A Boolean Inferential Approach to Mechanistic Models in Cognitive Science and Biology

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**Abstract**

The mechanistic approach in the cognitive and biological sciences emphasizes that scientific explanations succeed by analyzing the mechanisms underlying phenomena across multiple levels. In this paper, we propose a formal strategy to establish such multi-level mechanistic models, which are foundational to mechanistic explanations. Our objectives are twofold: First, we introduce the novel "mLCA" (multi-Level Coincidence Analysis) script, which transforms binary data tables from tests on mechanistic systems into mechanistic models consistent with those tables. Second, we provide several philosophical insights derived from the outcomes generated by this script and its underlying algorithm. Using illustrative examples, we defend the following claims: 1. Inference methods for generating mechanistic models generally require information on how causal factors are assigned to different levels within data tables generated by multi-level structures. 2. The mLCA script successfully produces appropriate mechanistic models from binary data tables, demonstrating the practical application of the philosophical mechanistic approach in the sciences. 3. The number of solutions generated by mLCA increases significantly as the number of relevant factors grows, reflecting adaptations in causal inference methods to meet the demands of multi-level mechanistic modeling. 4. Any further reduction of solutions, if possible, involves pragmatic considerations, a point that carries profound implications for the broader ambitions of the mechanistic approach. By addressing these points, our paper contributes both to the development of practical algorithmic tools and to a deeper philosophical understanding of multi-level mechanistic modeling.

1 Introduction

According to the mechanistic approach, scientific explanations succeed by analyzing the mechanisms that “constitute” a phenomenon on multiple levels (Bechtel and Richardson 1993; Glennan 1996; Machamer, Darden and Craver 2000; Bechtel and Abrahamsen 2005; Craver 2007b; Craver and Tabery 2017). Mechanisms are causal structures involving acting entities connected by causal relations. The disciplines in which mechanistic explanations are deemed particularly pertinent and potentially the only acceptable form of explanation are biology and the cognitive sciences. Others have also argued for the utilization of mechanistic explanations in the social sciences (Craver & Alexandrova 2008).

The epistemic norms underlying mechanistic explanations have garnered significant philosophical interest in the past three decades. Extensive research has been conducted on the conceptual analysis of the relation of mechanistic constitution (Craver 2007b; Harbecke 2010; Couch 2011), on the exclusivity of the mechanistic explanatory ideal and the existence of alternative forms of explanation (Huneman 2010; Chirimuuta 2014), as well as on the formal rules of constitutive inference (Harbecke 2015 a/b; Gebharter, 2017a; Baumgartner and Gebharter 2016; Baumgartner and Casini 2017; Baumgartner, Casini and Krickel 2020; Craver 2007a,b; Krickel 2018).

This paper focuses on the latter topic, namely the formal rules, methods, and algorithms for establishing mechanistic models, which form the core of mechanistic explanations. Our objectives are twofold: Firstly, we present a Boolean algorithm implemented in a functional Python script that returns all mechanistic models that are consistent with binary data tables derived from tests on multi-level mechanistic systems. Secondly, we advance several novel philosophical insights prompted by the solutions generated by this algorithm. Both aims are interconnected as the philosophical issues brought to light by the algorithm may in turn imply the necessity of pragmatic decisions in model selection.

Our motivation stems from three key observations. Firstly, to date there is virtually no connection between the ongoing mechanistic debate and the discourse surrounding Boolean inference methods for causal models. This absence is unexpected, considering the proven efficacy of Boolean methods in establishing causal models across various scientific disciplines. Although distinct in nature, mechanistic constitution and causation have been conceptually analyzed in similar terms. For instance, both have been treated as being tightly connected to regularities (cf. Harbecke 2010, Couch 2011, Baumgartner & Falk 2023). Moreover, many research projects in biology and the cognitive sciences effectively work with Boolean data.

Secondly, widely employed libraries such as Qualitative Comparative Analysis (QCA) and Coincidence Analysis (CNA) (cf. <https://cran.r-project.org/package=cna> and Dusa 2019) offer robust and compelling solutions for Boolean causal inference problems, which is the sole purpose for which they are designed. However, these existing configurational comparative methods cannot be adapted to generate adequate models for data generated by multi-level mechanistic structures observed in the real world. When fed with this specific type of data, none of the available parameter settings of these libraries yield mechanistically interpretable models. Therefore, at a minimum, an add-on is necessary if QCA or CNA is to be adapted for this purpose.

Thirdly, while some Bayesian constitutive inference algorithms have been proposed for continuous or probabilistic data (Gebharter 2017a/b), no such solution currently exists for binary data tables. In other words, the existing contributions that focus on the formal rules and potential challenges of constitutive inference methods from a theoretical perspective have not yet been substantiated with practical proposals on how to implement them. Consequently, due to the lack of well-developed alternatives, there is currently no methodological solution available to apply the philosophical mechanistic approach to binary data in scientific contexts.

As a response to these observations, we have developed the Python script “mLCA” (multi-level coincidence analysis) downloadable from the GitHub repository <https://github.com/user-jm/multi-lvl-Coincidence-Analysis>, which realizes our first objective. Based on a comparison of the output of mLCA with the existing QCA and CNA libraries relative to some prototypical examples of models and data tables, we defend the following claims as our second objective:

* 1. There are strong reasons to believe that inference methods for generating mechanistic models generally require information about the assignment of causal factors to various levels within data tables produced by multi-level structures. Without this additional qualitative information, it is not possible to retrieve multi-level mechanistic models solely from binary coincidence data. Merely having an ordering relation between causal factors is insufficient for distinguishing constitutive levels.
  2. The novel mLCA script successfully generates appropriate mechanistic models for data tables generated by multi-level mechanistic structures, showcasing the practical implementation of the philosophical mechanistic approach in the sciences.
  3. The number of solutions generated by mLCA significantly increases with the number of relevant causal factors listed in a data table due to the adaptations made to causal inference methods to meet the requirements of mechanistic modeling and the ability to generate multi-level models (as contended by claim 1). Additionally, the reduction of the solution set attainable with the information provided by coincidence data tables often fails to yield a unique solution.
  4. If further reductions are achievable at all, they involve an indispensable pragmatic element, which has significant implications for the realistic aspirations of mechanistic explanatory projects.

