INCORPORATING COMPLEX ADAPTIVE SYSTEMS CONCEPTS IN ONTOLOGY DRIVEN BAYESIAN NETWORK MODELS : TOWARDS RESOLVING WICKED PROBLEMS

DANIEL TEMBINKOSI SEMWAYO

Student Number: 2292902

A Ph.D. thesis submitted to the Faculty of Science, University of the Witwatersrand, in fulfillment of the requirements for the degree of Doctor of Philosophy in Computer Science

Doctor of Philosophy
Supervised by Prof. Ritesh Ajoodha
School of Computer Science and Applied Mathematics
The University of the Witwatersrand

August 26, 2024

Daniel Tembinkosi Semwayo: *Incorporating Complex Adaptive Systems Concepts in Ontology Driven Bayesian Network Models:Towards Resolving Wicked Problems*

SUPERVISOR:
Prof. Ritesh Ajoodha

LOCATION:
Johannesburg, South Africa

Dedication

This research project is dedicated to my parents, Aaron and Selina Semwayo for their undying belief in the power of education to change the world, and for their unwavering support.

Abstract

Wicked problems are complex ill defined problems very difficult to solve tractably using analytical methods and interventions. They include problems like pandemics, climate change effects, traffic jams, and financial market crashes. Attempts at solving such problems using analytical methods tend to produce counter-intuitive, unpredictable pathological outcomes. Wicked problems emerge, in part from the character of complex adaptive systems, and from stakeholder disagreements on their definition and resolution. We argue that baseline Bayesian models do not have adequate constructs to provide compact, and tractable modelling support for wicked problems. Applying an iterative and rigorous abductive design science research methodology, an ontology driven Bayesian modelling framework is applied to design the Granular Niche probabilistic Bayesian model, a formal, ontologically sound, and explainable artificial intelligence model, incorporating complex adaptive systems theory concepts: context; granularity; and perspective, as constructs. Using evaluation metrics from applicable kernel theories comparative evaluation of the model is carried against baseline Bayesian models. The results indicate that the novel model out-performs baseline Bayesian models against the following evaluation criteria: i) complex adaptive systems' representation accuracy and precision; ii) structure learning; iii) parameter estimation; iv) knowledge discovery; and v) explicitly modelling and reconciling divergent multiple stakeholder perspectives of a given wicked problem.

Key Words: Complex Adaptive Systems, Wicked Problems, Ontology Engineering, Bayesian Network Modeling, Explainable Artificial Intelligence, Machine Learning, Structure Learning, Parameter Estimation, Knowledge Discovery

Published Related Work

Excepts of the research work in this thesis has been published in the following peer reviewed conference paper :

Semwayo and Ajoodha [2021] Semwayo and Ajoodha.*Incorporating Complex Adaptive Systems Concepts in Ontology Driven Bayesian Network Models:Towards Resolving Wicked Problems. In 2021 IEEE International IOT, Electronics and Mechatronics Conference (IEMTRONICS), pages 1–8. IEEE, 2021.*

The experimentation results presented in the thesis have been submitted to the following journal for publication.

Semwayo and Ajodha.*Representing Complex Adaptive Systems Using Probabilistic Bayesian Models: Towards Resolving Wicked Problems*
Submitted for publication to the Journal of Artificial Intelligence Research, January 2024

Acknowledgements

I would like to thank my supervisor, Prof. Ritesh Ajoodha, for supporting me throughout this exciting journey of discovery with much needed good humour and patience. I would also like to thank my family for putting up with my extended periods of “non presence” even though I was physically present with them, as I explored the wonderful world of Artificial Intelligence and Machine Learning. I am most grateful to my fellow students and friends who encouraged me to soldier on through the times of the COVID19 pandemic and other challenges, particularly my daughter Chloe, my biggest fan, for meticulously editing the final thesis draft. I wish to acknowledge the mentorship support and guidance I received from my uncle and aunt Dr E.P. and Mrs S. Manyuchi from an early age, and right through the years on the pursuit for academic excellence. Special thanx goes to my wife Nokwanda for being my pillar of strength and encouragement throughout my research journey. Most importantly I would like to give thanx to God almighty for giving me strength and guidance in difficult and happy times to complete this journey.

Declaration

I, Daniel Tembinkosi Semwayo, student number 2292902 hereby declare the contents of this Ph.D. thesis to be my own work. This thesis is submitted for the degree of Doctor of Philosophy in Computer Science at the University of the Witwatersrand. This work has not been submitted to any other university, or for any other degree.

Johannesburg, South Africa

Daniel Tembinkosi Semwayo, August 26, 2024

Contents

1 Introduction **1**
1.1 Research Motivation . . . 2
1.2 Problem Statement . . . 3
1.3 Research Purpose . . . 4
1.4 Research Questions . . . 5
1.5 Hypothesis . . . 6
1.6 Research Methodology . . . 6
1.7 Novelty and Contribution to Science . . . 6
1.8 Research Limitations . . . 7
1.9 Thesis Structure . . . 8

2 Background **9**
2.1 Wicked Problems . . . 9
2.2 Link between Wicked Problems and Complex Adaptive Systems . . . 11
2.3 Formal Definition of Wicked Problems . . . 13
2.4 Context, Granularity and Perspective as Complexity Theory Concepts . . . 14
2.5 Ontology Engineering . . . 16
2.5.1 The Importance of Ontology Accuracy and Precision . . . 18
2.6 Bayesian Networks . . . 19
2.6.1 Hierarchical Bayesian Networks . . . 20
2.6.2 Dynamic Bayesian Networks . . . 20
2.6.3 Structure learning and parameter estimation . . . 21

3 Related Work **24**
3.0.1 Representation of complex adaptive systems in formal models . . . 24
3.0.2 Structure Learning and Parameter Estimation . . . 26

4 Research Methodology **29**
4.1 Conceptual Framework . . . 29
4.2 Research Methodologies and Methods . . . 30
4.3 Research Strategy . . . 30
4.3.1 The Granular Niche Bayesian Network Modelling Framework Design . . . 32
4.4 Probabilistic Graphical Model Artifacts Modeling . . . 35
4.5 Modeling Steps . . . 36
4.5.1 Granular Niche Bayesian Network Model Artifact Ontology Engineering . . . 37
4.5.2 Candidate Bayesian Probabilistic Bayesian Model Design . . . 40
4.5.3 Pre-processing and Synthetic Ground Truth Data Generation . . . 42
4.5.4 Structure Learning and Parameter Estimation Model Training . . . 43

4.5.5 Structure Learning and Parameter Estimation Model Validation 44

5 Results and Discussion **46**

5.1 Structure Learning and Model Performance Comparative Analysis 46

5.1.1 Bayesian Information Criterion Scores 47

5.2 Knowledge Discovery through Structure Learning 48

5.3 Parameter Estimation Model Comparative Performance Analysis 49

5.3.1 Bayesian Model Parameter Estimation Performance Comparison 49

5.3.2 Parameter Estimation Simulation 50

5.4 Discussion and Conclusion 51

5.4.1 Discussion 51

5.4.2 Conclusion 52

5.4.3 Research Limitations 53

5.5 Significance of the Study 53

5.6 Future Research 53

.1 Appendix A 55

references **64**

Chapter 1

Introduction

> "Natural science has discovered chaos, social science has encountered complexity. But chaos and complexity are not characteristic of our new reality; they are features of our perceptions and understanding. We see the world as increasingly complex and chaotic because we use inadequate tools to explain it. When we understand something, we no longer see it as chaotic or complex." [Gharajedaghi 2011, p.25]

The term *wicked problems* as attributed to Rittel and Webber [1973] describes complex problems which defy resolution despite numerous efforts at solving such problems. Such problems include, with increasing *wickedness*: i) traffic jams Brzica [2023], ii) design of emerging technologies like driveless cars Hoffmann [2020], iii) managing possible effects of climate change Peters [2017], iv) managing pandemics Auld *et al.* [2021] , v) unemployment vii), inequality Suoheimo *et al.* [2021], and vi) diagnosis and treatment of different types of cancer [Fleck 2024].

We argue that wicked problems (WP) are products of cognitive and computational limitations to understand complexity, its relationship to dimensionality, and, inherent uncertainty. Figure 1 shows that as phenomena becomes more complex, the many dimensions of related variables that make up that complexity increase exponentially. Our cognitive ability to understand complex phenomena from multiple perspectives given the available suite of computational tools and techniques to assist our understanding are thus challenged.

The close link between CAS and WPs has been noted by Zellner and Campbell [2015]. The authors have argued that understanding CAS from an ontological view point is a first step in understanding wicked problems. They posit that while knowledge of the characteristics of complex systems cannot in itself *solve* wicked problems in the conventional deterministic sense, the knowledge can be used to redefine wicked problems. This can be done, they further argue, while retaining diversity, interdependencies and *messiness* associated with wicked problems. They further argue that by replacing analytical approaches with more suitable statistical and mathematical analysis approaches complex systems can better computed and understood.

Gharajedaghi [2011] has suggested that the world is seen as increasingly complex and chaotic because the tools currently applied to analyse, explain, and understand it are inadequate. That it is not possible to solve current problems with same level of thinking that created those problems in the first place is attributed to Albert Einstein [1879 - 1955], which implies that we need a higher level of abstract thinking to rise above and resolve our current problems. In other words, it is more productive to imagine, build, test, and simulate alternative prototypical alternative new futures, as opposed to focusing on the problems themselves as a source of solutions.

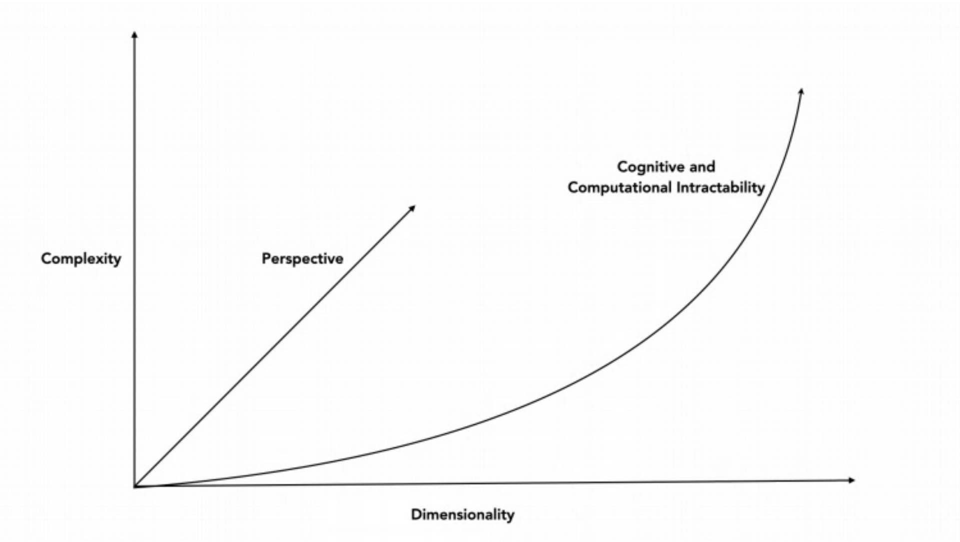


Figure 1.1: Wicked problems: Relationship between dimensionality, complexity perspectives and intractability

This research thesis embraces the views espoused by these authors and thinkers and is about incorporating new ways of seeing into computational modelling tools to: re-imagine; think about; describe; design; test; communicate; and compare alternative, prospective solutions in order to make informed choices in support of the resolution of wicked problems.

The research thesis contribution is in the form of a new set of conceptual and computational explainable artificial Intelligence (XAI) and machine learning (ML) tools and techniques to explore complexity and dimensionality in CASs.

We incorporate context, granularity and perspective, as explicit ontological constructs Semwayo and Ajoodha [2021] to represent complex theory concepts in a Bayesian network (BN) model and related computational ML algorithms. The aim being to improve the accuracy and precision of Bayesian models at representing and reasoning about complex adaptive systems.

The research work broadly seeks to provide explainable artificial intelligence Bayesian models and ML computational tools that are fit for purpose to enable the principled discovery of lever points for the resolution of wicked problems.

1.1 Research Motivation

Advances in the following scientific disciplines and technologies present opportunities to explore wicked problems differently: i) complex systems sciences modelling; ii) unprecedented growth of computational capacity; iii) growth in heuristic search approaches to deal with analytically intractable problems; iv) rapid prototyping and simulation of dynamic and counter-intuitive complex problems.

The complex systems sciences have provided kernel theories to help us better understand the character of wicked problems. Ontology Engineering Guizzardi [2005] and Bayesian modelling driven AI Gyftodimos and Flach [2002]; Potgieter and others [2005]; Pearl [2009] and ML Koller and Friedman [2009]; Faruqui *et al.* [2021] now provide us the necessary tools for the construction of explainable models to support tractable, rapid computation, simulation prediction, inference, and algorithmic machine learning.

Ontology Engineering (OE) involves the use of formal explicit terms representing a given domain to ensure the correct and precise representation phenomena from the real world into formal machine readable artifacts known as ontologies [Weber *et al.* 2012; Guizzardi *et al.* 2015]. A more formal definition is provided in section 2.5.

A Bayesian network modeling involves the use of probability graphical models (PGMs) to represent a joint distribution in a factorised way [Koller and Friedman 2009]. A more detailed formal definition is provided in section 2.6.

Machine learning techniques use heuristic search algorithms to learn the structure of complex phenomena and provide an estimation of the probability distributions of the parameters that make up PGMs.

To be able to fully access these benefits we believe the solution lies in incorporating complexity theory concepts [Manson 2001]. Smith and Klagges [2008] concepts as constructs in ontological and Bayesian models to obtain richer, more accurate and more precise Ontological models and BN models that better represent CAS and support reasoning and learning of wicked problems.

This research broadly seeks to contribute to a theory of CAS, a subset of complexity theory, that makes possible the exploration of lever points for the resolution of wicked problems [Holland 2006]. Such a theory, as posited by Holland [2006] could lead to great improvements in the resolution of wicked problems such as cancer treatment and drug design.

1.2 Problem Statement

While some effort has gone into developing and using non formal, formal models, and computational methods to represent and tractably simulate the behaviour of complex phenomena, wicked problems continue to be an unresolved challenge. We argue that this is because of the inadequacy of existing non formal and formal tools and techniques to address the challenge.

In the absence of appropriate tools and techniques to address wicked problems policy makers, political, public, and corporate decision makers are expected to make rational decisions and take decisive action on complex wicked problems given: (i) contesting multiple stakeholder perspectives and interests (ii) unintended counter intuitive pathological outcomes arising from some interventions; (iii) multiple dimensions and varying contexts, granularity, and perspectives of the problem; (iv) uncertainty about the full extent of the problem; (iv) incomplete data; and (v) an unknown fast, evolving present and future, which cannot rely entirely on past knowledge.

What results are ill informed decisions, typically driven by the voice of the loudest or the depth of the purse of the most influential pressure group, without full view of the problem and the linkages between the multiple sub-systems that make up the whole. Decisions made under these conditions typically have devastating impacts on some sectors of society and / or on society.

Non formal modeling frameworks and models quickly become unwieldy when the dimensionality of variables and complexity of variable interactions increases when applied to the resolution of wicked problems. Examples of such non formal modeling frameworks include: i) group concept mapping; ii) communicative planning; iii) systems thinking; iv) systems archetypes v) ; and vi) scenario and futures planning [Lich *et al.* 2017; Davies *et al.* 2015; Bar-Yam 2000; Senge 2006; Klein *et al.* 2006].

We argue that the success of these efforts has been limited by the their inability to: i) compactly represent complex adaptive systems and wicked problems in a way that is comprehensible; ii) tractably process the model variables parameters and outputs of interactions, and related data. In addition it is difficult to validate, and objectively test the models with data and to compare the accuracy and precision of these models.

While formal modeling approaches such as OE Whyte and Thompson [2012]; Nasim and Khan [2018]; Ruhl and Salzman [2020]and BN models, also known as belief networks and related ML algorithms Benjamin-Fink and Reilly [2017]; Marcot [2017] have been used to model and reason about complex phenomena, we argue that existing formal modeling frameworks from OE and BN models lack adequate constructs to provide compact, tractable, and resource inexpensive modelling support to represent, explore, and reason about complex phenomena, as viewed through the complex adaptive systems lens. Thus challenges still remain in providing adequate formal OE and BN models that transparently and accurately represent CAS and support the precise structure learning and parameter estimation of wicked problems.

We argue that this is because baseline BN models and related ML algorithms used to resolve WPs do not have adequate constructs to correctly and precisely represent such problems as CAS and accompanying ml algorithms with appropriate constructs to support their tractable computation. This research thesis addresses this challenge.

1.3 Research Purpose

The purpose of this research thesis is to demonstrate the effectiveness of incorporating complexity theory concepts, namely; i) context, ii) granularity, and iii) perspectives as constructs in a BN model to better support the representation of CAS and the resolution of wicked problems using machine learning algorithms. We shall call this novel BN model the Granular Niche Bayesian Network Model, the GNBN model in short, where granular niche refers to a sub-system delineated by context, hierarchical and temporal granularity, and perspective constructs.

By incorporating these complexity theory concepts in the proposed BN model we expect to improve the accuracy and precision of CAS representation models in domain ontologies and BN models. This should lead to improvements in Bayesian inference, structure learning, and parameter estimation accuracy and precision from data on complex phenomena, to support reasoning about wicked problems.

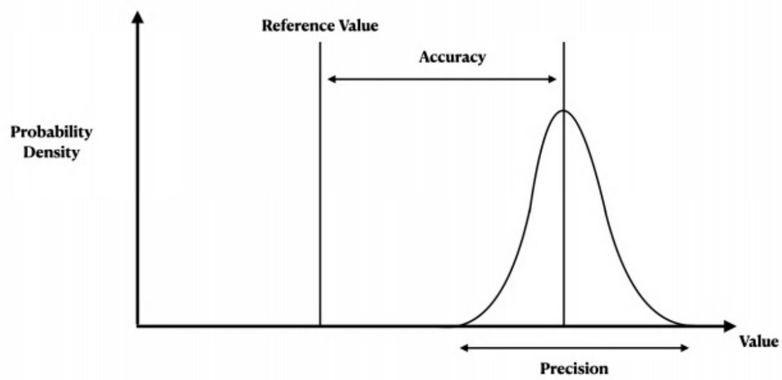


Figure 1.2: Probability Density Distribution: Relationship between accuracy and precision

Figure 1.2. shows the character of accuracy and precision with respect to the probability density of the variables in probability graphical models (PGMs). While we seek to improve the accuracy of domain CAS models through ontology engineering, we are also interested in the precision of the models, that is, deviation of the variables' probability density distributions from the mean.

1.4 Research Questions

Based on the discussion in the previous sections the principal research question is stated as follows:

How does the proposed novel ontology driven Granular Niche Bayesian Network model incorporating complexity concepts: context, granularity, and perspective, as foundational ontological modelling constructs, perform in comparison to baseline Bayesian models at recovering the structure of complex adaptive systems, estimating the model parameters, and knowledge discovery from ground truth data?

Following from the principal research question outlined above the following sub-research questions and research objectives are stated as follows in table 1.1:

Table 1.1: Research objectives and Research questions

	Research Question		**Research Objective**
RQ1	How does the proposed novel BN model, incorporating ontological CAS concepts as constructs, perform in comparison to baseline BN models at recovering the structure of complex adaptive systems from ground truth data?	R01	Use Bayesian Information Criterion (BIC) scores to compare the performance of the novel GNBN model to baseline Bayesian models at recovering the structure of complex adaptive systems from ground truth data.
RQ2	How does the proposed novel GNBN model compare with baseline BN models at approximating the true probability distribution of CAS model parameters from ground truth data?	RO2	Explore and compare, using synthetically generated ground truth data, how the designed novel GNBN model performs in comparison to baseline Bayesian models at minimising the relative entropy with the ground truth distribution using the Kullback-Leibler Divergence (KL Divergence) measure.
RQ3	How does the GNBN modeling framework support knowledge discovery about wicked problems?	RO3	Determine how learning of new knowledge about CAS and wicked problems can be improved by using the GNBN modelling framework and designed model, in comparison to baseline BN models.

In their review of Design Science research questions Thuan *et al.* [2019] identify three types of research questions. These are: i) problem solving; ii) gap spotting; and iii) problematization research questions. Problem solving questions focus on the identification of practical, and design problems and to build solution artifacts that address these. Gap-spotting research questions focus on under-researched or overlooked areas lacking a specific focus, and areas lacking empirical support. Finally problematization questions focus on in-house, root metaphor, paradigm, ideology, and field assumptions [Thuan *et al.* 2019].

This research thesis falls into the problem solving and gap spotting categories of research questions. Research questions (RQ1) and (RQ2) are built on the argument that there is a problem of inadequate formal, well-grounded design modelling artifacts for representing CAS to better understand and resolve wicked problems using explainable AI. Research question (RQ3) is a gap spotting research question, where the problem is in a well known but overlooked focus area by developing computational models to resolve wicked problems. We are seeking new improved ways of learning about, and discovering knowledge on the structure of given wicked problems.

1.5 Hypothesis

Our working hypothesis is that the GNBN model produced by our modeling framework out-performs baseline BN models at CAS structure learning (SL) and parameter estimation (PE), and knowledge discovery (KD) support of the nature and structure of wicked problems.

The null hypothesis is that the GNBN network model produced by our modeling framework does not perform better than baseline BN models at Bayesian structure learning and parameter learning and for knowledge discovery support of wicked problems.

1.6 Research Methodology

An iterative and rigorous abductive reasoning design science research methodology is applied in this research thesis where an ontology driven Bayesian modelling framework is applied to design the GNBN model, a formal, ontologically sound, and explainable artificial intelligence model, incorporating CAS theory concepts: context; granularity; and perspective, as constructs.

Qualitative approaches are applied to design ontologically sound models, and quantitative approaches are applied for experimentation with data to test our model against baseline BN models using ML algorithms.

1.7 Novelty and Contribution to Science

The novelty in our modeling framework, approach and model is that by incorporating context, granularity and perspectives as formal foundational ontological constructs in BN models we design BN models better suited to represent CAS and reason about wicked problems than baseline BN models.

We are able, using our modeling framework, to ensure the mapping of correct structural relationships between random variables within and across complex adaptive sub-systems to facilitate sensible belief propagation and Bayesian posterior updating within given contexts, granular levels and perspectives. We are also able to highlight the influence of GNBN properties (context, granularity, and perspective) on the probability distributions of the model parameters associated with any given set of beliefs by capturing these properties as prior knowledge. In essence our GNBN model extends the information space that baseline Bayesian inference can provide answers to with respect to CAS and WPs more accurately and more precisely.

