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# Appendix—Hypervolume Maximization: A Geometric View of Pareto Set Learning

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## 1 A Experiment Details

### 2 A.1 Metrics

3 As outlined in the main body of the paper, we utilize three metrics to evaluate the effectiveness of  
4 the learned solutions. In particular, we assess the performance of a Pareto neural model  $x_\beta(\cdot)$  by  
5 examining the output of the model for  $N$  angles that are uniformly distributed. The output solution  
6 set  $A = \{y^{(1)}, \dots, y^{(N)}\}$ , where  $A = f \circ x_\beta(\hat{\Theta})$ . The three metrics are:

- 7 1. The *Hypervolume* indicator [30], which measures both the diversity and convergence of  $A$ ;
- 8 2. The *Range* indicator, which measure the angular span of  $A$ ;
- 9 3. The *Sparsity* indicator [4], which measures the distances between adjacent points.

#### 10 A.1.1 The Hypervolume Indicator

11 The hypervolume indicator [30] used to measure  $A$  is standard, which has been defined in the main  
12 paper,

$$\mathcal{H}_r(A) = \Lambda(\{q \mid \exists p \in A : p \preceq q \text{ and } q \preceq r\}), \quad (11)$$

13 and  $r$  is a reference vector,  $r \succeq y^{\text{nadir}}$ . For bi-objective problems, the reference point  $r$  is set to [3.5,  
14 3.5], whereas for three-objective problems, the reference point is set to [3.5, 3.5, 3.5].

#### 15 A.1.2 The Range Indicator

16 The range indicator of a Pareto front is defined in polar coordinates and determines the angular span  
17 of the front. Let  $(\rho^{(i)}, \theta^{(i)})$  be the polar coordinate of objective vectors  $y^{(i)}$  with a reference point  $r$ .  
18 The relationship between of the Cartesian and polar coordinate is,

$$\begin{cases} y_1 = r_1 - \rho \sin \theta_1 \sin \theta_2 \dots \sin \theta_{m-1} \\ y_2 = r_2 - \rho \sin \theta_1 \sin \theta_2 \dots \cos \theta_{m-1} \\ \dots \\ y_m = r_m - \rho \cos \theta_1. \end{cases} \quad (12)$$

19 Then, the *Range* indicator is defined as,

$$\text{Range}(A) = \min_{i \in [m]} \max_{\substack{u \in [N], v \in [N], \\ u \neq v}} \left\{ |\theta_i^{(u)} - \theta_i^{(v)}| \right\}. \quad (13)$$

20 The *Range* indicator can be defined as the minimum angle span across all angles.

### 21 A.1.3 The Sparsity Indicator

22 The sparsity indicator first introduced in [4] measures how dense a set of solutions is. Small inter-  
 23 solution distances result in a small sparsity indicator indicating a dense Pareto front can be found by  
 24 the Pareto neural model. We make a modification for  $m = 2$  since we find that the maximization  
 25 operator is much more stable.

$$\text{Sparsity}(A) = \begin{cases} \max_{i \in [N-1]} \sum_{j=1}^m (\tilde{y}_j^{(i)} - \tilde{y}_j^{(i+1)})^2 & (m = 2) \\ \frac{1}{N-1} \sum_{j=1}^m \sum_{i=1}^{N-1} (\tilde{y}_j^{(i)} - \tilde{y}_j^{(i+1)})^2 & (m > 2). \end{cases} \quad (14)$$

26 where  $\tilde{y}_j^{(i)}$  is the  $i$ -th solution, and the  $j$ -th objective values in the sorted list by the non-dominating  
 27 sorting algorithm [9]. The unit of the Sparsity indicator is  $10^{-3}$  for bi-objective problems and  $10^{-7}$   
 28 for three objective problems.

### 29 A.2 Neural Model Architecture and Feasibility Guarantees

30 We use a 4-layer fully connected neural network similar to [37] for the Pareto neural model  $x_\beta(\cdot)$ .  
 31 We optimize the network using Stochastic Gradient Descent (SGD) optimizer with a batch size of  
 32 64. The first three layers are,

$$\begin{aligned} x_\beta(\cdot) : \theta &\rightarrow \text{Linear}(m, 64) \rightarrow \text{ReLU} \\ &\rightarrow \text{Linear}(64, 64) \rightarrow \text{ReLU} \\ &\rightarrow \text{Linear}(64, 64) \rightarrow \text{ReLU} \rightarrow x_{\text{mid}}. \end{aligned} \quad (15)$$

33 For constrained problems, to satisfy the constraint that the solution  $x_\beta(\lambda)$  must fall within the lower  
 34 bound ( $l$ ) and upper bound ( $u$ ), a sigmoid activation function is used to map the previous layer's  
 35 output to these boundaries,

$$\begin{aligned} x_{\text{mid}} &\rightarrow \text{Linear}(64, n) \rightarrow \text{Sigmoid} \\ &\rightarrow \odot(u - l) + l \rightarrow \text{Output } x_\beta(\lambda). \end{aligned} \quad (16)$$

36 For unconstrained problems, the output solution is obtained through a linear combination of  $x_{\text{mid}}$ ,

$$x_{\text{mid}} \rightarrow \text{Linear}(64, n) \rightarrow \text{Output } x_\beta(\lambda). \quad (17)$$

### 37 A.3 Benchmark Multiobjective Problems

38 **Standard Multiobjective Optimization (MOO) problems.** ZDT1-2 [42] and VLMOP1-2 [38]  
 39 are widely recognized as standard multi-objective optimization (MOO) problems and are commonly  
 40 employed in gradient-based MOO methods. ZDT1 exhibits a convex Pareto front described by  
 41 ( $y_2 = 1 - \sqrt{y_1}$ ,  $0 \leq y_1 \leq 1$ ). On the other hand, ZDT2 presents a non-convex Pareto front defined  
 42 by ( $y_2 = 1 - y_1^2$ ,  $0 \leq y_1 \leq 1$ ), and the LS-based PSL approach can only capture a single Pareto  
 43 solution.

44 **Real world designing problem.** Three real-world design problems with multi-objective optimiza-  
 45 tion are the Four Bar Truss Design (RE21), Hatch Cover Design (RE24), and Rocket Injector Design  
 46 (RE37). In order to simplify the optimization process, the objectives have been scaled to a range of  
 47 zero to one.

48 **Multiobjective Linear Quadratic Regulator.** The Multiobjective Linear Quadratic Regulator  
 49 (MO-LQR) problem is first introduced in [44]. MO-LQR is regarded as a specialized form of  
 50 multi-objective reinforcement learning, where the problem is defined by a set of dynamics presented  
 51 through the following equations:

$$\begin{cases} s_{t+1} = A s_t + B a_t \\ a_t \sim \mathcal{N}(K_{\text{LQR}} s_t, \Sigma). \end{cases} \quad (18)$$

Table 3: Problem information for multiobjective synthetic benchmarks, design, and LQR problems.

Problem	$m$	$n$
ZDT1	2	5
ZDT2	2	5
VLMOP1	2	5
VLMOP2	2	5
LQR2	2	2
Four Bar Truss Design	2	4
Hatch Cover Design	2	2
Rocket Injector Design	3	4
LQR3	3	3

52 In accordance with the settings discussed in the aforementioned work by Parisi et al. [44], the  
 53 identity matrices  $A$ ,  $B$ , and  $\Sigma$  are utilized. The initial state for the bi-objective problem is set to  $s_0 =$   
 54  $[10, 10]$ , whereas for the three-objective problem, it is set to  $s_0 = [10, 10, 10]$ . The reward function  
 55 is defined as  $r_i(s_t, a_t)$ , where  $i$  represents the respective objective. The function is formulated as  
 56 follows:

$$r_i(s_t, a_t) = -(1 - \xi)(s_{t,i}^2 + \sum_{i \neq j} a_{t,i}^2) - \xi(a_{t,i}^2 + \sum_{i \neq j} s_{t,i}^2). \quad (19)$$

57 Here,  $\xi$  is the hyperparameter value that has been set to 0.1. The ultimate objective of the MO-LQR  
 58 problem is to optimize the total reward while simultaneously taking into account the discount factor  
 59 of  $\gamma = 0.9$ . The objectives are scaled with 0.01 for better illustration purposes.