Our paper is organized as follows: Section 2 provides background information on the notion of a mechanistic explanation, mechanistic models, and constitutive inference. Section 3 outlines how configurational comparative methods generate complex causal models. Section 4 evaluates the effectiveness of the latest configurational comparative methods in handling multi-level data generated by mechanistic structures. It demonstrates that the latest QCA and CNA libraries in none of their parameter settings produce solutions that can be interpreted within the mechanistic framework when fed with multi-level data. Section 5 introduces our novel mLCA script and the algorithm it implements. Section 6 presents a defense of our philosophical claims. Section 7 summarizes the paper and highlights certain unresolved questions raised by our results.

2 Mechanistic Explanations and Constitutive Inference

A view common to authors such as Bechtel and Richardson (1993), Machamer et al. (2000), Bechtel and Abrahamsen (2005), and Craver (2002, 2007, 2008, 2009) is that explanatory goals notably in cognitive science, but potentially in various scientific disciplines, are achieved by modeling the mechanism responsible for a to-be-explained phenomenon and potentially additional information. Lawlike regularities subsuming the phenomenon play a secondary role in such explanations, if they play a role at all (see, however, Fazekas and Kertész 2011). The definition given by Machamer et al. describes a mechanism as consisting of “...entities and activities organized such that they are productive of regular changes from start or set-up to finish or termination conditions” (Machamer et al. 2000, 3). Bechtel and Abrahamsen extend this definition by characterizing a mechanism as “...a structure performing a function in virtue of its component parts, component operations, and their organization. The orchestrated functioning of the mechanism is responsible for one or more phenomena.” (Bechtel and Abrahamsen 2005, 423)

When mechanisms are characterized as producing a phenomenon, or as being responsible for it, they are believed to essentially overlap temporally with the phenomenon. This marks a key difference to causes, which are commonly understood to be diachronous with the phenomena at least in some cases. In this sense, mechanisms are taken to underlie, realize, instantaneously determine, or “constitute” the to-be-explained phenomenon.

A schematic illustration of a mechanistic model is the one offered by figure 1. A mechanistic model should be understood as a formal or graphic representation used to simulate or predict a mechanistic structure involving a to-be-explained phenomenon and the underlying mechanisms. While a mechanistic explanation often builds on a mechanistic model, it typically adds informal details to clarify how and why these mechanisms lead to the phenomenon in question. Since the explanation often relies on the model, the two are closely related.

In the model illustrated by figure 1, capital letters ***P***, ***A-C***, and ***D-J*** stand for specific kinds of entities realizing specific activities, which we will call “mechanistic factors” or “mechanistic types”.[[1]](#footnote-1) The model construes a to-be-explained phenomenon ***P*** via its inputs and outputs, and identifies the mechanism underlying ***P*** involving (in this case) mechanistic factors ***A-C*** along with their causal relations. Thus, mechanistic factors ***A-C*** are characterized as jointly sufficient for the to-be-explained phenomenon ***P***.[[2]](#footnote-2) For each of these mechanistic factors the model then offers a further analysis on a lower level. For instance, mechanistic factor ***A*** is analyzed in terms of the lower-level mechanism involving mechanistic factors ***D, E, H***, such that ***D, E, H*** are jointly sufficient for ***A***. And so on. The overall model characterizing mechanisms at different levels along with their constitution relations forms the basis of a satisfactory, possibly complete, mechanistic explanation of ***P***.

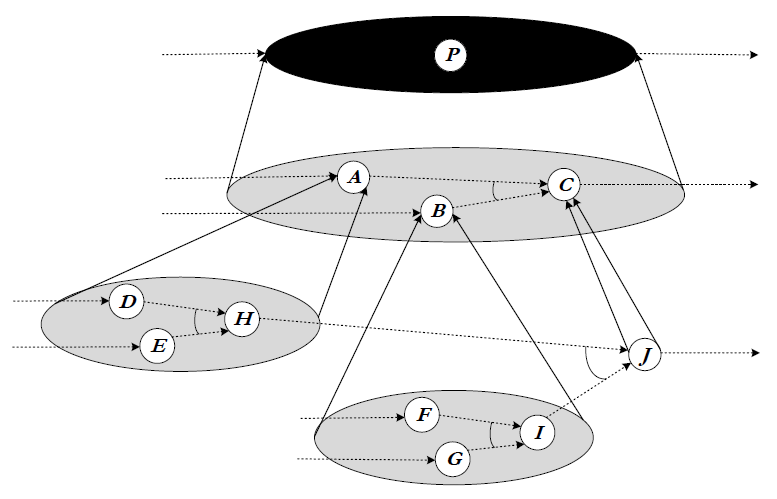


FIGURE 1: A three-level mechanistic model with a to-be-explained phenomenon ***P*** on the top level, mechanistic factors ***A-C*** on the intermediate level, and mechanistic factors ***D-J*** on the bottom level. Dotted arrows stand for causal relations, while solid arrows represent constitutive relations. Curved lines connecting dotted arrows stand for conjunctions of causal factors.

The general ideal of a mechanistic explanation leaves room for a range of positions on the metaphysical nature of the causal relation and the constitutive relation. As highlighted in section 1, a substantial amount of theoretical work has already been done on the nature of causation and constitution presupposed by mechanistic explanations as well as the question of how mechanistic models may be established for both binary and continuous data (Harbecke 2015 a/b; Gebharter 2017a; Baumgartner and Gebharter 2016; Baumgartner and Casini 2017; Baumgartner, Casini and Krickel 2020; Craver, 2007a, 2007b; Krickel, 2018).

In this paper, we side with Harbecke (2010) and Couch (2011) in their position that the notion of mechanistic constitution presupposed by explanations in the cognitive and biological sciences (cf. Harbecke 2020) often satisfies the conditions of a regularity. In consequence, our present focus is on binary data and the establishment of mechanistic models and mechanistic explanations based on these. Accordingly, mechanistic factors are conceived of as parts of minimally sufficient conditions of the constituted phenomena. Our aim is to go beyond the theoretical work on Boolean constitutive inference mentioned above and to develop an algorithm that automatically transforms data tables generated by mechanistic structures into mechanistic models in an adequate and reliable way.

Our project can build on existing research on Boolean causal inference methods and their implementations. Theoretical investigations rooted in the modern regularity theory of causation can be found in Graßhoff & May (2001), Baumgartner (2008, 2011), Falk (2020), Falk & Baumgartner (2023). The methods of Qualitative Comparative Analysis (QCA) and Coincidence Analysis (CNA) (cf. <https://cran.r-project.org/package=cna> and Dusa 2019) are implementations of this theoretical work. In principle, they allow establishing causal models at each level of a mechanistic model.

However, as we demonstrate in section 4, the existing computational implementations of these approaches cannot be adapted in any straightforward way to uncover mechanistic models. As an alternative, we introduce the novel mLCA script in section 5, which enables the establishment of comprehensive causal-constitutive models.

