UCB-driven Utility Function Search for Multi-objective Reinforcement Learning Supplementary Material

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1 Algorithms

Algorithm 1 Fixed-MOPPO

```
1: Input: State s_t, weights w
 2: Initialize: K weight-conditioned Actor-Critic Networks \pi_k / v^{\pi_k}, scalarisation-vector sub-
       spaces \mathbf{W}_k for k = 1, \dots, K, and memory buffer \mathcal{E} size of D.
      for k = 1 to K do
             for t = 1 to D do
 4:
                    \mathbf{w}_{pivot} \leftarrow \text{get pivot weight}(\mathbf{W}_k)
 5:
                    a_t \leftarrow \pi_k(s_t, \mathbf{w}_{pivot})
 6:
                   s_{t+1}, \mathbf{r_t} \leftarrow simulator(a_t)
 7:
                   \mathcal{E} \leftarrow \mathcal{E} \cup \langle s_t, a_t, \mathbf{w}_{pivot}, \mathbf{r_t}, s_{t+1} \rangle
 8:
 9:
                    s_t \leftarrow s_{t+1}
             end for
10:
11:
             sample \langle s_t, a_t, \mathbf{w}_{pivot}, \mathbf{r_t}, s_{t+1} \rangle \leftarrow \mathcal{E}
             \theta \leftarrow \theta + \eta \left( \nabla_{\theta} \log \pi_{\theta}(s_t, a; \mathbf{w}_{pivot}) \right) \left( A^{\pi}(s_t, a_t; \mathbf{w}_{pivot}) \right)
             \phi \leftarrow \phi + || \boldsymbol{V}^{\pi_k}(s_t; \mathbf{w}_{pivot}) - \boldsymbol{V}^{\pi_k}(s_{t+1}; \mathbf{w}_{pivot}) ||^2
13:
             clear \mathcal{E}
14:
15: end for
```

2 Benchmark Problems

This section provide detail objective return for each problems. Where C in the following equations is live bonus.

2.1 Swimmer-v2

Observation and action space: $S \in \mathbb{R}^8$, $A \in \mathbb{R}^2$. The first objective is forward speed in x axis:

$$R_1 = v_x \tag{1}$$

The second objective is energy efficiency:

$$R_2 = 0.3 - 0.15 \sum_{i} a_i^2, \quad a_i \in (-1, 1)$$
 (2)

Algorithm 2 Random-MOPPO

```
1: Input: State s_t, weights w
 2: Initialize: K weight-conditioned Actor-Critic Networks \pi_k / v^{\pi_k}, scalarisation-vector sub-
      spaces \mathbf{W}_k for k=1,\ldots,K, memory buffer \mathcal{E} size of D, and scalarisation-vector re-sampling
      frequency RF.
 3: for k = 1 to K do
            for t = 1 to D do
 4:
                  if t \% RF = 0 then
 5:
                        \mathbf{w}_t \leftarrow \text{uniform random sample}(\mathbf{W}_k)
 6:
 7:
                  a_t \leftarrow \pi_k(s_t, \mathbf{w_t})
 8:
                  s_{t+1}, \mathbf{r_t} \leftarrow simulator(a_t)
 9:
                  \mathcal{E} \leftarrow \mathcal{E} \cup \langle s_t, a_t, \mathbf{w}_t, \mathbf{r_t}, s_{t+1} \rangle
10:
11:
                  s_t \leftarrow s_{t+1}
12:
            end for
            sample \langle s_t, a_t, \mathbf{w}_t, \mathbf{r_t}, s_{t+1} \rangle \leftarrow \mathcal{E}
13:
            \theta \leftarrow \theta + \eta \left( \nabla_{\theta} \log \pi_{\theta}(s, a; \mathbf{w}_t) \right) \left( A^{\pi}(s_t, a_t; \mathbf{w}_t) \right)
            \phi \leftarrow \phi + ||\boldsymbol{V}^{\pi_k}(s_t; \mathbf{w}_t) - \boldsymbol{V}^{\pi_k}(s_{t+1}; \mathbf{w}_t)||^2
15:
            clear \mathcal{E}
16:
17: end for
```

2.2 HalfCheetah-v2

Observation and action space: $S \in \mathbb{R}^{17}$, $A \in \mathbb{R}^6$.

