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Towards Practical Multi-label Causal Discovery in High-Dimensional Event Sequences via One-Shot Graph Aggregation

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Abstract

Understanding causality in event sequences where outcome labels such as diseases or system failures arise from preceding events like symptoms or error codes is critical—yet remains an unsolved challenge across domains like healthcare or vehicle diagnostics. We introduce CARGO, a scalable multi-label causal discovery method for sparse, high-dimensional event sequences comprising of thousands of unique event types. Using two pretrained causal Transformers as domain-specific foundation models for event sequences—CARGO infers in parallel, per sequence one-shot causal graphs and aggregates them using an adaptive frequency fusion to reconstruct the global Markov boundaries of labels. This two-stage approach enables efficient probabilistic reasoning at scale while bypassing the intractable cost of full-dataset conditional independence testing. Our results on a challenging real-world automotive fault prediction dataset with over 29,100 unique event types and 474 imbalanced labels demonstrate CARGO's ability to perform structured reasoning.

1 Introduction

Understanding *why* specific events lead to particular outcomes is vital for effective diagnosis, predictions and overall decision making [23, 35]. For instance, "what serie of events captured by diagnostic led to this vehicle failure" or "what symptoms led to this disease" [26, 38, 14, 24, 33]. Here, an event sequence consists of a list of discrete events x_i recorded asynchronously over time, while labels $\boldsymbol{y}$ summarize outcomes associated with the full sequence (e.g, a diagnosed defect or condition).

A fundamental obstacle in these settings is dimensionality. Real-world systems often involve tens of thousands of possible events, which renders the causal discovery intractable for current algorithms [13]. To address this, we reinterpret multi-label causal discovery for event sequences as a form of Bayesian model averaging [15, 32], where each sequence is treated as a sample from a local causal model. Specifically, each sequence induces a one-shot causal graph (i.e., a directed acyclic graph (DAG)) [39]. Together they can be fused to form a unified global structure [6]. This process, known as structural fusion [31], aggregates local graphs into a consensus causal graph over all observed sequences.

To summarise our contributions: we introduce CARGO (Causal Aggregation via Regressive Graph Operations), the first method to provide scalable causal discovery across thousands of labelled event sequences, with theoretical guarantees under standard assumptions. It is divided into two phases: (1) One-shot graph extraction, where for each sequence CARGO infers the local Markov boundary

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of each label using two autoregressive Transformers as density estimators [47, 9] (2) Graph fusion, where the local graphs are aggregated via an adaptive thresholding function to provide global Markov Boundaries.

We empirically validate CARGO on a large-scale vehicular dataset composed of about $29,100$ events and 474 imbalanced labels, demonstrating for the first time, scalability and practical superiority over traditional causal discovery baselines. We also provide ablation on scoring criterions, frequency thresholds and the quality of the Transformers.

2 Preliminary & Related Work

A full description of the notations and definitions used throughout the paper can be found in Appendix A.

Event Sequence Modelling. Event sequences are typically represented as a series of time-stamped discrete events $S = \{(t_1, x_1), \ldots, (t_L, x_L)\}$ where $0 \leq t_1 < \ldots \leq t_L$ denotes the time of occurrence of event type $x_i \in \mathbb{X}$ drawn from a finite vocabulary $\mathbb{X}$. In multi-label settings, a binary label vector $\boldsymbol{y} \in \{0,1\}^{|\mathbb{Y}|}$ is attached to S and indicates the presence of multiple outcome labels chosen from $\mathbb{Y}$ occuring at the final time step t_L. Together, this results in a multi-labeled sequence $S_l = (S, (\boldsymbol{y}_L, t_L))$.

Event sequence modelling has been widely applied to predictive tasks. For instance, in the automotive domain, Diagnostic Trouble Codes (DTCs) [33] are logged asynchronously over time and used to infer failures or error patterns [27]. In healthcare, electronic health records encode temporal sequences of symptoms to perform predictive tasks [38, 19, 14]. A common modelling strategy [21, 28] separates such event types $\mathbb{X}$ from labels $\mathbb{Y}$.

Transformers [47, 37, 44] have emerged as the dominant architecture for sequence modelling. Recent work leveraged Transformers in high-dimensional event spaces for next-event and label prediction. Math et al. [27] proposed a dual Transformer architecture where one model predicts the next event type (DTC), and the other predicts label occurrence (e.g, error pattern). Through this paper, we repurpose this dual architecture for causal discovery.

Multi-label Causal Discovery seeks to identify the Markov Boundary (**MB**) of each label—its minimal set of parents, children, and spouses—such that the label is conditionally independent of all other variables given its **MB** [45] (Def. 3).

While classical constraint-based algorithms have shown success on low-dimensional tabular data [40, 51], their application to event sequences with multi-label outputs remains challenging due to: (1) *dimensionality*—thousands of event types increase super-exponentially the number of graphs (2) *sparsity*—multi-hot encodings often underrepresent rare but important events (3) *distributional assumptions*—such as linearity or Gaussian noise, which rarely hold in real-world sequences [11].

Contemporary works point toward dividing classical causal discovery for high-dimensional datasets into sub-problems and graph aggregation. Laborda et al. [20] introduce a ring-based distributed algorithm for learning high-dimensional BN, Dong et al. [6] explores a distributed approach for large-scale causal structure learning and Mokhtarian et al. [29] for Markov Boundaries.

Bayesian Network [32] has served as a modelling technique for a variety of decision problems. It is defined as a triplet $< \boldsymbol{U}, \mathbb{G}, P >$ with P the joint distribution over a variable set $\boldsymbol{U}$ of a directed acyclic graph $\mathbb{G} = (\boldsymbol{U}, E)$ with E as the set of directed edges. This triplet must satisfy the Markov Condition: every random variable U_i is independent of its non-descendant variables given its parents $\text{Pa}(U_i)$ in $\mathbb{G}$. The directed edge $(U_i \rightarrow U_j)$ encodes a probabilistic dependence. Thus, the joint probability distribution can be factorised as:

$$P(U_1, \cdots, U_n) = \prod_{i=1}^{n} P(U_i | \text{Pa}(U_i))$$

The DAG encodes a set of conditional independencies $\mathcal{I}(\mathbb{G})$, where each element corresponds to a conditional independence relation $U_i \perp U_j | \boldsymbol{Z}$, meaning that U_i and U_j are conditionally independent given the set of variables $\boldsymbol{Z}$. Formally, a DAG $\mathbb{G}_k$ is an I-map (or Independence map) of another $\mathbb{G}$ if

the set of conditional independencies encoded by $\mathbb{G}_k$ is a subset of those encoded by $\mathbb{G}$:

$$\mathcal{I}(\mathbb{G}_k) \subseteq \mathcal{I}(\mathbb{G})$$

$\mathbb{G}_k$ is a minimal I-map of $\mathbb{G}$ if removing any edge from it introduces a conditional dependence that would violate an independence in $\mathbb{G}$, i.e $\mathcal{I}(\mathbb{G}_k \backslash \{e\} \not\subseteq I(\mathbb{G}) \forall e \in E$.

Bayesian Model Averaging. Fusing BN has several direct applications. Either to average multiple models from different experts to learn a global and average representation [15]. Or to perform causal discovery in distributed settings with federated learning algorithms [49, 12].

Formally, Given a set of Bayesian Networks $\{B_k\}_{k=1}^m$ with associated DAGs $\{\mathbb{G}_k = (V_k, E_k)\}_{k=1}^m, V_k \in \boldsymbol{U}$ sharing the same finite set of node $\boldsymbol{U}$, structural fusion aim to construct the DAG $\mathbb{G}^* = (V, E), V \in \boldsymbol{U}$. Multiple fusion methods exist and leverage either the probability distribution p by doing Bayesian Model Averaging [15] or focus on the structural learning (Fig. 8) of $\mathbb{G}^*$ [5, 31, 10, 34, 12], which is an NP-hard [31] problem.

We will focus on the second element in this paper. Hence, we are seeking the merged edges $E = \bigcup_{i=1}^m E_i^\sigma$. The consistent node ordering σ ensures acyclicity. The fused DAG $\mathbb{G}^*$ is the minimal I-map of the intersection of the conditional independencies across all DAGs $\mathbb{G}_k = (V_k, E_k)\}_{k=1}^m$.

Greedy Equivalence Search. (GES) [2] is one of the most theoretically sound methods to recover a Markov equivalence class (MEC, Def. 4) of a DAG. Particularly in the context of large samples of data, GES provides theoretical guarantees of reaching the true graph. Formally, GES searches for the MEC of the graph $\mathbb{G}^*$ from the observational dataset $\boldsymbol{D}$ with distribution p. This defines the optimisation problem as:

$$\mathbb{G}^* = \arg_{\mathbb{G}} \max S(\mathbb{G}, \boldsymbol{D}) \tag{1}$$

Chickering [2] proved that under parametric assumption, a large number of samples and using the Bayesian Information Criterion (BIC) as criterion S, GES is guaranteed to recover a Markov Equivalence Class of $\mathbb{G}^*$.