3 Configurational Comparative Methods in Causal Modeling

Configurational comparative methods (CCMs) are popular tools for causal modeling of complex systems. These methods generate potential causal models based on Boolean coincidence tables[[3]](#footnote-3) that represent the investigated causal phenomena. Presently, two major CCMs, Qualitative Comparative Analysis (QCA) and Coincidence Analysis (CNA), continue to be actively maintained and developed.

QCA originated from the need for a scientific method in comparative social science to handle data on complex systems (cf. Ragin 1987). While QCA lacks a direct linkage to any specific concept of causation (cf. Haesebrouck and Thomann 2021), CNA was deliberately designed to align with the regularity theory of causation proposed by Baumgartner (2009) and developed further in Baumgartner and Falk (2023). This theory posits that causation between two factors, ***K*** and ***L*** requires ***K*** to be part of a minimally sufficient condition of ***L***,such that there are at least two non-identical minimally sufficient conditions of ***L*** and the total disjunction of minimally sufficient conditions of ***L*** is minimal as well. Due to its more fundamental approach to causation, Baumgartner (2014) raised several concerns about QCA, some of which have been addressed in subsequent revisions (Dusa 2019). Nonetheless, Swiatczak (2022) noted that disparities still exist between the results of CNA and different QCA packages in cases of noisy or incomplete data tables.

CNA generates causal models in two steps. It first derives all potential causal dependencies from the coincidence table. The obtained formulae have the form of equivalences with a disjunctive normal form (DNF)[[4]](#footnote-4) as one equivalent – the cause – and the effect as a second equivalent. These atomic solution formulae represent all possible causal dependencies between the analyzed causal factors. The second step is to combine them to causal models, or complex solution formulae in CNA’s terms, by conjunctively connecting atomic solution formulae. Currently, as of version 3.22, QCA only implements the first step.

For the bottom level of our example from figure 1, the atomic solution formulae contain the minimally sufficient conditions for the factors ***H***, ***I***, ***J*** (**\***=conjunction operator, **↔**=biconditional operator):

**(1) D\*E ↔ H**

**(2) F\*G ↔ I**

**(3a) D\*E\*F\*G ↔ J**

**(3b) D\*E\*I ↔ J**

**(3c) F\*G\*H ↔ J**

**(3d) H\*I ↔ J**

In order to arrive at a causal model for the outcome ***J***, the atomic solutions have to be connected. While the causal relations for the factors ***H*** and ***I*** are unambiguous, a causal model can only contain one formula from (3a)-(3d). The first case (3a) constitutes a common cause, or causal fork, whereas the fourth is a causal chain. In the CCM-literature, this kind of ambiguity is known as the “causal chain problem” (Baumgartner 2009) or as a “functional ambiguity” (Baumgartner & Falk 2023).

While this type of functional ambiguities can easily be detected by the existence of multiple equivalence relations to the same causal factor, the occurrence of structural redundancies is less obvious: Even if every conjunct is a minimally sufficient condition for a different variable, their conjunction can exhibit redundancies, namely if one equivalence relation can be deduced from the set of the others (Baumgartner & Falk 2023). The problem with such redundant conjuncts is that they involve causally upstream dependencies between factors which should not be interpreted as causal – hence, downstream – relations. Accordingly, an algorithm that generates complex causal models from minimally sufficient conditions for individual causal factors has to eliminate such redundant relations.

Thus, the construction of causal models from the equivalence formulae for the individual factors is non-trivial. In the next section we will show that establishing mechanistic models requires even further considerations and section 5 will present our solution to this problem.

4 Direct Application of Existing Configurational Comparative Methods to Mechanistic Modeling

In this section, we examine the ability of existing CCMs to derive mechanistic models from binary data tables. As will become clear, their design, specifically tailored for complex causal structures, presents challenges when applied directly to mechanistic modeling. Despite this limitation, the single-level causal models produced by CCMs provide a valuable starting point for the development of our algorithm for mechanistic models.

Both CNA and QCA are designed to analyze complex causal structures using binary data tables. As Harbecke (2010) and Couch (2011) have argued, causality and mechanistic constitution share important characteristics. These shared features include complex dependency relationships among sets of factors that can be represented using Boolean variables. This is the case despite the fact that causal relations hold among factors of a single level[[5]](#footnote-5), whilst constitution relations hold between a subset of the factors of one level and one factor at the next higher level. What sets constitutive inference apart from causal inference is that the former works with data generated by structures with multiple levels of causal substructures whilst the latter operates on data generated by a single causal level. Hence, we maintain that the same necessary condition applies to constitutive relations as to causal relations between causal factors. A factor is a constituent of another factor of a higher level only if it is part of an atomic solution formula of the latter. However, as we show in this section, not every atomic solution formula that is generated for a multi-level structure represents a causal or constitutive relation.

It is possible to manually incorporate information about causal ordering into both CNA and QCA. One could re-interpret this as hierarchical information regarding different constitutive levels. In the following, we will show that this proceeding does not yield adequate mechanistic models. Let us examine once again the causal-mechanistic structure illustrated in figure 1. The latest versions of CNA and QCA[[6]](#footnote-6) yield different number of solutions for the data table corresponding to the mechanistic structure represented by figure 1 (containing only data on the two levels below phenomenon ***P***).[[7]](#footnote-7) QCA emits 32 potential equivalences, some of which are:

**J <-> C**

**A\*B <-> C**

**A\*I <-> C**

**B\*H <-> C**

**H\*I <-> C**

**A\*F\*G <-> C**

**F\*G\*H <-> C**

**H <-> A**

**...**

CNA emits 160 solutions representing complex causal structures. Two examples are:

**(H <-> A)\*(I <-> B)\*(J <-> C)\*(D\*E <-> H)\*(G\*F <-> I)\*(F\*G\*H <-> J)**

**(D\*E <-> A)\*(G\*F <-> B)\*(A\*G\*F <-> C)\*(D\*E <-> H)\*(G\*F <-> I)\*(D\*E\*I <-> J)**

None of these outputs represents a multi-level mechanistic model since they either include a causal or a constitutive relation a mechanistic factor such as ***C*** bears to other factors, but not both. However, it is precisely the point of an adequate mechanistic model that it provides all the causal and constitutive relations a mechanistic factor bears to other factors. The exclusion happens because CNA does not make an explicit distinction between causation and constitution, even with the inclusion of a prior level assignment to each factor. Both QCA[[8]](#footnote-8) and CNA have been designed as tools for causal inference only. If applied to data generated by multi-level structures, they implicitly assimilate constitution and the level hierarchy to single-level causation.[[9]](#footnote-9) As a result, many of the generated causal models *blend* variables from different mechanistic levels into a single causal structure. According to many mechanistic theorists, such mixed models are misleading, as variables belonging to different mechanistic levels cannot be directly causally linked.

