

## SUPPLEMENTARY MATERIALS - AND/OR ALGORITHM

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### Algorithm 1: AOAS, a single probe

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**Require:** A graphical model  $\mathcal{M} = (\mathbf{X}, \mathbf{D}, \mathbf{F})$  over  $X = \{X_1, \dots, X_n\}$ , a pseudo-tree  $\mathcal{T}$ . An implicit AND/OR tree  $T_{\mathcal{T}}$  of  $\mathcal{M}$ .  $g(s)$  is the product of arc-costs from root to  $s$  and  $h(s)$  (heuristic function) An abstraction  $a$ .  $s_0$  is the root of the tree.

**Ensure:** A sampled subtree  $\tilde{T}_{\mathcal{T}} = (\tilde{N}, E, C)$  of  $T_{\mathcal{T}}$ . Each  $n \in \tilde{N}$  is a pair  $n = \langle s, w(s) \rangle$  where  $w(s)$  is a weight. Note that OR node weight is always 1.

- 1: **initialize**  $\tilde{T}_{\mathcal{T}} \leftarrow \{ \langle s_0, 1 \rangle \}$ ,
  - 2: **while** *OPEN* is not empty **do**
  - 3:    $\langle s, w(s) \rangle \leftarrow$  remove smallest  $a$  node in *OPEN*
  - 4:   Expand  $s$ , generating all its child nodes variables in the pseudo-tree  $\{X_1, \dots, X_r\}$ , each yielding OR nodes denoted  $s_1, \dots, s_r$  ( $var(s_j) = X_j$ ) and add them to  $\tilde{T}_{\mathcal{T}}$ .
  - 5:   **for** each OR child node  $s_j$  **do**
  - 6:     expand  $s_j$ , generating all its AND child nodes  $s_{j_i} = \langle X_j, x_{j_i} \rangle$ ,  $x_{j_i} \in D_{X_j}$  with  $w(s_{j_i}) = w(s)$ .
  - 7:     **for** each child  $s_{j_i}$  **do**
  - 8:       **if**  $\tilde{T}_{\mathcal{T}}$  contains a representative  $\langle s_{\{k\}}, w_{\{k\}} \rangle$  of abstraction  $\{k\}$ ,  $a(s_{j_i}) = k$  that shares the same configuration up to its branching variable (i.e., obeys properness) **then**
  - 9:          $p \leftarrow \frac{w(s_{j_i})g(s_{j_i})h(s_{j_i})}{w(s_j)g(s_j)h(s_j) + w_{\{k\}}g(s_{\{k\}})h(s_{\{k\}})}$
  - 10:        with probability  $p$  **do**:
  - 11:         remove  $s_{\{k\}}$  from  $\tilde{T}_{\mathcal{T}}$  and *OPEN*
  - 12:         add  $\langle s_{j_i}, \frac{w(s_{j_i})}{p} \rangle$  as a child of  $s_j$  in  $\tilde{T}_{\mathcal{T}}$  representing  $\{k\}$  and add it to *OPEN*
  - 13:         **else**
  - 14:          $w_{\{k\}} \leftarrow \frac{w_{\{k\}}}{1-p}$
  - 15:         **else**
  - 16:         add  $\langle s_{j_i}, w(s_{j_i}) \rangle$  as a child of  $s_j$  in  $\tilde{T}_{\mathcal{T}}$  representing  $\{k\}$  and add it to *OPEN*.
  - 17:  $\tilde{T}_{\mathcal{T}}$  is the final tree generated.
  - 18: **return**  $\hat{Z} \leftarrow$  compute  $Z$  of  $\tilde{T}$  AOAS-Z-estimator
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## SUPPLEMENTARY MATERIALS - EXTENDED UNBIASEDNESS PROOF

**THEOREM 1 (unbiasedness)** *Given a weighted directed AND/OR search tree  $T$  derived from a graphical model, the estimate  $\hat{Z}$  generated by AS is unbiased.*

**Proof.** (sketch) Clearly, for any node in the AND/OR tree the partition function it roots can be expressed recursively by:  $Z(n) = \prod_{n' \in ch(n)} \sum_{n'' \in ch(n')} c(n', n'') Z(n')$ ,  $Z(n) = 1$

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### Algorithm 2: AOAS-Z-estimator

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**Require:** A graphical model  $\mathcal{M} = (\mathbf{X}, \mathbf{D}, \mathbf{F})$  over  $X = \{X_1, \dots, X_n\}$ , a pseudo-tree  $\mathcal{T}$ . An AND/OR tree  $T_{\mathcal{T}}$  of  $\mathcal{M}$ ; its subtree  $\tilde{T}_{\mathcal{T}} = (\tilde{N}, E, C)$  of  $T_{\mathcal{T}}$ .  $c(s)$  is the cost of an OR-to-AND arc ( $parent(s), s$ ) in  $T_{\mathcal{T}}$ .

