}^0 \in \mathcal{X} \), we use the balance mode with the anchor direction from Lagrange’s identity (18) for every iteration until \( f^t \) is (nearly) proportional to \( r^{-1} \), i.e. until \( \mu(f^t, r^{-1}) < \epsilon \) for some small \( \epsilon > 0 \). Then we use the descent mode until convergence, i.e., when the magnitude of search direction vanishes.

When there are active constraints at \( \mathbf{x}^t \), i.e. \( \beta \) is not freely decided to minimize the quadratic cost (21), we further constrain it to ensure convergence (see lemma 3 and theorem 2). Let \( J^* \) be the index set of maximum relative objective values:

\[
J^* = \left\{ j \mid j = \arg \max_{j \in [m]} f_j r_j \right\}.
\]

(24)

The final \( m \) dimensional QP problem to be solved at \( \mathbf{x}^t \) is given as

\[
\beta^* = \arg \min_{\beta \in [-1, 1]^m} \| F F^T \beta - a \|^2
\]

(25a)

s.t. \( \beta^T F \nabla g_k \geq 0 \), for all \( k \in [p_a] \), if \( p_a > 0 \),

(25b)

\( \beta^T F \nabla h_k = 0 \), for all \( k \in [q_a] \), if \( q > 0 \),

(25c)

\( \beta^T F \nabla f_j \geq 0 \), for all \( j \in J^* \), if \( p_a + q > 0 \).

(25d)

Moving against the resulting search direction yields a solution \( \mathbf{x}^{t+1} \) that is not dominated by \( \mathbf{x}^t \), i.e. \( f^{t+1} \succeq f^t \). Therefore we call \( \mathbf{d}_{ad} = F^T \beta^* \) to be a non-dominating direction. Algorithm 1 summarizes the EPO Search Algorithm for random initialization. Some practically useful variations are discussed in Appendix B.

Note that when \( \mathbf{x}^t \) is in the interior of \( \mathcal{X} \), there will be no constraints in the QP problem (25) apart from \( \beta \in [-1, 1]^m \). The constraint in (25d) ensures that the search direction reduces the objective values of \( J^* \), irrespective of \( \mathbf{x}^t \in \text{Int}(\mathcal{X}) \) (interior) or \( \mathbf{x}^t \in \partial \mathcal{X} \) (boundary), under a regularity assumption. In the terminology of differentiable maps, \( \mathbf{x}^t \) is a regular point of the vector valued function \( \mathbf{f} \), if its Jacobian \( F(\mathbf{x}^t) \) is full rank.
Algorithm 1 EPO Search for Random initialization

1: **Input:** $x^0 \in \mathbb{X}$, $r \in \mathbb{R}^m$, $\eta$  
2: **while** maximum iterations not reached do  
3: **if** $\mu_r(f(x^t)) \sim 0$ then  
4: $a = \text{LaGrange anchor from (18)}$  
5: else  
6: $a = \text{Descending anchor from (19)}$  
7: $\mathbf{d}_{nd} = F^T \beta^*$, where $\beta^*$ is obtained by solving the QP in (25)  
8: $x^{t+1} = \pi(x^t - \eta \mathbf{d}_{nd})$  
9: **if** $\|\mathbf{d}_{nd}\| \sim 0$ then break  
10: **Output:** $(x^t, f^t)$

**Lemma 3.** If $x^t$ is a regular point of $f$, then the non-dominating direction makes positive angle with the gradients of objectives with maximum relative value

$$
\mathbf{d}_{nd}^T \nabla_x f^*_j \geq 0 \text{ for all } j \in J^*.
$$

A positive angle with the gradient means moving against $\mathbf{d}_{nd}$ will reduce the objective value. Beyond the mild full rank assumption of Jacobian, this lemma is true at certain points $x^t$ with rank deficient Jacobian as well (discussed in the proof).

5.2.1 Convergence.

We prove the convergence of Algorithm 1 in two steps. First we define an admissible set $\mathcal{A}_r f^t \in \mathbb{R}^m$ that contains potential objective vectors $f^{t+1} = f(x^{t+1})$ to which the EPO Search in Algorithm 1 can reach. Then we prove that the sequence of sets $\{\mathcal{A}_r f^t\}_t$ converges to $\mathcal{P}_r$, the set containing the EPO solutions.

To characterize the properties of $x^{t+1}$ obtained by moving against the search direction on $\mathbf{d}_{nd}$, we define some sets in $\mathbb{R}^m$ that are illustrated in figure 4. The set of all attainable objective vectors that dominate the $f^t$ is denoted as

$$
\mathcal{V}_{\leq f^t} = \{f \in \mathcal{O} \mid f \preceq f^t\}.
$$

The set of all attainable objective vectors that have better proportionality than $f^t$ is denoted as

$$
\mathcal{M}_{f^t} = \{f \in \mathcal{O} \mid \mu_r(f) \leq \mu_r(f^t)\}.
$$

During a descent mode $f^{t+1} \in \mathcal{V}_{\leq f^t}$, and in a balance mode $f^{t+1} \in \mathcal{M}_{f^t}$. For the $t^{th}$ iteration, we define a point $\tilde{f}^t = \lambda^t(1/r_1, \cdots, 1/r_m)$, where $\lambda^t = \max \{f^t_j/r_j \mid j \in [m]\}$.
\( \lambda^t \), and hence \( \tilde{\lambda}^t \), are bounded, as each \( r_j \) is positive. Using \( \tilde{\mathcal{F}} \) we define the admissible set as

\[
\mathcal{A}^*_{\mathcal{F}_t} = \left\{ \mathbf{f} \in \mathcal{O} \mid \mathbf{f} \leq \tilde{\mathbf{f}}^t \right\},
\]

which is also bounded. Note its relation with \( \mathcal{V}_{\leq t} \):

**Lemma 4.** When \( \mathcal{F}^t \) and the \( r^{-1} \) ray are not proportional, i.e. \( \mu(\mathbf{f}^t, r^{-1}) > 0 \), the set of dominating objective vectors is a subset of the admissible set \( \mathcal{V}_{\leq t} \subseteq \mathcal{A}^*_{\mathcal{F}_t} \). But when proportional, i.e. \( \mu(\mathbf{f}^t, r^{-1}) = 0 \), both sets are equal \( \mathcal{V}_{\leq t} = \mathcal{A}^*_{\mathcal{F}_t} \).

Using lemmas 3 and 4 we can show:

**Theorem 2.** If \( \mathbf{x}^t \) is a regular point of \( \mathcal{F} \), there exists a step size \( \eta_0 > 0 \), such that for every \( \eta \in [0, \eta_0] \), objective vector of the new solution point \( \mathbf{x}^{t+1} = \mathbf{x}^t - \eta \mathbf{d} \) lies in the \( t \)th admissible set

\[
\mathbf{f} \left( \mathbf{x}^{t+1} \right) \in \mathcal{A}^*_{\mathcal{F}_t}.
\]

Clearly, the admissible set contains all the points in \( \mathcal{O} \) that dominate the \( \mathcal{F}^t \), i.e. \( \mathcal{V}_{\leq t} \subseteq \mathcal{A}^*_{\mathcal{F}_t} \). Moreover, when \( \mu(\mathbf{f}^t) > 0 \), it also has points with better proportionality than \( \mathcal{F}^t \), i.e. \( \mathcal{A}^*_{\mathcal{F}_t} \cap \mathcal{M}^t_{\mathcal{F}} \neq \emptyset \).

Therefore, the admissible set contains the required solution for the next iteration, satisfying both proportionality to \( r^{-1} \) and dominating properties.

A natural consequence of Lemma 4 and Theorem 2 is the monotonicity of \( \lambda^t \) and \( \mathcal{A}^*_{\mathcal{F}_{t+1}} \).

**Corollary 1.** The sequence of relative maximum values \( \{\lambda^t\} \) is monotonic with \( \lambda^{t+1} \leq \lambda^t \), which means \( \mathcal{A}^*_{\mathcal{F}_{t+1}} \subset \mathcal{A}^*_{\mathcal{F}_t} \), and the sequence of bounded sets \( \{\mathcal{A}^*_{\mathcal{F}_t}\} \) converges.

Note that if an EPO solution does not exist for the given preference, i.e. \( r^{-1} \) ray does not intersect the Pareto front \( \mathcal{P} \), then EPO search finds the intersection point between \( r^{-1} \) ray and \( \partial \mathcal{O} \), the boundary of the attainable objective vectors. If the \( r^{-1} \) ray does not intersect \( \partial \mathcal{O} \), then EPO search finds the point in \( \partial \mathcal{O} \) that is maximally proportional to the \( r^{-1} \) ray.