In essence, neither QCA nor CNA have the capability to produce outputs that explicitly differentiate between causal and constitutive relationships. They are applicable only within a given level. Therefore, the knowledge of the level hierarchy is essential for CCMs to be applied in deriving mechanistic models. Nevertheless, we maintain that, despite these limitations, causal inference methods can play an invaluable role in establishing constitutive-causal models in principle.

In light of these technical limitations of QCA and CNA vis-à-vis data from multi-level structures, we conducted an extensive literature search for suggestions as to how CCMs can be used to generate multi-level mechanistic models on the basis of multi-level data. The literature on CCM’s and, in particular, on QCA has mushroomed over the last two decades. A broad search in November 2022 with Google Scholar using “(QCA OR CNA) AND Configurational Comparative Methods” yielded 11.900 results for the years between 2010 and 2023. For comparison, the same search phrase for the years between 1997 and 2010 only yielded 2.310 results. A similar comparative search with PubMed yielded 27 results for the years 2010-2022, and only 2 results for all the available years prior to and including 2010.

The articles available on PubMed predominantly focus on natural scientific fields such as medicine, cell biology, neuroscience, etc., with only a few philosophical papers discussing CCMs and best practices for complex causal inference (e.g., Whitaker et al., 2020; Baumgartner, 2021). On the other hand, the literature found on Google Scholar is more scattered. Among the identified papers, none provided a concrete proposal on how inference methods for causal-constitutive or multi-level models should be approached.

Based on this literature search, we have concluded that the specific topic of Boolean inference methods within the framework of the philosophical approach to mechanistic explanation still awaits exploration. Furthermore, while the literature on mechanistic explanations contains some initial theoretical attempts for constitutive inference algorithms, these ideas have not yet been substantiated by functional algorithms that could be tested. The few contributions we encountered that discuss both CCMs and “mechanistic explanations” understand the latter term to refer to causal explanations enriched by spatio-temporal information, rather than multi-level mechanistic explanations.

What is currently lacking is an approach to effectively implement constitutive inference and bridge the gap between theoretical discussion and practical implementation. In the following section, we introduce the algorithm that yields the desired results for mechanistic structures such as the one illustrated above, along with the results obtained.

5 An Algorithm for Boolean Causal-Constitutive Inference

In this section, we introduce an extension to QCA and CNA that allows for the generation of multi-level models consistent with a given Boolean data table obtained from a multi-level structure. The crucial change consists in the distinct treatment of causal and constitutive relations, both of which are established from the logical equivalences that are derived from the given data set and the level assignment of the factors. Thus, mLCA differs from QCA and CNA primarily with regard to the construction of complex models out of the atomic solutions. It is possible to start with the atomic solution formulae generated by QCA or CNA. Alternatively, mLCA features a function for deriving atomic solution formulae from a Boolean coincidence table that can be read from csv-files. However, in the current version the built-in function is restricted to noise-free ideal data sets.

Since both constitution and causation are treated in this context as certain kinds of regularities, a level assignment in addition to a coincidence table is necessary to derive multi-level mechanistic models. Without such an assignment, any constitution relation will be treated as a causal relation, and vice versa. If one chooses the option of reading the data from a csv-file, the level assignment can be given explicitly by adding a row to the table in which the entry “<<” in any cell indicates that the causal factor corresponding to that column is of a higher constitutive level than those left to it. Similarly “<” functions as separator between different causal orders within the same level. If atomic solution formulae generated by QCA or CNA are used, we interpret the optional causal ordering argument as level separation of the factors. This gives us a definite assignment of all causal factors to a specific constitutive level.

Based thereon, we can categorize all equivalence formulae into causal relations, constitution relations or mechanistically uninterpretable formulae, which are to be discarded. A necessary condition for an equivalence formulae being either interpretable as causal or constitution relation is that all factors on the left side (the complex term) inhabit the same constitutive level. This means that iff the right side term is a factor of the same level, the formula is categorized as a causal relation of that level. Elsewise, iff it is a factor of the next higher level, the formula is considered as a potential constitution relation.[[10]](#footnote-10) All further logical relations are rejected at this point – this avoids any undesired direct causation across levels.[[11]](#footnote-11)

In the next step, the individual causal relations are combined into complex causal models. This can be done for each constitutive level separately. As indicated in section 3, this basically consists in selecting a subset of causal relations from the full list obtained in the prior step. Three principles determine how mLCA selects:

1. at most one equivalence per factor is included
2. if it is possible without breaking causal connections, the causal relations should be reduced until a total causal ordering[[12]](#footnote-12) of the factors can be defined
3. the number of causal relations included is maximized respecting a. and b.

The first principle has already been addressed in section 3. No two sets of necessary and sufficient conditions can represent the direct causes of the same effect simultaneously. Therefore, only one can be included in any causal model. Because of principle b., it cannot be guaranteed to include exactly one equivalence formula per factor. As has been mentioned in section 3, not all atomic solutions correspond to downstream causal relations. A direct consequence of the occurrence of such an upstream relation among the equivalence relations interpreted as causal, is the impossibility of defining a total causal ordering of the factors involved. This observation motivates principle b. In order to obtain the most informative models for the given data set, we also impose principle c. In the following, we describe the concrete procedure of how mLCA generates causal models on the basis of these abstract principles.

At first only principles a. and c. are taken into account when gradually combining causal relations. The reason is that b. is a property of the entire complex. It will be ensured in a later step. For now all prospective causal relations of the particular constitutive level are divided into groups according to two decisions:

1. Are there further equivalence formulae with the same right-hand side term (the effect)?
2. Is the left-hand side term of the equivalence formulae (the cause) a complex or an atomic logical sub-formulae?

