

Integrating Large Language Models in Causal Discovery: A Statistical Causal Approach

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Abstract

In practical statistical causal discovery (SCD), embedding domain expert knowledge as constraints into the algorithm is significant for creating consistent meaningful causal models, despite the challenges in systematic acquisition of the background knowledge. To overcome these challenges, this paper proposes a novel methodology for causal inference, in which SCD methods and knowledge based causal inference (KBCI) with a large language model (LLM) are synthesized through “statistical causal prompting (SCP)” for LLMs and prior knowledge augmentation for SCD. Experiments have revealed that GPT-4 can cause the output of the LLM-KBCI and the SCD result with prior knowledge from LLM-KBCI to approach the ground truth, and that the SCD result can be further improved, if GPT-4 undergoes SCP. Furthermore, by using an unpublished real-world dataset, we have demonstrated that the background knowledge provided by the LLM can improve SCD on this dataset, even if this dataset has never been included in the training data of the LLM. The proposed approach can thus address challenges such as dataset biases and limitations, illustrating the potential of LLMs to improve data-driven causal inference across diverse scientific domains.

1 Introduction

1.1 Background

Understanding causal relationships is key to comprehending basic mechanisms in various scientific fields. The statistical causal inference framework, which is widely applied in areas such as medical science, economics, and environmental science, aids this understanding. However, traditional statistical causal inference methods generally rely on the assumed causal graph for determining the existence and strength of causal impacts. To overcome this challenge, data-driven algorithmic methods have been developed as statistical causal discovery (SCD) methods, both in non-parametric (Spirtes et al., 2000; Chickering, 2002; Silander & Myllymäki, 2006; Yuan & Malone, 2013; Huang et al., 2018; Xie et al., 2020) and semi-parametric (Shimizu et al., 2006; Hoyer et al., 2008; Shimizu et al., 2011; Rolland et al., 2022; Tu et al., 2022) approaches. In addition, benchmark datasets have been published for the evaluation of SCD methods (Mooij et al., 2016; Käding & Runge, 2023).

Despite advancements in SCD algorithms, data-driven acquisition of causal graphs without domain knowledge can be inaccurate. This is generally attributed to a mismatch between assumptions in SCD and real-world phenomena (Reisach et al., 2021). Moreover, obtaining experimental and systematic datasets sufficient for causal inference is difficult, whereas observational datasets, which are prone to selection bias and measurement errors, are more readily accessible (Abdullahi et al., 2020). Consequently, for more persuasive and reliable validation of causal models, the augmentation with domain knowledge plays a critical role (Rohrer, 2017).

In addition, with respect to efficiency and precision in SCD, the importance of incorporating constraints on trivial causal relationships into the SCD algorithms has been highlighted (Inazumi et al., 2010; Chowdhury et al., 2023). Causal learning software packages have been augmented with prior knowledge, as demonstrated in “causal-learn”¹, and “LiNGAM”² (Zheng et al., 2023; Ikeuchi et al., 2023).

¹<https://github.com/py-why/causal-learn>

²<https://github.com/cdt15/lingam>

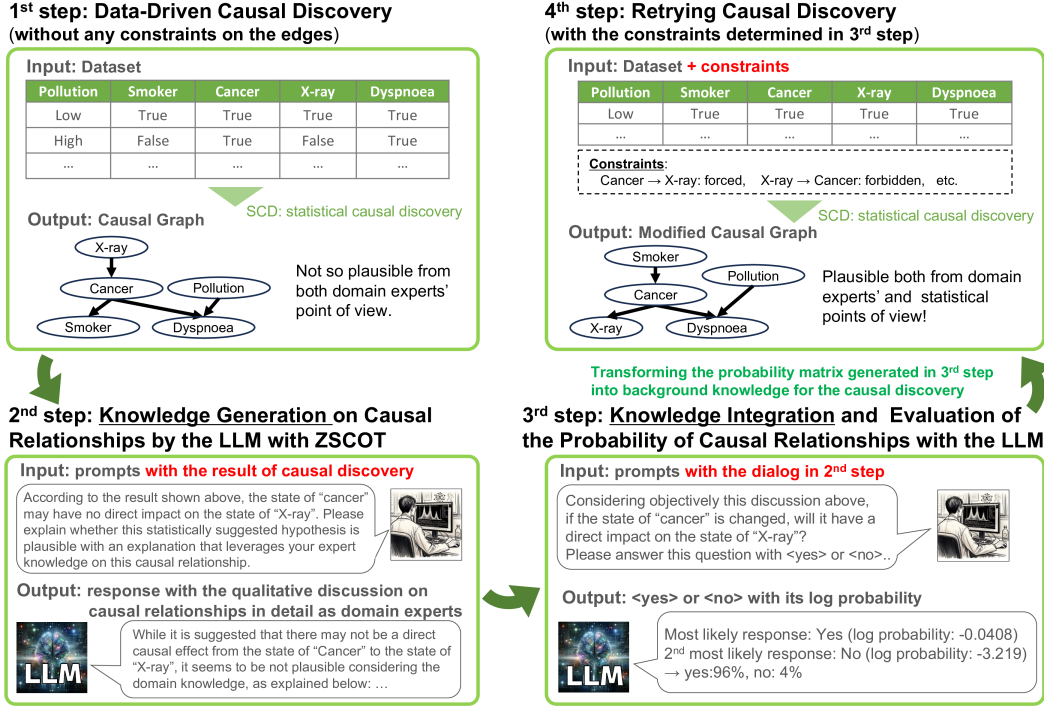


Figure 1: Overall framework of the statistical causal prompting in a large language model (LLM) and statistical causal discovery (SCD) with LLM-based background knowledge.

Moreover, the systematic acquisition of domain expert knowledge is a challenging task. Although there are several examples of constructing directed acyclic graphs (DAGs) by domain experts, as demonstrated in health services research (Rodrigues et al., 2022), practical methods for this process have not been proposed.

The scenario recently has been changed with the rapid progress in the development of high-end large language models (LLMs). With their high performances in the applications of their domain knowledge acquired from vast amounts of data in the pre-training processes (OpenAI, 2023; Touvron et al., 2023; Gemini Team, Google, 2023), LLMs can be expected to perform objective evaluation of causal relationships. Several studies have reported the trial results of LLM knowledge-based causal inference (LLM-KBCI) (Jiang et al., 2023; Jin et al., 2024; Kıcıman et al., 2023; Zečević et al., 2023; Jiralerspong et al., 2024; Zhang et al., 2024), and in particular, the performance enhancement in non-parametric SCD with the guides by LLMs was confirmed (Ban et al., 2023; Vashishtha et al., 2023; Khatibi et al., 2024). However, it remains unclear whether the enhancement in SCD accuracy with background knowledge augmented by LLMs is robustly observed in inference themes involving closed data uncontained in the pre-training datasets of LLMs, and whether it leads to more statistically valid causal models.

1.2 Central Idea of Our Research

Based on the rapidly evolving techniques in the context of causal inference with LLMs, a novel methodology for SCD is proposed in this paper, in which the LLM prompted with the results of SCD without background knowledge evaluates the probability of the causal relationships considering both the domain knowledge and the statistical characteristic suggested by SCD (Figure 1).

In the first step, an SCD is executed on a dataset without prior knowledge, and the results of the statistical causal analysis are outputted. To maximize the usage of the expert knowledge acquired in the pre-training process of the LLM, the method of generated knowledge prompting (Liu et al., 2022) is adopted, and then, the process of utilizing the LLM includes the second step (knowledge generation) and the third step (knowledge integration). In the second step, knowledge of the causal relationships between all pairs of variables is generated in detail from the domain knowledge of the LLM based on the zero-shot chain-of-thought (ZSCOT)

prompting technique (Kojima et al., 2022). Here, the LLM can be prompted with the results of SCD as supplemental information for LLM inference. We define this technique as “statistical causal prompting” (SCP). Thereafter, in the third step, the LLM judges whether there are any causal relationships between all pairs of variables with “yes” or “no,” thus objectively considering the dialogs of the second step. Here, the probabilities of the responses from the LLM are evaluated and transformed into the prior knowledge matrix. This matrix, the output of LLM-KBCI with SCP, is finally re-applied to SCD in the fourth step.

1.3 Our Contribution

The contributions through the demonstration of the proposed method in this paper are as follows:

(1) Realization of the Synthesis of LLM-KBCI and SCD in a Mutually-Referential Manner

The practical method for realizing the proposed concept of Figure 1 is detailed, and the SCP method is proposed. Experiments were demonstrated with several benchmark datasets, which are open and have been widely used for the evaluation of SCD algorithms. They all consist of continuous variables.

(2) Mutual Performance Enhancement of SCD and LLM-KBCI We demonstrated that the augmentation by the LLM with SCP, improved the performance of the SCD, and the performance of LLM-KBCI was also enhanced by SCP.

(3) Enhancement of SCD Performance by SCP In the experiments, we demonstrate the implication that the output of several SCD algorithms augmented by the LLM with SCP, can be a superior causal model to the pattern of prompting without SCP in terms of domain expertise and statistic.

(4) Improvement of SCD results with the background knowledge provided by LLMs even if the dataset is uncontained in the pre-training materials We prepared a closed health screening dataset that is uncontained in the pre-training materials for LLMs, and demonstrated the experiment on a sub-dataset that has been randomly sampled from the entire dataset. Through this experiment, we clearly confirmed that the proposed method robustly leads to more statistically valid causal models with the natural ground truths. This fact proved that the LLMs can indeed contribute to background knowledge augmentation for SCD algorithms in practical situations, even if the dataset used for SCD are not memorized by LLMs.

2 Related Works and Originality in Our Work

Augmentation of SCD Algorithms with Background Knowledge As introduced in Section 1.1, several SCD algorithms³ can be systematically augmented with background knowledge. Moreover, their software packages are open. For example, as a non-parametric and constraint-based SCD method, the Peter-Clerk (PC) algorithm (Spirtes et al., 2000) is augmented with the background knowledge of the forced or forbidden directed edges in “causal-learn.” “Causal-learn” also provides the Exact Search algorithm (Silander & Myllymäki, 2006; Yuan & Malone, 2013) as a non-parametric and score-based SCD method, which can be augmented with the background knowledge of the forbidden directed edges as a super-structure matrix. With respect to a semi-parametric approach, DirectLiNGAM (Shimizu et al., 2011) algorithm is augmented with prior knowledge of the causal order (Inazumi et al., 2010) in “LiNGAM” project (Ikeuchi et al., 2023).

Causal Inference in Knowledge-Driven Approach with LLMs In addition to the study on the causality detection from natural language texts using language models with additional training datasets (Khetan et al., 2022), the rapid growth of LLMs have made it possible to produce some valuable works on causality, including causal inference using LLMs. Attempts have been made to use LLMs for causal inference among a set of variables, prompting with the metadata such as the names of variables, and without the SCD process with the benchmark datasets (Kıcıman et al., 2023; Zečević et al., 2023; Jiralerspong et al., 2024; Zhang et al., 2024). Adopting the similar approach, the concept of causal modeling agents, which improves

³All of the algorithms adopted for the experiments in this paper can be used under the assumptions of DAG and with no hidden common causes.

the precision of the causal graphs through the iteration of hypothesis generation from LLMs and model fitting to the real-world data, has also been proposed (Abdulaal et al., 2024). There are also studies on incorporating LLMs in the process of SCD as an alternative tool for conditional independence tests in the PC algorithm (Cohrs et al., 2023), and for identifying the causal graphs beyond the Markov equivalent class (Long et al., 2023). In addition, researches have been conducted with focus on the use of LLMs to improve the SCD results (Ban et al., 2023; Vashishtha et al., 2023; Khatibi et al., 2024). However, all the experiments were conducted only on popular benchmark datasets, contained in the pre-training datasets of LLMs. Consequently, while acknowledging the valuable foundations laid by previous studies, it has remained uncertain whether the enhancements in SCD accuracy are truly driven by LLMs leveraging their vast knowledge for genuine causal inference, or merely by reproducing the memorized content of datasets (Vashishtha et al., 2023).

Originality in Our Work In contrast to the studies with similar focuses on LLM-guided SCD (Ban et al., 2023; Vashishtha et al., 2023; Khatibi et al., 2024), this study also focuses on the construction of the background knowledge in a quantitative manner based on the response probability of the LLM, which can reflect the credibility of the decision made by the LLM with SCP. In addition, in the case of a semi-parametric SCD method such as LiNGAM, we detail herein how to achieve both statistical validity and natural interpretation with respect to domain knowledge at a maximally high level, by prompting with the causal coefficients and bootstrap probabilities of all the patterns of directed edges.

Moreover, we validate the proposed method on an unpublished dataset. This approach has not only demonstrated the practical utility and robustness of our method, but also helped to confirm the applicability and validity of existing works (Ban et al., 2023; Vashishtha et al., 2023; Khatibi et al., 2024).

3 Materials and Methods

3.1 Algorithms and Elements for LLM-Augmented Causal Discovery

With respect to practicality, the method of Figure 1 is outlined as Algorithm 1. Following the notations in Algorithm 1, the the input elements in the demonstration are explained below.

Algorithms for Statistical Causal Discovery For the SCD method S , we adopted the PC algorithm (Spirtes et al., 2000), Exact Search based on the A* algorithm (Yuan & Malone, 2013), and DirectLiNGAM algorithm (Shimizu et al., 2011), which can all be optionally augmented with prior knowledge, and are open in “causal-learn” (Zheng et al., 2023) and “LiNGAM” (Ikeuchi et al., 2023). Furthermore, we also implement the bootstrap sampling function B of the SCD algorithm to investigate the statistical properties such as the bootstrap probabilities p_{ij} of the emergence of the directed edges from x_j to x_i . In our experiments, the number of bootstrap resamplings was fixed to 1000.

Conditions of the LLM and Prompting For utilizing the LLM as the domain expert, we adopted GPT-4-1106-`preview`⁴ developed by OpenAI; the temperature, a hyperparameter for adjusting the probability distribution of the output, was fixed to 0.7.

The template for the first prompting $q_{ij}^{(1)}$ for knowledge generation is shown in Table 1. This prompting template is based on the underlying principle of the ZSCOT technique⁵ (Kojima et al., 2022), which was reported as a potential method to enhance the performance of the LLM generation tasks; enhancement is performed

⁴We recognize that there have been various kinds of high-performance LLMs from several institutes, and that it is valuable to demonstrate that including a broader range of LLMs could provide valuable insights into the generalizability and scalability of our method across various LLM architectures. However, our goal in this work is to explore the effectiveness of integrating LLMs into SCD via SCP, requiring trials and comparisons of various SCP patterns and SCD algorithms, as described in Section 4. To maintain consistency and control across these trials, it is also important to fix the LLM in the experiments, which has advanced capabilities and state-of-the-art status in various domains. Moreover, we should adopt the LLMs that satisfy specific conditions for our experiments, such as the maximum input token capacity for the prompting processes, and the functionality to obtain log-probability of the output. For these strategic and technical reasons, we adopted GPT-4 in our experiments.

⁵Although the quality of the LLM outputs can be further enhanced, e.g., by fine-tuning with several datasets containing fundamental knowledge for causal inference or Retrieval-Augmented Generation (RAG), we adopt the idea of ZSCOT in order to establish low-cost and simple methods, which can be universally applied independent of the targeted fields of causal inference.

