Appendix: D-Struct

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A Additional experiments

Please find our (anonymous) online code repository at:

`https://anonymous.4open.science/r/d-struct`

Our code is based on code provided by Zheng et al. [36], and we annotated our code where we used their implementation.

A.1 Settings and details

In the interest of space, we left out a few details in our main text. Here we discuss hyperparameters (those in addition to the hyperparameters required for the selected DSFs), the evaluation metrics, and how we combine the different parallel DAGs.

Hyperparameters. D-Struct inherits hyperparameters from the chosen underlying DSFs. These hyperparameters act in the same way as they would in their original incarnation. For a discussion on these hyperparameters we refer to the relevant literature on these methods specifically.

However, D-Struct also adds two additional parameters: K and α. The impact of K is already discussed in the main text, recapitulated as: K implicitly determines the sizes of the subsets used to train the parallel DSFs, as such, *for high K we should have high n*. With both increasing, we report better performance (particularly in Scale-Free DAGs).

The impact of α is a bit more subtle, and also a function of K. First, consider Fig. 7, displaying the impact on each evaluation metric as a function of different α. What we find is that setting α is mostly

dependent on K as lower α tend to work better with higher K, and vice versa for lower K. This makes sense as we sum each $\mathcal{L}_{\text{MSE}}$, resulting in a higher value with more K. If α is large in a setting with large K, the regularisation effect would simply be too large. We set our hyperparameters to those which yielded best performance (deduced from Fig. 7 for α, and $K = 3$ when not varied over as this yielded most stable results overall).

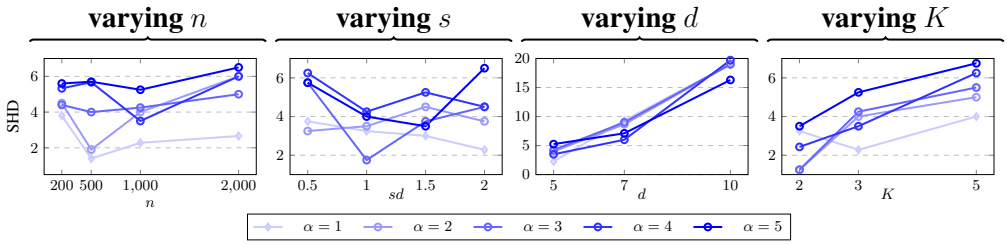


Figure 7: **Results showing the effect of α.** Depending on the nature of the problem the degree of regularization imposed by α can vary. This then changes the amount we enforce the similarity between the different D-Struct adjacency. matrices.

Evaluation metrics. The learned graphs from NOTEARS and D-Struct are assessed using four graph metrics namely: (1) Structural Hamming distance (SHD), (2) False discovery rate (FDR), (3) False positive rate (FPR) and (4) True positive rate (TPR). These values are standard when evaluating structure learning methods. We provide some insight into these evaluation metrics below.

Structural Hamming distance (SHD) SHD is the total number of edge additions, deletions, and reversals needed to convert the estimated DAG into the true DAG. That means that the worst case SHD is $d^2 - d$, as we bound the diagonal to be 0 at all times. As such, the reported SHD with varying d is expected to be higher, not due to hardness of the problem, but as a property of the SHD (see for example Fig. 6).

False discovery rate (FDR) Whenever an edge is suggested in the estimated DAG, which is incorrect, we add to the falsely discovered edges. As such, the FDR is defined as the number of reversed edges and edges that should not exist, divided by the number of edges in total. Of course, the exception being when no edges are suggested at all (which implies dividing by 0), which naturally has an FDR of zero.

False positive rate (FPR) We sum the edges that should have been reversed and those that should not exist, and divide by the total number of *non-edges* in the ground truth DAG. A non-edge is an edge that does not exist. With a more connected ground truth DAG, we expect this number to be lower automatically (as the numerator of the FPR would be higher). This is the reason why we let s be a function of d, as increasing the number of expected edges with d would somewhat counter this effect. Note that, in Table 1 we see the FPR increasing proportionate to the factor multiplied with d, which is as we would expect.

True positive rate (TPR) This signifies the number of correctly estimated edges, over the number of edges in the true graph. Note that, reversed edges are counted as wrong edges.

Combining graphs. Inference is done by combining the K internal graphs. In our implementation of D-Struct we combine graphs by averaging the adjacency matrices and apply a threshold to convert the average graph into a binary matrix. The latter is a similar strategy to most DSFs' strategies to convert a continuous matrix into a binary one. This is a relatively simple method with promising results, in line with what is currently done in literature.

However, given that D-Struct has multiple graphs, we can actually come up with different strategies (a potential topic for future research). Naturally, this would be more relevant with high K, which in turn requires a larger sample-size, as per our discussion above. Specifically, we enter the domain of ensemble learning. Like D-Struct, ensemble methods need to combine, potentially conflicting, outcomes and provide the user with only one outcome.

Table 3: **Results on Erdos-Renyì (ER) graphs.** *First block:* We sample five different ER random graphs, and accompanying non-linear structural equations using an index-model. From each system we then sample a varying number of samples, and evaluate NOTEARS-MLP *with* D-Struct (indicated as "✓") and *without* D-Struct (indicated as "✗"). *Second block:* For each row we sample a new ER graph with a varying degree of connectedness (s indicates the expected number of edges). In both cases, we report the average performance in terms of SHD, FPR, TPR, and FDR, with std in scriptsize.

metric	**SHD (↓)**		**FPR (↓)**		**TPR (↑)**		**FDR (↓)**	
D-Struct	✓	✗	✓	✗	✓	✗	✓	✗
n	*varying sample size*							
200	**3.60**±0.27	4.20±0.44	**2.00**±0.67	4.20±0.44	**0.67**±0.05	0.64±0.05	**0.25**±0.06	0.42±0.04
500	**3.20**±0.80	3.94±0.33	**1.20**±0.44	3.94±0.33	**0.66**±0.24	0.56±0.04	**0.18**±0.05	0.44±0.04
1000	**2.75**±0.47	3.67±0.82	**1.00**±0.37	2.67±0.63	**0.75**±0.08	0.63±0.13	**0.18**±0.03	0.39±0.11
s	*varying graph connectedness*							
$0.5d$	**3.75**±1.6	7.33±0.13	**0.50**±0.25	1.05±0.02	0.83±0.19	**0.88**±0.04	**0.42**±0.16	0.73±0.01
$1d$	**3.50**±0.86	7.67±0.45	**0.55**±0.22	1.53±0.09	**0.75**±0.09	0.46±0.09	**0.40**±0.09	0.77±0.07
$1.5d$	**3.00**±1.15	5.67±1.75	**1.00**±0.19	1.55±0.08	**0.89**±0.07	0.62±0.06	**0.32**±0.05	0.53±0.04
$2d$	**2.28**±0.80	3.67±0.82	**1.00**±0.32	2.67±0.63	0.67±0.17	**0.70**±0.09	**0.11**±0.03	0.32±0.08
d	*varying dimension count*							
5	**2.28**±0.80	3.67±0.82	**1.00**±0.32	2.67±0.63	0.67±0.17	**0.70**±0.09	**0.11**±0.03	0.32±0.08
7	**8.67**±0.56	12.88±0.15	**0.72**±0.05	1.07±0.01	**0.96**±0.02	0.83±0.01	**0.49**±0.01	0.63±0.01
10	**19.71**±0.72	30.82±0.98	**0.42**±0.13	1.18±0.04	0.70±0.16	**0.71**±0.06	**0.34**±0.08	0.70±0.02

One avenue is to not vote on a per-element basis, but on a per-graph basis. Imagine, two graphs in K that are exactly the same aspire more confidence in their accuracy. We could even relax similarity to an SHD across graphs, where we weight each graph's "vote" proportionally to their combined SHD. We believe this to be promising area of future research.

Experimental procedure. Here we explain how our experimental setup works, which steps we need to perform before starting an experiment, and which information each model is provided.

There are two main parts to an experimental setup: (i) we need a structure, (ii) we need a set of structural equations accompanying the structure of step (i).

(i) The structure. In our setup, a structure can only be a DAG. To reduce bias as much as possible, we do not determine structures up front, but sample random structures for each experimental run. Of course, the same random structure is presented for each benchmark. Sampling random structures happens in two ways: either we sample a random Erdös-Renyi graph, which requires a dimension count (d), and an expected number of edges (ds); or we use a scale-free graph which is generated using the process described in Barabási and Albert [69] as was also done in Zheng et al. [36], which needs a parameter $\beta = 1$ (the exponent for the preferential attachment process). The expected number of edges in our setup depends on d such that s resembles the ratio of edges versus non-edges in the random graph.