**Ensure:** An estimate  $\hat{Z}$  of the partition function  $Z$ .

- 1: Compute an estimate for each node in  $\tilde{T}_{\mathcal{T}}$ , bottom up, with the following rules
  - 2:   For leaf node  $\langle s, w(s) \rangle$ , its value is  $\hat{Z}(s) = w(s)c(s)$ .
  - 3:   For internal OR node  $s$ , its value is  $\hat{Z}(s) = \sum_{c \in ch(s)} \hat{Z}(c)$ .
  - 4:   For internal AND node  $\langle s, w(s) \rangle$ , its value is  $\hat{Z}(s) = \frac{w(s)}{w(parent(s))} c(s) \prod_{c \in ch(s)} \hat{Z}(c)$ .
  - 5: **return** Value of the root node  $\hat{Z}(r)$ .
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if  $n$  is a leaf AND node. At each step, the algorithm maintains the current, partially generated, AND/OR tree denoted  $\tilde{T}^{(t)}$  where  $t$  index the algorithm's steps. The partial tree  $\tilde{T}^{(t)}$  is a stochastic subtree of  $T$  whose nodes are assigned weights by the algorithm.

Let *OPEN* be the set of AND leaf nodes of the partial tree  $\tilde{T}^{(t)}$  and let *CLOSED* be the rest of the nodes in  $\tilde{T}^{(t)}$ . We define an intermediate estimator of  $Z$  at step  $t$  denoted  $\hat{Z}^{(t)}(n)$ , over  $\tilde{T}^{(t)}$  recursively as follows. For an AND node  $n \in \tilde{T}^{(t)}$ .

$$\hat{Z}^{(t)}(n) = \begin{cases} Z(n) & \text{if } n \in \text{OPEN} \\ \prod_{n' \in ch(n)} \sum_{n'' \in ch(n')} w(n'') c(n', n'') \hat{Z}^{(t)}(n'') & \text{if } n \in \text{CLOSED} \end{cases} \quad (1)$$

This recursive estimate combines information from the sampled nodes and estimated weights in  $\tilde{T}^{(t)}$  with exact values of  $Z$  for the nodes in *OPEN* at time  $t$ . We can show that at any step  $t$ ,  $E(\hat{Z}^{(t+1)}(r) - \hat{Z}^{(t)}(r) | \tilde{T}^t) = 0$ , where  $r$  is the root. Consequently the expected value of our successive approximation at the end of sampling is equal to its initial value:  $\hat{Z}^{(0)}(r) = Z(r) = Z$ . (For more details see supplement.)  $\square$

### DEFINITION 1 (recursive function on AND/OR trees)

*Given a weighted directed AND/OR tree, having costs,  $c$ , labeling its OR to AND arcs. We define a recursive value function denoted  $Z(n)$  for an AND node by:*

$$Z(n) = \prod_{n' \in ch(n)} \sum_{n'' \in ch(n')} c(n', n'') Z(n') \quad (2)$$

*The initial value for leaves:  $Z(n) = 1$  if  $n$  is a leaf AND node.*

**THEOREM 2** Given a weighted directed AND/OR search tree  $T$  derived from a graphical model, and a value function  $Z(n)$  defined recursively over  $T$  and given a proper abstraction function over  $T$ , the estimate generated by AOAS and AOAS-Z-estimator,  $\hat{Z}(r)$ , is unbiased. Namely  $E\hat{Z}(r) = Z(r)$ , when  $r$  is the dummy root AND node of  $T$ .

**Proof.** At each step, the algorithm maintains the current, partially generated, AND/OR tree denoted  $\tilde{T}^{(t)}$  (we drop the subscript of the pseudo-tree for simplicity), where  $t$  index the algorithm's steps in generating the sampled tree. The partial tree  $\tilde{T}^{(t)}$  is a stochastic subgraph of  $T$  whose nodes are assigned weights by the algorithm. Let  $OPEN$  be the set of AND leaf nodes of the partial tree  $\tilde{T}^{(t)}$  and let  $CLOSED$  be the rest of the nodes in  $\tilde{T}^{(t)}$ .