### 5.3 EPO Search for Tracing the Pareto Front from \( \mathbf{x}^0 \in \mathcal{P} \)

If the initialization \( \mathbf{x}^0 \) itself is a Pareto optimal solution, then we can modify the EPO search in Algorithm 1 to trace the Pareto front from \( \mathbf{x}^0 \) to \( \mathbf{x}^* \), an EPO solution w.r.t. preference vector \( r \), and obtain new Pareto optimal solutions along the trajectory. The QP problem solved in each iteration of the modified EPO search is given by

\[
\beta^* = \arg \min_{\beta \in [-1,1]^m} \| \mathbf{F}^T \beta - \mathbf{a} \|^2 \quad \text{s.t.} \quad \beta^T \mathbf{F} \nabla g_k \geq 0, \quad \text{for all } k \in [p_a], \quad \text{if } p_a > 0,
\]

\[
\beta^T \mathbf{F} \nabla h_k = 0, \quad \text{for all } k \in [q], \quad \text{if } q > 0.
\]

Note that we have excluded the constraint (32d) associated to objectives of \( \bar{\mathcal{J}}^* \). Because, if the objective vector \( \mathcal{F}^t \) is (approximately) on the Pareto front, then some objectives with highest relative value (\( r_j f_j^t \)) may require a further increase in their value to move towards an EPO solution.

In the modified algorithm we use Cauchy-Schwarz anchor direction (16) in the balance mode. Because it is orthogonal to the objective vector (see claim 2), and guarantees the escape of the local Pareto optimal at \( \mathbf{x}^* \) to a new point (formalized in theorem 3). However, if we use only the balance mode until \( \mu(\mathbf{f}^t, r^{-1}) \sim 0 \), the trajectory may drift away from the Pareto front, especially for convex objective functions (see appendix B.1.1). Therefore, to ensure that the objective vectors \( \mathcal{F}^t \) in EPO search trajectory stay close to the Pareto front, we alternate between the balance mode and descent mode in every iteration. But the stopping criteria is checked only in the balance mode; because the goal is to keep “balancing” the relative objective vector \( r \odot \mathbf{f} \) until it reaches uniformity 1. This EPO Search is summarized in Algorithm 2.

Note that both the \( m \)-dimensional QP problems (25) and (32) are convex, have at most \( p \) inequality constraints and \( q \) equality constraints, and are independent of \( n \). They can be solved efficiently, e.g., using interior point methods (Cai et al. [2013] [Zhang et al. 2021]). In deep networks, usually the dimension \( n \) of the gradients \( n \gg m \) and the per-iteration complexity of Algorithm 1 as well as Algorithm 2 is \( O(n) \).
With the tracing capability of our algorithm we can move from one Pareto optimal solution to another, and discover new ones in the path. We use this feature to generate a diverse set of optimal solutions by tracing towards the EPO solutions for different preference vectors. We adopt the Pattern Efficient Set

### 5.3.1 Convergence.

We prove the contra-positive: convergence is not achieved until the iterate \( x^t \) is close to \( x^* \) in \( P \), and \( \mu_r(f(x^t)) \) keeps decreasing.

At a point \( x^t \), the set of descent directions is given by

\[
D^f_{x^t} x = \{ d \in T_x x \mid d^T \nabla_{x} f_j \geq 0, \forall j \in [m] \}.
\]

At a local Pareto optimal point \( x^* \) there does not exist any non-zero feasible descent direction, i.e.,

\[
D^f_{x^*} x \cap J_{x^*} x = \{ 0 \}.
\]

Note that, if there are no active constraints at \( x^* \), \( D^f_{x^*} x = \{ 0 \} \). A necessary condition to check if a point \( x^t \) is Pareto optimal, i.e., \( D^f_{x^t} x \cap J_{x^t} x = \{ 0 \} \), is given by Pareto Criticality (see Hillemeier (2001) [Ch 4]):

\[
\begin{align*}
\text{there exists a } & \beta \in S^m, \ \alpha \in \mathbb{R}^p_+, \text{ and } \gamma \in \mathbb{R}^q, \ s.t. \ F^T \beta + G^T \alpha + H^T \gamma = 0, \\
\end{align*}
\]

where \( G \) and \( H \) are the Jacobians of inequality and equality constraints. When there are no active constraints at an optimal point \( x^* \) in \( P \), the Pareto criticality condition in (33) reduces to \( F^T \beta = 0 \) for some \( \beta \in S^m \), and \( x^* \) is called as a Regular Pareto optimal solution if its Jacobian \( F \) is of rank \( m - 1 \) (Zhang et al. (2008)).

Previous gradient-based methods such as Fliege and Svaiter (2000), Désidéri (2012) use the Pareto criticality condition (existence of such coefficient \( \beta \)) as a stopping criterion, since they focus on finding a descent direction in every iteration. As a result these MOO methods stop at any local Pareto optimal solution. In contrast, our proposed method is not designed to find \( \beta \) for a descent direction, hence is not stopped prematurely at any local Pareto optimal solution.

With a mild assumption, that is problem dependent and discussed further in [31], we can guarantee non-convergence at a non-EPO point when there are active constraints, i.e., \( x^* \in \partial \mathbb{R}^n \), and \( \mathbb{R}^n \). We assume there exists an \( \eta_0 > 0 \) such that \( f^* + \eta \tilde{f}^2 \in \text{Int}(O) \) for all \( \eta \in [0, \eta_0] \), where \( f^* = f(x^*) \).

In other words, an infinitesimal step along the direction of objective vector \( \tilde{f}^2 \) starting from \( f^* \in \partial \mathbb{O} \) will take it to the interior of \( \mathbb{O} \). We call this as \( \tilde{f}^2 \) penetrates \( \mathbb{O} \).

**Theorem 3.** Let \( x^* \in \mathbb{P} \) such that, if \( x^* \in \text{Int}(\partial \mathbb{R}^n) \) then it is a regular Pareto optimal solution, and if \( x^* \in \partial \mathbb{R}^n \) then it is a regular point of \( f \) and \( \tilde{f}^2 \) penetrates \( \mathbb{O} \). Then, at \( x^* \), the non-dominating direction \( d_{nd} = F^T \beta^* \) found by the QP (32) with Cauchy-Schwarz anchor (16) is \( 0 \in \mathbb{R}^n \) if and only if \( x^* \in \mathbb{P} \).

Theorem 3 shows that when an EPO solution exists, the algorithm does not stop prematurely at a local Pareto Optimal solution; it traces the Pareto front until an EPO solution is found. This also holds for cases when the regularity assumptions are not satisfied (discussed in the proof).

### 5.4 EPO for Diverse Preference vectors to Approximate Pareto Front

With the tracing capability of our algorithm we can move from one Pareto optimal solution to another, and discover new ones in the path. We use this feature to generate a diverse set of optimal solutions by tracing towards the EPO solutions for different preference vectors. We adopt the Pattern Efficient Set

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**Algorithm 2** EPO Search for Pareto Optimal Initialization

1: **Input:** \( x^0 \in \mathbb{X}, \ r \in \mathbb{R}^m, \ \eta \)  
2: mode = 0  
3: while \( \mu_r(f(x^t)) > 0 \) or \( t < \text{maximum iterations} \) do  
4: if mode = 0 then  
5: \( a = \text{Cauchy-Schwarz anchor from (15)} \)  
6: else  
7: \( d_{nd} = F^T \beta^* \), where \( \beta^* \) is obtained by solving the QP in (32)  
8: \( x^{t+1} = \pi(x^t - \eta d_{nd}) \)  
9: if mode = 0 and \( \|d_{nd}\| \sim 0 \) then break  
10: if mode = 1 - mode  
11: Output: \( \{(x^t, f^t)\}_{t=0}^\infty \)  

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Algorithm (PESA) by Stanojević and Glover (2020) for generating a diverse set preference vectors in the \( m - 1 \) dimensional Simplex \( S^m \).

In PESA, the preference vectors are sampled from \( S^m \) recursively to progressively fill the gaps among existing optimal solutions in the Pareto front. Instead of sampling \( r \), we directly sample the preference rays \( r_k^{-1} \) since it is directly (not inversely) associated with the anchor directions and EPO objective vector. The sampling process in PESA is as follows: given a set of \( m \) preference rays \( R^0 = \{ r_k^{-1} \in S^m \mid k \in [m] \} \), the next ray is sampled as a convex combination of rays in \( R^0 \):

\[
r_{k+1}^{-1} = \frac{1}{m} \sum_{k=1}^{m} r_k^{-1}.
\]

This new ray creates \( m \) more sets, \( R^0_j = R^0 \cup \{ r_{k+1}^{-1} \} - \{ r_j^{-1} \} \) for all \( j \in [m] \). Therefore one can recursively sample new rays and start “filling” the convex hull of the original set of preferences rays. If the original set consists of the axes of positive orthant in \( \mathbb{R}^m \), then this recursive sampling process approximates the entire simplex.

