

D. Algorithm tables

As introduced in Section 5, Trifle generally works in two phases: rejection sampling for action generation and beam search for action selection. The main algorithm is illustrated in Algorithm 1, where we take the current state s_t as well as the past trajectory $\tau_{<t}$ as input, utilize the specified value estimate f_v as a heuristic to guide beam search, and output the best trajectory. After that, we extract the current action a_t from the output trajectory to execute in the environment.

At the first step of the beam search, we will perform rejection sampling to obtain a candidate action set \mathbf{a}_t (line 4 of Algorithm 1). The concrete rejection sampling procedure for s-Trifle is detailed in Algorithm 2. The major modification of m-Trifle compared to s-Trifle is the adoption of a multi-step value estimate instead of the single-step value estimate, which is also shown in Algorithm 3.

Algorithm 1 Trifle with Beam Search

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1: Input: past trajectory  $\tau_{<t}$ , current state  $s_t$ , beam width  $N$ , beam horizon  $H$ , scaling ratio  $\lambda$ , sequence model  $\mathcal{M}$ ,
   value function  $f_v$   $\triangleright f_v = \mathbb{E}[V_t]$  for s-Trifle and  $\mathbb{E}[V_t^m]$  for m-Trifle
2: Output: The best trajectory
3: Let  $\mathbf{x}_t \leftarrow \text{concat}(\tau_{<t}, s_t).$ reshape(1, -1).repeat( $N$ , dim = 0)  $\triangleright$  Batchify the input trajectory and prepare for the beam search
4: Perform rejection sampling to obtain  $\mathbf{a}_t$   $\triangleright$  cf. Algorithm 2
5: Initialize  $X_0 = \text{concat}(\mathbf{x}_t, \mathbf{a}_t)$ 
6: for  $t = 1, \dots, H$  do
7:    $X_{t-1} \leftarrow X_{t-1}.$ repeat( $\lambda$ , dim = 0)  $\triangleright$  Scale the number of trajectories from  $N$  to  $\lambda N$ 
8:    $\mathcal{C}_t \leftarrow \{\text{concat}(\mathbf{x}_{t-1}, x) \mid \forall \mathbf{x}_{t-1} \in X_{t-1}, \text{sample } x \sim p_{\mathcal{M}}(\cdot \mid \mathbf{x}_{t-1})\}$   $\triangleright$  Candidate next-token prediction
9:    $X_t \leftarrow \text{topk}_{X \in \mathcal{C}_t}(f_v(X), k=N)$   $\triangleright$  keep  $N$  most rewarding trajectories
10: end for
11: return  $\text{argmax}_{X \in X_H} f_v(X)$ 

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Algorithm 2 Rejection Sampling with Single-step Value Estimate

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1: Input: past trajectory  $\tau_{<t}$ , current state  $s_t$ , dimension of action  $k$ , rejection rate  $\delta > 0$ 
2: Output: The sampled action  $a_t^{1:k}$ 
3: Let  $x_t \leftarrow \text{concat}(\tau_{<t}, s_t)$ 
4: for  $i = 1, \dots, k$  do
5:   Compute  $p_{\text{GPT}}(a_t^i \mid x_t, a_t^{<i})$  Note that  $a_t^{<1} = \emptyset$ .
6:   Compute  $p_{\text{TPM}}(V_t \mid x_t, a_t^{<i}) = \sum_{a_t^{i:k}} p_{\text{TPM}}(V_t \mid x_t, a_t^{1:k})$   $\triangleright$  The marginal can be efficiently computed by PC in linear time.
7:   Compute  $v_\delta = \max_v \{v \in \text{val}(V_t) \mid p_{\text{TPM}}(V_t \geq v \mid x_t, a_t^{<i}) \geq 1 - \delta\}$ , for each  $a_t^i \in \text{val}(A_t^i)$ 
8:   Compute  $\tilde{p}(a_t^i \mid x_t, a_t^{<i}; v_\delta) = \frac{1}{Z} \cdot p_{\text{GPT}}(a_t^i \mid x_t, a_t^{<i}) \cdot p_{\text{TPM}}(V_t \geq v_\delta \mid x_t, a_t^{<i})$   $\triangleright$  Apply Equation (2)
9:   Sample  $a_t^i \sim \tilde{p}(a_t^i \mid x_t, a_t^{<i}; v_\delta)$ 
10: end for
11: return  $a_t^{1:k}$ 

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Algorithm 3 Multi-step Value Estimate

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1: Input:  $\tau_{\leq t}$ , sequence model  $\mathcal{M}$ , terminal timestep  $t' > t$ , discount  $\gamma$ 
2: Output: The multi-step value estimate  $\mathbb{E}[V_t^m]$ 
3: Sample  $r_t, s_{t+1}, a_{t+1}, r_{t+1}, \dots, s_{t'}, a_{t'}, r_{t'}$  from  $\mathcal{M}$ 
4: Compute  $p_{\text{TPM}}(\text{RTG}_{t'} \mid \tau_{\leq t}, a_{t+1:t'}) = \sum_{s_{t+1:t'}} p_{\text{TPM}}(\text{RTG}_{t'} \mid \tau_{\leq t'})$   $\triangleright$  Marginalize over intermediate states  $s_{t+1:t'}$ 
5: compute  $\mathbb{E}[V_t^m] = \sum_{h=t}^{t'} \gamma^{h-t} r_h + \gamma^{t'+1-t} \mathbb{E}_{\text{RTG}_{t'} \sim p_{\text{TPM}}(\cdot \mid s_t, a_{t:t'})}[\text{RTG}_{t'}]$ 
6: return  $\mathbb{E}[V_t^m]$ 

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