

## Appendix

A common sampling technique often used in this setting is the Metropolis-Hastings algorithm, which is a Markov chain Monte Carlo (MCMC) method. The M-H acceptance probability for moving from state  $x$  to state  $x'$  is shown below, where each *state* is a DBN.

$$\alpha(x, x') = \min \left\{ 1, \frac{p(D|x')}{p(D|x)} \times \frac{p(x' \rightarrow x)}{p(x \rightarrow x')} \right\} = \min \left\{ 1, \underbrace{\frac{p(D|x')}{p(D|x)}}_{\text{likelihood ratio}} \times \underbrace{\frac{p(m')p(x|x', m')}{p(m)p(x'|x, m)}}_{\text{proposal ratio}} \right\}$$

where  $m$  is the move type that allows for a transition from state  $x$  to  $x'$  and  $m'$  is the reverse move type for a transition from state  $x'$  back to state  $x$ . The proposal ratio can be split into two terms: one is the ratio of the proposal probabilities for move types and the other is the ratio of selecting a particular state given the current state and the move type. The choice of scoring metric determines the likelihoods, and often  $p(m')$  and  $p(m)$  are chosen *a priori* to be simple to calculate or to actually cancel out.

Move type $M$	Proposal probability	$\frac{p(M')}{p(M)}$	$\frac{p(x x', M')}{p(x' x, M')}$	
$(M_1)$ add edge to $G_1$	$P_a$	$\frac{P_d}{P_a}$	$\frac{(E_1+1)^{-1}}{(np_{max}-E_1)^{-1}} = \frac{np_{max}-E_1}{E_1+1}$	<div style="display: flex; align-items: center;"> <div style="margin-right: 5px;">}</div> <div style="writing-mode: vertical-rl; transform: rotate(180deg);">KNKT</div> </div>
$(M_2)$ delete edge from $G_1$	$P_d$	$\frac{P_a}{P_d}$	$\frac{(np_{max}-E_1+1)^{-1}}{E_1^{-1}} = \frac{E_1}{np_{max}-E_1+1}$	
$(M_3)$ add edge to $\Delta g_i$	$P_{ae}$	$\frac{P_{de}}{P_{ae}}$	$\frac{m^{-1}(S_i+1)^{-1}}{m^{-1}(S_{max}-S_i)^{-1}} = \frac{S_{max}-S_i}{S_i+1}$	
$(M_4)$ delete edge from $\Delta g_i$	$P_{de}$	$\frac{P_{ae}}{P_{de}}$	$\frac{m^{-1}(S_{max}-S_i+1)^{-1}}{m^{-1}S_i^{-1}} = \frac{S_i}{S_{max}-S_i+1}$	
$(M_5)$ move edge from $\Delta g_i$ to $\Delta g_j$	$P_{me}$	1	$\frac{(m-1)^{-1}(\sum_i S_i)^{-1}}{(m-1)^{-1}(\sum_i S_i)^{-1}} = 1$	
$(M_6)$ locally shift $t_i$	$P_{st}$	1	$\frac{(2d+1)^{-1}}{(2d+1)^{-1}} = 1$	
$(M_7)$ merge $\Delta g_i$ and $\Delta g_{i+1}$	$P_m$	$\frac{P_s}{P_m}$	$\frac{(m-1)^{-1}2^{(S_i+S_{i+1})^{-1}}(S_i+S_{i+1})^{-1}}{(m-1)^{-1}} = \frac{2}{(S_i+S_{i+1})\binom{S_i+S_{i+1}}{S_i}}$	<div style="display: flex; align-items: center;"> <div style="margin-right: 5px;">}</div> <div style="writing-mode: vertical-rl; transform: rotate(180deg);">UNUT</div> </div>
$(M_8)$ split $\Delta g_i$	$P_s$	$\frac{P_m}{P_s}$	$\frac{(m-1)^{-1}}{(m-1)^{-1}(S_i/2)^{-1}\binom{S_i}{x}} = (S_i/2)\binom{S_i}{x}$	
$(M_9)$ create new $\Delta g_i$	$P_{ag}$	$\frac{P_{dg}}{P_{ag}}$	$\frac{(m+1)^{-1}}{(N-m)^{-1}n^{-2}} = \frac{(N-m)n^2}{m+1}$	
$(M_{10})$ delete $\Delta g_i$	$P_{dg}$	$\frac{P_{ag}}{P_{dg}}$	$\frac{(N-m-1)^{-1}n^{-2}}{m^{-1}} = \frac{m}{(N-m-1)n^2}$	

Table 1:  $E_1$  is the total number of edges in  $G_1$ ,  $S_{max}$  is the maximum number of transitions allowed in a single transition time,  $p_{max}$  is the maximum parent set size, and  $S_i$  is the number of edge changes in the set  $\Delta g_i$ . The proposal ratio is the product of the last two columns. The KNKT setting uses moves  $(M_1) - (M_5)$ , KNUT uses moves  $(M_1) - (M_6)$ , and UNUT uses moves  $(M_1) - (M_{10})$ , in each case with the proposal probabilities appropriately normalized to add to 1.

All of the F1-measures for the nsDBNs learned under the UNUT setting are shown in Table 2 below.

**A**

$\lambda_s$					
1	2	3	4	5	
0.4341	0.9423	0.9469	0.9738	<b>0.9912</b>	1
0.6760	0.9562	0.9553	0.9906	0.9909	2
0.9206	0.9553	0.9729	0.9731	0.9905	5
0.9264	0.9550	0.9657	0.9829	0.9791	10
0.8804	0.8806	0.9042	0.8922	0.8807	50

**B**

$\lambda_s$				
1	3	5		
0.9489	0.9510	0.9468	1	
0.9377	0.9521	0.9356	2	
<b>0.9531</b>	0.9459	0.9398	5	

Table 2: F1-measure for different values of  $\lambda_s$  and  $\lambda_m$  under the UNUT setting. F1-measures over 0.9 are shaded in light gray and the best score is shown in bold. **A**: F1-measures for the nine variable dataset defined by the nsDBN in Figure 1A. **B**: F1-measures for the large 100 variable dataset.