(ii) The equations. With a sampled structure from (i), we can now sample some structural equations. In our paper we use an index model to sample these. In short, an index model is randomly parameterised as: $f_j(X_{\text{pa}(j)}) = \sum_{m=1}^{3} h_m(\sum_{k\in\text{pa}(j)} \theta_{jmk} X_k)$, where $h_1 = \tanh$, $h_2 = \cos$, $h_3 = \sin$, and each θ_{jmk} is drawn uniformly from range $[-2, -0.5] \cup [0.5, 2]$. Exactly as was reported in Zheng et al. [36].

A.2 Completed results

Recall from Section 4 that we only reported a subset of the results. In Table 5 we report the remainder for NOTEARS-MLP and the D-Struct implementation on scale free graphs.

Table 4: **Results on Scale-Free (SF) graphs.** *First block:* We sample five different SF random graphs, and accompanying non-linear structural equations using an index-model. From each system we then sample a varying number of samples, and evaluate NOTEARS-SOB *with* D-Struct (indicated as "✓") and *without* D-Struct (indicated as "✗"). *Second block:* For each row we sample a new SF graph with a varying degree of connectedness (s indicates the expected number of edges). *Third block:* For each row we vary the feature dimension count (d). *Fourth block:* For each row we vary the number of subsets for D-Struct (s).In all cases, we report the average performance in terms of SHD, FPR, TPR, and FDR, with std in scriptsize.

metric	**SHD (↓)**		**FPR (↓)**		**TPR (↑)**		**FDR (↓)**	
D-Struct	✓	✗	✓	✗	✓	✗	✓	✗
n	*varying sample size*							
200	6.00±0.69	3.8±0.25	1.8±0.20	1.27±0.08	0.49±0.12	0.83±0.03	0.63±0.08	0.39±0.02
500	**3.40**±0.88	4.60±0.25	**0.67**±0.14	1.53±0.08	0.57±0.09	0.69±0.03	**0.41**±0.12	0.48±0.03
1000	**2.75**±0.86	4.33±0.50	**0.58**±0.22	1.44±0.17	0.61±0.15	0.76±0.05	**0.36**±0.15	0.44±0.05
s	*varying graph connectedness*							
$0.5d$	**14.11**±5.40	39.53±0.37	**0.31**±0.13	0.89±0.01	**0.22**±0.14	0.20±0.11	**0.42**±0.17	0.93±0.01
$1d$	**8.11**±3.96	39.46±0.38	**0.13**±0.09	0.89±0.01	**0.30**±0.18	0.16±0.09	**0.22**±0.15	0.99±0.01
$1.5d$	**15.20**±3.44	38.31±0.41	**0.32**±0.14	1.05±0.01	**0.58**±0.23	0.52±0.07	**0.40**±0.17	0.98±0.01
$2d$	**15.20**±3.44	38.25±0.44	**0.32**±0.14	1.04±0.01	**0.58**±0.23	0.50±0.07	**0.40**±0.17	0.89±0.01
d	*varying dimension count*							
5	**2.75**±0.86	4.33±0.50	**0.58**±0.22	1.44±0.17	0.61±0.15	0.76±0.05	**0.36**±0.15	0.44±0.05
7	**8.25**±3.09	15.00±0.22	**0.55**±0.21	1.00±0.01	**0.96**±0.08	0.78±0.02	**0.49**±0.16	0.76±0.01
10	**16.80**±4.21	35.75±0.33	**0.36**±0.17	0.99±0.01	0.58±0.24	0.67±0.03	**0.42**±0.17	0.85±0.01
K	*varying subset count*							
2	**3.00**±0.42	6.00±0.30	**0.53**±0.21	2.00±0.10	**0.66**±0.04	0.57±0.04	**0.21**±0.07	0.60±0.03
3	**2.75**±0.86	4.33±0.5	**0.58**±0.22	1.44±0.17	0.61±0.15	0.76±0.05	**0.36**±0.15	0.44±0.05
5	**2.80**±0.57	5.25±0.21	**0.73**±0.15	1.75±0.07	**0.74**±0.09	0.68±0.03	**0.31**±0.07	0.53±0.02

A.3 Other DSFs

We repeat the results above for NOTEARS-SOB which is a Sobolev based implementation of NOTEARS, in Table 4. The main difference here with NOTEARS-MLP is the nonparametric estimation of the structural equations in $\hat{\mathcal{G}}$. Note that, future implementations of DSFs broadly alter the way in which the structural equations are estimated, and much less on how the proposed structure is evaluated to be a DAG (as they are mostly based on eq. (3)). Overall, we find that NOTEARS-SOB behaves the same as NOTEARS-MLP: D-Struct vastly improves performance.

Note that code to reproduce above results is provided in the online code repository linked to above.

A.4 Subsampling datasets

We refer to Table 6 for the full results presented originally in Table 2. While FPR may be a little higher, using D-Struct still outperforms not using D-Struct in terms of the FPR– already shown in Table 1. Furthermore, as the subsampling routine forces D-Struct to learn on different distributions, it is possible that this increase in FPR is a result of initially more conflicting DAG structures. When combined, these structures include more edges which in turn result in more potential for a false positive edge discovery. In fact, we observe a lower necessary threshold when using our subsampling routine, necessary to transform the real-values matrix into a binary adjacency matrix.

We also report the same metrics as a function of the DAG-finding threshold in Fig. 8, where the threshold is applied to the adjacency matrix to produce a binary matrix on which we compute the metrics. Of course, a threshold will be selected in practice; however, we show that for a range of plausible threshold values and all metrics that subsampling with our routine is indeed beneficial, compared to randomized subsampling. From this, it seems that the results we find in Table 6 are consistent even with changing thresholds.

Table 5: **Results on Scale-Free (SF) graphs.** *First block:* We sample five different SF random graphs, and accompanying non-linear structural equations using an index-model. From each system we then sample a varying number of samples, and evaluate `NOTEARS-MLP` *with* D-Struct (indicated as "✓") and *without* D-Struct (indicated as "✗"). *Second block:* For each row we sample a new SF graph with a varying degree of connectedness (s indicates the expected number of edges). *Third block:* For each row we vary the feature dimension count (d). *Fourth block:* For each row we vary the number of subsets for D-Struct (s).In all cases, we report the average performance in terms of SHD, FPR, TPR, and FDR, with std in scriptsize.

metric	**SHD (↓)**		**FPR (↓)**		**TPR (↑)**		**FDR (↓)**	
D-Struct	✓	✗	✓	✗	✓	✗	✓	✗
n	*varying sample size*							
200	**2.80**±0.86	6.20±0.57	**0.73**±0.28	2.07±0.19	**0.80**±0.11	0.54±0.08	**0.26**±0.11	0.62±0.06
500	**2.20**±0.80	7.20±0.66	**0.27**±0.12	2.20±0.18	**0.77**±0.13	0.37±0.09	**0.14**±0.06	0.72±0.06
1000	**3.25**±1.49	5.33±0.61	**0.75**±0.43	1.78±0.20	**0.68**±0.15	0.66±0.08	**0.29**±0.18	0.53±0.06
s	*varying graph connectedness*							
$0.5d$	**3.33**±0.88	8.00±0.37	**0.50**±0.19	1.17±0.06	**0.92**±0.08	0.38±0.05	**0.41**±0.08	0.82±0.03
$1d$	**3.33**±0.89	8.00±1.00	**0.50**±0.19	1.17±0.17	**0.92**±0.08	0.38±0.13	**0.41**±0.08	0.82±0.07
$1.5d$	**3.25**±0.41	7.67±0.31	**0.50**±0.07	1.17±0.04	**0.94**±0.04	0.42±0.06	**0.43**±0.03	0.80±0.03
$2d$	**2.75**±1.03	5.00±1.00	**0.33**±0.23	1.22±0.22	**0.64**±0.15	0.50±0.07	**0.14**±0.09	0.48±0.12
d	*varying dimension count*							
5	**3.25**±1.49	5.33±0.61	**0.75**±0.43	1.78±0.20	**0.68**±0.15	0.66±0.08	**0.29**±0.18	0.53±0.06
7	**8.22**±1.31	15.67±0.14	**0.54**±0.09	1.04±0.01	**0.98**±0.02	0.83±0.03	**0.54**±0.04	0.76±0.01
10	**16.80**±4.21	35.75±0.33	**0.36**±0.17	0.99±0.01	0.58±0.24	0.67±0.03	**0.42**±0.17	0.85±0.01
K	*varying subset count*							
2	**2.40**±0.24	6.50±0.46	**0.53**±0.08	2.16±0.15	**0.83**±0.05	0.50±0.06	**0.21**±0.03	0.65±0.06
3	**2.00**±1.04	5.33±0.6	**0.33**±0.47	1.78±0.20	**0.68**±0.14	0.66±0.09	**0.14**±0.09	0.53±0.06
5	**0.75**±0.48	5.25±0.21	**0.25**±0.16	2.55±0.11	**1.00**±0.00	0.33±0.05	**0.09**±0.05	0.76±0.03

