

Appendix of “High-Dimensional Dueling Optimization with Preference Embedding”

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This appendix first shows the detailed proofs of Lemma 1, Theorem 1 and 2 in the main paper. Then, we describe the difference of implementation details between the original PBO and the improved PBO by us. This improvement enables the PBO method to be applied on high-dimensional optimization problems. Subsequently, we present the hyper-parameter analysis of the proposed PE-DBO on the real-world dataset. Finally, the implementation details of the comparison algorithms deployed on the fixed budget experiment are depicted.

A Proof of Lemma 1

Lemma 1 (Sufficient Condition). *If an objective function f has the optimal ϵ -effective dimension d_e , then the corresponding preference function π_f has the preferential intrinsic dimension $d_p \leq 2d_e$.*

Proof. If the objective function f has optimal ϵ -effective dimension with effective dimension d_e , one has $|f(\mathbf{x}) - f(\mathbf{x}_\epsilon)| \leq \epsilon$, and the following inequality holds for small enough ϵ .

$$\begin{aligned} & |\pi_f([\mathbf{x}; \mathbf{x}']) - \pi_f([\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon])| \\ &= \left| \frac{1}{1 + e^{-[f(\mathbf{x}) - f(\mathbf{x}')]}} - \frac{1}{1 + e^{-[f(\mathbf{x}_\epsilon) - f(\mathbf{x}'_\epsilon)]}} \right| \\ &= \frac{\left| e^{f(\mathbf{x})} (e^{f(\mathbf{x}_\epsilon)} + e^{f(\mathbf{x}'_\epsilon)}) - e^{f(\mathbf{x}_\epsilon)} (e^{f(\mathbf{x})} + e^{f(\mathbf{x}'_\epsilon)}) \right|}{(e^{f(\mathbf{x})} + e^{f(\mathbf{x}')})(e^{f(\mathbf{x}_\epsilon)} + e^{f(\mathbf{x}'_\epsilon)})} \\ &= \frac{e^{f(\mathbf{x}_\epsilon) + f(\mathbf{x}'_\epsilon)} |e^{f(\mathbf{x}) - f(\mathbf{x}_\epsilon)} - e^{f(\mathbf{x}') - f(\mathbf{x}'_\epsilon)}|}{(e^{f(\mathbf{x})} + e^{f(\mathbf{x}')})(e^{f(\mathbf{x}_\epsilon)} + e^{f(\mathbf{x}'_\epsilon)})} \\ &\leq \frac{e^{f(\mathbf{x}_\epsilon) + f(\mathbf{x}'_\epsilon)} |e^\epsilon - e^{-\epsilon}|}{(e^{f(\mathbf{x})} + e^{f(\mathbf{x}')})(e^{f(\mathbf{x}_\epsilon)} + e^{f(\mathbf{x}'_\epsilon)})} \\ &\leq \frac{e^{f(\mathbf{x}_\epsilon) + f(\mathbf{x}'_\epsilon)} (e^\epsilon - e^{-\epsilon})}{(e^{f(\mathbf{x}_\epsilon) - \epsilon} + e^{f(\mathbf{x}'_\epsilon) - \epsilon})(e^{f(\mathbf{x}_\epsilon)} + e^{f(\mathbf{x}'_\epsilon)})} \\ &= \frac{e^{f(\mathbf{x}_\epsilon) + f(\mathbf{x}'_\epsilon)} (e^\epsilon - e^{-\epsilon})}{e^{-\epsilon} (e^{f(\mathbf{x}_\epsilon)} + e^{f(\mathbf{x}'_\epsilon)})^2} \\ &\leq \frac{1}{4} (e^\epsilon - 1) \leq \epsilon, \end{aligned}$$

where the first and the second inequality is by $-\epsilon \leq f(\mathbf{x}) - f(\mathbf{x}_\epsilon) \leq \epsilon$ and $-\epsilon \leq f(\mathbf{x}') - f(\mathbf{x}'_\epsilon) \leq \epsilon$. The last inequality is by $(e^{f(\mathbf{x}_\epsilon)} + e^{f(\mathbf{x}'_\epsilon)})^2 \geq 4e^{f(\mathbf{x}_\epsilon) + f(\mathbf{x}'_\epsilon)}$.

