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Qualitative chain graphs and their application

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ABSTRACT

For many problem domains, such as medicine, chain graphs are more attractive than Bayesian networks as they support representing interactions between variables that have no natural direction. In particular, interactions between variables that result from certain feedback mechanisms can be represented by chain graphs. Using qualitative abstractions of probabilistic interactions is also of interest, as these allow focusing on patterns in the interactions rather than on the numerical detail. Such patterns are often known by experts and sufficient for making decisions. So far, qualitative abstractions of probabilistic interactions have only been developed for Bayesian networks in the form of qualitative probabilistic networks. In this paper, such qualitative abstractions are developed for chain graphs with the practical aim of using qualitative knowledge as constraints on the hyperspace of probability distributions. The usefulness of qualitative chain graphs is explored for modelling and reasoning about the interactions between diseases.

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1. Introduction

Probabilistic graphical models (PGMs) have been shown to be convenient and intuitive formalisms to capture the probabilistic independence information in many application fields. In a PGM, random variables are modelled as vertices connected by edges in a graph. These connections reflect the probabilistic dependences and independences between variables and one can associate a probability distribution to the graph that is faithful in some way to the dependences and independences. Popular PGMs include models based on undirected graphs (UGs), i.e., *Markov networks*, and based on directed acyclic graphs (DAGs), i.e., *Bayesian networks* [1]. However, both undirected and directed graphs have certain undesirable limitations when representing independence information for an actual problem domain. Hybrid graphs, containing both directed and undirected edges, such as *chain graphs*, offer an elegant generalisation of both Markov and Bayesian networks [2].

A chain graph (CG) uses potentials rather than straight probabilities to represent the probability distribution of variables and is, therefore, often seen as a blackbox model. Nevertheless, chain graphs have been shown to model equilibrium systems [3], which occur in many areas including biology, physics, chemistry, and economics. In fact, it was shown that particular sets of conditional independence statements, which cannot be modelled by a Bayesian network, can indeed be modelled with a chain graph; the ideal gas law and the price and demand model in economics are examples [4].

On the other hand, Bayesian networks have the advantage that both structure and parameters can be assessed from either expert knowledge, data, or both, which renders Bayesian networks whitebox rather than blackbox models. For the more expressive chain graphs, it is much more difficult to exploit human knowledge in assessing their parameters, and, as a consequence, these models do not share all the advantages of Bayesian networks as whitebox models. One of the aims of

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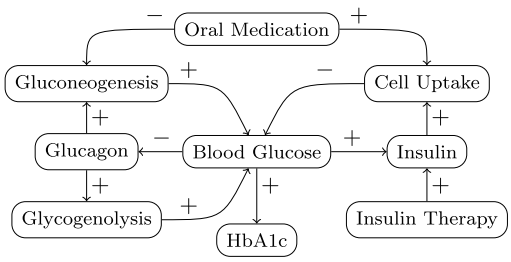

Fig. 1. Single disease modelling – a graphical representation of physiological processes involved in blood glucose regulation.

the research described in this paper is to come up with ways to move chain graphs closer to whitebox models, in particular by the use of qualitative probabilistic abstractions.

Probabilistic information is available in different forms, ranging from numerical, quantitative probabilistic values (possibly with a confidence interval) to qualitative information. Qualitative abstractions of Bayesian networks, called *qualitative probabilistic networks* (QPNs) [5], offer a useful method for exploiting qualitative constraints in assessing probabilistic information. Qualitative information in QPNs may consist of qualitative influences and synergies, and independence information. While it is well known that QPN theory has its limitation when it comes to qualitative reasoning – the main reason why QPN theory is not used in actual systems – qualitative knowledge may be quite useful when looked at as offering constraints that should be taken into account when estimating a probability distribution. Some algorithms have been proposed in the past to derive bounds [6] and qualitative influences [7] in the presence of both quantitative and qualitative knowledge, with applications in e.g. computer vision [8]. Furthermore, it has been proposed to derive marginal probability distributions in the presence of such hybrid knowledge [9]. If exact probabilistic information is not required, then such distributions, also called second-order distributions,[1] provide insight into the domain and could, e.g., be used to make decisions.

In the next section, we will first argue why chain graphs provide a good starting point for modelling feedback mechanisms. Here we explore three realistic examples drawn from the medical field. The needed theoretical basis underlying the work presented in this paper is provided in Section 3. In Section 4, we extend the known QPN theory towards chain graphs, which we call *qualitative chain graphs* (QCGs). In particular, we will formally discuss qualitative relationships, compare these to the relationships in QPNs, and prove their most important properties. In Section 5, we show that sign propagation, a qualitative variant of belief propagation, can be amended to qualitative chain graphs. In Section 6, we also demonstrate their usefulness in semi-qualitative reasoning and present experimental results supporting this claim. Although examples were drawn from the field of medicine, which offers a rich source of qualitative modelling, the results will be of value to many other domains. The work is rounded off by conclusions and plans for future research in Section 7.

2. Motivation from the medical field

Many regulatory mechanisms within the human body, described by its physiology, can be seen as causal feedback systems, in which some kind of equilibrium setpoint – called *homoeostasis* – is maintained. Diseases can be conceived as a derangement of one or more regulatory mechanisms and treatments typically interact with these systems in non-trivial ways. In non-healthy people the equilibrium setpoint typically differs from the healthy people, but therapeutic interventions can reset the equilibrium setpoint to a state that is closer to that of the healthy people.

Example 1 concerns a simplified model of the blood glucose level regulation, showing how different agents, natural and pharmacological, have their role in maintaining the blood sugar homoeostasis. The representation here is often found in medical textbooks. A plus-sign typically represents stimulation of a process, and a minus-sign typically represents inhibition.

Example 1. Blood sugar levels are regulated by negative feedback systems in order to keep the body in homoeostasis. High blood glucose levels stimulate the secretion of insulin by the pancreas, inducing glucose uptake in peripheral tissue. High blood glucose levels inhibit the secretion of glucagon by the pancreas, thereby also inhibiting glycogenolysis and gluconeogenesis, which both elevate blood sugar levels. Fig. 1 shows a graphical representation of the blood glucose regulation, as typically used in medical textbooks. Glycated hemoglobin (HbA1c) is a marker of average blood glucose levels over the previous months, and thus provides a valid measurement of the blood glucose equilibrium. In diabetics, elevated glucose levels are caused by either an impaired insulin production (type I), or an insulin resistance of peripheral cells (type II). Possible solutions to re-establish a healthy equilibrium are insulin therapy or oral medication.

The disturbance of the equilibrium of one physiological process might also alter the equilibrium setpoints of other regulatory systems, which might in turn induce new pathophysiology that deteriorates the patient's prognosis even further. In the interest of the physician, it is important to know the qualitative dynamics of such interactions, e.g., whether it is

[1] In this context, a second-order distribution yields a distribution over all possible probability distributions that obey a set of qualitative constraints.

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