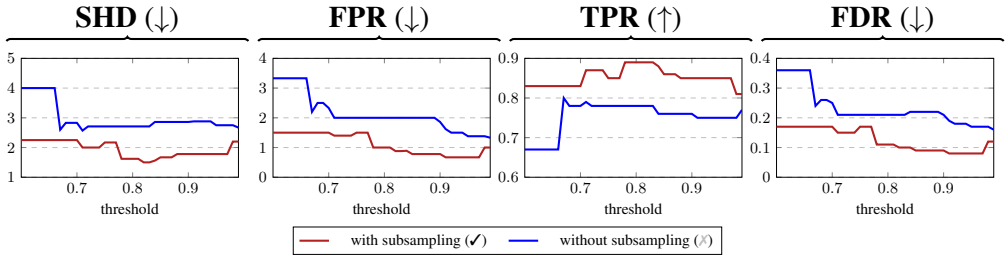


Figure 8: **Subsampling with different DAG-thresholds.** The DAG-threshold transforms the real-valued adjacency matrix, to a binary one. As the threshold increases, the amount edges that remain part of the DAG decreases. The above confirms our findings from Table 6 in different settings.

A.5 DAGs: D-Struct vs NOTEARS

We wish to also highlight that indeed what is recovered by D-Struct is different from NOTEARS. For this we refer to Figs. 9 and 10, each representing an independent run.

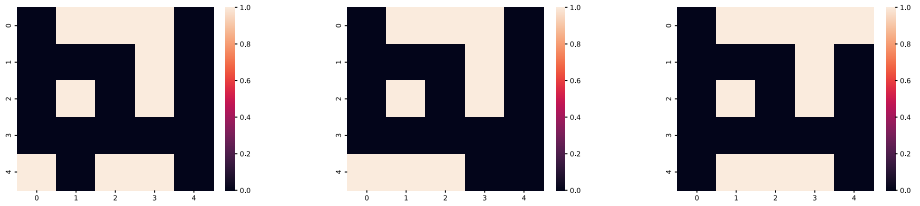
A.6 Gains from enforcing transportability

A key concept of D-Struct is to enforce transportability, which is done using our novel loss function.

$$\mathcal{L}(\mathcal{G}_k|\mathcal{D}_k) := \mathcal{L}_{\text{DSF}}(\mathcal{G}|\mathcal{D}_k) + \alpha\mathcal{L}_{\text{MSE}}(A(\mathcal{G}_k)),$$

Table 6: **Usefulness of our subsampling routine.** We sample ten different ER random graphs, and accompanying non-linear structural equations as in Zheng et al. [36]. From each system we then sample $n = 2000$ samples, and evaluate `NOTEARS-MLP` *with* our subsampling routine from Section 3.2 (indicated as "✓") and *without* the subsampling routine, using random splits instead (indicated as "✗"). For each row we repeat our experiment with different K. In both cases, we report the average performance in terms of SHD, FPR, TPR, and FDR, with std in scriptsize.

metric	**SHD (↓)**		**FPR (↓)**		**TPR (↑)**		**FDR (↓)**	
Subsample	✓	✗	✓	✗	✓	✗	✓	✗
K	*varying amount of splits*							
2	**2.80**±0.53	3.40±0.58	2.80±0.53	**2.60**±0.33	**0.80**±0.06	0.71±0.07	**0.28**±0.05	0.30±0.16
3	**3.00**±0.37	4.00±0.59	2.00±0.51	**1.60**±0.45	**0.73**±0.04	0.58±0.06	**0.22**±0.05	0.24±0.17
5	**2.80**±0.57	4.40±1.29	1.40±0.50	**0.60**±0.26	**0.71**±0.06	0.53±0.15	0.18±0.06	**0.07**±0.10

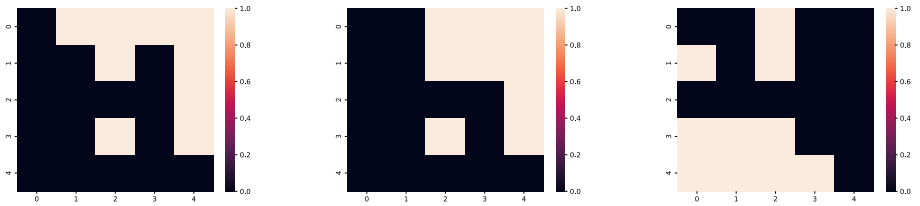


(a) True DAG.

(b) D-Struct estimated DAG. SHD=2, FDR=0.11, FPR=1.

(c) NOTEARS estimated DAG. SHD=2, FDR=0.2, FPR=2.

Figure 9: First independent run



(a) True DAG.

(b) D-Struct estimated DAG. SHD=2, FDR=0.11, FPR=1.

(c) NOTEARS estimated DAG. SHD=2, FDR=0.2, FPR=2.

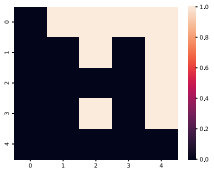
Figure 10: Second independent run

The question is what do we gain from the usage of the α term which is key to enforcing transportability. We conduct an experiment where we set $\alpha = 0$. This not only assesses the importance of this term, but also without $\mathcal{L}_{\text{MSE}}$ this amounts to assessing K *independent* versions of vanilla NOTEARS.

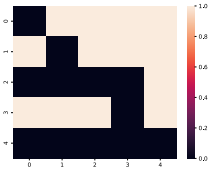
Results: When we combine the K DAGs by averaging them, the result is NOT a DAG.

This highlights that indeed that (1) transportability is key as part of this formulation and (2) that simply running parallel versions of NOTEARS is not a sufficient solution.

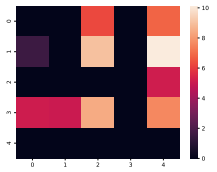
We highlight this by showing the independent DAGs discovered without transportability enforced, the average of the DAGs and the true DAG. These results are reported in Figs. 11 and 12



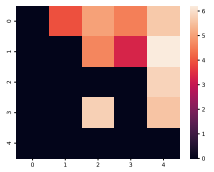
(a) True DAG.



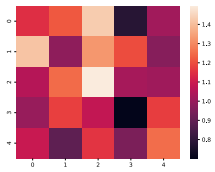
(b) **NOTEARS**: Mean. This is not a DAG!



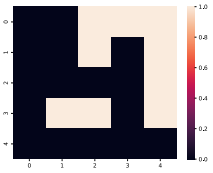
(c) **NOTEARS**: 1st DAG.



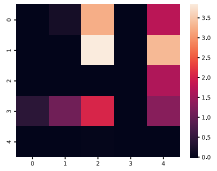
(d) **NOTEARS**: 2nd DAG.



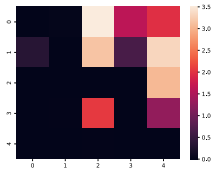
(e) **NOTEARS**: 3rd DAG.



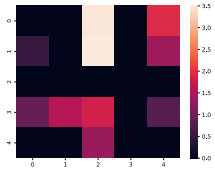
(f) **D-Struct**: Mean. This **is** a DAG!



(g) **D-Struct**: 1st DAG.



(h) **D-Struct**: 2nd DAG.



(i) **D-Struct**: 3rd DAG.

Figure 11: **First independent run.** Note the differences between the three DAGS on each partition for NOTEARS (Row 1), the average is also not a DAG. Whereas, for D-Struct note the similarities by enforcing transportability, the average is also a DAG.

B CAUSAL INTERPRETATION AND UNIQUENESS

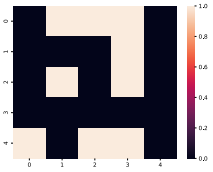
Causality. Causal relationships between variables are often expressed as DAGs [28]. While D-Struct is able to recover DAGs more reliably, there is actually no guarantee that the found DAG can be interpreted as a causal DAG. There is a simple reason for this: we do not make any additional identification assumptions on the structural equations when learning DAGs, at least not beyond what is already assumed in the used DSFs. Furthermore, should D-Struct be combined with a DSF that *is* able to recover a causal DAG[4], the way in which the K internal DAGs are combined may violate these assumptions (recall DAG combination from Appendix A.1).