60 Moreover, the control matrix  $K_{LQR}$  is assumed to be a diagonal matrix, and the diagonal elements  
 61 of this matrix are treated as decision variables. Table 3 highlights the number of decision variables  
 62 and objectives.

#### 63 A.4 Results on All Problems

64 The results for all the examined problems are depicted in Figures 10-18, and combined with the  
 65 results tabulated in Table 5 of the main paper, several conclusions can be made.

66 **Behavior of LS-based PSL.** A well-known fact of the linear scalarization method is, it can only  
 67 learn the convex part of a Pareto front. This fact is validated by Figure 11(e), where LS-based PSL  
 68 can only learn several solutions.

69 However, it is crucial to note that the connection between a solution and its corresponding preference  
 70 vector,  $\lambda(\theta)$ , is *non-uniform*, though it is rarely discussed in previous literature. Therefore, a uniform  
 71 sampling of preferences will not result in a uniform sampling of solutions. This observation is  
 72 supported by the results depicted in Figures 10(e), 13(e), and 15(e), where the learned solutions by  
 73 LS-based PSL are not uniformly distributed. And as a result, the sparsity indicators are rather high,  
 74 which indicates the learned front is sparse.

75 **Time Consumption of EPO-based PSL.** In comparison to our approach, the Exact Pareto Op-  
 76 timization [6] algorithm, which serves as the foundation for EPO-based PSL [14], exhibits low  
 77 efficiency due to two factors.

- 78 1. To execute the Exact Pareto Optimization (EPO) algorithm, it is necessary to compute  
 79 the gradients of all objectives,  $\nabla f_i(x)$ 's. This prerequisite entails performing  $m$  back-  
 80 propagation, resulting in higher computational costs. In contrast, our approach banks on  
 81 just one back-propagation operation, rendering it a more efficient option in comparison to  
 82 EPO.
- 83 2. For each iteration, the Exact Pareto Optimization (EPO) algorithm entails solving a com-  
 84 plicated optimization problem based on the specific value of  $f_i$ 's, utilizing the respective

Table 4: Licences.

Resource	Link	License
EPO	<a href="https://github.com/dbmptr/EPOSearch.git">https://github.com/dbmptr/EPOSearch.git</a>	MIT license
pymoo	<a href="https://pymoo.org/">https://pymoo.org/</a>	Apache License 2.0
reproblems	<a href="https://royjitanabe.github.io/reproblems/">https://royjitanabe.github.io/reproblems/</a>	None

85 gradients of  $\nabla f_i(x)$ 's. In contrast, our method does not rely on solving optimization prob-  
 86 lems for each iteration.

87 **Emphasis on Boundary Solutions.** Based on our empirical findings, it is crucial to put emphasis  
 88 on boundary solutions when aiming to recover a complete Pareto set. As shown in Figure 12 and 14,  
 89 if all coordinate  $\theta$  are dealt with equally important, the neural model can only recover a partial part  
 90 of the Pareto set. PSL-HV1 and PSL-HV2 have different behaviors on the three-objective Rocket  
 91 Injector Design problem, as shown in Figure 18. PSL-HV2 algorithm has a tendency to accurately  
 92 identify the complete boundary of the Pareto front, but it often overlooks intermediate solutions. In  
 93 contrast, although PSL-HV1 method may not always recover the complete boundary, it generates a  
 94 denser Pareto front.

## 95 A.5 Licences

96 In this paper, we utilized various licenses, which are outlined in Table 4. All methods were imple-  
 97 mented using Python and the PyTorch framework, with the SMS-EMOA algorithm being aggregated  
 98 in pymoo.

Table 5: Standard derivation (std) value of PSL results on all problems.

Method	ZDT1				ZDT2				VLMOP1			
	HV $\uparrow$	Range $\uparrow$	Sparsity $\downarrow$	Time(s) $\downarrow$	HV	Range	Sparsity	Time(s)	HV	Range	Sparsity	Time(s)
PSL-EPO	0.05	0.04	0.08	2.03	0.13	0.06	0.25	0.91	0.01	0.01	0.02	0.56
PSL-LS	0.0	0.0	0.2	0.43	0.0	0.0	0.0	0.36	0.0	0.0	0.05	0.76
PSL-Tche	0.01	0.0	0.01	0.56	0.01	0.0	0.22	0.79	0.01	0.01	0.02	0.54
PSL-HV1	0.01	0.0	0.05	0.22	0.03	0.01	0.04	0.2	0.0	0.0	0.03	0.48
PSL-HV2	0.01	0.0	0.04	0.29	0.01	0.0	0.21	0.95	0.01	0.0	0.04	1.15
Method	VLMOP2				Four Bar Truss Design				Hatch Cover Design			
	HV $\uparrow$	Range $\uparrow$	Sparsity $\downarrow$	Time(s) $\downarrow$	HV	Range	Sparsity	Time(s)	HV	Range	Sparsity	Time(s)
PSL-EPO	0.08	0.04	0.19	0.48	0.02	0.01	0.01	1.53	0.0	0.02	0.06	4.96
PSL-LS	0.03	0.01	8.69	0.06	0.0	0.0	0.08	0.12	0.0	0.0	0.31	1.21
PSL-Tche	0.01	0.0	0.04	0.49	0.02	0.01	0.02	1.71	0.0	0.01	0.02	2.99
PSL-HV1	0.0	0.0	0.19	1.32	0.01	0.0	0.03	0.38	0.02	0.02	1.41	1.18
PSL-HV2	0.01	0.0	0.13	0.15	0.0	0.0	0.01	1.79	0.0	0.0	0.11	1.42
Method	LQR2				Rocket Injector Design				LQR3			
	HV $\uparrow$	Range $\uparrow$	Sparsity $\downarrow$	Time(s) $\downarrow$	HV	Range	Sparsity	Time(s)	HV	Range	Sparsity	Time(s)
PSL-EPO	0.01	0.01	0.03	15.46	1.34	0.08	0.1	1.12	0.01	0.02	0.71	24.21
PSL-LS	0.0	0.0	0.08	3.7	0.0	0.0	0.02	0.11	0.0	0.01	0.05	5.79
PSL-Tche	0.01	0.01	0.1	4.63	0.01	0.0	0.02	1.17	0.01	0.01	0.27	8.9
PSL-HV1	0.0	0.0	0.22	1.83	0.09	0.01	0.18	0.14	0.0	0.02	0.68	1.34
PSL-HV2	0.0	0.0	0.13	9.86	0.03	0.01	1.53	1.31	0.0	0.01	0.72	11.95

## 99 B Characters of Hypervolume Maximization

### 100 B.1 The Notation Table

101 To enhance the clarity of the paper, we have included a summary of the main notations in Table 6.

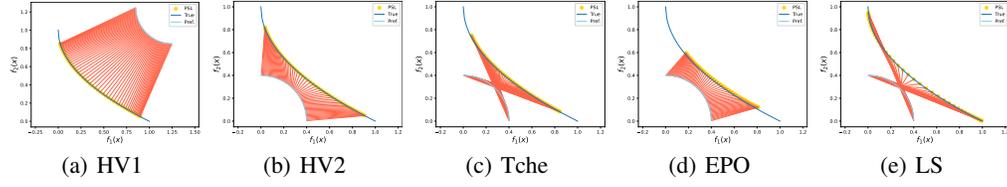


Figure 10: ZDT1.