Algorithm 1 Background knowledge construction with the LLM prompted with the results of the SCD

Input 1: Data X with variables $\{x_1, \dots, x_n\}$
Input 2: SCD method S
Input 3: Function for bootstrap B
Input 4: Response of the domain expert (GPT-4) ϵ_{GPT4}
Input 5: Log probability of the response $L(\epsilon_{\text{GPT4}})$
Input 6: Prompt function for knowledge generation $Q_{ij}^{(1)}$
Input 7: Prompt function for knowledge integration $Q_{ij}^{(2)}$
Input 8: Transformation from probability matrix to prior knowledge T
Input 9: Number of times to measure the probability M
Output: Result of SCD with prior knowledge \hat{G} on X

SCD result without prior knowledge $\hat{G}_0 = S(X)$

bootstrap probability matrix $\mathbf{P} = B(S, X)$

for $i = 1$ **to** n **do**

for $j = 1$ **to** n **do**

$\bar{p}_{i,i} = \text{NaN}$

if $i \neq j$ **then**

 prompt $q_{ij}^{(1)} = Q_{ij}^{(1)}(x_i, x_j, \hat{G}_0, \mathbf{P})$

 response $a_{ij} = \epsilon_{\text{GPT4}}(q_{ij}^{(1)})$

 prompt $q_{ij}^{(2)} = Q_{ij}^{(2)}(q_{ij}^{(1)}, a_{ij})$

for $m = 1$ **to** M **do**

$L_{ij}^{(m)} = L(\epsilon_{\text{GPT4}}(q_{ij}^{(2)})) = \text{"yes"}$

end for

 mean probability $\bar{p}_{ij} = \frac{\sum_{m=1}^M \exp(L_{ij}^{(m)})}{M}$

end if

end for

end for

probability matrix $\bar{\mathbf{p}} = (\bar{p}_{ij})$

prior knowledge $\mathbf{PK} = T(\bar{\mathbf{p}})$

return $\hat{G} = S(X, \mathbf{PK})$

by guiding logical inference and eliciting the background knowledge acquired through the pre-training process from the LLM. Furthermore, the SCD results, e.g., the causal structure and bootstrap probabilities, can be included in $\langle \text{blank 5} \rangle$ and $\langle \text{blank 9} \rangle$, which are defined as “statistical causal prompting” (SCP). Because the information used in SCP is partially dependent on the SCD algorithms, a brief description of the patterns for constructing the contents of $\langle \text{blank 5} \rangle$ and $\langle \text{blank 9} \rangle$ is presented in Section 3.2.

As shown in Table 2, generated knowledge is integrated in the second prompt, and GPT-4 is required to judge the existence of the causal effect from x_j on x_i from an objective point of view. Because the response from GPT-4 is required with “yes” or “no,” it is simple to quantitatively evaluate the level of GPT-4’s confidence regarding the existence of the causal relationship based on both the SCD result and domain knowledge. The probability p_{ij} of the assertion that there is a causal effect from x_j on x_i can be output by the optional function of GPT-4. Although p_{ij} can be evaluated readily from the log probability of the GPT-4 response as “yes,” there is a slight fluctuation in the log probability output from GPT-4 (Andriushchenko et al., 2024). Thus, we adopted the mean probability \bar{p}_{ij} of the single-shot measurement M times for the decision of prior knowledge matrix \mathbf{PK} , and we set $M = 5$ in the experiments. The combination of these prompting techniques can contribute to minimizing the risk of hallucination from the LLM, and it is expected that reliable probability of the response from the LLM for the causal relationship between a pair of variables is obtained.

Table 1: Prompt template of $Q_{ij}^{(1)}(x_i, x_j, \hat{G}_0, \mathbf{P})$ used for the generation of the expert knowledge of the causal effect from x_j on x_i . The “blanks” enclosed with $\langle \rangle$ are filled with description words. The word for $\langle \text{blank 6} \rangle$ is selected from “a” or “no,” depending on the content of $\langle \text{blank 5} \rangle$. The notations of the SCD result without prior knowledge \hat{G}_0 and the bootstrap probability matrix \mathbf{P} are same as those in Algorithm 1.

Prompt Template of $q_{ij}^{(1)} = Q_{ij}^{(1)}(x_i, x_j, \hat{G}_0, \mathbf{P})$

We want to carry out causal inference on $\langle \text{blank 1. The theme} \rangle$, considering $\langle \text{blank 2. The description of all variables} \rangle$ as variables.

First, we have conducted the statistical causal discovery with $\langle \text{blank 3. The name of the SCD algorithm} \rangle$, using a fully standardized dataset on $\langle \text{blank 4. The description of the dataset} \rangle$.

$\langle \text{blank 5. Including here the information of } \hat{G}_0 \text{ or } \mathbf{P}. \text{The detail of the contents depends on prompting patterns.} \rangle$

According to the results shown above, it has been determined that there may be $\langle \text{blank 6. a/no} \rangle$ direct impact of a change in $\langle \text{blank 7. The name of } x_j \rangle$ on $\langle \text{blank 8. The name of } x_i \rangle$ $\langle \text{blank 9. The value of causal coefficients or bootstrap probability} \rangle$.

Then, your task is to interpret this result from a domain knowledge perspective and determine whether this statistically suggested hypothesis is plausible in the context of the domain.

Please provide an explanation that leverages your expert knowledge on the causal relationship between $\langle \text{blank 7. The name of } x_j \rangle$ and $\langle \text{blank 8. The name of } x_i \rangle$, and assess the naturalness of this causal discovery result. Your response should consider the relevant factors and provide a reasoned explanation based on your understanding of the domain.

Table 2: Prompt template of $Q_{ij}^{(2)}(q_{ij}^{(1)}, a_{ij})$ used for the quantitative evaluation of the probability of GPT-4’s assertion that there is a causal effect from x_j on x_i .

Prompt Template of $q_{ij}^{(2)} = Q_{ij}^{(2)}(q_{ij}^{(1)}, a_{ij})$

An expert was asked the question below:

$\langle \text{blank 10. } q_{ij}^{(1)} \rangle$

Then, the expert replied with its domain knowledge:

$\langle \text{blank 11. } a_{ij} \rangle$

Considering objectively this discussion above, if $\langle \text{blank 12. The name of } x_j \rangle$ is modified, will it have a direct or indirect impact on $\langle \text{blank 13. The name of } x_i \rangle$?

Please answer this question with $\langle \text{yes} \rangle$ or $\langle \text{no} \rangle$.

No answers except these two responses are needed.

For the subsequent SCD with prior knowledge, the probability matrix $\bar{\mathbf{p}}$ is transformed with T , as expressed by Algorithm 2, into the background knowledge matrix. For the decision of forbidden or forced causal relationship from PK_{ij} , we prepare the probability criterion for the forbidden path as α_1 and that for the forced path as α_2 . In our experiments, α_1 is fixed at 0.05 and α_2 is fixed at 0.95, for common settings⁶.

Furthermore, the differences in the constraints that can be adopted depending on the SCD algorithms should be considered. In the Exact Search algorithm, the constraints of the forced edge cannot be applied. For the case of DirectLiNGAM, because prior knowledge is used for the decision of the causal order in the algorithm, the prior knowledge matrix must be an “acyclic” adjacency matrix when it is represented in the form of a network graph. Thus, when $S = \text{DirectLiNGAM}$ and \mathbf{PK} is cyclic, an additional transformation algorithm

⁶These heuristic thresholds follow the widely accepted conventions seen in statistical significance levels. Although the specific choice of threshold might influence the formation of the prior knowledge matrix, the probability outputs from LLMs for clear domain knowledge instances are either very high (close to 100 %) or very low (close to 0 %), ensuring that the essential insights are retained regardless of the threshold.

Algorithm 2 Transformation from the probability matrix into the prior knowledge matrix

```

Input 1: probability matrix  $\mathbf{p} = (p_{ij})$ 
Input 2: SCD method  $S \in \{ \text{PC}, \text{Exact Search}, \text{DirectLiNGAM} \}$ 
Input 3: probability criterion for the forbidden causal relationship  $\alpha_1$ 
Input 4: probability criterion for the forced causal relationship  $\alpha_2$ 
Output: prior knowledge matrix  $\mathbf{PK} = (PK_{ij})$ 
for  $i = 1$  to  $n$  do
  for  $j = 1$  to  $n$  do
     $PK_{ij} = \text{Unknown}$ 
    if  $i = j$  then
       $PK_{ij} = \text{Forbidden}$ 
    else
      if  $p_{ij} < \alpha_1$  then
         $PK_{ij} = \text{Forbidden}$ 
      else if  $(p_{ij} \geq \alpha_2)$  and  $(S \neq \text{Exact Search})$  then
         $PK_{ij} = \text{Forced}$ 
      end if
    end if
  end for
end for
if  $S = \text{DirectLiNGAM}$  then
   $\mathbf{PK} = A(\mathbf{PK})$  (acyclic transformation)
end if
return  $\mathbf{PK}$ 

```

A is required. In addition, there can be several acyclic transformation patterns; only one acyclic matrix with some criteria should be selected. The algorithm for the transformation and the matrix selection criterion in this study are explained in Appendix E.

3.2 Experiment Patterns of SCP

Related to the ⟨blank 5⟩ and ⟨blank 9⟩ in Table 1, we conducted experiments using several patterns of SCP. the notations of the prompting patterns in the experiments are presented with explanations below:

Pattern 0: without SCP This pattern corresponds to the reference for the comparison with the other patterns including SCD results in their prompts. Because the prompt template shown in Table 1 is not adequate for this pattern, we prepare a different template for Pattern 0, which is shown in Appendix B.

Pattern 1: with the list of edges that appeared in the first SCD Directed or undirected⁷ edges between x_i and x_j emerged in the SCD are listed.

Pattern 2: with the list of edges with their non-zero bootstrap probabilities Directed or undirected edges between x_i and x_j that emerged in the bootstrap process are listed with their bootstrap probabilities.

Pattern 3: with the list of edges that emerged in the first SCD with the calculated causal coefficients (only for DirectLiNGAM) Based on the property of DirectLiNGAM, that outputs the causal coefficients with the DAG discovered in the algorithm, this pattern is attempted to elucidate whether more information such as causal coefficients in addition to Pattern 1 can improve the performance of LLM-KBCI and the subsequent SCD with prior knowledge.

⁷In the PC algorithm, undirected edges that appear as $x_i - x_j$ with respect to a causal relationships between “ x_i and x_j ” in which the direction cannot be determined, can be detected. The prompt template for reflecting this difference from directed edges is shown in Appendix B.

Pattern 4: with the list of edges with their non-zero bootstrap probabilities and calculated causal coefficients for the full dataset (only for DirectLiNGAM) We also attempt this pattern with the most amount of information of 1st SCD as a mixture of Patterns 2 and 3.

3.3 Datasets for the Experiments

Although there are several widely-open benchmark datasets with well-known ground truths, particularly for Bayesian network-based causal structure learning (Scutari & Denis, 2014), several of them are fully or partially composed with categorical or discrete variables. However, considering Patterns 3 and 4 for the experiments in this study, because the basic structure causal model assumes the continuous properties of all variables, it is more effective to adopt benchmark datasets fully composed with continuous variables.

Consequently, we select three benchmark datasets for the experiments, as follows: 1. Auto MPG data (Quinlan, 1993) (five continuous variables) , 2. Deutscher Wetterdienst (DWD) climate data (Mooij et al., 2016) (six continuous variables) , 3. Sachs protein data (Sachs et al., 2005)(eleven continuous variables) .

Furthermore, to demonstrate that GPT-4 can aid SCD with its domain knowledge, even if the dataset used in the SCD process and analytics on the dataset are not contained in the pre-training data of GPT-4, the proposed methods are also applied on our dataset on health screening results, which has not been disclosed and therefore not learned by GPT-4. To demonstrate that the proposed methods can be applied when the dataset contains bias, which may lead to highly inaccurate SCD results, the health screening dataset for this experiment was sampled, and we deliberately chose a subset where certain biases are still present. Basic information on these datasets such as the first SCD results and the ground truths is presented in Appendix C.

4 Results and Discussions

4.1 Results in Benchmark Datasets

For the interpretation of the experimental results, we evaluate **PK** (for measuring the performance of LLM-KBCI with the prompts, including the first SCD results) and the adjacency matrix obtained in SCD with **PK** for each pattern (for measuring the performance of SCD augmented with LLM-KBCI), with the structural hamming distance (SHD), false positive rate (FPR), false negative rate (FNR), precision, and F1 score, using the ground truth adjacency matrix **GT** as a reference. As shown in Appendix D.3, all of these metrics can be calculated solely from the adjacency matrix and **GT**. In addition, this paper presents the evaluation of the comparative fit index (CFI) (Bentler, 1990), root mean square error of approximation (RMSEA) (Steiger & Lind, 1980) and Bayes information criterion (BIC) (Schwarz, 1978) of the causal structure obtained in SCD with **PK**, under the assumption of linear-Gaussian data⁸; to evaluate the results with respect to the statistical validity of calculated causal models. For evaluating the effect of **PK** augmentation by the LLM, the baseline result is that wo **PK** (Baseline A), as a reference for the comparison with the SCD results augmented with **PK**. In contrast, for evaluating the effect of SCP, the results with the prompting in Pattern 0 becomes the baseline (Baseline B), in the comparison with the results obtained in other SCP patterns. The indices for all patterns on the DWD, Auto MPG, and Sachs datasets are summarized in Table 3.

Enhancing the performance with prior knowledge augmentation by GPT-4 One of the characteristics in Table 3 is that in most of the cases, the result of SCD augmented with **PK** is more similar to **GT** than the first SCD result without prior knowledge (Baseline A). This behavior is interpreted as the knowledge-based improvement of the causal graph by GPT-4 as a domain expert, which is qualitatively consistent with other related works on LLM-guided causal inference (Ban et al., 2023; Vashishtha et al., 2023). Moreover, in many of the cases of Auto MPG and DWD data, the precision or F1 score are higher after the SCD augmented with **PK** than the pure **PK**, which are conclusions of LLM-KBCI, while they are almost comparable in the cases of Sachs data. From this comparison it is implied that even if LLM-KBCI is not optimal, the ground truths can be better approached by conducting SCD augmented with LLM-KBCI. In addition, BIC decreases in

⁸Although this assumption of linear-Gaussian data for the calculation of the CFI, RMSEA, and BIC, does not match the assumption of a non-Gaussian error distribution in LiNGAM, we adopt these indices to evaluate and compare the results with respect to the same statistical method, irrespective of the difference in the SCD algorithms.

Table 3: Comparison of the SCD results (and structural familiarity of **PK** with ground truths, for evaluation of the performance of LLM-KBCI) in all the experiment patterns we have conducted. Lower values are superior for SHD, FPR, FNR, RMSEA and BIC, and higher values for precision, F1score and CFI. The values in the blue font are the optimal results among all the prompting patterns, If the dataset and the SCD algorithm is fixed. Baseline A is used for the the comparison with the SCD results augmented with **PK** generated by the LLM, to evaluate the effect of **PK** augmentation by the LLM. Baseline B is used for the the comparison with the results obtained in other SCP patterns, to evaluate the effect of SCP. It is implied that in DWD and Sachs datasets, the outputs of LLM-KBCI in Patterns 1–4 are likely to approach the ground truths more closely than those in Pattern 0. It is also suggested that several of the outputs of Exact Search and DirectLiNGAM in Patterns 1–4 (with SCP), can be superior causal models than those in Pattern 0.