Let $\mathcal{X}_\epsilon = \mathcal{V}_\epsilon$ denote the ϵ -effective subspace of f . Then one has $[\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon] \in \mathcal{X}_\epsilon \times \mathcal{X}_\epsilon = \mathcal{T}$. The derivation process above means that the preference function has the preferential intrinsic dimensionality and a preferential intrinsic subspace \mathcal{T} . According to Definition 1 in the main paper, the preferential intrinsic dimension is no more than the dimension of \mathcal{T} , i.e., $d_p \leq 2d_e$, then the lemma holds. \square

B Proof of Theorem 1

Theorem 1 (Effectiveness on Unbounded Domains). *Suppose the preference function $\pi_f : \mathbb{R}^{2D} \rightarrow [0, 1]$ has preferential intrinsic dimension $d_p \leq 2d_e$. Then, with probability 1, for any $[\mathbf{x}; \mathbf{x}'] \in \mathbb{R}^{2D}$, there exists a $[\mathbf{y}; \mathbf{y}'] \in \mathbb{R}^{2d}$, s.t. $|\pi_f([\mathbf{x}; \mathbf{x}']) - \pi_f([\mathbf{y}; \mathbf{y}'])| \leq 2\epsilon$.*

Proof. Since $\pi_f([\mathbf{y}; \mathbf{y}']) = \pi_f(\mathbf{A}_p[\mathbf{y}; \mathbf{y}'])$, it suffices to prove $|\pi_f([\mathbf{x}; \mathbf{x}']) - \pi_f(\mathbf{A}_p[\mathbf{y}; \mathbf{y}'])| \leq 2\epsilon$. We adopt the same way as (Wang et al. 2016) to construct $[\mathbf{y}; \mathbf{y}']$. Since π_f has the preferential intrinsic dimension d_p , there exists an effective subspace $\mathcal{X}_\epsilon \times \mathcal{X}_\epsilon = \mathcal{T} \subset \mathbb{R}^{2D}$ such that $\dim(\mathcal{T}) = d_p$. By the definition of preferential intrinsic dimension, $|\pi_f([\mathbf{x}; \mathbf{x}']) - \pi_f([\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon])| \leq \epsilon$ holds. Hence, we only need to show that, for any $[\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon] \in \mathcal{T}$, there exists $[\mathbf{y}; \mathbf{y}'] \in \mathbb{R}^{2d}$ s.t. $|\pi_f([\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon]) - \pi_f(\mathbf{A}_p[\mathbf{y}; \mathbf{y}'])| \leq \epsilon$.

Let $\Phi \in \mathbb{R}^{D \times \frac{d_p}{2}}$ be a matrix whose columns form a set of standard orthogonal basis of \mathcal{X}_ϵ . One can concatenate a zero vector with dimension D before or after the orthonormal basis of \mathcal{X}_ϵ . This straightforward way extends the basis of \mathcal{X}_ϵ to the basis of \mathcal{T} . Let $\Phi_p \in \mathbb{R}^{2D \times d_p}$ be a matrix whose columns form a set of standard orthogonal basis of \mathcal{T} , since $\mathcal{T} = \mathcal{X}_\epsilon \times \mathcal{X}_\epsilon$, we have $\Phi_p = \begin{bmatrix} \Phi & \mathbf{0} \\ \mathbf{0} & \Phi \end{bmatrix}_{2D \times d_p}$. Thus, for any $[\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon] \in \mathcal{T}$, there exists a column vector $[\mathbf{z}; \mathbf{z}'] \in \mathbb{R}^{d_p}$ such that $[\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon] = \Phi_p[\mathbf{z}; \mathbf{z}']$.