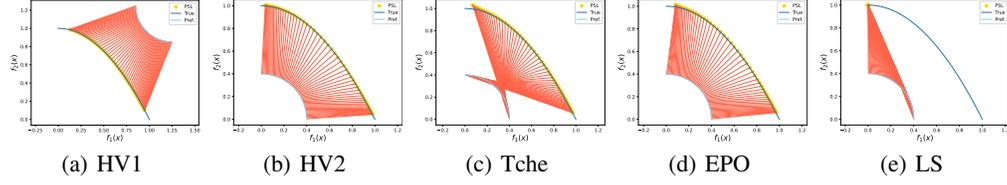


Figure 11: ZDT2.

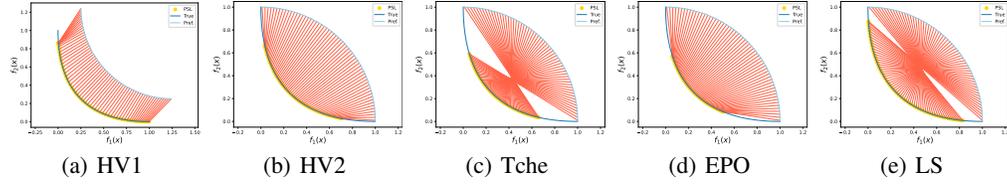


Figure 12: VLMOP1.

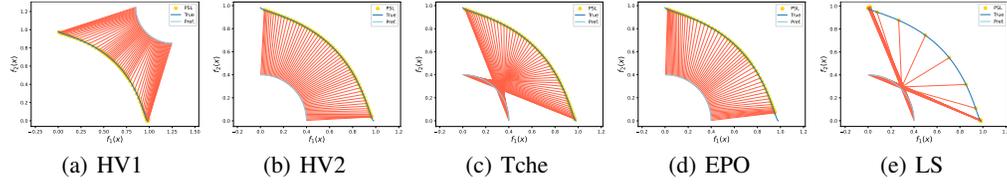


Figure 13: VLMOP2.

## 102 B.2 Hypervolume Calculation in the Polar Coordinate

103 *Proof.* In this subsection, we provide the proof for Equation (5).  $\mathcal{H}_r(\mathcal{F}^*)$  can be simplified by the  
 104 following equations,

$$\begin{aligned}
 \mathcal{H}_r(\mathcal{F}^*) &= \int_{\mathbb{R}^m} I_{\Omega} dy_1 \dots dy_m \\
 &= \underbrace{\int_0^{\frac{\pi}{2}} \dots \int_0^{\frac{\pi}{2}}}_{m-1} dv \\
 &= \underbrace{\int_0^{\frac{\pi}{2}} \dots \int_0^{\frac{\pi}{2}}}_{m-1} \bar{c}_m \cdot \frac{\rho_{\mathcal{X}}(\theta)^m}{2\pi \cdot \pi^{m-2}} \underbrace{d\theta_1 \dots d\theta_{m-1}}_{d\theta} \\
 &= \frac{\bar{c}_m}{2\pi^{m-1}} \underbrace{\int_0^{\frac{\pi}{2}} \dots \int_0^{\frac{\pi}{2}}}_{m-1} \rho_{\mathcal{X}}(\theta)^m d\theta \\
 &= \frac{\bar{c}_m}{2\pi^{m-1}} \cdot \left(\frac{\pi}{2}\right)^{m-1} \cdot \mathbb{E}_{\theta \sim \text{Unif}(\Theta)}[\rho_{\mathcal{X}}(\theta)^m] \\
 &= c_m \mathbb{E}_{\theta \sim \text{Unif}(\Theta)}[\rho_{\mathcal{X}}(\theta)^m].
 \end{aligned} \tag{20}$$

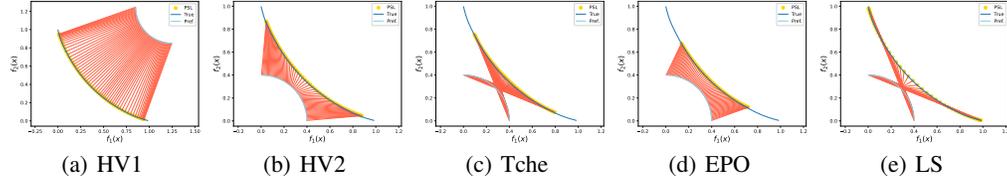


Figure 14: RE21.

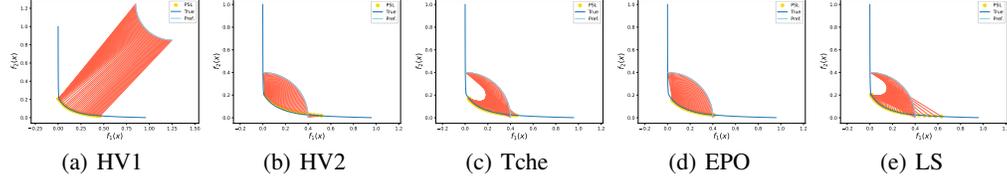


Figure 15: RE24.

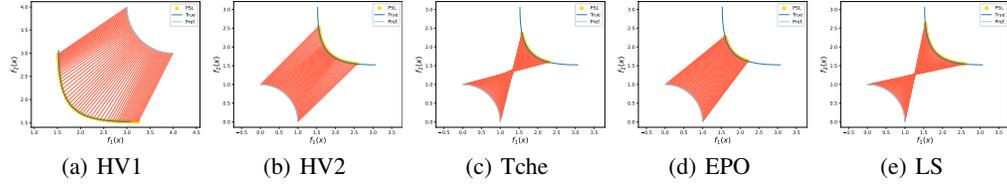


Figure 16: MO-LQR2.

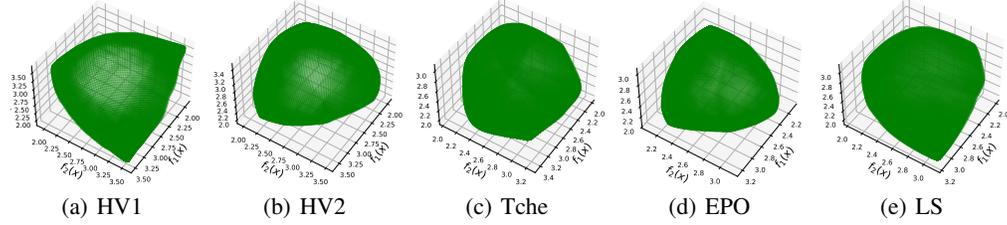


Figure 17: MO-LQR3.

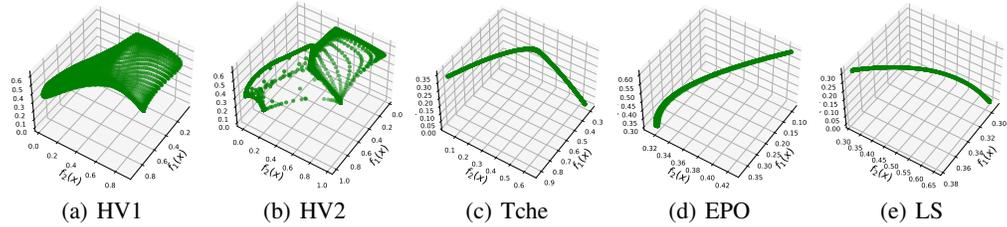


Figure 18: RE37.