SCD algorithm	Pattern	SHD↓	FPR↓	FNR↓	Precision↑	F1score↑	CFI↑	RMSEA↓	BIC↓
1. Auto MPG data with 5 continuous variables									
PC	wo PK (Baseline A)	8	0.40	0.80	0.11	0.14	1.00	0.00	71.65
	Pattern 0 (Baseline B)	3 (5)	0.15 (0.25)	0.20 (0.20)	0.57 (0.44)	0.67 (0.57)	1.00	0.07	65.62
	Pattern 1	4 (7)	0.15 (0.30)	0.20 (0.20)	0.57 (0.40)	0.67 (0.53)	1.00	0.00	59.71
	Pattern 2	3 (6)	0.15 (0.30)	0.20 (0.20)	0.57 (0.40)	0.67 (0.53)	1.00	0.07	65.62
Exact Search	wo PK (Baseline A)	5	0.25	0.40	0.38	0.46	1.00	0.07	71.61
	Pattern 0 (Baseline B)	4 (5)	0.20 (0.25)	0.20 (0.20)	0.50 (0.44)	0.62 (0.57)	1.00	0.09	71.59
	Pattern 1	5 (5)	0.20 (0.20)	0.20 (0.20)	0.50 (0.50)	0.62 (0.62)	1.00	0.07	65.62
	Pattern 2	4 (5)	0.20 (0.25)	0.20 (0.20)	0.50 (0.44)	0.62 (0.57)	1.00	0.09	71.59
DirectLiNGAM	wo PK (Baseline A)	8	0.40	0.80	0.11	0.14	1.00	0.05	77.61
	Pattern 0 (Baseline B)	3 (5)	0.15 (0.25)	0.20 (0.20)	0.57 (0.44)	0.67 (0.57)	1.00	0.07	65.62
	Pattern 1	3 (5)	0.15 (0.30)	0.20 (0.20)	0.57 (0.40)	0.67 (0.53)	1.00	0.07	65.62
	Pattern 2	3 (5)	0.15 (0.25)	0.20 (0.20)	0.57 (0.44)	0.67 (0.57)	1.00	0.07	65.62
	Pattern 3	4 (6)	0.20 (0.35)	0.20 (0.20)	0.50 (0.36)	0.62 (0.50)	1.00	0.00	71.65
	Pattern 4	3 (5)	0.15 (0.30)	0.20 (0.20)	0.57 (0.40)	0.67 (0.53)	1.00	0.07	65.62
2. DWD climate data with 6 continuous variables									
PC	wo PK (Baseline A)	9	0.20	0.83	0.14	0.15	0.90	0.22	69.32
	Pattern 0 (Baseline B)	5 (8)	0.03 (0.20)	0.67 (0.33)	0.67 (0.40)	0.44 (0.50)	0.71	0.36	32.70
	Pattern 1	5 (9)	0.03 (0.23)	0.67 (0.33)	0.67 (0.36)	0.44 (0.47)	0.71	0.36	32.70
	Pattern 2	5 (8)	0.03 (0.20)	0.67 (0.33)	0.67 (0.40)	0.44 (0.50)	0.71	0.36	32.70
Exact Search	wo PK (Baseline A)	6	0.20	0.17	0.45	0.59	0.91	0.28	92.87
	Pattern 0 (Baseline B)	5 (8)	0.10 (0.20)	0.33 (0.33)	0.57 (0.40)	0.62 (0.50)	0.98	0.12	58.38
	Pattern 1	5 (5)	0.10 (0.13)	0.33 (0.17)	0.57 (0.56)	0.62 (0.67)	0.91	0.19	57.73
	Pattern 2	6 (9)	0.13 (0.23)	0.33 (0.33)	0.50 (0.36)	0.57 (0.47)	0.91	0.20	63.58
DirectLiNGAM	wo PK (Baseline A)	10	0.33	0.67	0.17	0.22	1.00	0.00	99.53
	Pattern 0 (Baseline B)	4 (8)	0.07 (0.20)	0.33 (0.33)	0.67 (0.40)	0.67 (0.50)	1.00	0.00	52.67
	Pattern 1	8 (8)	0.10 (0.10)	0.83 (0.83)	0.25 (0.25)	0.20 (0.20)	0.64	0.43	38.03
	Pattern 2	4 (7)	0.03 (0.17)	0.50 (0.33)	0.75 (0.44)	0.60 (0.53)	0.98	0.09	40.80
	Pattern 3	5 (6)	0.10 (0.13)	0.33 (0.33)	0.57 (0.50)	0.62 (0.57)	0.93	0.16	57.90
	Pattern 4	5 (6)	0.10 (0.17)	0.33 (0.16)	0.57 (0.50)	0.62 (0.62)	0.92	0.18	57.80
3. Sachs' protein data with 11 continuous variables									
PC	wo PK (Baseline A)	24	0.16	0.47	0.38	0.44	0.99	0.05	294.15
	Pattern 0 (Baseline B)	15 (19)	0.04 (0.11)	0.58 (0.47)	0.67 (0.48)	0.52 (0.50)	0.89	0.16	166.91
	Pattern 1	25 (43)	0.17 (0.53)	0.68 (0.16)	0.26 (0.23)	0.29 (0.36)	0.97	0.11	284.58
	Pattern 2	23 (23)	0.13 (0.24)	0.74 (0.32)	0.28 (0.35)	0.27 (0.46)	0.97	0.09	231.27
Exact Search	wo PK (Baseline A)	31	0.26	0.68	0.18	0.23	0.99	0.07	374.35
	Pattern 0 (Baseline B)	17 (19)	0.07 (0.11)	0.58 (0.47)	0.53 (0.48)	0.47 (0.50)	0.91	0.16	202.97
	Pattern 1	17 (15)	0.05 (0.06)	0.68 (0.58)	0.55 (0.57)	0.40 (0.48)	0.87	0.20	158.26
	Pattern 2	16 (14)	0.11 (0.14)	0.53 (0.32)	0.45 (0.48)	0.46 (0.57)	0.95	0.12	257.53
DirectLiNGAM	wo PK (Baseline A)	29	0.25	0.47	0.28	0.36	1.00	0.01	410.23
	Pattern 0 (Baseline B)	17 (19)	0.07 (0.11)	0.53 (0.47)	0.56 (0.48)	0.51 (0.50)	0.91	0.16	203.02
	Pattern 1	15 (13)	0.07 (0.08)	0.47 (0.37)	0.59 (0.60)	0.56 (0.62)	0.88	0.18	220.32
	Pattern 2	22 (21)	0.14 (0.18)	0.63 (0.47)	0.33 (0.36)	0.35 (0.43)	0.70	0.31	269.76
	Pattern 3	22 (23)	0.15 (0.18)	0.53 (0.53)	0.38 (0.33)	0.42 (0.39)	0.92	0.16	301.51
	Pattern 4	20 (16)	0.12 (0.16)	0.53 (0.26)	0.43 (0.47)	0.45 (0.57)	0.89	0.19	264.97

almost all the patterns from the SCD result without **PK** (Baseline A). The aforementioned properties suggest that knowledge-based augmentation from GPT-4 can improve the performance of SCD, indeed, in terms of the consistency with respect to the domain expert knowledge and statistical causal structure. However, the amount of improvement can differ depending on the number of variables and the methods of SCD.

Dependence on the number of variables In the case of Auto MPG data with only five variables, the amount of improvement for each SCD method is almost constant among all the prompting patterns. One of

the possible reasons is that within relatively small numbers of variables, the amount of information in SCP becomes small, and the difference of inference performance of GPT-4 among the prompting patterns becomes subtle. Moreover, because the space for discovery becomes also smaller along with the network shrink, the SCD algorithm may reach a single optimal solution, even if **PK** is different.

On the other hand, in the cases of DWD data with six variables and Sachs data with eleven variables, the difference in the amount of improvement becomes more clear depending on the prompting patterns. From this fact, it is implied that the threshold of the number of variables over which the quality of **PK** and SCD results depend on the amount of information included. In SCP for GPT-4, it is around five.

Moreover, in many cases of DWD and Sachs data, in particular for Exact Search or DirectLiNGAM, the precision and F1 score of **PK** in Pattern 0 (Baseline B) are usually smaller than any of other patterns, in which GPT-4 experiences SCP. This supports the performance enhancement of LLM-KBCI by SCP.

Prompting pattern dependence on SCD methods On the other hand, considering the output of the SCD augmented with **PK**, Pattern 0 (Baseline B) stably indicates relatively higher performance among all the patterns in both terms of domain knowledge and statistical model fitting. Furthermore, the results of Patterns 0 and 1 are almost the same when the PC or the Exact Search algorithm is adopted, and in particular, the result of Pattern 0 with the PC algorithm on Sachs data is superior to that of Pattern 0.

Although it is difficult to explain the reason for this behavior, one of the possible reasons, if we focus only on the results on Sachs data, is that we adopted the ground truths partially determined by Bayesian network inference (Sachs et al., 2005). Indeed, the first SCD result in PC is already relatively close to **GT**, as shown in Figure 8 (a), and we interpret that in this situation, the performance of SCD with **PK** cannot be improved.

The scenario differs when DirectLiNGAM is adopted. The performance of the SCD with **PK** either in Pattern 1 or 2, remains totally superior to that of Pattern 0 (Baseline B) from both statistical and domain expert points of view. This implies that SCP can effectively improve the performance of DirectLiNGAM.

However, from the analysis of Patterns 3 and 4, in which GPT-4 is prompted with the causal coefficients of the first SCD results, it is also revealed that prompting with a greater amount of statistical information does not always lead to improved SCD results. In particular, while **PK** in Pattern 4 is closer to ground truth matrix than that in Pattern 0 in DWD or Sachs data ⁹, the final SCD result augmented with **PK** in Pattern 4 is inferior to that of Pattern 0. One of the possible reasons for this may be the pruning of the candidate edges suggested from **PK** in the SCD process. For elucidating this behavior, further research is required on what type and amount of information in SCP can truly maximize the performance of SCD.

4.2 Results in Randomly Selected Sub-sample of Health Screening Data Excluded from GPT-4 Pre-Training Dataset

It is difficult to assert that this improvement is solely due to the LLM’s high performance in KBCI from the experimental results on open benchmark datasets, because it cannot be determined whether the improvement stems from the LLM’s recall of the data obtained during the pre-training process on these datasets. Furthermore, assuming realistic situations, it is also important to confirm the robust effectiveness of this method, even if the range of the available dataset for statistical causal inference is limited to observation data, which may be statistically biased, and the trivial causal relationships are not apparent in SCD without prior knowledge. Therefore, we also apply the proposed methods on the sub-dataset of health screening results, which has been randomly sampled from the entire dataset¹⁰, and the natural ground truth is not presented in the SCD results without **PK**.

In Figure 2(a), the result of DirectLiNGAM without **PK** is shown, and unnatural directed edges to “Age” from other variables are suggested, although the parts of the ground truths from expert knowledge are reversed relationships from these edges, such as “Age”→“HbA1c”. However, when the causal discovery is assisted with **PK** generated from GPT-4 with SCP in Patterns 2 and 4, the causal graph becomes more natural: “Age” is not influenced by other variables, and the ground truth “Age”→“HbA1c”, which cannot be

⁹This fact reinforces the reliability of our interpretation that SCP enhance the performance of LLM-KBCI.

¹⁰The details of the sampling method for this experiment are presented in Appendix C

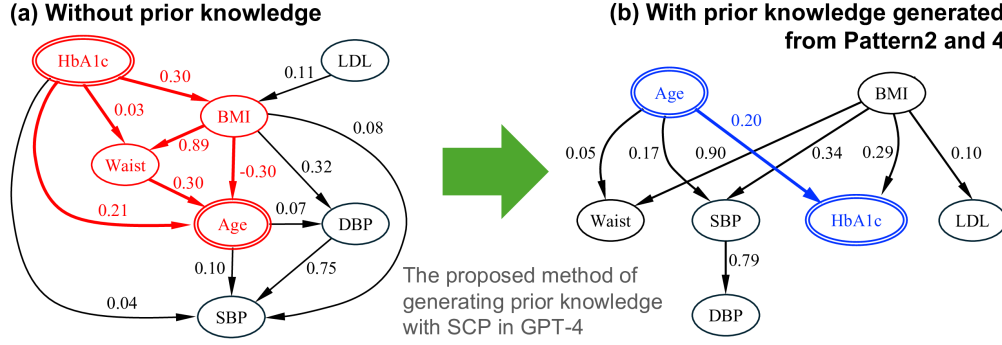


Figure 2: Results of DirectLiNGAM in the health screening data. (a) Result without prior knowledge. (b) Result with prior knowledge, which is generated from GPT-4 with SCP in Patterns 2 and 4. In this randomly selected subset, the DirectLiNGAM result without prior knowledge exhibits unnatural paths drawn in red in (a), which indicates that “Age” is influenced by “HbA1c.” However, using the proposed method, the unnatural behavior is clearly mitigated with the guide of prior knowledge generated from GPT-4 with SCP, including the value of causal coefficients in (a) or the bootstrap probabilities of the emergence of directed edges.

Table 4: Quantitative evaluation of characteristic results of SCD in the proposed methods on the subset of health screening data with certain biases.

A: The elements of \mathbf{P} generated in each prompting pattern for all the appropriate ground truth causal relationships in these variables. The values enclosed in parentheses are the bootstrap probabilities of the directed edges in the DirectLiNGAM algorithm without \mathbf{PK} . Moreover, all the probabilities of reversed, unnatural causal relationships in which “age” is influenced by other factors are extremely closed to zero.

B: CFI, RMSEA and BIC evaluated on the model fitting with the structure discovered by DirectLiNGAM, under the assumption of linear-Gaussian data. The values enclosed in parentheses are the statistics of the structure calculated without \mathbf{PK} .

It can be inferred that SCP with bootstrap probabilities in Patterns 2 and 4, have enhanced the confidence in “Age” \rightarrow “DBP” by GPT-4, and improved the BIC when compared with Pattern 0.

		Pattern 0	Pattern 1	Pattern 2	Pattern 3	Pattern 4
A. Probability of reproducing ground truth from GPT-4	“Age” \rightarrow “BMI” (0.166)	0.901	0.076	0.093	0.306	0.037
	“Age” \rightarrow “SBP” (0.550)	0.626	0.302	0.207	0.235	0.795
	“Age” \rightarrow “DBP” (0.308)	0.001	0.019	0.115	0.095	0.926
	“Age” \rightarrow “HbA1c” (0.327)	0.986	0.170	0.723	0.046	0.176
B. Statistics of linear-Gaussian fitting with the results of DirectLiNGAM	CFI \uparrow (1.002)	0.999	0.992	0.995	0.986	0.995
	RMSEA \downarrow (0.000)	0.018	0.054	0.032	0.057	0.032
	BIC \downarrow (124.332)	103.581	89.738	89.740	103.506	89.740

detected without \mathbf{PK} in this randomly selected subset, appears in the causal graph, as shown in Figure 2(b). Because this sub-dataset and the analysis results are not disclosed and have been completely excluded from the pre-training data for GPT-4, GPT-4 cannot respond to prompts asking for the causal relationships merely by reproducing the knowledge acquired from the same data. Based on the above, it is verified that the assist of GPT-4 with SCP can cause the result of SCD to further approach the ground truths to an extent, even when the dataset is not learned by GPT-4 and contains bias.

For further clarity regarding the behaviors of SCP, the mean probabilities of the positive response on the causal relationships from GPT-4 for ground truths in the health screening data, in addition to the statistics of the fitting results with the structure suggested by DirectLiNGAM with SCP are presented in Table 4. In Pattern 0 without SCP, the existence of “Age” \rightarrow “BMI” and “Age” \rightarrow “HbA1c” is supported in the probabilities over 0.90, and the probabilities decrease in other patterns with SCP. On the other hand, the opposite behavior

is also observed on “Age”→“DBP,” which is strongly denied from the GPT-4 domain knowledge without SCP in Pattern 0. It is reasonable to interpret that these probability changes with SCP in GPT-4 are induced by the results of SCD and bootstrap probabilities.

For example, focusing on the relationship “Age”→“BMI,” the lack of the direct edge in the SCD result with **PK** shown in Figure 2(b) and the relatively low bootstrap probability 0.166 in Table 4, may be the cause of lower probability in the SCP patterns than Pattern 0. By contrast, although the hypothesis of “Age”→“DBP” is not supported by the GPT-4 domain knowledge in Pattern 0, the appearance of the edge in Figure 2(a) and the bootstrap probability 0.308 are considered to be the cause of the increase in probability through SCP. Considering the aforementioned properties, the probability that the judgement rendered by GPT-4 regarding causal relationships can be influenced by the SCD results, particularly when the dataset with some significant biases is used in the causal discovery.

Finally, it is also confirmed that the BIC becomes smaller with the assistance by GPT-4 than without **PK**. In particular, the values in Patterns 1, 2, and 4 are lower than Pattern 0. This suggests that SCP can contribute to the discovery of the causal structure with more adequate statistical models.

5 Conclusion

In this study, a novel methodology of causal inference, in which SCD and LLM-KBCI are synthesized with SCP and prior knowledge augmentation was developed and demonstrated.

It has been revealed that GPT-4 can cause the output of LLM-KBCI and the SCD result with prior knowledge from LLM-KBCI to approach the ground truth, and that the SCD result can be further improved, if GPT-4 undergoes SCP. Furthermore, with an unpublished real-world dataset, we have demonstrated that GPT-4 with SCP can assist in SCD with respect to domain expertise and statistics, and that the proposed method is effective even if the dataset has never been included in the training data of the LLM and the sample size is not sufficiently large to obtain reasonable SCD results.

Limitation of this work

We have fixed the LLM in our experiment to GPT-4 for its extensive general knowledge and capabilities in common-sense reasoning, and our experiments on several real-world datasets, typically within the realm of common-sense reasoning, have illustrated the potential utility of the proposed method across various scientific domains. However, we recognize that deeper domain specificity might require employing optimal LLMs. Additionally, we also believe that incorporating techniques such as fine-tuning and RAG could also offer further enhancements to outcomes without changing LLMs. Therefore, systematic research in the context of optimal LLM-KBCI is also required on the selection of the optimal LLMs for each domain and on the techniques for utilizing the LLMs.

Furthermore, for generalization of the method we have proposed, we also have to remark that although SCP is indeed likely to enhance the performance of SCD more than the prompting without SCP, whether this improvement is observed can depend on the datasets used for SCD. In terms of the more reliable application of the proposed method, further basic research on the effect of causal coefficients or bootstrap probabilities on the results of LLM-KBCI is required.