The formulae for which i. Is answered negatively form the set of unique formulae. The unique formulae are the common core of all causal models to a given data table. Those non-unique formulae with complex cause-term are grouped according to their effect. For example, in the case of the lower level in the mechanism represented by figure 1, the set of unique formulae is ***{D\*E ↔ H,***  ***F\*G ↔ I}***, while ***D\*E\*F\*G ↔ J, D\*E\*I ↔ J, F\*G\*H ↔ J*** and ***H\*I ↔ J*** are conflicting formulae for the effect ***J***. They are conflicting in the sense that they cannot all correctly represent the actual causal structure. Formulae of the third type are equivalences between single factors, such as ***Fi ↔ Fj*** or ***~Fi ↔ Fj*** for i≠j. These form clusters of symmetric equivalences. For each cluster, mLCA takes the power set[[13]](#footnote-13) of the corresponding set of equivalence formulae and discards all of its elements that

1. give rise to circularities, such as ***{F1 ↔ F2,***  ***F2 ↔ F3, F3 ↔ F1}***, this would violate principle b.
2. contain more than one formula for an effect, such as ***{F1 ↔ F2,***  ***F3 ↔ F2}***, which violates principle a.
3. lacks at least one factor pertaining to the cluster, such as ***{F1 ↔ F2}***, this violates c. since a further relation like ***F2 ↔ F3*** could be added without being in conflict with a. or b.
4. breaks causal connections within the cluster, such as ***{F1 ↔ F2,***  ***F3 ↔ F4}*** likewise violating c.

Examples for valid elements of the cluster of co-extensive factors ***F1 – F4*** are ***{F1 ↔ F2,***  ***F2 ↔ F3, F3 ↔ F4}, {F4 ↔ F2,***  ***F2 ↔ F3, F3 ↔ F1}*** etc.

The set of all possible models of the considered constitutive level – prior to assessing for principle b. – can now be defined as the Cartesian product of ***{***set of unique formulae***}*** × conflicting formulae to factor ***A*** ×  … conflicting formulae to factor ***N*** × co-extensive group of cluster *1* ×  … co-extensive group of cluster *m*. Taking up once again the example from figure 1, the set of causal models for the bottom level is

***{{D\*E ↔ H,***  ***F\*G ↔ I, D\*E\*F\*G ↔ J}, {D\*E ↔ H,***  ***F\*G ↔ I, D\*E\*I ↔ J}, {D\*E ↔ H,***  ***F\*G ↔ I, F\*G\*H ↔ J}, {D\*E ↔ H,***  ***F\*G ↔ I, H\*I ↔ J}}***.

By now, it is certain that every model includes at most one equivalence relation per effect. However, the solutions possibly exhibit circularities. Due to the entirely formal logical analysis, we may mistakenly get the artifact that, according to the obtained models, an effect is a cause of one of its own causes. From the technical point of view, the error is that the model includes too many relations. In order to enforce principle b. and to determine the excess relations, the following recursive procedure is applied to every model for which no total causal ordering can be defined. Its objective is to obtain a non-circular minimal model: The recursive step *R* is to discard one relation from the model. If this breaks a causal connection, such that one causal factor becomes separated from the others, or if the reduced model is not logically equivalent to the initial one, this step is undone and it is continued with another relation until all relations have been examined once. Otherwise, if the elimination of the relation does not break the causal connections and maintains the equivalence to the initial set of formulae, mLCA checks whether this reduced model allows to define a total causal ordering. If this is the case, it has found the minimal model. Otherwise, it goes back to the recursive step *R* but this time with the reduced model and removes further relations until it finally finds the non-circular minimal model or until it has unsuccessfully tested every formula and has to conclude that the circularity cannot be resolved.

Once the individual causal models have been constructed for each level, mLCA connects them using the constitution relations. A causally connected part of the causal structure on level *m* constitutes a factor on level *m+1* iff the former form a minimally sufficient condition for the latter. Here the relation is inverse to the case of causation: multiple constitution relations to the same upper level factor can occur in one mechanistic model, but every lower level factor can be constitutive part of at most one upper-level factor – whereas in causal models a factor cannot be the effect in more than one, but occur as cause in various relations.

A disadvantage of QCA and CNA has been the lack of a unified visualization of the obtained results. Since multi-level causal models are usually particularly complex and the number of compatible solutions tends to be rather large, mLCA generates diagrammatic representations of the generated solutions that follow the standards of constitutive-mechanistic models.[[14]](#footnote-14) The output graphs should be read as follows:

* nodes are causal-constitutive factors
* diamond symbols at nodes express a negation of the respective factor
* straight, solid lines with arrows correspond to sufficient conditions
* curved lines meeting in a dot express conjunctions
* dotted lines with arrows represent connectives between lower and upper mechanisms (if bent to the left they represent a *causal start* of a sub-mechanism; if bent to the right, they represent a *causal end* of a sub-mechanism; if a line is vertical and straight, then the upper-level factor is constituted by a single lower-level factor, optionally the constituents of a higher order factor are highlighted in color).

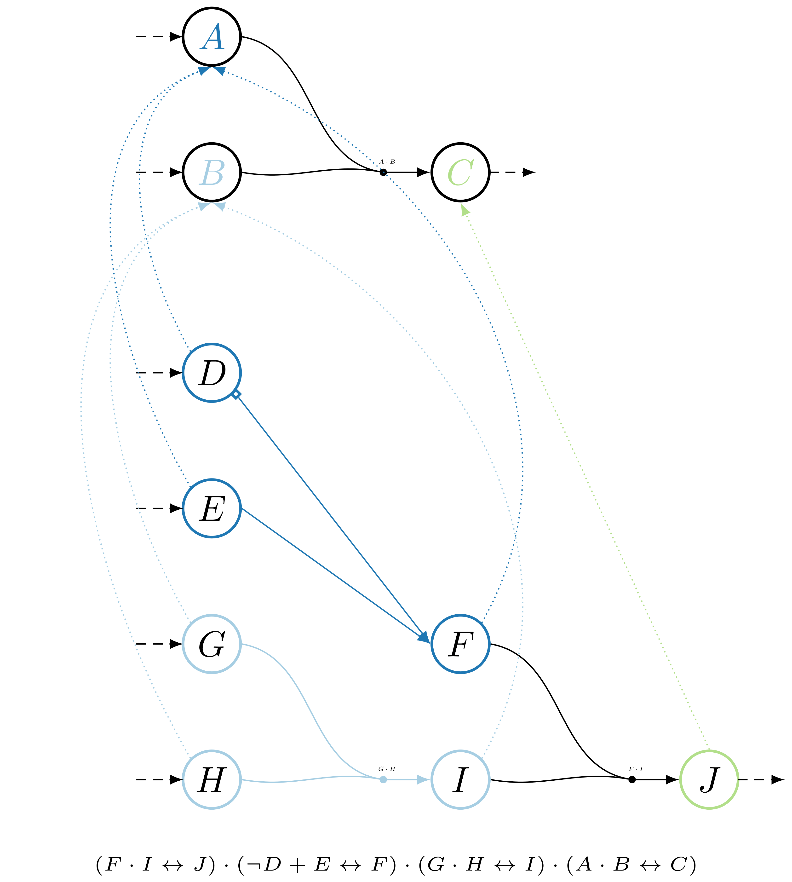


FIGURE 2: An example for a visualization of a multi-level model generated by mLCA.