105 Here,  $\Omega$  denotes the region dominated by  $\mathcal{F}^*$  with a reference point  $r$ ,  $\Omega = \{q \mid \exists p \in \mathcal{F}^* :$   
 106  $p \preceq q \text{ and } q \preceq r\}$ .  $I_\Omega$  is the indicator function of  $\Omega$ .  $\bar{c}_m$  is the volume of a  $m$ -D unit sphere,  
 107  $\bar{c}_m = \frac{\pi^{m/2}}{\Gamma(m/2+1)}$ .  $c_m$  is a constant defined in the main paper,  $c_m = \frac{\pi^{m/2}}{2^m \Gamma(m/2+1)}$ .  
 108 Line 2 holds since it represents the integral of  $\Omega$  expressed in polar coordinates, wherein the element  
 109  $dv$  corresponds to the volume associated with a segment obtained by varying  $d\theta$ .  
 110 Line 3 calculates the infinitesimal volume of  $dv$  by noticing the fact that the ratio of  $dv$  to  $\bar{c}_m$   
 111  $\frac{\rho_{\mathcal{X}}(\theta)^m}{2\pi \cdot \pi^{m-2}}$ . Line 4 is a simplification of Line 3. And Line 5 and 6 express the integral in its expectation  
 112 form.  $\square$

Table 6: The notation table.

Variable	Definition
$x$	The decision variable.
$n$	The number of the decision variables.
$N$	The number of samples.
$m$	The number of objectives.
$\theta$	The angular polar coordinate.
$\lambda(\theta)$	An $m$ -dimensional preference vector.
$\beta$	The model parameter.
$y^{\text{nadir}}/y^{\text{ideal}}$	The nadir/ideal point of a given MOO problem.
$\mathcal{F}^*$	The Pareto front, which is set of all Pareto non-dominated solutions.
$\mathcal{H}_r(A)$	The hypervolume of set $A$ w.r.t a reference .
$\mathcal{S}_+^{m-1}$	The $(m-1)$ -D positive unit sphere.

### 113 B.3 Proof of $\rho_{\mathcal{X}}(\theta)$ as a Max-Min Problem

We provide the proof of the following equation (Equation (6) in the main paper) in this subsection.

$$\rho_{\mathcal{X}}(\theta) = \max_{x \in \mathcal{X}} \rho(x, \theta) = \max_{x \in \mathcal{X}} \min_{i \in [m]} \left\{ \frac{r_i - f_i(x)}{\lambda_i(\theta)} \right\}.$$

114 *Proof.* Let  $x^*$  be one of the optimal solutions of Problem  $\max_{x \in \mathcal{X}} \rho(x, \theta)$ . To begin, we define  
 115 the attainment surface  $\mathcal{S}_{\text{attain}}$ , as detailed in [31], utilizing a reference point  $r$ . The sets of Pareto  
 116 solutions and weakly Pareto solutions are denoted as  $\mathcal{F}^*$  and  $\mathcal{F}_{\text{weak}}^*$ , respectively. Then,  $\mathcal{S}_{\text{attain}}$  is  
 117 defined as,

$$\mathcal{S}_{\text{attain}} = \mathcal{F}^* \cup \{p \mid p \preceq r, p \in \mathcal{F}_{\text{weak}}^*\}. \quad (21)$$

118 We denote  $P(\theta)$  as the intersection point of the ray from the pole  $r$  along angle  $\theta$  and the attainment  
 119 surface  $\mathcal{S}_{\text{attain}}$ .  $\rho_{\mathcal{X}}(\theta)$  is the distance from the reference point  $r$  to the intersection point  $P(\theta)$ . There  
 120 are two cases,  $x^*$  is a Pareto solution or a weakly Pareto solution. Else, by contradiction,  $f(x^*)$  can  
 121 be improved in all objectives,  $x^*$  cannot be a solution of Problem (6).

122 **When  $x^*$  is Pareto optimal.** In such case, we should prove that  $f(x^*) = P(\theta)$ . If  $x^* \neq P(\theta)$ ,  
 123 then there exist at least one element  $j$  such that,  $\frac{r_j - f_j(\theta)}{\lambda_j(\theta)} \leq \frac{r_i - P_i(\theta)}{\lambda_i(\theta)}$ ,  $\forall i = 1, \dots, m$ . This is a  
 124 contradiction with  $x^*$  is the optimal solution of Problem (6). So,  $x^* = P(\theta)$ .

125 **When  $x^*$  is weakly Pareto optimal.** In such case,  $f(x^*)$  does not necessary equals to  $P(\theta)$ .  
 126 In such case, since  $x^*$  is the solution of Problem (6), we have that there exist at least one index  
 127  $j$ , where  $j = \arg \min \frac{r_j - f_j(x^*)}{\lambda_j(\theta)}$  such that  $\frac{r_j - f_j(x^*)}{\lambda_j(\theta)} = \frac{r_i - P_i(\theta)}{\lambda_i(\theta)}$ ,  $i = 1, \dots, m$ . In such a case,  
 128  $\text{dist}(P(\theta), r) = \frac{r_j - f_j(x^*)}{\lambda_j(\theta)}$ . □

### 129 B.4 Proof of Proposition 2

130 This subsection provides the proof for Proposition 2, which builds the relationship between a polar  
 131 angle  $\theta$  and the corresponding solution of Problem (6).

132 *Proof.* There are two cases for  $x^*$ .  $x^*$  is Pareto optimal or  $x^*$  is weakly Pareto optimal. When  $x^*$  is  
 133 neither Pareto optimal nor weakly Pareto optimal, there exists a solution  $x'$  which is better than  $x^*$   
 134 for all objectives. In such case,  $x^*$  is not a solution for Problem (6), which is a contradiction.

135 **When  $x^*$  is Pareto optimal.** Since we have  $\rho_{\mathcal{X}}(\theta) = \frac{r_i - f_i(x^*)}{\lambda_i(\theta)}$ , which indicates that for any other  
 136 solution  $x'$ , there exist at least one index  $j$  such that,  $\frac{r_j - f_j(x')}{\lambda_j(\theta)} \leq \rho_{\mathcal{X}}(\theta)$ , then  $x'$  is not the optimal  
 137 solution of Problem (6). As a result  $x^*$  is the only solution of Problem (6),  $\mathcal{X}_{\theta} = \{x^*\}$ .

138 **When  $x^*$  is weakly Pareto optimal.** There  
 139 can exist one solution  $x'$  such that,  $x'_i \neq x_i^*$  for  
 140 some  $i$  and therefore,  $x' \in \mathcal{X}_\theta$ . As a result, we  
 141 can conclude that,  $x^* \in \mathcal{X}_\theta$ .  $\square$

## 142 B.5 Case of a Disjointed Pareto Front

143 In order to gain a more thorough comprehension  
 144 of our approach to optimizing loss functions for Pareto set learning (PSL), we investigate a scenario where the Pareto front is disjointed. In such a scenario, it is noted that the preference vector still has an intersection point with the attainment surface (defined in Equation (21)), as illustrated by the blue curve in Figure 19. Equation (6) now measures the volume within the attainment surface and the reference point  $r$ , which is just the hypervolume of a disjointed Pareto front  $\mathcal{H}_r(\mathcal{F}^*)$ .

154 For a disjointed Pareto front, the quantity  $\rho_{\mathcal{X}}(\theta)$  denotes the distance between  $r$  and the attainment surface associated with angle  $\theta$ . Specifically, in Figure 19, the black dot represents the solution for this scenario. The integral of the distance function  $\rho_{\mathcal{X}}(\theta)$  still returns the hypervolume of a disjointed Pareto front, which satisfies our purpose in this paper.

158 However, disjointed Pareto fronts in Pareto set learning overemphasize boundary solutions which may result in unpredictable outcomes. For disjointed Pareto fronts, it is recommended to adaptively adjust the preference distribution (which is set to be uniform in our experiments).