Following Theorem 2 in (Wang et al. 2016), since multiplying a matrix by a non-zero constant does not change its rank, $\Phi^\top \mathbf{A}$ still has rank $\frac{d_p}{2}$ with probability 1. Therefore, the rank of $\Phi_p^\top \mathbf{A}_p$ can be calculated by

$$\text{rank}(\Phi_p^\top \mathbf{A}_p) = \text{rank} \begin{pmatrix} \Phi^\top \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \Phi^\top \mathbf{A} \end{pmatrix} = 2 \cdot \text{rank}(\Phi^\top \mathbf{A}),$$

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i.e., with probability 1, $\text{rank}(\Phi_p^\top \mathbf{A}_p) = d_p$. This implies that there exists a point $[\mathbf{y}; \mathbf{y}'] \in \mathbb{R}^{2d}$ s.t. $\Phi_p^\top \mathbf{A}_p[\mathbf{y}; \mathbf{y}'] = [\mathbf{z}; \mathbf{z}']$. The orthogonal projection of $\mathbf{A}_p[\mathbf{y}; \mathbf{y}']$ onto \mathcal{T} is given by

$$\Phi_p \Phi_p^\top \mathbf{A}_p[\mathbf{y}; \mathbf{y}'] = \Phi_p[\mathbf{z}; \mathbf{z}'] = [\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon].$$

This means that $\mathbf{A}_p[\mathbf{y}; \mathbf{y}'] = [\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon] + [\mathbf{x}_\perp; \mathbf{x}'_\perp]$ for some $[\mathbf{x}_\perp; \mathbf{x}'_\perp] \in \mathcal{T}^\perp$, since $[\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon]$ is the projection of $\mathbf{A}_p[\mathbf{y}; \mathbf{y}']$ onto \mathcal{T} . According to the definition of the preferential intrinsic dimension, $|\pi_f([\mathbf{x}_\epsilon; \mathbf{x}'_\epsilon]) - \pi_f(\mathbf{A}_p[\mathbf{y}; \mathbf{y}'])| \leq \epsilon$, thus $|\pi_f([\mathbf{x}; \mathbf{x}']) - \pi_f(\mathbf{A}_p[\mathbf{y}; \mathbf{y}'])| \leq 2\epsilon$. \square

C Proof of Theorem 2

Theorem 2 (Effectiveness on Bounded Domains). *Suppose the preference function π_f has preferential intrinsic dimension d_p , the domain of f is $\mathcal{X} \subset \mathbb{R}^D$ and \mathcal{X} is centered around $\mathbf{0}$. Let $\mathbf{x}^* = \text{argmax}_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$ be an optimizer of f with the \mathcal{X} and $\mathbf{x}'_\epsilon \in \mathcal{X} \cap \mathcal{X}_\epsilon$ be the optimizer of f inside \mathcal{X}_ϵ . For any $\mathbf{x}' \in \mathcal{X}$, $\mathbf{x}'_\epsilon \in \mathcal{X} \cap \mathcal{X}_\epsilon$, there exists a duel $[\mathbf{y}^*; \mathbf{y}'] \in \mathbb{R}^{2d}$, s.t. $|\pi_{f_p}([\mathbf{y}^*; \mathbf{y}']) - \pi_f([\mathbf{x}^*; \mathbf{x}'_\epsilon])| \leq 2\epsilon$ and $\|[\mathbf{y}^*; \mathbf{y}']\|_2 \leq \sqrt{\frac{dd_p}{2\epsilon^2}} \|[\mathbf{x}^*; \mathbf{x}'_\epsilon]\|_2$ w.p. at least $1 - \epsilon$.*

