DESIGN DESCRIPTIONS IN THE DEVELOPMENT OF MACHINE LEARNING BASED DESIGN TOOLS

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ABSTRACT
Applications of machine learning technologies are becoming ubiquitous in many sectors and their impacts, both positive and negative, are widely reported. As a result, there is substantial interest from the engineering community to integrate machine learning technologies into design workflows with a view to improving the performance of the product development process. In essence, machine learning technologies are thought to have the potential to underpin future generations of data-enabled engineering design system that will deliver radical improvements to product development and so organisational performance. In this paper we report learning from experiments where we applied machine learning to two shape-based design challenges: in a given collection of designed shapes, clustering (i) visually similar shapes and (ii) shapes that are likely to be manufactured using the same primary process. Both challenges were identified with our industry partners and are embodied in a design case study. We report early results and conclude with issues for design descriptions that need to be addressed if the full potential of machine learning is to be realised in engineering design.

Keywords: Big data, Artificial intelligence, Design informatics

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1 INTRODUCTION

Despite major advances in computer science, computational support for engineering design practice remains limited. For example, applications such as that outlined by Cavalcantea et al. (2019), who report an application of machine learning for the selection of suppliers in manufacturing supply chains, have the potential to improve the effectiveness and efficiency of procurement processes, and so reduce time to market and costs. However, the impact of such improvements on design quality (e.g., creating a design that better meets its design requirements or is easier (and so quicker and cheaper) to manufacture or support through life) is limited. For design definition, e.g., in computer aided design, and design analysis and optimisation applications (collectively referred to as CAD here), design information captures the results of design processes. In mechanical design, this information includes geometric models of individual parts and geometric constraints between them, often attributed with further information such as material specifications. However, a given design can be described in many ways, typically driven by the preferences and capabilities of the CAD system used to create it and its users. As a result, the structure of a given shape model is user defined and there is no guarantee that, in a given collection of shape models, the logic behind the structures of the models will be meaningful or consistent.

This paper reports experiments using a machine learning application to address two shape-based challenges in engineering design practice: clustering of (i) similar part shapes in a given design and (ii) shapes that are likely to be manufactured using a given process. The focus of this paper is on the application of machine learning in design rather than the development of the machine learning system itself although, given the research was driven through the development of a series of prototypes, these two processes are intertwined. For this reason, the paper begins with a review of literature on applications of machine learning in engineering design (Section 2). This is followed, in Section 3 with an outline of the approach used and in Section 4 with a brief description of the machine learning system that was used in our design experiments. Results are provided in Section 5. The paper concludes, in Sections 6 and 7, by outlining issues that need to be addressed if the full potential of machine learning is to be realised in engineering design.

2 LITERATURE REVIEW

There are numerous models and manifestations of the engineering design process. Common features are their integration of divergent and convergent thinking and, in this context, cycles of synthesis, analysis and decision making (Suh, 1990). In mechanical design, design requirements are transformed into assemblies of parts where each part has a geometry that, coupled with geometric constraints between parts, govern the behaviours of the final design. Computational design tools are available to support many aspects of this process. However, while there are experimental systems that support conceptual design (Pokojski et al., 2019), the most widely used in design practice are those based on geometric models of a developing design. Human designers are critical to the process because they bring creativity, to generate new solution principles in response to design requirements, and innovation, where constraints inform the development of a design. Further complexity is added by the fact that real-world design processes are typically delivered by teams of designers, often working across networks of organisations. To support such ways of working, design problems are decomposed into system architectures and design requirements are allocated to specific subsystems (Blanchard and Fabrycky, 1990). Thus, the results of a given engineering design process are design descriptions of assemblies of parts (either references to models of standard parts or shape models and associated information of designed parts), assembly relationships between these parts, and product architectures (typically, a product decomposition with requirements allocated to each part and relationships, often geometric, between parts) (Shapiro and Voelcker, 1989). The research reported here focussed on component parts and associated shape models.

