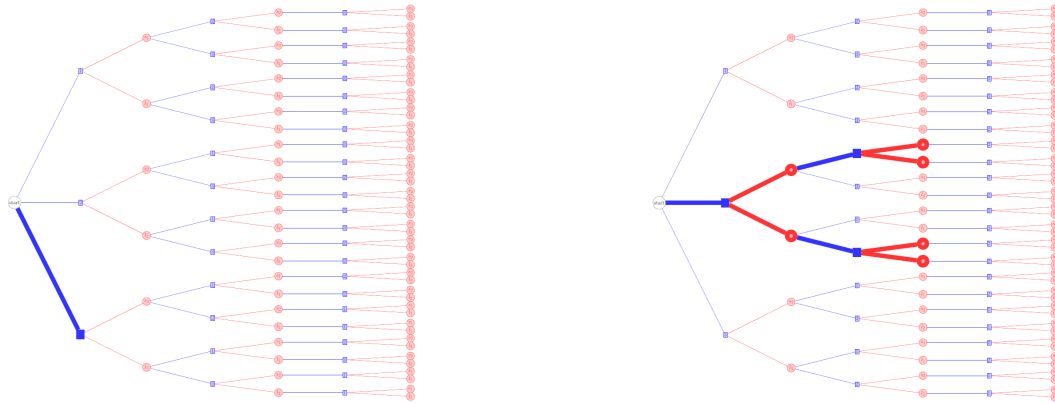


## Supplementary Material

### A Illustration of Policies



(a) A policy of just playing item 3. This policy has depth 1.

(b) A policy that plays item 2 first. If it is small, it plays item 1 whereas if it is large it plays item 3. After this, the final item is determined due to the fact that there are only 3 items in the problem. This policy has depth 2.

Figure 4: Examples of policies in the simple 3 item, 2 sizes stochastic knapsack problem. Each blue line represents choosing an item and the red lines represent the sizes of the previous items.

### B Illustration of Bounds

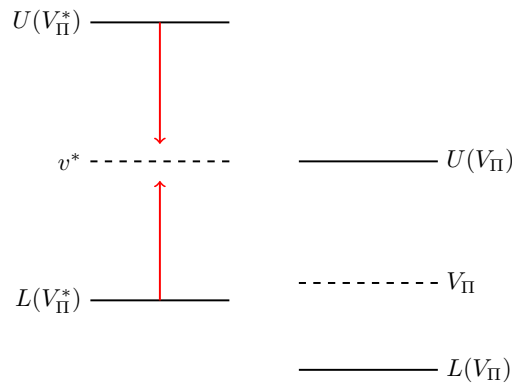


Figure 5: Example of where just looking at the optimistic policy might fail: If we always play the optimistic policy then, since  $U(V_{\Pi^*}^+) \geq U(V_{\Pi}^+)$ , we will always play  $\Pi^*$  and so the confidence bounds on  $\Pi$  will not shrink. This means that  $L(V_{\Pi^*}^+)$  will never be (epsilon) greater than the best alternative upper bound so there will not be enough confidence to conclude we have found the best policy.

### C Algorithms

In these algorithms **Generate**( $i$ ) samples a reward and item size pair from the generative model of item  $i$ , whereas **sample**( $A, k$ ) samples from a set  $A$  with replacement to get  $k$  samples. The notation  $i(d) = \Pi(d, b)$  indicates that item  $i(d)$  was chosen by policy  $\Pi$  at depth  $d$  when the remaining capacity was  $b$ .

**Algorithm 3: EstimateValue( $\Pi, m$ )**

**Initialization:** For all  $i \in I$ ,  $\mathcal{S}_i = \mathcal{S}_i^*$   
**1** for  $j = 1, \dots, m$  do  
**2**      $B_0 = B$ ;  
**3**     for  $d = 1, \dots, d(\Pi)$  do  
**4**          $i(d) = \Pi(d, B_{d-1})$ ;  
**5**         if  $|\mathcal{S}_{i(d)}| \leq 0$  then  $(r_{i(d)}, c_{i(d)}) = \text{Generate}(i(d))$ ,  $\mathcal{S}_i^* = \mathcal{S}_i^* \cup \{r_{i(d)}, c_{i(d)}\}$ ;  
**6**         else  $(r_{i(d)}, c_{i(d)}) = \text{sample}(\mathcal{S}_i, 1)$ , and  $\mathcal{S}_i = \mathcal{S}_i \setminus \{(r_{i(d)}, c_{i(d)})\}$ ;  
**7**          $B_d = B_{d-1} - c_{i(d)}$ ;  
**8**         if  $B_d < 0$  then  $r_{i(d)} = 0$ ;  
**9**     end  
**10**      $\overline{V}_\Pi^{(j)} = \sum_{d=1}^{d(\Pi)} r_{i(d)}$ ;  
**11** end  
**12** return  $(\overline{V}_{\Pi m} = \frac{1}{m} \sum_{j=1}^m \overline{V}_\Pi^{(j)}, \mathcal{S}^*)$