Proof. Since $\pi_{f_p}([\mathbf{y}; \mathbf{y}']) = \pi_f(\mathbf{A}_p[\mathbf{y}; \mathbf{y}'])$, it suffices to prove $|\pi_f([\mathbf{x}; \mathbf{x}']) - \pi_f(\mathbf{A}_p[\mathbf{y}; \mathbf{y}'])| \leq 2\epsilon$. By projecting $[\mathbf{x}^*; \mathbf{x}']$ to \mathcal{T} , one has $[\mathbf{x}^*_\epsilon; \mathbf{x}'_\epsilon] \in \mathcal{X}_\epsilon \times \mathcal{X}_\epsilon \cap \mathcal{T}$. Since $[\mathbf{x}^*; \mathbf{x}'] = [\mathbf{x}^*_\epsilon; \mathbf{x}'_\epsilon] + [\mathbf{x}_\perp; \mathbf{x}'_\perp]$ for some $[\mathbf{x}_\perp; \mathbf{x}'_\perp] \in \mathcal{T}^\perp$, $|\pi_f([\mathbf{x}^*; \mathbf{x}']) - \pi_f([\mathbf{x}^*_\epsilon; \mathbf{x}'_\epsilon])| \leq \epsilon$ holds.

Let Φ_p be a matrix whose columns form a set of standard orthogonal basis of \mathcal{T} . As the proof of Theorem 1, we have $\Phi_p = \begin{bmatrix} \Phi & \mathbf{O} \\ \mathbf{O} & \Phi \end{bmatrix}$ and the columns of Φ form a set of standard orthogonal basis of \mathcal{X}_ϵ . Without loss of generality, one can assume that $\Phi = [\mathbf{I}_{d_p/2} \ \mathbf{O}]^\top$. Then, as shown in the proof of Theorem 1, for $[\mathbf{x}^*_\epsilon; \mathbf{x}'_\epsilon]$, there exists $[\mathbf{y}^*; \mathbf{y}'] \in \mathbb{R}^{2d}$ s.t. $\Phi_p \Phi_p^\top \mathbf{A}_p[\mathbf{y}^*; \mathbf{y}'] = [\mathbf{x}^*_\epsilon; \mathbf{x}'_\epsilon]$. As same as Theorem 3 in (Wang et al. 2016), $\Phi \Phi^\top \mathbf{A} \mathbf{y}^* = \mathbf{x}^*_\epsilon$ is equivalent to $\sqrt{d}^{-1} \mathbf{B} \mathbf{y}^* = \bar{\mathbf{x}}^*_\epsilon$, where $\mathbf{B} \in \mathbb{R}^{\frac{d_p}{2} \times \frac{d_p}{2}}$ is a random matrix with independent standard Gaussian entries, and $\bar{\mathbf{x}}^*_\epsilon$ is a vector that contains the first $\frac{d_p}{2}$ entries of \mathbf{x}^*_ϵ and the rest entries are 0. The same analysis is applied to \mathbf{x}' . Therefore, $\Phi_p \Phi_p^\top \mathbf{A}_p[\mathbf{y}^*; \mathbf{y}'] = [\mathbf{x}^*_\epsilon; \mathbf{x}'_\epsilon]$ is equivalent to

$$\begin{aligned} \Phi_p \Phi_p^\top \mathbf{A}_p[\mathbf{y}^*; \mathbf{y}'] &= \begin{bmatrix} \Phi \Phi^\top \mathbf{A} & \mathbf{O} \\ \mathbf{O} & \Phi \Phi^\top \mathbf{A} \end{bmatrix} [\mathbf{y}^*; \mathbf{y}'] \\ &= \begin{bmatrix} \sqrt{d}^{-1} \mathbf{B} & \mathbf{O} \\ \mathbf{O} & \sqrt{d}^{-1} \mathbf{B} \end{bmatrix} [\mathbf{y}^*; \mathbf{y}'] \\ &= [\bar{\mathbf{x}}^*_\epsilon; \bar{\mathbf{x}}'_\epsilon], \end{aligned}$$

where $[\bar{\mathbf{x}}^*_\epsilon; \bar{\mathbf{x}}'_\epsilon]$ is a vector that contains the $\{1, \dots, \frac{d_p}{2}, D + 1, \dots, D + \frac{d_p}{2}\}$ entries of $[\mathbf{x}^*; \mathbf{x}'_\epsilon]$. Then, by Theorem 3.4 in (Sankar, Spielman, and Teng 2006), one has

$$\Pr \left[\|\mathbf{B}^{-1}\|_2 \geq \sqrt{\frac{d_p}{2\epsilon^2}} \right] \leq \epsilon.$$