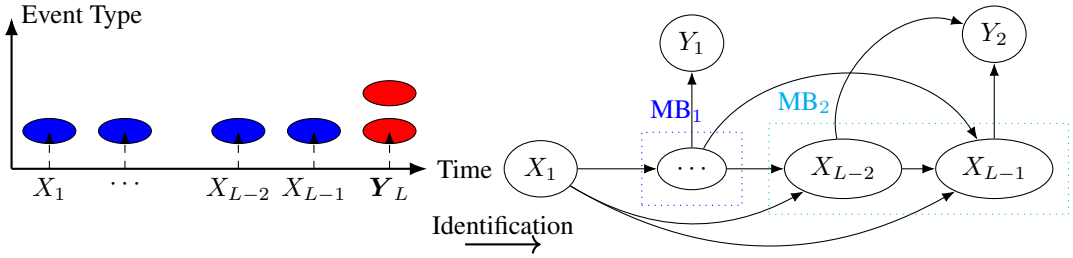
Frequency Based. Multiple heuristics have been developed to merge multiple BNs. One is edge frequency cutoff [42], other on estimating the proportion of false positive edges [7] and integer linear programming (ILP) [7] or a mix of both: [43]. As pointed out by [7], choosing a frequency cutoff τ is particularly challenging. Moreover, under class imbalance and long-tail problem in classification [52], the theoretical property of frequency approaches, such as the law of large numbers, might not hold.

We will now explain the two phases of CARGO, which are (1) One-shot causal discovery (2) Graph aggregation using adaptive thresholding. The Proofs of Lemmas and Theorems can be found in the Appendix B.

3 One-shot Causal Discovery

Let S_l^k be a multi-labeled sequence drawn from a dataset $D = \{S_l^1, \cdots, S_l^m\} \subset \mathbb{S}$ and $\mathbb{G}_k$ the sequential BN (Fig. 1) with attached labels. The goal of multi-label causal discovery is to identify the

Figure 1: An example of a causal graph extracted from a single multi-label event sequence where MB_1 represents the Markov Boundary of Y_1 and MB_2 the Markov Boundary of Y_2.



(a) Multi-label event sequence S_l (b) BN representation of S_l

Markov Boundary of each label $Y_j \in \boldsymbol{Y}$ present in S_l^k. To be able to access conditional independence (Def. 2) between X_i and Y_j conditioned on the past events $\boldsymbol{Z} = (x_1, \cdots, x_{i-1}) = S_{<i}$, we model the event apparitions using a sequential BN (Fig. 1).

We would like to assess how much additional information event X_i occurring at step i provides about label Y_j when we already know the past sequence of events $\boldsymbol{Z} = S_{<i}$. We essentially try to answer if:

$$P(Y_j|X_i, \boldsymbol{Z}) = P(Y_j|\boldsymbol{Z}) \Leftrightarrow D_{KL}(P(Y_j|X_i, \boldsymbol{Z})\|P(Y_j|\boldsymbol{Z})) = 0$$

where D_{KL} denotes the ***Kullback-Leibler divergence*** [3]. The distributional difference between the conditionals $P(Y_j|X_i, \boldsymbol{Z}), P(Y_j|\boldsymbol{Z})$ is akin to Information Gain I_G [36] conditioned on past events:

$$I_G(x_i, Y_j|z_i) \triangleq D_{KL}(P(Y_j|X_i = x_i, \boldsymbol{Z} = z_i))||P(Y_j|Z = z_i)) \tag{2}$$

Which is equals to the difference between the conditional entropies [3] denoted as H:

$$I_G(Y_j, x_i|z_i) = H(Y_j|z_i) - H(Y_j|x_i, z_i) \tag{3}$$

More generally, we can access the conditional independence of event X_i and label Y_j using the conditional mutual information (CMI) [3] which is simply the expected value over x_i, z_i of the information gain $I_G(Y_j, x_i|z_i)$ such as:

$$I(Y_j, X_i|\boldsymbol{Z}) \triangleq H(Y_j|\boldsymbol{Z}) - H(Y_j|\boldsymbol{Z}, X_i) = \mathbb{E}_{x_i,z_i}[I_G(Y_j, X_i = x_i|\boldsymbol{Z} = z_i)]) \tag{4}$$

Density Estimation. We used two pretrained Transformers (Tf_x, Tf_y) trained via maximum likelihood on a dataset of multi-labelled event sequences $D = \{S_l^1, \cdots, S_l^m\} \subset \mathbb{S}$. We assume that they perfectly model the true conditional distributions of events and labels (A4). While due to the strict equivalences between CI-tests and conditional independence, it is difficult to provide a theoretical guarantee under imperfect models, we acknowledge that this assumption may be violated. We note that most of the causal discovery methods either have strong parametric data assumptions or assume a perfect CI-test. We provide an ablation study on the impact of the NADE's quality on the one-shot phase in Appendix C.1, including number of parameters, context c and Tf_y performance.

Formally, the two Transformers infer the probability of the next event and label conditioned on the past events using the hidden states $\boldsymbol{h}_{i-1}^x, \boldsymbol{h}_i^y \in \mathbb{R}^d$, from Tf_x, Tf_y respectively:

$$\text{Tf}_x(S_{<i}) = \textit{Softmax}(\boldsymbol{h}_{i-1}^x) = P_{\theta_x}(X_i|\boldsymbol{Z}),\ \hat{x}_i^{(z)} \triangleq P_{\theta_x}(X_i = x_i|\boldsymbol{Z}) \tag{5}$$

$$\text{Tf}_y(S_{\leq i}) = \textit{Sigmoid}(\boldsymbol{h}_i^y) = P_{\theta_y}(Y|X_i, \boldsymbol{Z}), \hat{y}_{i+1,j}^{(z)} \triangleq P_{\theta_y}(Y = y_j|X_i = x_i, \boldsymbol{Z}) \tag{6}$$

Sequential One-shot Causal Discovery. The CMI using Eq.(4) is computable only with the posteriors $P(Y_j|\boldsymbol{Z}), P(Y_j|X_i, \boldsymbol{Z}))$. In practice a label-specific threshold $\theta_j \approx 0$ is applied to Eq (4) to identify conditional dependence:

$$Y_j \not\perp\!\!\!\perp X_i \mid \boldsymbol{Z} \quad \Leftrightarrow \quad I(Y_j, X_i \mid \boldsymbol{Z}) > \theta_j \approx 0. \tag{7}$$

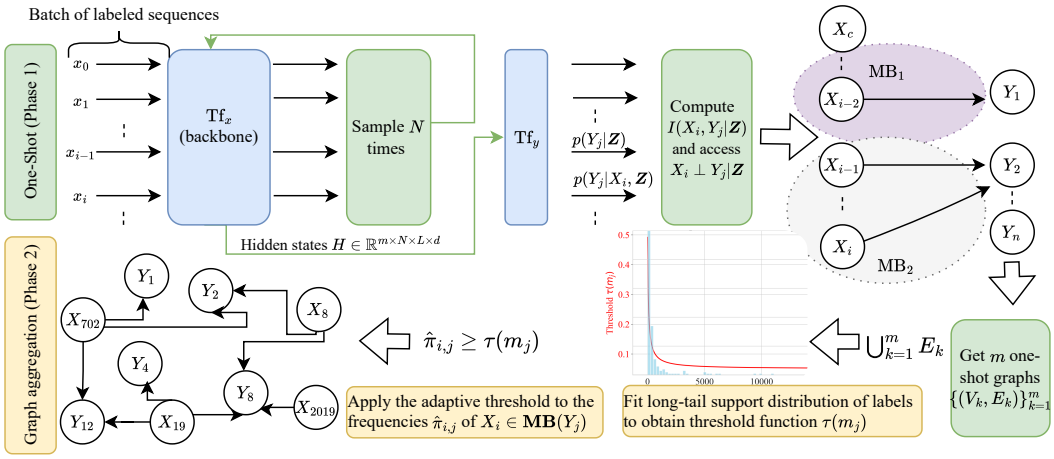
Hence, the expectation in Eq.(4) is computed using a Monte-Carlo simulation, by sampling N similar context $\boldsymbol{Z}$ from Tf_x. Such that for each position in the sequence, we generate N plausible next tokens using a combination top-k and nucleus sampling [16]. Ablation studies on the effect of the sampling method and thresholding are given in Appendix C.2, C.3.

Theorem 1 (Markov Boundary Identification in Event Sequences)**.** *If S_l^k a multi-labeled sequence drawn from a dataset $D = \{S_l^1, \cdots, S_l^m\} \subset \mathbb{S}$ where two Oracle Models Tf_x and Tf_y were trained on, then under causal sufficiency (A3), bounded lagged effects (A2) and temporal precedence (A1), the Markov Boundary of each label Y_j in the causal graph $\mathbb{G}$ can be identified using conditional mutual information for CI-testing.*

Theorem 1 enables us to sequentially recover the Markov Boundary of each label in a sequence. It provides a theoretical guarantee to recover the correct causes for each label Y_j.

Computation. A key advantage of our approach is its scalability. Unlike traditional methods whose complexity depends on the event and label cardinality $|\mathbb{X}|$ and $|\mathbb{Y}|$ [22], phase 1 is agnostic to both. Figure 2 shows all parallelised steps on GPUs. CMI estimations are independently performed for all

Figure 2: The overview of CARGO. Phase 1 (One-shot) is on top, and Phase 2 (Adaptive Thresholding) is on the bottom. d denotes the hidden dimension, L the sequence length, m the number of samples and MB_1, MB_2 the Markov Boundary of Y_1, Y_2. All green and blue areas are parallelised.



positions $i \in [c, L]$, with the sampling pushed into the batch dimension and results averaged across labels. This transitions the time complexity from $\mathcal{O}(\text{BS} \times N \times L)$ to $\mathcal{O}(1)$ per batch, with L being the sequence length.

