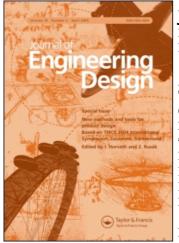
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Supporting knowledge exploration and discovery in multi-dimensional data with interactive multiscale visualisation

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Supporting knowledge exploration and discovery in multi-dimensional data with interactive multiscale visualisation

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Knowledge discovery in multi-dimensional data is a challenging problem in engineering design. For example, in trade space exploration of large design data sets, designers need to select a subset of data of interest and examine data from different data dimensions and within data clusters at different granularities. This exploration is a process that demands both humans, who can heuristically decide what data to explore and how best to explore it, and computers, which can quickly extract features that may be of interest in the data. Thus, to support this process of knowledge discovery, we need tools that can go beyond traditional computeroriented optimisation approaches and support advanced designer-centred trade space exploration and data interaction. This paper is an effort to address this need. In particular, we propose the interactive multiscalenested clustering and aggregation framework to support trade space exploration of multi-dimensional data common to design optimisation. A system prototype of this framework is implemented to allow users to visually examine large design data sets through interactive data clustering, aggregation, and visualisation. The paper also presents an evaluation study involving morphing wing design using this prototype system.

Keywords: trade space exploration; visualisation; multiscale visualisation; multi-dimensional data; multiscale data; nested clustering and aggregation

1. Introduction

Complex engineered systems such as automobiles, aircraft, and satellites usually consist of multiple, interacting sub-systems and components that are often designed by engineers from a variety of disciplines. The main challenge when designing such systems lies in resolving the inherent trade-offs that exist both within and between sub-systems and the overall system.

The design of such complex engineered systems is starting to experience a paradigm shift. More and more, designers want to go beyond single point solutions obtained from a fully automated optimisation process and explore trade space while 'shopping' for the best design that suits their needs and meets the customers' requirements. This paradigm shift from design *optimisation* to design *exploration* is being enabled by recent advances in computing power and speed and novel

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visualisation software; however, designers are encountering new problems such as information overload in that they have too many options from which to choose and become overwhelmed, not knowing which design is the best. Trade space here refers to the 'potential solution space' (Ross *et al.* 2004). This space consists of a set of multiple design alternatives, data attributes, or system parameters that designers can evaluate to satisfy various design objectives (Brantley *et al.* 2002).

Designers need help in analysing large data sets and generating knowledge from them. Usually, large data sets are multi-dimensional and stored in databases, and designers often choose part of a data set in certain dimensions and examine their behaviour in other dimensions. One of the primary challenges in the design of complex engineered systems, such as cars, is to identify interesting trends among many design alternatives. Designers explore multiple design alternatives to evaluate the impact of changes in the design parameters (e.g. car size, engine size, the number of cylinders, etc.) on the performance of the car (e.g. fuel efficiency, torque). To determine the best design(s) among thousands of simulated design alternatives – created by varying these design variables and storing the corresponding values of the performance variables for each alternative - designers need to compare the performance of each alternative to choose the best design variables. Designers need effective tools for choosing data of interest (often a subset of the whole data set), selecting the attributes to observe (e.g. engine size, weight in the aforementioned example), and determining which attributes to cluster during data analysis (e.g. fuel efficiency, torque). Furthermore, designers would benefit greatly from controlling the way in which they compare design alternatives, such as evaluating data clusters with different aggregation methods (e.g. mean, median, and sum) and changing the size of clusters. Current data analyses and visualisation tools in engineering design do not support these diverse needs well. Advanced visualisation techniques like the scatter plot matrix (Carr and Nicholson 1985) are largely *ad hoc* and often overwhelm designers with too much information.

To support trade space exploration for multi-dimensional data, we propose an interactive multiscale-nested clustering and aggregation (iMSNCA) framework in this paper. The novel framework puts design activities in the forefront and emphasises the role of computational tools in supporting such activities by considering the characteristics of design data. The next section reviews relevant literature. Section 3 introduces the framework, and a prototype system is described in Section 4. An evaluation study involving an aircraft wing design problem is presented in Section 5. Finally, the benefits and limitations of this research are discussed in Section 6.

2. Related work

The research questions we address in this paper are related to trade space exploration in engineering design, scientific and information visualisation, and multi-dimensional and multiscale data interaction. Each is reviewed in the following sections.