We evaluated the results of mLCA in two ways: As no alternative software package exists for the purpose of mechanistic modeling, we tested the multi-level case by examining the results for several mechanistic models which we transformed into coincidence tables that we used as input to mLCA. We have then confirmed that the original model is within mLCA’s results, checked the plausibility of the other solutions, and compared the number of models emitted with the possible combinations of ambiguities that arise from the Boolean data table.

Our second method of testing mLCA consisted in a benchmark test against CNA using only data for single level causal structures. To this end, we generated 10.000 random Boolean coincidence tables of six variables and compared the obtained complex solution formulae with the results from mLCA. The result of this benchmark test is that mLCA and CNA return the same results in all of the tested cases. All of CNA’s complex solution formulae are among the models generated by mLCA – after restricting CNA’s output to some conditions that are generally applied in mLCA but not in CNA (in particular, exhaustiveness and faithfulness have to be set to 1, for the details on the benchmark test see the Appendix), while all models identified by mLCA are also returned by CNA.

Thus, we can conclude that mLCA stands out by accurately distinguishing causal and constitutive relationships, as emphasized by claim 1 in section 1. Whilst QCA and CNA, which were designed for causal inference only, cannot be adapted in any straightforward way to handle multi-level mechanistic data adequately, mLCA offers a working solution for causal-constitutive inference. In consequence, mLCA can be a valuable tool for scientists in the cognitive and biological sciences who aim to establish mechanistic models using binary data.

However, it is important to note that even for the relatively simple data sets that we have used for the benchmark tests with six variables and one level only, mLCA yields a large number of solutions that are consistent with the coincidence data. In this sense, its job is mainly an *exploratory* one: it generates the often large set of all possible mechanistic models that are consistent with the data table. This observation prompts the philosophical discussion in the subsequent section on how to *justify* the choice of a particular model.

6 Reducing the Set of Possible Solutions and Philosophical Implications for the Mechanistic Approach

As mentioned in the previous section, coincidence data generated by multi-level mechanistic structures are often consistent with many alternative models. One reason is that the set of solutions consistent with coincidence data multiplies with every level of constitution. This observation invites several philosophical questions on the justification of how to model a particular phenomenon.

Among these is the question (i) how working cognitive and biological scientists manage to identify one mechanistic model as the only adequate one for an investigated brain or organism, whilst a purely formal approach to the matter would suggest high ambiguity and many empirically equivalent models.

Secondly (ii), it might be asked whether mLCA misses some important information found in the coincidence data, or whether it can be developed further to incorporate additional information that would eventually reduce the ambiguity and identify only a small set of solutions.

Thirdly (iii), in case the additional knowledge invoked by working scientists to reduce the set of solutions and minimize ambiguity is of a pragmatic nature, serious questions arise concerning the potential of the cognitive and biological sciences to establish intersubjective and generalizable knowledge of mechanistic structures.

In our discussion we will first elaborate on question (ii) before assessing the strategies and additional sources of information that might be applied by scientists when facing the ambiguity of coincidence data and the underdetermination of mechanistic models (questions (i) and (iii)).

The answer to question (ii) is that, without the availability of an extension of the factor set and additional coincidence data, the given data tables by themselves generally do not offer additional, or perhaps hidden information that would suggest further reductions that the algorithm could work with. The variables recognized by the algorithm are of a Boolean nature, and the only kind of information provided by them is an on/off information, or a bit. All dependencies among such variables are based on these bits only, and all the interrelations are identified and visualized by mLCA. Hence, the pure coincidence data do not contain hidden information that could mitigate the ambiguity.

Would a piecemeal procedure offer some relief? Such a strategy first identifies exactly one “adequate” or “correct” causal model on each single level, potentially based on additional and independent qualitative evidence, before it integrates all the mechanistic levels into one model. If practical and adequate, this would substantially reduce the ambiguity. The problem with this procedure is that the different levels can turn out to be inconsistent with one another. For instance, the data that is consistent with a common cause structure on a higher-level *j*can sometimes be consistent with a causal chain structure on lower than level *j-1*. If the common cause structure is declared the “correct model” on level *j*, whilst the causal chain is declared the best model for level *j-1*, both levels turn out to be inconsistent.

Things would be different if a particular level *k* is declared an *anchor* such that a causal model is declared to be correct for *k* and all models found on levels higher and lower than *k* are excluded if they are inconsistent with *k*’s structure. Whilst such a procedure would often reduce the number of acceptable solutions significantly, it struggles with at least two problems: Firstly, the data tables alone provide no information about which level should be chosen as the anchor level. Moreover, the more complex level *k*, the higher degree of ambiguity on levels lower than level *k*. Hence, there is no guarantee that such a procedure alone can generate the desired result of just a few or one most likely and adequate model.

The question then is whether mLCA could be extended so that it could incorporate more and additional information on the mechanistic structures investigated and observed. Whilst the introduction of additional constraints is technically unproblematic, the question is which kind of information this could be. In order to receive an answer to this question, it might be worthwhile to look at question (i) and the additional sources scientists typically use or may use.

A scientist might invoke additional prior spatial and causal knowledge when approaching the investigated structure. For instance, again referring to figure 1, the researcher might *see* from the start that factor ***B*** represents a brain network that projects into a neural configuration represented by factor ***C***. As a result, she can immediately exclude a causal chain solution in which ***A*** and ***B*** form a causal chain leading into ***C***.

mLCA could be extended in order to incorporate such information and allow a researcher to exclude, or set, certain causal connections from the start. It already incorporates the option to indicate a specific causal ordering within a constitution level.

The more such additional exclusive information is provided, the smaller becomes the number of solutions. Thus, additional causal information can reduce the ambiguity considerably. But it does so at a cost, because the additional information to be provided is precisely the kind of information that the algorithm is supposed to explicate. If much of the information about the causal structures at the different levels is already available, then the researcher is already in a comfortable epistemic position, and the search algorithm has little work to do.

The more interesting question is whether the ambiguity could be reduced by additional knowledge or information on the side of the researcher that is not itself causal or constitutive knowledge. In other words, can the researcher reduce the large set of options emitted by mLCA by employing some external, perhaps qualitative knowledge? Such knowledge or information may be which of the offered models is *simpler* or more *generalizable* than others whilst offering the same predictive and explanatory powers as these. The simpler model may be considered closer to the truth than more complex models. A more generalizable model may be considered more valuable.