## 161 B.6 Pareto Front Hypervolume Calculation (Type2)

162 In this subsection, we define region  $A$  as the set  
 163 of points dominating the Pareto front,

$$A = \{q \mid \exists p \in \mathcal{F}^* : p \leq q \text{ and } q \geq p^{\text{ideal}}\}. \quad (22)$$

164 To ensure consistency with the notation used in  
 165 the main paper, we use the notation  $\Lambda(\cdot)$  to represent the Lebesgue measure of a set. From a geometric perspective, as illustrated in Figure 20, it can be observed that:

$$\Lambda(A) + \mathcal{H}_r(\beta) = \prod_{i=1}^m (r_i - y_i^{\text{ideal}}). \quad (23)$$

169 The volume of  $A$  can be calculated in a polar  
 170 coordinate as follows,

$$\Lambda(A) = c_m \int_{(0, \frac{\pi}{2})^{m-1}} \bar{\rho}_{\mathcal{X}}(\theta)^m d\theta, \quad (24)$$

171 where  $c_m$  is a constant and  $\bar{\rho}_{\mathcal{X}}(\theta)$  represents the distance from the ideal point to the Pareto front  
 172 at angle  $\theta$ . This distance function  $\bar{\rho}_{\mathcal{X}}(\theta)$  is obtained by solving the optimization problem assuming  
 173 that any radius from  $\theta$  intersects with the Pareto front.

### Problem 1.

$$\bar{\rho}_{\mathcal{X}}(\theta) = \min_{x \in \mathcal{X}} \bar{\rho}_{\mathcal{X}}(\theta, x) = \min_{x \in \mathcal{X}} \max_{i \in [m]} \left\{ \frac{f_i(x) - y_i^{\text{ideal}}}{\lambda_i(\theta)} \right\}, \quad \theta \in (0, \frac{\pi}{2})^{m-1}. \quad (25)$$

174 The relationship between preference  $\lambda$  and the polar angle  $\theta$  is as follows:

$$\begin{cases} \lambda_1(\theta) = \sin \theta_1 \sin \theta_2 \dots \sin \theta_{m-1} \\ \lambda_2(\theta) = \sin \theta_1 \sin \theta_2 \dots \cos \theta_{m-1} \\ \dots \\ \lambda_m(\theta) = \cos \theta_1. \end{cases} \quad (26)$$

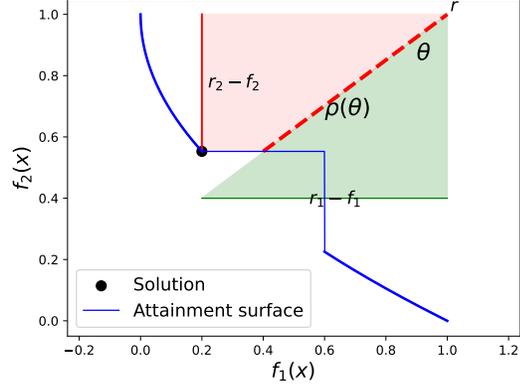


Figure 19: Case of a disjointed Pareto front.

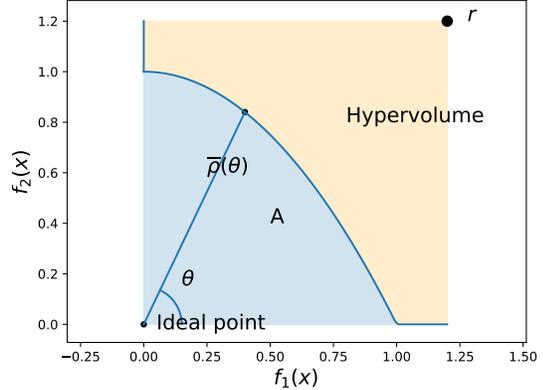


Figure 20: The hypervolume calculation (Type2).

175 Combining Equation (24) and (25) implies that  $\overline{\mathcal{H}}_r(\beta)$  can be estimated as an expectation problem,

$$\overline{\mathcal{H}}_r(\beta) = \prod_{i=1}^m (r_i - y_i^{\text{ideal}}) - \frac{1}{m} c_m \mathbb{E}_{\theta \sim \text{Unif}(\Theta)} [\overline{\rho}_{\mathcal{X}}(x_\beta(\theta), \theta)^m]. \quad (27)$$

### 176 B.7 Proof of Proposition 3

177 *Proof.* It can be observed that Equation (6) in the main paper implies the following equation,

$$-\rho(x, \theta) = \max_{i \in [m]} \left\{ \frac{f_i(x) - r_i}{\lambda_i(\theta)} \right\}. \quad (28)$$

178 When all objectives  $f_i$ 's are convex, function  $-\rho(x, \theta)$  is also convex yet non-smooth, and hence  
 179  $\rho(x, \theta)$  is concave. When  $f_i$ 's are differentiable,  $-\rho(x, \theta)$  possesses a natural subgradient denoted  
 180 as  $d$  that is formulated as  $d = \frac{\partial f_j(x)}{\partial x} \frac{1}{\lambda_j(\theta)}$ , where  $j = \arg \max_{i \in [m]} \left\{ \frac{f_i(x) - r_i}{\lambda_i(\theta)} \right\}$ . The subgradient  $d$   
 181 can be iteratively updated to converge on the global optima of  $\rho_{\mathcal{X}}(\theta)$  in a  $\mathcal{O}(1/\epsilon^2)$  rate, as described  
 182 in [48, 49].

183 When all objectives  $f_i$ 's are quasi-convex,  $-\rho(x, \theta)$ , which is a point-wise max of quasi-convex  
 184 functions, is quasi-convex. And, hence  $\rho(x, \theta)$  is quasi-concave.  $\square$

### 185 B.8 Proof of $\rho_\beta(\theta)$ is Quasi-Concave w.r.t. $x$

186 *Proof.* Proposition 3 rigorously demonstrates that the function  $-\rho(x, \theta)$  is convex for any given  
 187 value of  $\theta$ . Furthermore, consider the function  $h(x) : \mathbb{R} \rightarrow \mathbb{R}$  which may be defined as follows,

$$h(u) = \begin{cases} u^m & \text{if } u \geq 0 \\ u & \text{otherwise} \end{cases}. \quad (29)$$

188 It is clear  $h(x)$  is a non-decreasing function, and  $g(x) = -\rho_\beta(x) = h \circ (-\rho(x, \theta))$ . Since  $(-\rho(x, \theta))$   
 189 is convex, then, for any  $\alpha$ , the set  $S_\alpha(-\rho(x, \theta))$ , as defined as follows, is convex.

$$S_\alpha(-\rho(x, \theta)) = \{x \mid -\rho(x, \theta) \leq \alpha\}. \quad (30)$$

190 Let  $\gamma = h(\alpha)$ . Then for any  $\gamma$ , the set  $S_\gamma(h \circ (-\rho(x, \theta)))$ , which equals to  $S_\alpha(-\rho(x, \theta))$ , is convex.  
 191 This indicates that  $h \circ (-\rho(x, \theta))$  is quasi-convex, and as a result  $\rho_\beta(\theta)$  is quasi-convex w.r.t.  $x$ .  $\square$

### 192 B.9 Proof of Theorem 1

193 **Definitions and preliminaries.** The proof will heavily utilize the existing results on Rademacher  
 194 complexity of MLPs. We will first provide some useful definitions and facts. We start with the  
 195 definition of Rademacher complexity as follows:

