An Integrated Application of Inductive Learning Techniques in Intelligent Design Support Systems

Ming Xi Tang

Engineering Design Centre, Department of Engineering
University of Cambridge
Trumpington Street, Cambridge CB2 1PZ, UK

1. Introduction

Knowledge-based design systems stress the explicit use of design knowledge throughout the design process by the members of a design team. Without a learning capability, however, such systems are unable to reflect the designers' growing experience in the field and designers' ability to abstract useful knowledge from past design examples and other sources of information. The importance of Machine Learning in design has been widely recognised [Bratko 1993]. Persidis and Duffy argued that learning is *inextricably* linked to design and Machine Learning should become an integral part of research into intelligent CAD systems.

Many design systems contain components of learning. In the Edinburgh Designer System, for example, newly generated knowledge is transferred from the dynamic knowledge base (in the form of design description document) to the design knowledge base [Smithers *et al* 1993]. BRIDGER is a system that synthesises designs from initial design specifications using existing design examples [Reich 1993]. In prototype-based design systems, the creation of a design prototype is seen essentially as a learning task that generates conceptual knowledge in terms of functional, structural and behavioural properties of design components. In knowledge-based functional design, Brown and Spillane described an experimental evaluation of some design knowledge compilation mechanisms using constraint inheritance [Brown *et al* 1991]. Stroulia, Shankar and Goel used structure-behaviour-function models that capture a designer's comprehension of the way a device works in terms of causal explanations of how its structure results in its behaviours [Stroulia et al 1992]. Arciszewski, Mustafa, and Zoarko [Arciszewski *et al* 1987] used a supervised inductive learning method to differentiate between feasible and unfeasible designs. In case-based design systems, case-based reasoning is used for the automatic search and retrieval of past design cases to suit new requirements [Maher *et al* 1994].

Inductive learning methods are suitable for acquiring and structuring data in a way that facilitates efficient synthesis. Their potential in a knowledge-based design system as an integrated learning component is, however, yet to be fully explored. There is still limited understanding of the role of learning in design. Learning and designing as intelligent behaviour has not been effectively formalised either in theory or in computational form. In AI-based design research two fundamental problems about computational learning and design need to be addressed within an integrated computational environment:

1. How to utilise inductive learning techniques to support conceptual design tasks; and

2. How to capture design product as well as design process information within a knowledge-based design support system architecture.

This paper presents an approach to the development of intelligent design support system that incorporate inductive learning techniques. In particular this approach integrates heuristic design knowledge with inductive learning techniques to support design synthesis tasks in the early stage of the design process. This approach is demonstrated through the integration of a design concept learning system within a knowledge-based design support system architecture and two case studies.

3. The Development of a Design Concept Learning System

Traditional clustering analysis methods are suitable for classifying categories of data for which there is no prior knowledge [Fisher 1991]. These methods, however, impose a structure on the data set which may not necessarily be desirable for design purposes. The idea of concept formation is to use domain specific knowledge to restrict the output of cluster analysis to only those that are desirable. This idea is therefore particular relevant to early stage design the task of which is to derive the conceptual structure of a design problem from raw data or past design examples [Reich 1993]. However most current concept formation systems use simple attribute-value based representations, and few of them can deal with the kind of complex structural representations which are inherent in engineering design tasks. On the other hand, in AI in design community, few attempt has been made in utilising inductive learning techniques as part of an integrated design support system architecture.

In a knowledge-based design support system, learning and designing activities need to be supported in an integrated way in order for the system to demonstrate a level of learning behaviour that can be compared with experienced human designers. In such a system, the learning process should provide a suitable data structure for design exploration purposes whilst the results of the design exploration and the knowledge captured in the process should be transformed into something that can help future learning. In this context, a learning sub-system within a knowledge-based design support system needs to be developed for conceptual design tasks.

A design concept learning system has been developed by the author as an attempt to address the issue of integrating inductive learning techniques into a knowledge-based design support system architecture. This design concept learning system has been implemented using an object-oriented representation within a Lisp-based environment called GoldWorks III.

The design concept learning system adopts a unsupervised inductive learning approach and it integrates both non-incremental and incremental learning strategies to support the task in the early stage of the design process. It deals with both simple data structures (in the case where all the object instances have single value slots) and complex data structures (in the case where instances are linked to each other). The result of the learning process is a hierarchically structured design concept tree in which each node has a concept description associated with a subset of instances, as well as a performance evaluation score indicating the quality of that concept description. Nodes higher in the hierarchy represent more general (or more abstract) concepts. The learning process can be graphically displayed as the design concept tree is being built.

