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)
 - ightharpoonup eg f is a giant neural network

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
- ▶ Requires multiple evaluations, better with more compute
- ▶ Continuous relaxation, $x \approx g(\theta, \epsilon)$

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

- Biased, lower variance
- Requires low number of evals, less benefit from more compute
- Requires relaxable f
- Stochastic softmax tricks (SST)
- Focus on improving SFE
 - SFE under-explored

Rao-Blackwellization

- ▶ Too expensive to enumerate over all x (f is expensive)
- ► Reduce effective width of distribution via sub-sampling (red)
- ► Enumerate over green portion

Rao-Blackwellization of score function estimator

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

$$\nabla_{\theta} \sum_{x} p_{\theta}(x) f(x)$$

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

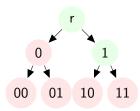
$$= \sum_{x \in S} p(x) f(x) \nabla \log p_{\theta}(x) + \mathbb{E}_{p_{\theta}(x \notin S)} [f(x) \nabla \log p_{\theta}(x)]$$

- ▶ Conditioning on all values f(x) =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

- In the flat setting, only cared about width
- In structured setting, can also approximate depth

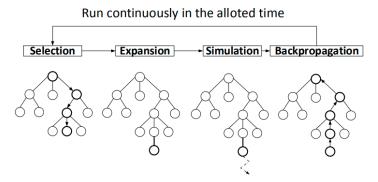
Flat Structured



Best-first Rao-Blackwellization

- Modern MCTS
 - Prior p(x) (limits width)
 - ightharpoonup Cost-to-go estimate $\tilde{V}(x)$ (limits depth)
 - 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)
 - Link the two by marginalization

BF RB



Minimal Experiment

Approximate DP when exact is tractable

- Depth approx: Learn cost-to-go estimate to bound depth in i 32k state HMM
 - HMM with forward algo that doesnt go all the way to end
 - Bounded width = prior not important
- Width approx: Utilize prior in large-state HMM
 - Limit num states considered at each time step
- Approximations for width + depth
 - Probably more useful in PCFGs

Citations I