With D-Struct, we recover a Bayesian network (BN), which is directed, yet the included directions are not necessarily meaningful. The only guarantee we have with BNs is that they resemble a distribution, which express some conditional distributions (as per the independence sets in Section 2.1). Order is not accounted for in these independence sets. For more information regarding this, we refer to Appendix D and Koller and Friedman [26].

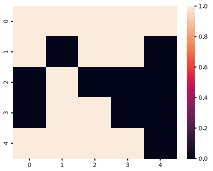
However, as is indicated in Koller and Friedman [26, Chapter 21], a "good" BN structure should correspond to causality, where edges $X \to Y$ indicated that X causes Y. Koller and Friedman [26] state that BNs with a causal structure tend to be sparser. Though, if queries remain probabilistic, it doesn't matter whether or not the structure is causal, the answers will remain the same. Only when we are interested in interventional queries (by using do-calculus) we have to make sure the DAG is a causal one.

Uniqueness. The above is a pragmatic view. To our knowledge, there is no real proof stating that sparser DAGs are (even more likely to be) causal. However, it could offer guidance to try and recover a causal DAG, assuming it to be sparse [72]. The latter of course is assuming that there exists a *unique* or *correct* DAG, which is something we implicitly assume to be true. Naturally, when

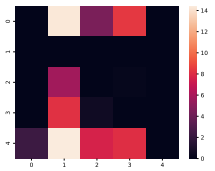
[4]We know of none that is able to.



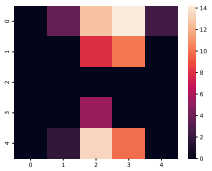
(a) True DAG.



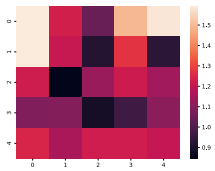
(b) **NOTEARS**: Mean. This is not a DAG!



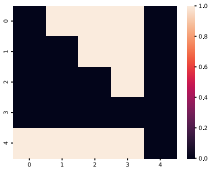
(c) **NOTEARS**: 1st DAG.



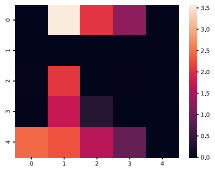
(d) **NOTEARS**: 2nd DAG.



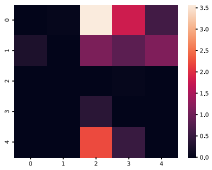
(e) **NOTEARS**: 3rd DAG.



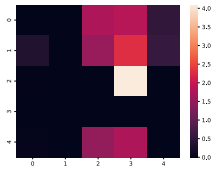
(f) **D-Struct**: Mean. This **is** a DAG!



(g) **D-Struct**: 1st DAG.



(h) **D-Struct**: 2nd DAG.



(i) **D-Struct**: 3rd DAG.

Figure 12: **Second independent run.** Note the differences between the three DAGS on each partition for NOTEARS (Row 1), the average is also not a DAG. Whereas, for D-Struct note the similarities by enforcing transportability, the average is also a DAG.

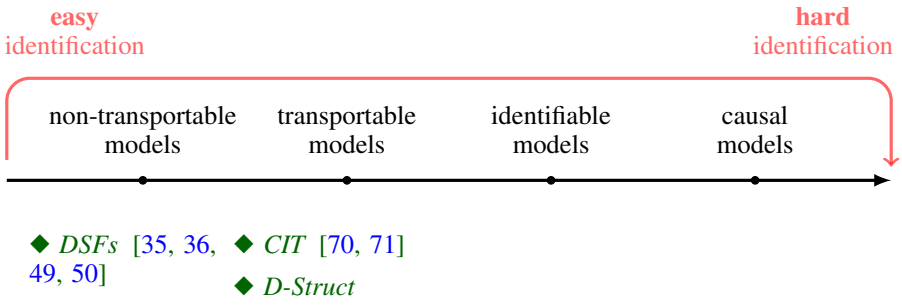


Figure 13: **Comparison of methods w.r.t. identification and uniqueness.** The ultimate goal of structure learning is to come up with unique and correct structures. Once we recover the one true DAG, we may interpret the structure as a causal model. However, discovering a causal structure using only observational data is not possible. Yet, we can *approach* it with methods that restrict the set of possible DAGs. From this illustration, we gather that D-Struct is an attempt to restrict the solution space of DSFs, going one step further towards unique solutions.

aiming to make a discovery, we aim to recover a *true* DAG, where a truthful DAG is corresponding with a DAG that can be uniquely recovered.

However, there is a difference between *a* unique DAG, and *the* unique DAG. Where the former is a matter of identifiability (discussed more below), the latter is one of causality. With the latter we mean: "can a method actually recover the unique causal DAG?" From Meek [37] and Meek [37] we learn that, from observational data alone, this is impossible and should thus not be a goal if one is not willing to make additional assumptions.

We stress that transportability is a weaker goal than identifiability. Enforcing transportability does not guarantee unique or repeatable results. Take CIT-based methods— which we know to be fully transportable. While it is true that the same set of independence statements will always result in the same DAG (i.e. transportability), it is not necessarily true that we will always recover the same independence statements. Depending on which independence test one uses to build the set of independence statements, the resulting DAG may look entirely different. Similar for D-Struct, while D-Struct does encourage similar DAGs (see for example Appendix A), we have no guarantee to recover the *same* DAG over different runs. The latter is a requirement for identifiability [73] as identifiability requires the model to always converge to the same set of parameters.

However, we do believe transportability is a vehicle to bring us closer to unique identification with DSFs. It is clear from our experiments that transportable learners greatly improve edge accuracy. As our synthetic setup is governed by one (and thus unique) graph, having a more accurate learner means a learner that discovers a DAG that is more like the unique, underlying graphical model. Consider Fig. 13 for an illustration comparing the relevant methods in terms of model identification.

C TRANSPORTABILITY IN NON-OVERLAPPING DOMAINS

Consider the multi-origin setting, where we have at least two datasets, each stemming from a different source. It is entirely possible that, given the different sources, these datasets are not comparable in terms of recorded features. We can recognise two major manifestations of this phenomenon: either (i) the supports of the datasets do not match, or (ii) the dimensions do not match.

(i) Different support. Recall from Section 2.1 that DAGs encode a set of independence statements. As such, it is mainly independence that governs structure. Transportability in the setting of conflicting support, thus requires some (mild) assumptions. Specifically, we require that independence holds, regardless of support. The is mostly a pragmatic assumption. If for example, we find that $\mathcal{X}_i \perp\!\!\!\perp \mathcal{X}_j$, where each component denotes a dimension in $\mathcal{X}$, we usually don't specify over what support this independence holds. Implicitly, we assume that independence holds, regardless of what area in $\{\mathcal{X}_i, \mathcal{X}_j\}$ we find ourselves in.

Note that the chosen distributions in $\mathcal{P}$ in Section 3.2 govern the entire domain $[N]$, and as a consequence $\mathcal{X}$. As such, the problem of conflicting support does not manifest in our solution of single-origin D-Struct. In case one chooses distributions that do not cover $[N]$ equally, we have to assume independence is constant across different supports (i.e. the assumption explained above).

(ii) Different dimensions. A more difficult setting of conflicting domains, is when we record different variables in each of the multi-origin datasets. In order for a DAG to be transportable, we *require* the variable sets to correspond. As such, we are only able to work with overlapping intersections of the non-overlapping domains. Doing so requires some additional assumptions on the noise: assuming we record some noise on each variable, we have to make the additional assumption that the noise is independent of the other variables, or at least the variables outside the intersection between domains. The latter is made quite often, and should not limit applicability of D-Struct in this setting too much (recall that applicability of D-Struct is mostly determined by the used DSF). The reason relates to the second assumption, below.

The second assumption is a bit stricter: any variables outside the intersection cannot be confounding variables inside the intersection. If two variables have no direct edges, and the nodes part of an indirect edge fall outside the domain-intersection, we have to expect the DSF to find an edge between these two nodes. While this direct edge is wrong, this is actually expected behaviour of most DSFs as the algorithms will find these variables to be correlated (due to the third, now unobserved, vari-

able). The only way to overcome these situations, is to use DSFs that naturally handle unobserved confounding.