To ensure stable conditional entropy estimates and reliable predictions from Tf$_y$, the CMI is computed after observing c events (*context*). This design choice also enables out-of-the-box parallelisation. By sampling N variations of the prefix sequence $S_{\leq c}$, the CMI is independently computed across positions $i \in [c, L]$. In our experiments, we set $c = 15, L = 192$. The implementation of Phase 1 in *Pytorch* [30] is provided in Appendix D.2.

4 Structural Fusion of Markov Boundaries

Let $\{\mathbb{G}_k = (V_k, E_k)\}_{k=1}^{m}, V_i \in \boldsymbol{U}$ be the set of DAGs generated by the Phase 1 from the dataset $\boldsymbol{D}$ containing m i.i.d sequences $\{S_l^k\}_{k=1}^{m}$ drawn from a joint distribution $p(x, y)$. Each graph $\mathbb{G}_k$ represents local Markov Boundaries identified within sequence S_l^k. Our objective is to fuse these local graphs into a single, global consensus graph $\mathbb{G}^* = (\boldsymbol{U}, E)$ (see Fig. 8) with the events always as parents of labels Y_j such as:

$$\text{Pa}(Y_j) \subseteq \{X_1, \cdots, X_n\}$$

A naive fusion approach, such as taking the simple union of all edges $E = \bigcup_{k=1}^{m} E_k^{\sigma}$ works iff the Oracle models yield the perfect CI-tests in Phase 1 and thus the local graphs $\mathbb{G}^k$ are faithful to $p(x, y)$ ([31], Theorem 4.). Here, the ordering σ doesn't matter since we are dealing with Markov Boundaries. Moreover, G^* is naturally a DAG because we considered previously that outcome labels are solely explained by events, which simplifies acyclicity. We define the Bernoulli variable $Z_{i,j}^k$ for each potential edge $(X_i \to Y_j)$ within each sequence S_l^k:

$$Z_{i,j}^k = \begin{cases} 1 \text{ if the edge } X_i \to Y_j \text{ is present in } \mathbb{G}_k \\ 0 \text{ otherwise} \end{cases}$$

Under the Oracle Models assumption (A4), our one-shot discovery phase acts as a perfect conditional independence tester. Consequently, the detection of an edge in a local graph $\mathbb{G}_k$ corresponds precisely to a true causal dependency in the global graph $\mathbb{G}^*$. The probability of this event $P(Z_{i,j}^k = 1)$ is therefore the true marginal probability of the edge's existence, which we denote as $\pi_{i,j}$.

The empirical frequency, $\hat{\pi}_{i,j}(m)$, of the edge $(X_i \to Y_j)$ after observing m sequences is the sample mean of these i.i.d Bernoulli variables $\hat{\pi}_{i,j}(m) = \frac{1}{m}\sum_{k=1}^{m} Z_{ij}^k$. By the Law of Large Numbers (LLN), as the number of i.i.d sequences m tends to infinity, the empirical frequency converges in

probability to the true expected value of the random variable:

$$\hat{\pi}_{i,j}(m) \xrightarrow{p} \mathbb{E}[Z_{i,j}^{(k)}] = \pi_{i,j}$$

Thus, given a sufficiently large number of sequences, the empirical frequency $\hat{\pi}_{i,j}(m)$ serves as a consistent estimator for the true probability of the edge's existence in the global DAG $\mathbb{G}^*$.

4.1 Aggregation under imperfect CI-tests

The assumption of an Oracle CI-tester, while necessary for initial theoretical guarantees, is invariably violated in practice due to factors like model capacity, limited data or class imbalance. The extracted one-shot graphs will most likely violate the independencies in $\mathbb{G}_k$ and thus $\mathbb{G}^*$.

Let us model the performance of our one-shot CI-test for any potential edge $X_i \to Y_j$ with the following error rates: (1) False Positive Rate (Type I Error): $\alpha = P(\text{detect} \mid \text{edge is spurious})$ (2) True Positive Rate (Sensitivity): $1 - \beta = P(\text{detect} \mid \text{edge is causal})$. We operate under the reasonable assumption that our one-shot classifier is significantly better than random, which implies that $1 - \beta \gg \alpha$. The expected value of our Bernoulli variable $Z_{i,j}^k$ is now:

$$\begin{aligned}\mathbb{E}[Z_{ij}^k] &= P(Z_{ij}^k = 1) \\ &= P(\text{detect} \mid \text{causal})P(\text{causal}) + P(\text{detect} \mid \text{spurious})P(\text{spurious}) \\ &= (1-\beta)\pi_{ij} + \alpha(1-\pi_{ij})\end{aligned}$$

The empirical frequency now converges to this new expectation. For a true edge ($\pi_{i,j} = 1$), the empirical frequency converges to a high value: $\hat{\pi}_{ij}(m) \xrightarrow{p} 1 - \beta$ and for spurious edge ($\pi_{i,j} = 0$) it converges to a low value: $\hat{\pi}_{ij}(m) \xrightarrow{p} \alpha$ This reveals the critical role of frequency aggregation as a mechanism for separating signal from noise.

4.2 Adaptive Fusion for Structural Discovery in Long-Tail Distributions

A primary challenge in real-world causal discovery is the long-tail distribution of outcome labels, where a few "head" labels possess abundant data while the vast majority of "tail" labels are data-sparse [52].

For rare labels, where empirical edge frequencies are high-variance estimators, a conservative high threshold is necessary to maintain precision against statistical noise. Conversely, for common labels where frequencies are reliable, a high threshold would be overly stringent, purging weaker but valid causal links. To resolve this, we introduce an adaptive thresholding strategy (Fig. 7) that tailors the edge inclusion criterion to the statistical power available for each label. We define a label-specific threshold τ_j, as a logistic decay function of its sample support m_j:

$$\tau_j(m_j) = (\tau_{\max} - \tau_{\min}) \cdot \frac{1}{1 + e^{k(\log m_j - \log m_0)}} + \tau_{\min} \tag{8}$$

This function smoothly interpolates between a user-defined maximum threshold, τ_{max} (prioritising precision for the tail), and a minimum, τ_{min} (prioritising recall for the head). Crucially, the function's behaviour is calibrated by the data's distribution. Such that decay midpoint m_0 is set to the median of all label supports, providing a robust anchor point against skew.

The decay rate, k is made inversely proportional to the log-inter-quartile range of supports such that $k = \frac{2 \log 3}{\log q_{75} - \log q_{25}}$. For rare labels with small m_j, the high variance of the frequency estimate necessitates a high threshold $\tau_j(m_j)$ that acts as a strong regularizer. For common labels with large m_j, the LLN guarantees the convergence of $\hat{\pi}_{i,j}$ to the true edge probability, justifying a lower threshold to capture a more complete causal structure. Hence, this strategy effectively functions as a data-driven denoising mechanism and shares theoretical parallels with ensembling methods [1, 54] to enhance the robustness and accuracy of the final fused graph.

5 Empirical Evaluation

Settings & Vehicle Dataset. We used a $g4dn.12xlarge$ instance from AWS Sagemaker to run comparisons. It contains 48 vCPUs and 4 NVIDIA T4 GPUs. We used a combination of F1-Score,

Figure 3: Example of an error pattern (y_1) defined as a boolean rules of diagnosis trouble codes (x_i)

$$y_1 = x_1 \ \& \ x_5 \ \& \ x_8 \ \& \ x_{18} \ \& \ x_{12} \ \& \ x_3 \ \& \ !x_{10} \ \& \ !x_{20}$$

Precision, and Recall with different averaging [53] to perform comparisons. We evaluated our method on a real-world vehicular test set of $m = 300,000$ sequences, with $|\mathbb{Y}| = 474$ different error patterns and $|\mathbb{X}| = 29,100$ different DTCs forming sequences of $\approx 100 \pm 35$ events. We used Tf_x and Tf_y with 90m and 15m parameters [27]. The two NADEs didn't see the test set during training. The error patterns are manually defined by domain experts as boolean rules between DTCs (Fig. 3). We set the elements of this rule as the correct Markov Boundary for each label y_j in the tested sequences.

Multi-label Causal Discovery Comparisons. We benchmark CARGO against local structure learning (LSL) algorithms that estimate Markov Boundaries. This includes established approaches such as CMB [8], MB-by-MB [48], PCD-by-PCD [50], IAMB [46] from the *PyCausalFS* package [51], as well as the more recent, state-of-the-art MI-MCF [25]. 6 random folds of the test data were created and converted into a multi-one-hot data-frame where one row represents one sequence and each column represents an event type or label $(\mathbb{X}, \mathbb{Y})$.

Ablation on Aggregation Criterions for Phase 2. We provide an Ablation of the different criterion used in the structural fusion of Markov Boundaries. Union stands for a simple union over all edges without any removal. Frequency or edge voting, counts how often is $X_i \in \text{MB}(Y_j)$. Then apply a static frequency threshold $\tau = [0.05, 0.25, 0.5, 0.8]$. MI uses the mutual information between events and label as criterion in a Background Equivalence Search [2]. Expected FPR (false positive ratio) [7] describes two beta distributions which are fitted using the distribution of the mutual information $I(X_i, Y_j)$ extracted from Phase 1. The lower tail is used for outlier detection. Different FPR are chosen $\beta = [0.01, 0.05, 0.15, 0.2]$. Detailed definitions can be found in Appendix C.4.

