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Observability and Approximate Observability of Boolean Control Networks from Finite Offline Data

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Appendix A Proof of Theorem 1

Proof. First, it is proved that Ω_T admits a recursive form $\Omega_{T+1} = \Omega_T \cup \mathcal{Q}(\Omega_T)$.

According to the definition of Ω_T, Ω_T including pairs are distinguishable within horizon T. Clearly, if a pair is distinguishable within horizon T, it is also distinguishable within $T+1$ by using the same input sequence, that is, $\Omega_T \subseteq \Omega_{T+1}$. Next, let $(s, s') \in \mathcal{Q}(\Omega_T)$, where $(s, s') \in \Omega$. By the definition of the operator $\mathcal{Q}$, there exists $k \in \mathbb{N}_{1\to M}$ such that $(L\delta_M^k s, L\delta_M^k s') \in \Omega_T$. Hence there are a input sequence $\tilde{u}(0 : T-1) = (\tilde{u}(0), \ldots, \tilde{u}(T-1))$ and $\tau \in \mathbb{N}_{0\to T}$ such that outputs generated from $L\delta_M^k s$ and $L\delta_M^k s'$ under $\tilde{u}(0 : T-1)$ differ at time τ. Prepending the input δ_M^k gives $\tilde{w}(0 : T) = (\delta_M^k, \tilde{w}(1), \ldots, \tilde{w}(T))$, then the outputs from s and s' differ at time time $\tau + 1 \leqslant T + 1$, so $(s, s') \in \Omega_{T+1}$. Therefore, $\Omega_T \cup \mathcal{Q}(\Omega_T) \subseteq \Omega_{T+1}$.

Conversely, $\forall (s, s') \in \Omega_{T+1}$, there always exists input sequence $u_{(s,s')}(0 : T)$ and $\tau_{(s,s')} \in \mathbb{N}_{0\to T+1}$ such that the outputs generated from s and s' under $u_{(s,s')}(0 : T)$ differ at time $\tau_{(s,s')}$. If $\tau_{(s,s')} \leqslant T$, then $(s, s') \in \Omega_T$. Otherwise write $u_{(s,s')}(0 : T) = (u_{(s,s')}(0), w(0), \ldots, w(T-1)) = (u_{(s,s')}(0), w(0 : T-1))$, where $w(i) = u_{(s,s')}(i+1), i \in \mathbb{N}_{0\to T-1}$. States $Lu_{(s,s')}(0)s$ and $Lu_{(s,s')}(0)s'$ are distinguished by $w(0 : T-1)$ at time $\tau_{(s,s')} - 1 \leqslant T$, hence $(Lu_{(s,s')}(0)s, Lu_{(s,s')}(0)s') \in \Omega_T$ and therefore $(s, s') \in \mathcal{Q}(\Omega_T)$. This proves $\Omega_{T+1} = \Omega_T \cup \mathcal{Q}(\Omega_T)$, and and in particular $\Omega_T \subseteq \Omega_{T+1}, \forall\, T \geqslant 0$.

Since the set Ω is a finite set and $\Omega_T \subseteq \Omega_{T+1}, \forall\, T \geqslant 0$, there will be a $T' \leqslant N(N-1)/2$ such that $\Omega_{T'} = \Omega_{T'+1}$. Then

$$\Omega_{T'+2} = \Omega_{T'+1} \cup \mathcal{Q}(\Omega_{T'+1}) = \Omega_{T'} \cup \mathcal{Q}(\Omega_{T'}) = \Omega_{T'+1},$$

by mathematical induction, it can be concluded that $\Omega_{T'+r} = \Omega_{T'}, \forall r \in \mathbb{N}_+$. Therefore there exists a minimal integer $T^* = T' \leqslant N(N-1)/2$ such that $\forall T \geqslant T^*$, $\Omega_T = \Omega_{T^*}$, which completes the proof.

Appendix B Algorithm of calculating structure based observability for $\mathcal{B}(L, H)$

Algorithm B1 structure-based observability for $\mathcal{B}(L, H)$

Input: Structure matrices pair (L, H), $N = 2^n$, $M = 2^m$.
Output: T^*, $\mathcal{O}_S(L, H)$.