The research questions in section 1.4 provide the basis for our contribution to scientific research wherein our proposed GNBN modeling framework contributes towards the design of semantically richer models for Bayesian SL and PE of CASs, see figure. 1.3 which shows our contribution, through a useful framework after [Pearl 2019].

where:

- *E_s is a mathematical formula that, based on the assumptions, provides a recipe for answering the query from any hypothetical data, whenever it is available*
- *$\hat{E}_s$ an actual estimate for the answer together with statistical estimates of confidence for that answer*
- *F represents fit indices that measure how compatible the data is with assumptions conveyed in the model.*

[Pearl 2009]

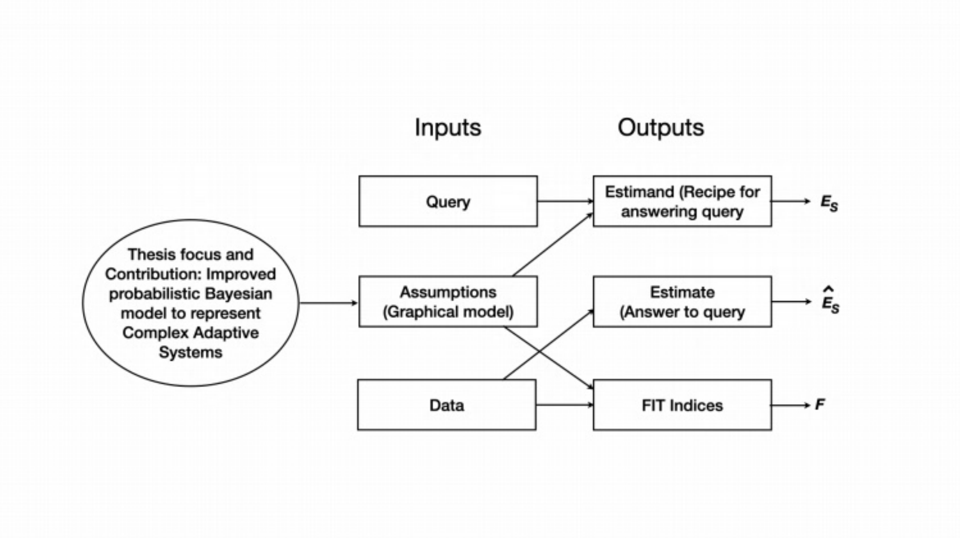


Figure 1.3: Research Contribution framework adapted from[Pearl 2009]

More broadly the GNBN modeling framework and designed GNBN model's contribution to scientific research is as follows:

1. Visual, ontologically transparent, structural and probabilistic graphical model representation of CAS to facilitate stakeholder collaboration and design of machine readable models. This has the effect of enhancing cross disciplinary communication between stakeholders, such as, mathematical modellers, domain experts, and decision makers;
2. A Bayesian model with an underlying Bayesian structure recovery and parameter estimation capability that out-performs baseline Bayesian models at supporting algorithmic learning from data generated by CAS's. This is made possible through the incorporation of knowledge about the systemic nature of the real world encoded as GNBN model constructs.
3. A Bayesian probabilistic modeling framework that performs better than baseline approaches at tractable, economic (time and cost), exploration and comparisons of various candidate wicked problems solution proposals through the use of Bayesian simulation.

1.8 Research Limitations

The research thesis uses a prototypical CAS example from literature to explore the design and application of the required artifact in an artificial setting through experimentation. Synthetically generated data is used to evaluate the utility and performance of the proposed designed artifacts. While this approach does provide proof of concept, the artifacts would need to be tested against case studies and empirical data from real world natural settings.

Our approach does not involve validation of our preliminary integrated ontological and Bayesian graphical model by experts. While consulting experts to validate the model at different stages would have been useful, it is outside of the scope of the contributions of this work.

Further, the level of expertise and perspectives of different experts on the same issue varies, making it difficult to arrive at a common problem definition and general level of accepted discipline knowledge, a feature of wicked problems itself. The author's domain knowledge of complex theory and complex adaptive systems is applied to generate synthetic data for structure learning and parameter estimation.

1.9 Thesis Structure

The rest of the thesis is set out as follows;

Background. The background chapter provides an overview of the character of wicked problems, the relevant complexity theory Semwayo and Ajoodha [2021], and the applicable modeling concepts and constructs from the fields of OE and Bayesian modeling.

Related Work. Provides a review and discussion of relevant previous research on the subject matter, that is modeling CAS using OE and Bayesian SL and PE.

Methodology. Discussion of the research philosophy and paradigm, the research method chosen, the formal definition of the modeling framework and modeling steps and the resultant model.

Results and Discussion. In this chapter SL and PE are carried out to compare the performance of the GNBN model against baseline Bayesian models, using synthetically generated data from a prototypical textbook CAS and wicked problem.

Significance of the Study. The significance of the study is highlighted in this chapter.

Conclusions and Future Research.This chapter provides summary conclusions from the research outcomes and directions for future research.

Chapter 2

Background

This chapter provides an outline of the background concepts from complexity theory and wicked problems used in this research paper. We also provide an overview of the concepts and terms from the fields of ontology engineering, Bayesian structure learning and parameter estimation, relevant to explainable artificial intelligence modeling and machine learning of complex adaptive systems and wicked problems.

2.1 Wicked Problems

Wicked problems are complex problems difficult to define and solve using analytical methods and interventions [Rittel and Webber 1973]. Attempts at resolving wicked problems by applying traditional stakeholder engagements and analytical methods tends to produce counter-intuitive outcomes, typically referred to as *unintended consequences* [Crowley and Head 2017; Levin *et al.* 2012; Xiang 2013].

The original full list of the ten wicked problems characteristics as provided by Rittel are available in Crowley and Head [2017] and summarised here as follows:

1. The problem is difficult to formulate definitively. The problem is usually only well defined after a solution has been found;
2. It is difficult to determine when an inquiry should be concluded;
3. Solution are only described as better or worse from different stakeholder perspectives;
4. The the quality of the solution is difficult; to determine;
5. The solutions cannot be verified in polynomial time;
6. There is no room for trial and error. Decisions. can have dire consequences;
7. There is no definitive algorithm to solve problems;
8. Solutions are not singular and are not well defined;
9. Applying learning from the past is not adequate because the future hardly resembles the past;
10. Wrong or inadequate solution are not tolerated because of their consequentially.

The character of wicked problems has since been revisited, with the most recent review provided by [Crowley and Head 2017]. Xiang [2013] provides a summarised useful characterisation of wicked problems, that is: i) divergent perspectives of the problem that arises from different experiences, goals;

ii) solutions are difficult to define Elia and Margherita [2018]; ii) non-solubility Xiang [2013]; iii) irreversible consequentiality, where trial and error strategies are not feasible [Xiang 2013].

Wicked problems emerge from: i) non-linear, dynamic complex and adaptive interactions between entities in a bounded system / sub-system and their external environment, producing positive and negative feedback loop mechanisms between the interacting entities; and ii) multiple divergent stakeholder perspectives of framing a given problem [Crowley and Head 2017]. The divergent perspectives influence the problem definition, and candidate solution proposals for such wicked problems. We shall refer to the first category, i), as Type I wicked problems causes and the second (ii), as Type II wicked problem causes.

Type II wicked problems causes are the product of: i) various philosophical and scientific positions with respect to complex phenomena; ii) methods applied to study them; iii) experiences; iv) culture; divergent stakeholder beliefs, interests and biases; v) context; vi) varying problem focus areas and levels of abstraction, and v) divergent conventions for naming and describing the world observed [Crowley and Head 2017; Levin *et al.* 2012; Xiang 2013]. Figure 2.1. provides a schematic representation of these author's ideas.

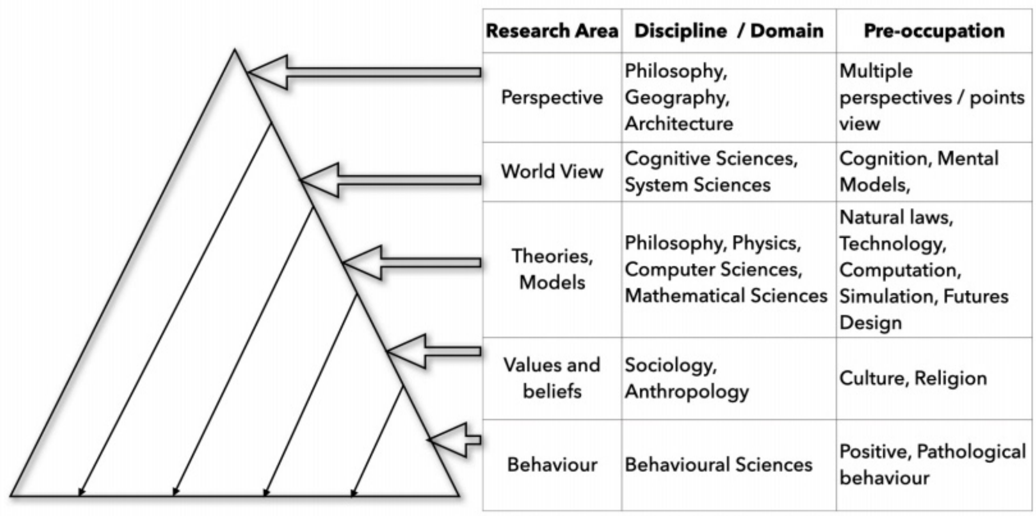


Figure 2.1: Influence Triangle

From the bottom up of the triangle (from Values and beliefs to Perspective) the elements at the bottom affect the development of elements of the research areas above them. Values and beliefs affect the development of theories and models, which in turn affect the development of world views, and finally the world views become perspectives, that is, enduring, entrenched beliefs about reality.

As one moves down the triangle the elements at the higher level have more influence on the elements below. For example, perspective, which is in effect the product of enduring world views, once entrenched in a group of people, influences their view of the world and the theories and models they use to explore reality. A typical example is the multiple divergent perspectives on climate change, where debates and disagreements on defining and handling the multiple dimensions of the problems rage on.

Munn and Smith [2013] define perspectivism as enduring different world views carried by different stakeholders, a product of past experience and knowledge and a major sources of disagreements about the character of a given reality. Raimbault [2017] advances a similar notion from a different angle. Here perspectivism refers to where different scientific knowledge enterprises are seen as perspectives with co-evolving components from complementary knowledge domains.

Farrell and Hooker [2013] isolated finitude, complexity, and normativity as the three cognitive processes that are responsible for wicked problems, where complexity refers to the emergent outcomes of multiple interactions within a system. Finitude refers to limitations in human cognition and knowledge. Normativity referees to different stakeholders norms and values [Farrell and Hooker 2013].

A useful mapping of the theoretical status of the wicked problems concept, the range of meanings associated with the concept, the epistemological assumptions that underlie the description of the concept, and the rhetorical functions formed by the concept is provided in [Lönngren and Van Poeck 2021]. The authors distinguish between 'tame problems' associated with the natural sciences, which are well defined and are solvable through linear reductionist approaches, as opposed to ill defined 'wicked problems' associated with the social sciences. A further useful typology breakdown of the spectrum between 'tame' and 'wicked' problems based on perceived intractability of modelling and problem resolution is provided by [Alford and Head 2017].

Resolving wicked problems is difficult primarily because of they are complex and dynamic [Xiang 2013]. It has been argued that the inherent complexity and pathological emergence from the structural relationships and numerous dynamic interactions of related entities within natural or artificially defined bounded systems (CAS) are the root cause that produce Type I wicked problems [Semwayo and Ajoodha 2021]. The numerous dynamic interactions of agents (variables) with feedback loops between them take place at varying levels of granularity, making natural and engineered systems unpredictable [Farrell and Hooker 2013].

Wicked problems have largely been considered non-soluble because of perceived modelling and computational intractability [Zellner and Campbell 2015]. The characterisation of wicked problems as pathological products of agent interactions in complex adaptive systems paints a picture of modeling intractability. Computational intractability has been attributed to such problems because 'they cannot be broken into parts' [Xiang 2013].

2.2 Link between Wicked Problems and Complex Adaptive Systems

The close similarity between CAS and wicked problems is noted by [Zellner and Campbell 2015]. The authors argue that understanding CAS is a first step to understanding wicked problems. Peters Peters [2017] goes as far as to argue that the study of complex adaptive systems was birthed by the need to understand the character of wicked problems. Wicked problems are thus best understood when viewed from a systems paradigm lens and have been defined as emergent behaviour from complex adaptive systems in (Wimsatt, 1994) and (Bar-Yam, 2000).

The view that wicked problems are best understood when viewed though the systems paradigm is also found in [Wimsatt 1994; Bar-Yam 2000]. The resolution of wicked problems as viewed through a systems paradigm lens is discussed in [Senge 2006; Klein *et al.* 2006; Akers 2015; Onik *et al.* 2017; Gharajedaghi 2011; Randle and Stroink 2018].

A complex system is characterised by Zellner and Campbell [2015] as being composed of multiple, heterogeneous parts which selectively interact with each other. The interaction can give rise to an emergent organisational whole with its own attributes, behaviours. Other characteristics of CAS include: i) feedback loops which are usually time-lagged and spanning spatial scales; ii) parallelism, wherein CAS are subject to sets of parallel simple rules that define the agents' behaviour which give rise to unpredictable future states. Thus the long term behaviour of CAS cannot be predicted by aggregating the behaviour of parts [Zellner and Campbell 2015].

Another characterisation of Complex Adaptive Systems (CAS) is provided by as a diverse collection of diverse parts inter-connected in a hierarchical manner such that organisations persist or grow over time without centralised control [Eidelson 1997]. Self organisation is considered a key component of CAS [Kauffman 1993]. Figure 2.2 captures the essence of complex adaptive systems.

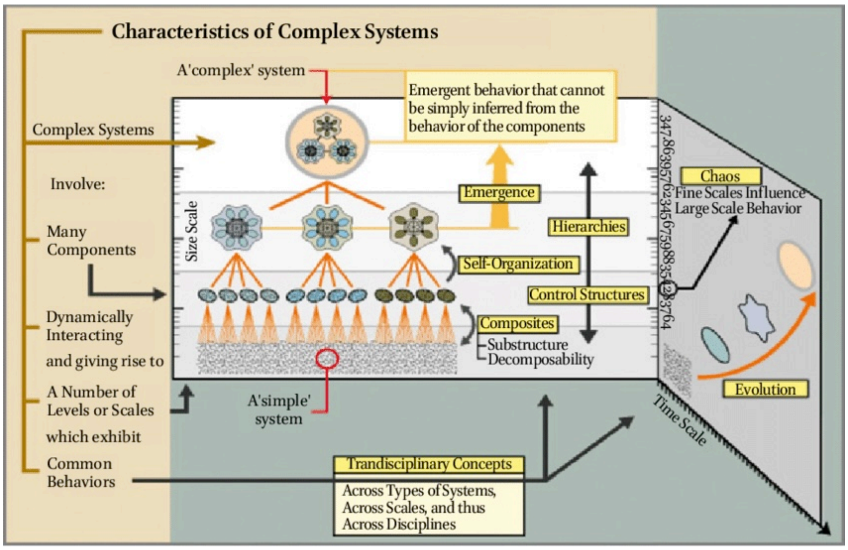


Figure 2.2: Characteristics of Complex Adaptive Systems [Clemens 2023]

Emergence is at the core of CAS and wicked problems. Emergence refers to system outcomes properties / products that 'emerge' from the CAS as a whole, through interaction between variables and cannot be attributed to individual variables within the system. Four types of emergence are defined by [Fromm 2005]. Type I, which the author defines as simple emergence, arises from simple intentional or unintentional emergence through feed forward relationships. Examples of intentional emergence provided by Fromm [2005] are: i) the function of a software system as an emergent property of its software code; ii) the function of a machine as an emergent property of its components. Examples of unintentional emergence include: i) thermodynamic properties like pressure, temperature and volume, and avalanches.

Type II, weak emergence, arises from positive and negative feedback, with negative feedback having a stabilising effect, while positive feedback has a destabilising pathological effect. Examples of positive feedback in Fromm [2005] are: i) Stock market bubbles and crashes; ii) fads; iii) social explosion of unrest, iv) path dependent lock in technology such as keyboard QWERTY arrangement.Examples of stability arising from negative emergence include: i) flocking behavior of birds, ii) the world wide web's self organisation.

Type III emergence is characterised by multiple short range positive feedback and long range negative feedback refereed to as activator-inhibitor systems [Fromm 2005]. According to Fromm [2005] this emergence appears in CAS and is responsible for the appearances of and dramatic changes in ecological niches. Examples include i) market stock movements, ii) metal and scientific breakthroughs.

Type IV, strong emergence, is associated with the emergent structures at higher levels of organisation such as life which emerges from genes, genetic code, and nucleic / amino acids [Fromm 2005]. Type IV emergence is characterised by emergence that arises at multiple levels and where the laws governing emergence at one level are not applicable at another level. Physics quantum and relativity theories fall into this category.

Type II through to type IV emergence are the ones of interest in this research paper, particularly where positive forward feedback is present, as it is associated with the emergence of wicked problems.

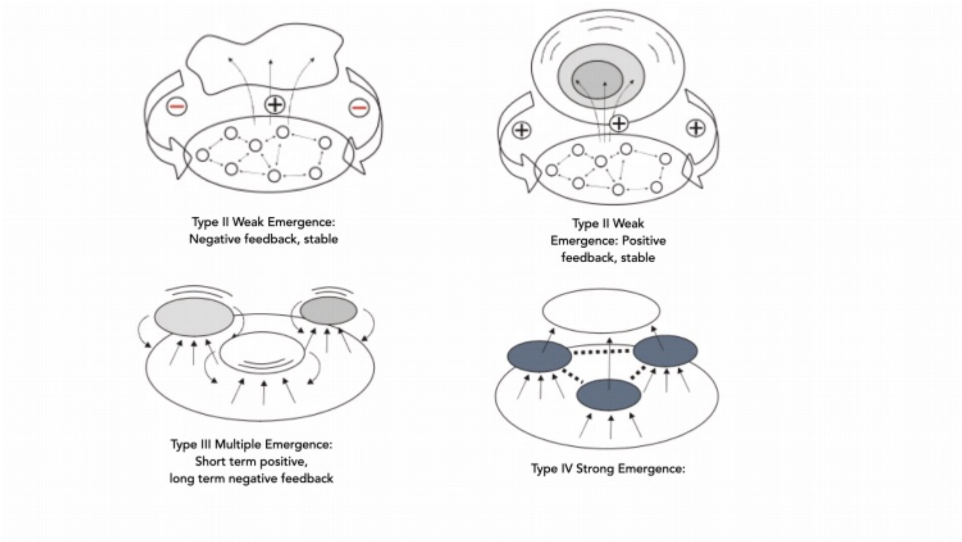


Figure 2.3: Types of emergence [Fromm 2005]

In summary a wicked problem can be defined from contributions by [Bar-Yam 2000; Zellner and Campbell 2015; Elia and Margherita 2018] as a tuple (P, F, V, C, S), where:

- **P**: may be defined as a set of parameters and variables that influence the problem's behavior and includes the space of potential problem states, encompassing the various factors, variables, and dimensions that contribute to the wicked problem.
- **F**: Feedback mechanisms that capture the interactions between the problem space, solution space, and contextual factors. These mechanisms represent how changes in one aspect of the system affect other aspects and may be modeled using mathematical relationships.
- **V**: encompasses the subjective values, preferences, and perspectives of various stakeholders involved in the wicked problem. This introduces a qualitative and human-centric element.
- **C**: These are social, economic, political, environmental, and cultural aspects that shape the problem and its potential solutions.
- **S**: represents the space of potential solutions or interventions to the wicked problem which includes the set of strategies, actions, or policy options that stakeholders might consider to address the problem.

We provide a more formal defintion of a wicked problem in the next section.

2.3 Formal Definition of Wicked Problems

The formal definition for emergence, as cast in the complex adaptive system framework is provided by Baas and Emmeche [1997] as follows:
Definition 1. ***Emergence***

Let $\{S_i\}_{i \in I}$ be a family of general systems or "agents". Let Obs^1 be "observation" mechanisms and Int^1 be interactions between agents.

The observation mechanisms measure the properties of the agents to be used in the interactions. The interactions then generate a new kind of structure, which is the result of the interactions:

$$S^2 = R\left(S_i^1, \mathrm{Obs}^1, \mathrm{Int}^1\right). \tag{2.1}$$

This could be a stable pattern or a dynamically interacting system. S^2 is an emergent structure which may be subject to new observational mechanisms, Obs^2 [Baas and Emmeche 1997].

This leads us to the definition of a wicked problem. The definition of a wicked problem from an emergence point of view is as follows:

Definition 2. ***Wicked problems***

P is a pathological emergent property (a wicked problem)

$$\Longleftrightarrow$$

$$P \in \mathrm{Obs}^2(S^2) \;\; \textit{and} \;\; ,P \notin \mathrm{Obs}^2, (S_i^1)$$

A property observed in S , but not in the S_i's could be said to have emergent explanation Baas and Emmeche [1997], wherein the emergent complex adaptive system property is pathological / undesirable, is refereed to as a wicked problem. This further extends to the definition of that of an unintended consequence which occurs when an intervention takes place on the interaction between interacting variables, resulting in an unexpected and undesirable emergent property.

Type I wicked problems refer to pathological emergence of $S^2 = R\left(S_i^1, \mathrm{Int}^1\right)$ and type II wicked problems emerge from divergent Obs^1 and / or Obs^2 perspectives of stakeholders.

2.4 Context, Granularity and Perspective as Complexity Theory Concepts

"There is only one Herbert (the frog) that we and the molecular biologist apprehend, but, depending upon our interests and our focus, we may each apprehend him from different granular perspectives". [Munn and Smith 2013, p. 12]

For any given context or sub-context, complex phenomena is abstracted cognitively and described at different levels of granularity and from a specific perspective [Semwayo and Ajoodha 2021].

Complexity theory, a field of theoretical Computer Science, provides the theoretical grounding to study complex adaptive systems, wicked problems, and computational complexity [Montiel *et al.* 2019]. Techniques such as the theory of chaos, cellular automata, and evolutionary computing have been applied to deal with complexity [Montiel *et al.* 2019]. Context, granularity and perspective are key complexity theory concepts used in the description of the environmental situation, hierarchical and dynamic character of CAS in literature [Frei *et al.* 2007].

Context

Context is determined by the focus of interest [Semwayo and Ajoodha 2021]. Pearl [2009] has argued the need to delimit the contextual endogenous and exogenous elements of a system under review. Ko and Sim [2008] in their work on context awareness modeling have shown that ontologies provide an effective way of representing syntactic and semantic knowledge.

Complex adaptive systems are defined by Mittal and Risco-Martín [2017] as systems that display adaptive behavior in addition to emergent behavior. The authors describes adaptive behavior as adaptable manifesting at the agent-environment system boundary where the agent is situated in an environment [Mittal and Risco-Martín 2017]. An adaptive system here is seen as a resilient system capable of change in the face of perturbations [Mittal and Risco-Martín 2017]. The authors explore the tools and techniques required for a multi-disciplinary systems engineering enterprise and identify Network Science as key to understand the structure of CAS.

Semantic context aware quality services that specifically incorporate context in models to support explicit multiple perspectives representation are discussed by [Alti *et al.* 2013]. The authors argue that semantic heterogeneity, disagreement about the meaning of terms amongst multiple stakeholder perspectives, remains an obstacle especially for modelling CAS, given different contexts. Our model seeks to address this shortcoming, and we thus incorporate context as a formal foundational ontology construct in our Bayesian probabilistic graphical model.

Granularity

Granularity is a concept relating to the cognitive, spatial, or temporal, level of abstraction of a phenomena from an observer's point of view [Semwayo and Ajoodha 2021; Santos 2015; Smith and Mark 1998]. It is also used to define the coarseness of an observation or an investigation [Semwayo and Ajoodha 2021].

The level of problem abstraction, *granularity*, is a key determinant in what is defined, 'seen' and investigated [Semwayo and Ajoodha 2021; Gignoux *et al.* 2017]. Jensen and Aven [2018] emphasises the importance of considering both, atomic elements within micro sub-systems, and the macro system that emerge from systems interactions to fully understand wicked problems.

While granularity has been said to influence what we 'see' with our mind's eye and the linguistic concepts we use describe what we see, our perspective Smith and Klagges [2008], the corollary is also true. The focus of interest or context influences at which level of granularity we carry out our investigation at, and the tools and techniques we apply. As one zooms in onto a subject of interest one gains detail, and as one zooms out one gains broad perspective.

Mittal and Risco-Martín [2017] have argued that perceptions of adaptation capacity are dependent on the observer's scale and granularity of abstraction . Climate change, for example can be viewed as human made phenomena if viewed from a lived human time scale but could be viewed as a natural phenomena if viewed from a coarse temporal granularity, covering millions of years.