An important prerequisite for applications of machine learning is the availability of training data on a scale large enough to train algorithms for a target activity. The only available design data on this scale are libraries of shape models such as the ABC and FabWave datasets (Koch et al., 2018; Starly et al., 2019) that were used in the experiments reported in this paper. However, in practice, design definition data is significantly richer than the shape models in such libraries. A second feature common to all engineering design processes lies in the broad categories of information that they use and produce. In essence, engineering design can be seen as a mapping process, from customer needs and design requirements (Suh’s customer and functional domains (Suh, 1990)) to design definitions (Suh’s physical domain) and associated processing information for, e.g., manufacturing, and lifecycle support.
and end of life processes (Suh’s process domain). As a result, engineering design information relates to all of these domains (McKay et al., 1996) along with information on the mappings themselves and rationale for decisions made (e.g., see Design Rationale editor (Bracewell, et al., 2009). Some authors report work using design analysis and optimisation approaches to generate training data (Pilarski et al., 2021; Sharpe et al., 2019; Tallman et al, 2019) but, again, this is limited to shape models and associated analysis parameters and objective functions that do not reflect the full richness of the design requirements being addressed. In addition, the problems addressed tend to be focussed on specific design problems for which it is possible to specify specific design parameters and goals. This research is more widely focussed and, given the available training data, our experiments explored applications of machine learning that could be trained using shape models.

The DeCoDE lab at MIT is doing work on the use of artificial intelligence to support engineering design activities and so-called “cognitive design assistants” are emerging as a means by which machine learning and other branches of artificial intelligence can support such activities. Maier et al. (2019) propose an ontology for cognitive assistants that includes categories covering degrees of natural language processing, and levels of functionality and learning. Zhang et al. (2021) report a study, using a model bridge design activity, which highlights the importance of considering human and team performance in the introduction of artificial intelligence to the design process. The long-term goal of the experiments reported in this paper is to inform the development of design assistants that can support real-world engineering design and development processes. While there are numerous opportunities, a limiting factor lies in the availability of suitable training data. The first experiment in this paper explored the use of machine learning to assist designers in finding shapes that are similar to the one they are working on. In the second experiment, the general problem addressed lay in identifying clusters of similar shapes to support, e.g., manufacturing planning. Corney et al. (2002) describe an early web-based search engine that finds shapes similar to a given shape and highlight the need for shape representations that support similarity detection as a major challenge. In this paper, representations of topology are used to identify clusters of topologically similar shapes.

3 APPROACH

The approach used is illustrated in Figure 1. Three key aspects are highlighted: the creation of a machine learning-based design system, the formulation of a design case study and the application of the machine learning-based system to the case study. The focus of this paper lies in the application of the systems to two design challenges (both of which were identified by industry partners as being important for improving product development process performance) and the learning, in the form of feedback to inform future generations of machine learning-based design system and potential design cases, which
was generated. Details of how the machine learning-based systems were created are reported elsewhere but a summary of key points necessary for this paper is provided in Section 4. This paper reports three research cycles using three different machine learning-based systems: two, trained with different training data, used shape similarity to cluster shapes from a case study and the third used training data that had been labelled by hand to cluster the same shapes based their primary manufacturing process.

A subsystem of a prototype 3D sintering machine (the cakebox shown in Figure 2) was used as the design case study. As a prototype machine, some design features were not as would be found in a production machine. For example, the prototype used Rexroth sections which would be unlikely to be used in a production machine. However, the sintering machine was selected as a suitable case study for two reasons: a full set of CAD models was available and the design definition was not subject to confidentiality constraints. CAD models for each mechanical part were provided as STEP (ISO10303-203, 1994) files that had been exported from PTC Creo.

From discussions with the case study owners and other industry partners, two design challenges were identified. The first aimed to reduce time and cost by reducing unnecessary design work on new parts when existing designs were available either for direct use or adaptation. To achieve this, the need to be able to identify parts with similar shapes, so that feasibility of reuse could be assessed, was identified. The second challenge related to improving quality in procurement processes: so reducing cost and time for manufacturing, and ultimately the production of scrap. Achieving this requires procurement teams, with limited design and manufacturing knowledge, to be able to identify parts likely to be made using the same primary manufacturing process. For both challenges all parts of the cakebox were selected that were not standard parts and whose primary manufacturing process could be one of: machined bar or other raw material with a constant cross-section (e.g., materials such as Rexroth), casting or forging, and sheet metal processes such as bending and stamping. A subset of 71 distinct parts were selected: bar (18 parts), casting or forging (28 parts), and sheet metal (25 parts).

A key conclusion from the first two research cycles (shape clustering with FabWave data and clustering by manufacturing process) was the need to improve the quality of the training data. In response, survey-based experiments (to be reported elsewhere) were carried out to assess how people perceive visual similarity of selected shapes. The survey used data from the ABC dataset. Survey results, on human perceptions of shape similarity, were used to train a third, shape clustering, system. In preparing the surveys, a need was identified to refine the ABC data used with a view to assuring its quality. This was done using a manual process where shapes from the data set were sifted so that only valid looking parts were included. The user, who kept a record of reasons for rejecting shapes, was offered one image at a time with options to accept or reject it. The sifting was done in 30 minute blocks to reduce the risk of bias. Details of reasons for rejection of shapes is provided later (in Section 5) along with the impact the use of the new training data set had on the results.