We integrate this sampling rule with EPO Search algorithm and develop the PESA-EPO Search algorithm for approximating the Pareto front. Given a set of \( m \) Pareto optimal objective vectors \( R = \{ \hat{f}_k^0 \mid k = 1, \ldots, m \} \), first we sample the next preference ray as

\[
r_{k+1}^{-1} = \frac{1}{m} \sum_{k=1}^{m} \hat{r}_k^2,
\]

where \( \hat{r}_k^2 \) is the \( \ell_1 \) normalized vector. We then run EPO search (Algorithm 2) to trace the Pareto front (PF) from each of \( \hat{f}_k^0 \) to \( r_{k+1}^{-1} \) ray. This produces \( m \) trajectories on the PF, wherein each end point is (approximately) an EPO solution. Let \( k \hat{f}_k^0 \) be the end point of a trajectory starting at \( \hat{f}_k^0 \). If the EPO solution exists, then all of \( k \hat{f}_k^0 \) will be close to each other near to \( r_{k+1}^{-1} \) ray, i.e. \( \mu(\hat{r}_{k+1}^{-1}, k \hat{f}_k^0) \sim 0 \).

If not, then instead of \( r_{k+1}^{-1} \), we use the end points \( k \hat{f}_k^0 \) to build \( m \) new sets: \( R \cup \{ k \hat{f}_k^0 \} - \{ \hat{r}_k^2 \} \) for all \( k \). The exact same procedure is recursively performed on these new \( m \) sets. Finally the recursion is stopped at a certain depth. In the collection of points obtained from the trajectories, there could be solutions that are dominated by others. In a post-processing step, the dominated solutions are removed to finally present the set of non-dominated solutions.

We conjecture that if the initial set of objective vectors are (closest to the) EPO solutions for the extreme preference rays, i.e. positive axes of \( \mathbb{R}^m \), and the boundary of attainable objective vectors \( \partial \mathcal{O} \) is connected, then one can arbitrarily approximate the Pareto front by increasing the depth of the above recursive procedure. Note that, the Pareto front \( f(\mathcal{P}) \subset \partial \mathcal{O} \) may be disconnected. But due to the connected boundary assumption the trajectories of EPO Search can move between different portions of \( \mathcal{P} \). In case of a bi-objective optimization with a connected Pareto front, a recursion depth of just 1 can approximate the Pareto front. Because for \( m = 2 \), the Pareto front will be at most a \( 1 \)– dimensional manifold, and the trajectories of traced EPO Search are also \( 1 \)– dimensional. This is further clarified through our empirical results in §6.3.

6. Experimental Results

We compare the performance of EPO Search in Algorithm 1 with that of PMTL (Lin et al. 2019), first on synthetic data in §6.1 and then on real data in §6.2. We examine both regression and classification in the multi-task setting where the solution space (weights of the neural network) is high dimensional. In §6.3, we evaluate Algorithm 2 used in PESA-EPO Search for approximating the Pareto front on benchmark multi-objective problems.

6.1 Exact Pareto Optimal Solutions: Synthetic Data

We use the toy problem introduced by Fonseca (1995) to illustrate the behavior of EPO Search in Algorithm 1. The two objectives to be minimized are non-convex functions where \( x \in \mathbb{R}^n \); figure 5 shows this function for \( n = 1 \). The
set of attainable objective values \( O \) is also non-convex in the objective space \( \mathbb{R}^2 \).

\[
f_1(x) = 1 - e^{-\frac{L(x)^2}{2}},
\]

\[
f_2(x) = 1 - e^{-\frac{L(x)^2}{2}},
\]

(36a)

(36b)

Figure 5: 1d solution space for (36)

We run PMTL with the same reference vectors that are given as preferences to EPO search. The set of Pareto optimal solutions \( P \) for the multi-objective functions in (36) is a subset of the hyper-box

\[
B = \{ x \in \mathbb{R}^n | -1/\sqrt{n} \leq x \leq 1/\sqrt{n} \},
\]

(37)

where \( \preceq_n \) denotes the partial ordering induced by the positive cone \( \mathbb{R}^n_+ \) in solution space. We test both the methods when initialization \( x^0 \) is randomly sampled from inside and outside this hyper-box. PMTL is run for 200 iterations while EPO Search is run for only 80 iterations.

When initialization is inside the hyperbox (figure 6a), we observe that PMTL, that does not use any notion of proportionality, descends in every step and reaches a Pareto optimal but not at the preference vectors. On the other hand, EPO search reaches the preference-specific solutions. When initialization is outside the hyperbox (figure 6b), we see that EPO Search both descends and ascends in a controlled manner. It traces the Pareto front to find the required solutions, which makes it robust to initialization. No updates are seen in phase 2 of PMTL, when initialization is outside the hyper-box and far from the preference vectors. It reaches the Pareto front only in 2 out of 4 runs.

We extend this example to create \( m \) loss functions and compare PMTL with EPO Search, with respect to their scalability, in Appendix C.1.

6.2 Multi Task Learning

We use three benchmark classification datasets: (1) MultiMNIST, (2) MultiFashion, and (3) MultiFashion+MNIST. In the MultiMNIST dataset (Sabour et al. 2017), two images of different digits are randomly picked from the original MNIST dataset (LeCun et al. 1998), and combined to form a new image, where one is in the top-left and the other is in the bottom-right. There is zero padding in the top-right and bottom-left. The MultiFashion dataset is generated in a similar manner from the FashionMNIST dataset (Xiao et al. 2017). In Multi-Fashion+MNIST dataset, one image is from MNIST (top-left) and the other image is from FashionMNIST (bottom-right). In each dataset, there are 120,000 samples in the training set and 20,000 samples in the test set.

For each dataset, there are two tasks: 1) classifying the top-left image, and 2) classifying the bottom-right image. Cross entropy losses are used for training. For a fair comparison with PMTL, we use
The results in figure 7 show that the per-task accuracy of EPO search is higher than that of PMTL in every single run (top). The test set losses (bottom) show that the solutions from EPO search are closer to the corresponding preference vectors, compared to the solutions from PMTL.

We observe that the performance of LinScalar is worse than both the MOO-based methods. Recall that search direction is a convex combination of the gradients. In PMTL and EPO search, this combination is optimally chosen in each iteration. In LinScalar it is fixed, in every iteration, to the input user preference (L1 normalized). This causes opposing gradients to cancel each other and decrease the magnitude of the resulting update. Thus, update magnitude of LinScalar is lesser than that of other methods in almost every iteration. With learning rate and number of iterations fixed across methods, update magnitude finally determines proximity to the Pareto front.

Another experiment on a regression problem with 8 tasks is discussed in Appendix C.2. We find that EPO Search outperforms PMTL, Linear scalarization as well as models trained on each task individually.

6.3 Approximating the Pareto Front by Tracing

We tested our algorithm on six multi-objective problems: ZDT1 ZDT2 ZDT3 from Zitzler et al. (2000), DTLZ2 and DTLZ7 from Deb et al. (2005), and TNK from Tanaka et al. (1995). In §6.3.1 we describe the problems and illustrate the Pareto fronts generated by EPO Search. In §6.3.2 we numerically compare the fronts generated by EPO-Search with those from competing approaches.

Figure 7: (Color Online) The top row show the accuracies, and the bottom row losses for 3 datasets. In each figure, x axis corresponds to task-1 while y axis corresponds to task-2. Different colors indicate different preference vectors, which are shown with corresponding $r^{-1}$ rays. EPO solutions have the highest per-task accuracy and are closest to the preference vectors.
6.3.1 Pareto front generated by EPO Search.

The ZDT series of problems minimize two objectives: $f_1(x) = x_1$ and $f_2(x) = g(x)h(f_1(x), g(x))$, where $g(x) = 1 + \frac{\sqrt{f_1(x)}}{n} \sum_{i=2}^{n} x_i$, and

$$h(f_1, g) = \begin{cases} 1 - \sqrt{f_1/g} & \text{for ZDT1}, \\ 1 - (f_1/g)^2 & \text{for ZDT2}, \\ 1 - \sqrt{f_1/g} - (f_1/g) \sin(10\pi f_1) & \text{for ZDT3}, \\ \end{cases}$$

and the argument $x$ is bounded as $0 \leq x_i \leq 1$ for $i = 1, \ldots, n$. Figures 8a, 8b, and 8c show results of applying PESA-EPO. In these results, the depth of PESA procedure is 1 for ZDT1 and ZDT2, and 2 for ZDT3. Note that although ZDT3 has a disconnected Pareto Front, but its boundary of attainable objective vectors $\partial V$ is connected. Therefore, while tracing, PESA-EPO connects the disconnected segments of the Pareto front by tracing the boundary $\partial V$ through $f_{trace}$. This is made possible due to the controlled gradient ascent within EPO Search.