The need to carry out ontology alignments at multiple granular levels to support semantic interoperation, towards unification of multiple perspectives, is discussed in [Semwayo and Berman 2004]. Natural, biological and social systems are examples of CAS with complex, dynamic, cause and effect interactions at varying levels of granularity [Santos 2015]. It has been argued by Ketter *et al.* [2015] that wicked problems transcend individuals, organisations, and markets and can only be fully understood by the exploration and analysis of a wide variety of data at many levels of abstraction.

It has been argued by several authors that patterns emerge at higher levels of complexity that are specific to that level emerging [Gleick 1998; Ball 2004; Bousquet and Curtis 2011]. Such properties, which cannot be deduced from the lower granular constituent parts, may manifest as wicked problems [Semwayo and Ajoodha 2021]. Incorporating these features as ontological constructs in modeling frameworks is key in improving the accuracy and precision of models representing CAS and their emergent problems Bousquet and Curtis [2011], the goal of the research presented in this paper.

Perspective

Munn and Smith propose embracing realist perspectivalism, a view that knowledge can be obtained by means of veridical granular partitions [Munn and Smith 2013]. They describe veridical partitioning as the representation of some aspect of reality in a model for a given purpose [Munn and Smith 2013]. The authors argue that the existence of multiple perspectives should not be seen as a hindrance but a means to deepen our understanding of reality [Munn and Smith 2013]. Raimbault [2017] advances a similar notion which he calls perspectivism, where the scientific knowledge enterprises are seen as perspectives with co-evolving components from complementary knowledge domains.

We argue, as pointed out by Raimbault [2017]; Munn and Smith [2013] that the existence of multiple perspectives should not be seen as a hindrance but a means to share our knowledge of a given reality and deepen our understanding of reality, in other words overcome finitude. Efforts at developing ways of surfacing and possibly unifying multiple perspectives have been attempted in the fields of Foresighting and Scenario planning [Hietanen *et al.* 2011].

The utility of incorporating additional constructs in foundational ontologies to improve the accuracy of domain ontologies is discussed by [Jansen 2008; Gangemi *et al.* 2001]. Incorporating different perspectives, contexts, and granular levels of abstraction as foundational ontology constructs, also refereed to as top level ontology constructs, for CAS representation presents an opportunity to represent complexity and handle multiple perspectives of wicked problems.

2.5 Ontology Engineering

Epistemology is defined by Tolk "as the theory of obtaining knowledge, knowledge validity, and scope, and methods applied to obtain it" [Tolk *et al.* 2018]. Knowledge here is defined as scientifically justified belief. The authors further posit that systems are governed by law-like generalizations within a special science. These laws, they argue, result in emergence, which is characteristic of the system and is hidden from the researcher, whereas the unpredictability of the system is a knowledge matter [Tolk *et al.* 2018]. This becomes the source of 'unintended consequences' when intervening on a system.

The view of CAS from an ontology perspective is premised upon the view that emergence in a CAS is independent of human knowledge Tolk *et al.* [2018] and that emergent properties are of the system and cannot be explained by the system components, their relations and interactions alone [Tolk *et al.* 2018]. Tolk argues that while epistemological emergence can be obtained through accessing more knowledge about the system, ontological emergence is an inherit part of the system and thus cannot be obtained through accessing more knowledge [Tolk *et al.* 2018].

For the reasons given above the absence of a common vocabulary for multiple stakeholders from various backgrounds to describe an observed world creates semantic heterogeneity problems. This is where stakeholders from diverse scientific backgrounds observing the same reality describe such a world using divergent vocabularies (concepts and terms) and divergent conventions for naming and describing the world. Rusty Schweickart, an Apollo 9 astronaut is quoted as having said that when he came back from space it took him five years to describe his experience of seeing earth from space. He simply could not find the right words in the commonly used language (concepts and terms) to describe and share his experience [Kaku 2012].

As René Descartes (1596-1650) succinctly put it, that "we do not describe the world we see, but rather we see the world that we can describe" [Descartes and Cress 1998]. A common ontological lexicon that unifies divergent conventions for naming and describing the world we observe is needed to accurately describe and communicate what we perceive.

Studer *et al.* [1998] define an ontology as *a formal, explicit specification of a shared conceptualization*, refereed to by Smith and Klagges [2008] as a computable lexicon . An ontology explicitly represents: i) the types of entities that can exist in the domain; ii) the properties these entities can have; iii) the relationships they can have to one another; iv) the roles they can play with respect to one another, v) how they are decomposed into parts, and vi) the events and processes in which entities can participate [Costa *et al.* 2006]. An important feature of an ontology is that it is a model that clarifies and specifies a set of meanings in a formal language Uschold [2015], opening the space for a shared multi-stakeholder view and conceptualisation of a given problem. Simply put, an ontology provides a common unambiguous language for shared meaning [Uschold 2015].

By making people's assumptions about the structure of a given world of interest explicit, the formal model is able to communicate and provide improved understanding, clarification of a particular view of the world [Guarino 1998]. Thus ontologies are particularly useful in representing domain knowledge unambiguously, useful for information sharing and communication between humans and machines. More formally an ontology, after Guizzardi [2007] is summarised in figure 2.4.

Definition 3:

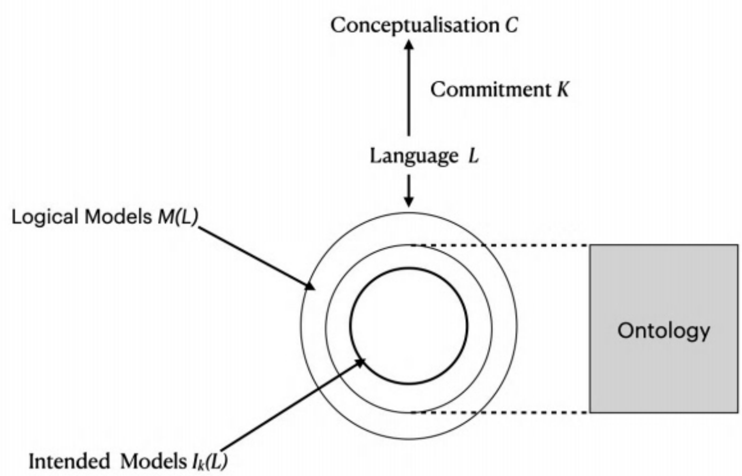


Figure 2.4: Relations between language(vocabulary),conceptualization,ontological commitment and ontology [Guizzardi 2007]

"where:

- C: is a conceptualization of the set of intended world structures, where each world structure is a set of individuals of the domain and a projection of existing concepts in a given world.

- L: is a given a logical language
- V: is a given vocabulary
- K: an Ontological Commitment"

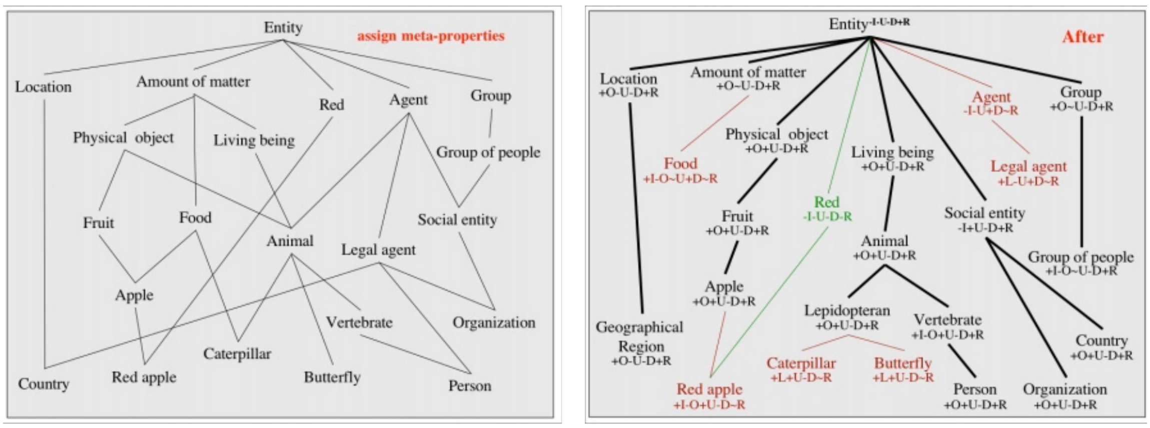
Representing of the structure of domain knowledge as ontologies is well documented in [Pai *et al.* 2017; Abuazab *et al.* 2017; Guarino 1998; Gignoux *et al.* 2017; Semwayo and Ajoodha 2021].

The primary role of formal ontology for domain ontology modeling, it has been argued, is not to enforce consensus among different stakeholders Borg *et al.* [2014]; Guarino and Welty [2004], but rather to achieve: (i) intra world-view consistency, and (ii) inter world-view interoperability [Borgo and others 2019; Semwayo and Ajoodha 2021].

2.5.1 The Importance of Ontology Accuracy and Precision

An incorrect representation of a given reality leads to incorrect inferences. Guarino [1998] emphasises the importance of accuracy and precision in designing robust and well founded ontologies. He argues that this is not only important for achieving a a common agreement but also making explicit and understanding the reasons for disagreement to support interoperability, across heterogeneous data systems.

Guarino and Guizzard have contributed to an ontological theory based on logical and philosophical principles to support clarity and precision in representing complex reality [Guarino 1998; Guizzardi *et al.* 2015; Gignoux *et al.* 2017]. A framework to ensure the correctness of abstraction of the structural relations between worldly entities is provided by [Weber *et al.* 2012], see figure 2.5.



A B

Figure 2.5: Ontology formalisms, after [Weber *et al.* 2012]

Ontological notions such as + R denoting Rigidity, + I denoting Identity, + O denoting global Identity, and $+U$ denoting Unity are used to bring order to semantic taxonomic relationships and avoid incorrect modeling of worldly concepts [Welty and Guarino 2001; Guizzardi *et al.* 2015]. Using these ontological notions, see figure 2.4 we can model relationships between entities such as that the *Person* concept is rigid + R, that is, must not change, whereas *Student* is non rigid - R, that is being a student may be transitory. This then means that we can define constraints such as that - R cannot subsume + R, that is, a non rigid concept *Student* cannot subsume a rigid concept *Person* in a taxonomic relationship.

The discipline of ontology engineering has emerged from the need to provide a robust method and meta-constructs to correctly and precisely represent the structure of complex phenomena as formal human and machine readable artifacts, domain ontologies as shown in figure 2.4 [Guizzardi *et al.* 2015; Weber *et al.* 2012; Spear *et al.* 2016; Simperl and Tempich 2006]. OntoClean Guarino and Welty [2004] and OntoUML Guizzardi [2005] are examples of methodological tool used developed to support ontology engineering.

A formal top level ontology, the Basic Foundational Ontology (BFO) which explores formal distinctions like time, space, and context, which are key features of complex systems, and lays the basis for designing domain ontologies to address inadequacies in formal conceptual modeling frameworks is proposed by [Munn and Smith 2013]. Such a top level ontology (TLO) is domain neutral and is intended to make explicit different perspectives and assumptions of a given complex reality in order to support human communication and machine level inter-operation. Our proposed complexity theory concepts of: context, granularity, and perspective, fall into this category.

2.6 Bayesian Networks

The Bayesian paradigm has been described as a paradigm where prior beliefs are updated each time there is an observation [Blei *et al.* 2017]. Here beliefs, based on perspectives, should always be mutable especially when the observed data is surprising. A belief is in this case is equivalent to a hypothesis. The paradigm is underlain by the Bayesian theorem which outlines the relationship between posterior probability, likelihood probability, prior probability and evidence as illustrated in figure 2.6.

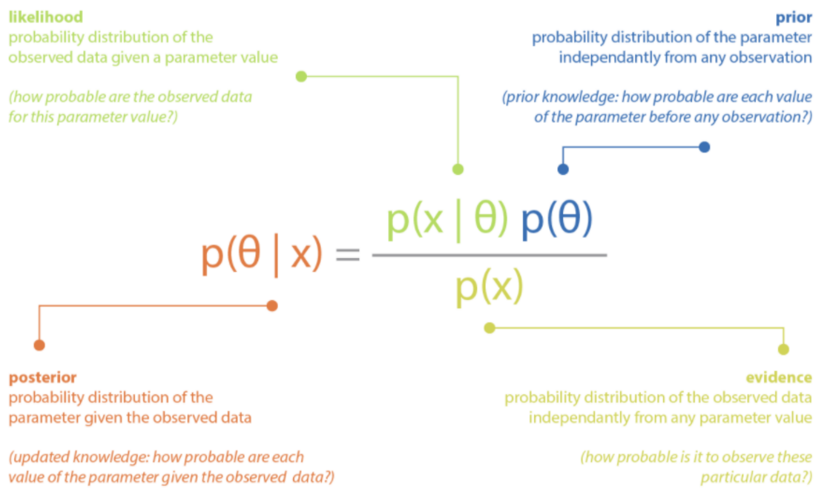


Figure 2.6: Illustration of the Bayes theorem applied to the inference of a parameter given observed data [Rocca 2019]

Bayesian formalism describes conditional probabilities, where:

- $P(A|B)$, which says belief in probability of A given knowledge of B.
- A and B are independent if $P(A|B) = P(A)$,

[Pearl 2009]

A Bayesian network graph G represents a domain D, and belongs to a group of graphic models referred to as probabilistic graphical models (PGM) . A PGM is a data structure skeleton for representing a joint distribution compactly in a factorized way [Koller and Friedman 2009]. It also provides a way to compactly represent a set of conditional independence assumptions about a distribution [Koller and Friedman 2009]. PGMs allow distributions to be written tractably even when the explicit representation of the joint distribution is astronomically large[Srihari 2014]. This feature is particularly key given our objective to manage exponentiality related to complexity (see figure 1.1).

d-separation

The challenges of exploring the relative strengths of connections between causal connections through representing joint distribution have been pointed out in [Koller and Friedman 2009]. The challenges are : i) the computational expense of data manipulation; ii) cognitive capacity of human expert to handle many parameters, and iii) the large amounts of data that would be required to statistically learn the distribution from data, and estimate many parameters robustly.

One key concept useful in understanding of probabilistic causal propagation information in Directed Acyclic Graphs (DAGs) representing probabilistic causal relationships between variables in complex systems is the concept of d-separation [Pearl 2009].

A set *Z* is said to d-separated *X* from *Y* *iff* *Z* blocks every path from a node in *X* to a node *Y* [Pearl 2009]. The concept of d-separation is important for our purposes in that it provides us with information on the structural implications of an intervention on a given variable on the whole complex system.

2.6.1 Hierarchical Bayesian Networks

Complex systems are made up of multiple levels of hierarchically organised entities and entity relationships [Smith and Klagges 2008]. Hierarchical Bayesian Networks provide for the representation of hierarchically structured systems [Gyftodimos and Flach 2002]. Hierarchical Bayesian Networks (HBN) are generalisations of standard Bayesian Networks, where a node in the network may be an aggregate data type. We view HBNs as critical for our proposed GN probabilistic Bayesian model because of their inbuilt capability to model sub-system intra-level and inter-level relations and and their quantitative probabilistic relations as illustrated by [Illari *et al.* 2011].

While the likes of Brown *et al.* [2010], and Burman *et al.* [2017] have argued that solutions to wicked problems are intractable, Simon [1996] has pointed out that tractable solutions can be achieved through modularising the exploration of solutions at the different granular levels at which hierarchical nested systems are perceived.

2.6.2 Dynamic Bayesian Networks

One of the key requirements of our proposed modeling framework is the ability to model temporal dynamism and temporal granularity. Dynamic Bayesian networks [DBNs] using Markov conditioning have been proposed for modeling CAS for this purpose in [Potgieter and others 2005].

The Markov assumption links graphs and their probability functions. Each variable is probabilistically independent of its non-descendants, conditional on its parents [Koller and Friedman 2009]

$$P(x_j|pa_j) = P(x_1, ...x_j - 1). \tag{2.2}$$

"Conditional probability x_j is thus sensitive only to a small subset of predecessors PA_j". This considerably simplifies and reduces input information handled [Pearl 2009]. In other words this leads to reduction in computational complexity.

Dynamic Bayesian Networks [DBNs] are defined as extended Bayesian Networks that relate variables to each other between adjacent time steps. DBNs thus include multiple copies of the same variables which represent different states of the variables over the time [Darwiche 2009].

Hidden Markov Chains are utilised to provide a method to discretize timelines into a set of time slices. Measurements of the system state are taken at pre-determined regularly spaced time intervals [Pearl 2011]. See figure 2.7. O represents observed variables while S nodes represent hidden (latent) variables.

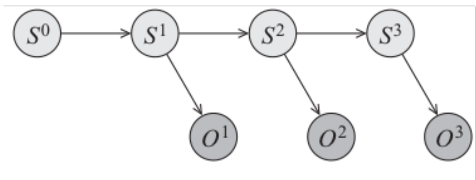


Figure 2.7: Unrolled DBN for four time slices, after [Koller and Pfeffer 1997]

2.6.3 Structure learning and parameter estimation

Bayesian networks are well suited for structure and parameter learning [Faruqui *et al.* 2021]. The application of Bayesian theory to these applications is well documented [Koller and Friedman 2009; Pearl 2011]. These applications are outlined in the next sub-section.

Structure Learning

Structure learning is carried to reconstruct network structure from data for the purpose of either knowledge discovery for a given domain or to perform density estimation, that is, estimate a statistical model of the underlying data distribution. This facilitates the reasoning about instances not in the training data [Koller and Friedman 2009]. The authors have argued for preference for a sparser structure with fewer edges at the expense of representing the true underlying structure.

Three types of structure learning approaches are documented in literature. Theses are: i) Constraint-based structure learning; ii) Score-based structure learning; and iii) Bayesian model averaging methods [Koller and Friedman 2009]. Constraint-based structure learning approaches view a Bayesian network as a representation of independencies between variables in data. These structure learning approaches attempt to the best minimal I-map for the domain, that is the network structure that best captures the independencies in a given domain [Koller and Friedman 2009].

Score based methods define a hypothesis space of potential structure models and a score that provides a measure how well the model fits the observed data with respect to training data [Koller and Friedman 2009]. Greedy search algorithms like Hill Climbing and Tableau search are common choices used as optimisation algorithms. Score based methods are particularly appropriate for this research where we need to compare the performance of our proposed model relative to Baseline Bayesian models.

The Bayesian information criterion (BIC) which is a statistical criterion used for model selection and model comparison in statistical modeling and machine learning will be used for model comparison in this research thesis. The BIC provides a way to balance the trade-off between model complexity and goodness of fit and aims to capture key features of posterior model uncertainty via a penalty that is motivated by the large sample properties of the marginal likelihood [Drton and Plummer 2017]. We use the BIC score to compare the performance of our model against Baseline models.

Parameter Estimation

The structure learning process outlined in the previous section produces a probabilistic graphical model. The probability distributions of the nodes in the structure are estimated using parameter estimation. Parameter estimation is a process of estimating conditional probability densities of variable parameters from data using a Bayesian model. Two main methods are used for this purpose, the Maximum Likehood and Bayesian estimation methods.

The Maximumlikehood is a frequentist approach which seeks to maximise the likelihood function of a point estimate without explicitly modeling uncertainty . The Bayesian estimate treats parameters as random variables and incorporates prior beliefs as prior probability distributions and produces posteriors which quantify uncertainty in the form of the posterior distribution[Koller and Friedman 2009]. Bayesian estimation can easily incorporate hypothesis testing which is useful for model comparison useful in our approach.

The Kullback–Leibler divergence (KL Divergence) is a basic measure to determine the divergence between an estimated distribution and a true one [Cano *et al.* 2020]. KL divergence is a distance measure or the relative entropy between two probability distributions [Koller and Friedman 2009]. The KL Divergence between two probability distributions P and Q is as follows:

$$KL(P \parallel Q) = \sum [P(x) * \log(\frac{P(x)}{Q(x)})], \tag{2.3}$$

where:

- P(x) represents the probability of an event x according to reference distribution P
- Q(x) represents the probability of the x according to the estimated distribution Q

The KL Divergence is used here to compare the performance of a given Bayesian probabilistic model at parameter estimation from P, the reference ground truth data based on a target variable.

Hyperparameters allow us to consider and encode prior knowledge of a given set of random variables. Weak informed priors of say $\alpha = 4, \beta = 6$ indicate low confidence in the precision as measured by σ , while $\alpha = 8, \beta = 2$ represent higher levels of confidence in priors. The narrower the the peak of the posterior distribution, see figure 2.8, the greater the precision of the distribution as measured by the standard deviation and the closer the measured distribution to the true distribution. Precision increases with the amount of data [Koller and Friedman 2009].

As argued by Martin *et al.* [2021] priors should be context dependent, that is, the choice of priors must be informed by the specific problems and the domain scientific field. This is consistent with our view of perspectives as entrenched world views, in other words perspective. We use the KL Dirvergence score to compare the performance of our model against Baseline models at parameter estimation relative to the ground truth.

Summary

The foregoing sections in chapter 2 provide an outline of the key theories, tools and techniques relevant to our research thesis [Zellner and Campbell 2015; Peters 2017; Senge 2006]. The systems paradigm with its complexity theory and systems thinking tools and techniques has provided science with insights into the character of wicked problems as complex adaptive systems' emergent pathological patterns [Frei *et al.* 2007; Elia and Margherita 2018].

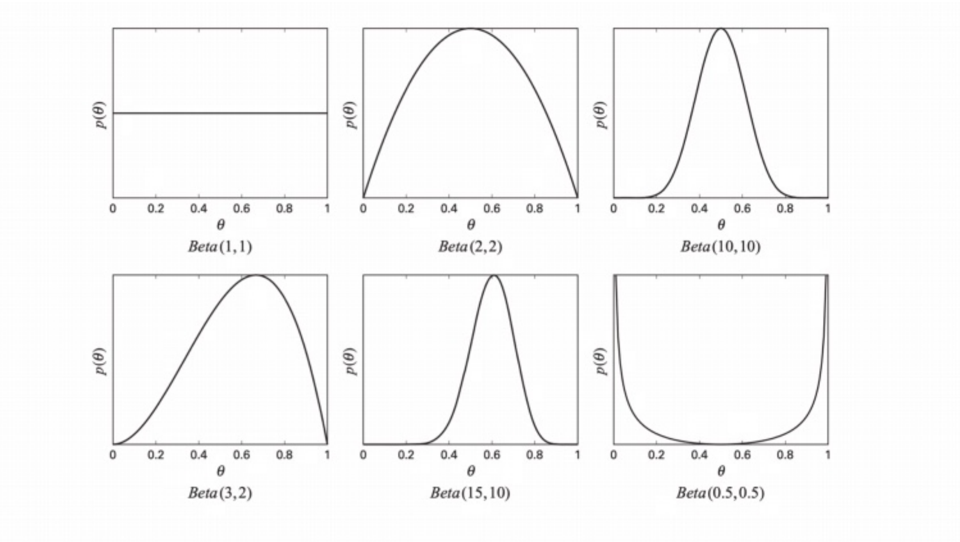


Figure 2.8: Examples of Beta distributions for different choices of hyperparameters [Koller and Friedman 2009]

Ontological engineering has provided tools to represent the structural architecture of complex adaptive systems and ways to ensure the correctness of abstraction and representation of a given reality, based on existing deterministic knowledge [Guarino and Welty 2000; Guizzardi *et al.* 2010].

Bayesian networks as probabilistic graphical models, the related Bayesian theorem, and information theory have provided science with the means to handle stochasticity, incomplete data, and the means to compare and evaluate the performance of different candidate and structure learning and parameter estimation techniques [Koller and Friedman 2009; Pearl 2009; Darwiche 2009].

These contributions together provide a solid trans-disciplinary suite of theories, tools, and techniques to support the development of models to comprehensively resolve wicked problems. The next chapter provides a review of recent related work carried out to develop Bayesian network models to support the resolution of wicked problems.