Broader Impact statement

This paper proposed a novel approach that integrates SCD methods with LLMs. This research has the potential to contribute to more accurate causal inference in fields where understanding causality is crucial, such as healthcare, economics, and environmental science. However, the use of LLMs such as GPT-4 necessitates the extensive consideration of data privacy and biases. This study highlights the responsible use of artificial intelligence, considering ethical implications and societal impacts. With appropriate guidelines and ethical standards, the proposed methodology can advance scientific understanding and provide extensive widespread benefits to society.

References

- Ahmed Abdulaal, adamos hadjivasiliou, Nina Montana-Brown, Tiantian He, Ayodeji Ijishakin, Ivana Drobnjak, Daniel C. Castro, and Daniel C. Alexander. Causal modelling agents: Causal graph discovery through synergising metadata- and data-driven reasoning. In *The Twelfth International Conference on Learning Representations*, 2024. URL <https://openreview.net/forum?id=pAoqRlTBtY>.
- Umar I. Abdullahi, Spyros Samothrakis, and M. Fasli. Causal inference with correlation alignment. In *Proc. 2020 IEEE International Conference on Big Data (Big Data)*, pp. 4971–4980, 2020. doi: 10.1109/BigData50022.2020.9378334.
- Dawn E. Alley, Luigi Ferrucci, Mario Barbagallo, Stephanie A. Studenski, and Tamara B. Harris. A Research Agenda: The Changing Relationship Between Body Weight and Health in Aging. *The Journals of Gerontology: Series A*, 63(11):1257–1259, 11 2008. ISSN 1079-5006. doi: 10.1093/gerona/63.11.1257. URL <https://doi.org/10.1093/gerona/63.11.1257>.
- Maksym Andriushchenko, Francesco Croce, and Nicolas Flammarion. Jailbreaking leading safety-aligned llms with simple adaptive attacks, 2024.
- Taiyu Ban, Lyuzhou Chen, Derui Lyu, Xiangyu Wang, and Huanhuan Chen. Causal structure learning supervised by large language model. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2311.11689.
- Peter M. Bentler. Comparative fit indexes in structural models. *Psychological bulletin*, 107 2:238–46, 1990. doi: 10.1037/0033-2909.107.2.238.
- Lu Cheng, Ruocheng Guo, Raha Moraffah, Paras Sheth, K. Selçuk Candan, and Huan Liu. Evaluation methods and measures for causal learning algorithms. *IEEE Transactions on Artificial Intelligence*, 3(6): 924–943, 2022. doi: 10.1109/TAI.2022.3150264.
- David Maxwell Chickering. Optimal structure identification with greedy search. *The Journal of Machine Learning Research*, 3:507–554, 2002. URL <https://dl.acm.org/doi/10.1162/153244303321897717>.
- Jawad Chowdhury, Rezaur Rashid, and Gabriel Terejanu. Evaluation of induced expert knowledge in causal structure learning by NOTEARS. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2301.01817.
- Philippa Clarke, Patrick M O’Malley, Lloyd D Johnston, and John E Schulenberg. Social disparities in BMI trajectories across adulthood by gender, race/ethnicity and lifetime socio-economic position: 1986–2004. *International Journal of Epidemiology*, 38(2):499–509, 10 2008. ISSN 0300-5771. doi: 10.1093/ije/dyn214. URL <https://doi.org/10.1093/ije/dyn214>.
- Kai-Hendrik Cohrs, Emiliano Diaz, Vasileios Sitokonstantinou, Gherardo Varando, and Gustau Camps-Valls. Large language models for constrained-based causal discovery. In *AAAI 2024 Workshop on "Are Large Language Models Simply Causal Parrots?"*, 2023. URL <https://openreview.net/forum?id=NEAoZRWHPN>.
- N. Dubowitz, W. Xue, Q. Long, J. G. Ownby, D. E. Olson, D. Barb, M. K. Rhee, A. V. Mohan, P. I. Watson-Williams, S. L. Jackson, A. M. Tomolo, T. M. Johnson II, and L. S. Phillips. Aging is associated with increased hba1c levels, independently of glucose levels and insulin resistance, and also with decreased hba1c diagnostic specificity. *Diabetic Medicine*, 31(8):927–935, 2014. doi: <https://doi.org/10.1111/dme.12459>.
- Gemini Team, Google. Gemini: A family of highly capable multimodal models. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2312.11805.
- Penny Gordon-Larsen, Natalie S. The, and Linda S. Adair. Longitudinal trends in obesity in the united states from adolescence to the third decade of life. *Obesity*, 18(9):1801–1804, 2010. doi: <https://doi.org/10.1038/oby.2009.451>.
- Michael Gurven, Aaron D. Blackwell, Daniel Eid Rodríguez, Jonathan Stieglitz, and Hillard Kaplan. Does blood pressure inevitably rise with age? *Hypertension*, 60(1):25–33, 2012. doi: 10.1161/HYPERTENSIONAHA.111.189100.

- Uzma Hasan, Emam Hossain, and Md Osman Gani. A survey on causal discovery methods for i.i.d. and time series data. *Transactions on Machine Learning Research*, 2023. ISSN 2835-8856.
- Patrik Hoyer, Dominik Janzing, Joris M Mooij, Jonas Peters, and Bernhard Schölkopf. Nonlinear causal discovery with additive noise models. In *Proc. NIPS 2008*, volume 21 of *Advances in Neural Information Processing Systems*, 2008. URL https://proceedings.neurips.cc/paper_files/paper/2008/file/f7664060cc52bc6f3d620bcdcd94a4b6-Paper.pdf.
- Biwei Huang, Kun Zhang, Yizhu Lin, Bernhard Schölkopf, and Clark Glymour. Generalized score functions for causal discovery. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (KDD '18)*, pp. 1551–1560, 2018. doi: 10.1145/3219819.3220104.
- Takashi Ikeuchi, Mayumi Ide, Yan Zeng, Takashi Nicholas Maeda, and Shohei Shimizu. Python package for causal discovery based on LiNGAM. *Journal of Machine Learning Research*, 24(14):1–8, 2023. URL <http://jmlr.org/papers/v24/21-0321.html>.
- Takanori Inazumi, Shohei Shimizu, and Takashi Washio. Use of prior knowledge in a non-Gaussian method for learning linear structural equation models. In *Proc. International Conference on Latent Variable Analysis and Signal Separation (LVA/ICA 2010)*, volume 6365 of *LNCTS (Lecture Notes in Computer Science)*, pp. 221–228, 2010. doi: 10.1007/978-3-642-15995-4_28.
- Haitao Jiang, Lin Ge, Yuhe Gao, Jianian Wang, and Rui Song. Large language model for causal decision making. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2312.17122.
- Zhijing Jin, Jiarui Liu, Zhiheng LYU, Spencer Poff, Mrinmaya Sachan, Rada Mihalcea, Mona T. Diab, and Bernhard Schölkopf. Can large language models infer causation from correlation? In *The Twelfth International Conference on Learning Representations*, 2024. URL <https://openreview.net/forum?id=vqIH00bdqL>.
- Thomas Jiralerspong, Xiaoyin Chen, Yash More, Vedant Shah, and Yoshua Bengio. Efficient causal graph discovery using large language models. *arXiv preprint*, 2024. doi: 10.48550/arXiv.2402.01207.
- Christoph Käding and Jakob Runge. Distinguishing cause and effect in bivariate structural causal models: A systematic investigation. *Journal of Machine Learning Research*, 24(278):1–144, 2023. URL <http://jmlr.org/papers/v24/22-0151.html>.
- Elahe Khatibi, Mahyar Abbasian, Zhongqi Yang, Iman Azimi, and Amir M. Rahmani. Alcm: Autonomous llm-augmented causal discovery framework, 2024.
- Vivek Khetan, Roshni Ramnani, Mayuresh Anand, Subhashis Sengupta, and Andrew E. Fano. Causal bert: Language models for causality detection between events expressed in text. In Kohei Arai (ed.), *Intelligent Computing*, pp. 965–980, Cham, 2022. Springer International Publishing. ISBN 978-3-030-80119-9.
- Takeshi Kojima, Shixiang (Shane) Gu, Machel Reid, Yutaka Matsuo, and Yusuke Iwasawa. Large language models are zero-shot reasoners. In *Proc. NeurIPS 2022*, volume 35 of *Advances in Neural Information Processing Systems*, pp. 22199–22213, 2022.
- Emre Kıcıman, Robert Ness, Amit Sharma, and Chenhao Tan. Causal reasoning and large language models: Opening a new frontier for causality. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2305.00050.
- Jiacheng Liu, Alisa Liu, Ximing Lu, Sean Welleck, Peter West, Ronan Le Bras, Yejin Choi, and Hannaneh Hajishirzi. Generated knowledge prompting for commonsense reasoning. In *Proceedings of the 60th Annual Meeting of the Association for Computational Linguistics (ACL 2022)*, volume 1 (Long Papers), pp. 3154–3169, May 2022. doi: 10.18653/v1/2022.acl-long.225.
- Stephanie Long, Alexandre Piché, Valentina Zantedeschi, Tibor Schuster, and Alexandre Drouin. Causal discovery with language models as imperfect experts. In *ICML 2023 Workshop on Structured Probabilistic Inference & Generative Modeling*, 2023. URL <https://openreview.net/forum?id=RXlvYZAE49>.

- Joris M. Mooij, Jonas Peters, Dominik Janzing, Jakob Zscheischler, and Bernhard Schölkopf. Distinguishing cause from effect using observational data: Methods and benchmarks. *Journal of Machine Learning Research*, 17(32):1–102, 2016. URL <http://jmlr.org/papers/v17/14-518.html>.
- OpenAI. GPT-4 technical report. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2303.08774.
- Lydie N. Pani, Leslie Korenda, James B. Meigs, Cynthia Driver, Shadi Chamany, Caroline S. Fox, Lisa Sullivan, Ralph B. D’Agostino, and David M. Nathan. Effect of Aging on A1C Levels in Individuals Without Diabetes: Evidence from the Framingham Offspring Study and the National Health and Nutrition Examination Survey 2001–2004. *Diabetes Care*, 31(10):1991–1996, 10 2008. ISSN 0149-5992. doi: 10.2337/dc08-0577. URL <https://doi.org/10.2337/dc08-0577>.
- R. Quinlan. Auto MPG. UCI Machine Learning Repository, 1993. doi: 10.24432/C5859H.
- P. RaviKumar, A. Bhansali, R. Walia, G. Shanmugasundar, and M. Ravikiran. Alterations in hba1c with advancing age in subjects with normal glucose tolerance: Chandigarh urban diabetes study (cuds). *Diabetic Medicine*, 28(5):590–594, 2011. doi: <https://doi.org/10.1111/j.1464-5491.2011.03242.x>.
- Alexander G. Reisach, Christof Seiler, and Sebastian Weichwald. Beware of the simulated DAG! causal discovery benchmarks may be easy to game. In *Proc. NeurIPS 2021*, volume 34 of *Advances in Neural Information Processing Systems*, 2021.
- Daniela Rodrigues, Noemi Kreif, Anna Lawrence-Jones, Mauricio Barahona, and Erik Mayer. Reflection on modern methods: constructing directed acyclic graphs (DAGs) with domain experts for health services research. *International Journal of Epidemiology*, 51(4):1339–1348, 06 2022. ISSN 0300-5771. doi: 10.1093/ije/dyac135.
- J. Rohrer. Thinking clearly about correlations and causation: Graphical causal models for observational data. *Advances in Methods and Practices in Psychological Science*, 1:27 – 42, 2017. doi: 10.1177/2515245917745629.
- Paul Rolland, Volkan Cevher, Matthäus Kleindessner, Chris Russell, Dominik Janzing, Bernhard Schölkopf, and Francesco Locatello. Score matching enables causal discovery of nonlinear additive noise models. In *Proceedings of the 39th International Conference on Machine Learning*, volume 162 of *PMLR (Proceedings of Machine Learning Research)*, pp. 18741–18753. PMLR, 17–23 Jul 2022. URL <https://proceedings.mlr.press/v162/rolland22a.html>.
- Karen Sachs, Omar Perez, Dana Pe’er, Douglas A. Lauffenburger, and Garry P. Nolan. Causal protein-signaling networks derived from multiparameter single-cell data. *Science*, 308(5721):523–529, 2005. doi: 10.1126/science.1105809.
- Gideon Schwarz. Estimating the Dimension of a Model. *The Annals of Statistics*, 6(2):461 – 464, 1978. doi: 10.1214/aos/1176344136.
- Marco Scutari and Jean-Baptiste Denis. *Bayesian Networks with Examples in R*. Chapman and Hall, Boca Raton, 2014.
- Shohei Shimizu, Patrik O. Hoyer, Aapo Hyvärinen, and Antti Kerminen. A linear non-Gaussian acyclic model for causal discovery. *Journal of Machine Learning Research*, 7(72):2003–2030, 2006. URL <https://dl.acm.org/doi/10.5555/1248547.1248619>.
- Shohei Shimizu, Takanori Inazumi, Yasuhiro Sogawa, Aapo Hyvärinen, Yoshinobu Kawahara, Takashi Washio, Patrik O. Hoyer, and Kenneth Bollen. DirectLiNGAM: A direct method for learning a linear non-gaussian structural equation model. *Journal of Machine Learning Research*, 12(33):1225–1248, 2011. URL <https://dl.acm.org/doi/10.5555/1953048.2021040>.
- Tomi Silander and Petri Myllymäki. A simple approach for finding the globally optimal Bayesian network structure. In *Proceedings of the Twenty-Second Conference on Uncertainty in Artificial Intelligence (UAI ’06)*, pp. 445–452, 2006.

- P. Spirtes, C. Glymour, and R. Scheines. *Causation, Prediction, and Search*. MIT press, 2nd edition, 2000.
- Peter Spirtes, Clark Glymour, Richard Scheines, and Robert Tillman. Automated Search for Causal Relations: Theory and Practice. In Rina Dechter, Hector Geffner, and Joseph Y. Halpern (eds.), *Heuristics, Probability and Causality: A Tribute to Judea Pearl*, chapter 28, pp. 467–506. College Publications, 2010.
- J. H. Steiger and J. C. Lind. Statistically based tests for the number of common factors. In *The Annual Meeting of the Psychometric Society*, 1980.
- Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, Dan Bikel, Lukas Blecher, Cristian Canton Ferrer, Moya Chen, Guillem Cucurull, David Esiobu, Jude Fernandes, Jeremy Fu, Wenyin Fu, Brian Fuller, Cynthia Gao, Vedanuj Goswami, Naman Goyal, Anthony Hartshorn, Saghar Hosseini, Rui Hou, Hakan Inan, Marcin Kardas, Viktor Kerkez, Madian Khabsa, Isabel Kloumann, Artem Korenev, Punit Singh Koura, Marie-Anne Lachaux, Thibaut Lavril, Jenya Lee, Diana Liskovich, Yinghai Lu, Yuning Mao, Xavier Martinet, Todor Mihaylov, Pushkar Mishra, Igor Molybog, Yixin Nie, Andrew Poulton, Jeremy Reizenstein, Rashi Rungta, Kalyan Saladi, Alan Schelten, Ruan Silva, Eric Michael Smith, Ranjan Subramanian, Xiaoqing Ellen Tan, Binh Tang, Ross Taylor, Adina Williams, Jian Xiang Kuan, Puxin Xu, Zheng Yan, Iliyan Zarov, Yuchen Zhang, Angela Fan, Melanie Kambadur, Sharan Narang, Aurelien Rodriguez, Robert Stojnic, Sergey Edunov, and Thomas Scialom. Llama 2: Open foundation and fine-tuned chat models. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2307.09288.
- Ruibin Tu, Kun Zhang, Hedvig Kjellstrom, and Cheng Zhang. Optimal transport for causal discovery. In *International Conference on Learning Representations*, 2022. URL <https://openreview.net/forum?id=qwBK94cP1y>.
- Aniket Vashishtha, Abbavaram Gowtham Reddy, Abhinav Kumar, Saketh Bachu, Vineeth N. Balasubramanian, and Amit Sharma. Causal inference using LLM-guided discovery. In *AAAI 2024 Workshop on "Are Large Language Models Simply Causal Parrots?"*, 2023. URL <https://openreview.net/forum?id=4B296hrTIS>.
- Feng Xie, Ruichu Cai, Biwei Huang, Clark Glymour, Zeng Hao, and Kun Zhang. Generalized independent noise condition for estimating latent variable causal graphs. In *Proc. NeurIPS 2020*, volume 33 of *Advances in Neural Information Processing Systems*, 2020.
- Yang Claire Yang, Christine E. Walsh, Moira P. Johnson, Daniel W. Belsky, Max Reason, Patrick Curran, Allison E. Aiello, Marianne Chanti-Ketterl, and Kathleen Mullan Harris. Life-course trajectories of body mass index from adolescence to old age: Racial and educational disparities. *Proceedings of the National Academy of Sciences*, 118(17):e2020167118, 2021. doi: 10.1073/pnas.2020167118. URL <https://www.pnas.org/doi/abs/10.1073/pnas.2020167118>.
- Changhe Yuan and Brandon Malone. Learning optimal Bayesian networks: A shortest path perspective. *Journal of Artificial Intelligence Research*, 48:23–65, 10 2013. doi: 10.1613/jair.4039.
- Matej Zečević, Moritz Willig, Devendra Singh Dhami, and Kristian Kersting. Causal parrots: Large language models may talk causality but are not causal. *Transactions on Machine Learning Research*, 2023. ISSN 2835-8856. URL <https://openreview.net/forum?id=tv46tCzs83>.
- Yuzhe Zhang, Yipeng Zhang, Yidong Gan, Lina Yao, and Chen Wang. Causal graph discovery with retrieval-augmented generation based large language models, 2024.
- Xun Zheng, Bryon Aragam, Pradeep K Ravikumar, and Eric P Xing. Dags with no tears: Continuous optimization for structure learning. In *Advances in Neural Information Processing Systems*, volume 31. Curran Associates, Inc., 2018. URL https://proceedings.neurips.cc/paper_files/paper/2018/file/e347c51419ffb23ca3fd5050202f9c3d-Paper.pdf.
- Yujia Zheng, Biwei Huang, Wei Chen, Joseph Ramsey, Mingming Gong, Ruichu Cai, Shohei Shimizu, Peter Spirtes, and Kun Zhang. Causal-learn: Causal discovery in python. *arXiv preprint*, 2023. doi: 10.48550/arXiv.2307.16405.