In the TNK problem, $m = n = 2$. The two objectives to minimize are $f_1(x) = x_1$ and $f_2(x) = x_2$ with bounds $0 \leq x_i \leq \pi$ and the inequality constraints

$$x_1^2 + x_2^2 - 1 - 0.1 \cos(16 \arctan \frac{x_1}{x_2}) \geq 0, \quad (x_1 - 0.5)^2 + (x_2 - 0.5)^2 \leq 0.5.$$ 

It has a discontinuous Pareto Front. Figure 8d shows the result of PESA-EPO for this problem.

The DTLZ series of problems have more than two objectives to minimize. Let the last $n - m + 1$ variables of $x \in [0, 1]^n$ be denoted as $x_m$. DTLZ2 is defined as

$$\min \ f_1(x) = (1 + g(x_m)) \cos(x_1 \pi/2) \cdots \cos(x_{m-2} \pi/2) \cos(x_{m-1} \pi/2)$$
$$\min \ f_2(x) = (1 + g(x_m)) \cos(x_1 \pi/2) \cdots \cos(x_{m-2} \pi/2) \sin(x_{m-1} \pi/2)$$
$$\min \ f_3(x) = (1 + g(x_m)) \cos(x_1 \pi/2) \cdots \sin(x_{m-2} \pi/2)$$
$$\vdots$$
$$\min \ f_m(x) = (1 + g(x_m)) \sin(x_1 \pi/2)$$

with $g(x_m) = \sum_{x_i \in x_m} (x_i - 0.5)^2$.

In DTLZ7, the first $m - 1$ objective vectors are $f_j = x_j$ for $j = 1, \ldots, m - 1$. The last objective is defined as

$$f_m(x) = (1 + g(x_m)) h(f_1, f_2, \cdots, f_{m-1}, g),$$

where $g(x_m) = 1 + \frac{9}{n - m + 1} \sum_{x_i \in x_m} x_i$,

$$h(f_1, f_2, \cdots, f_{m-1}) = m - \sum_{j=1}^{m-1} \frac{f_j}{1 + g(1 + \sin(3\pi f_j))}.$$ 

Figure 8e and 8f shows the result of PESA-EPO for DTLZ problems. Note that DTLZ7 has disconnected Pareto front but has a connected boundary of attainable objective vectors $\partial V$. Therefore, akin to ZDT3, here also our algorithm connects the Pareto fronts while tracing. For clarity of presentation, we show the solutions up to a depth of 3 in PESA-EPO for both the problems.

6.3.2 Evaluation of generated Pareto front.

We use Inverted Generational Distance (IGD), proposed by [Coello Coello and Reyes Sierra (2004)], as a performance indicator to measure how closely the obtained solutions approximate the Pareto Front. Let the ground truth Pareto front $P_g = \{y_1^*, \cdots, y_j^*, \cdots \}$ be finely discretized set of the actual Pareto front $P_a$, and $P_a = \{f_1^*, \cdots, f_j^*, \cdots \}$ be the set of points found by an algorithm. Then the performance indicator is defined as

$$\text{IGD}(P_g, P_a) = \frac{1}{|P_g|} \sum_{i=1}^{|P_g|} d(y_i^*, P_a) \quad \text{where} \quad d(y_i^*, P_a) = \min_{\tilde{f}_j^* \in P_a} \|y_i^* - \tilde{f}_j^*\|. \quad (38)$$
Figure 8: Result of PESA-EPO to approximate the Pareto front in six benchmark problems.

The ground truth Pareto fronts for the 6 test problems were obtained from the JMetal framework (Durillo et al. 2010, Durillo and Nebro 2014).

We compare the efficacy of our algorithm with two state-of-the-art algorithms: CTAEA (Li et al. 2019) and PESA-TDM (Stanojević and Glover 2020). CTAEA (Constrained Two-Archive Evolutionary Algorithm) is an evolutionary algorithm, whereas PESA-TDM (Pattern Efficient Search Algorithm with Targeted Directional Model) is a gradient-based algorithm. Empirically, CTAEA has been found to outperform several evolutionary algorithms for constrained MOO: C-MOEAD, C-NSGA-III (Jain and Deb 2013), C-MOEA/DD (Li et al. 2014), I-DBEA (Asafuddoula et al. 2014) and CMoEA (Woldesenbet et al. 2009); and the performance of PESA-TDM was found to be similar or better than NSGA-II (Deb et al. 2002) and four variants of MOEA/D (Zhang and Li 2007): MOEA/DDE, MOEA/D-UD1, MOEA/D-AWA, and MOEA/D-UD2. For CTAEA, we used the python package pymoo (Blank and Deb 2020), and for PESA-TDM we used the source code provided by the authors (Stanojević and Glover 2020). Each algorithm is used to obtain the Pareto front approximation of the 6 problems mentioned above and the IGD values and time of execution are shown in Table 1.

Table 1: Comparison among algorithms based on IGD and time of execution for MOO different problems.

| Algorithms | CTAEA | PESA-TDM | PESA-EPO |
|------------|-------|----------|----------|
| ZDT1 (m = 2, n = 30) | IGD: 0.0426, Time(s): 4.01 | IGD: 0.0088, Time(s): 1.71 | IGD: 0.0016, Time(s): 1.38 |
| ZDT2 (m = 2, n = 30) | IGD: 0.0404, Time(s): 4.05 | IGD: 0.0051, Time(s): 9.93 | IGD: 0.0016, Time(s): 1.14 |
| ZDT3 (m = 2, n = 30) | IGD: 0.0572, Time(s): 4.08 | IGD: 0.0217, Time(s): 20.23 | IGD: 0.0027, Time(s): 1.85 |
| DTLZ2 (m = 3, n = 12) | IGD: 0.0269, Time(s): 221.77 | IGD: 0.0681, Time(s): 40.38 | IGD: 0.0307, Time(s): 2.90 |
| DTLZ7 (m = 3, n = 12) | IGD: 0.0369, Time(s): 60.49 | IGD: 0.0439, Time(s): 41.74 | IGD: 0.0384, Time(s): 2.32 |
| TNK (m = n = p = 2) | IGD: 0.0922, Time(s): 1.64 | IGD: 0.0069, Time(s): 0.61 | IGD: 0.0061, Time(s): 0.83 |
The results indicate that PESA-EPO is able to efficiently (lower time of execution) achieve close approximation to the Pareto front (lower IGD). CTAEA uses the decomposition technique of PMTL (§3.3 and Appendix B.3). The computational complexity of decomposition strategy grows exponentially with the number of objectives. This is reflected in our experiment as well. The time required to reach an IGD value of same scale as that of the competing algorithms is significantly more in DTLZ2 and DTLZ7, where \( m = 3 \), as compared to the other bi-objective problems. PESA-TDM is efficient and suitable when the dimension of solution space is low: in TNK, it achieves as good an approximation as PESA-EPO with lesser execution time. However, for high dimensional solution spaces it is inefficient because, for every new reference vector in the PESA procedure, it has to solve an optimization problem (TDM) starting from a random initialization. On the other hand, PESA-EPO uses a previously obtained optimal solution as an initialization to solve an optimization problem (EPO). Moreover, the points in the trajectory of this optimization are Pareto optimal solutions. As a result, PESA-EPO efficiently achieves very good performance.

7 Conclusion

Our work advances the state-of-the-art in Multi-Objective Optimization and Multi-Task Learning. EPO Search is an efficient MOO-based MTL method to (i) find exact Pareto optimal solutions for input preferences, (ii) model constraints in the solution space and (iii) provide theoretical guarantees of convergence. To the best of our knowledge, no previous MOO-based MTL method offers these advantages. EPO search is robust to initialization and can systematically trace the Pareto front to reach an EPO solution; using this, we design an method to generate a diverse set of Pareto optimal solutions to approximate the Pareto front. Empirically we demonstrate the superior performance of EPO Search and its variants, over competing approaches, on benchmark problems in MTL and Pareto front approximation.