This design concept learning system is intended as a learning component within a knowledge-based design system architecture. Three different learning strategies have been implemented: 1) a non-incremental approach; 2) an incremental and divisive approach; and 3) a heuristic-based approach.

The first strategy adopts an improved agglomerative algorithm to cluster design examples into a design concept tree. In this approach, attributes of examples can be selected by the user for the system to generate clusters, each of which can be classified further using another set of selected attributes, thus forming the so-called nested clusters reflecting designer's views similar to the multi-perspective approach developed by Duffy and Kerr [Duffy *et al* 1993]. This strategy is suitable for organising data or past designs into a hierarchical or nested structure.

The second strategy builds a design concept tree in an incremental and divisive manner so that examples can be added to or deleted from the design concept tree, allowing the designers to observe the influence of particular examples to the features represented by the design concept tree. This strategy is necessary because of the incremental nature of the conceptual design process. Compared with the first strategy, this one cannot generate nested structures, but it allows examples to be processed incrementally.

The third (heuristic-based) approach uses design heuristic knowledge as background knowledge to sort design examples through a pre-defined or user specified conceptual structure. In this approach, the levels of concept represented by the design concept tree is influenced using the domain concepts and their relations already held in the system as *background knowledge*, thus providing a way for assessing the relevance of a set of design examples to an existing design concept already known to the system or a design concept suggested by a designer. Whilst the first two strategies are purely data driven, the third strategy is both data driven and knowledge driven. It is therefore more flexible in terms of integrating domain knowledge into the learning process.

3. Integration and Applications

The design concept learning system was first developed in the domain of small molecule drug design, in which a key task is to derive a structured description called *pharmacophore* from a set of known molecules in a knowledge base whose features are considered by the drug designers to be similar to that of the drug being designed. This paharmacophore is then used as a basis for designing a new molecule that has improved feature over those molecules that have been used to derive the pharmacophore [Smithers *et al* 1993]. A newly designed molecule can also be added to the knowledge base for future design. This process effectively keeps the knowledge base of molecules growing. In this domain design heuristics as background knowledge are used to build a design concept tree that is consistent with the concepts already known in the domain, but with features that are unique with the example molecules used [Tang 1995].

Figure 1 illustrates the inductive learning setting for this task in which feature patterns derived from the original example molecules and background knowledge about the relationships between various domain concepts are used as the input to the design concept learning system. In this application several approaches were investigated to tackle the problem of pharmacophore generation. The first and the second strategies as discussed in section 2 did not produce satisfactory results for two reasons: these two strategies cannot deal with the complex relationships of objects inherent in the domain and the generation of a pharmacophore by a designer is not just of a matter of induction but is largely influenced by the domain knowledge that already exists.

The heuristic-based approach, i.e., the third strategy, was successfully used to solve the problem of pharmacophore generation [Smithers *et al* 1993 and Tang 1995]. In this application the learning process involved the steps of pre-processing of molecule examples, ranking molecule examples using user-specified criteria, building the design concept tree incrementally, and evaluating and interpreting the concepts stored in the design concept tree. Design heuristics as background knowledge are tightly integrated with all these steps. This strategy provided a better basis for designing new drugs in this domain, compared with the level of complex in data analysis, size of the example molecule set, and the efficiency of the processing molecular examples that can be managed by human drug designers. This application also showed the importance of using background knowledge in the learning process in order to produce results relevant to design purposes.