D DEFINITIONS

Definition 2 (Markov blanket.)**.** *A Markov blanket of a random variable X_i in a random set $\mathcal{X} \coloneqq \{X_1, \ldots, X_d\}$ is any subset $\mathcal{X}' \subset \mathcal{X}$ where, when conditioned upon, results in independence between $\mathcal{X} \setminus \mathcal{X}'$ (the other variables) and X_i,*

$$X_i \perp\!\!\!\perp \mathcal{X} \setminus \mathcal{X}' | \mathcal{X}'. \tag{6}$$

We will denote the Markov blanket of X_i as $\mathcal{X}'(X_i)$.

In principle, Def. 2 means that $\mathcal{X}'$ contains all the information present in $\mathcal{X}$ to infer X_1. Note that this does not mean that $\mathcal{X} \setminus \mathcal{X}'$ contains *no* information to infer X_1, but variables in $\mathcal{X}'$ are sufficient to predict X_1.

One step further, is a *Markov boundary* [51]:

Definition 3 (Markov boundary.)**.** *A Markov boundary of a random variable X_i of a random set $\mathcal{X} \coloneqq \{X_1, \ldots, X_d\}$ is any subset $\mathcal{X}^- \subset \mathcal{X}$ which is a Markov blanket (Def. 2) itself, but does not contain any proper subset which itself is a Markov blanket. We will denote the Markov boundary of X_i as $\mathcal{X}^-(X_i)$.*

We can relate the Markov boundary (Def. 3) to probabilistic graphical modelling, as from a simplified factorisation (in eq. (1)), we can compose a Bayesian network. Specifically, each variable $X_j \in \mathcal{X}^-(X_i)$ depict one of three types of relationships: X_j is a parent of X_i, denoted as $\text{Pa}(X_i) = X_j$; X_j is a child of X_i, denoted as $\text{Ch}(X_i) = X_j$; or X_j is a parent of a child of X_i, denoted as $\text{Pa}(\text{Ch}(X_i)) = X_j$. Assuming that $\mathbb{P}_{\mathcal{X}}$ is governed by a Markov random field (rather than a Bayesian network) simplifies things, as the Markov boundary depicts only directly connected variables.

While the above may suggest that the Markov boundary only implies a vague graphical structure, doing this for ever variable in $\mathcal{X}$ will strongly constraint the possible graphical structures respecting any found independence statements. D-separation (Def. 4) is then used to further limit the set of potential DAGs [28, 34]. Relating above definitions to those discussed in Section 2.1. For more information regarding the above, we refer to Koller and Friedman [26].

Definition 4 (d-separation [34].)**.** *In a DAG $\mathcal{G}$, a path between nodes $\mathcal{X}_i$ and $\mathcal{X}_j$ is blocked by a set $\mathcal{X}_d \subset \mathcal{X}$ (which excludes $\mathcal{X}_i$ and $\mathcal{X}_j$) whenever there is a node $\mathcal{X}_k$, such that one of two holds:*

(1) $\mathcal{X}_k \in \mathcal{X}_d$ and

$$\begin{aligned} & \mathcal{X}_{k-1} \leftarrow \mathcal{X}_k \leftarrow \mathcal{X}_{k+1}, \\ \textit{or} \quad & \mathcal{X}_{k-1} \rightarrow \mathcal{X}_k \rightarrow \mathcal{X}_{k+1}, \\ \textit{or} \quad & \mathcal{X}_{k-1} \leftarrow \mathcal{X}_k \rightarrow \mathcal{X}_{k+1}. \end{aligned}$$

(2) neither $\mathcal{X}_k$ nor any of its descendants is in $\mathcal{X}_d$ and

$$\mathcal{X}_{k-1} \rightarrow \mathcal{X}_k \leftarrow \mathcal{X}_{k+1}.$$

Furthermore, in a DAG $\mathcal{G}$, we say that two disjoint subsets $\mathcal{A}$ and $\mathcal{B}$ are d-seperated by a third (also disjoint) subset $\mathcal{X}_d$ if every path between nodes in $\mathcal{A}$ and $\mathcal{B}$ is blocked by $\mathcal{X}_d$. We then write

$$\mathcal{A} \perp\!\!\!\perp_{\mathcal{G}} \mathcal{B} | \mathcal{X}_d.$$

When $\mathcal{X}_d$ d-seperates $\mathcal{A}$ and $\mathcal{B}$ in $\mathcal{G}$, we will denote this as d-sep$_{\mathcal{G}}(\mathcal{A}; \mathcal{B} | \mathcal{X}_d)$.

Definition 5 (Faithfulness from Peters et al. [34].)**.** *Consider a distribution $\mathbb{P}_{\mathcal{X}}$ and a DAG $\mathcal{G}$*

(i) $\mathbb{P}_{\mathcal{X}}$ is faithful to $\mathcal{G}$ if

$$\mathcal{A} \perp\!\!\!\perp \mathcal{B} | \mathcal{C} \Rightarrow \mathcal{A} \perp\!\!\!\perp_{\mathcal{G}} \mathcal{B} | \mathcal{C},$$

for all disjoint sets $\mathcal{A}, \mathcal{B}$ and $\mathcal{C}$.

(ii) a distribution satisfies causal minimality with respect to $\mathcal{G}$ if it is Markovian with respect to $\mathcal{G}$, but not to any proper subgraph of $\mathcal{G}$.

Part (i) posits an implication that is the opposite of the global Markov condition

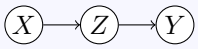
$$\mathcal{A} \perp\!\!\!\perp_{\mathcal{G}} \mathcal{B}|\mathcal{C} \Rightarrow \mathcal{A} \perp\!\!\!\perp \mathcal{B}|\mathcal{C},$$

for which we refer to Peters et al. [34, Def. 6.21].

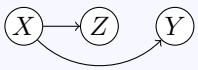
Part (ii) is actually implied when part (i) is satisfied, when $\mathbb{P}_{\mathcal{X}}$ is Markovian w.r.t. $\mathcal{G}$, as per Peters et al. [34, prop. 6.35]. To have an idea for when faithfulness is not satisfied, we refer to Zhang and Spirtes [74] and Spirtes et al. [70, Theorem 3.2].

E INCORPORATING PRIOR KNOWLEDGE ON $\mathcal{I}(\mathbb{P})$ USING L-BFGS-B

Consider the following, where we wish to discover a structure between 3 variables: X, Y, Z, where the ground truth satisfies $X \perp\!\!\!\perp Y|Z$. According to the rules of d-speration (cfr. Def. 4), we are always in a structure where X and Y are *only* directly connected to Z, i.e. no direct connection between X and Y exists. Let us further assume that the system is linear (as this is what vanilla NOTEARS assumes, but without loss of generality towards recent NOTEARS extensions), then we have the following,

structural equations	**structure**	**adjacency matrix**
$X \coloneqq \epsilon_X,$ $Z \coloneqq \beta_{Z,X}X + \epsilon_Z,$ $Y \coloneqq \beta_{Y,Z}Z + \epsilon_Y,$		$A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$

Naturally, using only conditional independence, the direction of the arrows are not identifiable as explained above. However, NOTEARS is unable to narrow it down to the equivalence classes expressed in Def. 4. The reason is simple, NOTEARS' three optimisation components (the h-measure, an L_2 loss, and an L_1 regularizer on A, [72]) are satisfied exactly the same with the following system:

structural equations	**structure**	**adjacency matrix**
$X \coloneqq \epsilon_X,$ $Z \coloneqq \beta_{Z,X}X + \epsilon_Z,$ $Y \coloneqq \beta_{Y,X}X + \epsilon'_Y,$		$A' = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$

where $\beta_{Y,X} = \beta_{Y,Z}\beta_{Z,X}$, and $\epsilon'_Y = \beta_{Y,Z}\epsilon_Z + \epsilon_Y$ resulting in Y being determined again by a simple linear equation. Both systems allow the same data to be generated, however under the constraint that $X \perp\!\!\!\perp Y|Z$ only the former is possible.

We argue that NOTEARS (and extensions) are unable to differentiate between them. Consider the components optimised by NOTEARS: both solutions propose a DAG (i.e. $h(A) = h(A') = 0$); each DAG has an equal amount of arrows, leading to the same L_1-loss across A and A'; and each equation is linear so NOTEARS is able to perfectly converge to each solution using its L_2 loss. Given that each component scores exactly the same, NOTEARS is unable to differentiate between these two results. Crucially however, in the latter system X is *always* dependent of Y, resulting in $X \not\perp\!\!\!\perp Y|Z$ (and even $X \not\perp\!\!\!\perp Y$ eliminating v-structures) which is completely opposite to the former system.