Chapter 3

Related Work

Our review of related research work in literature covers research on concepts, tools and techniques used to perceive, abstract, represent, learn the structure, and estimate the uncertainty parameters of complex adaptive systems (CAS) and wicked problems. We adopt a thematic approach to the review of research work relating to Type I wicked problems and those relating to Type II wicked problems using the following themes pertaining to CAS in general and and wicked problems in particular: i) representation of CAS in formal ontology and Bayesian models, ii) Bayesian machine learning tools for structure learning and and parameter estimation from data generated by underlying CAS processes.

Most wicked problems are not specifically labelled, or recognised as such [Alford and Head 2017]. This presents a problem in that the identification, perception, characterisation and representation of wicked problems in appropriate conceptual models is not done correctly, and by extension the understanding of the problems as emerging from adaptive complex systems and multiple stakeholder perceptions is stifled.

As a result proposed problem solving models and techniques applied to resolve wicked problems not only fail dismally but succeed in creating even bigger problems, typically labelled as unintended consequences [Burks-Copes and Kiker 2014]. We believe the main reason for this state of affairs is the fragmentation of knowledge of the problems, and the methods, techniques, and tools applied to resolve such problems across scientific disciplines.

3.0.1 Representation of complex adaptive systems in formal models

Table 3.1 provides a summary thematic review of related work contributing towards the formal representation of wicked problems in ontology and Bayesian modeling frameworks.

Wicked problems characterisation as complex systems as discussed by Zellner and Campbell [2015] provides the logical link between complex adaptive systems and wicked problems. Ko and Sim Ko and Sim [2008] in their work on context awareness modeling have shown that ontologies provide an effective way of representing syntactic and semantic knowledge in complex systems.

Granular levels of organisation of complex phenomena is discussed in-depth by [Smith and Klagges 2008; Santos 2015]. Granular level induced emergence is covered in [Gleick 1998; Munn and Smith 2013; Gignoux *et al.* 2017]. A convincing argument that portrays causation and emergence as products of relational interactions between variables across granular levels that not only changes the interacting variables quantitatively but quantitatively as well, is advanced by [Santos 2015].

Contributions from these authors provide a solid philosophical base to build engineered domain

Representation of complex adaptive systems in formal models	
Sub-theme	**Related Work**
Wicked problems characterization as complex systems	Zellner and Campbell [2015]
Granular level organization of complex adaptive phenomena	Santos [2015]; [Spear *et al.* 2016]
Granular level induced emergence	Gleick [1998]; Munn and Smith [2013]; Gignoux *et al.* [2017]; Crowley and Head [2017]
Ontology of complex systems	Wimsatt [1994]
Convergence of multiple perspectives through ontological mapping	Turnbull *et al.* [2018]; Phillips and Ritala [2019]
Ontologies as knowledge bases	Helsper and Van Der Gaag [2002]
Representation of confounding latent variables as being 'outside' a defined bounded system	Pearl [2009]
Representation of complex phenomena as hierarchical structures	Murphy and Russell [2002]; Gyftodimos and Flach [2002]

Table 3.1: Representation of complex adaptive systems in formal models

ontologies. The representation of CAS and wicked problems at varying granular levels of observation or abstraction for Type I wicked problems in formal conceptual models such as foundational ontologies and probabilistic Bayesian models is however limited [Semwayo and Ajoodha 2021].

The absence of a common vocabulary for multiple stakeholders from various backgrounds to describe an observed world creates semantic heterogeneity problems. This is where stakeholders observing the same reality of interest describe it using divergent vocabularies (concepts and terms) and divergent conventions for naming and describing the world. Domain ontologies are particularly useful at providing such a common formal vocabulary and can be utilised to represent domain knowledge.

Foundational ontology provides the meta-constructs to design domain ontologies. OntoUML has been used successfully to model domain ontologies [Guizzardi 2007]. OntoUML, is a compliant ontology modeling framework with ontological distinctions and axiomatization of a theoretically well-grounded foundational ontology based on the Unified Foundational Ontology (UFO), after [Guizzardi *et al.* 2015]. The OntoUML plug-in provides a solid platform to incorporate our modelling constructs to support modularization for the purposes of cognitive conceptual modeling of tractability, multiple view extraction, and semantic inter-operation between different perspectives of a given reality. Our proposed foundational CAS constructs can be incorporated into such a platform.

We note that a number of candidate effective formal Bayesian structuring theories and tools to compactly represent complex adaptive systems do exist and are covered in literature. These include: i) representing complex systems as hierarchical, dynamic structures, Murphy and Russell [2002] and Gyftodimos and Flach [2002]; ii) Use of Hidden Markov Models to model dynamic processes using dynamic structures as illustrated by Ajoodha and Rosman [2018]; iii) compact modularisation of complex structure using the d-separation principle as defined by Pearl [2011] and discussed in detail by [Koller and Friedman 2009]. The d-separation principle is particularly useful in managing complexity and can be applied to handle perceived 'non-solubility' and computational intractability in wicked problems.

There are two broad ontology and Bayesian integration approaches that have been applied to handle complexity. The first approach involves converting domain ontologies into Bayesian networks [Fenz 2012]. The second approach involves building ontologies from Bayesian networks [Mouenis *et al.*

2014]. Integrating ontologies and Bayesian networks has been attempted to take advantage of the relative strengths of the two modeling approaches [Mouenis *et al.* 2014]. Our approach involves incorporating foundational complexity concepts as constructs in an ontology engineering modeling framework described by Guizzardi *et al.* [2010] to support semantic and perspective reconciliation between diverse naming conventions and stakeholder perspectives. We then use the outputs of this process, domain ontologies, as candidate Bayesian model inputs for structure learning and parameter estimation.

Benjamin-Fink and Reilly [2017] provide an Object Oriented Bayesian Network (OOBN) to improve the modeling of complex Bayesian structures. We apply in this research paper the OOBN approach to modeling CAS to take advantage of the modularisation effect of OOBNs.

Advances in Bayesian network models and recent developments in the the integration of Bayesian network and other model forms to improve Bayesian classifiers and machine-learning algorithms for time-dynamic models are described by [Marcot and Penman 2019].

Machine learning algorithms for tractable heuristic search provide the means to carry out simulations for alternative candidate solutions, thus providing rational arguments for the choices of specific solutions by comparing the relative economic utility of various options [Korb and Nicholson 2010]. These algorithms, including Hill- Climbing heuristic, and variations thereof as described by Burke and Bykov [2012] can be used to resolve issue of irreversible consequentially in wicked problems [Zellner and Campbell 2015]. For example one cannot undo the construction of a harbour if decisions to locate the harbour are found to be ill informed. Here Bayesian models and associated ML algorithms can be used to generate virtual world simulations to explore various alternative scenarios, thus mitigating risky and costly real world experimentation [Mittal and Risco-Martín 2017].

While the aforementioned modeling techniques and tools from complexity sciences, ontology engineering, and Bayesian probabilistic graphical models, and Machine Learning can be combined and used to build tractable models for CAS to support reasoning about wicked problems, there is the outstanding need to enhance the transparency of stakeholder assumptions and the possible integration of multiple disciplinary granular perspectives about a given reality for human inspection and Bayesian inference and machine learning of wicked problems.

As noted by Munn and Smith [2013]specific representation of multiple contexts, granular levels, and multi-disciplinary perspectives as explicit complex adaptive systems representation constructs in Bayesian network models is still not adequately taken care of [Semwayo and Ajoodha 2021].

This represents the gap we intend to fill with our Bayesian model. We provide a framework for the design of explainable generative Artificial Intelligence (AI) models. We apply Bayesian models support for open, transparent, explainable underlying reality that is represented and computed. While other AI modeling approaches like Deep Neural Networks provide useful generative models, they are structured as black boxes where the results generated are not as explainable as in Bayesian probabilistic graphical models [Buhrmester *et al.* 2021].

3.0.2 Structure Learning and Parameter Estimation

We present in table 3.2 related work summaries in the application of Bayesian structure learning and parameter estimation of complex adaptive systems.

Bayesian learning has been described in Potgieter and others [2005] as the mining of the structure of a Bayesian network and the calculation of the conditional probability matrices from historical data. Structure learning has been developed to learn the structure between observable and latent variables and their parameters [Ajoodha 2018]. According to Koller and Friedman Koller and Friedman [2009] the need to learn structure and parameters of knowledge from data emanates from the difficulty in accessing

Structure Learning of Complex Adaptive Systems	
Sub-theme	**Related Work**
Challenges of machine learning of CAS structures for probability density distribution and knowledge discovery	Holland [2006]; Zhang *et al.* [2022]
Structure learning in traffic congestion prediction	Blackwell and Ajoodha [2022]
Discovery of new drug candidates	Hopkins [2008]
Discovering Alzheimer genetic biomarkers using Bayesian network	Sherif *et al.* [2015]
Using Bayesian networks to discover relations between genes, environment	Su *et al.* [2013]
Developing and applying object-oriented Bayesian networks to wicked problems	Benjamin-Fink and Reilly [2017]
Causal Bayesian Network Model for Resolving Complex Wicked Problems	Semwayo and Ajoodha [2021]
Bayesian networks for information synthesis in complex systems	Pitchforth [2015]
Complex Adaptive Systems modeling frameworks	Potgieter *et al.* [2005]
Geographical Information Systems, Spatial and Dynamic Bayesian Networks	Chee *et al.* [2016]
Parameter learning using Dynamic Bayesian Networks modelling architecture	Ajoodha and Rosman [2018]
Parameterisation and evaluation of a Bayesian network for use in an ecological risk assessment	Pollino *et al.* [2007]
Accurate parameter estimation for Bayesian network classifiers using hierarchical Dirichlet processes	Petitjean *et al.* [2018]

Table 3.2: Structure Learning and Parameter Estimation of Complex Adaptive Systems

experts and knowledge acquisition being an expensive exercise, while on the hand data is relatively cheap and plentiful.

Our approach generates synthetic data as opposed to soliciting expert knowledge as a way of bypassing difficulties with accessing domain experts and issues of finitude and indeterminacy. We use forward sampling, a reliable method to accurately predict full prior distributions, and Monte Carlo Markov Chains for modeling simulations as discussed by [Benjamin-Fink and Reilly 2017]. These modeling tools can be applied to address indeterminacy that arises from different expert perspectives of wicked problems.

Bayesian modeling frameworks and algorithms designed to manage computational complexity are discussed by [Pearl 2011; Xiang *et al.* 2003]. The models and techniques are key in managing computational complexity which arises from the fact that learning the structure of a Bayesian structure is NP-hard, that is, the search space for an optimal Bayesian structure is super-exponential [Chickering *et al.* 1994].

Machine learning algorithms such as the expectation maximization algorithm which have been used in parameterizing the probability values in Bayesian models Koller and Friedman [2009]. These algorithms can be used to provide the means to deal with issues of finitude arising from the dimensionality of variables which limit cognitive abilities to grasp the full extent of wicked problems .

The importance of the influence of latent variables to evaluate uncertainty of knowledge in the form of abstract concepts (latent variables) is discussed in [de Waal *et al.* 2016]. It is in the area of research with particular reference to complex adaptive systems and wicked problems that we have identified a need and where our research focus is. The proposed GN probabilistic Bayesian modeling framework is expected to significantly contribute to this category by providing a prior knowledge structure that includes latent variables to aid structure learning from data.

Integrated ontology and Bayesian Models developed for the purpose of improving parameter learning capability are discussed by [Marcot 2012]. Bayesian networks with underlying system dynamics, risk and decision management models to support enhanced inference over a range of resource management, most of which fit into the wicked problem definition are discussed by [Marcot and Penman 2019]. Our approach extends these ideas to apply a disciplined formal ontology engineering approach to elicit the structure of CAS models and wicked problems.

While Integrated Bayesian network modeling approaches perform better at providing explicit human and machine readable modeling schema and artefacts that support the generation of quick tractable outcomes than informal participatory systems modeling methods and regular Bayesian models, they still fall short at the efficient structure and parameter learning support given multi-context, multi-granular, and multi-perspectives.

The incorporation of these concepts as systemic meta-property constructs in Hierarchical Dynamic Bayesian Networks (HDBNs) the category the GN Bayesian probabilistic model belong is key in exploring and better understanding wicked problems and their resolution Smith and Mark [1998], the focus of this research thesis. Existing baseline Bayesian models for instance do not have adequate models to support and manage: i) forward and backwards Bayesian reasoning (inference) over CAS and wicked problems; ii) cognitive load induced by finitude, multi-dimensionality of variables and impact of confounding variables; iii) computational complexity induced by dynamic contexts, granularities, and perspectives.

Chapter 4

Research Methodology

This chapter presents the research conceptual framework, research strategy, research method, the modeling framework architecture, and modeling approach for this thesis.

4.1 Conceptual Framework

Different paradigms have different views about the structure of the world (ontology) and the ways in which that knowledge is obtained (epistemology). Venable [2006] identifies four types of paradigms applied in research.

The Positivist paradigm is associated with an ordered objective world perspective, where the laws and patterns of the world exist independently of any individual cognition [Hirschheim and Klein 1989; Venable 2006; Gioia and Pitre 1990]. Here the principal way of analysis is reductionist, that is, breaking reality into atomic component parts to gain insights about the world, refereed to as atomising in [Santos 2015]. Aggregating the components here is expected to give a clear understanding of higher level systems.

The Interpretivist paradigm views the perceived world as one that is constructed through multiple interpretations of the world based on experience and culture. Here it is assumed that there is no single version of the truth and that meaning is a dynamic social construction, transmitted via language and shared meanings and understanding [Oates 2005]. Consensus and rational choice are emphasised. The principal approach to obtaining knowledge for the Interpretivist paradigm is through induction, that is, observing a section of the world, and then based on those observations come up with a generalisations about what the word looks like.

The Critical Research paradigm like the interpretivist paradigm views reality as socially constructed and further argues that the predominant "objective" perspective is controlled by powerful, dominant players and advocates for changes in the structural relations that perpetuate the dominance of one view by a few [Oates 2005].

The Pragmatic paradigm is based on abstracting knowledge from established theory by making inferences about observations and then reflecting on the robustness of that theory [Oates 2005]. This research thesis is about incorporating concepts from kernel theories as model constructs in a novel Bayesian network model, which we shall call the Granular Niche probabilistic Bayesian network model, and refer to as the GNBN model for short. Using appropriate machine learning algorithms and synthetically generated ground truth data, the novel Bayesian network model is compared with baseline Bayesian models for performance with respect to accuracy in learning CAS probabilistic graphical model structures and precision at estimating the probability distributions of model parameters. The results are then reflected on against the kernel theories.

This research thesis fits in well with the pragmatic paradigm and thus the pragmatic paradigm is the principle paradigm applied in this research thesis. The pragmatic paradigm further allows for the simultaneous application of methodologies from the positivist, interpretivist, and action research as part of its arsenal of tools to model reality which is required for this research thesis [Oates 2005].

4.2 Research Methodologies and Methods

Research methodologies are typically classified into three categories, that is, induction, deduction, and abduction. Induction, from the interpretivist paradigm, is a reasoning method where some evidence from a sample and then generalising the outcome onto the full population without full confidence in the truth of the conclusion that is reached[Agterberg 2021]. Deduction reasoning, from the positivist paradigm, involves starting from premises that are assumed to be correct and lead to conclusions which are considered true [Agterberg 2021]. Finally abduction, from the pragmatic paradigm, is about drawing the simplest and most likely conclusion from observations [Agterberg 2021].

Medianovskyi and Pietarinen [2022] have argued that while abduction has not often been utilised in AI research, the research methodology provides the best approach to add to the body of knowledge with respect to developing explainable AI (XAI) models, given that "the successful generation of satisfactory, feasible and at best conclusive explanations is a touchstone of the truly novel abilities expected of future and emerging AI systems" [Medianovskyi and Pietarinen 2022]. This research thesis uses abduction as a research methodology to confirm the superiority of the proposed GNBN modeling framework at producing XAI models and ML algorithms that out-perform baseline Bayesian models at structure learning, parameter estimation and knowledge discovery.

Research methods can either be qualitative or quantitative. Qualitative methods use of observations, interviews, and published material for data collection and mostly thick descriptions for analysis, and for drawing insights and conclusions[Sardana *et al.* 2023]. Quantitative methods on the other hand use experiments, mathematics and surveys [Sardana *et al.* 2023]. The authors argue that quantitative research is useful to scientists for confirming or testing a theory or hypothesis.

Pilcher and Cortazzi [2024] have argued that the distinction between qualitative and quantitative research is often overdrawn and that it is difficult to avoid quantitative elements in the most qualitative subject matter and that quantitative components are crucial to most good qualitative research which begins with theories, concepts, and constructs.

This research thesis follows a mixture of qualitative and qualitative approaches to advance a theory and related concepts, and propose an a novel Bayesian modeling framework based on the granular niche theory and concepts. Qualitative approaches are applied to the design and evaluation of ontologically sound models. Quantitative approaches are applied for experimentation with data to test our model against baseline Bayesian models using machine learning algorithms.

4.3 Research Strategy

The Design Science research strategy after Hevner *et al.* [2004] of the pragmatic paradigm applies foundational / kernel theories, related frameworks, models, constructs, formalism, and validation criteria to ensure rigour of the design of model artifacts. The Design Science research strategy provides a comprehensive strategic framework suitable for the design, construction, and evaluation of the proposed model artifact.

For the GNBN modelling framework foundational theories from: i) foundational ontology; ii) information theory; iii) Bayesian theory; and iv) kernel theories from: systems theory; complexity theory; design theory, are applied to design and construct Bayesian model artifacts.

Vaishnavi and Kuechler [2015] propose a useful design science research step-wise methodological framework for designing, constructing, and evaluating model artifacts. We use the step-wise design-evaluate-construct-evaluate artifact development iterative cycle after Vaishnavi and Kuechler [2015] with the design strategy as proposed by Hevner *et al.* [2008] as the backdrop to ensure method rigour, see figure 4.1.

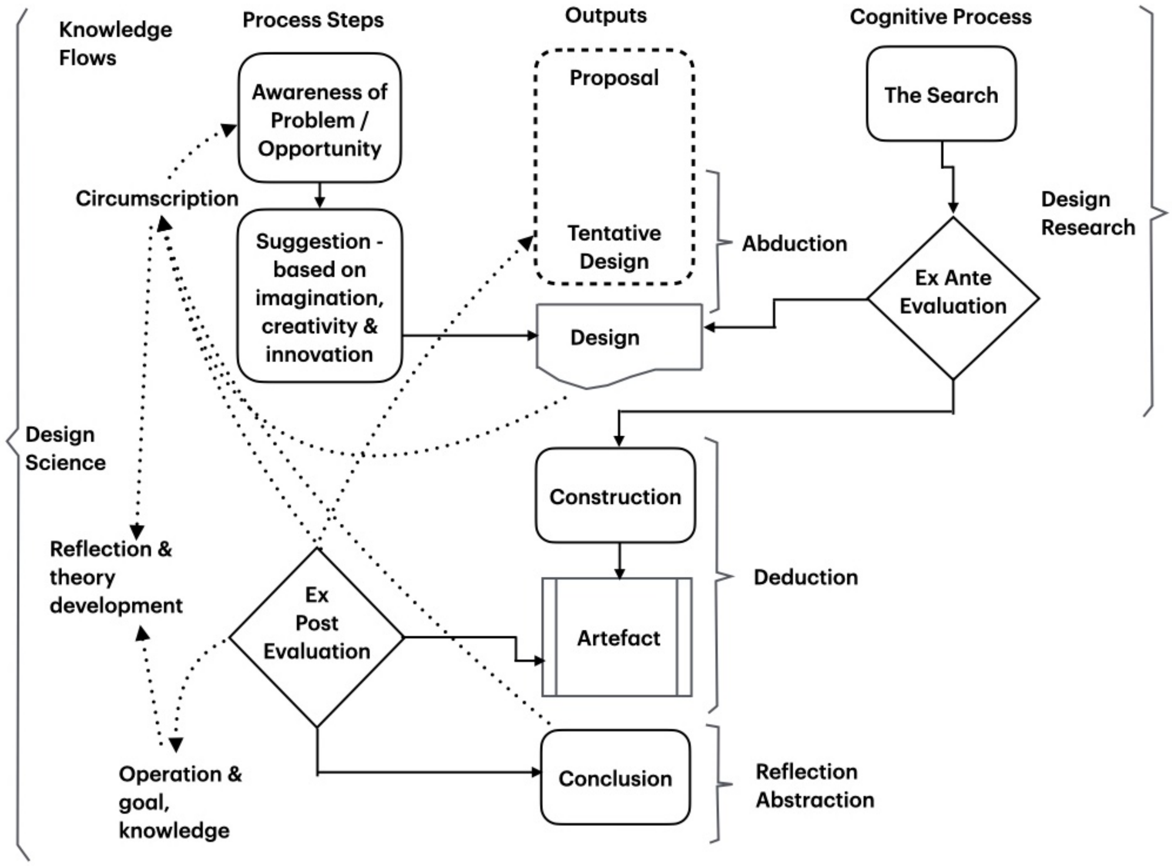


Figure 4.1: Design Science Research Strategy, and Method adapted from [Vaishnavi *et al.* 2004; Venable *et al.* 2012]

The first step in the research strategy is the design of the modeling framework which is achieved through an iterative process based on characterising the nature of wicked problems, and coming up with an innovative design modeling framework architecture and circumscription. Circumscription involves introspection on the proposed modeling framework design against kernel theories, which can result in revisiting the problem definition. In the context of this thesis the tentative design constructs, named granular niches representing CAS and incorporating complexity kernel theory concepts: granular contextual perspectives, were evaluated through circumscription for their validity and improved on. Once the validity of the design is deemed acceptable the next step involves the model construction artifact phase, see figure 4.1.

The GNBN modelling framework architecture obtained through this iterative process is described in detail in the next section. The constructed framework is itself evaluated indirectly, post ante, through the evaluation of performance of the designed GNBN model artifact against baseline Bayesian models using synthetic ground truth data.

4.3.1 The Granular Niche Bayesian Network Modelling Framework Design

The GNBN modelling framework is a formal representation of a natural or engineered CAS, within a given context at a given granular level of abstraction / observation, given a particular perspective. The term niche is borrowed from ecological science and refers to a complex adaptive system with specific characteristics that are a product of interactions of the variables within the internal system [Fromm 2005].

The term granularity refers to the hierarchical and temporal dimensions of the model abstraction, that is: macro; meso; base; micro; nano, for hierarchical abstraction and: short term; medium; and long term; for temporal granularity.

We show how the complexity theory modeling concepts: context, granularity and perspective are incorporated as formal constructs in the proposed GNBN modelling framework representing foundational ontology meta-constructs, for incorporating into domain CAS models.

For a given CAS, a granular niche is defined as the granular level of abstraction (hierarchical and temporal) of a CAS for a specified context, from a given observer's perspective. The formal definition of a granular niche here extends the definition of a granular niche by Semwayo and Berman [2004] and is defined as follows.