We define an intermediate estimator of  $Z$  at step  $t$  denoted  $\hat{Z}^{(t)}(n)$ , over  $\tilde{T}^{(t)}$  recursively as follows. For an AND node  $n \in \tilde{T}^{(t)}$ .

$$\hat{Z}^{(t)}(n) = \begin{cases} Z(n) & \text{if } n \in OPEN \\ \prod_{n' \in ch(n)} \sum_{n'' \in ch(n')} w(n'') c(n', n'') \hat{Z}^{(t)}(n'') & \text{if } n \in CLOSED \end{cases} \quad (3)$$

This recursive estimate combines information from the sampled nodes and estimated weights in  $\tilde{T}^{(t)}$  with exact values of  $Z$  for the nodes in  $OPEN$  at time  $t$ .

We will show that at any step  $t$ ,  $E(\hat{Z}^{(t+1)}(r) - \hat{Z}^{(t)}(r) | \tilde{T}^{(t)}) = 0$ . Consequently the expected value of our successive approximation at the end of sampling is equal to its initial value:  $\hat{Z}^{(0)}(r) = Z(r) = Z$ .

**Deterministic changes.** The algorithm performs deterministic steps of node expansions. These operations grow  $\tilde{T}^{(t)}$  but do not change the value of the estimator at all. According to EQ. (3), when the algorithm performs node expansion, namely expanding an AND node whose current estimate is  $Z(n)$  to its children and grandchildren and re-evaluate the resulting estimate at  $n$ , we will get back  $Z(n)$  because the recursion obeys the recursive definition of  $Z(n)$  (see EQ. (2) when  $w = 1$ , which are the initial weights). So, since the estimate does not change at the leaves of  $\tilde{T}^{(t)}$ , no change will be propagated up the tree, to the root. In other words in those cases we need no expectation. We have that:  $(\hat{Z}^{(t+1)}(r) - \hat{Z}^{(t)}(r) | \tilde{T}^{(t)}) = 0$ .

**Stochastic changes.** The only stochastic change occurs when an AND node,  $u$ , is examined (step 9) and the algorithm identifies a representative AND node  $v$  having the same abstraction in  $OPEN$ . We denote by  $s$  the first common ancestor of  $u$  and  $v$  in  $\tilde{T}^{(t)}$  through an OR tree. Since the abstraction is proper, the subtree of  $\tilde{T}^{(t)}$  rooted

at  $s$ , denoted by  $\tilde{T}_s^{(t)}$ , is an OR tree. Therefore, there would be no product in the second expression of EQ. (3) and we can see that the estimate at node  $s$  can be expressed by a sum over all paths from  $s$  to each leaf node in  $\tilde{T}_s^{(t)}$ . Noting explicitly the leaf nodes  $u$  and  $v$  we get, from recursing EQ. (3),

$$\begin{aligned} \hat{Z}^{(t)}(s) &= \sum_{\{n \neq u, v | \text{leaf } s \text{ in } \tilde{T}_s^{(t)}\}} \hat{Z}^{(t)}(n) \cdot \prod_{q \in path(s..n)} w(q) c(q) \\ &+ Z(u) \prod_{q \in path(s..u)} w(q) c(q) + Z(v) \prod_{q \in path(s..v)} w(q) c(q) \quad (4) \end{aligned}$$

The first term in EQ. (4) is not affected by the stochastic process. We denote this term by  $B$ :

Once node  $u$  is processed, the resulting graph  $\tilde{T}^{(t+1)}$  depends on the stochastic choice made. If  $u$  is selected, (which occurs with probability  $1 - p$ ) we get

$$\hat{Z}^{(t+1)}(s) = B + \frac{w(u)}{1-p} Z(u) c(u) \prod_{q \in path(s..par(u))} w(q) c(q)$$

else,  $v$  is selected with probability  $p$  then we get

$$\hat{Z}^{(t+1)}(s) = B + \frac{w(v)}{p} Z(v) c(v) \prod_{q \in path(s..par(v))} w(q) c(q)$$

By simple algebraic manipulation it is possible to show that for node  $s$  we get:  $E(\hat{Z}^{(t+1)}(s) - \hat{Z}^{(t)}(s) | \tilde{T}^{(t)}) = 0$ . Since at all the leaf nodes of  $\tilde{T}^{(t+1)}$ , excluding  $s$  and its subtree,  $\hat{Z}^{(t+1)}(n) - \hat{Z}^{(t)}(n) = 0$ , and since at  $s$ , we proved no change in expectation between the successive approximations. We get also at the root  $E(\hat{Z}^{(t+1)}(r) - \hat{Z}^{(t)}(r) | \tilde{T}^{(t)}) = 0$ .  $\square$

## SUPPLEMENTARY MATERIALS - FULL EXPERIMENTAL RESULTS

Table 1: Mean Error Aggregated Over Benchmark for a Given Scheme, Time and Abstraction Level ( $a_0, a_1, a_2$ ).  $a_0$  is 0-level abstraction, ( $a_1, a_2$ ) are: OR-RelCB:(4, 8), OR-RandCB:(16, 256), AO-RelCB:(1, 2.5), AO-RandCB:(2, 4.5). (#inst,  $\bar{n}$ ,  $\bar{w}$ ,  $\bar{k}$ ,  $|\bar{F}|$ ,  $\bar{s}$ ) are number of instances and averages of number of variables, induced width, max domain size, number of functions, max scope size.