Prior Markov independencies. We can however force known independence statements into DSFs a priori, using the L-BFGS-B optimizer. For example, consider the following $I = X_i \perp\!\!\!\perp X_j|Z$. If I is known a priori, then we also know there cannot (under any circumstance) exist a direct link between X_i and X_j as this would immediately contradict I which in turn would invalidate a structure proposing such a link.

As such, we propose to fix these directed edges to $0 \rightarrow \mathcal{A}_{ij}(\mathcal{G}), \mathcal{A}_{ji}(\mathcal{G})$, and exclude them from gradient calculation. This will not only constraint each DSL in step 2 above resulting in easier convergence, but it will also enforce any known $\mathcal{I}(\mathbb{P}_{\mathcal{X}})$ to be taken into account. Setting $A_{X,Y} = A_{Y,X} = 0$ would immediately restrict NOTEARS from converging to this false solution as the

solution would require $A_{X,Y}$ to be 1. The same approach is currently used in NOTEARS (and consequentially D-Structs parallel DSFs), by setting bounds of each diagonal element in A to $(0, 0)$.

Setting some elements to 0 using the L-BFGS-B bounds, we effectively limit the set of possible solutions. In fact, when applied to the above problems, the second solution would sit *outside* the set of possible solutions, ensuring that NOTEARS cannot converge to it.

F ADDITIONAL DETAILS ON SUBSAMPLING FROM DIFFERENT DISTRIBUTIONS

In Section 3.2 we introduced a method to sample subsets from a single-origin dataset such that the subsets correspond to distinct user-defined distributions. To provide some additional detail, we shall first discuss the general case, and then move on to discuss how we implemented this in D-Struct.

F.1 THE GENERAL WAY

A high-level view on our subsampling routine is provided in Fig. 3. From Fig. 3 we learn that we need two ingredients for our subroutine to work:

1. We need a dataset that spans some domain $\mathcal{X}$. We can retrieve this domain simply by calculating the maximum and minimum value of each dimension in $\mathcal{X}$. *We have illustrated a simple dataset in Fig. 3a.*
2. We need a set of K distinct distributions that span $\mathcal{X}$. In principle there is no constraint on these, besides them being different from one another, and each region in $\mathcal{X}$ having a non-zero probability of being sampled. *This is illustrated in Fig. 3b.*

Using the above two ingredients, we create K empty subsets. For each subset, we then define one distribution, illustrated in Fig. 3b. In Fig. 3 we used a Gaussian for each subset as they span the domain, and are simple to evaluate. Using these distributions, we will fill each subset using data from Fig. 3a. Each data point in our dataset is evaluated K times: using the user-defined distributions in Fig. 3b, we either include the sample in the corresponding subset, or not. When the probability of being sampled is *high enough*, it is included, when it is not high enough, it is excluded. High enough could be determined by something simple as a threshold, or something less parametric as a Bernoulli experiment. When finished, the subsamples look like Fig. 3c.

Alas, Gaussian distributions become more difficult to handle with increasing dimensionality as data is spread sparser in high dimensions. The provided high-level example may serve well as a (visual) explanation of our subroutine, it does not work well in practice. As such, we used a different implementation for D-Struct, which we explain in Section 3.2, and in more detail below.

F.2 HOW IT'S IMPLEMENTED IN D-STRUCT

Recall that the main issue with the simple Gaussian implementation above is that it does not scale well to high-dimensions. As such, we need a different implementation that scales to high-dimensions.

Defining the distributions. We do this using a very simple idea: rather than sampling in covariate-space, we sample the dataset's *indices*, which correspond to a sample's covariates. However, before we do this, we need to make sure that the indices are in some way correlated with the covariates, which is not the case for a standard dataset as they are sampled i.i.d.

To provide some correlation between index and covariates, we first sort the covariates and reindex the dataset. This way, a smaller set of covariates now corresponds with a smaller index-value. Note that it is unimportant whether we sort descending or ascending, the only thing that matters is that there is some *logical* ordering.

Having an index that is correlated with the covariates allows us to define a distribution over the indices (which are one-dimensional) rather than over the covariates (which are d-dimensional). We chose the beta distribution as our user-specified distribution, where each of the K distributions is given different parameters. The advantage a beta distribution has, is their flexibility to move its

density over the entire domain (contrasting Gaussian distributions which are symmetrical). This point is illustrated in Fig. 4.

Sampling data. Once we have defined our distributions, we can use them to sample data. As with our high-level idea in Appendix F.1, we will evaluate each data point K times to determine whether or not it should be included in each subset. However, rather than evaluating the chosen distributions using the covariates directly, we now use the index instead. Regardless of the number of dimensions we have, the index remains one-dimensional.

Evaluating a sample in D-Struct is done using a Bernoulli experiment: with the beta distributions we query the probability of being sampled and provide it to a Bernoulli experiment, the outcome determines inclusion or exclusion.

G CIT-BASED METHODS, SCORE-BASED METHODS AND FAITHFULNESS

G.1 CIT-BASED METHODS

CIT-based methods such as the well known PC-algorithm, the SGS algorithm, or the inductive causation (IC) algorithm all require faithfulness as per Def. 5. The reason is such that they render the Markov equivalence class identifiable. As we have explained in Section 3.1, using d-separation we have a one-to-one correspondence to this class of DAGs. Any query of a d-separation statement can therefore be answered by checking the corresponding conditional independence test [15].

Most CIT-based methods have 2 main phases, based on a set of conditional independence statements. Assuming the latter is a correct set (that is, we have correctly inferred all the independence statements present in $\mathbb{P}_{\mathcal{X}}$), we first infer a skeleton graph, and then orient the edges. After these two phases, we have either a fully identified DAG, or a Markov equivalence graphs in case there are edges we were not able to orient.

Phase 1: inferring a skeleton. Based on lem. 1 (below) introduced in Verma and Pearl [71], the SGS and IC algorithm build a skeleton from a completely unconnected graph.

Lemma 1. *The following two statements hold:*

> *(i) Two nodes X and Y in a DAG $(\mathcal{X}, \mathcal{E})$ are adjacent iff they cannot be d-separated by any subset $\mathcal{S} \subset \mathcal{X} \setminus \{X, Y\}$.*
>
> *(ii) If two nodes X and Y in a DAG $(\mathcal{X}, \mathcal{E})$ are not adjacent, then they are d-separated by either Pa_X or Pa_Y.*

Clearly, by using above lemma, SGS [70] and IC [28] *require* faithfulness. Contrasting methods that build from an unconnected graph, is the PC-algorithm which does the reverse: PC starts with a fully connected graph and step-by-step removes edges when they violate (ii) in lem. 1. While a different approach, both require d-separation, i.e. this too requires faithfulness to hold!

Phase 2: orienting the edges. As per Meek [37] there exists a set of graphical rules that is shown complete to correctly orient the edges based only on d-separation. Of course, this requires a *complete* set of correct independence statements which is arguably a much stricter assumption than faithfulness.

Essentially, we can relax the assumption of a complete set of independencies, but we'll have to replace it with other assumptions. One such example is assuming a $\mathbb{P}_{\mathcal{X}}$ to be Gaussian (which is also quite strict, but it serves our example). With the latter assumption, we can test for *partial correlation* [34, Appendices A.1 and A.2], which allows to identify the underlying Markov equivalence class [75]. Furthermore, by additionally assuming a condition called *strong faithfulness* [76, 77], we have uniform consistency [75]. We refer to Peters et al. [34, Ex. 7.9] for an example.

G.2 (DIFFERENTIABLE) SCORE-BASED METHODS

Contrasting CIT-based methods, are score-based methods. Score-based methods generalise our differentiable score based methods and non-differentiable methods. Contrasting CIT-based methods, which directly encode the independence statements governing $\mathbb{P}_{\mathcal{X}}$ into $\mathcal{G}$, a score-based method will

evaluate $\mathcal{G}$ on how well it fits the observed data. The rationale behind these score-based methods is that wrongly encoded independence statements will yield poor model fits [78, 79].

We can formalise a score-based method as a function S which is to be optimised over candidate DAGs:

$$\hat{\mathcal{G}} \coloneqq \underset{\mathcal{G} \text{ DAG over } \mathcal{D} \in \mathcal{X}}{\arg\max} S(\mathcal{D}, \mathcal{G}).$$

As such, there are two elements that comprise a score-based method: (i) the function S, and (ii) the way we optimise S. In our case, that is:

(i) S corresponds to eq. (5), which is in large part determined by the underlying DSF through $\mathcal{L}_{\text{DSF}}$.

(ii) S is optimised using gradient-optimisation, which has proven very efficient in this problem setting

Importantly, that rationale behind these methods does *not* require the faithfulness assumption for them to work. The latter may lead to violations against d-separation in case faithfulness does hold. However, in Appendix E we show how we can combat against this, by also incorporating any known independencies into our graph (which *does* require the faithfulness assumption to hold for those independence statements) using the L-BFGS-B optimisation algorithm.