Thus, with probability at least $1 - \epsilon$,

$$\begin{aligned} \|[\mathbf{y}^*; \mathbf{y}']\|_2 &\leq \left\| \begin{bmatrix} \sqrt{d}^{-1} \mathbf{B} & \mathbf{O} \\ \mathbf{O} & \sqrt{d}^{-1} \mathbf{B} \end{bmatrix}^{-1} \right\|_2 \|[\bar{\mathbf{x}}^*_\epsilon; \bar{\mathbf{x}}'_\epsilon]\|_2 \\ &\leq \|\sqrt{d} \mathbf{B}^{-1}\|_2 \|[\mathbf{x}^*_\epsilon; \mathbf{x}'_\epsilon]\|_2 \\ &\leq \sqrt{\frac{dd_p}{2\epsilon^2}} \|[\mathbf{x}^*; \mathbf{x}'_\epsilon]\|_2. \end{aligned}$$

\square

D Improvements on PBO

In the original version of PBO (González et al. 2017), it discretizes the dueling solution space to calculate the integration of the soft-Copeland score. The accuracy of this method depends on the number of points in the grid of each dimension. Since the total number of the grid is limited by the memory of the device, when the dimension increases, the number of points of each dimension decreases. Hence, the performance of the original PBO is affected by the dimension of the objective function severely and in (González et al. 2017) the original PBO can only be deployed on the 2-dimensional tasks. To improve the original PBO, the Monte-Carlo integration has been employed to estimate the soft-Copeland score, and now the improved PBO can be deployed on the high-dimensional tasks in our experiments. The acquisition function for $\mathbf{y}'_{\text{next}}$ is been substituted by the deviation of the fitted GP to reduce the calculation consumption.

To test whether the improved PBO can be deployed on the high-dimensional dueling optimization tasks, the improved PBO is deployed on the synthetic testing functions based on Bohachevsky, Bukin, Dixon, Levy and Zakhrov.¹ They have dimension $D = 10$ and optimal ϵ -effective dimension $d_e = 2$. These experiments set $M = 6$ duels to initialize and $N = 50$ duels to optimize. All experiments are repeated for 30 times. The number of points used to estimate the Monte-Carlo integration of π_f is $I = 300$ for both improved PBO and PE-DBO. We set the dimension of the low dimension subspace as $2d = 4$. The boundary of the low-dimensional subspace for PE-DBO is $[-1, 1]^4$. The result shown is in Figure 1.

Figure 1 indicates that, when the dimension of the dueling solution space is $2D = 20$, the improved PBO can have a comparable simple regret with other methods that fix one solution, such as the results on Bohachevsky, Bukin, and Zakhrov synthetic testing functions. Compared with that the original PBO is only deployed on 2-dimensional testing functions (González et al. 2017), the improved PBO can handle 10-dimension objective functions and thus can be deployed on the high-dimensional tasks as a comparison method of PE-DBO.