A Ethics Review

Ethical Considerations in Methodology and AI Use This paper proposes a novel approach that integrates SCD with LLMs. We have thoroughly considered the issues of data privacy and biases associated with the use of LLMs. The proposed methodology enhances the accuracy and efficiency of causal discovery; however, it does not introduce explicit ethical implications beyond those generally applicable to machine learning. We are committed to the responsible use of AI and welcome the scrutiny of the ethics review committee.

Institutional Review and Consent Compliance of Health Screening Data The institutional review board approved this study, and in accordance with the double-blind review process of TMLR, the name of the institution has been withheld. The identity of the institution will be disclosed upon successful completion of the peer review. As we only analyzed anonymized data from the database, the need for informed consent was waived.

B Detail of Contents in Each Prompting Pattern

In this section, the details of the prompting in each pattern are presented. For Pattern 0, another prompting template is detailed instead of the sentences shown in Table 1. Moreover, for Patterns 1, 2, 3, and 4, the contents filled in $\langle \text{blank 5} \rangle$ and $\langle \text{blank 9} \rangle$ of the prompt template for SCP shown in Table 1 are described.

For Pattern 0 Compared with other patterns of SCP, Pattern 0 does not include any results of SCD without prior knowledge. As a result, the prompt template in Table 1 is not suitable for Pattern 0, as it includes the blanks filled with the description of the dataset and SCD result. Thus, we prepare another prompt template for Pattern 0, which is completely independent of the SCD result, and require GPT-4 to generate the response solely from its domain knowledge. Table 5 presents the prompt template in Pattern 0, which is composed mainly from the ZSCOT concept. Because it does not include information on the SCD method and relies solely on the domain knowledge in GPT-4, the probability matrix from the process of GPT-4 in Pattern 0 is applied independently of the SCD method.

Table 5: The prompt template of $Q_{ij}^{(1)}(x_i, x_j)$ for Pattern 0 for the generation of the expert knowledge of the causal effect from x_j on x_i . The “blanks” enclosed with $\langle \rangle$ are filled with description words of the theme of the causal inference and variable names.

Prompt Template of $q_{ij}^{(1)} = Q_{ij}^{(1)}(x_i, x_j)$ in Pattern 0 (for all SCD methods)

We want to carry out causal inference on $\langle \text{blank 1. theme} \rangle$, considering $\langle \text{blank 2. The description of all variables} \rangle$ as variables.

If $\langle \text{blank 7. The name of } x_j \rangle$ is modified, will it have a direct impact on $\langle \text{blank 8. The name of } x_i \rangle$?

Please provide an explanation that leverages your expert knowledge on the causal relationship between $\langle \text{blank 7. The name of } x_j \rangle$ and $\langle \text{blank 8. The name of } x_i \rangle$.

Your response should consider the relevant factors and provide a reasoned explanation based on your understanding of the domain.

For Patterns 1–4 (in the case of Exact Search and DirectLiNGAM) Following the concept of each SCP pattern, the contents filled in $\langle \text{blank 5} \rangle$ shown in Table 1 are summarized in Table 6. In this table, the names of the causes and effected variables are represented as $\langle \text{cause } i \rangle$ and $\langle \text{effect } i \rangle$ respectively, and the bootstrap probability of this causal relationship in SCD P_i and the causal coefficient of LiNGAM b_i can be included in Patterns 2–4. In Patterns 2 and 4, only the causal relationships with $P_i \neq 0$ are listed in $\langle \text{blank 5} \rangle$. In Pattern 3, the causal relationships with $b_i \neq 0$ are listed in $\langle \text{blank 5} \rangle$.

The contents filled in $\langle \text{blank 6} \rangle$ and $\langle \text{blank 9} \rangle$ also depend on the SCP patterns, and are shown in Table 7. Here, we define the bootstrap probability of $x_j \rightarrow x_i$ as P_{ij} . we also define the causal coefficient of $x_j \rightarrow x_i$ in LiNGAM as b_{ij} , because the structural equation of LiNGAM is usually defined as¹¹:

$$x_i = \sum_{i \neq j} b_{ij} x_j + e_i \quad (1)$$

Prompt Template in case of PC algorithm Although the causal relationships are ultimately represented only as directed edges in Exact Search and DirectLiNGAM, the situation changes slightly when we adopt the PC algorithm along with the codes in “causal-learn.” This is because the PC algorithm can also output undirected edges, when the causal direction between a pair of variables cannot be determined. Therefore, we have tentatively decided to include not only directed edges but also undirected edges in SCP. Additionally, we have prepared another prompting template for SCP in the case of PC, as shown in Table 8. This template is

¹¹Here, the error distribution function e_i is also assumed to be non-Gaussian.

Table 6: Contents filled in ⟨blank 5⟩ shown in Table 1, when Exact Search or DirectLiNGAM is adopted for the SCD process.

SCP Pattern	Content in ⟨blank 5⟩
Pattern 1 Directed edges	All of the edges suggested by the statistical causal discovery are below: $\langle \text{cause } 1 \rangle \rightarrow \langle \text{effect } 1 \rangle$ $\langle \text{cause } 2 \rangle \rightarrow \langle \text{effect } 2 \rangle$ \vdots
Pattern 2 Bootstrap probabilities of directed edges	All of the edges with non-zero bootstrap probabilities suggested by the statistical causal discovery are below: $\langle \text{cause } 1 \rangle \rightarrow \langle \text{effect } 1 \rangle$ (bootstrap probability = P_1) $\langle \text{cause } 2 \rangle \rightarrow \langle \text{effect } 2 \rangle$ (bootstrap probability = P_2) \vdots
Pattern 3 (DirectLiNGAM Only) Non-zero causal coefficients of directed edges	All of the edges and their coefficients of the structural causal model suggested by the statistical causal discovery are below: $\langle \text{cause } 1 \rangle \rightarrow \langle \text{effect } 1 \rangle$ (coefficient = b_1) $\langle \text{cause } 2 \rangle \rightarrow \langle \text{effect } 2 \rangle$ (coefficient = b_2) \vdots
Pattern 4 (DirectLiNGAM Only) Non-zero causal coefficients and bootstrap probabilities of directed edges	All of the edges with non-zero bootstrap probabilities and their coefficients of the structural causal model suggested by the statistical causal discovery are below: $\langle \text{cause } 1 \rangle \rightarrow \langle \text{effect } 1 \rangle$ (coefficient = b_1 , bootstrap probability = P_1) $\langle \text{cause } 2 \rangle \rightarrow \langle \text{effect } 2 \rangle$ (coefficient = b_2 , bootstrap probability = P_2) \vdots

Table 7: Contents filled in ⟨blank 6⟩ and ⟨blank 9⟩ shown in Table 1, when Exact Search or DirectLiNGAM is adopted for the SCD process.

SCP Pattern	Case Classification	⟨blank 6⟩	Content in ⟨blank 9⟩
Pattern 1 Directed edges	$x_j \rightarrow x_i$ emerged	a	- (No values are filled in)
	$x_j \rightarrow x_i$ not emerged	no	- (No values are filled in)
Pattern 2 Bootstrap probabilities of directed edges	$P_{ij} \neq 0$	a	with a bootstrap probability of P_{ij}
	$P_{ij} = 0$	no	- (No values are filled in)
Pattern 3 (DirectLiNGAM Only) Non-zero causal coefficients of directed edges	$b_{ij} \neq 0$	a	with a causal coefficient of b_{ij}
	$b_{ij} = 0$	no	- (No values are filled in)
Pattern 4 (DirectLiNGAM Only) Non-zero causal coefficients and bootstrap probabilities of directed edges	$P_{ij} \neq 0$ and $b_{ij} \neq 0$	a	with a bootstrap probability of P_{ij} , and the coefficient is likely to be b_{ij}
	$P_{ij} \neq 0$ and $b_{ij} = 0$	a	with a bootstrap probability of P_{ij} , but the coefficient is likely to be 0
	$P_{ij} = 0$	no	- (No values are filled in)

slightly modified from the one in Table 1. The description for ⟨blank 5⟩ in each SCP pattern is augmented by Table 9, and the description for ⟨blank 6⟩ is similarly augmented by Table 10.

As shown in Table 9, the directed and undirected edges are separately listed and clearly distinguished by the edge symbols of “ \rightarrow ” for directed edges and “ $—$ ” for undirected edges. These are then filled in ⟨blank 5⟩. The pairs of variables connected by undirected edges are represented as ⟨cause or effect $i-1$ ⟩ and ⟨cause or effect $i-2$ ⟩, and the bootstrap probability of the emergence of these relationships is represented as P_i^d . On the other hand, the bootstrap probability of ⟨cause i ⟩ \rightarrow ⟨effect i ⟩ is represented as P_i^d .

The division of the descriptions in ⟨blank 6⟩ is shown in Table 10. The bootstrap probabilities of the appearance of $x_j \rightarrow x_i$ and $x_j — x_i$ are respectively represented as P_{ij}^d and P_{ij}^u .

Table 8: The prompt template of $Q_{ij}^{(1)}(x_i, x_j, \hat{G}_0, \mathbf{P}^d, \mathbf{P}^u)$ in case of the PC algorithm. The “blanks” enclosed with $\langle \rangle$ are filled with description words considering the theme of the causal inference, variable names, and the SCD result with the PC algorithm.

Prompt Template of $q_{ij}^{(1)} = Q_{ij}^{(1)}(x_i, x_j, \hat{G}_0, \mathbf{P}^d, \mathbf{P}^u)$ for PC
<p>We want to carry out causal inference on $\langle \text{blank 1. The theme} \rangle$, considering $\langle \text{blank 2. The description of all variables} \rangle$ as variables.</p> <p>First, we have conducted the statistical causal discovery with the PC (Peter-Clerk) algorithm, using a fully standardized dataset on $\langle \text{blank 4. The description of the dataset} \rangle$.</p> <p>$\langle \text{blank 5. Including here the information of } \hat{G}_0 \text{ (for Pattern 1), or } \mathbf{P}^d \text{ and } \mathbf{P}^u \text{ (for Pattern 2). The detail of the contents depends on prompting patterns, both for directed and undirected edges.} \rangle$</p> <p>According to the results shown above, it has been determined that $\langle \text{blank 6. The detail of the interpretation on whether there is a causal relationship between } x_j \text{ and } x_i \text{ from the result shown in blank 5} \rangle$.</p> <p>Then, your task is to interpret this result from a domain knowledge perspective and determine whether this statistically suggested hypothesis is plausible in the context of the domain.</p> <p>Please provide an explanation that leverages your expert knowledge on the causal relationship between $\langle \text{blank 7. The name of } x_j \rangle$ and $\langle \text{blank 8. The name of } x_i \rangle$, and assess the naturalness of this causal discovery result. Your response should consider the relevant factors and provide a reasoned explanation based on your understanding of the domain.</p>

Table 9: Contents filled in ⟨blank 5⟩ shown in Table 8.

SCP Pattern	Content in ⟨blank 5⟩
Pattern 1 Directed and undirected edges	All of the edges suggested by the statistical causal discovery are below: ⟨ cause 1 ⟩ → ⟨ effect 1 ⟩ ⟨ cause 2 ⟩ → ⟨ effect 2 ⟩ ⋮ In addition to the directed edges above, all of the undirected edges suggested by the statistical causal discovery are below: ⟨ cause or effect 1-1 ⟩ — ⟨ cause or effect 1-2 ⟩ ⟨ cause or effect 2-1 ⟩ — ⟨ cause or effect 2-2 ⟩ ⋮
	All of the edges with non-zero bootstrap probabilities suggested by the statistical causal discovery are below: ⟨ cause 1 ⟩ → ⟨ effect 1 ⟩ (bootstrap probability = P_1^d) ⟨ cause 2 ⟩ → ⟨ effect 2 ⟩ (bootstrap probability = P_2^d) ⋮ In addition to the directed edges above, all of the undirected edges suggested by the statistical causal discovery are below: ⟨ cause or effect 1-1 ⟩ — ⟨ cause or effect 1-1 ⟩ (bootstrap probability = P_1^u) ⟨ cause or effect 2-1 ⟩ — ⟨ cause or effect 2-2 ⟩ (bootstrap probability = P_2^u) ⋮

Table 10: Contents filled in ⟨blank 6⟩ shown in Table 8.

SCP Pattern	Case Classification	Content in ⟨blank 6⟩
Pattern 1 Directed and undirected edges	$x_j \rightarrow x_i$	there may be a direct impact of a change in ⟨blank 7. The name of x_j ⟩ on ⟨blank 8. The name of x_i ⟩
	$x_j - x_i$	there may be a direct causal relationship between ⟨blank 7. The name of x_j ⟩ and ⟨blank 8. The name of x_i ⟩, although the direction has not been determined
	no edge between x_i and x_j	there may be no direct impact of a change in ⟨blank 7. The name of x_j ⟩ on ⟨blank 8. The name of x_i ⟩
Pattern 2 Bootstrap probabilities of directed and undirected edges	$P_{ij}^d \neq 0$ and $P_{ij}^u \neq 0$	there may be a direct impact of a change in ⟨blank 7. The name of x_j ⟩ on ⟨blank 8. The name of x_i ⟩ with a bootstrap probability of P_{ij}^d . In addition, it has also been shown above that there may be a direct causal relationship between ⟨blank 7. The name of x_j ⟩ and ⟨blank 8. The name of x_i ⟩ with a bootstrap probability of P_{ij}^u , although the direction has not been determined
	$P_{ij}^d \neq 0$ and $P_{ij}^u = 0$	there may be a direct impact of a change in ⟨blank 7. The name of x_j ⟩ on ⟨blank 8. The name of x_i ⟩ with a bootstrap probability of P_{ij}^d
	$P_{ij}^d = 0$ and $P_{ij}^u \neq 0$	there may be a direct causal relationship between ⟨blank 7. The name of x_j ⟩ and ⟨blank 8. The name of x_i ⟩ with a bootstrap probability of P_{ij}^u , although the direction has not been determined
	$P_{ij}^d = 0$ and $P_{ij}^u = 0$	there may be no direct impact of a change in ⟨blank 7. The name of x_j ⟩ on ⟨blank 8. The name of x_i ⟩

C Details of Datasets used in Demonstrations

In this section, the details of the dataset used in the main body and the appendix are clarified. The ground truths set for the evaluation of the SCD and LLM-KBCI results for each dataset are presented.

