Chapter 7

Conclusions and Future Work

Let us return again to the "Domain-Knowledge Grand Challenge" [STN+20], first introduced in Chapter 1 as follows:

> "ML and AI are generally domain-agnostic... Off-the-shelf practice treats [each of these] datasets in the same way and ignores domain knowledge that extends far beyond the raw data itself—such as physical laws, available forward simulations, and established invariances and symmetries—that is readily available... Improving our ability to systematically incorporate diverse forms of domain knowledge can impact every aspect of AI . . . "

This dissertation has been about addressing the challenge of inclusion of complex symbolic domain-knowledge into some kinds of deep neural networks to analyse relational data. The domain-knowledge in all cases "extends the data" used by the deep neural networks, either by non-uniform sampling of relational features; or by inclusion of relational information in a simplified form; or by inclusion of all the relational information through the use of techniques developed in Inductive Logic Programming (ILP). In all cases, we find empirical evidence supporting the principal conjecture investigated in the dissertation, namely:

- Inclusion of domain-knowledge can significantly improve the performance of a deep neural network.

Here we reiterate the main contributions and findings, and then sketch a broad outline of future research directions.

7.1 Summary of the Dissertation

7.1.1 The Main Contributions

The principal contributions made in this dissertation are as follows:

Concepts. Hide-and-seek sampling for relational features; a simplified technique for treating domain-relations as hyperedges for inclusion in graph-based neural networks (GNNs); a general technique for the inclusion of relational domain-knowledge into GNNs through the use of mode-directed inverse entailment;

Implementations. Techniques that combine neural networks and symbolic representations resulting in Deep Relational Machines (DRMs), Vertex-Enriched Graph Neural Networks (VEGNNs), Bottom-Graph Neural Networks (BotGNNs); and a modular end-to-end neuro-symbolic system for generation of novel molecules for drug-design; and

Applications. Large-scale empirical testing, using nearly 75 datasets in the broad area of drug discovery and with domain-knowledge containing nearly 100 relations and over 200,000 relational data instances; and large-scale generation of molecules outside the space of compounds in known chemical databases.

7.1.2 The Main Findings

Some of the findings obtained during the course of these contributions are as follows:

DRMs. DRMs equipped with hide-and-seek sampling of relational features are simple, yet powerful. The predictive performance of a DRM increases with increase in number of relational features. However, constructing a reasonably powerful predictive model with DRM can be computationally expensive, often requiring a large number of logically expressive relational features.

VEGNNs. VEGNNs learn effectively using domain-relations represented as hyperedges. However, the vertex-enrichment technique results in loss of domain information, that is, enriched vertex labels do not convey information such as a vertex is a member of two different hyperedges of the same type. Therefore, this technique results simplified inclusion of domain-knowledge into GNNs.

BotGNNs. BotGNN is a general technique for complete inclusion of relational information into GNNs. BotGNNs are better than BCP-based MLPs. DRMs with hide-and-seek sampling can perform better than BotGNNs, but only with significant computational effort (several 1000s of input features, which can require sampling and evaluating many more features). BotGNNs are better than VEGNNs in terms of predictive performance and the amount of domain-information they can include into a GNN. BotGNNs appear to be at least as good as optimised ILP and probably better if no parameter optimisation is performed for the ILP engine (as is often the case in practice).

Novel Molecule Generation. A molecule generation system that has two deep generative models and a BotGNN acting as discriminator is found to benefit from the inclusion of symbolic domain-knowledge. The system is able to generate a diverse set of molecules, with novel scaffolds that can act as inhibitors for a well-studied target protein.

7.2 Challenges and Future Work

It is possible to consider representing domain-knowledge not as logical or numeric constraints, but through statements in natural language. Recent rapid progress in the area of language models, for example, the models based on attention [VSP+17, BMR+20] raises the possibility of incorporating domain-knowledge through conversations. While precision of these formal representations may continue to be needed for the purpose of construction of deep models with domain-knowledge, the flexibility of natural language may be especially useful in communicating commonsense knowledge to day-to-day machine assistants that need an informal knowledge of the world [TVdM18, ZKK+21]. Progress in this is being made (see, for example, https://allenai.org/aristo), but there is much more that needs to be done to make the language models required accessible to everyday machinery.

In this dissertation, we have not been concerned with how the domain-knowledge to be acquired from domain experts. Instead, our focus has been on the methods of their inclusion into DNNs. The work has further been restricted to inclusion by changing the input data. As we described in Chapter 2, domain-knowledge can also be about the loss function, the structure or parameters of the deep neural network. How any of these forms of domain-knowledge are to be acquired remains an important question to be addressed.

As this dissertation is being written, the field of deep neural networks is proceeding at a rapid pace. We have developed principled ways in which domain-knowledge can be included in just two kinds of neural networks, albeit with wide applicability (MLPs and GNNs). Do these same techniques apply to other kinds of DNNs and will the results be similarly positive? This remains to be studied.

The empirical results in the dissertation are all from molecular datasets, which we have used as classic representatives of relational data. However there are clearly many other problems where data are much more diverse in their relational structure; and where the tasks may not be "object-centred", but may involve relations between multiple relational objects (link-prediction tasks are an example). BotGNNs are not restricted to object-centred relations, since the graph it constructs is a representation of relations that hold between any number of objects. The power of BotGNNs as a deep neural-symbolic network has thus not been fully explored by the experimental work here.

Finally, we note that this dissertation has been focussed entirely on using domain-knowledge to improve the predictive performance of a deep neural network. Developing a mapping of internal representations of the deep-network's model to concepts provided as domain-concepts will be necessary for acceptable explanations for the model's predictions. One route for developing trust in the model comes through understanding of how decisions are made by the model, and what are the determining factors in these decisions. An important requirement of machine-models in workflows with humans-in-the-loop is that the models are human-understandable. Domain-knowledge can be used in two different ways to assist this. First, it can constrain the kinds of models that are deemed understandable. Secondly, it can provide concepts that are meaningful for use in a model. The role of domain-knowledge in constructing explanations for deep neural network models has not been addressed in this dissertation. However, the development of explanatory deep neural network models that identify true causal connections based on concepts provided as domain-knowledge remains an open question.

7.3 Closing Remarks

The overarching position in this dissertation is "Domain-Knowledge Matters". This position apparently runs against a school of machine-learning that takes the view that all necessary concepts can be discovered automatically from low-level data. However, this is not a true reflection of our position. It is indeed important for a machine-learning approach to be able to discover new concepts, especially if it is used as a part of an autonomous agent. However, for the use of machine-learning systems as tools for decision-support, our position is that it is inefficient, and altogether unfair, not to provide a machine-learning system all the information that may be relevant to the construction of good models. In this dissertation we have sought to develop concepts and implementations that allow us to explore this position more fully by combining the expressiveness of logical forms domain-knowledge with the predictive power of deep neural networks. We hope the results obtained provide encouragement to the development of neural-symbolic machine-learning for prediction and explanation.