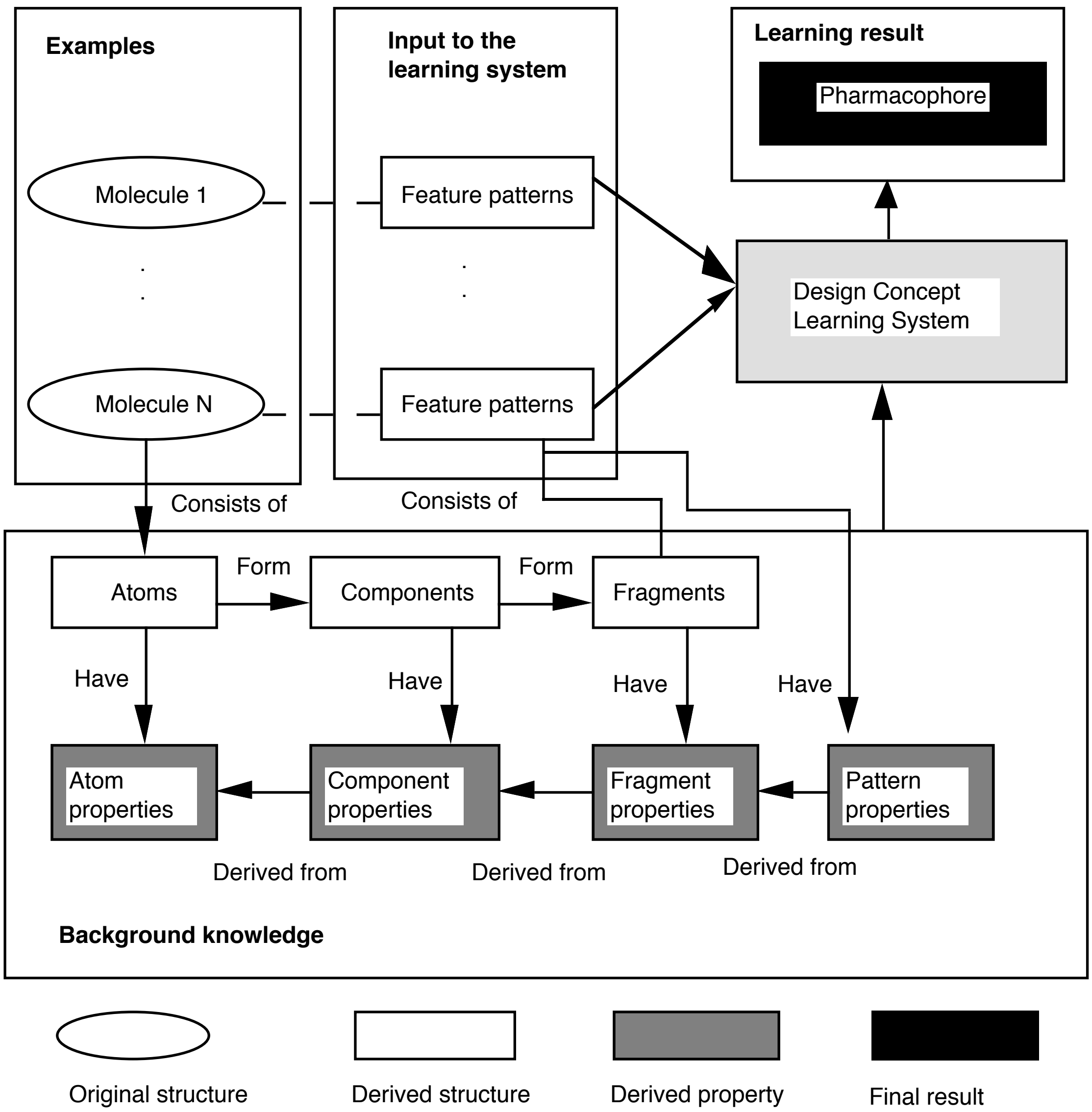

Figure 1: An Inductive Learning Setting for Drug Design

The design concept learning system is currently being tested in the domain of mechanical engineering design. In this domain, the design concept learning system is used in the design synthesis stage to organise the ideas generated by a *functional synthesiser*. The functional synthesiser generates a large number of *abstract conceptual solutions* from a user specified functional requirement and a selected set of examples (functional components with known input/output behaviour). In order for the designer to make the effective use of these abstract solution concepts, the design concept learning system is used to cluster them into higher level or lower level concepts using the clustering criteria specified by the designers [Chakrabarti *et al* 1996]. In a case study, a number of experienced designers have been asked to run the system and suggest the clustering criteria. These clustering criteria are used to characterise the abstract solution concepts which are subsequently classified using the design concept learning system. As a result of this case study, ten clustering criteria specific to mechanical engineering design have been identified and these are currently being tested. In this domain the first strategy adopted within the design concept learning system has so far appeared to be sufficient. Again in this domain the design concept learning system is used as a part of a design support system for the task of clustering initial conceptual solutions. The clustered conceptual solutions can then be further explored by the designers using an embodiment design support system.

4. Conclusions

As an initial attempt to integrate inductive learning techniques and knowledge-based design techniques, the development of the design concept learning system provided limited general facilities to support early design tasks with a particular emphases on the use of design heuristics as background knowledge. Future research on the topic will focus on the issue of testing the design concept learning system with more case studies and building a knowledge-based design support system architecture within which inductive learning techniques as well as other machine learning techniques can be utilised to support the learning from design principles, past design cases and documented design results.

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