C.1 Auto MPG data

Auto MPG data were originally open in the UCI Machine Learning Repository (Quinlan, 1993), and used as a benchmark dataset for causal inference (Spirtes et al., 2010; Mooij et al., 2016). This dataset consists of the variables around the fuel consumption of cars. We adopt five variables: “Weight”, “Displacement”, “Horsepower”, “Acceleration” and “Mpg”(miles per gallon). Moreover, the number of points of this dataset in the experiment is 392. The ground truth of causal relationships we adopt in this paper is shown in Figure 3; the original has been shown as the example of the kPC algorithm (Spirtes et al., 2010). The differences from the original study (Spirtes et al., 2010) are presented below:

(1) Loss of “Cylinders” Although there is also a discrete variable of “Cylinders” in the original data (Quinlan, 1993), it is omitted in the experiments to focus solely on the continuous variables.

(2) Directed edge from “Weight” to “Displacement” The “Weight” and “Displacement” are connected with an undirected edge, which indicates that the direction cannot be determined in the kPC algorithm, although a causal relationship between these two variables is suggested. However, it is empirically acknowledged that large and heavy vehicles use engines with larger displacement to provide sufficient power to match their size. Thus, we temporally set the direction of the edge between these two variable as “Weight” → “Displacement.”

We also recognize that another ground truth was interpreted in the process of reconstructing the Tübingen database for causal-effect pairs (Mooij et al., 2016)¹², and “Mpg” and “Acceleration” were interpreted as effected variables from other elements. This ground truth seems to be reliable, if we do not significantly discriminate between direct and indirect causal effects and targeting the identification of cause and effect from a pair of variables. However, we adopt the ground truth based on the result from the kPC algorithm, because our target is to approach the true causal graph, including multi-step causal relationships.

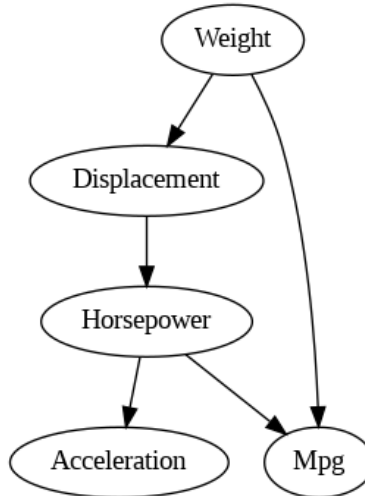


Figure 3: Causal graph of ground truth adopted for Auto MPG data in this study.

In Figure 4, the results of basic causal structure analysis by the PC, Exact Search, and DirectLiNGAM algorithms without prior knowledge are presented. Several reversed edges from ground truths such as “Mpg” → “Weight” are observed.

¹²<https://webdav.tuebingen.mpg.de/cause-effect/>

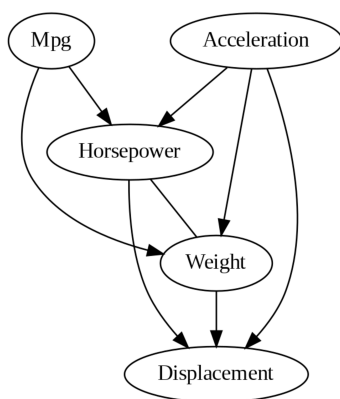
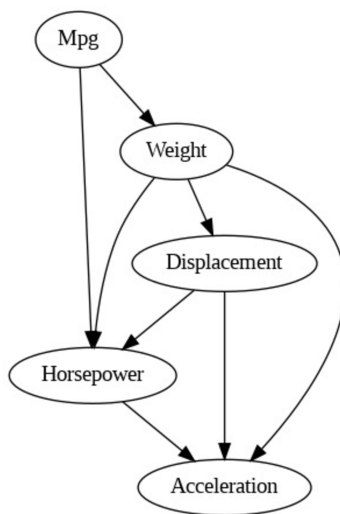
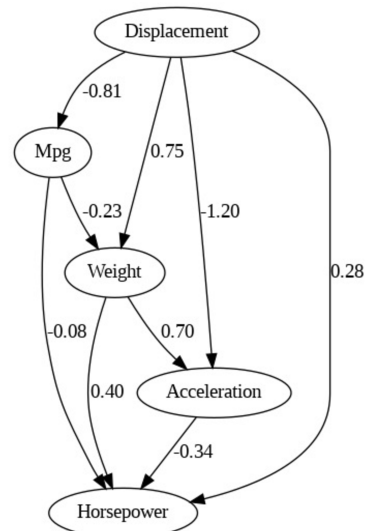
(A) PC**(B) Exact Search****(C) DirectLiNGAM**

Figure 4: Results of SCD on Auto MPG data with (A) PC, (B) Exact Search, and (C) DirectLiNGAM.

C.2 DWD climate data

The DWD climate data were originally provided by the DWD ¹³, and several of the original datasets were merged and reconstructed as a component of the übingen database for causal-effect pairs (Mooij et al., 2016). This dataset consists of six variables: “Altitude”, “Latitude”, “Longitude”, “Sunshine” (duration), “Temperature” and “Precipitation”. The number of points of this dataset is 349, which corresponds to the number of weather stations in Germany without missing data.

Because there is no ground truth on this dataset advocated, except for that in the übingen database for causal-effect pairs (Mooij et al., 2016), we adopt it temporally in this experiment, as shown in Figure 5.

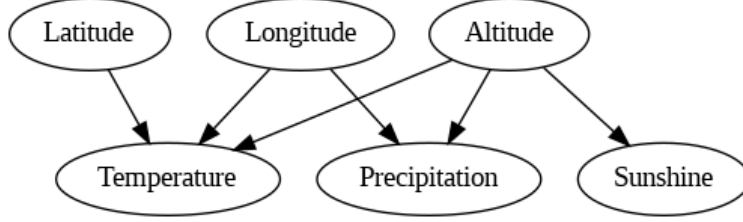
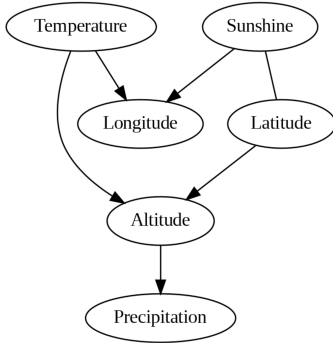


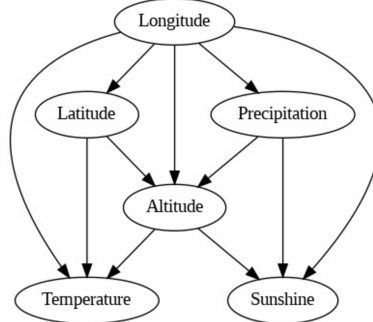
Figure 5: Causal graph of ground truth adopted for DWD climate data in this study.

In Figure 6, the results of basic causal structure analysis by the PC, Exact Search, and DirectLiNGAM algorithms without prior knowledge are presented. In all the causal graphs in Figure 6, several unnatural behaviors are observed, such as “Altitude” being effected by other climate variables, which we interpret as reversed causal relationships from the ground truths.

(A) PC



(B) Exact Search



(C) DirectLiNGAM

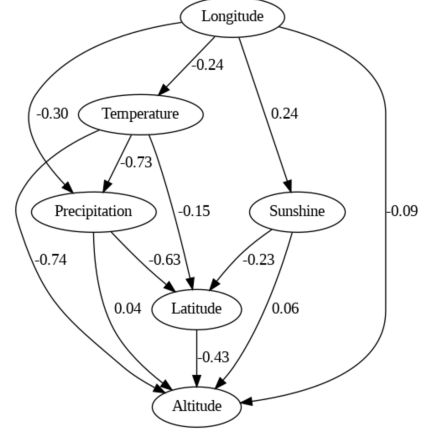


Figure 6: Results of SCD on DWD climate data with (A) PC, (B) Exact Search, and (C) DirectLiNGAM.

¹³<https://www.dwd.de/>

C.3 Sachs protein data

This dataset consists of the variables of the phosphorylation level of proteins and lipids in primary human immune cells, which were originally constructed and analyzed with the non-parametric causal structure learning algorithm by Sachs et al. (2005). It contains 11 continuous variables: “raf”, “mek”, “plc”, “pip2”, “pip3”, “erk”, “akt”, “pka”, “pkc”, “p38” and “jnk”. The number of points of this dataset is 7466.

The ground truth adopted in this study is almost the same as the interpretation shown in the study by Sachs et al. (2005). The differences from the causal graph visually displayed in the original paper are presented below:

(1) **Reversed edge between “pip3” and “plc”** Although the directed edge “plc” \rightarrow “pip3” was detected in the original study, it was denoted as “reversed,” which may be the reversed direction from the expected edge. Thus, we adopt the causal relationship of “pip3” \rightarrow “plc” which Sachs *et al.* anticipated as true from an expert point of view.

(2) **Three missed edges in the original study** In the study by Sachs *et al.*, “pip2” \rightarrow “pkc”, “plc” \rightarrow “pkc,” and “pip3” \rightarrow “akt” did not appear in the Bayesian network inference result, although they were expected to be direct causal relationships from the domain knowledge. We adopt these three edges for the ground truth considering that they may not appear under certain SCD conditions and assumptions.

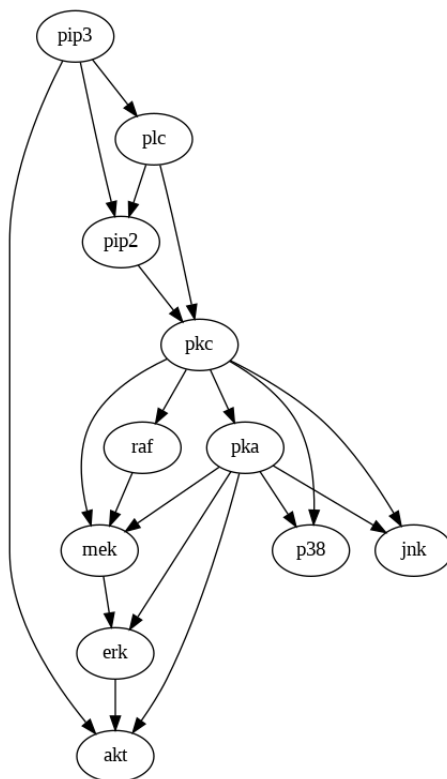


Figure 7: Causal graph of ground truth adopted for Sachs protein data in this study.

In Figure 8, the results of the basic causal structure analysis by the PC, Exact Search, and DirectLiNGAM algorithms without prior knowledge are shown.

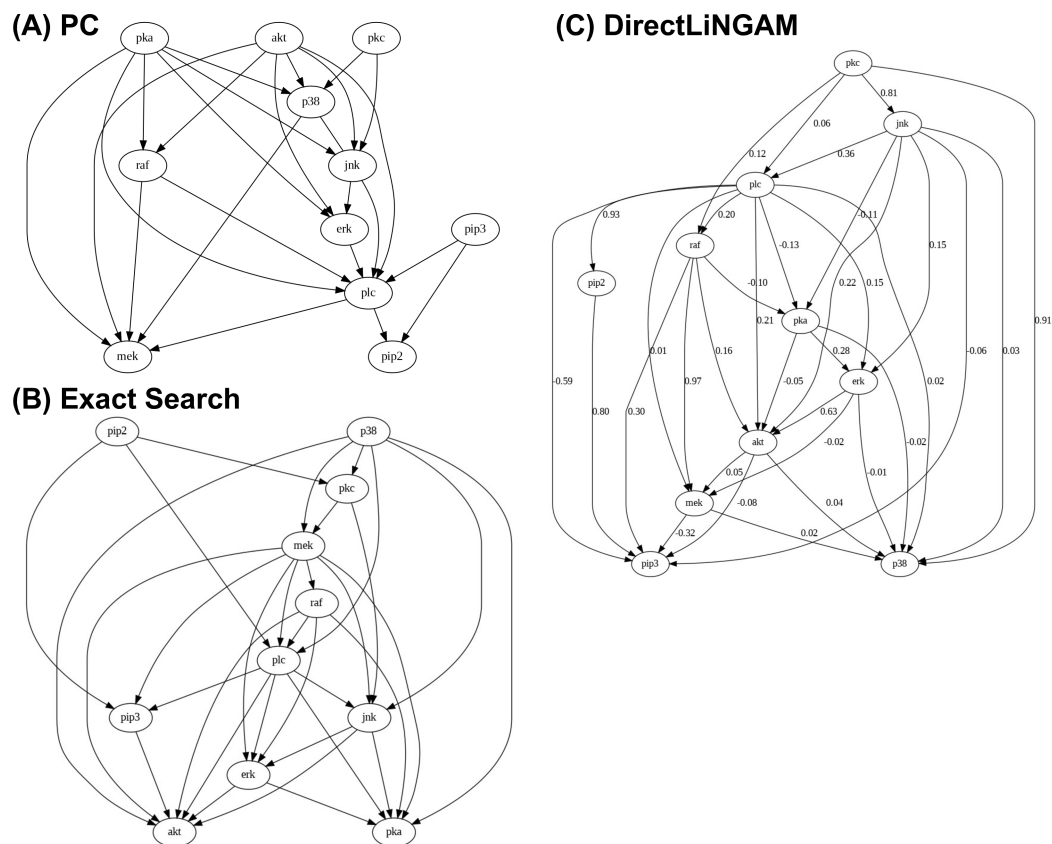


Figure 8: Results of SCD on Sachs data with (A) PC, (B) Exact Search, and (C) DirectLiNGAM.

C.4 Health screening data (closed data and not included in GPT-4’s pre-training materials)

To confirm that GPT-4 can adequately judge the existence of causal relationships with SCP, even if the dataset used in SCD is not included in the pre-training dataset of GPT-4, we have additionally prepared the health screening dataset of workers in engineering and construction contractors, which is not disclosed because of its sensitive nature from personal handling and other private aspects. It contains seven continuous variables: body mass index (“BMI”), waist circumference (“Waist”), Systolic blood pressure (“SBP”), Diastolic blood pressure (“DBP”), hemoglobin A1c (“HbA1c”), low density lipoprotein cholesterol (“LDL”), and age (“Age”). The number of total points of this dataset is 123 151.

Although the causal relationships between all pairs of variables are not completely determined, we set two types of ground truths.

(1) Directed edges interpreted as ground truths We empirically set four directed edges below as ground truths.

- “Age”→“BMI”(Clarke et al., 2008; Alley et al., 2008; Gordon-Larsen et al., 2010; Yang et al., 2021)
- at least one of “Age”→“SBP” and “Age”→“DBP”(Gurven et al., 2012)
- “Age”→“HbA1c”(Pani et al., 2008; RaviKumar et al., 2011; Dubowitz et al., 2014)

(2) Variable interpreted as a parent for all other variables “Age” is an unmodifiable background factor. Furthermore, it has been clearly demonstrated in numerous medical studies that aging affects “BMI,” “SBP,” “DBP,” and “HbA1c.” Based on this specialized knowledge, we interpret “Age” as a parent for all other variables.

The ground truths introduced above also appear in the result of DirectLiNGAM without prior knowledge, as shown in Figure 9. Although “Age”→“HbA1c” is confirmed in this result, the causal coefficient of this edge is relatively small. Thus, depending on the number of data points or the bias of the dataset, it is possible that this edge does not appear in all SCD methods without prior knowledge. For the experiment, to confirm that GPT-4 can supply SCD with adequate prior knowledge, even if a direct edge of the ground truth is not apparent, we have repeated the sampling of 1000 points from the entire dataset, until we obtained a subset on which PC, Exact Search, and DirectLiNGAM cannot discern the causal relationship “Age”→“HbA1c” without prior knowledge.

The results of the SCD on the subset are shown in Figure 10, and this subset is adopted to confirm the effectiveness of the proposed method. It is confirmed in all SCD results that “Age” → “HbA1c” does not appear, and “Age” is directly influenced by other variables, which we interpret as an unnatural behavior from the domain knowledge.