A further simplification can be made in the number of constitutive levels. We may ask how many and which levels are necessary to model and explain a particular phenomenon. For example, we could decide to remove the intermediate level with factors ***A-C*** from figure 1 in order to obtain the simpler model illustrated by figure 3.

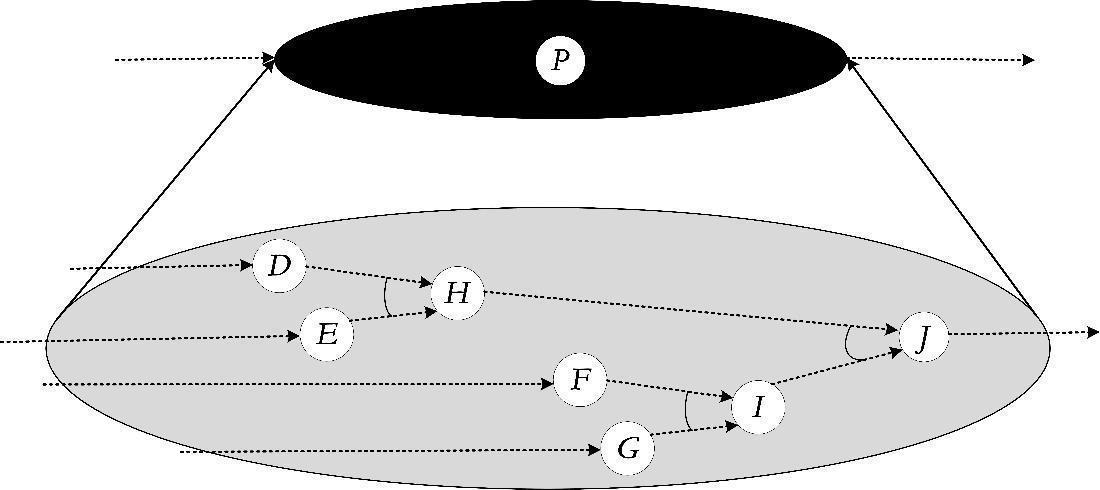


FIGURE 3: A mechanistic model simpler than, but input-output equivalent to, the one illustrated by figure 1. The illustration uses the same graphic elements as figure 1.

As discussed in section 3, QCA and CNA already comprise such simplicity norms to some extent as, under default parameter settings, they delete equivalent factors or variables entirely from the causal analysis.

The challenge with categorical simplicity norms, as discussed in section 3, is that they can sometimes conflict with explanatory adequacy. When investigating real-world structures that encompass modules such as individual neurons or neural populations that function as equivalent factors, these factors should ideally appear in at least one of the output solutions of the search algorithm. The inclusion is important, as it may be relevant for both explanation and interventions. Different types of interventions may target mesoscopic variables rather than microscopic ones. Furthermore, the mesoscopic level often provides a necessary level of understanding for human scientists in the explanatory process.

These considerations underscore the challenge of narrowing the set of solutions based solely on simplicity norms. Qualitative and pragmatic measures are likely to interact with simplicity criteria in determining the correct, best, and ideal explanatory model. Exploring the precise nature and application of these additional measures goes beyond the scope of this paper and warrants further investigation. Nonetheless, recognizing the need for potentially unknown qualitative and pragmatic measures to identify adequate mechanistic models of a certain complexity has important philosophical implications for the overall mechanistic project in the cognitive and biological sciences.

The crucial point is that regardless of the specific form and implementation of these measures and constraints, they will inherently possess an observer-relative component. They will encompass the researcher's ability to detect, identify, or perceive the presence of a real-world constituent or module corresponding to a particular factor within the mechanistic model. Additionally, the dimension of understanding associated with the mechanistic explanatory project is likely to be influenced by the researcher's abilities, interests, goals, and environment.

Consequently, determining the ideal or best mechanistic model may not be achievable through fully objective or intersubjective means. Given the vast number of solutions consistent even with small sets of coincidence data, these aspects of the mechanistic explanatory project raise doubts about the cognitive and biological sciences' ability to provide mechanistic knowledge in a robust and objective manner when dealing with binary data. Unless a radically different method distinct from existing CCMs is discovered, these findings present a rather pessimistic outlook for the broader philosophical endeavor of the mechanistic ideal of explanation.

Nevertheless, it is important to emphasize that regardless of the calibration of additional qualitative and pragmatic criteria, researchers are justified in assuming that the adequate and true model lies within the set of solutions generated by the search algorithm. However, they may need to accept the fact that they may never definitively know which model it is.

This insight holds significant importance within the broader discourse surrounding the mechanistic approach, and its implications should not be underestimated. It aligns with previous contributions that have emphasized the existence and value of non-mechanistic explanations (cf. Huneman 2010; Chirimuuta 2014). In a more general sense, it has the potential to challenge the foundational principles and expansive goals of the mechanistic project.

The original contributions to the mechanistic debate often carry a pioneering tone. In many scientific disciplines, mechanistic explanations are deemed as the only adequate explanations, with the belief that they alone can ensure the objectivity and truthfulness of the cognitive and biological sciences (cf. Machamer et al. 2000, 7-8; Bechtel and Abrahamsen 2005; Craver & Alexandrova 2008, sec. 2 Craver and Piccinini 2011, 284). However, if the aforementioned insights are indeed accurate, achieving this objectivity and truthfulness through mechanistic explanations, especially those of a certain level of complexity and beyond, is far from straightforward.

7 Conclusion

In this paper, our investigation focused on the formal rules necessary for establishing mechanistic models. Our objective was two-fold: Firstly, to develop a functional Python script that employs an algorithm to transform data tables derived from tests conducted on multi-level systems into mechanistic models that conform to these tables. Secondly, to defend several philosophical insights that emerged from the practical challenges we encountered when constructing causal models for multi-level structures. We asserted that these aims are interconnected.

Our main findings were the following:

* 1. Inference methods generating mechanistic models require information about level assignments of the causal factors listed in the data tables produced by multi-level structures.
  2. The novel mLCA script generates adequate mechanistic models for multi-level causal-constitutive data tables.
  3. Mechanistic modeling requires certain adaptations to the methods for causal inference compared to the strategies of the existing configurational comparative methods. These modifications lead to a significant increase of generated models to given data sets.
  4. Therefore, further reductions are necessary. They will have to involve an ineliminable pragmatic ingredient, which has sharp consequences for the realistic ambitions of mechanistic explanatory projects.