**Algorithm 4: SampleBudget( $\Pi, S$ )**

**Initialization:**  $B_0 = B$  and for all  $i \in I$ ,  $\mathcal{S}_i = \mathcal{S}_i^*$   
**1** for  $d = 1, \dots, d(\Pi)$  do  
**2**      $i(d) = \Pi(d, B_{d-1})$ ;  
**3**     if  $|\mathcal{S}_{i(d)}| \leq 0$  then  $(r_{i(d)}, c_{i(d)}) = \text{Generate}(i(d))$ ,  $\mathcal{S}_i^* = \mathcal{S}_i^* \cup \{r_{i(d)}, c_{i(d)}\}$ ;  
**4**     else  $(r_{i(d)}, c_{i(d)}) = \text{sample}(\mathcal{S}_i, 1)$ , and  $\mathcal{S}_i = \mathcal{S}_i \setminus \{(r_{i(d)}, c_{i(d)})\}$ ;  
**5**      $B_d = B_{d-1} - c_{i(d)}$ ;  
**6** end  
**7**  $\overline{\Psi}(B_\Pi)^{(j)} = \Psi(\max\{B - \sum_{d=1}^{d(\Pi)} c_{i(d)}, 0\})$ ;  
**8** return  $(\overline{\Psi}(B_\Pi)^{(j)}, \mathcal{S}^*)$

## D Proofs of Theoretical Results

For convenience we restate any results that appear in the main body of the paper before proving them.

### D.1 Bounding the Value of a Policy

**Lemma 7** (Lemma 1 in main text) *Let  $(\Omega, \mathcal{A}, P)$  be the probability space from Section 2, then for  $m_1 + m_2$  independent samples of policy  $\Pi$ , and  $\delta_1, \delta_2 > 0$ , with probability  $1 - \delta_1 - \delta_2$ ,*

$$\overline{V}_{\Pi m_1} - c_1 \leq V_\Pi^+ \leq \overline{V}_{\Pi m_1} + \overline{\Psi}(B_\Pi)_{m_2} + c_1 + c_2.$$

Where  $c_1 := \sqrt{\frac{\Psi(B)^2 \log(2/\delta_1)}{2m_1}}$  and  $c_2 := \sqrt{\frac{\Psi(B)^2 \log(1/\delta_2)}{2m_2}}$ .

*Proof:* Consider the average value of policy  $\Pi$  over  $m_1$  many trials. By Hoeffding's Inequality,  $P(|\overline{V}_{\Pi m_1} - E[V_\Pi]| > c_1) \leq \delta_1$  and, similarly,  $P(|\overline{\Psi}(B_\Pi)_{m_2} - E[\Psi(B_\Pi)]| > c_2) \leq \delta_2$ . We are interested in the probability,

$$\begin{aligned} P(|\overline{V}_{\Pi m_1} - V_\Pi^+| > t) &\leq P(|\overline{V}_{\Pi m_1} - E[V_\Pi]| + |E[V_\Pi] - V_\Pi^+| > t) \\ &\leq P(|\overline{V}_{\Pi m_1} - E[V_\Pi]| + E[\Psi(B_\Pi)] > t). \end{aligned}$$

where the first line follows from the triangle inequality and the second from the definition of  $\overline{\Psi}(B_\Pi)$ . From the Hoeffding bounds and defining  $t = \overline{\Psi}(B_\Pi)_{m_2} + c_1 + c_2$ , we consider  $P(|\overline{V}_{\Pi m_1} - E[V_\Pi]| + E[\Psi(B_\Pi)] > \overline{\Psi}(B_\Pi)_{m_2} + c_1 + c_2)$ . Define the events

$$A_1 = \{|\overline{V}_{\Pi m_1} - V_\Pi| + E[\Psi(B_\Pi)] \leq E[\Psi(B_\Pi)] + c_1\} \text{ and } A_2 = \{|\overline{\Psi}(B_\Pi)_{m_2} - E[\Psi(B_\Pi)]| \leq c_2\}.$$

Then,

$$\begin{aligned} P\left(\overline{V_{\Pi m_1}} - E[V_{\Pi}] + E[\Psi(B_{\Pi})] > \overline{\Psi(B_{\Pi})}_{m_2} + c_1 + c_2\right) &\leq P(\Omega \setminus (A_1 \cap A_2)) \\ &\leq P(\Omega \setminus A_1) + P(\Omega \setminus A_2) \\ &\leq \delta_1 + \delta_2. \end{aligned}$$

Hence,

$$P\left(\overline{V_{\Pi m_1}} - V_{\Pi}^+ > c_1\right) \leq P\left(\overline{V_{\Pi m_1}} - V_{\Pi} > c_1\right) \leq \delta_1 < \delta_1 + \delta_2$$

which gives the left hand side of the result. For the right hand side,

$$\begin{aligned} P\left(\overline{V_{\Pi m_1}} - V_{\Pi}^+ < -\overline{\Psi(B_{\Pi})}_{m_2} - c_1 - c_2\right) \\ \leq P\left(\overline{V_{\Pi m_1}} - E[V_{\Pi}] - E[\Psi(B_{\Pi})] < -\overline{\Psi(B_{\Pi})}_{m_2} - c_1 - c_2\right) \\ \leq \delta_1 + \delta_2. \end{aligned}$$

□

**Lemma 8** Let  $\{Z_m\}_{m=1}^{\infty}$  be a martingale with  $Z_m$  defined on the filtration  $\mathcal{F}_m$ ,  $E[Z_m] = 0$  and  $|Z_m - Z_{m-1}| \leq d$  for all  $m$  where  $Z_0 = 0$ . Then,

$$P\left(\exists m \leq n; \frac{Z_m}{m} \geq 2d^2 \sqrt{\frac{2}{m} \log\left(\frac{n}{m} \frac{4}{\delta}\right)}\right) \leq \delta$$

*Proof:* The proof is similar to that of Lemma B.1 in Perchet, Rigollet, Chassang, and Snowberg (2016) and will make use of the following standard results:

**Theorem 9** Doob's maximal inequality: Let  $Z$  be a non-negative submartingale. Then for  $c > 0$ ,

$$P\left(\sup_{k \leq n} Z_k \geq c\right) \leq \frac{E[Z_n]}{c}.$$

*Proof:* See, for example, Williams (1991), Theorem 14.6, page 137. □

**Lemma 10** Let  $Z_n$  be a martingale such that  $|Z_i - Z_{i-1}| \leq d_i$  for all  $i$  with probability 1. Then, for  $\lambda > 0$ ,

$$E[e^{\lambda Z_n}] \leq e^{\frac{\lambda^2 D^2}{2}},$$

where  $D^2 = \sum_{i=1}^n d_i^2$ .