Definition 3. ***Granular Niche***

A Granular Niche (GN) is defined as an 9-tuple $(s, t, m, n, g, c, a, e, pv)$
[Semwayo and Ajoodha 2021]
where:

- (s) *is a spatial or virtual location occupied by the CAS;*
- (t) *is a time interval granularity;*
- *(m) is a non-empty set of member entities, present at location s for part of time interval t, each representing a role;*
- (n) *is a non-empty set of interactions between entity roles, the normal behaviour in that CAS;*
- (g) *is a hierarchical structuring of the entities, m based on relative granularity of abstraction / observation / manifestation i.e. g is a function mapping every m in m onto a granular level g i.e. g(m) = G;*
- (c) *is a description of contextual character for a given granular niche;*
- (pv) *is a description of the world view that holds for a given GN, a product of stakeholder belief system, knowledge, experience and culture. Each GN is observed by multiple stakeholders at various levels of granularity of abstractions;*
- (a) *is a set of emergent attributes of the GN sub-system which are not direct attributes of its members M;*
- (e) *is a possibly empty set of environmental parameters that hold at location S during time t*

[Semwayo and Ajoodha 2021]

The following constraints are applicable for Granular Niches:

- If $m \in M$ then $g(m)$ *is unique i.e. every entity playing a specific role has exactly one granular level in a GN.*
- *If* $m_1 \in M$ *and* $m_2 \in M$ *and* m_1 *is-part-of* m_2 *then* $Gl(m_1) \leq G(m_2)$
- *If* $m_1 \in M$*,* $m_2 \in M$*,*$G \in n$ *and g* $(m_1, m_2))$ *then* $\exists t \in T$ *s.t. In*(s, t, m_1) *and In*(s, t, m_2) *i.e. for two entities to interact in a GN sub-system they must exist in that sub-system at the same time.*
- *For all* $m \in M$*,* $\exists$ $t \in T$ *s.t. In(s,t,m) = false i.e. an entity's role does not have to remain in a GN sub-system throughout its existence. Roles of entities may change but the entities (variable) values do not change.*

[Semwayo and Berman 2004; Semwayo and Ajoodha 2021]

Figure 4.2 shows a high level architecture of the Granular Niche Bayesian modeling framework depicted as a 2 time step unrolled dynamic Hidden Markov Models (HMM) representation of two separate Granular Niches (GN), that is, complex adaptive systems and sub-systems A and B and an integrating GN system C [Semwayo and Ajoodha 2021]. Each GN is modeled as a system template, where the key ontological notions of granularity, context, and perspective are incorporated as template variables, see definition 4 [Semwayo and Ajoodha 2021]. See also Koller and Friedman [2009] for a detailed definition of templates as representational model frameworks.

The GNBN model is defined formally as as a plate model, after Koller and Friedman [2009] as follows:

Definition 4. ***Granular Niche Plate Model***

A Plate model M_Plate *defines, for each template attribute A* $\in \aleph$ *with argument signature* $U_1, ..., U_k$ *[Koller and Friedman 2009]:*

- *A set of template parents* Pa_A = $\{(B_1(U_1)..., B_l(U_l)\ \}$*, such that for each* $B_i(U_i)$ *we have that* $U_i \subseteq \{U_1.., U_k\ \}$*. The variables* U_i *are the argument signature of the parent* B_i*.*
- *A template CPD P*$(A|Pa_A)$

[Semwayo and Ajoodha 2021]

The set of template parents B_i, $A_{1..n}, B_{1..n}, C_{1..n}$, the template parents, in the GNBN model, and $\{granularity, context, perspective\}$, being instances of the argument signature, U_i. [Semwayo and Ajoodha 2021]

Within each GN sub-system entities and their attributes are modelled as observable, semi-observable and latent random variables and values [Semwayo and Ajoodha 2021]. Observable variables are colored grey. The relationships between the variables represent causal links between world entities, concepts, and their conditional probabilities [Semwayo and Ajoodha 2021].

Typical dynamic Hierarchical Bayesian Network models, and the GNBN model designed using our modeling framework, differ in that while the variables propagated and observed over time are the same for dynamic Hierarchical Bayesian Network models, represented by a single GN sub-system, say GN A in the GN causal BN model model, each GN template contains a set of interacting random variables which although persistent play different roles for each GN or interact in a unique way as their existence and behaviour is determined or influenced by the parent sub-system meta-properties:

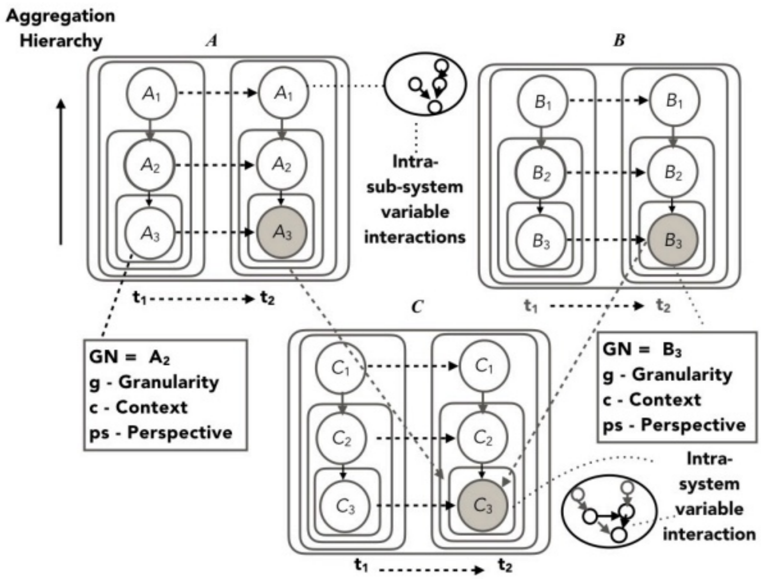


Figure 4.2: Granular Niche Probabilistic Bayesian Framework Model Architecture

granularity, context, and perspective [Semwayo and Ajoodha 2021]. Each variable in a GN subsystem is essentially an entity playing a role defined by the GN sub-system [Semwayo and Ajoodha 2021].

Further, intra - GN sub-system variable interactions produce emergent patterns and properties at the sub-system level which are greater or smaller than the sum of their parts. The proposed GNBN model artifacts are intended, on the one hand to specifically abstract an *objective* ontological structure and uncertain stochastic processes character of a complex world, while on the other hand, surface, and lay bare, the various granular contextual perspectives and assumptions held by stakeholders about a given wicked problem [Semwayo and Ajoodha 2021].

The GNBN modelling framework is thus expected to support the design of model artifacts that more accurately and precisely represent complex reality and provide richer probabilistic reasoning and learning capabilities with respect to CAS and their emergent wicked problems than baseline Bayesian modeling frameworks [Semwayo and Ajoodha 2021].

The basic Bayesian model incorporates prior knowledge as a probabilistic distribution which is updated each time there is an observation as shown in equation 4.1 [Pearl 2011].

$$p(\theta|x) = \frac{p(x|\theta)\, p(\theta)\,,}{p(x)} \tag{4.1}$$

where:

- $p(\theta)$ represents the prior belief, that is the prior probability distribution of the parameter independent of any observation,
- $p(\theta|x)$ represents the posterior probability of the parameter given the observed data,
- $p(x|\theta)$ likelihood probability distribution of the observed data given a parameter value, and
- $p(x)$ is the evidence probability distribution of the observed data independent of any parameter value, used as a normalizing constant.

We extend the basic expressions in the Bayesian formalism, after Pearl [2011] to incorporate CAS statements about conditional probabilities:

$$p(\theta|x) = \frac{p(x|\theta|gn|pv|)\, p(\theta)\,,}{p(x)} \tag{4.2}$$

where:

- *gn* is the granular niche representing knowledge of the contextual granular level of abstraction
- *pv* stands for the perspective of the observer, influenced by world view and prior knowledge
- $p(\theta|x)$, which says belief in probability of θ given observation of the data x.
- θ and x are said to be independent if $P(\theta|x) = p(\theta)$, that is, θ remains unchanged upon learning the truth about x.
- If $p(\theta|gn|pv) = p(x|gn|pv)$ this means θ and x are conditionally independent given gn and pv ; that is, once we know gn and pv , learning x would not change our belief in θ

4.4 Probabilistic Graphical Model Artifacts Modeling

The artifact modeling process starts with a description of a wicked problem, or opportunity, see figure 4.1. In the context of this research project the need is to correctly represent the Bunce Farm dilemma, a hypothetical prototypical wicked problem example from literature after Korb and Nicholson [2010], in a Bayesian model, in order to support the reasoning about the dilemma towards resolving the wicked problem.

The dilemma is stated as follows: Having observed a tree or trees in an orchard losing leaves, (see tree sub-system, observed random variable colored grey), the farmer has to figure out whether this is the result of sickness or water deficiency in order to make the corrective intervention to either spray the tree/s or irrigate the orchard soil given the financial implications, that is cost versus benefit of each chosen remedial intervention, see figure 4.3.

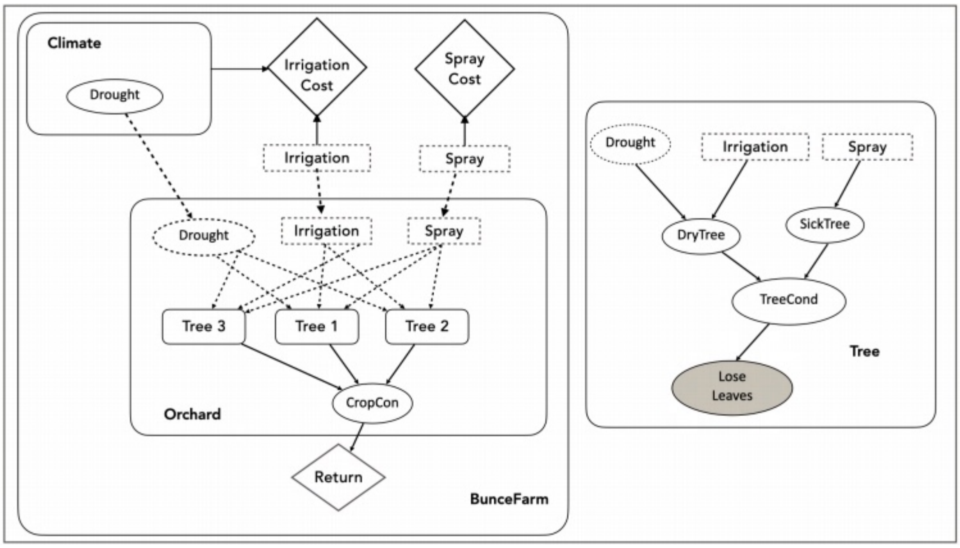


Figure 4.3: Prototypical Complex Adaptive System: Bunce Farm, after[Korb and Nicholson 2010]

While the utility of any action is represented in the *return* in figure 4.3 is important in making the decision, our focus here is on the correct and precise modeling of the probabilistic graphical model representing the problem and the stakeholder contestation on the character (structure) of the problem variables and related uncertainties surrounding the probability distribution of the values of the random variables.

4.5 Modeling Steps

Using the GNBN modelling framework as defined and outlined in section 4.2.1, a step wise approach to design and evaluate the model artifact is adopted. Figure 4.4 provides a summary outline of the modelling development and models performance comparison steps. Detailed graphic step wise inputs, processes, and outputs are provided under each process step sub-heading.

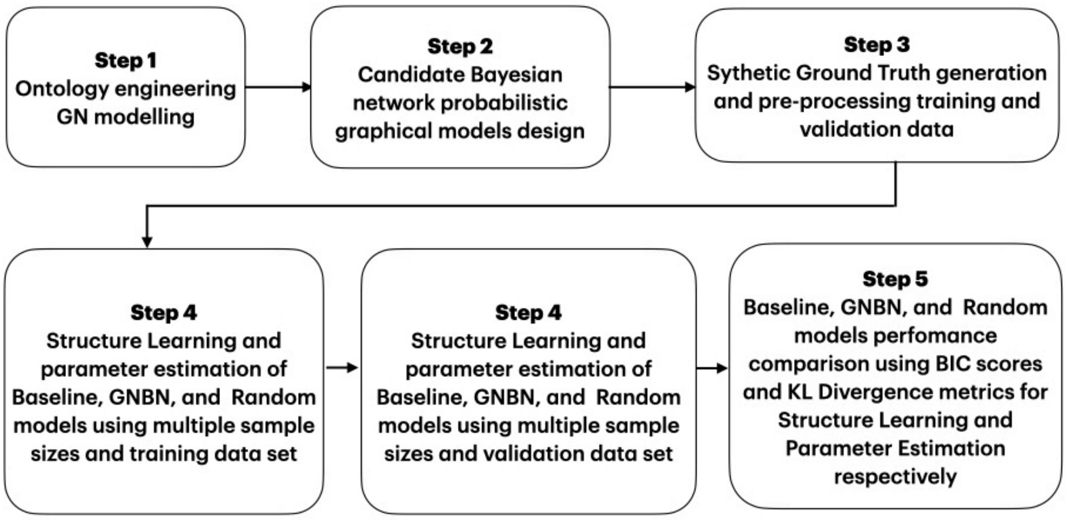


Figure 4.4: Summary model development and models performance comparison process steps

The modeling process steps cover: i) ontology engineering using the GNBN modeling framework defined and outlined in 4.3.1 to identify and resolve modeling anti-patterns (see Sales and Guizzardi [2015]) and resolve semantic heterogeneity amongst stakeholders; ii) Bayesian probabilistic graphical model candidate directed acyclic graphs structure design for the Ground Truth, GNBN ontology, Baseline and Random Bayesian models; iii) ground truth synthetic data generation; iv) training the probabilistic graphical models for structure learning and parameter estimation; v) validating and tuning the learned structures and the probability distribution of the estimated parameters; and vi) carrying out a comparative analysis of the validated model structures and parameters.

The GNBN model is expected to perform better than baseline and random models at more accurately recovering the structure of CAS and more precisely estimating the parameters of the Bunce Farm complex adaptive systems prototypical example to support the resolution of wicked problems.

4.5.1 Granular Niche Bayesian Network Model Artifact Ontology Engineering

As pointed out in section 2.5.1 the discipline of ontology engineering emerged from the need to provide a robust method and meta-constructs to correctly and precisely represent the structure of complex phenomena as formal human and machine readable artifacts [Sales and Guizzardi 2015].

An incorrect representation of a given reality leads to incorrect inferences [Guarino 1998]. As discussed in section 2.5.1 it is important to design robust, accurate, and precise well founded ontologies [Guarino 1998]. This is not only important for achieving a common agreement but also making explicit and understanding the reasons for disagreement to support interoperability across heterogeneous information systems.

Figure 4.5 provides details of the ontology engineering process steps, inputs, iterations, and outputs.

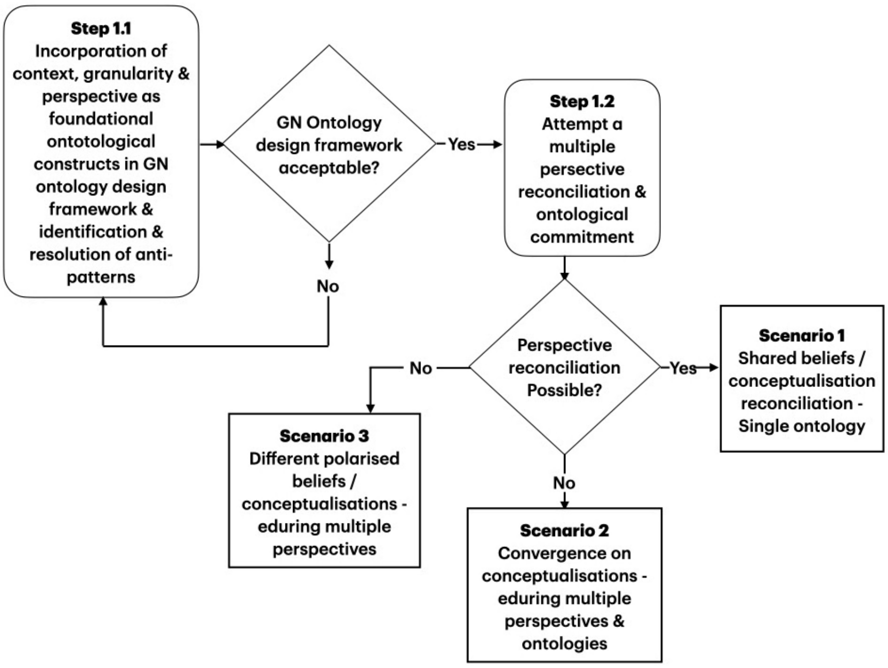


Figure 4.5: Ontology Engineering process steps and outputs

Ontological theory based on logical and philosophical principles adds to clarity and precision in abstracting complex reality [Guarino 1998; Guizzardi 2012]. A framework is provided byWand and Weber [1993] to ensure the correctness of abstraction of the structural relations between worldly entities. Our process involves the validation of the wicked problem ontological architecture using ontology engineering formalism after [Wand and Weber 1993]. For example Ontological notions such as + *R* denoting Rigidity, + *I* denoting Identity, + *O* denoting global Identity, and +*U* denoting Unity are used to bring order to semantic taxonomic relationships Welty and Guarino [2001] and avoid incorrect modeling of worldly concepts.

The formalism includes use of anti-patterns, after Sales and Guizzardi [2015] to detect and rectify incorrect relationship. Examples of such anti-patterns from figure 4.6 *A* are *Person* concept is rigid + *R*, that is, must not change, whereas *Customer* is non rigid - *R*, that is, being a customer may be transitory. This then means that we can define constraints such as that - *R* cannot subsume + *R*, that is, a non rigid concept *Customer* and *Organisation* cannot subsume a rigid concept *Person* in a taxonomic relationship. Figure 4.6 shows how the anti-patterns are resolved.

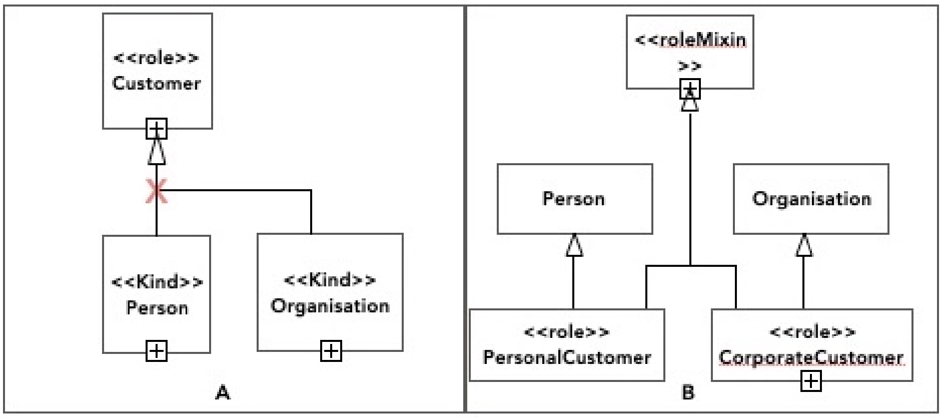


Figure 4.6: Detecting and resolving anti-patterns

Adding the Granular Niche foundational ontology concepts to the body of knowledge of ontology engineering formalisms, where each Granular Niche represents a CAS and has the following context / sub-context and granular level as explicit ontological constructs, we provide the following additional hierarchical taxonomic relationships to detect and correct anti-patterns: i) *GN*(g) denoting a base contextual granular level in a schema of granular levels, ii) *GN*(g^{+}) denoting a contextual meso granular level relative to *GN*(G), iii) *GN*(g^{++}) denoting a contextual macro granular level relative to the baseline , iv) *GN*(g^{-}) denoting a contextual micro granular level relative to *GN*(g), and finally v) *GN*(g^{--}) denoting a contextual nano granular level relative.

The following constraints apply. *GN*$(g^{++}) \neq$ *GN*(g^{+++}), which says the two Granular Niches are not equivalent (unequal granular levels) and therefore variables from within the two separate granular niches cannot interact directly, for example, see figure 4.7 where 'Drought' cannot interact directly with 'DryTree'.

The red *X* between 'Drought' and 'Tree' indicates that an anti-pattern exists between the relationships. Having a direct link between the variables violates the granular niche principle that two variables at different granular levels cannot interact directly. To resolve this anti-pattern two intermediary entities 'DryFarm' and 'SoilMoisture' are identified to normalise the relationship, see figure 4.8. Further, the hierarchical ordering is enforced by: variables in *GN*(g^{++}) cannot interact directly with variables *GN*(g^{-}), without a path through *GN*(g^{+}). The identification of 'DryFarm' and 'SoilMoisture' represents discovery of a new requisite variables in the model.

Intuitively this makes sense. By introducing the mediator variables 'DryFarm', 'SoilMoisture' we are saying that to know whether a tree is dry we get a more accurate inference by measuring soil moisture levels on the farm than from knowing whether there is a drought or not. Similarly 'irrigation' and 'tree' cannot interact directly as one does not irrigate the tree but the soil or any other medium the tree is in. This is a contextual violation, hence an anti-pattern. Anti-patterns thus facilitate knowledge discovery and innovation.

Similarly, we use temporal granularity to extend the representation of dynamic time intervals (t1...tn)

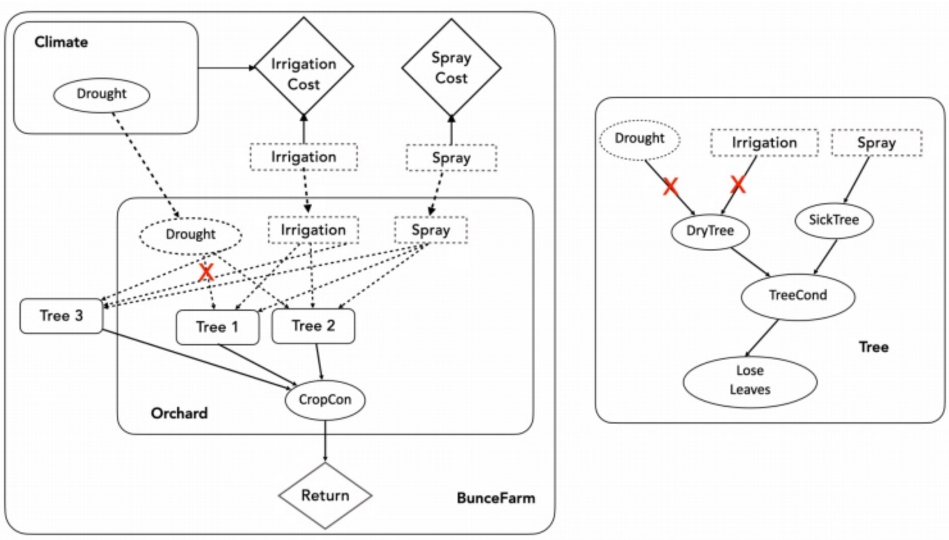


Figure 4.7: Bunce Farm Baseline Bayesian model: Detecting and resolving Anti-patterns

with $GN(t^{+})$ denoting a short term time horizon, $GN(t^{++})$, denoting a medium term time horizon, and $GN(t^{+++})$ a long term horizon. These constructs can be applied as constraints to detect anti-patterns. We can then exploit Hidden Markov Chains and the related Markovian assumption Koller and Friedman [2009] to track changes in the value of variables in Granular Niches and related probability distributions over time.

The process of anti-pattern identification and resolution is carried out iteratively, as shown in figure 4.8 until the model is acceptable. For instance an even more accurate model might introduce a granular niche 'Field' to normalise the relationships between the Granular Niches 'RegionalNiche', 'Farm' and 'Tree'.

By applying the ontological constraints detailed above we can improve on the accuracy of the Bayesian model in figure 4.7 to that of the GN Bayesian model in figure 4.8. The outcome is a well formed ontology representing a stakeholder shared conceptualisation of the structure of the CAS and type I wicked problem causal structure. In other words indeterminacy, caused by disagreement about the nature and structural causation pathways is resolved, (see section 2.3.1 for a discussion on indeterminacy).

The resolution of ontological anti-patterns primarily deals with the network causal structure associated with Type I wicked problems causal structural issues. Type II wicked problems causes associated with divergent multiple perspectives are more difficult to resolve. As a result three scenarios are possible with respect to the structure of the problem and perspectives on the inherent uncertainty surrounding the individual random variable parameters in the model, representing different perspectives (enduring beliefs), see figure 4.5.