![Figure 2: Sintering machine cakebox from case study](https://doi.org/10.1017/pds.2023.123)
4 MACHINE LEARNING-BASED DESIGN SYSTEMS

The machine learning based systems used in this research were developed using a two-step process: (1) common features in large volumes of input data (so-called "training data") are identified; and (2) these features are used to form an n-dimensional latent space into which all items from the training data are embedded. In our case, each system had a 16-dimensional latent space. Given its latent space, the system can then embed new input data (in our case, shapes from the cakebox) into the latent space. The remainder of this section is structured around the three steps needed to create a machine learning-based design system shown on the left-hand side of Figure 1.

4.1 Acquire training data

Given the focus of this paper on design descriptions, the method for developing the latent space is out of scope and reported elsewhere (DCS, 2022). Three prototype systems were built, each with distinct training data described in Table 1. For version 1, the FabWave dataset was used which contains around 4,500 CAD models, each labelled with one of 43 part categories. For version 2, a human based similarity study was carried out using hand selected models from the ABC dataset which is more general than FabWave.

<table>
<thead>
<tr>
<th>Shape clustering goal</th>
<th>Training data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Visual similarity (Version 1)</td>
<td>Raw FabWave data</td>
</tr>
<tr>
<td>Same primary manufacturing process</td>
<td>Labelled cakebox parts</td>
</tr>
<tr>
<td>Visual similarity (Version 2)</td>
<td>ABC data with human perception</td>
</tr>
</tbody>
</table>

Table 1: Summary of design systems and training data used

4.2 Extract training data

CAD models with STEP file formats were used because this format makes explicit the geometry of faces and their topological connectivity. The category labels from the FabWave data set allowed a simple measure of similarity to be defined though, on detailed examination, there were inconsistencies in the category labels. A widely recognised issue with CAD systems is that a given shape can be defined in multiple ways. This means that two shapes that are visually the same (e.g., a circle of radius $R$ and an ellipse with both minor and major radii $R$) are not the same in their definition. To avoid this, a graph representation of the topology of each CAD model was used. As a result, as the first stage of mapping to a latent space, each CAD model was converted into a graph with $n$ nodes, where each node represents a face in the CAD model and each edge represents a connection between a pair of faces that are in contact with one another. Nodes have a single attribute: type of face. Edges have four attributes: the angle between the connected surfaces, the ratio of the sizes of the two surfaces, the type of the curve of the edge, and the relative edge size compared to size of face. Results for three example shapes are illustrated in Figure 3.
4.3 Train design system

A given machine learning-based system is underpinned by a neural network. Given the different goals, different neural networks were required for the two design challenges. The Fabwave data was used to train the neural networks for clustering similar shapes, by providing triplets of models, an anchor model, a similar model, i.e., one in the same category and a dissimilar model, one in a different category. Later, when training the network on the human obtained similarity data, the direct results of the study were used in the same way. For the manufacturing process challenge, a small dataset of labels for the putative manufacturing processes for 71 parts was provided; this enabled further training based on the FabWave dataset. Our approach was to use the latent space for shape similarity as an intermediate representation for parts and to train a conventional fully connected neural network with three hidden layers on this space, instead of attempting to train a classifier on the original model graphs. Here the mapping into a low-dimensional latent space that has been optimised is leveraged on a large dataset of part models (from FabWave). This is an instance of transfer learning. The classifier was trained on 90% of the data (71 models) over 100 epochs and tested on the remaining 10% (7 models). 10-fold cross-validation was used to obtain an estimate of 70.53% for classification accuracy with a standard deviation of 6.69. Further details of the training process are outside the scope of this paper but available at (DCS, 2022).

5 RESULTS

Results from the three research cycles, each using the cakebox case study, are presented in this section followed by results of the sifting process used to prepare the ABC data for the human perception survey. Figure 4 shows the way in which the shapes from the cakebox were clustered by the machine learning system using topological features but trained using two different datasets: the Fabwave dataset in 4(a) and the ABC dataset augmented by human perceptions of shape similarity from the survey in 4(b). In both cases an emergent clustering of parts can be seen to the human eye though, again with the human eye, shapes such as those at the top of the plot in Figure 4(b) seem to be better clustered with the second dataset. Further work is needed to quantify the quality of the clustering and the level of quality needed in engineering design applications. However, a practical application of this is that, given a part mapped into the latent space, a search can be carried out for the closest vectors in that space to find parts with similar shapes. Figure 5 shows a different clustering that incorporates the manufacturing processes from the labelled dataset. The clustering of the whole dataset is shown in 5(a) and a screen capture from the interactive plot (see caption for link) is shown in 5(b) to highlight some clustered
shapes themselves. As with Figure 4, a visual assessment of the interactive plot shows that most shapes were categorised appropriately though further work is needed to quantify the quality of the clustering.