*Proof:* See the proof of the Azuma-Hoeffding inequality in Azuma (1967). □

Then, for the proof of Lemma 8, we first notice that since  $\{Z_m\}_{m=1}^{\infty}$  is a martingale, by Jensen's inequality for conditional expectations, it follows that for any  $\lambda > 0$ ,

$$E[e^{\lambda Z_m} | \mathcal{F}_{m-1}] \geq e^{\lambda E[Z_m | \mathcal{F}_{m-1}]} = e^{\lambda Z_{m-1}}.$$

Hence, for any  $\lambda > 0$ ,  $\{e^{\lambda Z_m}\}_{m=1}^{\infty}$  is a positive sub-martingale so we can apply Doob's maximal inequality (Theorem 9) to get

$$P\left(\sup_{m \leq n} Z_m \geq c\right) = P\left(\sup_{m \leq n} e^{\lambda Z_m} \geq e^{\lambda c}\right) \leq \frac{E[e^{\lambda Z_n}]}{e^{\lambda c}}.$$

Then, by Lemma 10, since  $|Z_i - Z_{i-1}| \leq d$  for all  $i$ , it follows that

$$P\left(\sup_{m \leq n} Z_m \geq c\right) \leq \frac{E[e^{\lambda Z_n}]}{e^{\lambda c}} \leq \frac{e^{\lambda^2 D^2/2}}{e^{\lambda c}} = \exp\left\{\frac{\lambda^2 D^2}{2} - \lambda c\right\}. \quad (5)$$

Minimizing the right hand side with respect to  $\lambda$  gives  $\hat{\lambda} = \frac{c}{D^2}$  and substituting this back into (5) gives,

$$P\left(\sup_{m \leq n} Z_m \geq c\right) \leq \exp\left\{-\frac{c^2}{2D^2}\right\}.$$

Then, since we are considering the case where  $d_i = d$  for all  $i$ ,  $D^2 = nd^2$  and so,

$$P\left(\sup_{m \leq n} Z_m \geq c\right) \leq \exp\left\{-\frac{c^2}{2nd^2}\right\}.$$

Further, if we are interested in  $P(\sup_{k \leq m \leq n} Z_m \geq c)$ , we can redefine the indices to get

$$P\left(\sup_{k \leq m \leq n} Z_m \geq c\right) = P\left(\sup_{m' \leq n-k+1} Z_m \geq c\right) \leq \exp\left\{-\frac{c^2}{2(n-k+1)d^2}\right\}. \quad (6)$$

We then define  $\varepsilon_m = 2d\sqrt{\frac{1}{m} \log\left(\frac{n}{m} \frac{8}{\delta}\right)}$  and use a peeling argument similar to that in Lemma B.1 of Perchet et al. (2016) to get

$$\begin{aligned} P\left(\exists m \leq n; \frac{Z_m}{m} \geq \varepsilon_m\right) &\leq \sum_{t=0}^{\lfloor \log_2(n) \rfloor + 1} P\left(\bigcup_{m=2^t}^{2^{t+1}-1} \left\{\frac{Z_m}{m} \geq \varepsilon_m\right\}\right) && \text{(by union bound)} \\ &\leq \sum_{t=0}^{\lfloor \log_2(n) \rfloor + 1} P\left(\bigcup_{m=2^t}^{2^{t+1}-1} \left\{\frac{Z_m}{m} \geq \varepsilon_{2^{t+1}}\right\}\right) && \text{(since } \varepsilon_m \text{ decreasing in } m) \\ &\leq \sum_{t=0}^{\lfloor \log_2(n) \rfloor + 1} P\left(\bigcup_{m=2^t}^{2^{t+1}-1} \{Z_m \geq 2^t \varepsilon_{2^{t+1}}\}\right) && \text{(as } m \geq 2^t) \\ &\leq \sum_{t=0}^{\lfloor \log_2(n) \rfloor + 1} \exp\left\{-\frac{(2^t \varepsilon_{2^{t+1}})^2}{2^{t+1} d^2}\right\} && \text{(from (6))} \\ &\leq \sum_{t=0}^{\lfloor \log_2(n) \rfloor + 1} \frac{2^{t+1} \delta}{8n} && \text{(substituting } \varepsilon_{2^{t+1}}) \\ &\leq \frac{2^{\log_2(n)+3} \delta}{8n} = \delta. && \text{(since } \sum_{i=1}^k 2^i = 2^{k+1} - 1) \end{aligned}$$

□

**Proposition 11** (Proposition 2 in main text) *The Algorithm `BoundValueShare` (Algorithm 2) returns confidence bounds,*

$$L(V_{\Pi}^+) = \overline{V}_{\Pi m_1} - \sqrt{\frac{\Psi(B)^2 \log(2/\delta_1)}{2m_1}} \quad U(V_{\Pi}^+) = \overline{V}_{\Pi m_1} + \overline{\Psi(B_{\Pi})}_{m_2} + \sqrt{\frac{\Psi(B)^2 \log(2/\delta_1)}{2m_1}} + 2\Psi(B) \sqrt{\frac{1}{m_2} \log\left(\frac{8n}{\delta_2 m_2}\right)}$$

which hold with probability  $1 - \delta_1 - \delta_2$ .