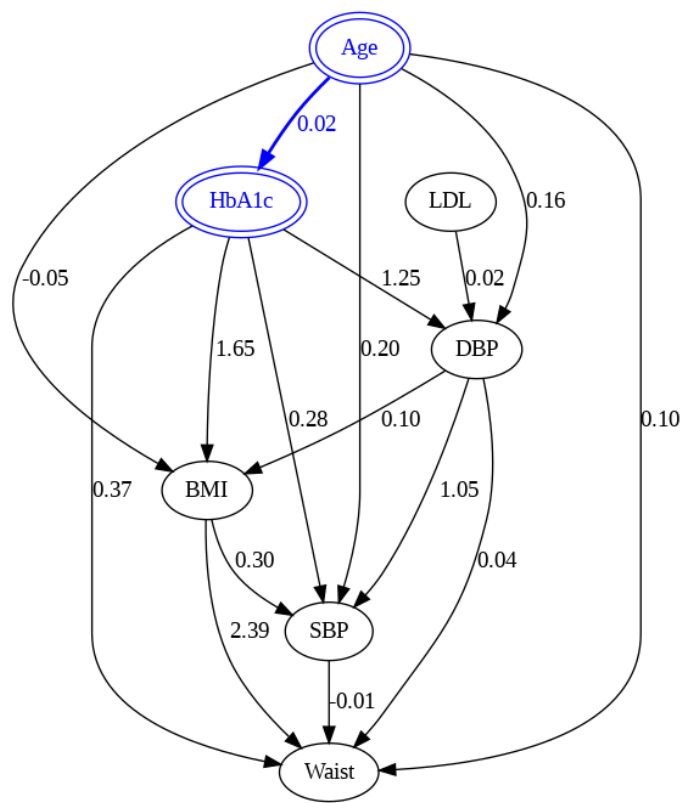
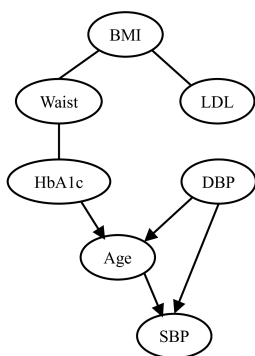
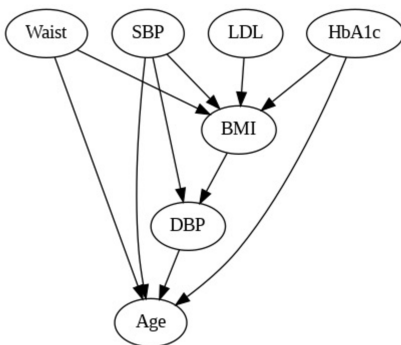


Figure 9: Causal graph suggested by DirectLiNGAM using full points of the health screening data.

(A) PC



(B) Exact Search



(C) DirectLiNGAM

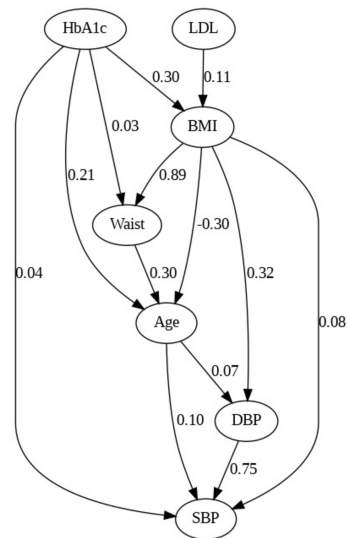


Figure 10: Results of SCD on the randomly selected subsample in the health screening dataset with (A) PC, (B) Exact Search, and (C) DirectLiNGAM.

D Composition of Adjacency Matrices Representing Causal Structure and Evaluation

D.1 Composition of Prior Knowledge Matrices

As shown in Algorithm 2, the composition rule of \mathbf{PK} depends on the type of SCD method adopted, and the decision criteria of forced and forbidden edges are tentatively set at 0.95 and 0.05, respectively. While PC and DirectLiNGAM can be augmented with constraints for both forced and forbidden directed edges or paths, Exact Search can only be augmented with the constraints for forbidden directed edges. In this section, the composition rule for \mathbf{PK} is described in detail for all the SCD algorithms we have adopted in this work.

For PC As for the matrix representation of \mathbf{PK} , the values of the matrix elements are determined as follows:

- Case 1. If $x_i \rightarrow x_j$ is forced (i.e., $p_{ij} \geq 0.95$), then PK_{ij} is set to 1.
- Case 2. If $x_i \rightarrow x_j$ is forbidden (i.e., $p_{ij} < 0.05$), then PK_{ij} is set to 0.
- Case 3. If the existence of $x_i \rightarrow x_j$ cannot be determined immediately from the domain knowledge generated by GPT-4 (i.e., $0.05 \leq p_{ij} < 0.95$), then PK_{ij} is set to -1 .

This ternary matrix composition is based on the constraints of the prior knowledge matrix DirectLiNGAM, which will be explained later, to apply the generated \mathbf{PK} to DirectLiNGAM as quickly as possible. Although prior knowledge is represented as a matrix in the PC algorithm widely open in “causal-learn,” both forced and forbidden edges can be set and the possibility of other unknown edges are explored. This similar properties with DirectLiNGAM means that the prior knowledge for this PC algorithm can be represented in ternary matrix, if we need to do. Therefore, the composition rule of \mathbf{PK} for PC is set to be the same as that for DirectLiNGAM in this work, to treat it consistently as possible.

For DirectLiNGAM Although the criteria of setting the values in \mathbf{PK} are the same as those for PC, the definition of the value becomes slightly different. Although the prior knowledge for the PC algorithm in the “causal-learn” package corresponds to the existence of directed edges between pairs of variables, the prior knowledge for DirectLiNGAM is determined with the knowledge on directed paths. The values of the matrix elements are determined as below:

- Case 1. If the directed path from x_i to x_j is forced (i.e., $p_{ij} \geq 0.95$), then PK_{ij} is set to 1.
- Case 2. If the directed path from x_i to x_j is forbidden (i.e., $p_{ij} < 0.05$), then PK_{ij} is set to 0.
- Case 3. If the existence of the directed path from x_i to x_j cannot be determined immediately from the domain knowledge generated by GPT-4 (i.e., $0.05 \leq p_{ij} < 0.95$), then PK_{ij} is set to -1 .

This ternary matrix composition, using 1, 0 and -1 is indeed implemented in the software package “LiNGAM.”

For Exact Search While \mathbf{PK} in cases of PC and DirectLiNGAM is a ternary matrix, one must be careful that \mathbf{PK} in Exact Search is a binary matrix. The values of the matrix elements are determined as below:

- Case 4. If $x_i \rightarrow x_j$ is forbidden (i.e., $p_{ij} < 0.05$), then PK_{ij} is set to 0.
- Case 5. If $x_i \rightarrow x_j$ is forced, or the existence of this causal relationship cannot be determined immediately from the domain knowledge generated by GPT-4 (i.e., $0.05 \leq p_{ij}$), then PK_{ij} is set to 1.

It must be carefully noted that, although the definition of $PK_{ij} = 0$ in Case 4 for Exact Search is exactly the same as that in Case 2 for PC and DirectLiNGAM, the definition of $PK_{ij} = 1$ in Case 5 for Exact Search encompasses the both Case 1 and Case 3 for PC and DirectLiNGAM. This difference must be taken into account when evaluating \mathbf{PK} in comparison with the ground truths, to interpret the results in a unified manner regardless of the SCD methods used.

D.2 Composition of Ground Truth Matrix

The representation of ground truths in matrix form can be simply realized using a binary matrix, provided that it is determined whether a directed edge exists for every possible pair of variables in the system. The composition rule for the ground truth matrix \mathbf{GT} is as follows:

- If $x_j \rightarrow x_i$ exists, then GT_{ij} is set to 1.
- If $x_j \rightarrow x_i$ does not exist, then GT_{ij} is set to 0.

The matrix representations of the ground truth of the benchmark datasets of Auto MPG, DWD, and Sachs shown in Appendix C are expressed as follows:

$$\mathbf{GT}_{\text{AutoMPG}} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (2)$$

$$\mathbf{GT}_{\text{DWD}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (3)$$

$$\mathbf{GT}_{\text{Sachs}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{pmatrix} \quad (4)$$

D.3 Calculation of Metrics for Evaluation of Structural Consistency with Ground Truths (SHD, FPR, FNR, Precision, F1 Score)

Structural metrics such as SHD, FPR, FNR, precision, and F1 score are commonly calculated for performance evaluation in various machine learning and classification contexts, and are compared with the ground truth data. In a similar context, the causal structures inferred by LLM-KBCI and SCD, especially for the benchmark datasets with known ground truths, can also be evaluated using these metrics.

For the practical evaluation of the SCD results in this study, we use the ground truth matrices defined for the benchmark datasets in Eq.(2), (3) and (4) as references, and we measure these metrics using the adjacency matrices that are calculated directly in SCD algorithms or easily transformed from the output causal graphs. Similarly, the calculation of these metrics for the evaluating LLM-KBCI outputs is carried out using \mathbf{PK} .

However, it must be noted that there can be some arguments on the definition of metrics for \mathbf{PK} based on \mathbf{GT} , because the definition of the matrix elements of \mathbf{PK} shown in Appendix D.1 is partially different from that of \mathbf{GT} described in Appendix D.2. In particular, although GT_{ij} is a binary variable completely determined with whether $x_j \rightarrow x_i$ exists or not, PK_{ij} can be set to -1 for PC and DirectLiNGAM and to 1 for Exact Search. This indicates or includes the case where it is not impossible to definitively assert the presence or absence of $x_j \rightarrow x_i$.

Therefore, although there may be a discussion that a reasonable extension of the definitions of these metrics is required for the case above, in this study, we evaluate these metrics from $|\mathbf{PK}|$, in which both $PK_{ij} = 1$ and $PK_{ij} = -1$ are interpreted as a “tentative assertion of the presence of $x_j \rightarrow x_i$ ” and are treated identically. This processing of \mathbf{PK} can also be interpreted as that of temporarily adopting the composition rule of \mathbf{PK} for Exact Search as it is for the evaluation of SHD, FPR, FNR, precision, and F1 score, for all SCD methods. With this processing, \mathbf{PK} is handled in a unified manner regardless of the SCD methods used. We believe this approach is the best way to maintain the original concept of composing \mathbf{PK} , while aiming for consistent discussion across all SCD methods.

Calculation of SHD According to the original concept of the structural hamming distance (SHD), this metric is represented as the total number of edge additions, deletions, or reversals that are needed to convert the estimated graph G' into its ground truth graph G (Zheng et al., 2018; Cheng et al., 2022; Hasan et al., 2023). As in our study, if network graphs G and G' are represented by binary matrices \mathbf{G} and \mathbf{G}' , respectively, where all elements are either 0 or 1, then the total number of edge additions (A), deletions (D), and reversals (R) can be simply calculated as follows:

$$A(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \mathbf{1}(G_{ij})\mathbf{1}(G_{ji})\mathbf{1}(G'_{ij} - 1) \quad (5)$$

$$D(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \mathbf{1}(G'_{ij})\mathbf{1}(G'_{ji})\mathbf{1}(G_{ij} - 1) \quad (6)$$

$$R(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \mathbf{1}(G_{ij})\mathbf{1}(G_{ji} - 1)\mathbf{1}(G'_{ij} - 1)\mathbf{1}(G'_{ji}) \quad (7)$$

Here, we introduce the indicator function $\mathbf{1}(x)$, expressed as follows:

$$\mathbf{1}(x) = \begin{cases} 1 & \text{if } x = 0, \\ 0 & \text{otherwise } (x \neq 0). \end{cases} \quad (8)$$

As SHD is defined as $SHD = A + D + R$, it is easily evaluated as follows:

$$SHD(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \left\{ \mathbf{1}(G_{ij})\mathbf{1}(G_{ji})\mathbf{1}(G'_{ij} - 1) + \mathbf{1}(G'_{ij})\mathbf{1}(G'_{ji})\mathbf{1}(G_{ij} - 1) + \mathbf{1}(G_{ij})\mathbf{1}(G_{ji} - 1)\mathbf{1}(G'_{ij} - 1)\mathbf{1}(G'_{ji}) \right\} \quad (9)$$

For the evaluation of SHD of LLM-KBCI outputs, $SHD(|\mathbf{PK}|, \mathbf{GT})$ is calculated with Eq. (9).

Calculation of FPR, FNR, Precision, and F1score In the similar context to SHD, for calculation of the metrics such as false positive rate (FPR) and false negative rate (FNR), we prepare the equation for evaluating the number of true positive (TP), false positive (FP), true negative (TN), and false negative (FN) edges as follows:

$$TP(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \mathbf{1}(G_{ij} - 1)\mathbf{1}(G'_{ij} - 1) \quad (10)$$

$$FP(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \mathbf{1}(G_{ij})\mathbf{1}(G'_{ij} - 1) \quad (11)$$

$$TN(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \mathbf{1}(G_{ij})\mathbf{1}(G'_{ij}) \quad (12)$$

$$FN(\mathbf{G}', \mathbf{G}) = \sum_{i,j} \mathbf{1}(G_{ij} - 1)\mathbf{1}(G'_{ij}) \quad (13)$$

Then, using Eq. (10)– (13), the definition of FPR, FNR, precision, and F1 score can be expressed as follows:

$$FPR(\mathbf{G}', \mathbf{G}) = \frac{FP(\mathbf{G}', \mathbf{G})}{TN(\mathbf{G}', \mathbf{G}) + FP(\mathbf{G}', \mathbf{G})} \quad (14)$$

$$FNR(\mathbf{G}', \mathbf{G}) = \frac{FN(\mathbf{G}', \mathbf{G})}{TP(\mathbf{G}', \mathbf{G}) + FN(\mathbf{G}', \mathbf{G})} \quad (15)$$

$$Precision(\mathbf{G}', \mathbf{G}) = \frac{TP(\mathbf{G}', \mathbf{G})}{TP(\mathbf{G}', \mathbf{G}) + FP(\mathbf{G}', \mathbf{G})} \quad (16)$$

$$F_1score(\mathbf{G}', \mathbf{G}) = \frac{2 TP(\mathbf{G}', \mathbf{G})}{2 TP(\mathbf{G}', \mathbf{G}) + FN(\mathbf{G}', \mathbf{G}) + FP(\mathbf{G}', \mathbf{G})} \quad (17)$$

For the evaluation of structural metrics such as FPR of LLM-KBCI outputs, $FPR(|\mathbf{PK}|, \mathbf{GT})$, $FNR(|\mathbf{PK}|, \mathbf{GT})$, $Precision(|\mathbf{PK}|, \mathbf{GT})$ and $F_1score(|\mathbf{PK}|, \mathbf{GT})$ are calculated with Eq. (14)–(17).

E Algorithm A for Transformation of Cyclic PK into Acyclic Adjacency Matrices and Selection of the Optimal Matrix

As briefly described in Section 3.1, for the case of DirectLiNGAM, acyclicity of PK is also required. Thus, if the PK directly calculated from the probability matrix is cyclic, it must be transformed into an acyclic form. One possible method is to delete the minimum number of edges included in cycles to transform PK into an acyclic matrix. However, it is possible that there are several solutions transformed from the same PK with the minimum manipulation of deleting edges. Therefore, we have decided to carry out causal discovery with DirectLiNGAM for every possible acyclic prior knowledge matrix to select the best acyclic prior knowledge matrix PK_A in terms of statistical modeling. The dataset is again fitted with a structural equation model under the constraint of the causal structure explored with DirectLiNGAM, assuming linear-Gaussian data, and the Bayes Information Criterion (BIC) is calculated. After repeating this process, the acyclic prior knowledge matrix with which the BIC becomes the lowest is selected as PK_A .

The overall transformation process is described in Algorithm 3. However, in the practical application of this method, it must be noted that completing the list of acyclic prior knowledge matrices A incurs significant computational costs. Hence, as the number of variables increases, completing this calculation algorithm in a realistic time frame becomes more challenging.

For the future generalization and application of our inference method using DirectLiNGAM, the development of more efficient algorithms for transforming a cyclic matrix into an acyclic one is anticipated.