In the third research cycle, a survey was conducted to build understanding of how people perceive shape similarity. Results from the survey were then used to provide a training dataset that included human perceptions of similarity. In the survey participants were given three models from which to pick the two most similar. Each triplet of models was presented to three different participants to confirm results. Answers that did not agree were left in the dataset as this ambiguity is something that was desirable in the trained network; however this means 100% accuracy is not achievable. In preparing the survey it was noticed that a significant proportion of the shapes in the training data were unsuitable for use in engineering design of component parts. For this reason, a manual sift of the shapes was carried out to ensure that survey participants were only provided with appropriate shapes.

A summary of the results from this selection process is shown in Table 2 along with reasons for rejecting shapes.

<table>
<thead>
<tr>
<th>Shapes considered</th>
<th>Shapes kept</th>
<th>Shapes rejected</th>
<th>% kept</th>
<th>% rejected</th>
<th>Primary reason (1st option from left used when multiple reasons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Not a single discrete solid</td>
<td>Standard part</td>
<td>Abstract or invalid 3D shape</td>
<td>Assembly modelled as a solid</td>
<td>Not producible with our processes</td>
<td></td>
</tr>
<tr>
<td>Shapes</td>
<td>6687</td>
<td>2010</td>
<td>4843</td>
<td>28%</td>
<td>72%</td>
</tr>
</tbody>
</table>

As can be seen from Table 2, of the 6687 shapes (from the ABC dataset) that were candidates for use in the survey, only 28% were regarded as being suitable for use. Five reasons for rejecting shapes, based on a visual assessment of individual shapes, were identified. 12% of shapes did not look like a single discrete solid because they included more than one shape that was not physically connected to other shapes. As a result, these shapes could not be regarded as the shapes of single discrete parts.
25% of rejected shapes were rejected because they looked like standard parts, e.g., nuts, bolts & screws, pins, spacers, bushes, bearings, pulleys, wheels, springs, gears and splines. Such parts are typically mass-produced and a design engineer would use these parts rather than generate new designs for them. 23% of rejected shapes were rejected because they appeared to be abstract or invalid 3D shapes. For example, these included shapes that looked odd (e.g., a cylinder intersected with a curved surface); shapes where the visible detail was insufficient to judge; and shapes such as chess and Lego pieces. A further 34% of rejected shapes were rejected because they looked like assemblies modelled as solids. For example, this group included products that were obvious assemblies, e.g., mechanisms, architectural products (though some of these may have been Lego buildings), process plants, electronic circuits and fabricated shapes such as welded structures. Finally, 7% were rejected because they could not reasonably be manufactured with our target processes: i.e., casting/forging, sheet metal, bar/section.

6 DISCUSSION

The experiments reported in this paper are promising in that they demonstrate the potential value of machine learning-based design systems in improving the time, cost and quality performance of activities within product development processes that require engineering expertise coupled with representations of designed shapes. In particular, the use of topology, which is a lighter weight representation of shape than a full CAD model but which can be computed from a STEP file, was important because, for a given shape, it remains constant regardless of how the shape was initially defined. However, a number of issues for design description have been identified; these need to be addressed if the full potential of machine learning is to be realised in engineering design. This section draws together learning from the experiments to identify issues in design description that need to be addressed for the effective deployment of machine learning in engineering design. Section 6.1 outlines primarily technical issues related to the availability and quality of training data for shape-based systems. In Section 6.2 issues related to the development of machine learning systems for wider design processes are considered. This feeds into Section 6.3 which discusses wider business issues related to the quality assurance of such systems and their suitability for use, especially in highly regulated application areas.