Benchmark #inst, $\bar{n}$ , $\bar{w}$ , $\bar{k}$ , $ \bar{F} $ , $\bar{s}$	scheme	#nodes per probe $a_0, a_1, a_2$	1 min $a_0, a_1, a_2$	20 min $a_0, a_1, a_2$	60 min $a_0, a_1, a_2$
DBN-small 60, 70, 30, 2, 16950, 2	OR-RelCB	141, 1963, 22687	1.18, 1.93, 2.58	0.88, 1.86, 1.77	0.78, 1.43, 1.65
	OR-RandCB-1	141, 1611, 13449	1.18, 1.04, 0.81	0.88, 0.71, 0.63	0.78, 0.42, 0.54
	OR-RandCB-2	141, 1624, 12656	1.18, 2.15, 1.77	0.88, 1.42, 1.23	0.78, 1.17, 1.07
	OR-RandCB-3	141, 1684, 14579	1.18, 1.34, 0.84	0.88, 1.05, 0.77	0.78, 0.78, 0.61
	WMB-IS		9.40	5.69	3.27
	IJGP-SS				1.22
Grids-small 7, 271, 24, 2, 791, 2	OR-RelCB	180, 2774, 42184	6.68, 5.19, 5.07	6.06, 4.71, 4.25	4.94, 4.31, 3.39
	OR-RandCB-1	180, 2755, 34101	6.68, 5.05, 1.97	6.06, 4.10, 1.55	4.94, 3.83, 1.41
	OR-RandCB-2	180, 2746, 33650	6.68, 4.29, 2.77	6.06, 3.98, 1.93	4.94, 3.27, 2.02
	OR-RandCB-3	180, 2748, 33898	6.68, 4.23, 3.27	6.06, 4.04, 3.38	4.94, 3.34, 2.24
	AO-RelCB	224, 13388, 91154	5.46, 3.84, 4.70	5.43, 3.68, 3.74	4.83, 2.97, 3.83
	AO-RandCB-1	224, 9418, 65423	5.46, 1.97, 4.27	5.43, 1.72, 3.36	4.83, 0.84, 2.77
	AO-RandCB-2	224, 8938, 84428	5.46, 3.16, 3.87	5.43, 3.10, 3.81	4.83, 2.82, 3.48
	AO-RandCB-3	224, 11291, 82649	5.46, 4.28, 3.77	5.43, 3.43, 3.41	4.83, 3.23, 3.50
	WMB-IS		2.94	1.94	1.21
	IJGP-SS				38.81
Pedigree-small 22, 917, 26, 5, 917, 4	OR-RelCB	270, 6115, 271925	0.17, 0.19, 0.26	0.17, 0.17, 0.19	0.17, 0.17, 0.16
	OR-RandCB-1	270, 4967, 75980	0.17, 0.20, 0.25	0.17, 0.17, 0.19	0.17, 0.17, 0.19
	OR-RandCB-2	270, 4967, 75841	0.17, 0.20, 0.25	0.17, 0.18, 0.18	0.17, 0.16, 0.16
	OR-RandCB-3	270, 4975, 76055	0.17, 0.19, 0.20	0.17, 0.17, 0.18	0.17, 0.17, 0.16
	AO-RelCB	294, 10286025, 337777	0.18, 0.47, 0.21	0.15, 0.36, 0.17	0.16, 0.20, 0.16
	AO-RandCB-1	294, 1171192, 92627	0.18, 0.24, 0.18	0.15, 0.19, 0.16	0.16, 0.18, 0.16
	AO-RandCB-2	294, 725005, 93194	0.18, 0.20, 0.18	0.15, 0.20, 0.17	0.16, 0.17, 0.16
	AO-RandCB-3	294, 2292328, 82475	0.18, 0.21, 0.18	0.15, 0.18, 0.16	0.16, 0.18, 0.16
	WMB-IS		-	-	1.06
	IJGP-SS				11.10
Promedas-small 41, 666, 26, 2, 674, 3	OR-RelCB	115, 1091, 12801	0.68, 0.77, 1.59	0.33, 0.44, 0.70	0.16, 0.34, 0.47
	OR-RandCB-1	115, 2174, 28712	0.69, 0.69, 0.62	0.33, 0.28, 0.38	0.16, 0.15, 0.21
	OR-RandCB-2	115, 2172, 28850	0.68, 0.64, 0.65	0.33, 0.28, 0.30	0.16, 0.13, 0.21
	OR-RandCB-3	115, 2172, 29017	0.68, 0.59, 0.73	0.33, 0.28, 0.36	0.16, 0.15, 0.19