$\Omega_0 \leftarrow \{(i, j) \mid 1 \leqslant i < j \leqslant N,\ H\delta_N^i \neq H\delta_N^j\}, \quad T \leftarrow 0.$ ▷ Initialize distinguishable pairs
loop
  $\Omega_{T+1} = \Omega_T \cup \mathcal{Q}(\Omega_T)$ ▷ Update pair set
  if $\Omega_T = \Omega_{T+1}$ **then**
    $T^* = T$; **break** ▷ Fixed point reached
  else
    $T \leftarrow T + 1$ ▷ Increase horizon
  end if
end loop
for $i = 1$ **to** N **do**
  $\widehat{\mathcal{X}}(\delta_N^i) \leftarrow \{\delta_N^i\} \cup \{\delta_N^j \neq \delta_N^i \mid (i, j) \notin \Omega_{T^*}\}.$ ▷ States indistinguishable from δ_N^i
  $err(\delta_N^i) \leftarrow \max_{\delta_N^j \in \widehat{\mathcal{X}}(\delta_N^i)} dist(\delta_N^i, \delta_N^j).$ ▷ Worst Hamming distance
end for
$\mathrm{Err}((L, H)) \leftarrow \dfrac{1}{n \cdot N} \sum_{i=1}^{N} err(\delta_N^i)$; $\mathcal{O}_S(L, H) = 1 - \mathrm{Err}((L, H)).$ ▷ Compute structure-based observability

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Remark 1. By Theorem 1, for any given pair $\mathcal{B}(L,H)$ the recursion $\Omega_{T+1}=\Omega_T\cup\mathcal{Q}(\Omega_T)$ stabilizes at a minimal horizon T^*, hence the maximal indistinguishable set Ω_{T^*} is obtained in finite time. Proposition 1 then recovers $\mathrm{Err}(L,H)$ from Ω_{T^*} and yields the structure based observability index $\mathcal{O}_S(L,H)$, so $\mathcal{O}_S(L,H)$ is computable in finite time for any $\mathcal{B}(L,H)$. In particular, let $N=2^n$ and $M=2^m$ denote the numbers of states and inputs. Algorithm 1 computes the error index $\mathrm{Err}(L,H)$ and the structure based observability $\mathcal{O}_S(L,H)$ from the structure matrix pair (L,H) with worst case time complexity $O(MN^2T^*)$, where T^* is the minimal horizon at which Ω_T stabilizes. The space complexity is dominated by the storage of indistinguishable pairs and the transition and is of order $O(N^2+MN)$. Thus, the computational complexity of the proposed method limits its applicability to large-scale networks, which remains an important direction for future research.

Appendix C Proof of Proposition 1

Proof. If $\delta_N^j\in\hat{\mathcal{X}}(\delta_N^i)$, $j\neq i$, then then no input sequence of any finite length can distinguish δ_N^i from δ_N^j. Therefore, $(\delta_N^i,\delta_N^j)\notin\Omega_T$, $\forall T\geqslant 0$. This can be deduced that $(\delta_N^i,\delta_N^j)\notin\Omega_{T^*}$, so $\hat{\mathcal{X}}(\delta_N^i)/\{\delta_N^i\}\subseteq\{\delta_N^j\neq\delta_N^i|(\delta_N^i,\delta_N^j)\notin\Omega_{T^*}\}$, that is, $\hat{\mathcal{X}}(\delta_N^i)\subseteq\{\delta_N^i\}\cup\{\delta_N^j\neq\delta_N^i|(\delta_N^i,\delta_N^j)\notin\Omega_{T^*}\}$

Conversely, if $(\delta_N^i,\delta_N^j)\notin\Omega_{T^*}$, $i\neq j$, by Theorem 1, $\Omega_T=\Omega_{T^*}$, $\forall T\geqslant T^*$. Thus $(\delta_N^i,\delta_N^j)\notin\Omega_T$ holds for every finite T, meaning that no finite input sequence distinguishes the two initial states. Hence $\delta_N^j\in\hat{\mathcal{X}}(\delta_N^i)$ and $\delta_N^i\in\hat{\mathcal{X}}(\delta_N^i)$. It can be concluded that $\{\delta_N^i\}\cup\{\delta_N^j\neq\delta_N^i|(\delta_N^i,\delta_N^j)\notin\Omega_{T^*}\}\subseteq\hat{\mathcal{X}}(\delta_N^i)$. Therefore, $\hat{\mathcal{X}}(\delta_N^i)=\{\delta_N^i\}\cup\{\delta_N^j\neq\delta_N^i|(\delta_N^i,\delta_N^j)\notin\Omega_{T^*}\}$, $\delta_N^i,\delta_N^j\in\Delta_N$ can be obtained by combining the two results, which completes the proof.