5.1 Results

Comparisons. We performed comparaisons on Table 1 with $n = 50,000$ random sequences. We found out that even under this reduced setup, LSL algorithms failed to compute the Markov Boundaries within multiple days (3 days timeout), far exceeding practical limits for deployment. This behaviour highlights the current infeasibility of multi-label causal discovery in high-dimensional event sequences. Current algorithms are cursed under high-dimensional data since they rely on expensive CI testing that scales quadratically with the number of nodes [11]. This positions CARGO as a more feasible approach for large-scale, multi-label causal discovery.

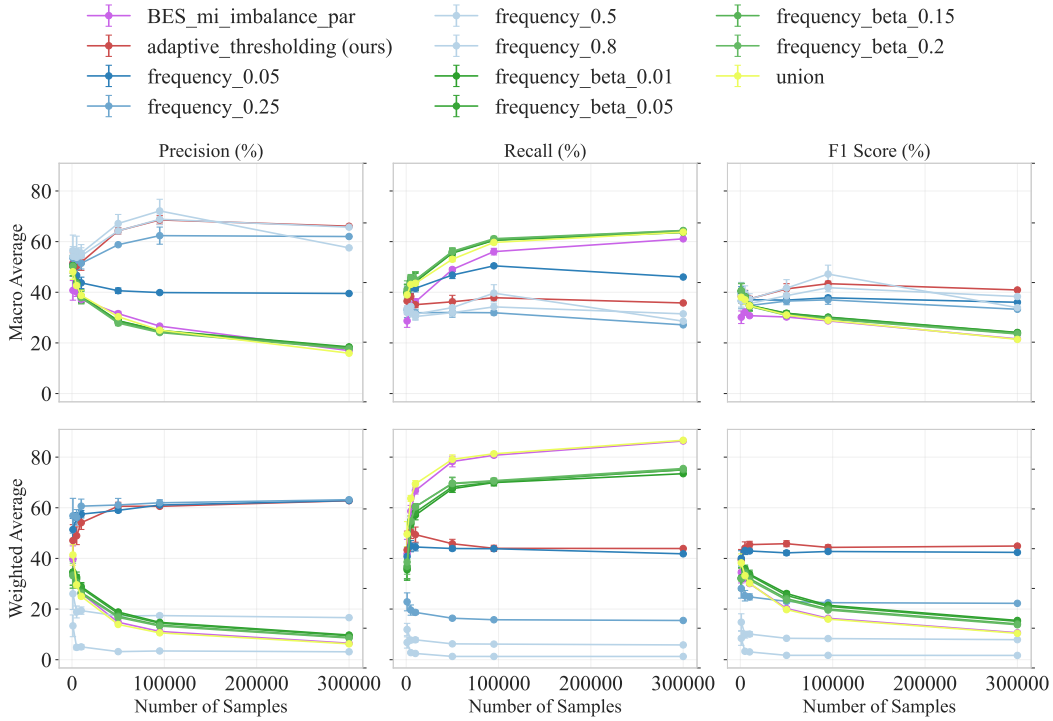
Table 1: Comparisons of **MB** retrieval with $m = 50,000$ samples averaged over $6-$folds with $|Y| = 474, |X| = 29,100$ nodes. Averaging is 'weighted'. The symbol '-' indicates that the algorithm didn't output the **MBs** within 3 days. Metrics are given in $\%$.

Algorithm	Precision↑	Recall↑	F1↑	Running Time (min)↓
IAMB	-	-	-	> 4320
CMB	-	-	-	> 4320
MB-by-MB	-	-	-	> 4320
PCDbyPCD	-	-	-	> 4320
MI-MCF	-	-	-	> 4320
CARGO	$\mathbf{60.6 \pm 1.5}$	$\mathbf{45.8 \pm 1.7}$	$\mathbf{45.8 \pm 1.2}$	$\mathbf{11.7}$

Criterions. Figure 4 illustrates the impact of aggregation choices during Phase 2. A naïve Union maximizes recall (84% for weighted) but suffers from poor precision. When optimising a local scoring criterion as the mutual information BES mi, didn't enhance significantly the performance over a basic Union.

Moreover, instead of optimising a score, fitting Beta distributions to detect outliers using their mutual information seems to work better; hence frequency beta is ahead, particularly with a lower FPR ratio. Frequency approaches with a static threshold confirms the analysis in Section 4.1. When a large number of samples per class m_j is available, the frequency cut-off τ needs to be lower to not penalise classes with big support. Thus, we see that frequency with $\tau = [0.5, 0.8]$ have the lower

Figure 4: Comparison of different criterions for the structural fusion (Phase 2) in function of the number of samples m. With $|Y| = 474, |X| = 29,100$ nodes.



weighted f1 score of all criterions. On the otherhand, a small cut-off $\tau = [0.05, 0.25]$ enables a huge improvement in the weighted average ($+40\%$ precision), but decrease its macro average metrics (-20% in precision).

Finally, our adaptive thresholding criterion leverages a small threshold for big supports and a big threshold for small supports, which takes advantage of the long-tail distribution. As a result, it is first on both averagings, with respectively 44.88% and 40.9% for weighted and macro f1 score, and 62.8% and 66.1% for weighted and macro precision.

6 Conclusion

We introduced CARGO, a novel framework for multi-label causal discovery in high-dimensional event sequences. By combining one-shot causal discovery with adaptive frequency-aware aggregation, CARGO successfully recovers interpretable causal structures from noisy observational data—achieving results in minutes where classical methods fail to scale.

CARGO could scale further by leveraging general-purpose foundation models for sequences (e.g., time-series transformers pretrained across domains). Such models could extend the applicability beyond automotive diagnostics to healthcare, cybersecurity, and other structured domains.

Under the temporal assumptions, large samples, faithfulness and perfect CI-test, CARGO recovers the true set of Markov Boundaries. However, we underlined the practical limitations, in particular long-tail distributions, a common trait in high-dimensional labeled data. Future work should extend this framework to support event-to-event causality and possibly relax assumptions such as bounded lagged effects or temporal precedence.

Ultimately, CARGO demonstrates how structured probabilistic methods can bridge the gap between causal discovery theory and scalable, practical deployment in complex industrial systems.

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Justification: The data characteristics, such as the number of sequences, events, labels, mean and standard deviation of the sequence length, are provided in the experiment section. Hyperparameters such as the sampling number N or the confidence parameter k are provided as ablation studies in Appendix C.2, C.3, as well as the NADEs configuration in Table 2.

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Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

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Justification: Results of the experiments are reported using mean and one standard deviation after 6 runs on 6 random data samples (Table 1). The classification performance as a function of the number of samples is reported using 1-sigma error bars in Figure 4 and shown for two different averaging methods across several runs on the same data sample. Ablation studies are also given using 1-sigma error bars to appropriately choose the hyperparameters in Section C.2, C.3.

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A Notations and Definitions

A.1 Notations

We use capital letters (e.g., X) to denote random variables, lower-case letters (e.g., x) for their realisations, and bold capital letters (e.g., $\boldsymbol{X}$) for sets of variables. Let $\boldsymbol{U}$ denote the set of all (discrete) random variables. We define the event set $\boldsymbol{X} = \{X_1, \ldots, X_n\} \subset \boldsymbol{U}$, and the label set $\boldsymbol{Y} = \{Y_1, \ldots, Y_n\} \subset \boldsymbol{U}$. When explicitly said, event $X_i^{(t_i)}$ represent the occurrence of X_i at the sequence step i and time t_i. Similarly for $Y_{i+1}^{(t_{i+1})}$.

A.2 Definitions

Definition 1 (Faithfulness)**.** *Spirtes et al. [41]. Given a BN $< \boldsymbol{U}, \mathbb{G}, P >$, $\mathbb{G}$ is faithful to P if and only if every conditional independence present in P is entailed by $\mathbb{G}$ and the Markov condition holds. P is faithful if and only if there exist a DAG $\mathbb{G}$ such that $\mathbb{G}$ is faithful to P.*

Definition 2 (Conditional Independence)**.** *Variables X and Y are said to be conditionally independent given a variable set $\boldsymbol{Z}$, if $P(X, Y|\boldsymbol{Z}) = P(X|\boldsymbol{Z})P(Y|\boldsymbol{Z})$, denoted as $X \perp Y|\boldsymbol{Z}$. Inversely, $X \not\perp Y|\boldsymbol{Z}$ denotes the conditional dependence. Using the conditional mutual information [3] to measure the independence relationship, this implies that $\boldsymbol{I}(X, Y|\boldsymbol{Z}) = 0 \Leftrightarrow X \perp Y|\boldsymbol{Z}$.*

Definition 3 (Markov Boundary)**.** *Tsamardinos and Aliferis [45]. In a faithful BN $< \boldsymbol{U}, \mathbb{G}, P >$, for a set of variables $\boldsymbol{Z} \subset \boldsymbol{U}$ and label $Y \in \boldsymbol{U}$, if all other variables $X \in \{\boldsymbol{X} - \boldsymbol{Z}\}$ are independent of Y conditioned on $\boldsymbol{Z}$, and any proper subset of $\boldsymbol{Z}$ do not satisfy the condition, then $\boldsymbol{Z}$ is the Markov Boundary of Y: $\boldsymbol{MB}(Y)$.*