A limitation of EPO Search is that the tracing procedure can approximate the entire Pareto front starting from the extreme solutions only if the set \( \mathcal{O} = \{ \mathbf{f}(\mathbf{x}) \mid \mathbf{x} \in \mathcal{X} \} \) is connected, i.e., there are paths connecting the discontinuous segments of \( \mathcal{P} \). Note that this is the case for disconnected Pareto fronts, in problems ZDT3, TNK and DTLZ7 in §6.3. If \( \mathcal{O} \) is not connected, e.g. in MOOPs of Wang et al. (2019b), then more initial seed points are required in each connected component of \( \mathcal{O} \). This can be addressed in future work by, for example, techniques to add relevant non-extreme seed points by detecting discontinuities in the Pareto front during tracing in EPO Search. Balancing search directions and the ability to trace the Pareto front in a principled manner, that give EPO Search its unique advantages, could be explored in the future in other settings. For instance, in Interactive MOO (Xin et al. 2018) where preference vectors are progressively varied until a satisfactory solution is obtained and other multi-criteria decision-making applications.
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Appendix

A Proofs of Lemmas and Theorems

Lemma 1. If all the objective functions are differentiable, then for any direction \( d \in \mathbb{R}^n \) satisfying \( a^T F d \geq 0 \), where \( F \) is the Jacobian of \( f \), and \( \max_j \{ d^T \nabla_x f_j \} > 0 \), there exists a step size \( \eta_0 > 0 \) such that

\[
\mu(f(x - \eta d), r^{-1}) \leq \mu(f(x), r^{-1}) \quad \text{and} \quad f(x - \eta d) \Rightarrow f(x) \quad \text{for all} \ \eta \in [0, \eta_0].
\]

(39a)

Proof. We first prove \( 39a \) by considering \( \mu(f(x), r^{-1}) \) as a function of \( x \), \( \mu_r^f(x) \). Taylor’s expansion of this function can be written with the Peano’s form of remainder as

\[
\mu_r^f(x - \eta d) = \mu_r^f(x) - \eta \frac{\partial \mu_r^f}{\partial x} d + o(\eta),
\]

(40)

where \( \frac{\partial \mu_r^f}{\partial x} \) is the transpose of gradient \( \nabla_x \mu_r^f \) and the asymptotic notation little-o(\( \eta \)) represents a function that approaches 0 faster than \( \eta \). In particular, for every \( \epsilon > 0 \), there exists an \( \eta_0 > 0 \) such that

\[
\left| \frac{o(\eta)}{\eta} \right| < \epsilon, \ \text{for} \ |\eta| < \eta_0.
\]

(41)

Applying chain rule of differentiation on \( \mu_r \), we get

\[
\frac{\partial \mu_r^f}{\partial x} = \frac{\partial \mu_r}{\partial T} \frac{\partial T}{\partial x} = a^T F.
\]

We know that \( a^T F d \) is non-negative from the statement of the lemma 1. Therefore, when positive, we treat \( a^T F d \) as \( \epsilon \), and use the property of \( o(\eta) \) as mentioned in \( 41 \) to conclude there exists a step size \( \eta_0 > 0 \) such that

\[
|o(\eta)| < \epsilon, \ \forall \eta \in [0, \eta_0],
\]

(42)

and hence \( \mu_r^f(x - \eta d) \leq \mu_r^f(x) \); equality holds when \( a^T F d = 0 \). That proves \( 39a \).

The above strategy can be applied to prove there exists a step size \( \eta_0 > 0 \) such that

\[
f_j(s)(x - \eta d) \leq f_j(s)(x), \quad \forall \eta \in [0, \eta_0],
\]

(43)

where \( j^* = \arg \max_{j \in [m]} d^T \nabla_x f_j \).

(44)

This is true because of the assumption in lemma 1 that \( d^T \nabla_x f_{j^*} > 0 \). And that proves \( 39b \).

Lemma 2. If \( \mu \) is such that the anchor direction is scale invariant to the preference vector, i.e. \( \overline{a}(f, sr) = \overline{a}(f, r) \) for all \( s > 0 \), where \( \overline{a} = \frac{a}{|a|} \) then

\[
\sum_{j=1}^m f_j a_j = \langle f, a \rangle \geq 0 \geq \langle r^{-1}, a \rangle = \sum_{j=1}^m \frac{a_j}{r_j}.
\]

(45)

Proof. We use the second property of \( \mu_r \), stated in 2 i.e. \( \mu_r(r^{-1} + \lambda(f - r^{-1})) \) increases monotonically with \( \lambda \geq 0 \). In other words, \( \mu_r^f(\lambda) = \frac{\partial \mu_r}{\partial \lambda} \geq 0 \), for \( \lambda \geq 0 \). At \( \lambda = 1 \), the chain rule reveals

\[
\mu_r^f(1) = \langle f - r^{-1}, a(f, r^{-1}) \rangle \geq 0
\]

(46)

\[
= \langle f - r^{-1}, a(f, r^{-1}) \rangle \geq \langle r^{-1}, \overline{a}(f, r^{-1}) \rangle.
\]

(47)

We apply the scale invariance property of the anchor direction to the preference vector in \( 47 \)

\[
\langle f, \overline{a}(f, sr^{-1}) \rangle \geq \langle sr^{-1}, \overline{a}(f, sr^{-1}) \rangle
\]

(48)

\[
= \langle f - r^{-1}, a(f, r^{-1}) \rangle \geq \langle sr^{-1}, \overline{a}(f, r^{-1}) \rangle \quad \forall s > 0.
\]

(49)

Applying \( \lim_{s \to 0} \) to \( 49 \), we get \( \langle f, \overline{a} \rangle \geq 0 \). Therefore, applying \( \lim_{s \to \infty} \) to \( 49 \), we get \( \langle r^{-1}, \overline{a} \rangle \leq 0 \), i.e. must not be positive. \( \square \)
Theorem 1. If the anchor direction is scale invariant to preference vector \( \mathbf{r} \), and all the objective functions are differentiable at \( \mathbf{x}^t \), then moving against a direction \( \mathbf{d} \in \mathbb{R}^n \) with \( \mathbf{F} \mathbf{d} = s \mathbf{a} \), for some \( s > 0 \), yields a non-dominated solution \( \mathbf{x}^{t+1} \) whose objective vector \( \mathbf{f}^{t+1} \) is closer to the \( \mathbf{r}^{-1} \) ray than that of \( \mathbf{f}^t \).

Proof. From lemma 2, we know \( \langle \mathbf{f}, \mathbf{a} \rangle > 0 \). Therefore, \( a_{j+} > 0 \) for at least one \( j^+ \in [m] \), because \( f_j > 0 \) for all \( j \in [m] \). As \( \mathbf{F} \mathbf{d} = s \mathbf{a} \) for some \( s > 0 \), we can write

1. \( 0 < sa_{j+} = \mathbf{d}^T \nabla_{xf_j} < \max_j \{ \mathbf{d}^T \nabla_{xf_j} \} \), and
2. \( \mathbf{a}^T \mathbf{F} \mathbf{d} = s \| \mathbf{a} \|^2 > 0 \)

So lemma 3 is applicable, and that concludes the proof.

Lemma 3. If \( \mathbf{x}^t \) is a regular point of \( \mathbf{f} \), then the non-dominating direction makes positive angle with the gradients of objectives with maximum relative value

\[
\mathbf{d}_{nd}^T \nabla_{xf_j} > 0 \quad \text{for all } j \in J^*.
\]

Proof. When \( \mathbf{x}^t \in \partial \mathcal{X} \), boundary of the domain, i.e. \( p_a + q > 0 \), then this is true by design of the QP in (25). The constraint in (25d) ensures that \( \beta^* \mathbf{F} \nabla_{xf_j} = \mathbf{d}_{nd}^T \nabla_{xf_j} > 0 \) for all \( j \in J^* \).