The first objective is forward speed in x axis:

$$R_1 = \min(v_x, 4) + C \tag{3}$$

The second objective is energy efficiency:

$$R_2 = 4 - \sum_i a_i^2 + C, \quad a_i \in (-1, 1)$$
 (4)

$$C = 1 \tag{5}$$

2.3 Walker2d-v2

Observation and action space: $S \in \mathbb{R}^{17}$, $A \in \mathbb{R}^6$.

The first objective is forward speed in x axis:

$$R_1 = v_x + C \tag{6}$$

The second objective is energy efficiency:

$$R_2 = 4 - \sum_i a_i^2 + C, \quad a_i \in (-1, 1)$$
 (7)

$$C = 1 \tag{8}$$

2.4 Ant-v2

Observation and action space: $S \in \mathbb{R}^{27}$, $A \in \mathbb{R}^8$.

The first objective is forward speed in x axis:

$$R_1 = v_x + C \tag{9}$$

The second objective is forward in y axis:

$$R_2 = v_y + C \tag{10}$$

$$C = 1 - 0.5 \sum_{i} a_i^2, \quad a_i \in (-1, 1)$$
(11)

Algorithm 3 UCB-MOPPO

```
1: Input: State S_t, weights w
 2: Initialize: K weight-conditioned Actor-Critic Networks \pi_k / v^{\pi_k}, predetermined sub-space W_k size
      of M, current working weight space \widetilde{W}_k size of M, each objective has m dimensions, warm-up it-
      erations Q, objective value collection interval in every C iterations, a set of linear surrogate models
      \{f_{\psi}^{k,j}\}_{k=1...K,j=0...M}, and dynamic weight experience pool \mathcal{E} size of D.
 3: for t = 0 to T do
 4:
           ► Warm-up Stage
 5:
           for k = 1 to K do
 6:
                 W_k \leftarrow \text{get pivot weights}(W_k)
                \pi_k^* \leftarrow \text{Fix Weight Optimisation}(\pi_k, W_k)
 7:
 8:
 9:

ightharpoonup Collect objective value from simulator
10:
           if t \mod C = 0 then
                for k = 1 to K do
11:
                     for w in \widetilde{W}_k do
12:
                           V^{\pi_k} \leftarrow simulator(\pi_k, \mathbf{w})
13:
                     end for
14:
15:
                end for
           end if
16:
           if t > Q then
17:
                ► Construct Training Data for Prediction Model:
18:
                for k = 1 to K do
19:
20:
                     for w in W_k do
                           for z = 0 to \frac{t}{C} do
21:
                                \begin{array}{l} \mathbf{for} \ j = 0 \ \mathsf{to} \ m \ \mathbf{do} \\ \Delta V_{j,\mathbf{w}}^{k,(z \to z+1)} \leftarrow V_{j,\mathbf{w}}^{\pi^k,z+1} - V_{j,\mathbf{w}}^{\pi^k,z} \end{array}
22:
23:
                                     D_{surrogate}^{k,j} \leftarrow append\left(\mathbf{w}, \Delta V_{j,\mathbf{w}}^{k,(z \rightarrow z+1)}\right)
24:
25:
                                end for
26:
                           end for
27:
                     end for
                     ► Update Surrogate Model:
28:
                     for k = 1 to K do
29:
                           for j = 0 to m do
30:
                                for w in W_k do
31:
                                     \psi \leftarrow \psi + \text{grid search}(f_{\psi}, D_{surrogate}^{k,j})
32:
                                end for
33:
                           end for
34:
                           \blacktriangleright Scalarisation\text{-}vector\ Search:
35:
36:
                           for w in W_k do
                                for w in W_k do
37:
                                      V_{\mathbf{w}}^{\pi_k} \leftarrow simulator(\pi_k, \mathbf{w})
38:
39:
                                     L \leftarrow append(V_{\mathbf{w}}^{\pi_k})
40:
                                end for
                                for j = 0 to m do
41:
                                     \hat{V}_{j,\mathbf{w}}^{\pi_k} = V_{j,\mathbf{w}}^{\pi_k} + f_{bagging}^{k,j}(\mathbf{w})
\tilde{V}_{j,\mathbf{w}}^{\pi_k} \leftarrow \hat{V}_{j,\mathbf{w}}^{\pi_k} + \sigma_{k,j}^2(\mathbf{w})
42:
43:
                                end for
44:
                                CCS \leftarrow \{\widetilde{V}_{i,\mathbf{w}}^{\pi_k}\} \bigcup L \setminus \{V_{i,\mathbf{w}}^{\pi_{k,z}}\}
45:
                                \mathcal{D} \leftarrow append(\langle \mathbf{w}, HV(CCS) \rangle)
46:
47:
48:
                           ► Update Working Preference Pool:
                           \{\mathbf{w}_i, k \in (0, M)\} \leftarrow \text{Sort } \mathcal{D} \text{ by } HV(CCS) \text{ in descending order}
49:
                           \widetilde{\boldsymbol{W}}_{\boldsymbol{k}} \leftarrow \{ \mathbf{w}_i, k \in (0, M) \}
50:
51:
                      end for
                end for
52:
53:
           end if
54: end for
```