Ethics Statement. We envisage D-Struct as a tool to *help* the scientific endeavour, however emphasise the discovered structures and links would need to be further verified by a human expert or in an experimental setting. Furthermore, the data used in this work is synthetically generated from given random graphical models, and no human-derived data was used.

Reproducibility Statement. To ensure reproducibility, we include experimental details in Appendix A.1. These details include: (1) hyperparameter settings, (2) evaluation metrics, (3) the synthetic data generation procedure, and (4) additional implementation details of D-Struct. Finally, all code is readily available at our anonymous online code repository: `https://anonymous.4open.science/r/d-struct`. Beyond documentation and instructions, this code includes benchmark models, synthetic data generation, and our D-Struct implementation.

REFERENCES

[1] Rohan Bhardwaj, Ankita R Nambiar, and Debojyoti Dutta. A study of machine learning in healthcare. In *2017 IEEE 41st Annual Computer Software and Applications Conference (COMPSAC)*, volume 2, pages 236–241. IEEE, 2017.

[2] Jeroen Berrevoets, James Jordon, Ioana Bica, Mihaela van der Schaar, et al. Organite: Optimal transplant donor organ offering using an individual treatment effect. *Advances in neural information processing systems*, 33:20037–20050, 2020.

[3] Mihaela van der Schaar, Ahmed M Alaa, Andres Floto, Alexander Gimson, Stefan Scholtes, Angela Wood, Eoin McKinney, Daniel Jarrett, Pietro Lio, and Ari Ercole. How artificial intelligence and machine learning can help healthcare systems respond to covid-19. *Machine Learning*, 110(1):1–14, 2021.

[4] Alvin Rajkomar, Jeffrey Dean, and Isaac Kohane. Machine learning in medicine. *New England Journal of Medicine*, 380(14):1347–1358, 2019.

[5] Jeroen Berrevoets, Ahmed Alaa, Zhaozhi Qian, James Jordon, Alexander ES Gimson, and Mihaela Van Der Schaar. Learning queueing policies for organ transplantation allocation using interpretable counterfactual survival analysis. In *International Conference on Machine Learning*, pages 792–802. PMLR, 2021.

[6] Susan Athey et al. The impact of machine learning on economics. *The economics of artificial intelligence: An agenda*, pages 507–547, 2018.

[7] Susan Athey and Guido W Imbens. Machine learning methods that economists should know about. *Annual Review of Economics*, 11:685–725, 2019.

[8] Sendhil Mullainathan and Jann Spiess. Machine learning: an applied econometric approach. *Journal of Economic Perspectives*, 31(2):87–106, 2017.

[9] Giuseppe Carleo, Ignacio Cirac, Kyle Cranmer, Laurent Daudet, Maria Schuld, Naftali Tishby, Leslie Vogt-Maranto, and Lenka Zdeborová. Machine learning and the physical sciences. *Reviews of Modern Physics*, 91(4):045002, 2019.

[10] Alexander Radovic, Mike Williams, David Rousseau, Michael Kagan, Daniele Bonacorsi, Alexander Himmel, Adam Aurisano, Kazuhiro Terao, and Taritree Wongjirad. Machine learning at the energy and intensity frontiers of particle physics. *Nature*, 560(7716):41–48, 2018.

[11] Sankar Das Sarma, Dong-Ling Deng, and Lu-Ming Duan. Machine learning meets quantum physics. *arXiv preprint arXiv:1903.03516*, 2019.

[12] George Em Karniadakis, Ioannis G Kevrekidis, Lu Lu, Paris Perdikaris, Sifan Wang, and Liu Yang. Physics-informed machine learning. *Nature Reviews Physics*, 3(6):422–440, 2021.

[13] Philip G Breen, Christopher N Foley, Tjarda Boekholt, and Simon Portegies Zwart. Newton versus the machine: solving the chaotic three-body problem using deep neural networks. *Monthly Notices of the Royal Astronomical Society*, 494(2):2465–2470, 2020.

[14] Silviu-Marian Udrescu and Max Tegmark. Ai feynman: A physics-inspired method for symbolic regression. *Science Advances*, 6(16):eaay2631, 2020.

[15] Jan Reinhard Peters. *Machine learning of motor skills for robotics*. University of Southern California, 2007.

[16] Xue Bin Peng, Marcin Andrychowicz, Wojciech Zaremba, and Pieter Abbeel. Sim-to-real transfer of robotic control with dynamics randomization. In *2018 IEEE international conference on robotics and automation (ICRA)*, pages 3803–3810. IEEE, 2018.

[17] Ben Kehoe, Sachin Patil, Pieter Abbeel, and Ken Goldberg. A survey of research on cloud robotics and automation. *IEEE Transactions on automation science and engineering*, 12(2): 398–409, 2015.

[18] Pieter Abbeel, Adam Coates, and Andrew Y Ng. Autonomous helicopter aerobatics through apprenticeship learning. *The International Journal of Robotics Research*, 29(13):1608–1639, 2010.

[19] Yanir Kleiman, Simon Pabst, and Patrick Nagle. Boosting vfx production with deep learning. In *ACM SIGGRAPH 2019 Talks*, pages 1–2. 2019.

[20] Dan Ring, Johanna Barbier, Guillaume Gales, Ben Kent, and Sebastian Lutz. Jumping in at the deep end: how to experiment with machine learning in post-production software. In *Proceedings of the 2019 Digital Production Symposium*, pages 1–5, 2019.

[21] Yi Wang. Film and television special effects production based on modern technology: from the perspective of statistical machine learning. In *2022 4th International Conference on Smart Systems and Inventive Technology (ICSSIT)*, pages 833–836. IEEE, 2022.

[22] Alex Davies, Petar Veličković, Lars Buesing, Sam Blackwell, Daniel Zheng, Nenad Tomašev, Richard Tanburn, Peter Battaglia, Charles Blundell, András Juhász, et al. Advancing mathematics by guiding human intuition with ai. *Nature*, 600(7887):70–74, 2021.

[23] John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, et al. Highly accurate protein structure prediction with alphafold. *Nature*, 596(7873):583–589, 2021.

[24] Kathryn Tunyasuvunakool, Jonas Adler, Zachary Wu, Tim Green, Michal Zielinski, Augustin Žídek, Alex Bridgland, Andrew Cowie, Clemens Meyer, Agata Laydon, et al. Highly accurate protein structure prediction for the human proteome. *Nature*, 596(7873):590–596, 2021.

[25] Kiersten M. Ruff and Rohit V. Pappu. Alphafold and implications for intrinsically disordered proteins. *Journal of Molecular Biology*, 433(20):167208, 2021. ISSN 0022-2836. doi: https://doi.org/10.1016/j.jmb.2021.167208. URL https://www.sciencedirect.com/science/article/pii/S0022283621004411. From Protein Sequence to Structure at Warp Speed: How Alphafold Impacts Biology.

[26] Daphne Koller and Nir Friedman. *Probabilistic graphical models: principles and techniques*. MIT press, 2009.

[27] Sewall Wright. The method of path coefficients. *The annals of mathematical statistics*, 5(3): 161–215, 1934.

[28] Judea Pearl. *Causality*. Cambridge university press, 2009.

[29] Clark Glymour, Kun Zhang, and Peter Spirtes. Review of causal discovery methods based on graphical models. *Frontiers in genetics*, 10:524, 2019.

[30] Dan Geiger and Judea Pearl. On the logic of causal models. In *Machine Intelligence and Pattern Recognition*, volume 9, pages 3–14. Elsevier, 1990.

[31] Christopher Meek. Strong completeness and faithfulness in bayesian networks. *arXiv preprint arXiv:1302.4973*, 2013.

[32] Frederick Eberhardt. Introduction to the foundations of causal discovery. *International Journal of Data Science and Analytics*, 3(2):81–91, 2017.

[33] Max Chickering, Dan Geiger, and David Heckerman. Learning bayesian networks: Search methods and experimental results. In *Proceedings of the fifth international workshop on artificial intelligence and statistics*, 1995.

[34] Jonas Peters, Dominik Janzing, and Bernhard Schölkopf. *Elements of causal inference: foundations and learning algorithms*. The MIT Press, 2017.

[35] Xun Zheng, Bryon Aragam, Pradeep Ravikumar, and Eric P. Xing. DAGs with NO TEARS: Continuous Optimization for Structure Learning. In *Advances in Neural Information Processing Systems*, 2018.