Definition 4. *(Markov Equivalence Class). Two distinct graph $\mathbb{G}, \mathbb{G}'$ are said to belong to the same Markov Equivalence Class (MEC) if they have the same set of conditional independencies i.e $I(\mathbb{G}) = I(\mathbb{G}')$.*

Definition 5. *(Decomposable Criterion). We say that a scoring criterion $S(\mathbb{G}, D)$ is decomposable if it can be written as a sum of measures, each of which is a function only of one node and its parents. In other words, a decomposable scoring criterion $\mathbb{S}$ applied to a DAG $\mathbb{G}$ can always be expressed as:*

$$S(\mathbb{G}, \boldsymbol{D}) = \sum_{i}^{n} s(X_i, \boldsymbol{Pa}_i^{\mathbb{G}}) \tag{9}$$

Definition 6 (Score equivalent)**.** *Chickering [2]. A score S is score equivalent if it assigns the same score to all the graphs in the same MEC.*

Definition 7 (Local Consistency)**.** *Chickering [2] Let $\boldsymbol{D}$ contain m iid samples from some distribution $p(.)$. Let $\mathbb{G}$ be any possible DAG and $\mathbb{G}'$ a different DAG obtained by adding the edge $i \to j$ to $\mathbb{G}$. A score S is locally consistent if both hold:*

- *If $X_i \not\perp_p X_j|Pa_j^{\mathbb{G}}$, then $S(\mathbb{G}', \boldsymbol{D}) > S(\mathbb{G}, \boldsymbol{D})$*
- *If $X_i \perp_p X_j|Pa_j^{\mathbb{G}}$, then $S(\mathbb{G}', \boldsymbol{D}) < S(\mathbb{G}, \boldsymbol{D})$*

A.3 Assumptions

Assumption 1 (Temporal Precedence)**.** *Given a perfectly recorded sequence of events $((x_1, t_1), \cdots, (x_L, t_L))$ with labels $(\boldsymbol{y}_L, t_L)$ and monotonically increasing time of occurrence $0 \leq t_1 \leq \cdots \leq t_L$, an event x_i is allowed to influence any subsequent event x_j such that $t_i \leq t_j$ and $i < j$. Formally, the graph $\mathbb{G} = (\boldsymbol{U}, \boldsymbol{E})$, $(x_i, x_j) \in \boldsymbol{E} \implies t_i \leq t_j$ and step $i < j$*

It allows us to remove ambiguity in causal directionality, and is a widely used assumption across time-series and sequential data [11].

Assumption 2 (Bounded Lagged Effects)**.** *Once we observed events up to timestamp t_i and step i as $\boldsymbol{Z}_{\leq t_i} = ((x_1, t_1), \cdots, (x_i, t_i))$, any future lagged copy of event $X_i^{(t_i+\tau)}$ is independent of Y_j conditioned on $\boldsymbol{Z}_{\leq t_i}$:*

$$Y_j \perp X_i^{(t_i+\tau)} | \boldsymbol{Z}_{\leq t_i}$$

Where $\tau = t_{i+1} - t_i$ is a finite bound on the allowed time delay for causal influence.

In other words, we allow the causal influence of event X_i on Y_j until the next event X_{i+1} is observed. We note that for data with strong lagged effects (e.g., financial transactions), this might not hold well, but for log-based and error code-based data this is usually correct.

Assumption 3 (Causal Sufficiency for Labels)**.** *All relevant variables are observed, and there are no hidden confounders affecting the labels.*

Assumption 4 (Oracle Models)**.** *We assume that two autoregressive Transformer models, Tf_x and Tf_y, are trained via maximum likelihood on a dataset of multi-labeled event sequences $D = \{S_l^1, \cdots, S_l^m\} \subset \mathbb{S}$, and can perfectly approximate the true conditional distributions of events and labels:*

$$P(X_i|Pa(X_i)) = P_{\theta_x}(X_i|Pa(X_i)) = Tf_x(S_{<i}),\ P(Y_j|Pa(Y_j)) = P_{\theta_y}(Y_j|Pa(Y_j)) = Tf_y(S_{\leq i}) \tag{10}$$

A.4 Lemmas

Lemma 1 (Identifiability of $\mathbb{G}$)**.** *Assuming the faithfulness condition holds for the true causal graph $\mathbb{G}$. Let Tf_x and Tf_y be oracle models that model the true conditional distributions of events and labels, respectively. The joint distribution P_{θ_x,θ_y} can then be constructed, and any conditional independence detected from the distributions estimated by Tf_x and Tf_y corresponds to a conditional independence in $\mathbb{G}$:*

$$X_i \perp_{\theta_x,\theta_y} Y_j \mid \boldsymbol{Z} \quad \Longrightarrow \quad X_i \perp_{\mathbb{G}} Y_j \mid \boldsymbol{Z}.$$

Where $\perp_{\theta_x,\theta_y}$ denotes the independence entailed by the joint probability P_{θ_x,θ_y}.

Lemma 2 (Markov Boundary Equivalence)**.** *In a multi-label event sequence S_l and under the temporal precedence assumption A1, the Markov Boundary of each label Y_j is only its parents such that $\forall X \in \{\boldsymbol{U} - Pa(Y_j)\}, X \perp Y_j|Pa(Y_j) \Leftrightarrow MB(Y_j) = Pa(Y_j)$.*

B Proofs

We provide proofs for the results described in Section 3

B.1 Proof of Lemma 1

Proof. We assume that the data is generated by the associated causal graph $\mathbb{G}$ following the sequential BN from a multi-labelled sequence S. And that the faithfulness assumption holds [32], meaning that all conditional independencies in the observational data are implied by the true causal graph $\mathbb{G}$.

Given that the Oracle models Tf_x and Tf_y are trained to perfectly approximate the true conditional distributions, for any variable U_i in the graph, we have:

$$P(U_i|\text{Pa}(U_i)) = \begin{cases} P(Y_j|\text{Pa}(Y_j)) = P_{\theta_y}(Y_j|\text{Pa}(Y_j)), & \text{if } U_i \in \boldsymbol{Y} \\ P(X_i|\text{Pa}(X_i)) = P_{\theta_x}(X_i|\text{Pa}(X_i)), & \text{otherwise.} \end{cases}$$

The joint distribution P_{θ_x,θ_y} can then be constructed using the chain rule $P_{\theta_x,\theta_y}(X_1, \cdots, X_i, Y_1, \cdots, Y_c) = \prod_{k=0}^{i} P(X_k|Pa(X_k)) \prod_l^c P(Y_l|\text{Pa}(Y_l)$. By the faithfulness assumption [32], if the conditional independencies hold in the data, they must also hold in the causal graph $\mathbb{G}$:

$$X_i \perp Y_j|\boldsymbol{Z} \implies X_i \perp_{\mathbb{G}} Y_j|\boldsymbol{Z}$$

Since we can approximate the true conditional distributions, it follows that:

$$X_i \perp_{\theta_x,\theta_y} Y_j|\boldsymbol{Z} \implies X_i \perp Y_j|\boldsymbol{Z} \implies X_i \perp_{\mathbb{G}} Y_j|\boldsymbol{Z}$$

Where $\perp_{\theta_x,\theta_y}$ denotes the independence entailed by the joint probability P_{θ_x,θ_y}. Thus, the graph $\mathbb{G}$ can be identified from the observational data. □

B.2 Proof of Lemma 2

Proof. Let $< \boldsymbol{U}, \mathbb{G}, P >$ be the sequential BN composed of the events from the multi-labeled sequence $S_l = (\{(t_1, x_1, \cdots, (t_L, x_L)\}_{i=1}^{L}, (\boldsymbol{y}_L, t_L))$. Following the temporal precedence assumption

A1, the labels $\boldsymbol{y_L}$ can only be caused by past events $(x_1, \cdots, x_L)$; moreover by definition, labels do not cause any other labels. Thus, Y_j has no descendants, so no children and spouses. Therefore, together with the Markov Assumption we know that $\forall X \in \{\boldsymbol{U} - Pa(Y_j)\} : Y_j \perp X | Pa(Y_j)$. Which is the definition of the MB (Def. 3). Thus, $\mathbf{MB}(Y_j) = Pa(Y_j)$.

□

B.3 Proof of Theorem 1.

Proof. By recurrence over the sequence length L of the multi-label sequence S_l^k, we want to show that under temporal precedence A1, bounded lagged effects A2, causal sufficiency A3, Oracle Models A4 the Markov Boundary of label Y_j can be identified in the causal graph $\mathbb{G}$.

Let's define $\mathcal{M}_j^L$ as the estimated Markov Boundary of Y_j after observing L events.