	AO-RelCB	110, 825, 5818	0.56, 0.59, 0.66	0.30, 0.34, 0.40	0.15, 0.23, 0.23
	AO-RandCB-1	110, 753, 6162	0.56, 0.32, 0.28	0.30, 0.19, 0.15	0.15, 0.10, 0.10
	AO-RandCB-2	110, 769, 6453	0.56, 0.43, 0.39	0.30, 0.17, 0.20	0.15, 0.12, 0.15
	AO-RandCB-3	110, 753, 6218	0.56, 0.36, 0.29	0.30, 0.19, 0.16	0.15, 0.11, 0.10
	WMB-IS		-	1.77	1.15
	IJGP-SS				3.06
DBN-large 48, 216, 78, 2, 66116, 2	OR-RelCB	434, 6586, 91881	366.77, 368.29, 369.59	365.32, 366.49, 367.44	363.93, 365.04, 366.20
	OR-RandCB-1	434, 4858, 71545	366.77, 365.56, 365.14	365.32, 364.04, 363.53	363.93, 363.14, 362.88
	OR-RandCB-2	434, 4804, 71036	366.77, 365.58, 364.49	365.32, 364.19, 363.02	363.93, 363.17, 362.53
	OR-RandCB-3	434, 4774, 70421	366.77, 365.70, 364.04	365.32, 363.84, 362.97	363.93, 363.20, 362.36
	WMB-IS		-	-	-
	IJGP-SS				356.91
Grids-large 19, 3432, 117, 2, 10244, 2	OR-RelCB	2827, 45112, 719763	966.46, 925.86, 927.60	933.64, 900.71, 909.37	928.35, 889.53, 894.59
	OR-RandCB-1	2827, 45104, 710675	966.46, 945.98, 918.19	933.64, 912.19, 907.30	928.35, 900.01, 894.15
	OR-RandCB-2	2827, 45097, 711566	966.46, 938.20, 917.92	933.64, 904.34, 910.19	928.35, 897.03, 895.12
	OR-RandCB-3	2827, 45100, 709978	966.46, 937.50, 923.23	933.64, 909.52, 915.99	928.35, 898.47, 890.60
	AO-RelCB	3326, 5485338, 2849697	949.25, 875.81, 910.60	925.85, 863.23, 892.96	918.74, 854.53, 885.18
	AO-RandCB-1	3326, 3896561, 2826722	949.25, 860.66, 885.97	925.85, 845.20, 876.74	918.74, 841.84, 871.05
	AO-RandCB-2	3326, 3846042, 2820388	949.25, 853.83, 880.27	925.85, 843.66, 874.03	918.74, 840.39, 868.61
	AO-RandCB-3	3326, 4276589, 2818713	949.25, 865.29, 882.50	925.85, 846.33, 871.89	918.74, 842.33, 865.49
	WMB-IS		-	-	-
	IJGP-SS				-
Promedas-large 88, 962, 48, 2, 974, 3	OR-RelCB	194, 2092, 25156	-, -, -	30.29, -, -	29.54, 30.28, 31.89
	OR-RandCB-1	194, 3586, 54901	-, -, 30.24	30.29, -, 29.27	29.54, 29.26, 28.59
	OR-RandCB-2	194, 3587, 54904	-, -, -	30.29, -, 29.36	29.54, 29.47, 28.47
	OR-RandCB-3	194, 3585, 54859	-, -, 30.21	30.29, 30.50, 29.20	29.54, 29.35, 28.55
	AO-RelCB	158, 1561, 10840	-, 30.45, 30.55	30.00, 29.31, 29.32	29.06, 28.67, 28.44
	AO-RandCB-1	158, 1319, 12082	-, 29.23, 28.97	30.00, 28.47, 28.06	29.06, 27.89, 27.66
	AO-RandCB-2	158, 1259, 11381	-, 29.24, 28.81	30.00, 28.56, 28.11	29.06, 27.96, 27.66
	AO-RandCB-3	158, 1377, 11704	-, 29.50, 28.82	30.00, 28.45, 28.07	29.06, 27.83, 27.68
	WMB-IS		-	-	-
	IJGP-SS				35.50