2.5 Hopper-v2

Observation and action space: $S \in \mathbb{R}^{11}$, $A \in \mathbb{R}^3$. The first objective is forward speed in x axis:

$$R_1 = 1.5v_x + C (12)$$

The second objective is jumping height:

$$R_2 = 12(h - h_{init}) + C (13)$$

$$C = 1 - 2e^{-4} \sum_{i} a_i^2, \quad a_i \in (-1, 1)$$
(14)

2.6 Hopper-v3

Observation and action space: $S \in \mathbb{R}^{11}$, $A \in \mathbb{R}^3$. The first objective is forward speed in x axis:

$$R_1 = 1.5v_x + C (15)$$

The second objective is jumping height:

$$R_2 = 12(h - h_{init}) + C (16)$$

The third objective is energy efficiency:

$$R_3 = 4 - \sum_i a_i^2 + C \tag{17}$$

$$C = 1 \tag{18}$$

3 PPO Hyperparameters

Table 1: Hyper-parameter configuration of MOPPO algorithms.

Hyperparameters	Value
Policy Number	10
Max Training Iterations	2×10^{6}
Number of Cells	64
Actor Learning Rate	3×10^{-4}
Critic Learning Rate	3×10^{-4}
Memory Size	2500
K Epochs	10
Gamma	0.99
Lambda	0.95
C1 Coefficient	0.5
C2 Coefficient	0
Epsilon Clip	0.2
Minibatch Size	64

4 Convex Coverage Set Expansion

In this section, we illustrate the expansion of the Convex Coverage Set (CCS) throughout the training process using our proposed UCB-MOPPO algorithm. The graphs are arranged sequentially from left to right and top to bottom, showing the progressive evolution of the CCS. Each graph depicts 100 sub-space vectors representing a two-objective optimization problem.

As training progresses, a clear trend of CCS growth emerges, characterized by an increasing spread and coverage of vectors across the objective space. Notably, the distribution of vectors provides valuable insights: regions where vectors are more widely scattered indicate areas with fewer vectors dominated by others, reflecting an expansion toward a more optimal and comprehensive CCS. This separation demonstrates the growing diversity and coverage of the vectors over time, effectively showcasing the CCS's ability to capture a wider range of trade-offs between objectives. Consequently, this illustrates the effectiveness of UCB-MOPPO in thoroughly exploring the objective space and improving the set of solutions throughout the training process.