Appendix D Proof of Theorem 2

Proof. Let $\mathcal{O}_S(L,H)=1-\mathrm{Err}((L,H))$ denote the structure based observability of the structure matrix pair (L,H). For this dataset $\mathcal{D}$, let $\mathcal{M}(\mathcal{D})$ be the set of all models compatible with $\mathcal{D}$. According to Definition 6, data observability lower bound of $\mathcal{D}$ is defined as

$$\mathcal{O}_D^l(\mathcal{D})=1-\max_{(L,H)\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L,H)).$$

Suppose $\mathcal{B}(L,H)$ is ϵ-approximately observable. From Definition 4, the error rate of the $\mathcal{B}(L,H)$ satisfies $\mathrm{Err}((L,H))\leqslant\epsilon$. Therefore, a dataset $\mathcal{D}^*$ including all information of state transition of $\mathcal{B}(L,H)$ is selected, and the cardinality of dataset $\mathcal{D}^*$ is NM. Since data in the dataset has been deduplicated and each state–input pair can fix the corresponding column of L, all columns of L are fixed. With the structure matrix H known, the dataset $\mathcal{D}^*$ can identify the structure matrix pair (L,H) uniquely. Consequently,

$$\mathcal{O}_D^l(\mathcal{D}^*)=1-\mathrm{Err}((L,H))\geqslant 1-\epsilon.$$

Conversely, assume there exists a dataset $\mathcal{D}$ such that $\mathcal{O}_D^l(\mathcal{D})\geqslant 1-\epsilon$. By definition,

$$\max_{(L',H')\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L',H'))\leqslant\epsilon.$$

Since the true structure matrix pair (L,H) is compatible with the dataset $\mathcal{D}$, this is, $(L,H)\in\mathcal{M}(\mathcal{D})$, hence $\mathrm{Err}((L,H))\leqslant\epsilon$. Therefore $\mathcal{B}(L,H)$ is ϵ-approximately observable. As both implications hold, the equivalence is proved.

Remark 2. Recently, the reinforcement learning approach has been widely used in the analysis and control of `BNs`. Related methods have achieved progress in stabilization [1], controllability [2], and observability [2]. Building on the recent progress in data-driven control for nonlinear systems [3], the data-informativity paradigm has emerged as a powerful tool for providing a unified viewpoint on the control of `BNs`. For example, in [4], output stabilization of `BCNs` has been examined under conditions where complete knowledge of the internal dynamics is not required. In this paper, within the data informativity paradigm, data-driven observability is discussed, with necessary and sufficient criteria are established.

Appendix E Proof of Proposition 2

Proof. Classical observability is the special case of ϵ-approximate observability with $\epsilon=0$. Hence $B(L,H)$ is observable if and only if it is 0-approximate observable.

On the other hand, Theorem 2 states that for any $\epsilon\in[0,1]$ the `BCN` $B(L,H)$ is ϵ-approximate observable if and only if there exists a dataset D collected from this `BCN` such that

$$O_D^l(D)\geqslant 1-\epsilon.$$

Setting $\epsilon=0$ gives that $B(L,H)$ is observable if and only if there exists a dataset D such that $O_D^l(D)\geqslant 1$. By definition of $O_D^l(D)$, $O_D^l(D)=1-\max_{(L,H)\in M(D)}\mathrm{Err}((L,H))$. Since $0\leqslant\mathrm{Err}((L,H))\leqslant 1$ for any (L,H), we always have $O_D^l(D)\leqslant 1$ for any dataset D. Therefore the condition $O_D^l(D)\geqslant 1$ is equivalent to $O_D^l(D)=1$.

Thus $B(L,H)$ is observable if and only if there exists a dataset D collected from this `BCN` such that $O_D^l(D)=1$, which completes the proof.