Scenario I is where perspectives converge and the ontology is incorporated as a singular candidate GNBN model. Scenario II is where there is convergence of agreement on the wicked problem's causal structural character, but no convergence on perspectives as influenced perspectivism, finitude, and normativity [Farrell and Hooker 2013].

Scenario III represents a polarised stakeholder position where despite the logic and outcomes presented by the ontology engineering process some stakeholders choose to maintain their 'baseline' view of the world. Recent global events here come to mind, that is, entrenched positions on the non existence

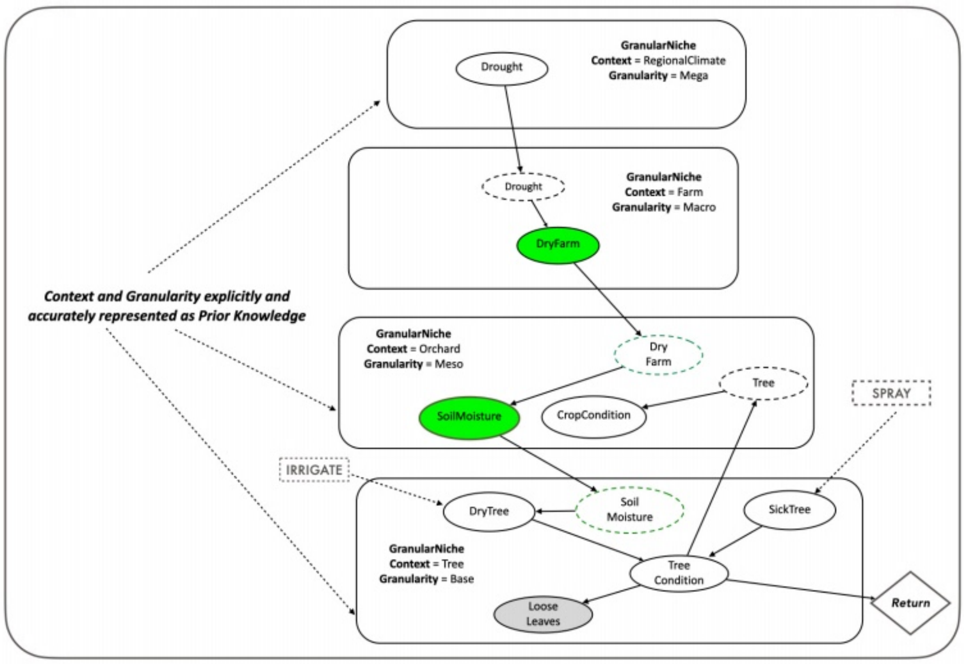


Figure 4.8: GN Bayesian candidate PGM Structure

of climate change and doubts on the efficacy of Covid19 vaccines. Farrell and Hooker [2013] argue that this is a result of finitude, that is, limited cognition and knowledge of the wicked problem by a stakeholder group. Robert *et al.* [2017] refer to a similar concept, bounded rationality, to describe limited cognition and knowledge. We discuss this in more detail in the next section. The ontology /ies designed become candidate probabilistic graphical models for structure learning in the next step.

4.5.2 Candidate Bayesian Probabilistic Bayesian Model Design

The output ontology/ies and the baseline Bayesian network model from the scenarios described in the previous section are used as inputs to design GNBN, and baseline Bayesian candidate probabilistic model structures. See figure 4.9.

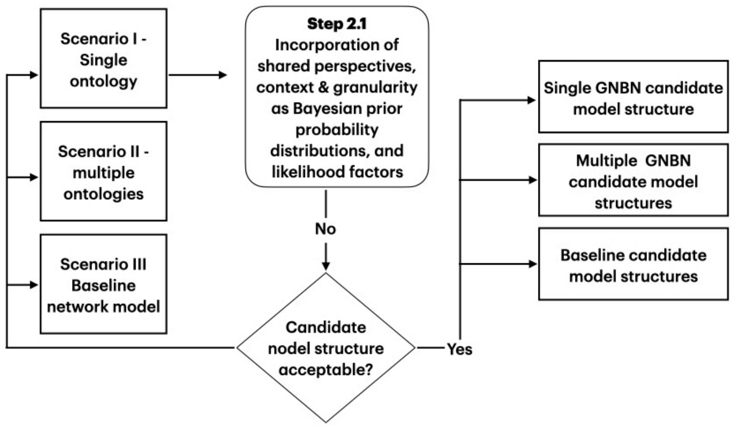


Figure 4.9: Candidate Bayesian model structures

The Bayesian mathematical notation for the candidate structure for scenarios I is shown as model 'A' in figure 4.10, while the GNBN candidate structure for scenarios II is shown as model 'B'. The Baseline Bayesian candidate structure model, representing scenario III is of the form of the normal Bayesian equation 4.1. A random Bayesian model candidate model is also included for control in experiments comparing the GN Bayesian models' performance of Baseline Bayesian models, detailed in chapter 5.

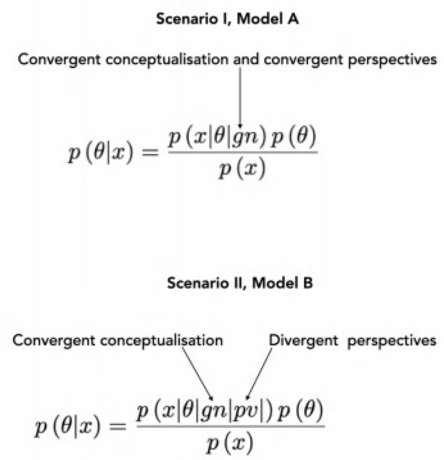


Figure 4.10: GN probabilistic Bayesian model scenarios notation

4.5.3 Pre-processing and Synthetic Ground Truth Data Generation

A candidate Ground Truth model structure obtained by adding random latent variables to the GNBN model, see figure 4.11, is used as an input into the synthetic training and validation data sets.

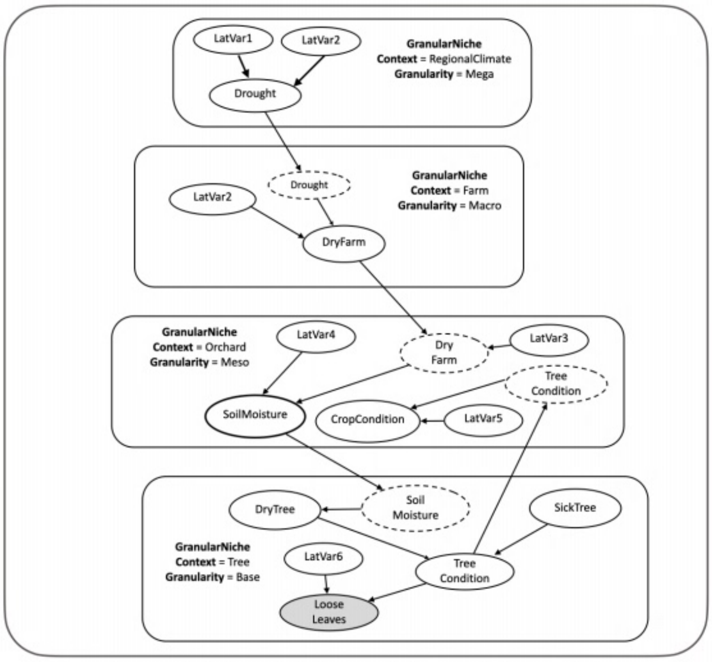


Figure 4.11: Ground Truth Structure

The sample data is generated using the Forward sampling algorithm, an algorithm used for sampling from a Bayesian network [Koller and Friedman 2009]. The sampling process involves generating random samples where:

$$\xi[1], \ldots, \xi[M] \sim \text{P(X)}.$$

The Bayesian priors used in the forward sampling are an approximation based on the knowledge of the authors of the precision farming domain. After a series of iterations 240,000 samples were deemed sufficient to represent the ground truth data. This is the number of samples at which the data produced a structure approximate to the ground truth structure.

The generated samples are split into a 70 / 30 split with 70 to be used as training data and 30 set aside as model validation data for structure learning and parameter estimation. Figures 4.12 shows the input, processes, and outputs for generating synthetic training and validation data. The python code snippet used to generate synthetic data and the splitting of sample data into training and validation data is available via a link in appendix A.

This approach is preferred to consulting experts from the relevant domain. Typically domain experts do not have the time to participate in model design. Issues of finitude, normativity, perspectivism, indeterminancy discussed in section 2.1 further compound problems of disagreements about the character of the wicked problem in a given domain.

The rationale is that the ground truth probability graphical model and its joint probability distribution used to generate synthetic data represents a good approximation of the processes that generate the

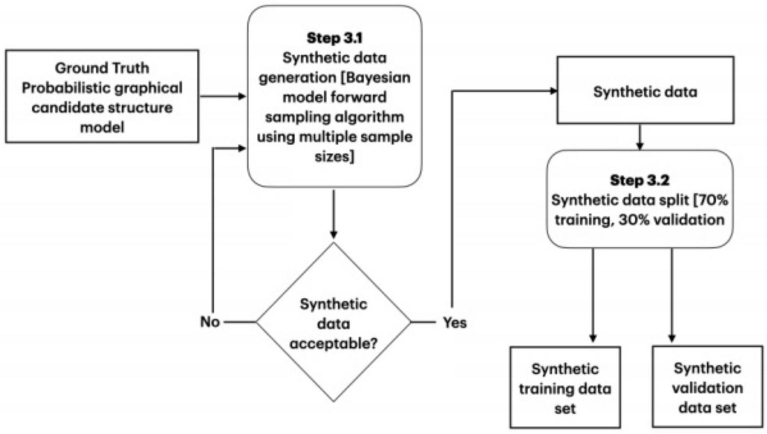


Figure 4.12: Synthetic data generation steps

data in the specific domain, see Ajoodha [2018] for a discussion. Latent variables are introduced to the candidate GNBN model to take into account unknown variables and their probability distributions.

With synthetic data we also have the liberty to explore multiple literature sources and perspectives, and incorporate these into our model. We are then able to experiment with the data generated, and may even discover additional knowledge from structure learning using heuristic machine learning techniques such as the Hill-Climbing search, and Bayesian parameter estimation.

4.5.4 Structure Learning and Parameter Estimation Model Training

Structure learning is carried out on the training data sets for the True, Baseline, GN model A, GNBN model B and random Bayesian models. The random Bayesian model is to be used later as a control model for performance comparison between the different model structures.

The greedy hill-climb search, a heuristic search is chosen for its simplicity and ability to progressively reach the largest improvement in the search score [Koller and Friedman 2009]. Applying sample size analysis Koller and Friedman [2009], multiple sample sizes are used to calibrate the models using an iterative process with the mean of 10 iterations per sample size. The accepted model structures are then used as the basis for model parameter estimation using the Bayesian Parameter estimation algorithm [Koller and Friedman 2009]. See figure 4.13 for the structure learning and parameter probability distribution estimation steps.

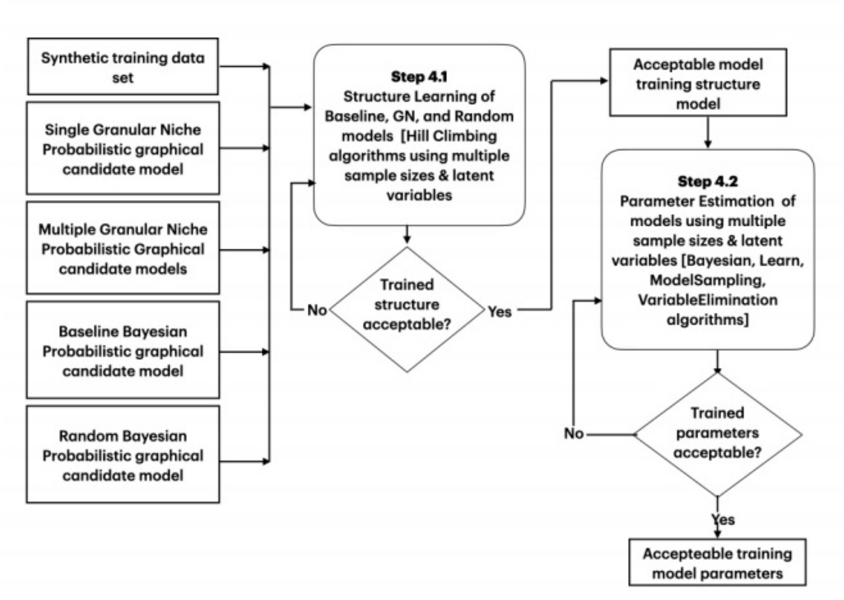


Figure 4.13: Training structure learning and parameter estimation

4.5.5 Structure Learning and Parameter Estimation Model Validation

The trained learned structure, once acceptable is used as an input into structure learning and parameter estimation using the validation data set. Structure learning and parameter estimation is then carried out iteratively to tune the structure and parameter probability distributions until acceptable. See figure 4.14.

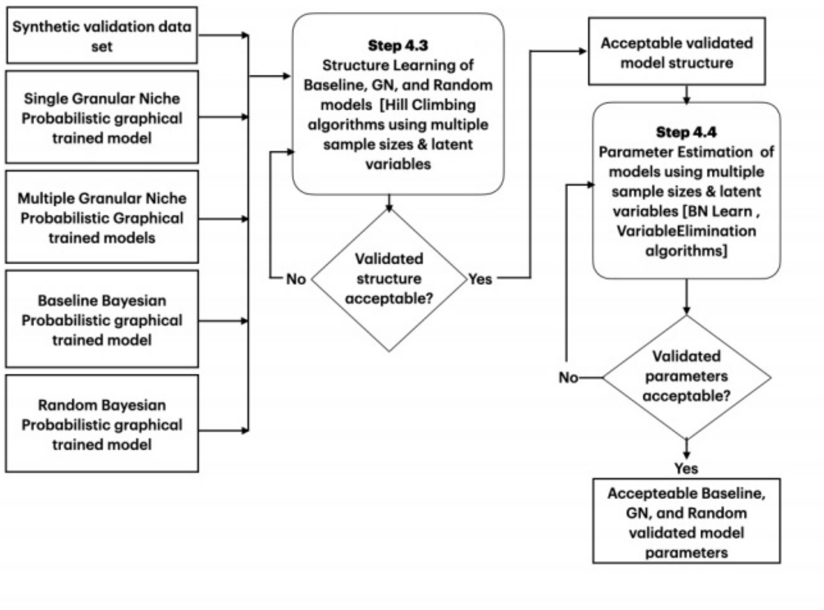


Figure 4.14: Structure learning and parameter estimation tuning and validation

The results of the performance comparison between the validated model structures learning and parameter learning processes for the GNBN, Baseline, and Random Baseline models against the Ground Truth structure and parameters are provided and discussed in the next chapter.

Chapter 5

Results and Discussion

In this chapter we provide details of the experimentation process undertaken to learn the structures and parameters of the candidate baseline and GN probabilistic models designed using the modeling framework.

5.1 Structure Learning and Model Performance Comparative Analysis

In the structure learning experiments undertaken, at 5000 samples, the learned structures from the validation data set appeared to be at their best relative to the candidate Bayesian structures provided and minimum relative entropy. We present the graphical model outputs from this experiment in figure 5.1.

Figure 5.1 depicts the learned structures from the ground truth validation data set. The learned structures depict the True model candidate structure accurately albeit with the directionality of the edges reversed between the random variables *Drought* and *LatVar2*, and between *CropCondition* and *LatVar5*. Figure 5.1 also depicts the learned structure from the ground truth validation data set using the GNBN model structure as the candidate Bayesian model. As can be seen from the image, the learned structure of the GNBN model Bayesian candidate probabilistic graphical model structure was recovered accurately albeit with the directionality of the edges reversed between the random variables *LowSoilMoisture* and *DryTree*, and between *DryFarm* and *LowSoilMoisture*.

The Baseline model structure though less accurate than the GNBN model does depict a reasonably accurate structure relative to the True model with much fewer nodes recovered and one dimentionality reversed, from *Drought* to *DryTree*. The Random model with no candidate definitive structure is used as a control Bayesian model . The learned structure of the Random model performed poorly at recovering the True model represented by the ground truth data.

The learned structures suggest that the GNBN model performs better than the Baseline and Random Bayesian models at structure learning as it provides the best approximation to the 'True' model structure Semwayo and Ajoodha [2021] from ground truth data. By observing the dimensionality of the resultant validated model nodes, the edges and direction of the edges between the nodes, see figure 5.1, we can discover latent (hidden) knowledge surfaced by the structure learning processes using the machine learning algorithms applied. A more detailed account of the knowledge discovery process is provided in section 5.2.

In the next section the performance at structure learning between the models is further evaluated using a more precise evaluation metric, the Bayesian Information Criterion (BIC) score.

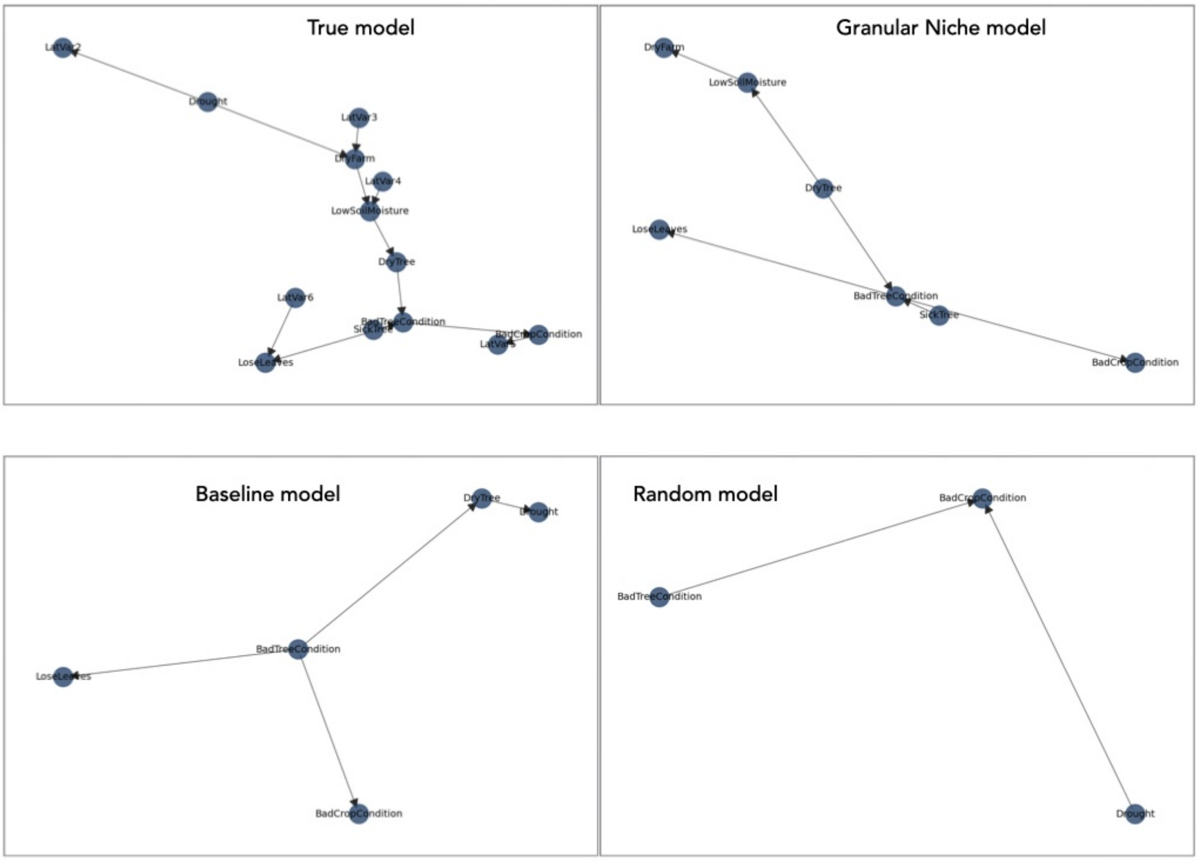


Figure 5.1: Learned structures using validation data set

5.1.1 Bayesian Information Criterion Scores

The BIC is a reliable statistical criterion used for model selection and model comparison in statistical modeling and machine learning [Drton and Plummer 2017]. See chapter 2, section 2.6.3. for a detailed discussion. The Bayesian information criterion (BIC) is used here to compare the performance of the GNBN model to that of the Baseline Bayesian, Random, and True distribution models.

Table 5.1 presents a comparative analysis of BIC scores.TD stands for True Distribution; BL stands for Baseline Bayesian Network; GN stands for the Granular Niche Bayesian Network; and RND stands for Random network. Figure 5.2 presents a plot of the BIC scores.

In comparing the models using the BIC score a model with a lower score indicates a better and preferred structure [Koller and Friedman 2009]. In table 5.1 and in figure 5.2 the GNBN model has lower BIC scores across the different sample sizes in comparison to the Baseline and Random models. This means that the GNBN model out performs the Baseline and Random models at learning the ground truth structure from synthetically generated ground truth data.

Research question 1, (See Chapter 1, sub-section 4.1), sort to answer the question on the performance of the GNBN model's probabilistic graphical model structure (PGM) relative to that of Baseline Bayesian (PGM) models at recovering the structure of complex adaptive systems from ground truth data. The foregoing results clearly show that the GNBN probabilistic graphical model performs better than the Baseline model and the Random Bayesian models at recovering the structure of complex adaptive systems from ground truth data.

Sample Size	TD Mean BIC	BL Mean BIC	GN Mean BIC	RND Mean BIC
500	-3798.0226	-1686.5140	-1962.0131	-848.8133
1000	-8112.5578	-3164.1487	-3932.4824	-1725.4863
1500	-11596.5166	-4545.9620	-5839.9927	-2640.9770
2000	-15453.4469	-5737.0663	-7945.2042	-3414.2126
2500	-19174.2895	-6894.3436	-9746.7931	-4311.4421
3000	-23018.8987	-8100.8495	-11796.7039	-5163.2694
3500	-26966.2309	-9290.5231	-13701.8399	-6054.7917
4000	-30704.1325	-10331.5588	-15629.1034	-6833.7801
4500	-34549.9188	-11687.0487	-17592.8567	-7804.3068
5000	**-38331.7205**	**-12682.8214**	**-19635.4139**	**-8652.3383**

Table 5.1: Models BIC Scores

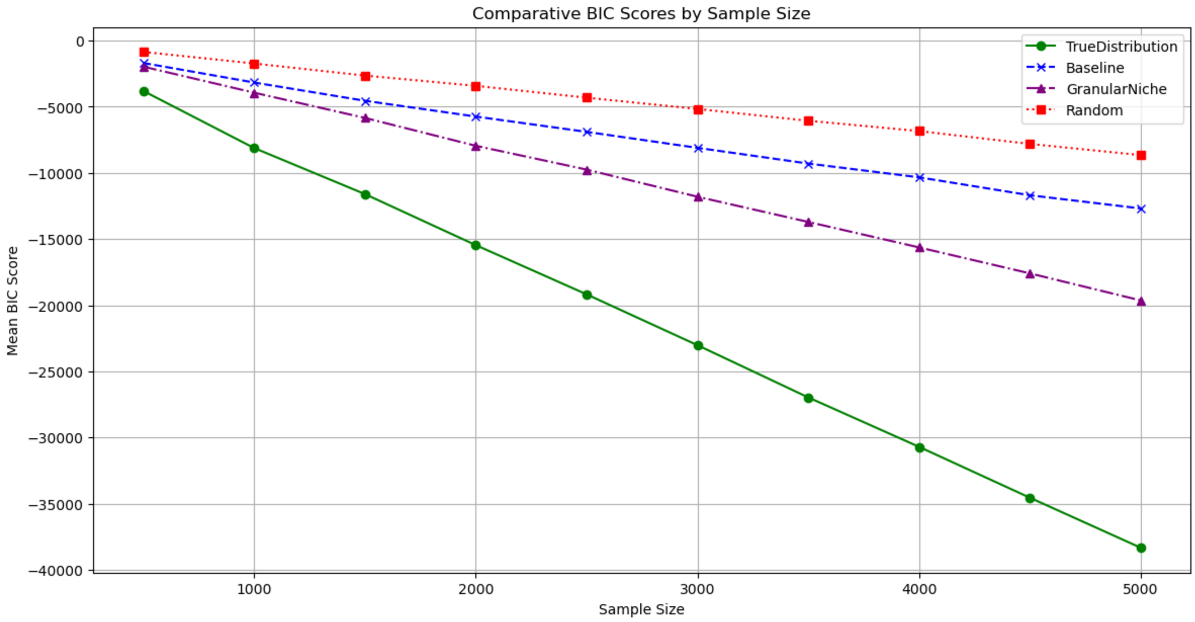


Figure 5.2: Model BIC Scores

5.2 Knowledge Discovery through Structure Learning

Figure 5.3 provides a comparison of the candidate True model and the learned True model structure from ground truth data. By examining the learned structures we can gain insights into the structure of the true model and possibly discover novel structural relationships in the data previously unknown, answering research question 3 (See Chapter 1, subsection 4.1.). Domain experts would be required to examine the learned structures to verify such new knowledge learned. This is beyond the scope of this research thesis.