*Proof:* We begin by noting that our samples of item size are dependent since in each iteration we construct a bound based on past samples and we use this bound to decide if we need to continue sampling or if we can stop. To model this dependence let us introduce a stopping time  $\tau$  such that  $\tau(\omega) = n$  if our algorithm exits the loop at time  $n$ . Consider the sequence

$$\overline{\Psi(B_{\Pi})}_{1 \wedge \tau}, \overline{\Psi(B_{\Pi})}_{2 \wedge \tau}, \dots$$

and define for  $m \geq 1$

$$M_m = (m \wedge \tau) (\overline{\Psi(B_{\Pi})}_{m \wedge \tau} - E[\Psi(B_{\Pi})]) \quad \text{with} \quad M_0 = 0.$$

Furthermore, define the filtration  $\mathcal{F}_m = \sigma(B_{\Pi,1}, \dots, B_{\Pi,m})$  then for  $m \geq 1$

$$E[M_m | \mathcal{F}_{m-1}] = E[M_m | \mathcal{F}_{m-1}, \tau \leq m-1] + E[M_m | \mathcal{F}_{m-1}, \tau > m-1].$$

Now

$$E[M_m | \mathcal{F}_{m-1}, \tau \leq m-1] = E[M_{m-1} | \tau \leq m-1].$$

and due to independence of the samples  $B_{\Pi,1}, \dots, B_{\Pi,m}$

$$\begin{aligned} & E[M_m | \mathcal{F}_{m-1}, \tau > m-1] \\ &= E[m(\overline{\Psi(B_{\Pi})})_m - E[\Psi(B_{\Pi})] | \mathcal{F}_{m-1}, \tau > m-1] \\ &= E \left[ \sum_{j=1}^{m-1} \Psi(B_{\Pi,j}) + \Psi(B_{\Pi,m}) - mE[\Psi(B_{\Pi})] \middle| \mathcal{F}_{m-1}, \tau > m-1 \right] \\ &= (m-1)E[\overline{\Psi(B_{\Pi})}_{m-1} - E[\Psi(B_{\Pi})] | \mathcal{F}_{m-1}, \tau > m-1] \\ &\quad + E[\Psi(B_{\Pi,m}) - E[\Psi(B_{\Pi})] | \mathcal{F}_{m-1}, \tau > m-1] \\ &= E[M_{m-1} | \tau > m-1] + E[\Psi(B_{\Pi,m})] - E[\Psi(B_{\Pi})] = E[M_{m-1} | \tau > m-1]. \end{aligned}$$

Hence,  $E[M_m | \mathcal{F}_{m-1}] = M_{m-1}$  and  $M_m$  is a martingale with increments  $|M_m - M_{m-1}| \leq |\Psi(B_{\Pi,m}) - E[\Psi(B_{\Pi})]| \leq \Psi(B)$ . We could apply the Azuma-Hoeffding inequality to gain guarantees for individual  $m$ -values. Alternatively, we can use Lemma 8 to get,

$$P \left( \sup_{m \leq n} \frac{M_m}{m} \geq 2\Psi(B) \sqrt{\frac{1}{m} \log \left( \frac{8n}{\delta m} \right)} \right) \leq \delta_2.$$

Combining this with the argument in Lemma 1 gives

$$\overline{V_{\Pi m_1}} - c_1 \leq V_{\Pi}^+ \leq \overline{V_{\Pi m_1}} + \overline{\Psi(B_{\Pi})}_{m_2} + c_1 + c_2,$$

where  $c_1 := \sqrt{\frac{\Psi(B)^2 \log(2/\delta_1)}{2m_1}}$  and  $c_2 := 2\Psi(B) \sqrt{\frac{1}{m_2} \log \left( \frac{8n}{\delta_2 m_2} \right)}$  and these bounds hold with probability  $1 - \delta_1 - \delta_2$ .  $\square$

**Lemma 12** *With probability  $1 - \delta_{0,1} - \delta_{0,2}$ , the bounds generated by BoundValueShare with parameters  $\delta_{1,d} = \frac{\delta_{0,1}}{d^*} N_d^{-1}$  and  $\delta_{2,d} = \frac{\delta_{0,2}}{d^*} N_d^{-1}$  hold for all policies  $\Pi$  of depth  $d = d(\Pi) \leq d^*$  simultaneously.*

*Proof:* The probability that all bounds hold simultaneously is  $P(\bigcap_{\Pi \in \mathcal{P}} \{L(V_{\Pi}^+) \leq V_{\Pi} \leq U(V_{\Pi}^+)\})$  where  $\mathcal{P}$  is the set of all policies. From Proposition 2, for any policy  $\Pi$  of depth  $d = d(\Pi)$ ,  $P(L(V_{\Pi}^+) \leq V_{\Pi} \leq U(V_{\Pi}^+)) \geq 1 - \delta_{d,1} - \delta_{d,2}$ . Then,

$$\begin{aligned} P \left( \bigcap_{\Pi \in \mathcal{P}} \{L(V_{\Pi}^+) \leq V_{\Pi} \leq U(V_{\Pi}^+)\} \right) &= 1 - P \left( \bigcup_{\Pi \in \mathcal{P}} \{L(V_{\Pi}^+) \leq V_{\Pi} \leq U(V_{\Pi}^+)\}^c \right) \\ &\geq 1 - \sum_{\Pi \in \mathcal{P}} P(\{L(V_{\Pi}^+) \leq V_{\Pi} \leq U(V_{\Pi}^+)\}^c) \\ &\geq 1 - \sum_{\Pi \in \mathcal{P}} (\delta_{d(\Pi),1} + \delta_{d(\Pi),2}) \\ &= 1 - \sum_{d=1}^{d^*} N_d (\delta_{d,1} + \delta_{d,2}) \\ &\geq 1 - \sum_{d=1}^{d^*} N_d \left( \frac{\delta_{0,1}}{d^*} N_d^{-1} + \frac{\delta_{0,2}}{d^*} N_{d(\Pi_t)}^{-1} \right) \\ &= 1 - \sum_{d=1}^{d^*} \frac{1}{d^*} (\delta_{0,1} + \delta_{0,2}) = 1 - \delta_{0,1} - \delta_{0,2} \end{aligned}$$