Appendix F Proof of Proposition 3

Proof. By construction of $\mathcal{M}(\mathcal{D})$, the true structure matrix pair (L,H) of this BCN is compatible with its own data, hence $(L,H)\in\mathcal{M}(\mathcal{D})$. Therefore,

$$\max_{(L',H')\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L',H'))\geqslant\mathrm{Err}((L,H))\geqslant\min_{(L',H')\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L',H')).$$

By construction of $\mathcal{O}_S(L,H)$, $\mathcal{O}_D^l(\mathcal{D})$ and $\mathcal{O}_D^u(\mathcal{D})$, the stated inequality is obtained as follows:

$$1-\mathcal{O}_D^l(\mathcal{D})\geqslant 1-\mathcal{O}_S(L,H)\geqslant 1-\mathcal{O}_D^u(\mathcal{D}),$$

$$\mathcal{O}_D^l(\mathcal{D})\leqslant\mathcal{O}_S(L,H)\leqslant\mathcal{O}_D^u(\mathcal{D}).$$

If $\mathcal{O}_D^l(\mathcal{D})=\mathcal{O}_S(L,H)=\mathcal{O}_D^u(\mathcal{D})$, then it means

$$\max_{(L',H')\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L',H'))=\mathrm{Err}((L,H))=\min_{(L',H')\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L',H')).$$

Hence the error rate of all structure matrix pair (L,H) in $\mathcal{M}(\mathcal{D})$ is $\mathrm{Err}((L,H))$. On the contrary, if the error rate attains the same value for all models in $\mathcal{M}(\mathcal{D})$, then the error rate of all structure matrix pair (L,H) in $\mathcal{M}(\mathcal{D})$ is $\mathrm{Err}((L,H))$, this is, $\mathcal{O}_D^l(\mathcal{D})=\mathcal{O}_D^u(\mathcal{D})=\mathcal{O}_S(L,H)=1-\mathrm{Err}((L,H))$.

Appendix G Proof of Proposition 4

Proof. By Definition 1, the set $\mathcal{M}(\mathcal{D})$ collects all structure matrix pairs that satisfy every column constraint induced by $\mathcal{D}$. Since $\mathcal{D}_1\subseteq\mathcal{D}_2$, the constraint induced by $\mathcal{D}_2$ contains that of $\mathcal{D}_1$. It means that any structure matrix pair compatible with $\mathcal{D}_2$ is therefore compatible with $\mathcal{D}_1$, and hence $\mathcal{M}(\mathcal{D}_2)\subseteq\mathcal{M}(\mathcal{D}_1)$. Maximization over a smaller feasible set cannot increase the maximum, and minimization cannot decrease the minimum:

$$\max_{(L',H')\in\mathcal{M}(\mathcal{D}_2)}\mathrm{Err}((L',H'))\leqslant\max_{(L',H')\in\mathcal{M}(\mathcal{D}_1)}\mathrm{Err}((L',H')),$$

$$\min_{(L',H')\in\mathcal{M}(\mathcal{D}_2)}\mathrm{Err}((L',H'))\geqslant\min_{(L',H')\in\mathcal{M}(\mathcal{D}_1)}\mathrm{Err}((L',H')).$$

By definition $\mathcal{O}_D^u(\mathcal{D})=1-\min_{(L',H')\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L',H'))$ and $\mathcal{O}_D^l(\mathcal{D})=1-\max_{(L',H')\in\mathcal{M}(\mathcal{D})}\mathrm{Err}((L',H'))$. Combining the definitions with the above inequalities yields $\mathcal{O}_D^u(\mathcal{D}_1)\geqslant\mathcal{O}_D^u(\mathcal{D}_2)$ and $\mathcal{O}_D^l(\mathcal{D}_1)\leqslant\mathcal{O}_D^l(\mathcal{D}_2)$.