This approach has been successfully applied to the discovery of relationships between genes Su *et al.* [2013] and discovery of Alzheimer biomarkers Hopkins [2008], where in examining the learned structures domain experts discovered new previously unknown relationships. We see our research efforts at designing better representation of CAS through the Granular Niches probabilistic Bayesian models adding to this body of knowledge.

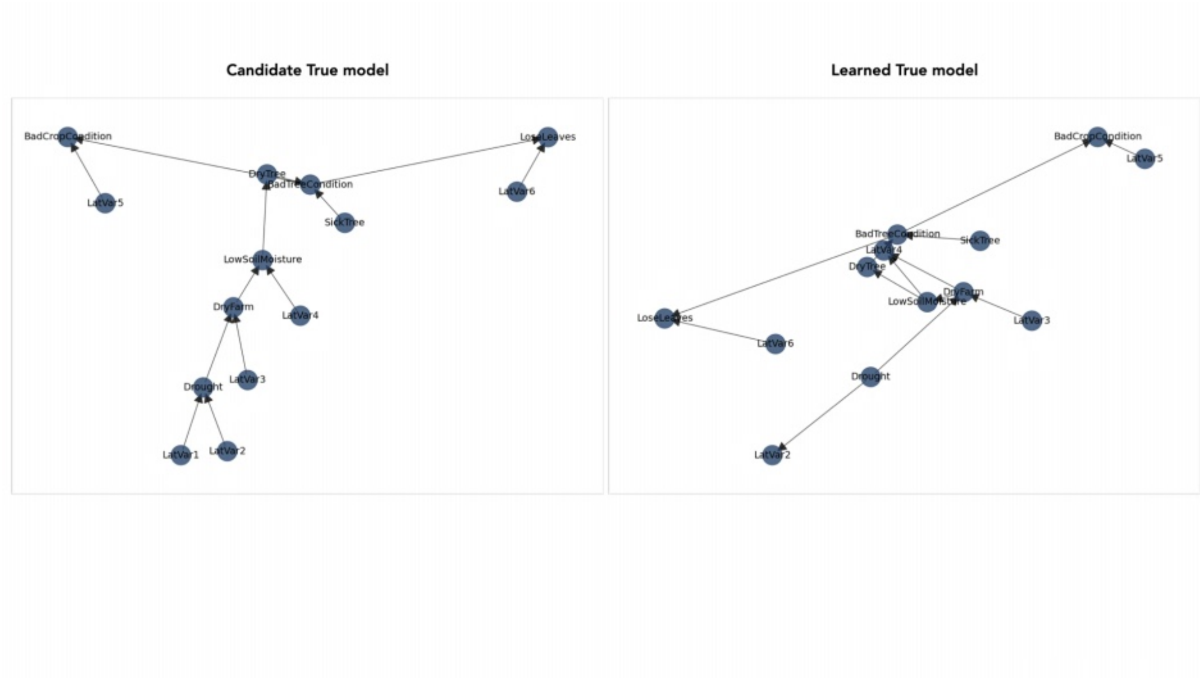


Figure 5.3: Knowledge Discovery through Structure Learning

5.3 Parameter Estimation Model Comparative Performance Analysis

The learned validated Bayesian structures are used to determine the conditional probability distributions between the nodes in the structure. We use the Kullback-Leibler (KL) divergence to compare the parameter estimation performance between the GNBN, Baseline and Random PGM models on the validation data set. See equation 2.3 section 2.6.3.

5.3.1 Bayesian Model Parameter Estimation Performance Comparison

We carry out first a comparative analysis of the GNBN model, the True, Baseline and Random PGM models. Figure 5.4 shows KL divergence plots of the different models. The GNBN model is characterised by a prior dichilect distribution with informative hyper-parameters where $\alpha = 80$ and $\beta = 20$. The Baseline candidate model is characterised by a prior dichilect distribution with non-informative hyper-parameters with $\alpha = 0.5$ and $\beta = 0.5$ and with no granularity and perspective incorporated as knowledge. The random candidate model has no hyper parameters on the prior distribution values.

As can be seen from figure 5.4 the GNBN model (abbreviated to GN in figure 5.4) performs better than the Baseline (BL) and Random (RND) Bayesian models at estimating the parameters' probability conditional distributions relative to the True (TD) model. Given that KL Divergence can be thought of as a measure of *loss* of information when one distribution is used to approximate the other, our GNBN model loses the least information in comparison to the Baseline and Random Bayesian models during the parameter estimation process. This experiment result thus provides an answer to research question 2 (see subsection 1.4).

The convergence of the graphs as the number of samples increase is an indication that as we get more data the different prior beliefs held by divergent stakeholder perspectives (as represented by Bayesian priors) have less influence on the posterior conditional distribution. In other words as we get more data the true character of the data generating processes become apparent. Prior beliefs of the nature of reality,

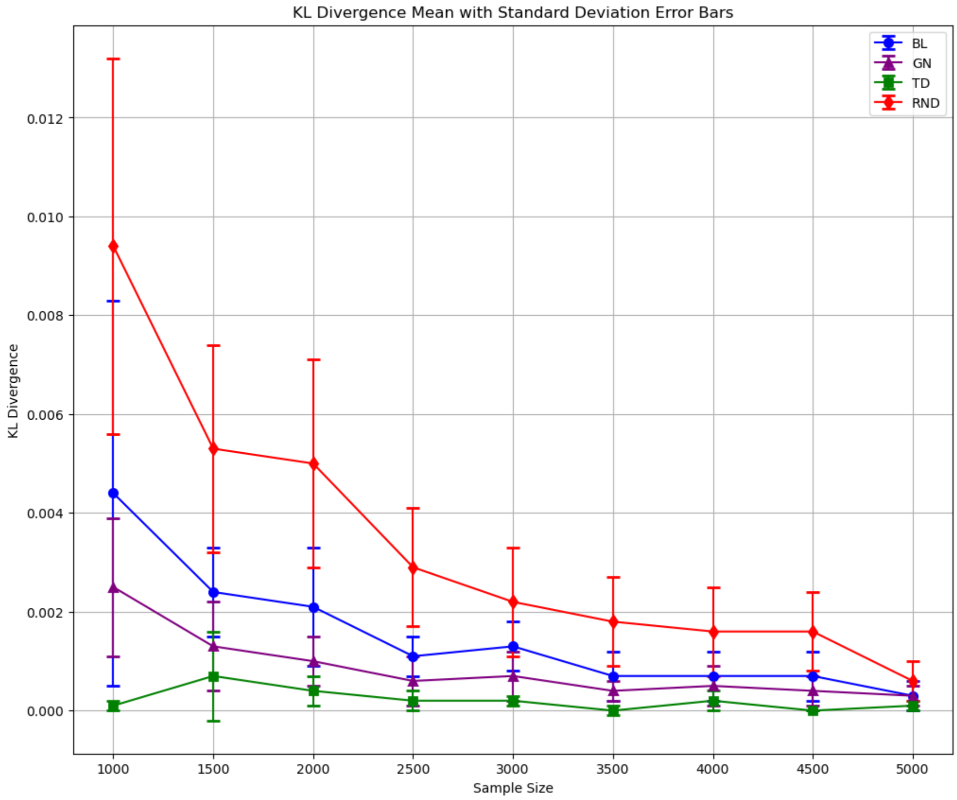


Figure 5.4: Model KL Divergence Comparison

that is, divergent stakeholder perspectives, or biases become less important with respect to the ground truth.

5.3.2 Parameter Estimation Simulation

Next we carry out a comparative analysis of scenario II where a shared conceptualisation (an ontology) of type I wicked problem causes component occurs while converge in perspective does not occur and divergence in perspective persists.

Assuming that one group of stakeholders, based on the output of the ontology engineering exercise and the ontology designed (see section 4.4.1), is very sure of the precision of their beliefs with respect to the probability distribution parameters, the hyper parameters are provided as ($\alpha = 80$ and $\beta = 20$). We refer to the model representing this perspective as *GNA*. The other group believes that based on their prior knowledge their confidence in the precision of the prior is low and settles for $\alpha = 40$ and $\beta = 60$. We refer to the Bayesian model representing this group this stakeholder group as *GNB*. We compare the performance of these 2 distributions against the ground truth using the KL divergence scores across a range of sample sizes. See figure 5.5.

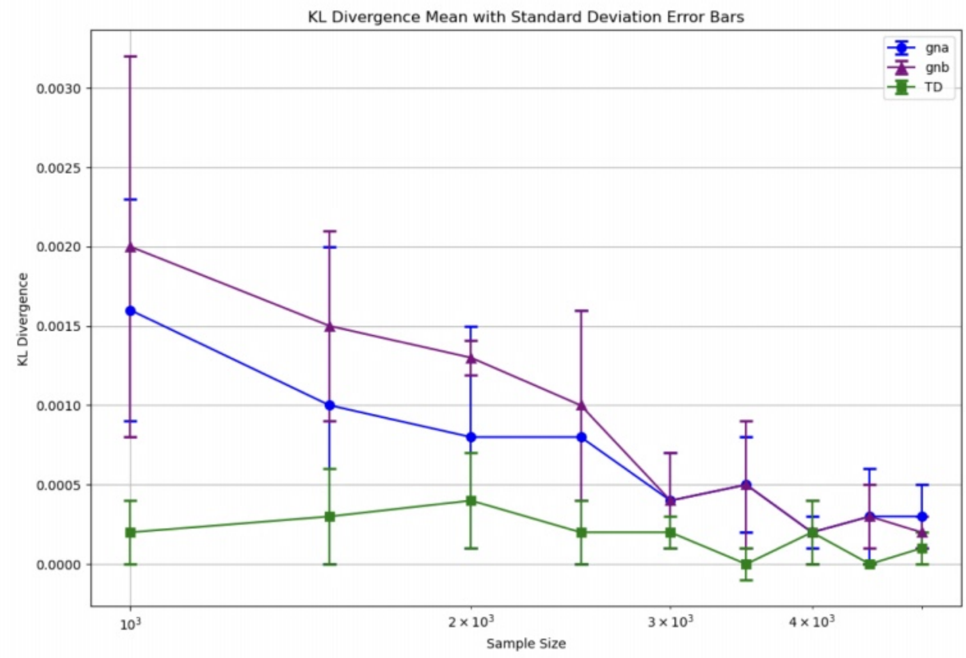


Figure 5.5: GN Models Divergent Perspectives Comparison

As can be seen from figure 5.5 model *GNA* out-performs model *GNB* across most sample sizes with respect to KL Divergence and Standard Deviation. This means that the perspective carried by stakeholder group A is more accurate and more precise with respect to the data generated by the underlying model. Note that as we get more data samples there is convergence in the KL divergence between the models as the posterior distribution of all models approximates the true distribution.

While not originally intended as an area of research to answer research question 3, the insights in parameter estimation simulation sub-section above represents knowledge discovery in that by simulation experiments on different perspectives, knowledge on the perspective closer to the truth is discovered.

5.4 Discussion and Conclusion

We provide a discussion of the research findings and draw conclusions with respect to the research purpose, objective, and research questions.

5.4.1 Discussion

This thesis started by making a bold statement, quoting Gharajedaghi [2011], that "we see an increasingly complex and chaotic world simply because use inadequate and in appropriate tools to explain it". We have shown in this research thesis that by incorporating complex adaptive concepts as constructs in an integrated ontology engineering, an explainable Bayesian network AI model, and machine algorithms we are able to provide adequate and appropriate tools to better understand, reason about, and carry out tractable computations about complexity and chaos in polynomial time.

This research thesis has provided an ontology engineering driven Bayesian modeling framework for complex adaptive systems. Our modeling framework and resultant GNBN model is able to handle features of complexity like emergence which confound clear understanding of complexity using deductive reasoning.

Through the ontology engineering component of the modelling framework a modeling framework to support semantic inter-operation required to better understand the character of wicked problems, given divergent multiple stakeholder perspectives is provided. Further, the ontology engineering process surfaces novel random variables required to adequately represent complex adaptive systems in an ontological model, thus supports knowledge discovery.

Using synthetically generated data from a sound ontological CAS True model as ground truth data, the Bayesian Information Criterion (BIC) and KL divergence metrics are used as model performance metrics for structure learning and parameter estimation parameters respectively.

A comparative analysis of the performance of the GNBN model at structure learning and estimating parameters from synthetic ground truth data against baseline hierarchical Bayesian and random Bayesian models shows that the GNBN model out-performs baseline Bayesian and random models. This is because the GNBN model incorporates constructs that faithfully represent complex adaptive systems' internal interactions and system emergence , missing in the two other models.

A further comparative analysis of the performance of two GNBN models representing agreement on the CAS structure but with no reconciliation of perspectives is carried out. One of the models, model *GNA* perspective performed better than model *GNB* at parameter estimation. Thus it has been demonstrated that we can, through simulation, compare the plausibility of two divergent perspectives of a given wicked problem with respect to accuracy and precision against a ground truth distribution. We have further illustrated how new knowledge can be discovered through the ontology engineering and Bayesian structure learning processes of the GNBN modelling framework.

5.4.2 Conclusion

The thesis set out to answer the following broad principal question; "*How does the proposed novel Granular Niche Bayesian Network model incorporating complexity concepts: context, granularity, and perspective, as foundational ontological modelling constructs, perform in comparison to baseline Bayesian models at recovering the structure and estimating the parameters of complex adaptive systems from ground truth data?* "

Research question 1 was set out as follows: "*How does the proposed novel GNBN model, incorporating ontological CAS concepts as constructs, perform in comparison to baseline Bayesian Network models at recovering the structure of complex adaptive systems from ground truth data?*" The research objective here was to compare the performance of the novel GNBN to baseline models at recovering the structure of complex adaptive systems from ground truth data. We have shown, using recovered structure images and BIC scores that the GNBN model out-performs baseline Bayesian models at recovering the structure of complex adaptive systems.

Research question 2 was set out as follows: " *How does the proposed novel GNBN model compare to baseline Bayesian models at approximating the true probability distribution of CAS model parameters from ground truth data?*" The research objective was to explore and compare, using synthetically generated ground truth data, how the designed novel GNBN model performs in comparison to baseline Bayesian models at minimising the relative entropy with the ground truth distribution.

We have, using the KL divergence measure, shown that the proposed novel GNBN model out-performs baseline Bayesian models at minimising the relative entropy with the ground truth distribution when estimating parameter distributions from synthetic data and candidate structures, using Hill Climbing and Bayesian Learning algorithms.

The working hypothesis of this thesis is that the GNBN model produced by our GNBN modeling framework out-performs Baseline probabilistic bayesian models at complex adaptive systems structure learning, parameter estimation, and knowledge discovery of the structure and nature of wicked problems. The null hypothesis is that the GNBN models produced by our modeling framework does not perform better than Baseline probabilistic model at Bayesian structure learning, parameter learning, and knowledge discovery in support of wicked problems resolution.

From the foregoing it is clear that the research thesis has proven that the working hypothesis of this thesis that the GNBN model produced by our modeling framework out-performs baseline probabilistic Bayesian models at complex adaptive systems structure learning and parameter estimation, and knowledge discovery support for wicked problems. The null hypothesis has thus been rejected.

5.4.3 Research Limitations

This thesis has used synthetically generated data by applying the forward sampling algorithm on the trained and validated underlying true model structure and estimated parameters, to prove that, the GNBN model produced by our modeling framework out-performs baseline probabilistic Bayesian models at complex adaptive systems structure learning, parameter estimation, and knowledge discovery, to support wicked problems resolution. While these findings provide proof of concept, this represents a limitation in that the model has not been tested on real world data.

5.5 Significance of the Study

This research thesis makes several inter-disciplinary contributions. By incorporating complexity systems theory concepts, namely: context, granularity and perspective, as explicit foundational ontological constructs in a Bayesian model and machine learning algorithms, we have provided a common ontological lexicon that unifies divergent naming conventions and describing the world we observe, to more accurately describe and communicate what we perceive, and surface our flawed assumptions about reality. This results in improved accuracy and precision for Bayesian models representing CASs, where accuracy is measured through the $\bar{x}$ and precision is measured the σ.

We have through Granular Niches as CAS Modeling constructs provided a way to manage the exponential model variables dimensionality explosion and inherent computational intractability that comes with increasing natural and engineered complexity. We have thus provided a Bayesian modeling framework to handle dimensionality and support the tractable, cost effective analysis of the character of complex adaptive systems and emergent wicked problems.

The research results further provide, using explainable artificial intelligence Bayesian modeling and machine learning tools, a framework to represent and explore complexity, and compare option solutions available, through simulation, to resolve wicked problems given divergent perspectives of the problem.

We have contributed to the broad framework for an advanced inference engine provided in Pearl [2009], see figure 1.3 by adding to the scope of inferences that can be made to CAS through the incorporation of granular contextual perspectives as modelling constructs.

5.6 Future Research

We have argued that wicked problems are as much a product of the innate complexity of the problem itself as it is about stakeholder perspective and semantic heterogeneity. We have shown how complexity concepts can be incorporated as constructs in a combined Ontology Engineering and Bayesian modeling framework to design more accurate and more precise domain ontology driven Bayesian models than existing baseline models, for applications in modeling CAS to support the resolution of wicked problems.

Future research will focus on comparing the performance of our modelling framework and generated Bayesian models using real world wicked problems and data. The motivation is to further explore how the GNBN modeling framework can be used to enhance domain knowledge discovery.

We also envisage future research in potential application areas for GN probabilistic Bayesian models such as Internet of things (IoT), autonomous driver-less cars, and bio-informatics, where context and granularity constructs are key in facilitating the exchange of accurate and precise information across dynamic contextual environments (CAS) at various levels of granularity.

.1 Appendix A

The Python code for this research thesis is available via the following GitHub repository link:

https://github.com/2292902/Research-files/blob/main/README.md

Bibliography

[Abuazab *et al.* 2017] Alaa Aldeen Ismail Abuazab, Harihodin Bin Selamat, Rasimah Bt Che Mohd Yusoff, and Ahmed N Abdalla. Ontology-driven bayesian network model for semantic expression. *DEStech Transactions on Computer Science and Engineering*, (cmee), 2017.

[Agterberg 2021] Frits Agterberg. Induction, deduction, and abduction. In *Encyclopedia of mathematical geosciences*, pages 1–12. Springer, 2021.

[Ajoodha and Rosman 2018] Ritesh Ajoodha and Benjamin Rosman. Learning the influence structure between partially observed stochastic processes using iot sensor data. In *Workshops at the Thirty-Second AAAI Conference on Artificial Intelligence*, 2018.

[Ajoodha 2018] Ritesh Ajoodha. *Influence modelling and learning between dynamic bayesian networks using score-based structure learning*. PhD thesis, 2018.

[Akers 2015] Walter Lee Akers. An approach for the development of complex systems archetypes. 2015.

[Alford and Head 2017] John Alford and Brian W Head. Wicked and less wicked problems: a typology and a contingency framework. *Policy and society*, 36(3):397–413, 2017.

[Alti *et al.* 2013] Adel Alti, Abbdellah Boukerram, and Philippe Roose. Ontology and tool support for quality service management. *Journal of Systems and Information Technology*, 15(1):4–23, 2013.

[Auld *et al.* 2021] Graeme Auld, Steven Bernstein, Benjamin Cashore, and Kelly Levin. Managing pandemics as super wicked problems: lessons from, and for, covid-19 and the climate crisis. *Policy sciences*, 54:707–728, 2021.

[Baas and Emmeche 1997] Nils Andreas Baas and Claus Emmeche. On emergence and explanation. *Intellectica*, 25(2):67–83, 1997.

[Ball 2004] Philip Ball. *Critical mass: How one thing leads to another*. Macmillan, 2004.

[Bar-Yam 2000] Yaneer Bar-Yam. *Complexity rising: From human beings to human civilization, a complexity profile*, 2000.

[Benjamin-Fink and Reilly 2017] Nicole Benjamin-Fink and Brian K Reilly. A road map for developing and applying object-oriented bayesian networks to “wicked” problems. *Ecological Modelling*, 360:27–44, 2017.

[Blackwell and Ajoodha 2022] Darren Blackwell and Ritesh Ajoodha. A bayesian approach to understanding the influence of traffic congestion given the road structure. In *Proceedings of Sixth International Congress on Information and Communication Technology: ICICT 2021, London, Volume 4*, pages 271–279. Springer, 2022.

[Blei *et al.* 2017] David M Blei, Alp Kucukelbir, and Jon D McAuliffe. Variational inference: A review for statisticians. *Journal of the American statistical Association*, 112(518):859–877, 2017.

[Borg *et al.* 2014] Audun Borg, Henrik Bjelland, and Ove Njå. Reflections on bayesian network models for road tunnel safety design: A case study from norway. *Tunnelling and underground space technology*, 43:300–314, 2014.

[Borgo and others 2019] Ontology Makes Sense S Borgo et al. Taking it to the next level: Nicola guarino, formal ontology and conceptual modeling. *Ontology Makes Sense: Essays in honor of Nicola Guarino*, 316:223, 2019.

[Bousquet and Curtis 2011] Antoine Bousquet and Simon Curtis. Beyond models and metaphors: complexity theory, systems thinking and international relations. *Cambridge review of international affairs*, 24(01):43–62, 2011.

[Brown *et al.* 2010] Valerie A Brown, John Alfred Harris, and Jacqueline Y Russell. *Tackling wicked problems through the transdisciplinary imagination*. Earthscan, 2010.

[Brzica 2023] Daneš Brzica. Urban transformation: environmental issues, wicked problems, and transport development in the context of circular economy. *European Journal of Social Impact and Circular Economy*, 4(1):19–26, 2023.

[Buhrmester *et al.* 2021] Vanessa Buhrmester, David Münch, and Michael Arens. Analysis of explainers of black box deep neural networks for computer vision: A survey. *Machine Learning and Knowledge Extraction*, 3(4):966–989, 2021.

[Burke and Bykov 2012] Edmund K Burke and Yuri Bykov. The late acceptance hill-climbing heuristic. *University of Stirling, Tech. Rep*, 2012.

[Burks-Copes and Kiker 2014] Kelly A Burks-Copes and Gregory A Kiker. Uncovering lines of evidence hidden in complex problems: using conceptual models to inform ecosystem-based management of the missouri river cottonwoods. *Environment Systems and Decisions*, 34(3):425–442, 2014.

[Burman *et al.* 2017] CJ Burman, MA Aphane, and NM Mollel. The taming wicked problems framework: Reflections in the making. *Journal for New Generation Sciences*, 15(1):51–73, 2017.