The central remaining question is what this ineliminable ingredient consists in, whether its general structure is generalizable, and whether it can be quantified at least in some instances. Providing an answer to this question will have to be left for future research.

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Appendix: Benchmark test

To evaluate the models generated by mLCA, we ran a benchmark test against the single-level causal models obtained from CNA (version 3.5.6). In the first step, we generated 10.000 (noise-free) Boolean coincidence tables of six variables (A, B, C, D, E, F). In order to avoid that the majority of these test tables yield no complex causal models and are thus worthless for our purpose, we derived them as truth tables from randomly generated logical formulae with the following characteristics:

Every formula is a conjunction of

* 2-5 equivalence formulae,
* the right-hand term of the n-th equivalence is our (7-n)-th variable – thus the right equivalent in the first conjunct is always the variable F, in the second E, if there is a third one, it would be D and so forth,
* the left equivalents are in all cases DNFs of the variables whose letters alphabetically precede the one on the right side,
* the DNFs are generated randomly according to the following rules: (m being the number of variables that might appear in a formula):
  + the number of disjunctions is a random number o in the range of 1 to m-1 (in case of o=1 the formula is in fact no disjunction, since at least two disjuncts would be needed)
  + for each disjunct, a random number p in the range of 1 to min{m-1, n-1} determines the number of conjuncts that form the respective disjunct
  + the p conjuncts are randomly selected from the m possible variables
  + each conjunct is negated with a probability of 0.5

This procedure is motivated by the fact that the formulae generated in this way have the same form as complex solution formulae, and the choice of variables avoids circularities. The formulae are generally not complex solution formulae themselves since the occurring DNFs are not transformed into minimally sufficient conditions. However, this is not a problem for us. What is important, though, is that causal models can be found for most cases. And in fact we had only 411 formulae for which no causal model has been found. If we had started with genuinely randomized truth tables, this number would have been much higher.

The Boolean tables to every of these formulae are then used as input for CNA using the options:

* maxstep = c(5,5,11) – sets the highest complexity of atomic solution formulae to five conjuncts, five disjuncts and six variables
* details = FALSE – we are not interested in verbose output
* acyclic.only = TRUE – mLCA returns by default only non-circular causal models
* nsolutions = “all” – we want all solutions
* n.init = 1.000.000 – setting the number of conjunctions that are considered for constructing atomic solution formulae

We exported the output of CNA into a separate text file for every data table and ran mLCA with the option to read the atomic solution formulae from these files and saved the mLCA-generated models. We have to note that even for our relatively small test samples the generation of models by mLCA could take several minutes because the algorithm contains several functions that do not run in polynomial-time. Therefore, we sorted the CNA-output files by size and stopped after 9.539 of the 10.000 data tables.

In order to make the results of mLCA and CNA comparable, we imposed three conditions on CNA’s complex solution formulae that are always satisfied by models from mLCA but not necessarily from CNA:

1. A solution must not be a fragment of another solution. Since solution formulae are generally conjunctions of equivalence relations, we discard every formula whose conjuncts are all contained in another solution. This means in practical terms that we are not looking for sub-models to models that we have already obtained.
2. All factors that are causally relevant to others have to appear in every solution.
3. Solutions have to be logically equivalent to the truth table they are derived from.

Conditions 1. and 3. are met by all CNA results whose faithfulness and exhaustiveness parameters are equal to 1. After filtering out CNA’s complex solution formulae that violate any of these conditions, all remaining solutions match exactly one obtained from mLCA for the respective data set and vice versa. All files of this benchmark test are available on the mLCA GitHub page.

1. Conceptually, the notion of a mechanistic factor or type is inspired by that of a specific variable as proposed in Spohn (2006). [↑](#footnote-ref-1)
2. To be more precise, each stage of the causal structure containing ***A-C*** is characterized as minimally sufficient for ***P*** (cf. Harbecke 2019). [↑](#footnote-ref-2)
3. A Boolean coincidence table is a tabular representation of systematic variation of sets of binary factors. Each column corresponds to a specific variable, whilst its rows represent possible states of the structure. [↑](#footnote-ref-3)
4. A disjunctive normal form is a disjunction of arbitrarily many conjunctions of either variables or negated variables. [↑](#footnote-ref-4)
5. Here, we exclude the possibility of inter-level causation in the context that interests us here, namely explanations in the cognitive and the biological sciences. [↑](#footnote-ref-5)
6. Our results are based on the R-packages CNA version 3.5.6 and QCA version 3.22. [↑](#footnote-ref-6)
7. In order to include the information on the constitutive levels, we used the non-strict causal ordering ***D***, ***E***, ***F***, ***G***, ***H, I, J < A, B, C***, which ensures that the factors to the right of “<” cannot be causes of factors on the left. [↑](#footnote-ref-7)
8. QCA offers no function to generate complex solutions that integrate the causal conditions of the factors into one model. Since the solutions for the atomic conditions are the same as CNA’s in the case of complete and correct data tables, the following observations hold for both likewise. [↑](#footnote-ref-8)
9. Note that neither strict, nor non-strict causal ordering is sufficient to separate causal factors of different constitutional levels as required for mechanistic modeling. In case of a strict ordering, only factors of a lower causal order are eligible to be a cause to a given factor. However, according to the mechanistic doctrine, causal relations occur exclusively between factors of the same constitutional level. Therefore, choosing strict ordering implies losing all causal relations.

   On the other hand, for a non-strict ordering, factors of equal or lower order can be causes. This leads to conditions that mix factors of different levels, which have no constitutive-causal interpretation. The only meaningful relations are between factors of the same level (causal relations) and equivalences of conditions of factors of one level to a factor of a higher level (constitutive relations). Most solutions of CNA and QCA under non-strict ordering are neither of these. [↑](#footnote-ref-9)
10. This is a rather strict conception of constitution. It is conceivable to make this principle more liberal. [↑](#footnote-ref-10)
11. As already mentioned above, in the current context we side with Craver & Bechtel (2007) in that causation happens only within levels, and not across levels. [↑](#footnote-ref-11)
12. An order relation on a set is a total order if any two elements of the set – here the set of causal factors – are comparable. [↑](#footnote-ref-12)
13. The power set of a set ***A*** is the set of all subsets of ***A*** including the empty set and ***A*** itself. [↑](#footnote-ref-13)
14. Since mLCA includes a function to convert CNA-syntax into ours, its functions can also be used to visualize CNA’s complex solution formulae, however, currently with the restriction to non-circular solutions. [↑](#footnote-ref-14)