Appendix H Proof of Proposition 5

Proof. Picking a special structure matrix pair (L',H'), where $L'=\delta_{2^n}[1,1,1,...,1,1,1]\in\mathbb{L}_{2^n\times 2^{n+m}}$ and $H'=\delta_2[\underbrace{1,...,1}_{2^{n-1}},\underbrace{0,...,0}_{2^{n-1}}]\in\mathbb{L}_{2\times 2^n}$. Assume that only the transition data of $2^{n+m}-th$ column of L' are unknown, then the cardinality of the dataset $\mathcal{D}'$ is $NM-1$. Let $\tilde{L}'=\delta_{2^n}[1,1,1,...,1,1,2^n]\in\mathbb{L}_{2^n\times 2^{n+m}}$. By definition of $\mathcal{M}(\mathcal{D})$, both (L',H') and $(\tilde{L}',H')$ are compatible with the dataset $\mathcal{D}'$, this is, (L',H'), $(\tilde{L}',H')\in\mathcal{M}(\mathcal{D}')$. Because of the special nature of the structural matrix L', apart from the first node, which H distinguishes at the beginning, all subsequent outputs are identical. Therefore, the error rate of (L',H') is 1/2. Due to $H'\tilde{L}'\delta_{2^m}^{2^m}\delta_{2^n}^{2^n}=0\neq H'\tilde{L}'\delta_{2^m}^{2^m}\delta_{2^n}^{i}=1,\ i\in\mathbb{N}_{2^{n-1}+1\to 2^n-1}$, the error rate of $(\tilde{L}',H')$ will be less than the error rate of (L',H'). Moreover, owing to the definition of $\mathcal{O}_D^u(\mathcal{D})$,

$$\mathcal{O}_D^u(\mathcal{D}')=1-\min_{(L'',H'')\in\mathcal{M}(\mathcal{D}')}\mathrm{Err}((L'',H''))\geqslant 1-\mathrm{Err}((\tilde{L}',H'))>1/2=\mathcal{O}_S(L',H'),$$

and the equality $\mathcal{O}_D^l(\mathcal{D}')=\mathcal{O}_S(L,H)=\mathcal{O}_D^u(\mathcal{D}')$ cannot be certified with $|\mathcal{D}'|=NM-1$. Hence, in the worst case, the minimal dataset size required to ensure the equality is NM.

Conversely, if H can reveals the full state such as $y_i=x_i,\ i\in\mathbb{N}_{1\to n}$, then $\mathrm{Err}(L,H)=0$ for every L, so with $|\mathcal{D}|=0$ one has $\mathcal{O}_D^l(\mathcal{D})=\mathcal{O}_S(L,H)=\mathcal{O}_D^u(\mathcal{D})$.

Appendix I Simulation: p53-mdm2 Model

Consider a BCN model of the human tumor suppressor gene p53 pathways in [5], whose logical dynamics are given as:

$$\begin{cases} x_1(t+1)=\neg x_3(t)\wedge(x_1(t)\vee u(t)),\\ x_2(t+1)=\neg x_4(t)\wedge(x_1(t)\vee x_3(t)),\\ x_3(t+1)=x_2(t),\\ x_4(t+1)=\neg x_1(t)\wedge(x_2(t)\vee x_3(t)). \end{cases}\tag{I1}$$

Here, x_1, x_2, x_3 and x_4 denote ATM, P53, Wip1 and Mdm2, respectively. The control variable u denotes the external signal is dna_dsb, the DNA damage input. Additionally, the observer for this biological network is $y(t) = x_2(t)$. The structure matrices of BCN (I1) can be calculated as follows:

$$L = \delta_{16}[14, 10, 6, 2, 16, 12, 8, 4, 13, 9, 5, 5, 15, 11, 8, 8, 14, 10, 6, 2, 16, 12, 8, 4, 13, 9, 13, 13, 15, 11, 16, 16],$$

$$H = \delta_2[1, 1, 1, 1, 2, 2, 2, 2, 1, 1, 1, 1, 2, 2, 2, 2].$$

By Algorithm B1, the structure based observability of this $\mathcal{B}(L, H)$ is 0.797 and $T^* = 3$. Unlike the previous synthetic three nodes BCN, the structure based observability of this BCN (I1) $\mathcal{O}_S(L, H)$ is less than 1. Accordingly, eight datasets are provided to illustrate the convergence of the data observability bounds. For each $i \in \mathbb{N}_{1\to 8}$, the dataset $\mathcal{D}_i$ consists of transition data from δ_{16}^{2i-1} and δ_{16}^{2i} under input δ_2^1 and δ_2^2. For example, dataset $\mathcal{D}_3$ consists of transition data

$$\{\delta_{16}^5 \xrightarrow{\delta_2^1} \delta_{16}^{12}; \delta_{16}^5 \xrightarrow{\delta_2^2} \delta_{16}^{16}; \delta_{16}^6 \xrightarrow{\delta_2^1} \delta_{16}^{8}; \delta_{16}^6 \xrightarrow{\delta_2^2} \delta_{16}^{12}\}.$$