Base Case: $\mathbf{L = 1}$: Consider the BN for step $L = 1$ following the Markov assumption [32] with two nodes X_1, Y_j. Using Tf_x, Tf_y as Oracle Models A4, we can express the conditional probabilities for any node U:

$$P(U|\text{Pa}(U)) = \begin{cases} P(X_1) = P_{\theta_x}(X_1|[CLS]) \text{ if } U \in \boldsymbol{X} \\ P(Y_j|X_1) = P_{\theta_y}(Y_j|X_1) \text{ otherwise} \end{cases} \tag{11}$$

Assuming that P is faithful (A1) to $\mathbb{G}$, no hidden confounders bias the estimate (A3) and temporal precedence (A1), we can estimate the CMI 4 such that iif $I(X_1, Y_j)|\emptyset) > 0 \Leftrightarrow Y_j \not\perp_{\theta_x,\theta_y} X_1 \implies Y_j \not\perp_{\mathbb{G}} X_1$ (Lemma 1).

Since we assume temporal precedence A1, we can orient the edge such that X_1 must be a parent of Y_j in $\mathbb{G}$. Using Lemma 2, we know that $Par(Y_j) = \mathbf{MB}(Y_j) \implies X_1 \in \mathbf{MB}(Y_j)$, thus we must include X_1 in M_j^1, otherwise not.

Heredity: For $L = i$, we obtained M_j^i with the sequential BN up to step $L = i$. Now for $L = i + 1$, the sequential BN has $i + 2$ nodes denoted as $\boldsymbol{U'} = (X_1, \cdots, X_i, X_{i+1}, Y_j)$. Using the Oracle Models A4 and following the Markov assumption [32], we can estimates the following conditional probabilities for any nodes $U \in \boldsymbol{U'}$:

$$P(U|\text{Pa}(U)) = \begin{cases} P(Y_j|\text{Pa}(Y_j)) \approx P_{\theta_y}(Y_j|\text{Pa}(Y_j)), & \text{if } U \in \boldsymbol{Y} \\ P(X|\text{Pa}(X)) \approx P_{\theta_x}(X|\text{Pa}(X)), & \text{otherwise.} \end{cases} \tag{12}$$

By bounded lagged effects (A2) we know that the causal influence of past $X_{\leq i}$ on Y_j has expired. Moreover, no hidden confounders (A3) bias the independence testing. Finally, using Eq. (4) we can estimate the CMI such that iif $I(Y_j, X_{i+1}|\boldsymbol{Z}) > 0 \Leftrightarrow Y_j \not\perp_{\theta_x,\theta_y} X_{i+1}|\boldsymbol{Z} \implies Y_j \not\perp_{\mathbb{G}} X_{i+1}|\boldsymbol{Z}$ (Lemma 1).

Since we assume temporal precedence A1, we can orient the edge so that X_{i+1} must be a parent of Y_j in $\mathbb{G}$. Using Lemma 2, we know that $Par(Y_j) = \mathbf{MB}(Y_j) \implies X_{i+1} \in \mathbf{MB}(Y_j)$. Thus $X_{i+1} \in M_j^{i+1}$ which represent the $\mathbf{MB}(Y_j)$ for step $i + 1$.

Finally, $\mathcal{M}_j^{i+1}$ still recovers the Markov Boundary of Y_j such that

$$\forall U \in \{\boldsymbol{U'} - \mathcal{M}_j^{i+1}\}, Y_j \perp U | \mathcal{M}_j^{i+1}$$

□

C Ablations

C.1 NADEs Quality.

We did several ablations on the quality of the NADEs and their impact on the one-shot causal discovery phase. In particular, Table 2 presents multiple Tf_x, Tf_y with respectively 90 and 15 million parameters or 34 and 4 million parameters. We also varied the context window (conditioning set $\boldsymbol{Z}$), trained on different amounts of data (tokens) and reported the classification results on the test set of Tf_y alone. We didn't output the running time since it was approximately the same for all NADEs: 1.27 minutes of 50,000 samples and 0.14 for 5000.

We observe that scaling up the NADEs model size and the trained data show the biggest improvements. After, it is via the context c, which after $c = 15$ shows declined performance for a larger number of samples. We then choose the backbone with 1.5B Tokens, 105m parameters and a context $c = 15$ for our experiments.

Table 2: Ablations of the performance of Phase 1 (One-shot **MB** retrieval) in function of different NADEs with $m = 50{,}000$ and $m = 500$ samples averaged over 6-folds. Classification metrics use weighted averaging. Metrics are given in $\%$.

Tokens	**Parameters**	**Context**	**Precision (↑)**	**Recall (↑)**	**F1 Score (↑)**	**Tfy F1 (↑)**
			For $n = 50{,}000$ *samples*			
1.5B	105m	$c = 4$	47.95 ± 1.05	30.65 ± 0.51	37.39 ± 0.67	88.6
1.5B	105m	$c = 12$	54.62 ± 1.03	29.88 ± 0.73	38.63 ± 0.85	90.43
1.5B	105m	$c = 15$	$\mathbf{55.26 \pm 1.42}$	$\mathbf{31.37 \pm 0.82}$	$\mathbf{40.02 \pm 1.03}$	90.57
1.5B	105m	$c = 20$	49.52 ± 1.59	$\mathbf{31.76 \pm 0.85}$	36.54 ± 1.10	91.19
1.5B	105m	$c = 30$	36.65 ± 1.18	22.75 ± 0.78	26.57 ± 0.91	**92.64**
300m	47m	$c = 20$	39.49 ± 1.77	26.30 ± 0.89	29.01 ± 1.10	83.6
			For $n = 500$ *samples*			
1.5B	105m	$c = 12$	54.84 ± 4.55	$\mathbf{31.45 \pm 2.23}$	$\mathbf{39.95 \pm 2.83}$	90.43
1.5B	105m	$c = 15$	55.04 ± 3.36	29.90 ± 1.78	38.74 ± 2.24	90.57
1.5B	105m	$c = 20$	48.84 ± 4.01	$\mathbf{31.65 \pm 2.37}$	36.19 ± 2.65	**91.19**
300m	47m	$c = 20$	38.23 ± 2.91	25.31 ± 2.39	27.92 ± 2.25	83.6

C.2 Sampling Number

We experimented with different numbers of n for the sampling method across different averaging (micro, macro, weighted), Fig. 5. We performed 8 different runs and reported the average, standard deviation and elapsed time. We can say that generally, sampling with a bigger N tends to decrease the standard deviation and give more reliable Markov Boundary estimation. Moreover, as we process more samples, the model is gradually improving at a logarithmic growth until it converges to a final score. We also verify that our time complexity is linear with the number of samples N. Based on these results, we choose generally $N = 68$ as the number of samples.

C.3 Dynamic Thresholding

We performed ablations on the effect of k during the dynamic thresholding of the CMI (Eq. (7)) to access conditional independence in Fig. 6. To balance the classification metrics across the different averaging, we set $k = 2.75$.

Figure 5: Evolution of several classification metrics (one-shot) and elapsed time per sample in function of the number of samples N chosen. Results are reported using 1-sigma error bar.

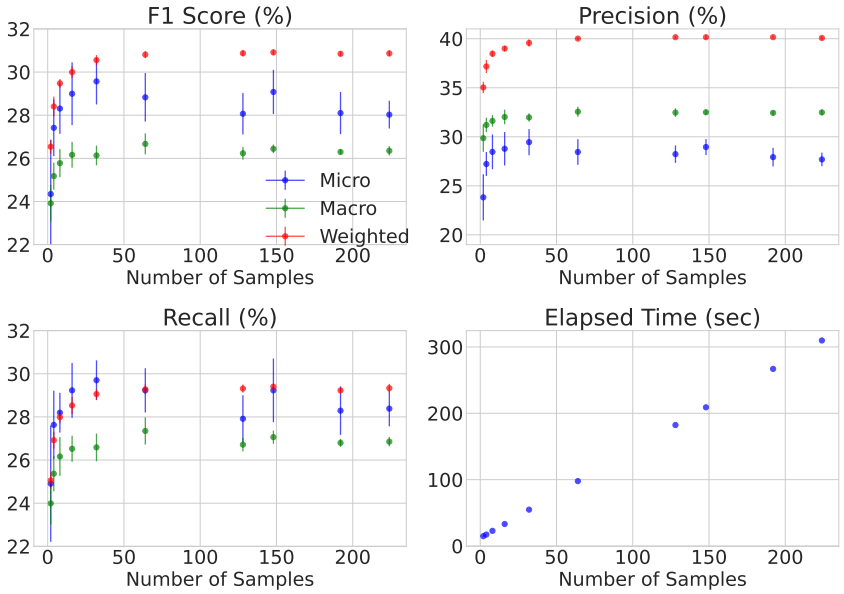
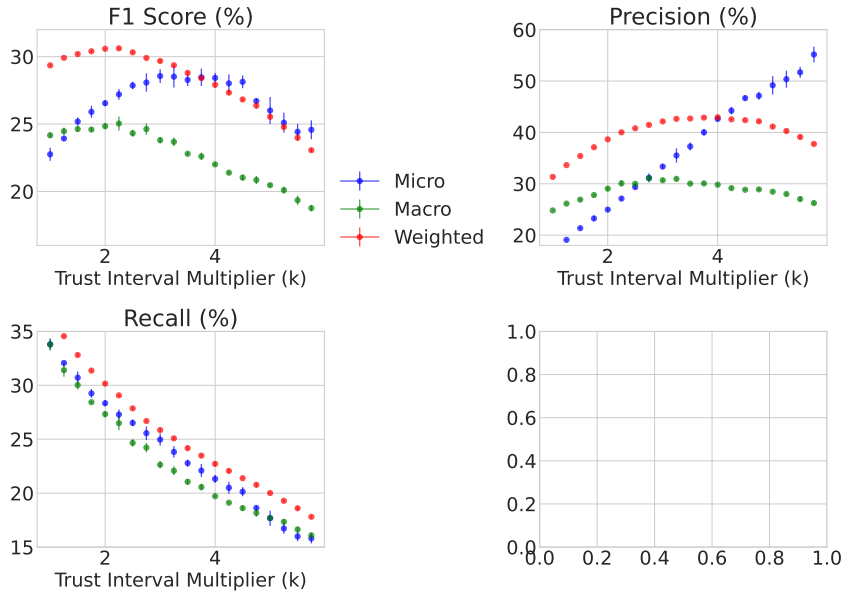


Figure 6: Evolution of one-shot F1 Score, Precision and Recall in function of coefficient k. Results are reported using 1-sigma error bar.