2.1. Visualisation in engineering design

Much of the research in the design of complex engineered systems has focused on novel formulations and algorithms for solving optimisation problems (Chen *et al.* 2000, Deb 2001, Sobieszczanski-Sobieski *et al.* 2003); approximation methods to reduce the computational expense of these analyses (Haftka *et al.* 1998, Simpson *et al.* 2001); and computational frameworks to integrate analyses from multiple disciplines (Phoenix Integration 1999, Koch *et al.* 2002). Despite the advances and developments over the past two decades, design optimisation still has several shortcomings and challenges (Papalambros 2002). Balling (1999) has noted that the traditional optimisation-based design process of '(1) formulate the design problem, (2) obtain/develop analysis models, and (3) execute an optimisation algorithm' often left designers unsatisfied with their results because the problem is usually improperly formulated: 'the objectives and constraints used in optimisation were not what the owners and stakeholders really wanted ... in many cases, people don't know what they really want until they see some designs'. Similar findings have occurred in other fields. For instance, Shanteau (1992) observed that when people are dissatisfied with the results of a rational decision-making process, they often change their ratings to make it come out the way they want. Wilson and Schooler (1991) have shown that people do worse at some decision tasks when asked to analyse the reasons for their preferences or to evaluate all the attributed of their choices.

Consequently, there is an emerging paradigm of design exploration whereby designers 'shop' for the best solution using visualisation tools instead of relying solely on optimisation. This design by shopping process, introduced by Balling (1999), allows designers to explore the design space first and then choose an optimal solution from a set of possible designs after 'forming realistic expectations of what is possible'. This approach can be classified as an *a posterior* articulation of preferences to solve a multi-objective optimisation (Hwang and Masud 1979) in that designers first form their preferences based on visualisation of the entire design space and then choose an optimal design that is based on their formed preference. The basic steps to such an approach include (1) creating a simulation model to analyse the system being designed, (2) generating thousands of simulated design alternatives by varying design variables and storing the corresponding values of the performance variables for each alternative, and (3) using visualisation tools to explore these design alternatives and 'shop' for the best design (Stump *et al.* 2003, 2004).

To date, trade space exploration has focused primarily on developing virtual environments and visualisation tools to support such an approach. For instance, spherical mechanism design has benefited greatly from virtual reality advancements (Evans et al. 1999, Furlong et al. 1999, Kihonge et al. 2002), as have large-scale manufacturing simulations (Kesavadas and Sudhir 2000, Kelsick et al. 2003). Several researchers have also looked at effective interface development for virtual environments (Mulder et al. 1998, Volkov and Vance 2001, Balijepalli and Kesavadas 2004). Virtual reality has supported a wide variety of engineering design problems (Jayaram et al. 2001); however, such environments tend not to support trade space exploration since they are used to visualise a single point solution, not explore the entire trade space. Cloud visualisation (Eddy and Lewis 2002), the visual design steering methods (Winer and Bloebaum 2001, Winer and Bloebaum, 2002a, 2002b), the ATSV system (Stump et al. 2003, 2004), and the U.S. Naval Research Laboratory's visual steering methods in their Virtual Reality Lab and High Performance Computing Center (Smith et al. 1999) are exceptions to this, but these methods are used in an ad hoc manner to support design decision-making – none of the research in engineering design has investigated the knowledge discovery process during trade space exploration or formalised systematic procedures to support it. Meanwhile, efforts to simplify the visualisation of n-dimensional Pareto frontiers (Agrawal et al. 2004) and group uncertainty-related data into 'bricks' (Kanukolanu et al. 2006) provide good intentioned, yet still ad hoc, solutions to the problem of overwhelming designers with too much information as they are put 'back in the loop' as part of the trade space exploration process.

2.2. Scientific and information visualisation

Research on using visualisation to facilitate information and knowledge processing has advanced greatly in the past two decades. Card *et al.* (1999) classify visualisation techniques into two categories – scientific visualisation and information visualisation – based on the nature of the data being visualised. Scientific visualisation usually deals with physical data. In scientific visualisation projects, such as flow vector visualisation (Shahnawaz *et al.* 1999, Wasfy and Wasfy 2003, Laidlaw *et al.* 2005), the spatial relationship of physical objects is accurately mapped (often re-scaled to fit

the screen) into that of visual components so that scientific phenomena can be accurately measured and clarified. Information visualisation extends beyond physical data and usually focuses on helping people analyse and make sense of more abstract phenomena. For example, Card *et al.* (1991) proposed a 3D-based visualisation technique for information visualisation where the 3D space is used to expand people's information workspace and reduce the cognitive costs in dealing with complex data, rather than just as a habitat to show 3D data.