When \( \mathbf{x}^t \in \mathcal{X} \setminus \partial \mathcal{X} \), interior of the domain, i.e. \( p_a = q = 0 \), then

\[
\mathbf{F} \mathbf{d}_{nd} = \mathbf{F} \mathbf{F}^T \beta^* = s \mathbf{a},
\]

for some \( s > 0 \); because \( \mathbf{F} \) is full rank. Therefore we need to prove that

\[
\mathbf{d}_{nd}^T \nabla_{xf_j} = sa_j > 0 \quad \text{for all } j \in J^*,
\]

i.e. the \( \text{Sign}(a_j) \) is non-negative for all \( j \in J^* \). This is trivially true in the descent mode as \( \mathbf{a} = \mathbf{f} \geq 0 \). In the balance mode, the anchor direction used in the EPO Search algorithm, either from Cauchy-Schwarz inequality or from Lagrange’s identity, are linear combination of \( \mathbf{f} \) and the \( \mathbf{r}^{-1} \) ray. The \( \mathbf{a} \) is in the same direction as \( \mathbf{f} \) – \( \mathbf{cr}^{-1} \), for some \( c > 0 \). So, \( \mathbf{r} \odot \mathbf{a} \) is in same direction as that of \( \mathbf{r} \odot \mathbf{f} \). As \( r_j \)'s are positive, we can write \( \text{Sign}(a_j) = \text{Sign}(r_j a_j) = \text{Sign}(f_j r_j - c) \). By assuming, without loss of generality, that \( f_1 r_1 \geq f_2 r_2 \geq \cdots \geq f_m r_m \), we now only have to prove \( a_1 \geq 0 \); because \( f_1 r_1 = f_2 r_2 \) for all \( j \in J^* \), and therefore \( \text{Sign}(f_1 r_1 - c) = \text{Sign}(f_1 - cr_1^{-1}) = \text{Sign}(a_1) = \text{Sign}(a_j) \) for all \( j \in J^* \). Next, we find the bounds of \( c \) by applying the properties of anchor direction proved in lemma 2.

\[
\langle \mathbf{r}^{-1}, \mathbf{a} \rangle \leq 0 \leq \langle \mathbf{f}, \mathbf{a} \rangle
\]

\[
\Rightarrow \langle \mathbf{r}^{-1} \mathbf{f} - cr_1^{-1} \rangle \leq 0 \leq \langle \mathbf{f} - cr^{-1} \rangle
\]

\[
\Rightarrow \langle \mathbf{f}, \mathbf{r}^{-1} \rangle \leq c \leq \frac{\| \mathbf{f} \|^2}{\| \mathbf{r}^{-1} \|^2},
\]

So, we only need to prove \( \text{Sign}(a_1) = \text{Sign}(f_1 - cr_1^{-1}) \) is non-negative for the upper bound of \( c \):

\[
\frac{\| \mathbf{f} \|^2 \mathbf{r}_1^{-1}}{\langle \mathbf{f}, \mathbf{r}^{-1} \rangle} = \frac{f_1^2 r_1^{-1} + f_2^2 r_2^{-1} + \cdots + f_m^2 r_m^{-1}}{\langle \mathbf{f}, \mathbf{r}^{-1} \rangle} \leq \frac{f_1^2 r_1^{-1} + f_2 f_1 r_2^{-1} + \cdots + f_m f_1 r_m^{-1}}{\langle \mathbf{f}, \mathbf{r}^{-1} \rangle} = f_1
\]

\[
\Rightarrow f_1 - cr_1^{-1} \geq 0
\]

\[
\therefore \, a_1 \geq 0,
\]

where the inequality in (56) comes from the fact that \( f_j r_j \leq f_1 r_1 \) \( \Rightarrow \) \( f_j r_j^{-1} \leq f_1 r_1^{-1} \) for all \( j \in [m] \). In fact, when \( \mu(\mathbf{f}, \mathbf{r}^{-1}) > 0, a_1 > 0 \). □

Lemma 3 can be true even without the full rank assumption of \( \mathbf{F} \). In particular, when \( \mathbf{x}^t \) is in the interior of the domain, \( \mathbf{a} \in \text{Col}(\mathbf{FF}^T) \), the column space of \( \mathbf{FF}^T \),
Lemma 4. When $f^i$ and the $r^{-1}$ ray are not proportional, i.e. $\mu(f^i, r^{-1}) > 0$, the set of dominating objective vectors is a subset of the admissible set $\mathcal{V}_{\leq f^i} \subseteq \mathcal{A}_{f^i}$. But when proportional, i.e. $\mu(f^i, r^{-1}) = 0$, both sets are equal $\mathcal{V}_{\leq f^i} = \mathcal{A}_{f^i}$.

Proof. Proof. When $\mu(f^i, r^{-1}) > 0$,
\[
f \in \mathcal{V}_{\leq f^i} \implies f \preceq f^i \implies r \odot f \preceq r \odot f \implies r \odot f \preceq \lambda^i 1 \implies f \preceq \tilde{f}^i \implies f \in \mathcal{A}_{f^i}.
\]
When $\mu(f^i, r^{-1}) = 0$, $\tilde{f}^i = f^i$. Therefore $\mathcal{V}_{\leq f^i} = \mathcal{A}_{f^i}$. \hfill \Box

Theorem 2. If $x^i$ is a regular point of $f$, there exists a step size $\eta_0 > 0$, such that for every $\eta \in [0, \eta_0]$, objective vector of the new solution point $x^{i+1} = x^i - \eta d_{nd}$ lies in the $i$th admissible set
\[
f(x^{i+1}) \in \mathcal{A}_{f^i}.
\]

Proof. Proof. We prove divide our analysis into descent mode and balance mode.

In the descent mode, i.e. $a = f^i$. The QP in (25), produces a search direction that makes non-negative angle with each gradient, i.e. $d_{nd}^T \nabla f_j \geq 0$ for all $j \in [m]$. As a result, by applying the Taylor’s expansion with Peano form of remainder to each $f_j$ along with the property of little-o notation, one can deduce that for every $j \in [m]$ there exists a step size $\eta_0 > 0$ such that $f_j(x^i - \eta d_{nd}) \leq f_j(x^i)$ for all $\eta \in [0, \eta_0]$. If we choose $\eta_0 = \min_j \{\eta_0^j\}$, then for all $\eta \in [0, \eta_0]$, we have
\[
f(x^i - \eta d_{nd}) \leq f(x^i)
\implies f(x^{i+1}) \in \mathcal{V}_{\leq f^i}.
\]
(60)

From Lemma 4 and 60, we conclude that $f^{i+1} \in \mathcal{A}_{f^i}$ for all $\eta \in [0, \eta_0]$.

Now let us analyse the case when $d_{nd}$ is not a descent direction. Let $J^+ = \{j \mid d_{nd}^T \nabla f_j \geq 0\}$ be the index set for descending objectives and $J^- = [m] - J$ for ascending ones. So, there exists an $\eta_{0j} > 0$ for all $j \in J^+$ such that
\[
f_j(x^i - \eta d_{nd}) = f_j^{i+1} \leq f_j^i
\]
for all $\eta \in [0, \eta_{0j}]$. Let $\eta_0^+ = \min_{j \in J^+}\{\eta_{0j}\}$, and $\eta_0 = \min\{\eta_0^-, \eta_0^+\}$, where $\eta_0^+$ is the maximum step size one can take so that $\mu_r(f^{i+1}) \leq \mu_r(f^i)$. Then for all $\eta \in [0, \eta_0]$, and $f^{i+1} = f(x^i - \eta d_{nd})$
\[
\mu_r(f^{i+1}) \leq \mu_r(f^i), \quad \text{and} \quad f^{i+1} \leq f^i, \quad \forall j \in J^+.
\]
\[
\implies r_j f_j^{i+1} \leq r_j f_j^i \leq \lambda^i
\]
\[
\implies f^{i+1} \leq \tilde{f}^i, \quad \forall j \in J^+
\]
Lemma 3 ensures that $J^+ \subseteq J^+$. If all the other objectives in $J^-$ also satisfy
\[
r_j f_j^{i+1} \leq \lambda^i, \forall j \in [0, \eta_0]
\]
then $\eta_0$ can be used as the step size as it is. If this is not the case, i.e. there exists some $j' \in J^-$ such that
\[
r_j f_j(x^i - \eta d_{nd}) > \lambda^i,
\]
then continuity of the objective functions ensures that there must exists some $\eta_{0j'} < \eta_0$ such that
\[
r_j f_j^{i+1} \leq \lambda^i, \forall j \in [0, \eta_{0j'}].
\]
So choosing $\eta_0 = \min_{j'} \{\eta_{0j'}\}$ we finally get
\[
r \odot f(x^i - \eta d_{nd}) = r \odot f^{i+1} \leq \lambda^i r
\]
\[
\implies f^{i+1} \leq \tilde{f}^i
\]
\[
\implies f^{i+1} \in \mathcal{A}_{f^i}
\]
for all $\eta \in [0, \eta_0]$. \hfill \Box
Theorem 3. Let $x^* \in \mathcal{P}$ such that, if $x^* \in \text{Int}(\mathcal{X})$ then it is a regular Pareto optimal solution, and if $x^* \in \partial \mathcal{X}$ then it is a regular point of $f$ and $f^* \neq 0$ penetrates $\mathcal{O}$. Then, at $x^*$, the non-dominating direction $d_{nd} = F^T \beta^*$ found by the QP (32) with Cauchy-Schwarz anchor (16) is $0 \in \mathbb{R}^n$ if and only if $x^* \in \mathcal{P}$.