6.1 Training data requirements

Given available data, especially for use in safety critical design applications, approaches for the validation and verification of the data will be necessary. This will include ensuring both the quality of data and that data are used in appropriate settings. With respect to the quality of design data, the engineering design community currently has very limited ways of evaluating this. For example, in the training dataset used in these experiments, there were numerous models that gave attractive looking renderings of part shapes but where the defined assembly structure was either incoherent or only sufficient for shape visualisation purposes. Current practice in assessing the quality of design descriptions tends to consider wider factors, such as data provenance (e.g., the level of expertise and competency of the person who created it) and the after-effects of a given design description (e.g., the number of queries generated from downstream processes to design and the amount of rework it generates). These approaches are effective in current practice but the necessary data to support such analyses is not available in current archives. For machine learning applications, further work is needed to (a) measure the inherent quality of given shape models and (b) establish the sensitivities of machine learning algorithms to weaknesses in the training data. An alternative, and perhaps more viable, source of shape data could be in organisations’ own design archives, from which training data could be harvested. However, as highlighted by Raina et al. (2022), regardless of the training data used, it will be important to ensure that machine learning-based design systems are not biased, through their training, by existing solutions.

6.2 Machine learning in engineering design

A prerequisite for any machine learning application lies in the data used to train the algorithms that underpin it. In engineering design, the only data currently available on the necessary scale are large databases of shape models. However, shape models are just part of the result of a design process. The design process itself is a creative and iterative one that translates design requirements into design
solutions that include shape in addition to other product-related knowledge and information. While there is literature that provides data formats for non-shape data, this work is at a very early stage in its development and standard, neutral formats to enable sharing of non-shape data created in different vendor systems do not exist. For this reason, the potential for machine learning-based applications in mechanical design, where shape and material combinations govern function and so are closely aligned to design requirements, is likely to be limited to applications that can be driven from shape models. At first sight this seems narrow. However, beyond design analyses such as FEA and CFD that predict the behaviour of a design against functional requirements, there are opportunities to generate training data, e.g., employing approaches currently used in design optimisation (Sharpe et al., 2019). This paper has shown just one, where manufacturing methods, implied by but not specified in shape models, can be gleaned.

6.3 Verification, validation and maintenance of applications using the data

Given a trained design system, especially if it is to be used in highly regulated sectors such as aerospace where, e.g., the chief engineer in the prime contractor is responsible for the whole design and the processes used to create it, there is a need to be able to establish its capability to ensure that it is used appropriately. Lavin et al. (2021) define technology readiness levels for machining learning systems that will be essential in assuring the quality of such systems. Further, if a system were able to continue to learn, this would need to be a continuous – and so, ideally, automated – quality assurance process. For example, even in less heavily regulated sectors, it would be important that the training status of the design system be kept up to date, e.g., with new manufacturing processes that become available to manufacturers. This, in turn, is linked to wider data sources than shape, e.g., it relates to the manufacturing capabilities of the supply chain to which the manufacturer has access. An opportunity here, however, is that a given design could be evaluated with respect to the capabilities in multiple supply bases and so support decisions related to production strategies. However, open questions remain, e.g., “How should results from a machine learning-based design system be verified and validated?” and “If learning is taking place, are there learning outcomes to be achieved and, if so, what are they?” Zhang et al. (2021) highlight differences in how design systems enhance (or not) the performance of novice and experienced designers using a simple design test case. Again, this points to a need for design system to be developed for, or able to adapt to, the needs, capabilities and preferences of specific users which, in turn, points to a need for better ways of assessing such things.

7 CONCLUSIONS

This paper has shown how machine learning-based design systems have the potential to improve the productivity of product development processes by reducing redesign work and errors e.g., in manufacturing planning. However, in line with Lavin et al. (2021), more controlled development processes are needed if such systems are to be integrated into engineering practice. As a prerequisite to this, there is a need for more advanced approaches to assuring the quality of training data used. Our research has highlighted three specific concerns: two related to the quality of geometric models and supplementary information associated with this data in available repositories, and a third in assessing the appropriateness of training data. For example, while there are similarities, data used to train an aircraft designer is very different to that used to train a car designer.

Despite these difficulties, there is a growing body of evidence demonstrating the potential value of machine learning in design and its potential to lead to a new generation of shape-based design tools. However, in addition to the demands this places of the computer science community where underlying methods or machine learning are under development, there are also significant demands emerging for design descriptions in the engineering design community. Firstly, shape is just one of two intrinsic characteristics of any mechanical piece part: the other being its material (McKay et al, 2015). Current repositories do not include material specifications and there is significant further work needed if such information is to be used to train machine learning algorithms. Further complexities relate to assembly information which, along with the shapes of individual parts, influence product functionalities and behaviour; such data are not captured in repositories but are critical in any design process (e.g., see Shapiro and Voelcker, 1989). In considering design for manufacturing and later lifecycle processes, further training data from these processes would be needed. While there is substantial anecdotal evidence that such data is being captured, significant further work is needed to
ensure that such data is captured in sharable formats and associated with descriptions of the designs the data relate to.

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