[Cano *et al.* 2020] Andrés Cano, Manuel Gómez-Olmedo, and Serafín Moral. Learning sets of bayesian networks. In *International Conference on Information Processing and Management of Uncertainty in Knowledge-Based Systems*, pages 151–164. Springer, 2020.

[Chee *et al.* 2016] Yung En Chee, Lauchlin Wilkinson, Ann E Nicholson, Pedro F Quintana-Ascencio, John E Fauth, Dianne Hall, Kimberli J Ponzio, and Libby Rumpff. Modelling spatial and temporal changes with gis and spatial and dynamic bayesian networks. *Environmental Modelling & Software*, 82:108–120, 2016.

[Chickering *et al.* 1994] David M Chickering, Dan Geiger, David Heckerman, et al. *Learning Bayesian networks is NP-hard*. Technical report, Citeseer, 1994.

[Clemens 2023] Marshall Clemens. *Characteristcs of Complex Systems Kernel Description*, 2023.

[Costa *et al.* 2006] Paulo CG Costa, Kathryn B Laskey, and Ghazi AlGhamdi. Bayesian ontologies in ai systems. 2006.

[Crowley and Head 2017] Kate Crowley and Brian W Head. The enduring challenge of 'wicked problems': revisiting rittel and webber. *Policy Sciences*, 50(4):539–547, 2017.

[Darwiche 2009] Adnan Darwiche. *Modeling and reasoning with Bayesian networks*. Cambridge university press, 2009.

[Davies *et al.* 2015] Kathryn K Davies, Karen T Fisher, Mark E Dickson, Simon F Thrush, and Richard Le Heron. Improving ecosystem service frameworks to address wicked problems. *Ecology and Society*, 20(2), 2015.

[de Waal *et al.* 2016] Alta de Waal, Hildegarde Koen, Pieter de Villiers, Henk Roodt, Nyalleng Moorosi, and Gregor Pavlin. Construction and evaluation of bayesian networks with expert-defined latent variables. In *2016 19th International Conference on Information Fusion (FUSION)*, pages 774–781. IEEE, 2016.

[Descartes and Cress 1998] René Descartes and Donald A Cress. *Discourse on method*. Hackett Publishing, 1998.

[Drton and Plummer 2017] Mathias Drton and Martyn Plummer. A bayesian information criterion for singular models. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 79(2):323–380, 2017.

[Eidelson 1997] Roy J Eidelson. Complex adaptive systems in the behavioral and social sciences. *Review of general psychology*, 1(1):42–71, 1997.

[Elia and Margherita 2018] Gianluca Elia and Alessandro Margherita. Can we solve wicked problems? a conceptual framework and a collective intelligence system to support problem analysis and solution design for complex social issues. *Technological Forecasting and Social Change*, 133:279–286, 2018.

[Farrell and Hooker 2013] Robert Farrell and Cliff Hooker. Design, science and wicked problems. *Design studies*, 34(6):681–705, 2013.

[Faruqui *et al.* 2021] Syed Hasib Akhter Faruqui, Adel Alaeddini, Jing Wang, Carlos A Jaramillo, and Mary Jo Pugh. A functional model for structure learning and parameter estimation in continuous time bayesian network: An application in identifying patterns of multiple chronic conditions. *IEEE Access*, 9:148076–148089, 2021.

[Fenz 2012] Stefan Fenz. An ontology-based approach for constructing bayesian networks. *Data & Knowledge Engineering*, 73:73–88, 2012.

[Fleck 2024] Leonard M Fleck. Precision medicine and rough justice: Wicked problems. *Cambridge Quarterly of Healthcare Ethics*, 33(1):1–4, 2024.

[Frei *et al.* 2007] Regina Frei, José Barata, and G Serugendo. A complexity theory approach to evolvable production systems. In *Proceedings of 3rd International Workshop on Multi-Agent Robotic Systems in conjunction with ICINCO*, pages 44–53, 2007.

[Fromm 2005] Jochen Fromm. Types and forms of emergence. *arXiv preprint nlin/0506028*, 2005.

[Gangemi *et al.* 2001] Aldo Gangemi, Nicola Guarino, Claudio Masolo, and Alessandro Oltramari. Understanding top-level ontological distinctions. *OIS@ IJCAI*, 47, 2001.

[Gharajedaghi 2011] Jamshid Gharajedaghi. *Systems thinking: Managing chaos and complexity: A platform for designing business architecture*. Elsevier, 2011.

[Gignoux *et al.* 2017] Jacques Gignoux, Guillaume Chérel, Ian D Davies, Shayne R Flint, and Eric Lateltin. Emergence and complex systems: The contribution of dynamic graph theory. *Ecological Complexity*, 31:34–49, 2017.

[Gioia and Pitre 1990] Dennis A Gioia and Evelyn Pitre. Multiparadigm perspectives on theory building. *Academy of management review*, 15(4):584–602, 1990.

[Gleick 1998] James Gleick. *Chaos: The amazing science of the unpredictable*. Vintage, 1998.

[Guarino and Welty 2000] Nicola Guarino and Christopher Welty. Ontological analysis of taxonomic relationships. In *International Conference on Conceptual Modeling*, pages 210–224. Springer, 2000.

[Guarino and Welty 2004] Nicola Guarino and Christopher A Welty. An overview of ontoclean. In *Handbook on ontologies*, pages 151–171. Springer, 2004.

[Guarino 1998] Nicola Guarino. *Formal ontology in information systems: Proceedings of the first international conference (FOIS'98), June 6-8, Trento, Italy*, volume 46. IOS press, 1998.

[Guizzardi *et al.* 2010] Giancarlo Guizzardi, Fernanda Baião, Mauro Lopes, and Ricardo Falbo. The role of foundational ontologies for domain ontology engineering: An industrial case study in the domain of oil and gas exploration and production. *International Journal of Information System Modeling and Design (IJISMD)*, 1(2):1–22, 2010.

[Guizzardi *et al.* 2015] Giancarlo Guizzardi, Gerd Wagner, João Paulo Andrade Almeida, and Renata SS Guizzardi. Towards ontological foundations for conceptual modeling: The unified foundational ontology (ufo) story. *Applied ontology*, 10(3-4):259–271, 2015.

[Guizzardi 2005] Giancarlo Guizzardi. Ontological foundations for structural conceptual models. 2005.

[Guizzardi 2007] Giancarlo Guizzardi. On ontology, ontologies, conceptualizations, modeling languages, and (meta) models. *Frontiers in artificial intelligence and applications*, 155:18, 2007.

[Guizzardi 2012] Giancarlo Guizzardi. Ontological foundations for conceptual modeling with applications. In *International Conference on Advanced Information Systems Engineering*, pages 695–696. Springer, 2012.

[Gyftodimos and Flach 2002] Elias Gyftodimos and Peter A Flach. Hierarchical bayesian networks: A probabilistic reasoning model for structured domains. In *Proceedings of the ICML-2002 Workshop on Development of Representations*, pages 23–30. Citeseer, 2002.

[Helsper and Van Der Gaag 2002] Eveline M Helsper and Linda C Van Der Gaag. Building bayesian networks through ontologies. In *ECAI*, volume 2002, page 15th, 2002.

[Hevner *et al.* 2004] Alan R Hevner, Salvatore T March, Jinsoo Park, and Sudha Ram. Design science in information systems research. *MIS quarterly*, pages 75–105, 2004.

[Hevner *et al.* 2008] Alan R Hevner, Salvatore T March, Jinsoo Park, and Sudha Ram. Design science in information systems research. *Management Information Systems Quarterly*, 28(1):6, 2008.

[Hietanen *et al.* 2011] Olli Hietanen, David Lefutso, Mario A Marais, Neeshal Munga, Barend Taute, Mphathi Nyewe, and Thembinkosi Daniel Semwayo. How to create national foresight culture and capacity: case study south africa. 2011.

[Hirschheim and Klein 1989] Rudy Hirschheim and Heinz K Klein. Four paradigms of information systems development. *Communications of the ACM*, 32(10):1199–1216, 1989.

[Hoffmann 2020] Michael HG Hoffmann. Reflective consensus building on wicked problems with the reflect! platform. *Science and Engineering Ethics*, 26(2):793–819, 2020.

[Holland 2006] John H Holland. Studying complex adaptive systems. *Journal of systems science and complexity*, 19:1–8, 2006.

[Hopkins 2008] Andrew L Hopkins. Network pharmacology: the next paradigm in drug discovery. *Nature chemical biology*, 4(11):682–690, 2008.

[Illari *et al.* 2011] Phyllis Illari, Lorenzo Casini, Federica Russo, and Jon Williamson. Models for prediction, explanation and control: Recursive bayesian nets. *THEORIA*, 2011.

[Jansen 2008] Ludger Jansen. Categories: The top-level ontology. *Applied ontology: An introduction*, pages 173–196, 2008.

[Jensen and Aven 2018] Anders Jensen and Terje Aven. A new definition of complexity in a risk analysis setting. *Reliability Engineering & System Safety*, 171:169–173, 2018.

[Kaku 2012] Michio Kaku. *Physics of the future: How science will shape human destiny and our daily lives by the year 2100*. Anchor, 2012.

[Kauffman 1993] Stuart A Kauffman. *The origins of order: Self-organization and selection in evolution*. Oxford University Press, USA, 1993.

[Ketter *et al.* 2015] Wolfgang Ketter, Markus Peters, John Collins, and Alok Gupta. Competitive benchmarking: an is research approach to address wicked problems with big data and analytics. *MIS quarterly*, 2015.

[Klein *et al.* 2006] Mark Klein, Hiroki Sayama, Peyman Faratin, and Yaneer Bar-Yam. The dynamics of collaborative design: Insights from complex systems and negotiation research. In *Complex Engineered Systems*, pages 158–174. Springer, 2006.

[Ko and Sim 2008] Kwang-Eun Ko and Kwee-Bo Sim. Development of context aware system based on bayesian network driven context reasoning method and ontology context modeling. In *2008 International Conference on Control, Automation and Systems*, pages 2309–2313. IEEE, 2008.

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

[Koller and Pfeffer 1997] Daphne Koller and Avi Pfeffer. Representations and solutions for game-theoretic problems. *Artificial intelligence*, 94(1-2):167–215, 1997.

[Korb and Nicholson 2010] Kevin B Korb and Ann E Nicholson. *Bayesian artificial intelligence*. CRC press, 2010.

[Levin *et al.* 2012] Kelly Levin, Benjamin Cashore, Steven Bernstein, and Graeme Auld. Overcoming the tragedy of super wicked problems: constraining our future selves to ameliorate global climate change. *Policy sciences*, 45(2):123–152, 2012.

[Lich *et al.* 2017] Kristen Hassmiller Lich, Jennifer Brown Urban, Leah Frerichs, and Gaurav Dave. Extending systems thinking in planning and evaluation using group concept mapping and system dynamics to tackle complex problems. *Evaluation and program planning*, 60:254–264, 2017.

[Lönngren and Van Poeck 2021] Johanna Lönngren and Katrien Van Poeck. Wicked problems: A mapping review of the literature. *International Journal of Sustainable Development & World Ecology*, 28(6):481–502, 2021.

[Manson 2001] Steven M Manson. Simplifying complexity: a review of complexity theory. *Geoforum*, 32(3):405–414, 2001.

[Marcot and Penman 2019] Bruce G Marcot and Trent D Penman. Advances in bayesian network modelling: Integration of modelling technologies. *Environmental modelling & software*, 111:386–393, 2019.

[Marcot 2012] Bruce G Marcot. Metrics for evaluating performance and uncertainty of bayesian network models. *Ecological modelling*, 230:50–62, 2012.

[Marcot 2017] Bruce G Marcot. Common quandaries and their practical solutions in bayesian network modeling. *Ecological Modelling*, 358:1–9, 2017.

[Martin *et al.* 2021] Osvaldo A Martin, Ravin Kumar, and Junpeng Lao. *Bayesian modeling and computation in python*. CRC Press, 2021.

[Medianovskyi and Pietarinen 2022] Kyrylo Medianovskyi and Ahti-Veikko Pietarinen. On explainable ai and abductive inference. *Philosophies*, 7(2):35, 2022.

[Mittal and Risco-Martín 2017] Saurabh Mittal and José L Risco-Martín. Simulation-based complex adaptive systems. In *Guide to Simulation-Based Disciplines*, pages 127–150. Springer, 2017.

[Montiel *et al.* 2019] Oscar Montiel, Yoshio Rubio, Cynthia Olvera, and Ajelet Rivera. Quantum-inspired acromyrmex evolutionary algorithm. *Scientific reports*, 9(1):12181, 2019.

[Mouenis *et al.* 2014] Anouar Tadlaoui Mouenis, Khaldi Mohamed, and Aammou Souhaib. Towards probabilistic ontology based on bayesian networks. 2014.

[Munn and Smith 2013] Katherine Munn and Barry Smith. *Applied ontology: An introduction*, volume 9. Walter de Gruyter, 2013.

[Murphy and Russell 2002] Kevin Patrick Murphy and Stuart Russell. Dynamic bayesian networks: representation, inference and learning. 2002.

[Nasim and Khan 2018] Zarmeen Nasim and Imran Khan. Solving poverty using ontology. In *KEOD*, pages 269–276, 2018.

[Oates 2005] Briony J Oates. *Researching information systems and computing*. Sage, 2005.

[Onik *et al.* 2017] Mohammad Fakhrul Alam Onik, Erwin Fielt, and Guy G Gable. Complex adaptive systems theory in information systems research: A systematic literature review. In *Proceedings of the 21st Pacific Asia Conference on Information Systems (PACIS 2017)*, pages Paper–271, 2017.

[Pai *et al.* 2017] Fang-Ping Pai, Lee-Jang Yang, and Yeh-Ching Chung. Multi-layer ontology based information fusion for situation awareness. *Applied Intelligence*, 46(2):285–307, 2017.

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

[Pearl 2011] Judea Pearl. Bayesian networks. 2011.

[Pearl 2019] Judea Pearl. The seven tools of causal inference, with reflections on machine learning. *Communications of the ACM*, 62(3):54–60, 2019.

[Peters 2017] B Guy Peters. What is so wicked about wicked problems? a conceptual analysis and a research program. *Policy and Society*, 36(3):385–396, 2017.

[Petitjean *et al.* 2018] François Petitjean, Wray Buntine, Geoffrey I Webb, and Nayyar Zaidi. Accurate parameter estimation for bayesian network classifiers using hierarchical dirichlet processes. *Machine Learning*, 107(8-10):1303–1331, 2018.

[Phillips and Ritala 2019] Mark A Phillips and Paavo Ritala. A complex adaptive systems agenda for ecosystem research methodology. *Technological Forecasting and Social Change*, 148:119739, 2019.

[Pilcher and Cortazzi 2024] Nick Pilcher and Martin Cortazzi. 'qualitative'and'quantitative'methods and approaches across subject fields: implications for research values, assumptions, and practices. *Quality & Quantity: International Journal of Methodology*, 58(3):2357–2387, 2024.

[Pitchforth 2015] Jegar Oliver Pitchforth. *Bayesian networks for information synthesis in complex systems*. PhD thesis, Queensland University of Technology, 2015.

[Pollino *et al.* 2007] Carmel A Pollino, Owen Woodberry, Ann Nicholson, Kevin Korb, and Barry T Hart. Parameterisation and evaluation of a bayesian network for use in an ecological risk assessment. *Environmental Modelling & Software*, 22(8):1140–1152, 2007.

[Potgieter and others 2005] Anna Elizabeth Gezina Potgieter et al. *The engineering of emergence in complex adaptive systems*. PhD thesis, University of Pretoria, 2005.

[Potgieter *et al.* 2005] Anet Potgieter, Kurt April, and Judith Bishop. Complex adaptive enterprises. In *Encyclopedia of Information Science and Technology, First Edition*, pages 475–480. IGI Global, 2005.

[Raimbault 2017] Juste Raimbault. An applied knowledge framework to study complex systems. *arXiv preprint arXiv:1706.09244*, 2017.

[Randle and Stroink 2018] Jason M Randle and Mirella L Stroink. The development and initial validation of the paradigm of systems thinking. *Systems Research and Behavioral Science*, 35(6):645–657, 2018.

[Rittel and Webber 1973] Horst WJ Rittel and Melvin M Webber. Dilemmas in a general theory of planning. *Policy sciences*, 4(2):155–169, 1973.

[Robert *et al.* 2017] Verónica Robert, Gabriel Yoguel, and Octavio Lerena. The ontology of complexity and the neo-schumpeterian evolutionary theory of economic change. *Journal of Evolutionary Economics*, 27(4):761–793, 2017.

[Rocca 2019] Rocca. *Bayesian inference problem, MCMC and variational inference*. https://towardsdatascience.com/bayesian-inference-problem-mcmc-and-variational-inference-25a8aa9bce29, 2019.

[Ruhl and Salzman 2020] JB Ruhl and James Salzman. Introduction: Governing wicked problems. *Vanderbilt Law Review*, 73:1561, 2020.

[Sales and Guizzardi 2015] Tiago Prince Sales and Giancarlo Guizzardi. Ontological anti-patterns: Empirically uncovered error-prone structures in ontology-driven conceptual models. *Data & Knowledge Engineering*, 99:72–104, 2015.

[Santos 2015] Gil C Santos. Upward and downward causation from a relational-horizontal ontological perspective. *Axiomathes*, 25(1):23–40, 2015.

[Sardana *et al.* 2023] Nitish Sardana, Sahar Shekoohi, Elyse M Cornett, and Alan David Kaye. Qualitative and quantitative research methods. In *Substance use and addiction research*, pages 65–69. Elsevier, 2023.

[Semwayo and Ajoodha 2021] Daniel T Semwayo and Ritesh Ajoodha. A causal bayesian network model for resolving complex wicked problems. In *2021 IEEE International IOT, Electronics and Mechatronics Conference (IEMTRONICS)*, pages 1–8. IEEE, 2021.

[Semwayo and Berman 2004] Daniel T Semwayo and Sonia Berman. Representing ecological niches in a conceptual model. In *International Conference on Conceptual Modeling*, pages 31–42. Springer, 2004.

[Senge 2006] Peter M Senge. The fifth discipline: The art and practice of the learning organization (rev. ed.). *New York, NY: Currency Doubleday*, 2006.

[Sherif *et al.* 2015] Fayroz F Sherif, Nourhan Zayed, and Mahmoud Fakhr. Discovering alzheimer genetic biomarkers using bayesian networks. *Advances in bioinformatics*, 2015, 2015.

[Simon 1996] HA Simon. *The architecture of complexity. Reprinted in his The Sciences of the Artificial*, 1996.

[Simperl and Tempich 2006] Elena Paslaru Bontas Simperl and Christoph Tempich. Ontology engineering: a reality check. In *OTM Confederated International Conferences" On the Move to Meaningful Internet Systems"*, pages 836–854. Springer, 2006.

[Smith and Klagges 2008] Barry Smith and Bert Klagges. Philosophy and biomedical information systems. 2008.

[Smith and Mark 1998] Barry Smith and David M Mark. Ontology and geographic kinds. 1998.

[Spear *et al.* 2016] Andrew D Spear, Werner Ceusters, and Barry Smith. Functions in basic formal ontology. *Applied Ontology*, 11(2):103–128, 2016.

[Srihari 2014] Sargur N Srihari. *Probabilistic Graphical Models.*, 2014.

[Studer *et al.* 1998] Rudi Studer, V Richard Benjamins, and Dieter Fensel. Knowledge engineering: principles and methods. *Data & knowledge engineering*, 25(1-2):161–197, 1998.

[Su *et al.* 2013] Chengwei Su, Angeline Andrew, Margaret R Karagas, and Mark E Borsuk. Using bayesian networks to discover relations between genes, environment, and disease. *BioData mining*, 6(1):1–21, 2013.

[Suoheimo *et al.* 2021] Mari Suoheimo, Tang Tang, and Tarja Juvonen. A visual tool for understanding wicked problems in design research: A case study of marginalized youth unemployment. *The Design Journal*, 24(6):955–976, 2021.

[Thuan *et al.* 2019] Nguyen Hoang Thuan, Andreas Drechsler, and Pedro Antunes. Construction of design science research questions. *Communications of the Association for Information Systems*, 44(1):20, 2019.

[Tolk *et al.* 2018] Andreas Tolk, Matthew TK Koehler, and Michael D Norman. Epistemological constraints when evaluating ontological emergence with computational complex adaptive systems. In *Unifying Themes in Complex Systems IX: Proceedings of the Ninth International Conference on Complex Systems 9*, pages 1–10. Springer, 2018.

[Turnbull *et al.* 2018] Laura Turnbull, Marc-Thorsten Hütt, Andreas A Ioannides, Stuart Kininmonth, Ronald Poeppl, Klement Tockner, Louise J Bracken, Saskia Keesstra, Lichan Liu, Rens Masselink, et al. Connectivity and complex systems: learning from a multi-disciplinary perspective. *Applied network science*, 3(1):11, 2018.

[Uschold 2015] Michael Uschold. Ontology and database schema: What's the difference? *Applied Ontology*, 10(3-4):243–258, 2015.

[Vaishnavi and Kuechler 2015] Vijay K Vaishnavi and William Kuechler. *Design science research methods and patterns: innovating information and communication technology*. Crc Press, 2015.

[Vaishnavi *et al.* 2004] Vijay Vaishnavi, William Kuechler, and Stacie Petter. Design science research in information systems. *January*, 20:2004, 2004.

[Venable *et al.* 2012] John Venable, Jan Pries-Heje, and Richard Baskerville. A comprehensive framework for evaluation in design science research. In *International Conference on Design Science Research in Information Systems*, pages 423–438. Springer, 2012.

[Venable 2006] John Venable. The role of theory and theorising in design science research. In *Proceedings of the 1st International Conference on Design Science in Information Systems and Technology (DESRIST 2006)*, pages 1–18. Citeseer, 2006.

[Wand and Weber 1993] Yair Wand and Ron Weber. On the ontological expressiveness of information systems analysis and design grammars. *Information Systems Journal*, 3(4):217–237, 1993.

[Weber *et al.* 2012] Philippe Weber, Gabriela Medina-Oliva, Christophe Simon, and Benoît Iung. Overview on bayesian networks applications for dependability, risk analysis and maintenance areas. *Engineering Applications of Artificial Intelligence*, 25(4):671–682, 2012.

[Welty and Guarino 2001] Christopher Welty and Nicola Guarino. Supporting ontological analysis of taxonomic relationships. *Data & Knowledge Engineering*, 39(1):51–74, 2001.

[Whyte and Thompson 2012] Kyle Powys Whyte and Paul B Thompson. Ideas for how to take wicked problems seriously. *Journal of Agricultural and Environmental Ethics*, 25:441–445, 2012.

[Wimsatt 1994] William C Wimsatt. The ontology of complex systems: levels of organization, perspectives, and causal thickets. *Canadian Journal of Philosophy*, 24(sup1):207–274, 1994.

[Xiang *et al.* 2003] Tao Xiang, Shaogang Gong, and Dennis Parkinson. On the structure of dynamic bayesian networks for complex scene modelling. In *Proc. Joint IEEE International Workshop on Visual Surveillance and Performance Evaluation of Tracking and Surveillance (VS-PETS)*, pages 17–22, 2003.

[Xiang 2013] Wei-Ning Xiang. Working with wicked problems in socio-ecological systems: Awareness, acceptance, and adaptation. *Landscape and Urban Planning*, (110):1–4, 2013.

[Zellner and Campbell 2015] Moira Zellner and Scott D Campbell. Planning for deep-rooted problems: What can we learn from aligning complex systems and wicked problems? *Planning Theory & Practice*, 16(4):457–478, 2015.

[Zhang *et al.* 2022] Liwei Zhang, Dayou Liu, Zheng Wang, and Xinlu Wang. Bayesian network structure learning and application. *Mobile Information Systems*, 2022, 2022.