E Hyper-Parameter Analysis

To investigate the effect of key hyper-parameters on the optimization performance of PE-DBO, we set the hyper-parameters with different values, and verify the robustness on

¹<http://www.sfu.ca/~ssurjano/optimization.html>

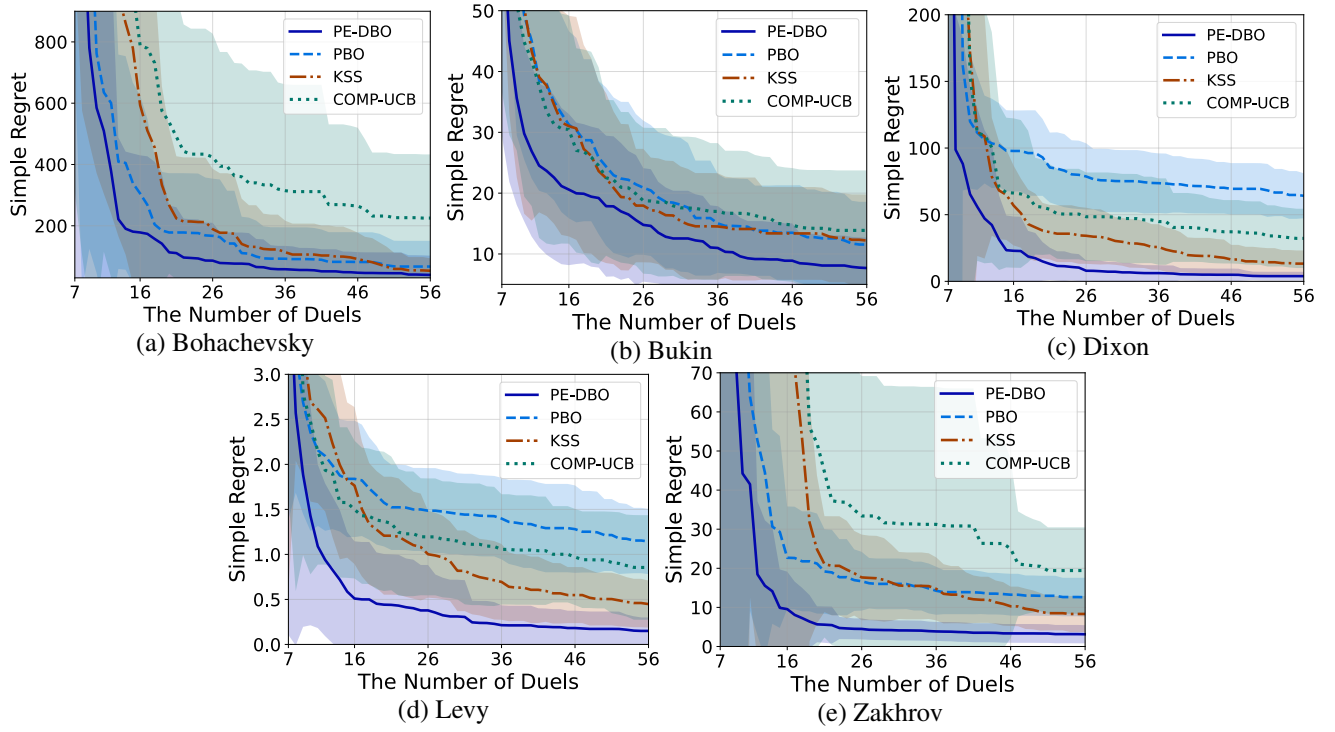


Figure 1: The simple regret (mean and standard deviation) on five synthetic testing functions with $D = 10$. Six duels are used to initialize all algorithms, and fifty duels are used for the optimization process. All experiments are repeated for 30 times.

Table 1: Hyper-parameter analysis on the real-world MSLR dataset. There are three hyper-parameters ($2d$, I , L_b) in PE-DBO, and we fix two of them while keeping the rest tunable for each experiment. The result is the mean of the returned objective function value and the standard deviation under each hyper-parameter setting. The mean is bold if it is the best among different tunable hyper-parameter values. Other settings are as same as that in Figure 3(b) in the main paper. All experiments are repeated for 20 times.