Proof. The necessity prove is trivial; because if $x^* \in \mathcal{P}$, then the Cauchy-Schwarz anchor direction $a$ in (16) is $0_m \in \mathbb{R}^m$, resulting a $0_m$ coefficient $\beta$ from the QP (32), and $0_m$ search direction.

For the sufficiency, we prove the contra-positive: if $x^* \notin \mathcal{P}$, then the Cauchy-Schwarz anchor direction $a$ in (16) is $0_m \in \mathbb{R}^m$, resulting a $0_m$ coefficient $\beta$ from the QP (32), and $0_m$ search direction.

Now let us consider the case $x^* \in \partial \mathcal{X}$. Since $\mathcal{F} \mathcal{F}^T$ is full rank due to the regularity of $x^*$, we know $f^* \in \text{Col}(\mathcal{F} \mathcal{F}^T)$. So there is a $d_{fs} = F^T \beta_{fs}$, where $\beta_{fs} \in [-1, 1]^m - \{0_m\}$, such that $\beta_{fs} \neq -F \delta d_{fs}$. Using the assumption $\beta_{fs}$ penetrates $\mathcal{O}$ and first order Taylor’s expansion, we can conclude there exists an $\eta_0 > 0$ such that $x^* \in \text{Null}(\mathcal{F} \mathcal{F}^T)$ for all $\eta \in [0, \eta_0]$. Therefore $-d_{fs}$ is a feasible direction, and $d_{fs}$ lies in the relative interior of the first order cone of feasible directions against which we can move: $d_{fs} \in \text{RelInt}(\mathcal{F})$. Now let $d_{s} = F^T \beta_{s}$, where $\beta_{s} \in [-1, 1]^m - \{0_m\}$, such that $\alpha = Fd_{s}$, and

$$\lambda^* = \max \{ \lambda \in [0, 1] \mid (1 - \lambda) d_{fs} + \lambda d_{s} \in \mathcal{F} \} .$$

As $d_{fs} \in \text{RelInt}(\mathcal{F})$, we can say that $\lambda^* > 0$, and the direction $d_{\lambda^*} = (1 - \lambda^*) d_{fs} + \lambda^* d_{s}$ satisfies

$$\langle a, Fd_{\lambda^*} \rangle = \langle a, Fd_{fs} \rangle + \lambda^* \langle a, Fd_{s} \rangle = \lambda^* \langle a, Fd_{s} \rangle + \lambda^* \langle a, Fd_{s} \rangle = \lambda^* \langle a, Fd_{s} \rangle + \lambda^* \langle a, Fd_{s} \rangle > 0 .$$

Moreover, $\beta_{\lambda^*} = (1 - \lambda^*) \beta_{fs} + \lambda^* \beta_{s} \in [-1, 1]^m$, which is non-zero. Therefore existence of such a coefficient $\beta_{\lambda^*}$ and a direction $d_{\lambda^*}$ confirms that the search direction from the solution of QP (32) is non-zero.

In general, this theorem is true even without the regularity assumptions when the orthogonal projection of Cauchy-Schwarz anchor $a$ onto the cone $\text{Col}(\mathcal{F} \mathcal{F}^T) \cap \mathcal{F} \mathcal{F}$ is non-zero, where $\mathcal{F} \mathcal{F} = \{ Fd \mid d \in \mathcal{F} \}$.\hfill \square

B Useful variations in EPO Search

In practice, for high dimensional solution space $\mathcal{X} \subset \mathbb{R}^n$, e.g. DNN parameters, we use a fixed step size instead of adaptively deciding by line search. So, for proper movement in the objective space, we introduce few variations in the EPO search algorithm.

B.1 Momentum in Anchor While Tracing

While tracing the Pareto front, i.e. starting from a Pareto optimal $x^0 \in \mathcal{P}$, we use the Cauchy-Schwarz anchor direction (16), which is always perpendicular to the objective vector (see claim 2). The first order change in the objective space created by the search direction found from QP (32) is $\delta f = Fd_{nd} = \mathcal{F} \mathcal{F}^T \beta^*$. This change $\delta f$ is same as the orthogonal projection of $a$ onto the cone $\text{Col}(\mathcal{F} \mathcal{F}^T) \cap \mathcal{F} \mathcal{F}$. When the Pareto front is connected, at any point on the Pareto front, $a \in \text{Col}(\mathcal{F} \mathcal{F}^T) \cap \mathcal{F} \mathcal{F}$, so the magnitude of $\delta f$ is significant enough to move the iterate with a small step size. But when, the Pareto front is disconnected, e.g. ZDT3 in figure 8c and the iterate is at a boundary point outside the Pareto front, $f^t \in \partial \mathcal{O} - f(\mathcal{P})$, then $a \notin \text{Col}(\mathcal{F} \mathcal{F}^T) \cap \mathcal{F} \mathcal{F}$, and the
magnitude of its projection $\delta f$ may not be enough to propel the iterate ahead with a small step size. The movements in objective slows down. To mitigate this we use a momentum term in the anchor,

$$a_m = a + (f^t - f^{t-1}),$$ (65)

and use $a_m$ in the QP. Using this anchor if the next iterate $f^{t+1} \sim f^t + \eta \delta f$ is dominated by the current one, i.e. $f^{t+1} > f^t$, then we conclude that $f^t \in \partial \mathcal{O} - \mathcal{f}(\mathcal{P})$, and don’t enter the descent mode in the subsequent iterations and only operate in the balance mode. As soon as a non-dominated iterate is found, i.e. $f^{t+1} \nmid f^t$, we resume alternating the modes of operation.

### B.1.1 Importance of Alternating Mode of Operation While Tracing:

It is important to use the descent mode of operation in every other iteration to keep the iterate close to the Pareto front, especially in case of convex objectives. Otherwise the trajectory will drift away from the Pareto front. This is shown in figure 9 for ZDT1 problem.

![Figure 9: Tracing the Pareto front of ZDT1 without the descent mode: the trajectory drifts away from PF.](image)

### B.2 Restricting Trajectory in Descent Mode When not Tracing

When reaching the EPO solution starting from an arbitrary initialization, ideally the algorithm should enter the descent mode only when the iterate $f^t$ reaches exactly onto the $r^{-1}$ ray. Because, when $\mu_r(f^t) = 0$, the anchor direction of descent becomes $\overline{a} = \overline{f^t} = r^{-1}$, and the iterates descent along the $r^{-1}$ to reach the EPO solution. But achieving $\mu_r(f^t) = 0$ while using a fixed step size is less likely. Therefore we perform a descent mode operation whenever the objective vector $f^t$ lies in the cone

$$\mathcal{M}^r_\epsilon = \{ f \in \mathbb{R}^m_+ \mid \mu_r(f) \leq \epsilon \},$$ (66)

for a small $\epsilon > 0$. As a result, the descending anchor direction, and hence the first order change in objective space $\delta f = FF^T \beta^*$, will no longer be aligned with the $r^{-1}$ ray. This causes oscillations around the $r^{-1}$ ray while descending, as shown in figure 10a. To mitigate this, we add the following equality constraint to the QP (25):

$$\delta f = r^{-1} \langle r^{-1}, \delta f \rangle \Rightarrow FF^T \beta = r^{-1} r^{-1}^T FF^T \beta$$

$$\Rightarrow (I_m - r^{-1} r^{-1}^T)FF^T \beta = 0,$$ (67)

where $r^{-1}$ is the $\ell_2$ normalized vector, and $I_m$ is the $m \times m$ identity matrix. This constraint ensures that the movement in the objective space will be aligned with $r^{-1}$ ray. We apply this equality constraint only when there are no active constraints, i.e. $x^t \in \text{Int}(\mathcal{X})$. The restriction in (67) makes the trajectory of descent mode non-oscillatory as shown in figure 10b. The objective functions used in figure 10 is described in section 6.1.

29
Figure 10: Restricting the QP with the constraint 67 eliminates fluctuations in descent mode.

B.3 Comparison with Pareto MTL

The restricted descent approach appears to be similar to Pareto MTL [Lin et al. (2019)] (described in section 3.3), where in the first phase one finds a solution $x^*_k \in \Omega_k$ such that the EPO solution is in $\omega_k$, and in the second phase one does pure descent. Their construction of $\Omega_k$ is such that $f(\Omega_k)$ is also a cone.