196 **Definition 2** (Rademacher complexity, Definition 13.1 in [50]). *Given a set of vectors  $V \subseteq \mathbb{R}^n$ , we  
 197 define the (unnormalized) Rademacher complexity as*

$$\text{URad}(V) := \mathbb{E} \sup_{u \in V} \langle \epsilon, u \rangle,$$

198 where each coordinate  $\epsilon_i$  is an i.i.d. Rademacher random variable, meaning  $\Pr[\epsilon_i = +1] = \frac{1}{2} =$   
 199  $\Pr[\epsilon_i = -1]$ . Furthermore, we can accordingly discuss the behavior of a function class  $\mathcal{G}$  on  $S =$   
 200  $\{z_i\}_{i=1}^N$  by using the following set:

$$\mathcal{G}_{|S} := \{(g(z_1), \dots, f(z_N)) : g \in \mathcal{G}\} \subseteq \mathbb{R}^N,$$

201 and its Rademacher complexity is

$$\text{URad}(\mathcal{G}_{|S}) = \mathbb{E} \sup_{\epsilon} \sup_{u \in \mathcal{G}_{|S}} \langle \epsilon, u \rangle = \mathbb{E} \sup_{\epsilon} \sup_{g \in \mathcal{G}} \sum_i \epsilon_i g(z_i).$$

202 Utilizing Rademacher complexity, we can conveniently bound the generalization error via the fol-  
 203 lowing theorem:

204 **Theorem 2** (Uniform Generalization Error, Theorem 13.1 and Corollary 13.1 in [50]). Let  $\mathcal{G}$  be  
 205 given with  $g(z) \in [a, b]$  a.s.  $\forall g \in \mathcal{G}$ . We collect i.i.d. samples  $S = \{z_i\}_{i=1}^N$  from the law of random  
 206 variable  $Z$ . With probability  $\geq 1 - \delta$ ,

$$\sup_{g \in \mathcal{G}} \mathbb{E}g(Z) - \frac{1}{N} \sum_i g(z_i) \leq \frac{2}{N} \text{URad}(\mathcal{G}_{|S}) + 3(b-a) \sqrt{\frac{\ln(2/\delta)}{2N}}.$$

207 Specifically, the Rademacher complexity in using MLP is provided by the following theorem:

208 **Theorem 3** (Rademacher complexity of MLP, Theorem 1 in [51]). Let 1-Lipschitz positive homo-  
 209 geneous activation  $\sigma_i$  be given, and

$$\mathcal{G}^{MLP} := \{\theta \mapsto \sigma_L(W_L \sigma_{L-1}(\cdots \sigma_1(W_1 \theta) \cdots)) : \|W_i\|_F \leq B_w\}$$

210 Then

$$\text{URad}(\mathcal{G}_{|S}^{MLP}) \leq B_w^L \|X_\theta\|_F (1 + \sqrt{2L \ln(2)}).$$

211 We can then utilize the following composition character of Rademacher complexity, to help induce  
 212 the final Rademacher complexity of hypervolume.

213 **Lemma 2** (Rademacher complexity of compositional function class, adapted from Lemma 13.3 in  
 214 [50]). Let  $g : \Theta \rightarrow \mathbb{R}^n$  be a vector of  $n$  multivariate functions  $g^{(1)}, g^{(2)}, \dots, g^{(n)}$ ,  $\mathcal{G}$  denote the  
 215 function class of  $g$ , and further  $\mathcal{G}^{(j)}$  be the function class of  $g^{(j)}$ ,  $\forall j$ . We have a “partially Lipschitz  
 216 continuous” function  $\ell(g(\theta), \theta)$  so that  $|\ell(g_1(\theta), \theta) - \ell(g_2(\theta), \theta)| \leq L_\ell \|g_1(\theta) - g_2(\theta)\|$  for all  
 217  $g_1, g_2 \in \mathcal{G}$  and a certain  $L_\ell > 0$ ; the associated function class of  $\ell$  is denoted as  $\mathcal{G}^\ell$ . We then have

$$\text{URad}(\mathcal{G}_{|S}^\ell) \leq \sqrt{2} L_\ell \sum_{j=1}^n \text{URad}(\mathcal{G}_{|S}^{(j)}).$$

218 *Proof.* This proof extends Lemma 13.3 in [50] for vector-valued  $g$  and “partially Lipschitz continu-  
 219 ous”  $\ell$ . We first similarly have

$$\begin{aligned} \text{URad}(\mathcal{G}_{|S}^\ell) &= \mathbb{E} \sup_{g \in \mathcal{G}} \sum_i \epsilon_i \ell(g(\theta_i), \theta_i) \\ &= \frac{1}{2} \mathbb{E} \sup_{f, h \in \mathcal{G}} \left( \ell(f(\theta_1), \theta_1) - \ell(h(\theta_1), \theta_1) + \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right) \\ &\leq \frac{1}{2} \mathbb{E} \sup_{f, h \in \mathcal{G}} \left( L_\ell \|f(\theta_1) - h(\theta_1)\| + \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right) \\ &\leq \frac{1}{2} \mathbb{E} \sup_{\epsilon, f, h \in \mathcal{G}} \left( L_\ell \sqrt{2} \left| \sum_{j=1}^n \epsilon_1^{(j)} (f^{(j)}(\theta_1) - h^{(j)}(\theta_1)) \right| + \right. \\ &\quad \left. \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right), \end{aligned}$$

220 where  $\epsilon_1^{(j)}$ 's are new i.i.d. Rademacher variables; the last inequality comes from Proposition 6 in [52]  
 221 (see Equations (5)-(10) in [52] for more details). We can then get rid of the absolute value by

222 considering swapping  $f$  and  $h$ ,

$$\begin{aligned}
& \sup_{f,h \in \mathcal{G}} \left( \sqrt{2}L_\ell \left| \sum_{j=1}^n \epsilon_1^{(j)} (f^{(j)}(\theta_1) - h^{(j)}(\theta_1)) \right| + \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right) \\
&= \max \left\{ \sup_{f,h \in \mathcal{G}} \left( \sqrt{2}L_\ell \sum_{j=1}^n \epsilon_1^{(j)} (f^{(j)}(\theta_1) - h^{(j)}(\theta_1)) + \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right), \right. \\
& \quad \left. \sup_{f,h \in \mathcal{G}} \left( \sqrt{2}L_\ell \sum_{j=1}^n \epsilon_1^{(j)} (h^{(j)}(\theta_1) - f^{(j)}(\theta_1)) + \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right) \right\} \\
&= \sup_{f,h \in \mathcal{G}} \left( \sqrt{2}L_\ell \sum_{j=1}^n \epsilon_1^{(j)} (f^{(j)}(\theta_1) - h^{(j)}(\theta_1)) + \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right).
\end{aligned}$$

223 We can thus upper bounded  $\text{URad}(\mathcal{G}_{|S}^\ell)$  by

$$\begin{aligned}
& \frac{1}{2} \mathbb{E}_\epsilon \sup_{f,h \in \mathcal{G}} \left( \sqrt{2}L_\ell \sum_{j=1}^n \epsilon_1^{(j)} (f^{(j)}(\theta_1) - h^{(j)}(\theta_1)) + \sum_{i=2}^N \epsilon_i (\ell(f(\theta_i), \theta_i) + \ell(h(\theta_i), \theta_i)) \right) \\
&= \mathbb{E}_\epsilon \sup_{g \in \mathcal{G}} \left( \sqrt{2}L_\ell \sum_{j=1}^n \epsilon_1^{(j)} g^{(j)}(\theta_1) + \sum_{i=2}^N \epsilon_i \ell(g(\theta_i), \theta_i) \right),
\end{aligned}$$

224 Repeating this procedure for the other coordinates, we can further have

$$\text{URad}(\mathcal{G}_{|S}^\ell) \leq \sqrt{2}L_\ell \mathbb{E}_\epsilon \sup_{g \in \mathcal{G}} \left( \sum_{i=1}^N \sum_{j=1}^n \epsilon_i^{(j)} g^{(j)}(\theta_i) \right) \leq \sqrt{2}L_\ell \sum_{j=1}^n \mathbb{E}_\epsilon \sup_{g^{(j)} \in \mathcal{G}^{(j)}} \left( \sum_{i=1}^N \epsilon_i^{(j)} g^{(j)}(\theta_i) \right),$$

225 which leads to our claim in the lemma.  $\square$

226 **Proof of Theorem 1.** We are now geared up for the complete proof.