C.4 Criterions

This section presents the different criteria used for comparison in the experimental evaluation.

C.5 Frequency

Frequency-based heuristics that apply fixed thresholds τ to the empirical frequency of the occurrence of X_i in each of the Markov Boundary $\mathbf{MB}(Y_j)$. Formally, For each label Y_j, after merging all local edge sets into a global set $E = \bigcup_{i=1}^{m} E_i$, we evaluate each candidate variable $X_i \in \mathbf{MB}_j$ based on

its frequency of appearance across the local models. If this frequency exceeds the threshold τ, the variable is retained in the final merged $\mathbf{MB}_j$; otherwise, it is discarded.

C.5.1 Expected FPR Adjustment

Same principle as in [7] except that we fit the two Beta distributions on the mutual information of $I(Y_j, X_i)$ instead of the raw frequencies.

C.5.2 Mutual Information

BES The BES is the second phase of GES [2], where edges are removed one after the other to maximise a criterion S. Heuristics approaches [34, 5] aim to solve this problem by optimizing:

$$E = \underset{E_i \in \varepsilon}{\arg\max} \sum_{e \in E_i} S(e) \tag{13}$$

Where ε denotes the search space (all possible edges over $\boldsymbol{U}$) and $S(e)$ a criterion function for edge relevance (e.g. edge frequency, thresholds, $\cdots$). This formulation takes into account the underlying edges' characteristics but not the overall network structure, complexity and missing data [31], leading to a *consensus fusion approach* [43].

Estimating Mutual Information in Event Sequences. We would like to reuse the estimated conditional mutual information, Eq. (4) and profit from the parallelised inference of Phase 1 (Fig. 2).

As argued out by Janzing et al. [17], a causal strength measure (or criterion) $C_{X_i \to Y_j}$ should possess multiple properties. Notably that if $C_{X_i \to Y_j} = 0$, then the joint distribution satisfies the Markov condition with respect to the DAG obtained by removing the arrow $X_i \to Y_j$. Moreover, the true DAG reads $X_i \to Y$ iff $C_{X_i \to Y_j} = I(X_i, Y_j)$.

It comes as a natural criterion to merge edges from multiple causal graphs. However, it remains tricky to estimate [18]. Using the chain rule of conditional mutual information [3], we can rewrite it as:

$$I(Y_j, X_i | \boldsymbol{Z}) = I(Y_j, X_i) - I(Y_j, X_i, \boldsymbol{Z}) \tag{14}$$

Where $I(Y_j, X_i, \boldsymbol{Z})$ is the interaction information [4], which tells us wether knowing $\boldsymbol{Z}$ explains away the dependency between X_i and Y_j (negative interaction), or enhances it (positive interaction):

$$I(Y_j, X_i, \boldsymbol{Z}) \triangleq I(Y_j, \boldsymbol{Z}) - I(Y_j, \boldsymbol{Z} | X_i)$$

$I(Y_j, \boldsymbol{Z})$ can be estimated using the same Monte-Carlo sampling as for $I(Y_j, X_i | \boldsymbol{Z})$ (4). Since $I(Y_j, \boldsymbol{Z}) = H(Y_j) - H(Y | \boldsymbol{Z_j})$, the marginal $p(y)$ is needed. Fortunately, the dataset $\boldsymbol{D}$ is large enough, hence the frequencies of y_j are recovered empirically and an estimate $\hat{p}(y)$ which we assume to be equal to the true marginal $p(y)$. We acknowledge that under a restricted dataset, $\hat{p}(y)$ might differ from $p(y)$. This yields to:

$$I(Y_j, \boldsymbol{Z}) = \mathbb{E}_z D_{KL}(P(Y_j | \boldsymbol{Z}) || \hat{P}(Y_j)) = \mathbb{E}_z I_G(Y_j, z) \tag{15}$$

Formally, we assume that for long sequences i.e $i \to +\infty$, our event sequences form a stationary ergodic stochastic process and $I(Y_j, \boldsymbol{Z} | X_i)$ is negligible compare to $I(Y_j, \boldsymbol{Z})$ since $\boldsymbol{Z}$ is containing most of the information to predict Y_j. This reduces the mutual information to

$$I(Y_j, X_i) \approx I(Y_j, X_i | \boldsymbol{Z}) + I(Y_j | \boldsymbol{Z})$$

Criterion. We propose a **Class-Aware Information Gain (CAIG)** score for evaluating candidate edges during Phase 2 of CARGO. Given m i.i.d. samples from a dataset $\boldsymbol{D}$, CAIG balances three key factors: mutual information derived from information gain, class imbalance, and network complexity.

For each label node Y_j, with candidate parent set $\mathbf{Pa}_j^{\mathbb{G}}$, the CAIG score is:

$$S(\mathbb{G}', \boldsymbol{D}) = \sum_{j=1}^{n} s_I(Y_j, \mathbf{Pa}_j^{\mathbb{G}}) - \alpha \cdot |\mathbf{Pa}_j^{\mathbb{G}}| \cdot \log\left(\frac{m}{m_j} + 1\right) \tag{16}$$

With $s_I(Y_j, \mathbf{Pa}_j^{\mathbb{G}}) = \sum_{X_i \in \mathbf{Pa}_j^{\mathbb{G}}} I(Y_j, X_i)$, α is a regularization hyperparameter, m_j is the number of positive instances for class Y_j.

This formulation encourages informative yet parsimonious graph structures, correcting for underrepresented labels via the regularisation term. It is also efficient since CAIG is decomposable [2] like BIC with the local s_I. This criterion is denoted as BES mi imbalance par in our experiments in Fig. 4.

D Implementation

D.1 Computation.

A key advantage of our approach is its scalability. Unlike traditional methods whose complexity depends on the event and label cardinality $|\mathbb{X}|$ and $|\mathbb{Y}|$ [22], our method is agnostic to both. As illustrated in Figure 2, all steps are parallelised on GPUs. CMI estimations are independently performed for all positions $i \in [c, L]$, with the sampling pushed into the batch dimension and results averaged across labels, leading to BS $\times N \times L$ CI-tests per batch $D = \{S_l^0, \ldots, S_l^m\}$. Consequently, time complexity transitions from $\mathcal{O}(\text{BS} \times N \times L)$ to $\mathcal{O}(1)$ per batch due to GPU parallelism. The complexity is bounded by the Transformers' inference part, where it scales quadratically with the sequence length $\mathcal{O}(L^2)$ if one uses vanilla self-attention [47].

D.2 Phase 1

The following is the implementation of the one-shot phase in PyTorch [30].

```
def topk_p_sampling(z, prob_x, c: int, n: int = 64, p: float = 0.8, k: int = 35,
                    cls_token_id: int = 1, temp: float = None):
    # Sample just the context
    input_ = prob_x[:, :c]

    # Top-k first
    topk_values, topk_indices = torch.topk(input_, k=k, dim=-1)

    # Top-p over top-k values
    sorted_probs, sorted_idx = torch.sort(topk_values, descending=True, dim=-1)
    cum_probs = torch.cumsum(sorted_probs, dim=-1)
    mask = cum_probs > p

    # Ensure at least one token is kept
    mask[..., 0] = 0

    # Mask and normalize
    filtered_probs = sorted_probs.masked_fill(mask, 0.0)
    filtered_probs += 1e-8  # for numerical stability
    filtered_probs /= filtered_probs.sum(dim=-1, keepdim=True)

    # Unscramble to match the original top-k indices
    # Need to reorder the sorted indices back to the original top-k
    reorder_idx = torch.argsort(sorted_idx, dim=-1)
    filtered_probs = torch.gather(filtered_probs, -1, reorder_idx)

    batched_probs = filtered_probs.unsqueeze(1).repeat(1, n, 1, 1)
        # (bs, n, seq_len, k)
    batched_indices = topk_indices.unsqueeze(1).repeat(1, n, 1, 1)
        # (bs, n, seq_len, k)

    sampled_idx = torch.multinomial(batched_probs.view(-1, k), 1)
        # (bs*n*seq_len, 1)
    sampled_idx = sampled_idx.view(-1, n, c).unsqueeze(-1)