Algorithm 3 Transformation of Cyclic PK into Acyclic Adjacency Matrices and Selection of the Optimal Matrix

Input 1: Cyclic prior knowledge matrix PK_C
Input 2: Data X with variables $\{x_1, \dots, x_n\}$
Input 3: DirectLiNGAM Algorithm $L(X, PK)$
Output: Optimal acyclic matrix PK_A
Initialize the temporal set for matrices $T \leftarrow \{PK_C\}$
Initialize the temporal set for number of the cycles $N \leftarrow \{\}$
Initialize the temporal set for acyclic matrices $A \leftarrow \{\}$
repeat
 for matrix $T_m \in T$ **do**
 Count the number of cycles in T_m as N_m
 Add N_m to N
 end for
 if $\exists N_m \in N, N_m = 0$ **then**
 Detect all T_m , which satisfies $N_m = 0$ and add them to A
 else
 Initialize the temporal set for modified matrices $T' \leftarrow \{\}$
 for $T_m \in T$ **do**
 Initialize the set for edges included in cycles $E_m \leftarrow \{\}$
 Initialize the set for edges to be removed $F_m \leftarrow \{\}$
 Detect all cycles in T_m
 For each detected cycle, identify all the edges that form the cycle
 Add these edges to a set of edges to be removed E_m
 Detect the most frequent edges " $x_i \leftarrow x_j$ " in E_m as $(i, j)_f$
 $\forall (i_f, j_f)$ add (i_f, j_f) to F_m
 for $(i_f, j_f) \in F_m$ **do**
 $T'_m = T_m$
 $T'_m(i_f, j_f) \leftarrow 0$
 Add T'_m to T'
 end for
 end for
 Replace T with T'
 end if
until A is not empty
Initialize the optimal BIC value $B = \text{None}$
Initialize the optimal acyclic matrix for prior knowledge in DirectLiNGAM $A_{\text{optimal BIC}} = \text{None}$
for $A_m \in A$ **do**
 Calculate adjacency matrix (with the components 0 or 1) of the causal discovery result $Adj = L(X, PK = A_m)$
 Fit X with the structural causal equation model represented in Adj assuming linear-Gaussian data
 Calculate BIC with Adj and X as B_{temp}
 if $B > B_{\text{temp}}$ **or** $B = \text{None}$ **then**
 $B \leftarrow B_{\text{temp}}$
 $A_{\text{optimal BIC}} = A_m$
 end if
end for
return $A_{\text{optimal BIC}}$ as PK_A

F Details of LLM-KBCI Results

It is also valuable to examine the details of the probability matrices generated by LLM-KBCI, both for the basic discussion on whether LLMs can generate a valid interpretation of causality from a domain expert’s point of view, and for understanding the characteristics of SCP. In this section, the probability matrices generated by GPT-4 for Auto MPG data and DWD climate data, which are relatively easy to interpret within common daily knowledge, are shown and briefly interpreted. For comparison among various SCP patterns (Patterns 1–4) using the same SCD method as much as possible, the probability matrices generated by GPT-4 with SCP are shown only for DirectLiNGAM. We also briefly present the probability matrices of LLM-KBCI for the sampled sub-dataset of health screening results.

F.1 LLM-KBCI for Auto MPG data

In Table 11, the probabilities of causal relationships of pairs of variables in Auto MPG data are shown. The cells highlighted in green are the ones in which the directed edges are expected to appear from the ground truths shown in Figure 3.

For all the prompting patterns, although the probability of “Weight”→“Displacement”, which is interpreted as one of the ground truth directed edges, is 0, the probability of reversed edge “Displacement”→“Weight” is non-zero and over 0.95 in Patterns 1–4. For understanding this behavior and elucidating the true causal relationship between these two variables, further discussion is required, including the possibility of the hidden common causes that are excluded from the dataset we have used.

In addition to that, although we do not believe the existence of the directed edge of “Displacement”→“Acceleration,” the probability of this causal relationship is over 0.85 for all the prompting patterns. This may be due to the property of the prompting for evaluating the probability. As shown in Table 2, GPT-4 is allowed to judge the existence of both direct and indirect causal relationships, to acquire a positive answer even if any intervening variables are not included in the dataset. However, for example, considering that the probabilities of both “Displacement”→“Horsepower” and “Horsepower”→“Acceleration,” which are part of the ground truths, are relatively high, it is also possible that GPT-4 supports the hypothesis of some impact from “Displacement” on “Acceleration” partially due to the confidence in the indirect causal relationship of “Displacement”→“Horsepower”→“Acceleration”. If one wants to distinguish the direct and indirect causal relationships in the interpretation of the probability matrix, investigation of the response from LLMs for the first prompting may lead to further understanding.

Some differences that can be related to the prompting patterns can also be observed. For example, the probability of “Horsepower”→“Mpg” in Pattern 1 is much smaller than other patterns. Moreover, the probabilities of “Horsepower”→“Acceleration” in Patterns 1 and 3 are smaller than other patterns, in which the probability of this edge is almost 1. A possible explanation of these behaviors is that the decision-making of GPT-4 is unsettled with SCP, in which the causal structure inferred by DirectLiNGAM shown in Figure 4 (c) is included. As neither “Horsepower”→“Acceleration” nor “Horsepower”→“Mpg” appears in Figure 4 (c), despite the confidence in the existence of these edges only from the domain knowledge, the decision-making of GPT-4 may become more careful, taking into account the result of SCD. It is desired to elucidate what kinds of decision-making of LLMs are likely to be affected by SCP in future work.

F.2 LLM-KBCI for DWD climate data

In Table 12, the probabilities of the causal relationships of pairs of variables in DWD climate data are shown. The cells highlighted in green are the ones in which the directed edges are expected to appear from the ground truths shown in Figure 5.

For all the prompting patterns, it is confirmed that all of the probabilities of the causal effects on “Altitude,” “Longitude,” and “Latitude” from other variables are 0. As these three variables are geographically given and fixed, the interpretation by GPT-4 that they act as parent variables that are not influenced by other factors is completely reasonable. Although “Altitude” and “Latitude” are somehow influenced according to the result of DirectLiNGAM without prior knowledge as shown in Figure 6 (c), SCP including these unnatural results

Table 11: Probabilities of the causal relationships suggested by GPT-4 in Auto MPG data. The cells in which the directed edges are expected to appear from the ground truths as shown in Figure 3 are highlighted in green.

Pattern 0					
EFFECTED\CAUSE	“Displacement”	“Mpg”	“Horsepower”	“Weight”	“Acceleration”
“Displacement”	-	0.000	0.000	0.000	0.000
“Mpg”	0.999	-	0.997	1.000	1.000
“Horsepower”	0.999	0.000	-	0.000	0.000
“Weight”	0.635	0.000	0.000	-	0.000
“Acceleration”	0.996	0.023	0.998	0.998	-

Pattern 1					
EFFECTED\CAUSE	“Displacement”	“Mpg”	“Horsepower”	“Weight”	“Acceleration”
“Displacement”	-	0.000	0.000	0.000	0.000
“Mpg”	1.000	-	0.128	0.484	0.058
“Horsepower”	1.000	0.056	-	0.001	0.000
“Weight”	0.994	0.000	0.000	-	0.000
“Acceleration”	0.859	0.000	0.828	0.998	-

Pattern 2					
EFFECTED\CAUSE	“Displacement”	“Mpg”	“Horsepower”	“Weight”	“Acceleration”
“Displacement”	-	0.000	0.000	0.000	0.000
“Mpg”	1.000	-	0.999	1.000	0.984
“Horsepower”	1.000	0.000	-	0.000	0.000
“Weight”	0.997	0.000	0.000	-	0.000
“Acceleration”	0.995	0.002	0.996	0.999	-

Pattern 3					
EFFECTED\CAUSE	“Displacement”	“Mpg”	“Horsepower”	“Weight”	“Acceleration”
“Displacement”	-	0.000	0.000	0.000	0.000
“Mpg”	0.977	-	0.969	0.754	0.547
“Horsepower”	1.000	0.051	-	0.696	0.010
“Weight”	0.954	0.000	0.000	-	0.000
“Acceleration”	0.981	0.000	0.435	0.809	-

Pattern 4					
EFFECTED\CAUSE	“Displacement”	“Mpg”	“Horsepower”	“Weight”	“Acceleration”
“Displacement”	-	0.000	0.000	0.000	0.000
“Mpg”	0.995	-	0.994	0.997	0.940
“Horsepower”	0.999	0.314	-	0.006	0.000
“Weight”	0.999	0.000	0.012	-	0.000
“Acceleration”	0.964	0.000	0.989	0.814	-

has not affected the decision-making by GPT-4. From this behavior, it is inferred that the response regarding axiomatic and self-evident matters from GPT-4 is robust and not likely to be affected by SCP, even if the SCD result exhibits obviously unnatural behaviors.

In addition, while “Longitude”→“Temperature,” which are assumed to be a ground truth, is not likely to be asserted by GPT-4, “Temperature”→“Precipitation,” which is not expected to be a ground truth, is likely to be asserted by GPT-4, across all the prompting patterns. For further interpretation of these unexpected behaviors from our ground truths, investigation of the response generated in the first prompting process is recommended. It is also interesting that although the probabilities of “Longitude”→“Precipitation” are 0 in Patterns 0–2, they become non-zero finite values in Patterns 3 and 4, in which the causal coefficient of this

directed edge calculated with DirectLiNGAM is included in SCP. This behavior may be a glimpse that SCP can assist the decision-making of GPT-4 even if it generates an incomplete response on causal relationships with its background knowledge.

Table 12: Probabilities of the causal relationships suggested by GPT-4 in DWD climate data. The cells in which the directed edges are expected to appear from the ground truths as shown in Figure 5 are highlighted in green.

Pattern 0

EFFECTED\CAUSE	“Altitude”	“Temperature”	“Precipitation”	“Longitude”	“Sunshine”	“Latitude”
“Altitude”	-	0.000	0.000	0.000	0.000	0.000
“Temperature”	1.000	-	0.891	0.000	1.000	1.000
“Precipitation”	1.000	0.999	-	0.000	0.001	0.995
“Longitude”	0.000	0.000	0.000	-	0.000	0.000
“Sunshine”	1.000	0.000	0.998	0.000	-	1.000
“Latitude”	0.000	0.000	0.000	0.000	0.000	-

Pattern 1

EFFECTED\CAUSE	“Altitude”	“Temperature”	“Precipitation”	“Longitude”	“Sunshine”	“Latitude”
“Altitude”	-	0.000	0.000	0.000	0.000	0.000
“Temperature”	0.384	-	0.034	0.000	0.856	0.011
“Precipitation”	0.025	0.999	-	0.000	0.036	0.026
“Longitude”	0.000	0.000	0.000	-	0.000	0.000
“Sunshine”	0.006	0.011	0.008	0.000	-	0.596
“Latitude”	0.000	0.000	0.000	0.000	0.000	-

Pattern 2

EFFECTED\CAUSE	“Altitude”	“Temperature”	“Precipitation”	“Longitude”	“Sunshine”	“Latitude”
“Altitude”	-	0.000	0.000	0.000	0.000	0.000
“Temperature”	0.997	-	0.007	0.000	0.999	0.989
“Precipitation”	0.739	0.999	-	0.000	0.000	0.384
“Longitude”	0.000	0.000	0.000	-	0.000	0.000
“Sunshine”	0.874	0.010	0.976	0.000	-	0.981
“Latitude”	0.000	0.000	0.000	0.000	0.000	-

Pattern 3

EFFECTED\CAUSE	“Altitude”	“Temperature”	“Precipitation”	“Longitude”	“Sunshine”	“Latitude”
“Altitude”	-	0.000	0.000	0.000	0.000	0.000
“Temperature”	0.919	-	0.016	0.003	0.615	0.973
“Precipitation”	0.585	0.996	-	0.175	0.002	0.008
“Longitude”	0.000	0.000	0.000	-	0.000	0.000
“Sunshine”	0.039	0.000	0.001	0.875	-	0.199
“Latitude”	0.000	0.000	0.000	0.000	0.000	-

Pattern 4

EFFECTED\CAUSE	“Altitude”	“Temperature”	“Precipitation”	“Longitude”	“Sunshine”	“Latitude”
“Altitude”	-	0.000	0.000	0.000	0.000	0.000
“Temperature”	0.982	-	0.023	0.029	0.990	0.958
“Precipitation”	0.826	0.987	-	0.927	0.010	0.797
“Longitude”	0.000	0.000	0.000	-	0.000	0.000
“Sunshine”	0.534	0.021	0.387	0.013	-	0.638
“Latitude”	0.000	0.000	0.000	0.000	0.000	-

F.3 LLM-KBCI for Dataset of Health Screening Results

In Table 13, the probabilities of the causal relationships of pairs of variables in our sampled sub-dataset of health screening results are shown. The cells highlighted in red are the ones in which the directed edges are expected to appear as described in Appendix C.4. In contrast, since “Age” is an unmodifiable background factor, it can be concluded that it is not a descendant of any other variables. Therefore, the probabilities in the cells highlighted in blue are expected to be 0.

Across all the prompting patterns, it is confirmed that all of probabilities of the causal effects on “Age” from other variables are indeed 0. From this fact, it is likely to be regarded by GPT-4 as axiomatic and self-evident that “Age” cannot be affected from other variables, and the judge of the causal relationships is not influenced by SCP, even if the SCD result exhibits obviously unnatural behaviors as shown in Figure 10.

Table 13: Probabilities of the causal relationships suggested by GPT-4 in the sampled sub-dataset of health screening results. The cells in which the directed edges are expected to appear from the ground truths are highlighted in red. In contrast, the probabilities in the cells highlighted in blue, are expected to be zero, since “Age” is expected to be a parent variable for all other variables.

Pattern 0							
EFFECTED\CAUSE	“BMI”	“Waist”	“SBP”	“DBP”	“HbA1c”	“LDL”	“Age”
“BMI”	-	0.994	0.000	0.000	0.000	0.000	0.901
“Waist”	1.000	-	0.000	0.000	0.000	0.000	0.353
“SBP”	0.999	0.962	-	0.998	0.987	0.000	0.626
“DBP”	0.998	0.995	0.993	-	0.000	0.000	0.001
“HbA1c”	0.998	0.998	0.000	0.000	-	0.000	0.986
“LDL”	0.988	0.967	0.000	0.000	0.000	-	0.002
“Age”	0.000	0.000	0.000	0.000	0.000	0.000	-

Pattern 1							
EFFECTED\CAUSE	“BMI”	“Waist”	“SBP”	“DBP”	“HbA1c”	“LDL”	“Age”
“BMI”	-	0.312	0.000	0.000	0.014	0.000	0.076
“Waist”	1.000	-	0.000	0.000	0.023	0.000	0.043
“SBP”	0.999	0.912	-	0.999	0.997	0.000	0.302
“DBP”	0.998	0.421	0.050	-	0.000	0.000	0.019
“HbA1c”	0.517	0.503	0.101	0.000	-	0.000	0.170
“LDL”	0.008	0.527	0.000	0.000	0.000	-	0.517
“Age”	0.000	0.000	0.000	0.000	0.000	0.000	-

Pattern 2							
EFFECTED\CAUSE	“BMI”	“Waist”	“SBP”	“DBP”	“HbA1c”	“LDL”	“Age”
“BMI”	-	0.998	0.001	0.001	0.996	0.000	0.093
“Waist”	0.999	-	0.000	0.003	0.959	0.007	0.099
“SBP”	0.998	0.994	-	0.983	0.994	0.040	0.207
“DBP”	0.997	0.975	0.984	-	0.983	0.002	0.115
“HbA1c”	0.982	0.608	0.002	0.000	-	0.000	0.723
“LDL”	0.994	0.946	0.000	0.000	0.452	-	0.171
“Age”	0.000	0.000	0.000	0.000	0.000	0.000	-

Pattern 3							
EFFECTED\CAUSE	“BMI”	“Waist”	“SBP”	“DBP”	“HbA1c”	“LDL”	“Age”
“BMI”	-	0.003	0.000	0.000	0.868	0.923	0.306
“Waist”	1.000	-	0.000	0.000	0.983	0.000	0.076
“SBP”	1.000	0.855	-	0.959	0.999	0.000	0.235
“DBP”	1.000	0.032	0.140	-	0.021	0.000	0.095
“HbA1c”	0.967	0.634	0.000	0.000	-	0.000	0.046
“LDL”	0.562	0.165	0.000	0.000	0.085	-	0.013
“Age”	0.000	0.000	0.000	0.000	0.000	0.000	-

Pattern 4							
EFFECTED\CAUSE	“BMI”	“Waist”	“SBP”	“DBP”	“HbA1c”	“LDL”	“Age”
“BMI”	-	0.993	0.000	0.000	0.024	0.006	0.037
“Waist”	1.000	-	0.000	0.000	0.957	0.000	0.395
“SBP”	0.999	0.982	-	0.001	0.998	0.000	0.795
“DBP”	0.994	0.204	0.985	-	0.408	0.000	0.926
“HbA1c”	0.824	0.391	0.000	0.000	-	0.000	0.176
“LDL”	0.485	0.403	0.000	0.000	0.000	-	0.027
“Age”	0.000	0.000	0.000	0.000	0.000	0.000	-