

# 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  $f(x)$ 
  - ▶ 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,  $x \approx g(\theta, \epsilon)$

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

- ▶ 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
  - ▶ Better with more compute is attractive

# 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

$p(1)$	$p(2)$	$p(3)$	$p(4)$
$f(1)$	$f(2)$	$f(3)$	$f(4)$

# 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  $f(x)$  = 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

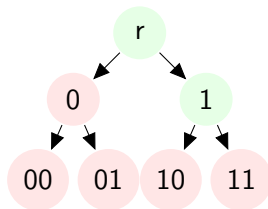
- ▶ In the flat setting, only cared about width
- ▶ In structured setting, can also approximate depth

Flat

p(1) p(2) p(3) p(4)

f(1) f(2) f(3) f(4)

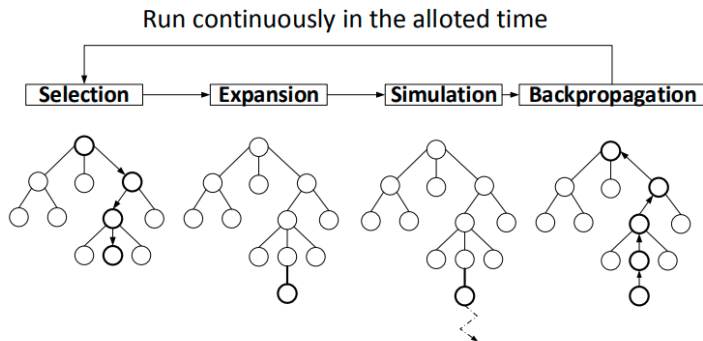
Structured



# Best-first Rao-Blackwellization

- ▶ Modern MCTS
  - ▶ Prior  $p(x)$  (limits width)
  - ▶ 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 (learned value function approx)
  - ▶ 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 32k state HMM
  - ▶ HMM with forward algo that doesn't go all the way to end
  - ▶ Bounded width = prior not important
  - ▶ Experiment with continuous relaxation + learned  $\tilde{V}$  for suffix
- ▶ 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 or other more interesting models (massive switching)

# Random thoughts

- ▶ For exp fam, is this an instance of hypernetworks (ie predicting gradient)?

# Citations I