```

```
    sampled_tokens = torch.gather(batched_indices, -1, sampled_idx).squeeze(-1)
    sampled_tokens[..., 0] = cls_token_id

    # Reconstruct full sequence
    z_expanded = z.unsqueeze(1).repeat(1, n, 1)[..., c:]
    return torch.cat((sampled_tokens, z_expanded), dim=-1)

from torch import nn
def OneShotCD(tfe: nn.Module, tfy: nn.Module, batch: dict[str, torch.Tensor], c: int, n: int, eps: float=1e-6, topk: int=20, k: int=2.75, p=0.8) -> torch.Tensor:
    """ tfe, tfy: are the two autoregressive transformers (event type and label)
        batch: dictionary containing a batch of input_ids and attention_mask of shape (bs, L) to explain.
        c: scalar number defining the minimum context to start inferring, also the sampling interval.
        n: scalar number representing the number of samples for the sampling method.
        eps: float for numerical stability
        topk: The number of top-k most probable tokens to keep for sampling
        k: Number of standard deviations to add to the mean for dynamic threshold calculation
        p: Probability mass for top-p nucleus
    """
    o = tfe(attention_mask=batch['attention_mask'], input_ids=batch['input_ids'])['prediction_logits'] # Infer the next event type
    x_hat = torch.nn.functional.softmax(o, dim=-1)

    b_sampled = topk_p_sampling(batch['input_ids'], x_hat, c, k=topk, n=n, p=p) # Sampling up to (bs, n, L)
    n_att_mask = batch['attention_mask'].unsqueeze(1).repeat(1, n, 1)

    with torch.inference_mode():
        o = tfy(attention_mask=n_att_mask.reshape(-1, b_sampled.size(-1)), input_ids=b_sampled.reshape(-1, b_sampled.size(-1))) # flatten and infer
        prob_y_sampled = o['ep_prediction'].reshape(b_sampled.size(0), n, batch['input_ids'].size(-1)-c, -1) # reshape to (bs, n, L-c)

        # Ensure probs are within (eps, 1-eps)
        prob_y_sampled = torch.clamp(prob_y_sampled, eps, 1 - eps)

        y_hat_i = prob_y_sampled[..., :-1, :] # P(Yj|z)
        y_hat_iplus1 = prob_y_sampled[..., 1:, :] # P(Yj|z, x_i)

        # Compute the CMI & CS and average across sampling dim
        cmi = torch.mean(y_hat_iplus1*torch.log(y_hat_iplus1/y_hat_i)+(1-y_hat_iplus1)*torch.log((1-y_hat_iplus1)/(1-y_hat_i)), dim=1)
        # (BS, L, Y)
        cs = y_hat_iplus1 - y_hat_i
        cs_mean = torch.mean(cs, dim=1)
        cs_std = torch.std(cs, dim=1)

        # Confidence interval for threshold
        mu = cmi.mean(dim=1)
        std = cmi.std(dim=1)
        dynamic_thresholds = mu + std * k

        # Broadcast to select an individual dynamic threshold
        cmi_mask = cmi >= dynamic_thresholds.unsqueeze(1)

        cause_token_indices = cmi_mask.nonzero(as_tuple=False)
```

```
        # (num_causes, 3) --> each row is [batch_idx, position_idx, label_idx]
        return cause_token_indices, cs_mean, cs_std, cmi_mask
```

Remark. *Since tfy contains tfe as backbone, in practice we need only one forward pass from tfy and extract also $\hat{x}$, so tfe is not needed. We let it to improve understanding and clarity.*

D.3 Phase 2.

```
import random
def create_auto_adaptive_threshold_fn(all_m_j, tau_max=0.5, tau_min=0.05, k=None, m0="median"):
    m_0 = np.median(all_m_j)

    if k == None:
        q25, q75 = np.percentile(all_m_j, [25, 75])
        if q75 == q25:
            k = 1.0
        else:
            log_iqr = np.log(q75) - np.log(q25)
            k = (2 * np.log(3)) / log_iqr

    def threshold_function(m_j):
        log_m_j = np.log(m_j + 1e-9)
        log_m_0 = np.log(m_0)
        logistic_decay = 1 / (1 + np.exp(k * (log_m_j - log_m_0)))
        return (tau_max - tau_min) * logistic_decay + tau_min

    return threshold_function

def adaptive_thresholding_frequency(graphs: list,
                present_labels: dict,
                frequency_threshold: float = 0.5,
                k: float=None,
                tau_min: float=0.05,
                tau_max: float=0.5,
                m0: str="median",
                verbose=False,
                **kwargs):
    """
    Frequency voting: keep edges appearing with frequency > threshold across samples.

    :param graphs: list of local graphs (e.g., from Phase 1). Each graph is a dict[label][token] = list of stats.
    :param present_labels: labels present in evaluation
    :param frequency_threshold: e.g. 0.5 for majority, 0.8 for conservative
    :return: filtered_labels, sample_per_label, elapsed_time
    """
    start_time = datetime.now()
    # Step 1: Aggregate graphs
    labels, sample_per_label = union(graphs)  # user-defined union function
    old_labels = labels.copy()
    nodes = count_nodes(labels)
    samples = len(graphs)

    # Create threshold function
    auto_threshold_fn = create_auto_adaptive_threshold_fn(list(sample_per_label.values()), k=k, tau_max=tau_max, tau_min=tau_min, m0=m0)

    # Step 2: Frequency voting with dynamic thresholds
```

```
    edge_counts = defaultdict(lambda: defaultdict(int))  # edge_counts[label][token] = count

    for g in graphs:
        for label, token_dict in g.items():
            if label not in labels:
                continue
            for token in token_dict:
                edge_counts[label][token] += 1

    # Step 3: Keep edges above frequency threshold
    filtered_labels = defaultdict(dict)
    for label in labels:
        total = sample_per_label.get(label, samples)  # fallback to total graphs if missing
        for token, count in edge_counts[label].items():
            freq = count / total
            if freq >= auto_threshold_fn(sample_per_label.get(label, 1)):
                filtered_labels[label][token] = {'frequency': freq}
                if verbose:
                    print(f"[{label}] token {token} kept (freq={freq:.2f})")

    nb_of_edges = sum(len(v) for v in filtered_labels.values())
    print(f"Time: {(datetime.now() - start_time).total_seconds():.2f}s")
    return filtered_labels, sample_per_label, (datetime.now() - start_time).total_seconds()
```

E Figures

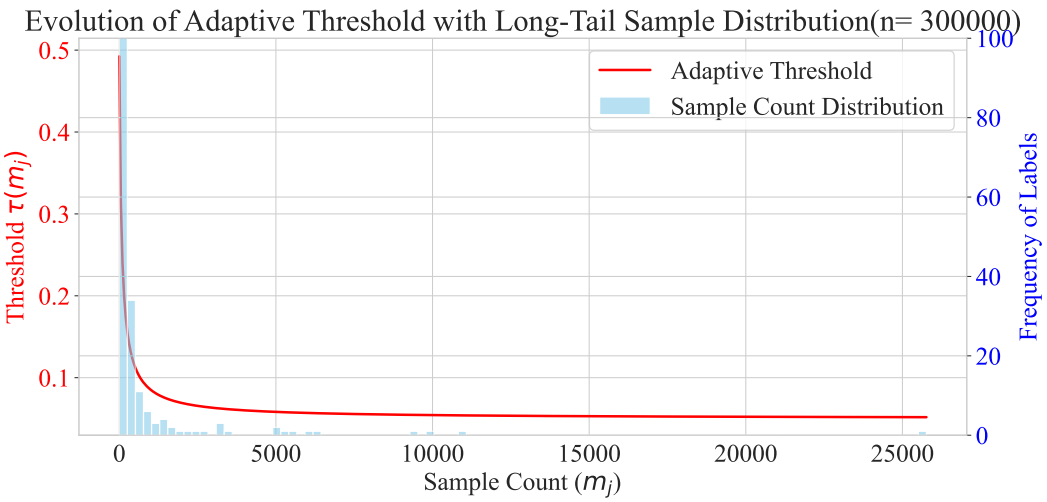


Figure 7: Adaptive thresholding function $\tau_j(m_j)$ across varying label frequencies m_j, illustrating the logistic decay from $\tau_{\max}$ to $\tau_{\min}$.

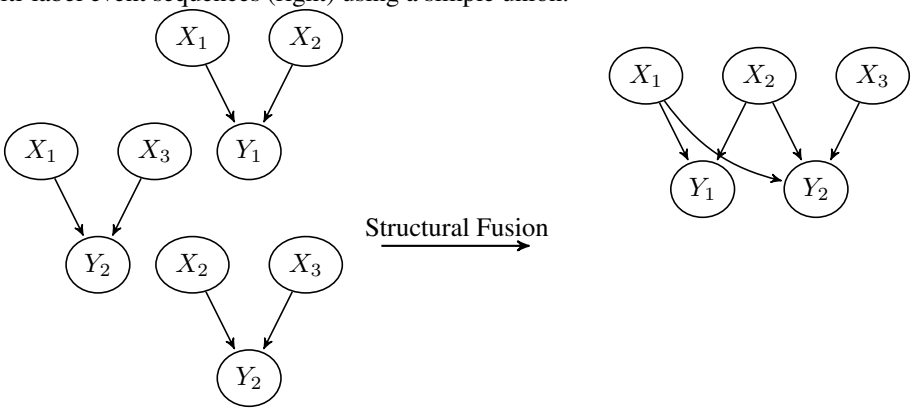



Figure 8: Illustration of structural fusion: individual causal graphs (left) aggregated into a fused DAG for multi-label event sequences (right) using a simple union.