

# Best-First Rao-Blackwellization

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# Gradient Estimation

- ▶ Goal: optimize

$$\max_{\theta} \sum_x p_{\theta}(x) f(x)$$

(optimizing wrt parameters of  $f$  is easy)

- ▶ Discrete  $x$ , expensive evaluation of  $f(x)$

# Gradient Estimators

- ▶ Score-function estimator (SFE)

$$\nabla_{\theta} \sum_x p_{\theta}(x) f(x) = \mathbb{E}_{p_{\theta}(x)} [f(x) \nabla \log p_{\theta}(x)]$$

- ▶ High variance, consistent
- ▶ Continuous relaxation,  $x \approx g(\theta, \epsilon)$

$$\nabla_{\theta} \sum_x p_{\theta}(x) f(x) \approx \mathbb{E}_{p(\epsilon)} [\nabla_{\theta} f(g_{\theta}(\theta, \epsilon))]$$

- ▶ Biased, lower variance
  - ▶ Requires relaxable  $f$
  - ▶ Stochastic softmax tricks (SST)
- ▶ Focus on improving SFE
  - ▶ Total error most important, but SFE under-explored

# Rao-Blackwellization of score function estimator

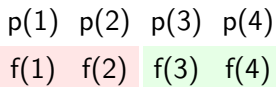
- ▶ Condition on values of  $f(x)$  for  $x \in S$

$$\begin{aligned} & \nabla_{\theta} \sum_x p_{\theta}(x) f(x) \\ &= \mathbb{E}_{p_{\theta}(x)} [f(x) \nabla \log p_{\theta}(x)] \\ &= \sum_{x \in S} p(x) f(x) \nabla \log p_{\theta}(x) + \mathbb{E}_{p_{\theta}(x \notin S)} [f(x) \nabla \log p_{\theta}(x)] \end{aligned}$$

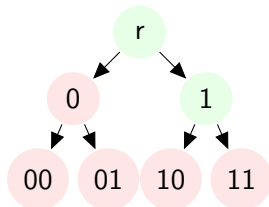
- ▶ Conditioning on all values  $f(x) = \text{no variance}$
- ▶ Want  $S$  to have  $x$  with high  $p(x)f(x)$ 
  - ▶ Need to compromise with high  $p(x)$
  - ▶ Use heuristic estimate of  $f(x)$ ?
  - ▶ What if  $x$  is structured?

# Structured Setting

Flat



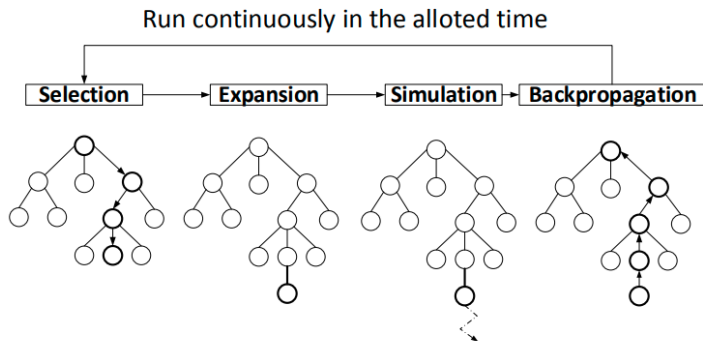
Structured



# Best-first Rao-Blackwellization

- ▶ Modern MCTS
  - ▶ Prior  $p(x)$  (forward)
  - ▶ Cost-to-go estimate  $\tilde{V}(x)$  (backward)
  - ▶ Search procedure that links the two
- ▶ Proposal
  - ▶ In many cases, already have the prior  $p(x)$
  - ▶ Estimate cost-to-go with continuous relaxation or cheaper problem-dependent weaker model (Markov transformer)
  - ▶

# BF RB



# Citations I