However, their method does not guarantee that the outcome of second phase $x^*$ also lies in $\Omega_k$. Because while descending, the objective vector may go outside the cone $f(\Omega_k)$. On the other hand, our method guarantees that the objective vector of the final solution will be inside the cone $M^\epsilon_\tau$ in 66. Because, if in some iteration the $f^i \notin M^\epsilon_\tau$, then a balancing anchor direction is used in the QP to bring it back inside the cone $M^\epsilon_\tau$ in the subsequent iterations.

Moreover, the angular fineness of their cone $f(\Omega_k)$, which dictates the accuracy of the final solution, is dependent on how many reference vectors $\hat{u}^k$, $k = 1, \cdots, K$ are used, which increases exponentially with the number of objectives $m$. On other hand, the angular fineness of our cone $M^\epsilon_\tau$ can be set by merely choosing a small value of $\epsilon$.

C Additional Experimental Results

C.1 Scalability to Many Objectives

Figure 11: Comparison for how the algorithms scale with increasing number of objective functions. Figure 11a is for the quality of preference specific optimal solution, and figure 11b is for run time for 200 iterations.

We test how our algorithm scale with increasing number of objectives and compare that with Pareto MTL. We create $m$ loss functions as

$$f_j(x) = 1 - \exp \left( - \|x - \hat{x}^j\|_2^2 \right), \quad j \in [m],$$

where the entries of $\hat{x}^j \in \mathbb{R}^n$ are sampled uniformly in $[-1/n, 1/n]$. For every $m$, we run both the algorithms for 20 different $n$, dimension of solution space, randomly sampled within 20 and 100.
We randomly select a preference vector in \( \mathbb{R}^m \) for every \((m, n)\) pair. In addition to a preference vector, the PMTL algorithm requires \( K \) reference vectors, which, according to the authors, should be increased exponentially with the increasing \( m \). However, for a fair comparison, we provide \( K = 2m \) (maximum number of constraints in EPO search in this problem) reference vectors, which are again randomly \( \mathbb{R}^m \).

We use \( \mu_r \) from Lagrange identity \((\ref{eq:lagrangian})\) as a measure of the quality of preference-specific Pareto optimal solutions found by the algorithms; result shown in figure \((\ref{fig:rlp})\). Clearly, EPO search scales better with increasing number of objectives as compared to the Pareto MTL method. For every \((m, n)\) pair, both the algorithms were run for 200 iterations with equal step size. The comparison of overall run time (in seconds) is shown in figure \((\ref{fig:run_time})\).

C.2 Multi-Task Learning: Regression

We use the River Flow dataset \cite{Spyromitros-Xioufis2016} that has \( m = 8 \) tasks: predicting the flow at 8 sites in the Mississippi River network. Each sample contains, for each site, the most recent and time-lagged flow measurements from 6, 12, 18, 24, 36, 48, 60 hours in the past. Thus, there are 64 features and 8 target variables. We remove samples with missing values and use 6,300 samples for training and 2,700 for testing. We use a fully connected feed-forward neural network (FNN) with 4 layers (layerwise sizes: 64 \( \rightarrow 32 \rightarrow 16 \rightarrow 8 \rightarrow 8 \)) with \( n = 6,896 \) parameters to fit the data. We randomly choose 20 input preference vectors \( \mathbf{r} \in \mathbb{R}^8 \) (with \( \sum_j r_j = 1 \)) and train the FNN using EPO search, PMTL and LinScalar. We use each of the 8 objectives trained separately as baselines. The same hyper-parameters are used for each method as done in the previous experiment. We used Mean Squared Error (MSE) as the loss for each task. Since visualization is difficult for 8 dimensions, we compare the methods using the relative loss profile (RLP) \( \mathbf{r} \odot \mathbf{f} \) on the test data as shown in figure \((\ref{fig:rlp})\).

We observe that EPO Search outperforms the other methods, indicating that it complies better with the input user preferences; the RLP of EPO search is more uniform (in the sense of definition \((\ref{def:uniformity})\)). Compared to the previous experiment with 2 tasks, the improvement over PMTL is higher. This is expected since the number of reference vectors required by PMTL, to reach a desired preference, grows exponentially with \( m \). Interestingly, our method also improves over the baseline which shows the advantage of MTL for correlated tasks over learning each task independently: predicting river flow at one site helps improving the prediction at other sites as all the sites are from the same river.

D Our Penetration Assumption

We consider the penetration assumption to be mild because, when the range set \( \mathcal{O} \) is \( m \) dimensional and its boundary \( \partial \mathcal{O} \) is \( m - 1 \) dimensional, almost all points in \( \partial \mathcal{O} \) that violate the penetration assumption are not Pareto optimal, not even locally. Figure \((\ref{fig:penetration})\) illustrates a scenario where it is
Figure 13: Penetration assumption is violated at $f^2$. Therefore EPO search for tracing in Algorithm 2 will not be able to trace from $f^1$ to $f^4$; the iterations will converge (stop prematurely) at $f^2$. But it can trace from $f^3$ to $f^4$. Note that the set of points on boundary $\partial O$ from $f^2$ to $f^3$ is not locally Pareto Optimal.

violated. If a point $\hat{f} \in \partial O$ violates penetration along with the points in any of its $m - 1$ dimensional (relative) open neighbourhoods in $\partial O$, then $-\hat{f}$ penetrates $O$, and thus $\hat{f}$ is dominated by $\hat{f} - \eta \hat{v}$ for some small $\eta$. The assumption of $m - 1$ dimensional boundary is fairly general since it is similar to the assumption of regular Pareto optimal in the unconstrained case.

E Notations

Table 2: Notations used in sections 4 and 5

| Notations | Description |
|-----------|-------------|
| $n$, and $m$ | number of variables in the solution space, and number of objectives |
| $f$ | $\mathbb{R}^m$-valued objective function, or a vector in $\mathbb{R}^m$ |
| $S^m$ | $m - 1$ dimensional simplex |
| $r \in S^m$, $r^{-1} \in \mathbb{R}^m$ | preference vector, and its point-wise inverse |
| $x^\ast, x^\ast_0 \in \mathbb{R}^m$ | a Pareto optimal solution, an Exact Pareto optimal solution w.r.t $r$ |
| $x^\ast, f^\ast$ | solution and its objective vector at $t^{th}$ iteration |
| $b^\ast, b^\ast_0 \in \mathbb{R}^m$ | lower and upper bounds (box constraint) on solution variable: $b^\ast_i \leq x_i \leq b^\ast_0$ |
| $\pi : \mathbb{R}^m \rightarrow \mathbb{R}^m$ | Projection function that brings $x$ inside the box constraints element-wise |
| $p, q$ | number of inequality and equality constraints |
| $g, h$ | $\mathbb{R}^p$-valued inequality and $\mathbb{R}^q$ valued equality constraints |
| $p_a, q_a$ | number of active inequality and equality constraints |
| $F, G, H$ | Jacobians of objectives, active inequality and and equality constraints |
| $X \subset \mathbb{R}^m$, $O \subset \mathbb{R}^m$ | Set of feasible solutions, and range of $\mathbb{R}^m$-valued objective function $f$ |
| $\partial X, \partial O$ | Boundaries of domain and range of $f$ respectively |
| $\text{Int}(X), \text{Int}(O)$ | Interior of domain and range of $f$ respectively |
| $P^\ast, P_r$ | Set of Pareto optimal solutions, and Exact Pareto optimal solutions w.r.t $r$ |
| $P^\ast, P^\ast_r, D^\ast$ | Tangent plane/cone, set of feasible directions, descent directions at $x$ |
| $d, d_{nd} \in P^\ast_r$ | a general search direction, non-dominating search direction |
| $\beta \in \mathbb{R}^m$, $\alpha \in \mathbb{R}^{pn}$, $\gamma \in \mathbb{R}^{qn}$ | coefficients for gradients of objectives, active inequality and equality constraints |
| $\mu_r(f) = \mu(f, r^{-1})$ | A measure of proportionality of $f$ w.r.t. $r^{-1}$ |
| $a(f, r)$ or simply $a$ | Anchor direction at point $f \in \mathbb{R}^m$ w.r.t. preference $r$ |
| $\lambda$ | maximum relative value of objectives: $\max_j r_j f_j$ |
| $J^\ast$ | index set of objectives with maximum relative value |
| $A_r, V_{<f}$ | set of attainable objective vectors dominated by $\lambda^\ast r^{-1}$ and $f$ |
| $M_r$ | set of attainable objective vectors with measure of proportionality $< \mu_r(f)$ |
| $\mathbb{R}^m, \mathbb{R}^{m+1}$ | discrete sets of $m$ preference vectors at start, and after 3 recursion in PESA |