Tunable hyper-parameter: $2d$. With $I = 600$, $L_b = \sqrt{d}$ fixed.							
$2d$	4	20	60	100	140	200	272
Result	7.533 \pm 1.456	8.632 \pm 0.129	8.656 \pm 0.116	8.687 \pm 0.123	8.689 \pm 0.127	8.688 \pm 0.136	8.675 \pm 0.091
Tunable hyper-parameter: I . With $2d = 100$, $L_b = \sqrt{d}$ fixed.							
I	1	50	100	300	600	900	
Result	8.644 \pm 0.130	8.667 \pm 0.107	8.669 \pm 0.112	8.637 \pm 0.096	8.687 \pm 0.123	8.669 \pm 0.128	
Tunable hyper-parameter: L_b . With $2d = 100$, $I = 600$ fixed.							
L_b	0.5	1	1.5	2	5	$\sqrt{50}$	10
Result	8.271 \pm 0.183	8.476 \pm 0.139	8.579 \pm 0.136	8.632 \pm 0.131	8.665 \pm 0.129	8.687 \pm 0.123	8.686 \pm 0.116

the real-world MSLR dataset. The tunable hyper-parameters in PE-DBO include the dimension of the low-dimensional subspace $2d$, the integration number of points I that are used to estimate the soft-Copeland score via the Monte-Carlo integration, and the boundary of the low-dimensional subspace L_b . In this experiment, we fix two hyper-parameters while keeping the rest hyper-parameter tunable to realize the different hyper-parameter value settings for PE-DBO. We use $M = 25$ duels to initialize the GP in PE-DBO. Each experiment is iterated for $N = 50$ steps and repeated for 20 times. The result is shown in Table 1.

In Table 1, the top part shows the effect of hyper-parameter $2d$ on the optimization performance of PE-DBO. From the main paper, we know that the optimal ϵ -effective dimension of the MSLR dataset is nearly 50, thus when $2d$ gradually rises to 100, the mean of the function value improves, and when $2d$ is larger than 100, the result rarely varies. The top part in Table 1 shows that, if $2d < d_p$, the low-dimensional subspace may not contain the optimal solution of the objective function, thus the result becomes poor. When $2d \geq d_p$, the low-dimensional subspace is large enough to contain the optimal solution, and the best solution found by PE-DBO approaches the global optima of the objective function. It can also be observed that, when $2d = 272 = 2D$, the standard deviation is the smallest across different d , due to the low-dimensional subspace being a linear transformation of the original solution space. Thus all the low-dimensional subspaces contain the global optima with high probability, and the preference embeddings rarely fail. However, setting $2d = 2D$ is the opposite of our motivation since this cannot solve the scalability problem that PBO is encountered, i.e., fitting a GP with dimension $2D$. The middle part of Table 1 shows the effect of hyper-parameter I on the optimization performance of PE-DBO. The result indicates that this hyper-parameter does not affect the performance of PE-DBO much. Since too many sample points increase the computational time of the soft-Copeland score via the Monte-Carlo integration, choosing a not too large I is sufficient. The bottom part of Table 1 shows the effect of hyper-parameter L_b . From the analysis of the MSLR dataset, the global optima is near the boundary of the domain of the objective function. Hence, the performance is improved when L_b expands. However, when the boundary is large, the search space for the optimization algorithm is vast, and the exploration cost increases. This may hurt the result of PE-DBO, and setting L_b in a reasonable way is meaningful.

F Details of the Fixed Budget Experiment

This section describes the details of experiment in Figure 3(d) in the main paper. The comparison algorithms are GP-UCB (Srinivas et al. 2010) and REMBO (Wang et al. 2016). We use the Bayesian optimization toolkit (Nogueira 2014) to implement these algorithms. The hyper-parameters of GP-UCB and REMBO are defaults in the Bayesian optimization toolkit except for the boundary of low-dimensional space of REMBO. For fairness, we set this boundary $[-\sqrt{d}, \sqrt{d}]^d$ just like the L_b of PE-DBO, which is $[-\sqrt{d}, \sqrt{d}]^{2d}$.

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