Let $\tilde{\mathcal{D}}_0 = \varnothing$ and $\tilde{\mathcal{D}}_j = \tilde{\mathcal{D}}_{j-1} \cup \mathcal{D}_j,\ j \in \mathbb{N}_{1\to 8}$. The data observability upper and lower bounds are computed separately for each of these datasets. Figure I1 shows how the data observability upper and lower bounds vary as the dataset size increases.

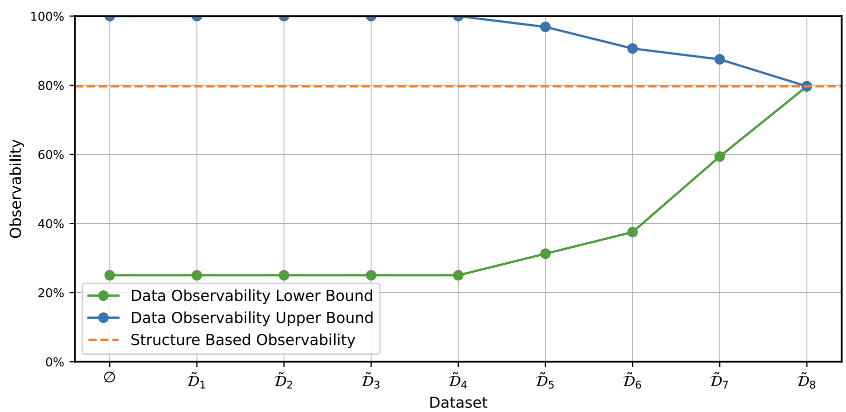

Figure I1 Data observability bounds as the dataset grows from the empty set to the full set

The figure shows a decrease in the observability upper bound and an increase in the observability lower bound as the dataset grows, thereby verifying Propositions 3 and 4. Since this case is a series of given datasets and cannot fully reflect the properties of limited data-driven, a random case is given next.

Appendix J Simulation: Randomly Generated BCNs

In this part, randomly generated BCNs with outputs are studied. The number of nodes n is prescribed, and the number of control inputs m is randomly selected from $\{1, 2\}$. For each node, the in-degree is uniformly selected from $\{2, 3, 4\}$. The number of observed nodes is set to $p = \lfloor n/2 \rfloor$. Due to structural properties of BNs, when $n > 3$, the number of transition samples is a multiple of 8. Therefore, for a Boolean control network with n nodes and m inputs, each round of data collection, $(2^{n+m}/8)$ data pairs are sampled. The code to randomly generate these BCNs and datasets is provided in our GitHub repository https://github.com/GG-ontorller/Random-BCN-with-output.

Figure J1 shows that, for each network size, the data observability lower bound increases monotonically with the data ratio and approaches the structure based observability. The shaded ellipses are minimum ellipses that summarize points that denote each experiment.

Figure J2(a) shows that, for each network size, the median tightness versus data ratio, with shaded bands indicating the confidence interval across trials, where tightness is $\mathcal{O}_D^u(\mathcal{D}) - \mathcal{O}_D^l(\mathcal{D})$ for a dataset $\mathcal{D}$. Figure J2(b) reports the mean gaps to the structure based observability for $n = 6$ and $n = 8$, showing Δ_{upper} and Δ_{lower} as functions of data ratio, where Δ_{upper} and Δ_{lower} denote $\mathcal{O}_D^u(\mathcal{D}) - \mathcal{O}_S(L, H)$ and $\mathcal{O}_S(L, H) - \mathcal{O}_D^l(\mathcal{D})$, respectively.