Information visualisation also provides a means for exploratory analysis (Nagel 2006). While scientific visualisation emphasises confirmatory analysis (i.e. confirm or reject hypotheses), information visualisation can also help people identify new hypotheses through cognitive amplification and user-centred interactive designs (Card *et al.* 1999). Cognitively, information visualisation benefits users by increasing available spatial (e.g. large workspace) and cognitive resources (e.g. less demand for information recall mentally), improving searching processes (e.g. colour-coded visual search), enhancing pattern recognition (e.g. visual icons), etc. Interactively, information visualisation, control the mapping between data and visual forms (e.g. hierarchical visualisation as discussed later), and modify the views on visual forms (e.g. zooming). Cognitive amplification and flexible interaction facilitate a knowledge crystallisation process that provides 'the most compact description possible' of complicated data and information (Card *et al.* 1999).

Making sense of large data sets often involves creating structures and putting data into structures (Russell et al. 1993), and this 'sense-making' process is often a critical component in the knowledge crystallisation process. The famous 'knowledge hierarchy' of Lucky (1989) argues that knowledge is built upon information, which is in turn built upon data. In this sense, knowledge is the result of aggregating information, and knowledge discovery arises from organising fragmental information into structured knowledge schemas. However, finding appropriate structures to organise available information is a complicated yet cognitively costly process, because possible structures must be mentally searched and modified to fit all information of interest. Such searching and fitting activities are conceptual and involve an analysis of the attributes of both knowledge structures and information pieces. To reduce the cognitive costs of 'sense-making', researchers have proposed a variety of structures for organising information (Qu and Furnas 2005). Among these structures, hierarchies are frequently used to organise information and knowledge: they provide semantic descriptions with different levels of detail and allow users to navigate through the different levels with context and content as needed. Techniques for visualising hierarchies include treemaps (Shneiderman 1992), Cone Trees (Robertson et al. 1991), and hyperbolic views (Lamping and Rao 1994), which use nested boxes, 3D space and interactive animation, and hyperbolic representations, respectively.

Although information visualisation is regarded as a means to crystallise knowledge, visualisation-based methods to support knowledge discovery in engineering design are not well understood. Among the extensive literature on information visualisation, we are particularly interested in research on multi-dimensional and multiscale data visualisation because design data for complex engineered systems is usually multi-dimensional and designers often need to examine data at different levels of analysis when designing different sub-systems.

It should be pointed out that data visualisation is a broad topic that has been researched by scientists from many disciplines. For example, researchers in statistics also have developed powerful tools to assist the analysis of multi-dimensional data (Unwin *et al.* 2006, Cook and Swayne 2007). However, these tools are often built upon specialised statistics software packages (e.g. R), making it impractical to integrate them into general-purpose, stand-alone visualisation systems. Also, the focus of such tools is on visualising general statistical characteristics of large data sets and need to be further enhanced to support trade space exploration, which often concerns both general data distributions of data at a global level and potential data anomalies at local levels.

2.3. Multi-dimensional and multiscale data interaction

Extensive research has been done in visualising multi-dimensional data. Although these techniques are not targeted at in-depth analysis, such as quantitatively comparing a few dimensions, their focus on visualising overall relationships does serve as the entry point to understanding of multidimensional data. Parallel coordinates (Inselberg 1985) represent individual dimensions as parallel lines and plot a multi-dimensional record as a poly-line across parallel coordinates, revealing cross-dimension patterns and trends. There are also some variations derived from this technique (Hoffman et al. 1999) by positioning individual dimensions in different ways. These techniques are effective to present overall trends, but lack detailed descriptions of between-dimension relationships and aggregated information of individual dimensions. Scatter plot matrices (Carr and Nicholson 1985) use a matrix to organise scatter plots between each pair of dimensions and help users quickly grasp the overall trends and relationships between each pair of dimensions and then pick those of interest. Recently, this technique was improved by the rank-by-feature (Seo and Shneiderman 2005) method, which colour-codes the matrix cells based on the magnitude of correlation between each pair of dimensions. However, these techniques largely focus on between-dimension relationships, and they do not provide sufficient support for detailed analysis within dimensions of interest. The Table Lens technique (Rao and Card 1995) uses a simple 2D table to hold data for in-depth, within-dimensional data analysis, but the tools are largely about ranking and sorting data, which are not sufficient for engineering design. Recently, some commercial software packages (e.g. http://www.tableausoftware.com/, http://www.ilog.com, and http://www.grantadesign.com/products/ces/) provide comprehensive tools for multi-dimensional data visualisation. However, their support for in-depth data analysis within the same dimension is insufficient to enable designers to examine how designs may vary at different levels of analysis.