227 *Proof.* We first introduce the sketch of the proof. We mainly utilize Theorem 2 to attain the  
228 claimed results in Theorem 1. Specifically, we set the random sample set  $S = \{\theta_i\}_{i=1}^N$ , the  
229 function class  $\mathcal{G}$  as  $\{\theta \mapsto c_m \rho(x_\beta(\theta), \theta)^m\}$  (the assumption  $r_i - f_i(x) \in [b, B]$  indicates that  
230  $\rho(x, \theta) = \min_{i \in [m]} \left\{ \frac{r_i - f_i(x)}{\lambda_i(\theta)} \right\} \geq b \geq 0$  and by the definition in Equation (7),  $\rho_\beta(\theta)$  is thus al-  
231 ways  $\rho(x(\theta), \theta)^m$ ;  $x_\beta(\cdot)$  is an  $L$ -layer MLP to be specified later). Applying Theorem 2, we can  
232 obtain that with probability at least  $1 - \frac{\delta}{2}$ ,

$$\sup_{g \in \mathcal{G}} \mathbb{E}_\theta g(\theta) - \frac{1}{N} \sum_i g(\theta_i) \leq \frac{2}{N} \text{URad}(\mathcal{G}_{|S}) + 3c_m (B\sqrt{m})^m \sqrt{\frac{\ln(4/\delta)}{2N}},$$

233 where the definition of  $\text{URad}$  and  $\mathcal{G}_{|S}$  can be found in Definition 2. Simply replacing  $\mathcal{G}$  with  
234  $-\mathcal{G} := \{-g : g \in \mathcal{G}\}$ , we can have the inequality of the other direction with probability at least  
235  $1 - \frac{\delta}{2}$ :

$$\begin{aligned}
& \sup_{g \in -\mathcal{G}} \mathbb{E}_\theta g(\theta) - \frac{1}{N} \sum_i g(\theta_i) \leq \frac{2}{N} \text{URad}(-\mathcal{G}_{|S}) + 3c_m (B\sqrt{m})^m \sqrt{\frac{\ln(4/\delta)}{2N}} \\
& \Rightarrow \sup_{g \in \mathcal{G}} \mathbb{E}_\theta -g(\theta) - \frac{1}{N} \sum_i -g(\theta_i) \leq \frac{2}{N} \text{URad}(-\mathcal{G}_{|S}) + 3c_m (B\sqrt{m})^m \sqrt{\frac{\ln(4/\delta)}{2N}} \\
& \Rightarrow \sup_{g \in \mathcal{G}} \frac{1}{N} \sum_i g(\theta_i) - \mathbb{E}_\theta g(\theta) \leq \frac{2}{N} \text{URad}(\mathcal{G}_{|S}) + 3c_m (B\sqrt{m})^m \sqrt{\frac{\ln(4/\delta)}{2N}},
\end{aligned}$$

236 where we apply the property  $\text{URad}(-\mathcal{G}_{|S}) = \text{URad}(\mathcal{G}_{|S})$ . We thus, with probability at least  $1 - \delta$   
 237 (as a result of union bound), can upper bound  $\sup_{g \in \mathcal{G}} |\mathbb{E}_\theta g(\theta) - \frac{1}{N} \sum_i g(\theta_i)|$  by

$$\begin{aligned} & \max \left\{ \sup_{g \in \mathcal{G}} \mathbb{E}_\theta g(\theta) - \frac{1}{N} \sum_i g(\theta_i), \sup_{g \in \mathcal{G}} \frac{1}{N} \sum_i g(\theta_i) - \mathbb{E}_\theta g(\theta) \right\} \\ & \leq \frac{2}{N} \text{URad}(\mathcal{G}_{|S}) + 3c_m (B\sqrt{m})^m \sqrt{\frac{\ln(4/\delta)}{2N}}. \end{aligned}$$

238 For the next step, we will upper bound  $\text{URad}(\mathcal{G}_{|S})$  by analyzing the structure of  $c_m \rho(x_\beta(\theta), \theta)^m$   
 239 and utilizing the existing bound (see Theorem 3) for Rademacher complexity of MLP  $x_\beta$ .

240 The main idea of controlling  $\text{URad}(\mathcal{G}_{|S})$  is to obtain the ‘‘partially Lipschitz continuity’’ that  
 241  $|\rho(x_\beta(\theta), \theta) - \rho(x_{\beta'}(\theta), \theta)| \leq L_\rho \|x_\beta(\theta) - x_{\beta'}(\theta)\|$  for a certain  $L_\rho > 0$ ; with the ‘‘partially  
 242 Lipschitz continuity’’ we can apply Lemma 2 and obtain the desired bound. For simplicity, we de-  
 243 note  $x_\beta(\theta), x_{\beta'}(\theta)$  respectively as  $x, x'$ , and use  $\lambda_j$ 's as shorthand for  $\lambda_j(\theta)$ 's. We now expand the  
 244 difference  $|\rho(x_\beta(\theta), \theta) - \rho(x_{\beta'}(\theta), \theta)|$  as:

$$\begin{aligned} & \left| \min_{j \in [m]} \frac{r_j - f_j(x)}{\lambda_j} - \min_{k \in [m]} \frac{r_k - f_k(x')}{\lambda_k} \right| \\ & = \max \left\{ \min_{j \in [m]} \frac{r_j - f_j(x)}{\lambda_j} - \min_{k \in [m]} \frac{r_k - f_k(x')}{\lambda_k}, \min_{k \in [m]} \frac{r_k - f_k(x')}{\lambda_k} - \min_{j \in [m]} \frac{r_j - f_j(x)}{\lambda_j} \right\}. \end{aligned}$$

245 If we respectively denote the minima index of the two finite-term minimization as  $j^*$  and  $k^*$ , we can  
 246 then upper bound  $|\rho(x_\beta(\theta), \theta) - \rho(x_{\beta'}(\theta), \theta)|$  by

$$\begin{aligned} & \max \left\{ \frac{r_{k^*} - f_{k^*}(x)}{\lambda_{k^*}} - \frac{r_{k^*} - f_{k^*}(x')}{\lambda_{k^*}}, \frac{r_{j^*} - f_{j^*}(x')}{\lambda_{j^*}} - \frac{r_{j^*} - f_{j^*}(x)}{\lambda_{j^*}} \right\} \\ & = \max \left\{ \frac{f_{k^*}(x') - f_{k^*}(x)}{\lambda_{k^*}}, \frac{f_{j^*}(x) - f_{j^*}(x')}{\lambda_{j^*}} \right\} \leq \max_{j \in \{j^*, k^*\}} \frac{|f_j(x) - f_j(x')|}{\lambda_j} \\ & \leq \max_{j \in \{j^*, k^*\}} \frac{L_f |x - x'|}{\lambda_j}. \end{aligned}$$

247 We note there is a special property for  $\lambda_j$  when  $j$  is the minima index: as  $\|\lambda\| = 1$ , there must be a  
 248 certain  $\lambda_j \geq 1/\sqrt{m}$ , and since  $b \leq r_j - f_j(x) \leq B, \forall j$ , we have

$$\frac{b}{\lambda_{j^*}} \leq \frac{r_{j^*} - f_{j^*}(x')}{\lambda_{j^*}} \leq \frac{B}{1/\sqrt{m}} \Rightarrow \lambda_{j^*} \geq \frac{b}{\sqrt{m}B}.$$