$\square$

## D.2 Theoretical Results for Optimistic Stochastic Knapsacks (OpStoK)

**Proposition 13** (Proposition 4 in main text) *With probability at least  $(1 - \delta_{0,1} - \delta_{0,2})$ , the algorithm OpStoK returns a policy with value at least  $v^* - \epsilon$ .*

*Proof:* The proof follows from the following lemma.

**Lemma 14** *For every round of the algorithm and incomplete policy  $\Pi$ , let  $D(\Pi)$  be the set of all descendants of  $\Pi$ . Define the event  $A = \bigcap_{\Pi' \in D(\Pi)} \{V_{\Pi'} \in [L(V_{\Pi}^+), U(V_{\Pi}^+)]\}$ . Then  $P(A) \geq 1 - \delta_{0,1} - \delta_{0,2}$ .*

*Proof:* When BoundValueShare is called for a policy  $\Pi$  with  $d(\Pi) = d$ , it is done so with parameters  $\delta_{d,1} = \frac{\delta_{0,1}}{d^*} N_d^{-1}$  and  $\delta_{d,2} = \frac{\delta_{0,2}}{d^*} N_d^{-1}$ , where  $\delta_{d,1}$  and  $\delta_{d,2}$  are used to control the accuracy of the estimated value of  $V_{\Pi}$  and  $E\Psi(B_{\Pi})$  respectively. It follows from Proposition 2, that for any active policy  $\Pi$ , the probability that the interval  $[\overline{V_{\Pi}^{m_1}} - c_1, \overline{V_{\Pi}^{m_1}} + \overline{\Psi(B_{\Pi})}_{m_2} + c_1 + c_2]$  generated by BoundValueShare does not contain  $V_{\Pi}^+$  is less than  $\delta_{d,1} + \delta_{d,2}$ . Furthermore, from standard Hoeffding bounds, the probability that  $V_{\Pi}$  is outside the interval  $[V_{\Pi} - c_1, V_{\Pi} + c_1]$  is less than  $\delta_{d,1}$ . Since any descendant policy  $\Pi'$  of  $\Pi$  consists of adding at least one item to the knapsack and item rewards are all  $\geq 0$ , it follows that  $V_{\Pi} \leq V_{\Pi'} \leq V_{\Pi}^+$ . Hence, the probability of the value of a descendant policy being outside the interval  $[L(V_{\Pi}^+), U(V_{\Pi}^+)]$  is less than  $\delta_{d,1} + \delta_{d,2}$ . By the same argument as in Lemma 12, it can be shown that  $P(A) > 1 - \sum_{d=1}^{d^*} (\delta_{d,1} + \delta_{d,2}) N_d = 1 - \delta_{0,1} - \delta_{0,2}$ .  $\square$

The result of the proposition follows by noting that the true optimal policy  $\Pi^{OPT}$  will be a descendant of  $\Pi_i$  for some  $i \in I$ . Let  $\Pi^*$  be the policy outputted by the algorithm. By the stopping criterion,  $L(V_{\Pi^*}^+) + \epsilon \geq \max_{\Pi \in \text{ACTIVE} \setminus \{\Pi^*\}} \geq U(V_{\Pi}^+)$  for any  $\Pi \in \text{ACTIVE}$ . From the expansion rule of OpStoK, it follows that either  $\Pi^{OPT} \in \text{ACTIVE}$  or there exists some ancestor policy  $\Pi'$  of  $\Pi^{OPT}$  in ACTIVE. In the first case,  $V_{\Pi^{OPT}} = v^* \leq U(V_{\Pi^{OPT}}^+)$  whereas in the latter  $V_{\Pi^{OPT}} = v^* \leq U(V_{\Pi'}^+)$  with high probability from Lemma 14. In either case, it follows that  $L(V_{\Pi^*}^+) + \epsilon \geq v^*$  and so  $V_{\Pi^*} + \epsilon \geq v^*$ .  $\square$

**Lemma 15** *If  $\Pi$  is a complete policy then,  $U(V_{\Pi}^+) - L(V_{\Pi}^+) \leq \epsilon$ , otherwise  $U(V_{\Pi}^+) - L(V_{\Pi}^+) \leq 6E\Psi(B_{\Pi}) - \frac{3}{4}\epsilon$ .*

*Proof:* By the bounds in Proposition 2,  $U(V_{\Pi}^+) - L(V_{\Pi}^+) \leq \overline{\Psi(B_{\Pi})}_{m_2} + c_2 + 2c_1 = U(\Psi(B_{\Pi})) + 2c_1$ . For a complete policy,  $U(\Psi(B_{\Pi})) \leq \frac{\epsilon}{2}$  and according to BoundValueShare,  $m_1$  is chosen such that  $2c_1 \leq \frac{\epsilon}{2}$  which implies  $U(V_{\Pi}^+) - L(V_{\Pi}^+) \leq \epsilon$ .