4.1 Swimmer-V2

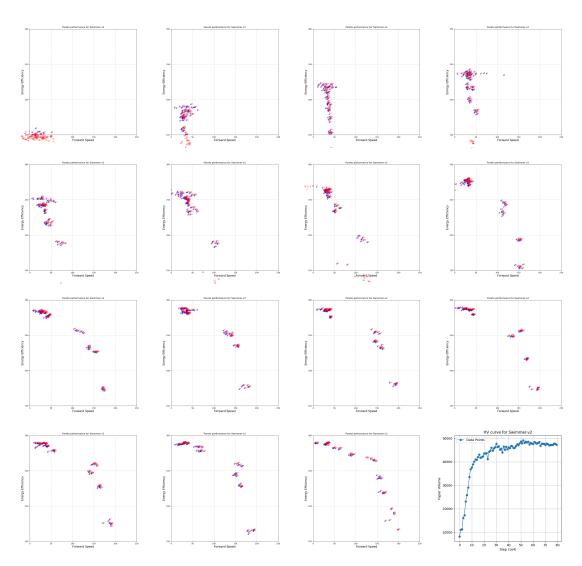


Figure 1: CCS expansion in Swimmer-V2 with one seed. Last graph shows the Hypervolume growth.

4.2 HalfCheetah-v2

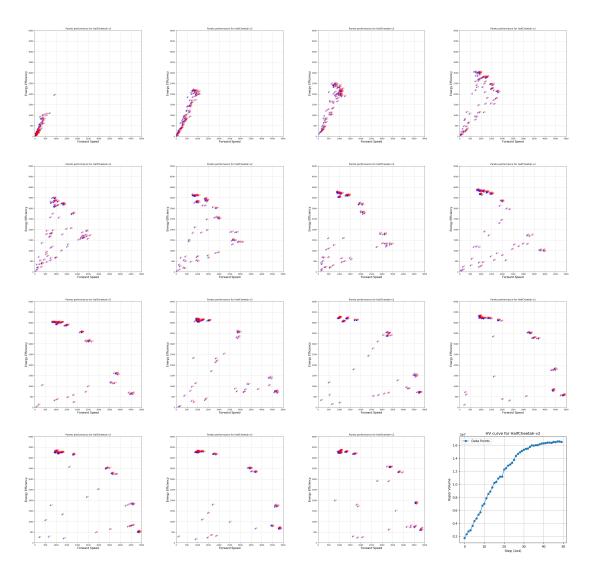


Figure 2: CCS expansion in HalfCheetach-V2 with one seed. Last graph shows the Hypervolume growth.

4.3 Hopper-V2

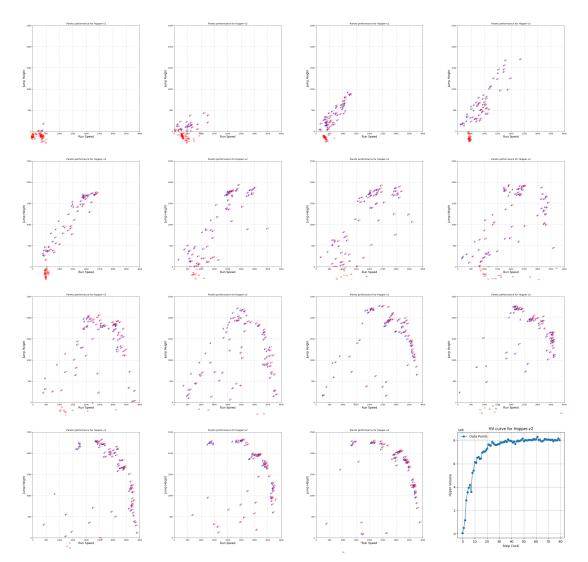


Figure 3: CCS expansion in Hopper-V2 with one seed. Last graph shows the Hypervolume growth.