249 With this special property, we obtain

$$|\rho(x_\beta(\theta), \theta) - \rho(x_{\beta'}(\theta), \theta)| \leq \frac{\sqrt{m}B}{b} L_f |x - x'|.$$

250 We further have

$$\begin{aligned} & |c_m \rho(x_\beta(\theta), \theta)^m - c_m \rho(x_{\beta'}(\theta), \theta)^m| \\ & = c_m |\rho(x_\beta(\theta), \theta) - \rho(x_{\beta'}(\theta), \theta)| \left( \sum_{k=1}^m \rho(x_\beta(\theta), \theta)^{m-k} \rho(x_{\beta'}(\theta), \theta)^{k-1} \right) \\ & \leq c_m \frac{\sqrt{m}B}{b} L_f |x - x'| m (B\sqrt{m})^{m-1} = c_m \frac{m}{b} (B\sqrt{m})^m L_f |x - x'|, \end{aligned}$$

251 which establishes the ‘‘partially Lipschitz continuity’’. We can then apply Lemma 2 and have

$$\begin{aligned} \text{URad}(\mathcal{G}_{|S}) & \leq \sqrt{2} c_m \frac{m}{b} (B\sqrt{m})^m L_f n \text{URad}(\mathcal{G}_{|S}^{\text{MLP}}) \\ & \leq \sqrt{2} c_m \frac{m}{b} (B\sqrt{m})^m L_f n \cdot B_w^L \|X_\theta\|_F (1 + \sqrt{2L \ln(2)}). \end{aligned}$$

252 Combining the pieces above, we finally have

$$\begin{aligned}
& \sup_{g \in \mathcal{G}} |\mathbb{E}_{\theta} g(\theta) - \frac{1}{N} \sum_i g(\theta_i)| \\
& \leq \frac{2}{N} \text{URad}(\mathcal{G}_{|S}) + 3c_m (B\sqrt{m})^m \sqrt{\frac{\ln(4/\delta)}{2N}} \\
& \leq c_m (B\sqrt{m})^m \left( \frac{2\sqrt{2}mn}{Nb} L_f \cdot B_w^L \|X_{\theta}\|_F (1 + \sqrt{2L \ln(2)}) + 3\sqrt{\frac{\ln(4/\delta)}{2N}} \right),
\end{aligned}$$

253 which is the generalization error bound we claim.  $\square$

### 254 B.10 Upper Bound of $\rho_{\mathcal{X}}(\theta)$

255 In this subsection, we prove that the distance function  $\rho_{\mathcal{X}}(\theta)$  is bounded by the following inequality,

$$256 \rho_{\mathcal{X}}(\theta) \leq Bm^{1/2}, \quad (31)$$

256 when  $r_i - f_i(x) \leq B, \forall x \in \mathcal{X}, \forall i \in [m]$  and  $\|\lambda(\theta)\| = 1$ .

257 *Proof.* We show that the following inequalities hold,

$$\begin{aligned}
\rho_{\mathcal{X}}(\theta) & \leq \max_{x \in \mathcal{X}, \|\lambda(\theta)\|=1} \left( \min_{i \in [m]} \left\{ \frac{r_i - f_i(x)}{\lambda_i(\theta)} \right\} \right) \\
& \leq \max_{\|\lambda(\theta)\|=1} \left( \min_{i \in [m]} \left\{ \frac{B}{\lambda_i(\theta)} \right\} \right) \\
& \leq \frac{B}{m^{-1/2}} = Bm^{1/2}.
\end{aligned} \quad (32)$$

258 The transition from line one to line two is due to the fact that the inequality  $r_i - f_i(x) \leq B$   
259 holds for all  $x \in \mathcal{X}$  and for all  $i \in [m]$ . The transition from line two to line three is  
260  $\max_{\|\lambda(\theta)\|=1} \left( \min_{i \in [m]} \left\{ \frac{B}{\lambda_i(\theta)} \right\} \right)$  is an optimization problem under the constraint  $\|\lambda(\theta)\| = 1$ .  
261 The upper bound for this optimization is when  $\lambda_i = \dots = \lambda_m = m^{-1/2}$ .  $\square$   
262 Let  $\mathcal{Z}(\theta) = c_m \rho_{\mathcal{X}}(\theta)^m$ , as a corollary,  $\mathcal{Z}(\theta) \leq c_m B^m m^{m/2}$ .

### 263 B.11 Gradients of HV-PSL

264 In this subsection, we present the analytical expression for  $\nabla_{\beta} \mathcal{H}_r(\beta)$  to ensure completeness. The  
265 gradient for PSL-HV1 can be computed using the chain rule, which yields:

$$\nabla_{\beta} \mathcal{H}_r(\beta) = \begin{cases} mc_m \mathbb{E}_{\theta \sim \text{Unif}(\Theta)} [\rho(x_{\beta}(\theta), \theta)^{m-1} \underbrace{\frac{\partial \rho(x_{\beta}(\theta), \theta)}{\partial x_{\beta}(\theta)}}_{1 \times n} \underbrace{\frac{\partial x_{\beta}(\theta)}{\partial \beta}}_{n \times d}], & \rho(x_{\beta}(\theta), \theta) \geq 0. \\ c_m \mathbb{E}_{\theta \sim \text{Unif}(\Theta)} \left[ \underbrace{\frac{\partial \rho(x_{\beta}(\theta), \theta)}{\partial x_{\beta}(\theta)}}_{1 \times n} \underbrace{\frac{\partial x_{\beta}(\theta)}{\partial \beta}}_{n \times d} \right], & \text{Otherwise.} \end{cases} \quad (33)$$

266 The gradient of PSL-HV2 can be calculated by,

$$267 \nabla_{\beta} \mathcal{H}_r(\beta) = -mc_m \mathbb{E}_{\theta \sim \text{Unif}(\Theta)} \left[ \bar{\rho}_{\mathcal{X}}(x_{\beta}(\theta), \theta)^{m-1} \underbrace{\frac{\partial \bar{\rho}_{\mathcal{X}}(x_{\beta}(\theta), \theta)}{\partial x_{\beta}(\theta)}}_{1 \times n} \underbrace{\frac{\partial x_{\beta}(\theta)}{\partial \beta}}_{n \times d} \right]. \quad (34)$$

### 267 B.12 Relationship between Hypervolume and Decomposition based Multiobjective 268 Optimization

269 In this subsection, we will explore the fundamental relationship between hypervolume-based  
270 and decomposition-based multiobjective optimization. Prior to our study, it was commonly ac-  
271 knowledged that there were three primary multiobjective optimization methods: Pareto-based [9],  
272 hypervolume-based [30], and decomposition-based methods [8].

273 The present paper yields a result by establishing a correlation between hypervolume and  
 274 decomposition-based approach in scenarios where the number of preference  $\lambda(\theta)$  is considerably  
 275 high. Previous methods mainly consider two decomposition functions, namely linear scalarization  
 276 and Tchebycheff. Actually, we only need to make two modifications for the classical decomposition-  
 277 based method in [8],

- 278 1. Sampling the polar angles  $\theta^{(i)}$  from  $S_+^{m-1}$ .
- 279 2. For each sampled angle  $\theta^{(i)}$ , maximizing the scalarization function  $\rho_{\mathcal{X}}(\theta^{(i)}) =$   
 280  $\max_{x_i \in [m]} \left\{ \frac{r_i - f_i(x)}{\lambda_i(\theta^{(i)})} \right\}$ .

281 Subsequently, upon optimizing each scalarization function, it becomes feasible to constrain the de-  
 282 viation between the empirical mean of  $c_m \rho_{\mathcal{X}}(\theta^{(i)})^m$  and the hypervolume of the Pareto front to a  
 283 small value with a high level of certainty. This is elaborated by Equation (9) in the main manuscript.

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