If  $\Pi$  is not complete, by the sampling strategy in BoundValueShare, we continue sampling the remaining budget until  $L(\Psi(B_{\Pi})) \geq \frac{\epsilon}{4}$ . In this setting, the maximal width of the confidence interval of  $E\Psi(B_{\Pi})$  will satisfy

$$2c_2 \leq E\Psi(B_{\Pi}) - \frac{\epsilon}{4}. \quad (7)$$

Hence,

$$\begin{aligned} U(V_{\Pi}^+) - L(V_{\Pi}^+) &\leq U(\Psi(B_{\Pi})) + 2c_1 \\ &\leq 3U(\Psi(B_{\Pi})) \end{aligned} \quad (8)$$

$$\begin{aligned} &\leq 3(E\Psi(B_{\Pi}) + 2c_2) \\ &\leq 3\left(E\Psi(B_{\Pi}) + E\Psi(B_{\Pi}) - \frac{\epsilon}{4}\right) \\ &\leq 6E\Psi(B_{\Pi}) - \frac{3}{4}\epsilon. \end{aligned} \quad (9)$$

Where (8) follows since, when  $L(\Psi(B_{\Pi})) \geq \frac{\epsilon}{4}$ , we sample the value of policy  $\Pi$  until  $c_1 \leq U(\Psi(B_{\Pi}))$ , and (9) by substituting in (7).  $\square$

**Lemma 16** (Lemma 3 in main text) *Assume that  $L(V_{\Pi}^+) \leq V_{\Pi} \leq U(V_{\Pi}^+)$  holds simultaneously for all policies  $\Pi \in \text{ACTIVE}$  with  $U(V_{\Pi}^+)$  and  $L(V_{\Pi}^+)$  as defined in Proposition 2. Then,  $\Pi_t \in \mathcal{Q}^{\epsilon}$  for every policy selected by OpStoK at every time point  $t$ , except for possibly the last one.*

*Proof:* Since, when we expand a policy, we replace it in ACTIVE by all its child policies, at any time point  $t \geq 1$  there will be one ancestor of  $\Pi^*$  in the active set, denote this policy by  $\Pi_t^*$ . If  $\Pi_t = \Pi_t^*$ , then by Lemma 14,  $V_{\Pi^*} \in [L(V_{\Pi_t^*}^+), U(V_{\Pi_t^*}^+)]$ . Hence,

$$V_{\Pi} + 6E\Psi(B_{\Pi}) + \frac{3}{4}\epsilon \geq U(V_{\Pi}^+) \geq v^* \geq v^* - 6E\Psi(B_{\Pi}) - \frac{3}{4}\epsilon + \epsilon.$$

Where the last inequality will hold for any incomplete policy (since for an incomplete policy  $L(B_{\Pi}) \geq \frac{\epsilon}{4}$ ) and so,  $\Pi_t \in \mathcal{Q}^\epsilon$ . For  $\Pi_t = \Pi^*$ , since  $\frac{6}{4}\epsilon \geq \epsilon$ ,  $\Pi_t \in \mathcal{Q}^\epsilon$ .

Assume  $\Pi_t \neq \Pi_t^*$ . If  $\Pi_t$  is a complete policy,  $U(V_{\Pi_t}^+) - L(V_{\Pi_t}^+) \leq \epsilon$ . For a complete policy  $\Pi$  to be selected, it must have the largest  $U(V_{\Pi}^+)$ , since most alternative policies will have larger  $U(\Psi(B_{\Pi}))$ . Hence  $\Pi_t^{(1)} = \Pi_t$  and

$$L(V_{\Pi_t^{(1)}}^+) + \epsilon \geq U(V_{\Pi_t^{(1)}}^+) \geq \max_{\Pi \in \text{ACTIVE} \setminus \{\Pi_t^{(1)}\}} U(V_{\Pi}^+),$$

so the algorithm stops.

Assume  $\Pi_t = \Pi_t^{(1)} \neq \Pi_t^*$  is an incomplete policy. By Lemma 15, for an incomplete policy,

$$U(V_{\Pi}^+) - L(V_{\Pi}^+) \leq 3U(\Psi(B_{\Pi})) \leq 6E\Psi(B_{\Pi}) - \frac{3}{4}\epsilon. \quad (10)$$

Then, if the termination criteria is not met,

$$\begin{aligned} V_{\Pi_t} \geq L(V_{\Pi_t}^+) &\implies V_{\Pi_t} + 6E\Psi(B_{\Pi}) - \frac{3}{4}\epsilon - \epsilon \geq L(V_{\Pi_t}^+) + 6E\Psi(B_{\Pi}) - \frac{3}{4}\epsilon - \epsilon \\ &\geq U(V_{\Pi_t}^+) - \epsilon \\ &\geq \max_{\Pi \in \text{ACTIVE} \setminus \{\Pi_t\}} U(V_{\Pi}^+) - \epsilon \\ &\geq L(V_{\Pi_t}^+) \\ &\geq U(V_{\Pi_t}^+) - 6E\Psi(B_{\Pi}) + \frac{3}{4}\epsilon \\ &\geq U(V_{\Pi_t}^+) - 6E\Psi(B_{\Pi}) + \frac{3}{4}\epsilon \\ &\geq v^* - 6E\Psi(B_{\Pi}) + \frac{3}{4}\epsilon \end{aligned}$$

which follows since  $\Pi_t^{(1)}$  is chosen to be the policy with largest upper bound. Therefore,  $\Pi_t \in \mathcal{Q}^\epsilon$ .