[36] Xun Zheng, Chen Dan, Bryon Aragam, Pradeep Ravikumar, and Eric P. Xing. Learning sparse nonparametric DAGs. In *International Conference on Artificial Intelligence and Statistics*, 2020.

[37] Christopher Meek. Strong completeness and faithfulness in bayesian networks. In *Proceedings of the Eleventh Conference on Uncertainty in Artificial Intelligence*, 1995.

[38] Ann Becker, Dan Geiger, and Christopher Meek. Perfect tree-like markovian distributions. In *Proceedings of the Sixteenth Conference on Uncertainty in Artificial Intelligence*, 2000. URL https://arxiv.org/abs/1301.3834.

[39] Monya Baker. 1,500 scientists lift the lid on reproducibility. *Nature*, 533(7604), 2016.

[40] Colin F Camerer, Anna Dreber, Eskil Forsell, Teck-Hua Ho, Jürgen Huber, Magnus Johannesson, Michael Kirchler, Johan Almenberg, Adam Altmejd, Taizan Chan, et al. Evaluating replicability of laboratory experiments in economics. *Science*, 351(6280):1433–1436, 2016.

[41] Robert K Merton. *The sociology of science: Theoretical and empirical investigations*. University of Chicago press, 1973.

[42] Victoria Stodden. The scientific method in practice: Reproducibility in the computational sciences. 2010.

[43] Rohit Bhattacharya, Tushar Nagarajan, Daniel Malinsky, and Ilya Shpitser. Differentiable causal discovery under unmeasured confounding. In *International Conference on Artificial Intelligence and Statistics*, pages 2314–2322. PMLR, 2021.

[44] Trent Kyono, Yao Zhang, and Mihaela van der Schaar. Castle: Regularization via auxiliary causal graph discovery. *Advances in Neural Information Processing Systems*, 33:1501–1512, 2020.

[45] Roxana Pamfil, Nisara Sriwattanaworachai, Shaan Desai, Philip Pilgerstorfer, Konstantinos Georgatzis, Paul Beaumont, and Bryon Aragam. Dynotears: Structure learning from time-series data. In *International Conference on Artificial Intelligence and Statistics*, pages 1595–1605. PMLR, 2020.

[46] Trent Kyono, Yao Zhang, Alexis Bellot, and Mihaela van der Schaar. Miracle: Causally-aware imputation via learning missing data mechanisms. *Advances in Neural Information Processing Systems*, 34, 2021.

[47] Boris van Breugel, Trent Kyono, Jeroen Berrevoets, and Mihaela van der Schaar. Decaf: Generating fair synthetic data using causally-aware generative networks. *Advances in Neural Information Processing Systems*, 34, 2021.

[48] Sébastien Lachapelle, Philippe Brouillard, Tristan Deleu, and Simon Lacoste-Julien. Gradient-based neural dag learning. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=rklbKA4YDS.

[49] Yue Yu, Tian Gao, Naiyu Yin, and Qiang Ji. Dags with no curl: An efficient dag structure learning approach. In Marina Meila and Tong Zhang, editors, *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pages 12156–12166. PMLR, 18–24 Jul 2021. URL https://proceedings.mlr.press/v139/yu21a.html.

[50] Yue Yu, Jie Chen, Tian Gao, and Mo Yu. DAG-GNN: DAG structure learning with graph neural networks. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 7154–7163. PMLR, 09–15 Jun 2019. URL https://proceedings.mlr.press/v97/yu19a.html.

[51] Judea Pearl. *Probabilistic reasoning in intelligent systems: networks of plausible inference*. Morgan kaufmann, 1988.

[52] Martin J Wainwright, Michael I Jordan, et al. Graphical models, exponential families, and variational inference. *Foundations and Trends® in Machine Learning*, 1(1–2):1–305, 2008.

[53] Judea Pearl. Fusion, propagation, and structuring in belief networks. *Artificial intelligence*, 29 (3):241–288, 1986.

[54] Thomas Verma and Judea Pearl. Causal networks: Semantics and expressiveness. In *Machine intelligence and pattern recognition*, volume 9, pages 69–76. Elsevier, 1990.

[55] Dan Geiger, Thomas Verma, and Judea Pearl. d-separation: From theorems to algorithms. In *Machine Intelligence and Pattern Recognition*, volume 10, pages 139–148. Elsevier, 1990.

[56] Dan Geiger, Thomas Verma, and Judea Pearl. Identifying independence in bayesian networks. *Networks*, 20(5):507–534, 1990.

[57] Ronald A Howard and James E Matheson. The principles and applications of decision analysis. *Strategic Decisions Group, Palo Alto, CA*, pages 719–762, 1984.

[58] JQ Smith. Influence diagrams for statistical modeling. *The Annals of Statistics*, 1, 1989.

[59] Dan Geiger and Judea Pearl. Logical and algorithmic properties of conditional independence and graphical models. *The annals of statistics*, 21(4):2001–2021, 1993.

[60] Robert W Robinson. Counting unlabeled acyclic digraphs. In *Combinatorial mathematics V*, pages 28–43. Springer, 1977.

[61] Matthew J Vowels, Necati Cihan Camgoz, and Richard Bowden. D'ya like dags? a survey on structure learning and causal discovery. *ACM Computing Surveys (CSUR)*, 2021.

[62] Xinshi Chen, Haoran Sun, Caleb Ellington, Eric Xing, and Le Song. Multi-task learning of order-consistent causal graphs. *Advances in Neural Information Processing Systems*, 34: 11083–11095, 2021.

[63] Dimitri P. Bertsekas. *Nonlinear Programming*. Athena Scientific, 3rd edition, 2016. ISBN 978-1-886529-05-2.

[64] Richard H Byrd, Peihuang Lu, Jorge Nocedal, and Ciyou Zhu. A limited memory algorithm for bound constrained optimization. *SIAM Journal on scientific computing*, 16(5):1190–1208, 1995.

[65] Marcus Kaiser and Maksim Sipos. Unsuitability of NOTEARS for causal graph discovery when dealing with dimensional quantities. *Neural Processing Letters*, pages 1–9, 2022.

[66] Alexander G Reisach, Christof Seiler, and Sebastian Weichwald. Beware of the simulated dag! varsortability in additive noise models. *arXiv preprint arXiv:2102.13647*, 2021.

[67] Michael Irwin Jordan. *Learning in graphical models*. MIT press, 1999.

[68] Steffen L Lauritzen. *Graphical models*, volume 17. Clarendon Press, 1996.

[69] Albert-László Barabási and Réka Albert. Emergence of scaling in random networks. *science*, 286(5439):509–512, 1999.

[70] Peter Spirtes, Clark N Glymour, Richard Scheines, and David Heckerman. *Causation, prediction, and search*. MIT press, 2000.

[71] Thomas S. Verma and Judea Pearl. Equivalence and synthesis of causal models. In *Proceedings of the Sixth Conference on Uncertainty in Artificial Intelligence*, 1990.

[72] Ignavier Ng, AmirEmad Ghassami, and Kun Zhang. On the role of sparsity and dag constraints for learning linear dags. In H. Larochelle, M. Ranzato, R. Hadsell, M.F. Balcan, and H. Lin, editors, *Advances in Neural Information Processing Systems*, volume 33, pages 17943–17954. Curran Associates, Inc., 2020. URL https://proceedings.neurips.cc/paper/2020/file/d04d42cdf14579cd294e5079e0745411-Paper.pdf.

[73] Eric Walter. *Identifiability of parametric models*. Elsevier, 2014.

[74] Jiji Zhang and Peter Spirtes. Detection of unfaithfulness and robust causal inference. *Minds and Machines*, 18(2):239–271, 2008.

[75] Markus Kalisch and Peter Bühlman. Estimating high-dimensional directed acyclic graphs with the pc-algorithm. *Journal of Machine Learning Research*, 8(3), 2007.

[76] Jiji Zhang and Peter L Spirtes. Strong faithfulness and uniform consistency in causal inference. *arXiv preprint arXiv:1212.2506*, 2012.

[77] Caroline Uhler, Garvesh Raskutti, Peter Bühlmann, and Bin Yu. Geometry of the faithfulness assumption in causal inference. *The Annals of Statistics*, pages 436–463, 2013.

[78] Dan Geiger and David Heckerman. Learning gaussian networks. In *Uncertainty Proceedings 1994*, pages 235–243. Elsevier, 1994.

[79] David Heckerman, Christopher Meek, and Gregory Cooper. A bayesian approach to causal discovery. In *Innovations in Machine Learning*, pages 1–28. Springer, 2006.