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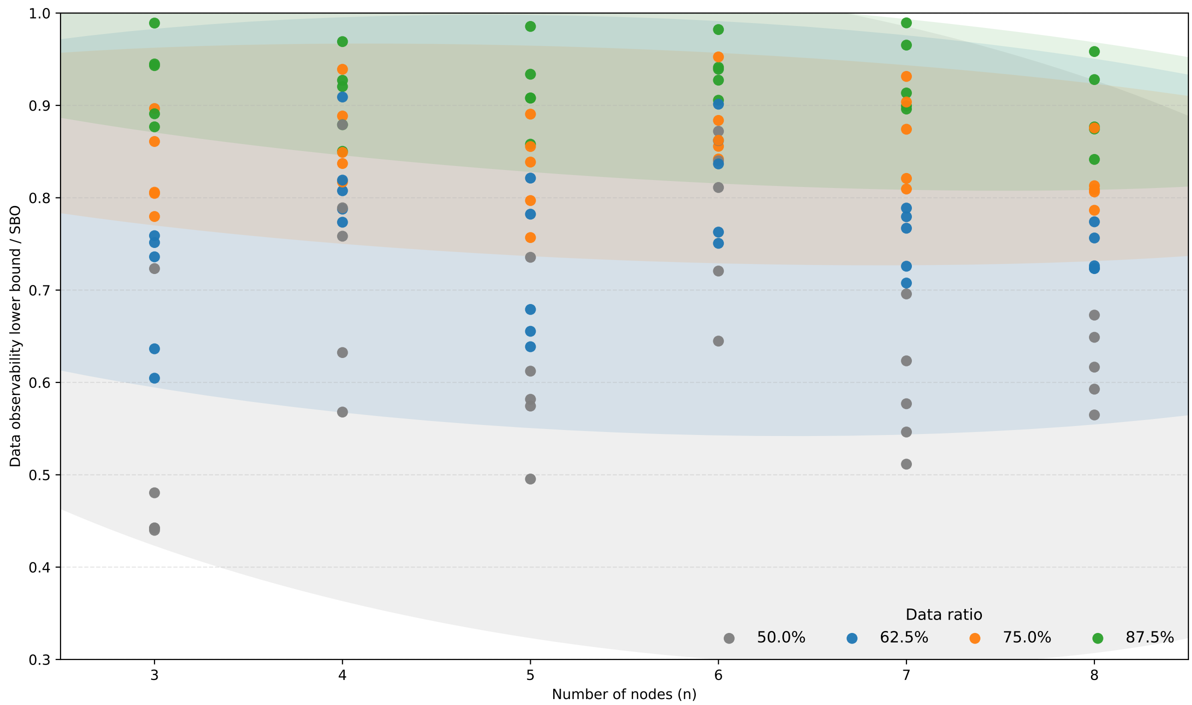
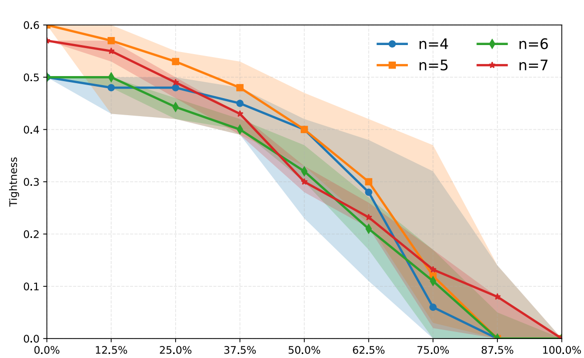
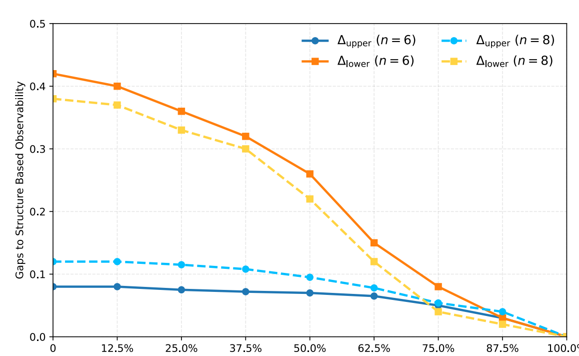


Figure J1 Comparison of the data observability lower bound distribution across network sizes and data ratios



(a) The variation of tightness with data ratio at different network sizes



(b) Gaps to structure based observability curves for $n = 6$ and $n = 8$ showing Δ_{upper} and Δ_{lower} as functions of data ratio

Figure J2 Effect of data ratio on observability metrics