By the stopping criteria of OpStoK, if the algorithm does not stop and select  $\Pi_t^{(1)}$  as the optimal policy, then  $\Pi_t = \Pi_t^{(2)}$  and

$$L(V_{\Pi_t^{(1)}}^+) + \epsilon < \max_{\Pi \in \text{ACTIVE} \setminus \{\Pi_t^{(1)}\}} U(V_{\Pi}^+) = U(V_{\Pi_t^{(2)}}^+).$$

By equation (10),

$$L(V_{\Pi_t^{(1)}}^+) + 6E\Psi(B_{\Pi}) - \frac{3}{4}\epsilon \geq U(V_{\Pi_t^{(1)}}^+).$$

and by the selection criterion  $U(\Psi(B_{\Pi_t^{(2)}})) \geq U(\Psi(B_{\Pi_t^{(1)}}))$ . Therefore, for  $\Pi_t = \Pi_t^{(2)} \neq \Pi_t^*$ ,

$$\begin{aligned}
 V_{\Pi_t} + 12E\Psi(B_{\Pi}) - \frac{6}{4}\epsilon - \epsilon &\geq L(V_{\Pi_t}^+) + 6E\Psi(B_{\Pi_t}) - \frac{3}{4}\epsilon + 6E\Psi(B_{\Pi_t}) - \frac{3}{4}\epsilon - \epsilon \\
 &\geq U(V_{\Pi_t}^+) + 6E\Psi(B_{\Pi_t}) - \frac{3}{4}\epsilon - \epsilon \\
 &\geq U(V_{\Pi_t}^+) + 3U(\Psi(B_{\Pi_t})) - \epsilon \\
 &\geq U(V_{\Pi_t}^+) + 3U(\Psi(B_{\Pi_t^{(1)}})) - \epsilon \\
 &\geq L(V_{\Pi_t^{(1)}}^+) + 3U(\Psi(B_{\Pi_t^{(1)}})) \\
 &\geq U(V_{\Pi_t^{(1)}}^+) \\
 &\geq U(V_{\Pi_t^*}^+) \\
 &\geq v^*.
 \end{aligned}$$

Hence  $\Pi_t \in \mathcal{Q}^\epsilon$ . □

**Theorem 17** (Theorem 5 in main text) *The total number of samples required by `OpStoK` is bounded from above by,*

$$\sum_{\Pi \in \mathcal{Q}^\epsilon} (m_1(\Pi) + m_2(\Pi)) d(\Pi),$$

with probability  $1 - \delta_{0,2}$ .

*Proof:* The result follows from the following three lemmas.

**Lemma 18** *For  $\Pi \in \mathcal{A}^\epsilon$  of depth  $d = d(\Pi)$ , then, with probability  $1 - \delta_{d,2}$ , the minimum number of samples of the value and remaining budget of the policy  $\Pi$  are bounded by*

$$m_1(\Pi) = \left\lceil \frac{8\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{\epsilon^2} \right\rceil \quad \text{and} \quad m_2(\Pi) = m^*,$$

where  $m^*$  is the smallest integer satisfying  $\frac{16\Psi(B)^2}{(E\Psi(B_{\Pi}) - \epsilon/2)^2} \leq \frac{m}{\log(\frac{8n}{m\delta_2})}$  with  $n$  defined as in (2).

*Proof:* When  $E\Psi(B_{\Pi}) \leq \frac{\epsilon}{4}$ , the event  $\{U(\Psi(B_{\Pi})) \leq \frac{\epsilon}{2}\}$  will eventually occur with enough samples of the remaining budget of the policy. With probability greater than  $1 - \delta_{d,2}$ , this will happen when  $2c_2 \leq \frac{\epsilon}{2} - E\Psi(B_{\Pi})$ , since by Hoeffding's Inequality we know  $\overline{\Psi(B_{\Pi})}_{m_2} \in [E\Psi(B_{\Pi}) - c_2, E\Psi(B_{\Pi}) + c_2]$  where  $c_2$  is as defined in Lemma 1. From this, it follows that  $U(\Psi(B_{\Pi})) \in [E\Psi(B_{\Pi}), E\Psi(B_{\Pi}) + 2c_2]$ . We want to make sure that  $U(\Psi(B_{\Pi})) \leq \frac{\epsilon}{2}$  will eventually happen so we need to construct a confidence interval such that  $c_2$  satisfies  $E\Psi(B_{\Pi}) + 2c_2 \leq \frac{\epsilon}{2}$ . Therefore we select  $m_2$  such that,

$$\begin{aligned}
 2c_2 &\leq \frac{\epsilon}{2} - E\Psi(B_{\Pi}) \\
 \implies 4\Psi(B) \sqrt{\frac{2 \log(\frac{8n}{m_2 \delta_{d,2}})}{m_2}} &\leq \frac{\epsilon}{2} - E\Psi(B_{\Pi}) \\
 \implies \frac{16\Psi(B)^2}{(E\Psi(B_{\Pi}) - \epsilon/2)^2} &\leq \frac{m_2}{\log(\frac{4n}{m_2 \delta_2})}.
 \end{aligned}$$

Defining,  $m_2(\Pi) = m^*$ , where  $m^*$  is the smallest integer satisfying the above, is therefore an upper bound on the minimum number of samples necessary to ensure that  $U(\Psi(B_{\Pi})) \leq \frac{\epsilon}{2}$  with probability greater than  $1 - \delta_{d,2}$ .

When  $U(\Psi(B_{\Pi})) \leq \frac{\epsilon}{2}$ , `BoundValueShare` requires  $m_1(\Pi) = \left\lceil \frac{2\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{\epsilon^2} \right\rceil$  samples of the value of the policy to ensure  $2c_1 \leq \frac{\epsilon}{2}$ . □



**Lemma 19** For  $\Pi \in \mathcal{B}^\epsilon$  of depth  $d = d(\Pi)$ , then, with probability  $1 - \delta_{d,2}$ , the minimum number of samples of the value and remaining budget of the policy  $\Pi$  are bounded by

$$m_1(\Pi) \leq \left\lceil \frac{\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{2E\Psi(B_\Pi)^2} \right\rceil \quad \text{and} \quad m_2(\Pi) = m^*,$$

where  $m^*$  is the smallest integer satisfying  $\frac{16\Psi(B)^2}{(E\Psi(B_\Pi) - \epsilon/4)^2} \leq \frac{m}{\log(8n/m\delta_2)}$  with  $n$  defined as in (2).

*Proof:* When  $E\Psi(B_\Pi) \geq \frac{\epsilon}{2}$ , by noting that the event  $\{L(\Psi(B_\Pi)) \geq \frac{\epsilon}{4}\}$  will eventually happen and using a very similar argument to Lemma 18, it follows that  $m_2(\Pi)$  is the smallest integer solution to

$$\frac{16\Psi(B)^2}{(E\Psi(B_\Pi) - \epsilon/4)^2} \leq \frac{m}{\log(8n/m\delta_2)},$$

with probability greater than  $1 - \delta_{d,2}$ . Whenever  $L(\Psi(B_\Pi)) \geq \frac{\epsilon}{4}$ , `BoundValueShare` requires  $m_1(\Pi) = \left\lceil \frac{2\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{(U(\Psi(B_\Pi)))^2} \right\rceil$  samples of the value of policy  $\Pi$ . Since  $U(\Psi(B_\Pi)) \in [E\Psi(B_\Pi), E\Psi(B_\Pi) + 2c_2]$  with probability  $1 - \delta_{0,2}$ ,  $U(\Psi(B_\Pi)) \geq E\Psi(B_\Pi)$ , and so,

$$m_1(\Pi) = \left\lceil \frac{2\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{(U(\Psi(B_\Pi)))^2} \right\rceil \leq \left\lceil \frac{2\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{E\Psi(B_\Pi)^2} \right\rceil$$

and the result holds.  $\square$

**Lemma 20** For  $\Pi \in \mathcal{C}^\epsilon$  of depth  $d = d(\Pi)$ , then, with probability  $1 - \delta_{d,2}$ , the minimum number of samples of the value and remaining budget of the policy  $\Pi$  are bounded by

$$m_1(\Pi) \leq \max \left\{ \left\lceil \frac{8\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{\epsilon^2} \right\rceil, \left\lceil \frac{\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{2E\Psi(B_\Pi)^2} \right\rceil \right\}$$

and  $m_2(\Pi) = m^*$ , where  $m^*$  is the smallest integer satisfying  $\frac{16\Psi(B)^2}{(\epsilon/4)^2} \leq \frac{m}{\log(8n/m\delta_2)}$  with  $n$  defined as in (2).

*Proof:* When  $\frac{\epsilon}{4} < E\Psi(B_\Pi) < \frac{\epsilon}{2}$ , then the minimum width we will need a confidence interval to be is  $\epsilon/4$ . By an argument similar to Lemma 18, we can deduce that  $m_2(\Pi)$  will be the smallest integer satisfying  $\frac{16\Psi(B)^2}{(\epsilon/4)^2} \leq \frac{m}{\log(8n/m\delta_2)}$ .

In order to determine the number of samples of the value required by `BoundValueShare`, we need to know which of  $\{U(\Psi(B_\Pi)) \leq \frac{\epsilon}{2}\}$  or  $\{L(\Psi(B_\Pi)) \geq \frac{\epsilon}{4}\}$  occurs first. However, when  $\Pi \in \mathcal{C}^\epsilon$ , we do not know this so the best we can do is bound  $m_1(\Pi)$  by the maximum of the two alternatives,

$$m_1(\Pi) \leq \max \left\{ \left\lceil \frac{2\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{\epsilon^2} \right\rceil, \left\lceil \frac{2\Psi(B)^2 \log(\frac{2}{\delta_{d,1}})}{E\Psi(B_\Pi)^2} \right\rceil \right\}.$$

$\square$

The result of the theorem then follows by noting that for any policy  $\Pi$  of depth  $d(\Pi)$ , it will be necessary to have  $m_1(\Pi)$  samples of the value of the policy and  $m_2(\Pi)$  samples of the value of the policy. This requires  $m_1(\Pi)d(\Pi)$  samples of item rewards,  $m_1(\Pi)d(\Pi)$  samples of item sizes (to calculate the rewards) and  $m_2(\Pi)d(\Pi)$  samples of item sizes (to calculate remaining budget), thus a total of  $(m_1(\Pi) + m_2(\Pi))d(\Pi)$  calls to the generative model. From Lemma 3, any policy expanded by `OpStoK` will be in  $\mathcal{Q}^\epsilon$  so it suffices to sum over all policies in  $\mathcal{Q}^\epsilon$ . This result assumes that all confidence bounds hold, whereas we know that for any policy  $\Pi$  of depth  $d(\Pi)$ , the probability of the confidence bound holding is greater than  $1 - \delta_{d,2}$ . By an argument similar to Lemma 12, the probability that all bounds hold is greater than  $1 - \delta_{0,2}$ . Note that, since  $|\mathcal{Q}^\epsilon| \leq |\mathcal{P}|$ , the probability should be considerably greater than  $1 - \delta_{0,2}$ .  $\square$