Multiscale user interfaces, also called zoomable user interfaces, allows users to control the levels of detail in visualising and interacting with large data sets. Benefits of multiscale tools include helping users obtain desired context and content information and showing important characteristics of data at various scales at the same workspace (Perlin and Fox 1993, Furnas and Bederson 1995, Bederson *et al.* 1996). However, most systems that use multiscale tools, such as PhotoMesa (Bederson 2001), are targeted at data sets that are already hierarchically structured. Few designs can support interaction with raw data sets that do not have hierarchical structures or are not structured at all.

Semantic zooming is a powerful tool in multiscale user interfaces for visualising different data properties across scales. For example, with semantic zooming, designers can examine what factors affect the characteristics of a new material by seeing features from the atomic level (e.g. the strength of atomic bonds) to the microscopic level (e.g. the tangle of molecules) and to the macroscopic level (e.g. mechanical stress). However, how to generate semantic representations across scales is still a challenge. Some efforts have been made to interactively construct semantic representations for a small set of objects (Furnas and Zhang 1998), but it is still difficult to deal with large data sets with thousands or even millions of data records.

Another stream of relevant research is multi-facet information visualisation and navigation. Originating from the area of library science, a facet refers to an aspect in which information is organised (Hearst 2006) and can be regarded as equivalent to dimension, but with different focus. While dimension tends to be used to describe the intrinsic aspect of data, facet emphasises the perspective of people's understanding of data. Often, dimension and facet are inter-exchangeable (Hearst 2006), but in some situations, such as visualising unstructured data, data dimension may be difficult to identify, but data facets can be generated with the help of tools like data mining. Designs have been explored to combine different data and visual facets in support of information search and knowledge visualisation (Hearst 2006, Dachselt *et al.* 2008). Usability studies have

shown that multiscale faceted designs are effective in assisting navigation in large information space (Dachselt and Frisch 2007). It has also been found that facet-based visualisation tools need to provide users with accurate and appropriate facet descriptions in support of information exploration (Hearst 2009). This finding echoes an argument on effective view navigation (Furnas 1997), which suggests that visual information should be sufficient for users to see where to go and at the same time should be succinct to avoid making views cluttered. This issue is even more challenging in dealing with multi-dimensional engineering data, because unlike data sets in these facet-based visualisation tools, which usually already have had pre-defined hierarchical facet structures, multi-dimensional engineering data usually do not have finer structures within individual data dimensions to describe the characteristics of possible data clusters.

In summary, while visually guided knowledge exploration in complex data becomes increasingly important, existing research has not sufficiently addressed the user needs concerning multiscale data clustering of multi-dimensional data.

3. The iMSNCA framework

The iMSNCA framework is an effort to address this issue. This framework has been developed based on our rich experiences in developing visualisation-based knowledge exploration systems (Stump *et al.* 2003, 2004, Zhang *et al.* 2008, Wu *et al.* 2009) and our observations of the design of complex engineering systems (e.g. car, airplane) that involve extensive use of simulation-based design and struggle with visualising the results.

3.1. Framework development

When designers visualise large data sets, one of the primary goals is to identify interesting trends among thousands, if not millions, of design alternatives. For vehicle design, for instance, we may be interested in understanding how car size, car type, engine size, etc., affect vehicle performance characteristics such as torque, fuel efficiency, weight, etc. Designers might also want to know how these performance characteristics are correlated; so, a designer might, for instance, construct a scatter plot of available design alternatives to see how torque and highway efficiency are related (Figure 1(a)). From this figure, the designer might see that the points tend to concentrate in the middle torque region, and a savvy designer might want to explore the data more to identify how this relates to the size of the car (i.e. compact, mid-size, large). After viewing the scatter matrix in Figure 1(b), the values can be grouped by size and groups can be represented by different glyphs to create Figure 1(c), which provides valuable insight among three groups: designs in a size group with lower torques (represented by +) lead to better results than those in other two size groups with higher torques. The designer can review these three size groups in more detail by comparing the average highway efficiency for each group as seen in Figure 1(d). During the exploration, the designer can change the viewing scale of any graph at any time to see general patterns or detailed data.

This example exploration process demonstrates several major tasks in the trade space exploration process. First, the designer selects three dimensions (highway efficiency, torque, and size) out of those available data dimensions and then clusters the data based on the dimension(s) of interest (car size in this case). Next, the designer uses different graph types, a scatter plot and a histogram in this case, to compare data clusters of interest. Some graph types (e.g. histogram) show the aggregate descriptions of data clusters, while some (e.g. scatter plot) do not. Finally, the designer explores design alternatives at different levels of analysis by manipulating the viewing scale of the graphs (e.g. zooming out on the scatter matrix to browse the overall pattern or zooming in the matrix to examine the relationship between any two dimensions).

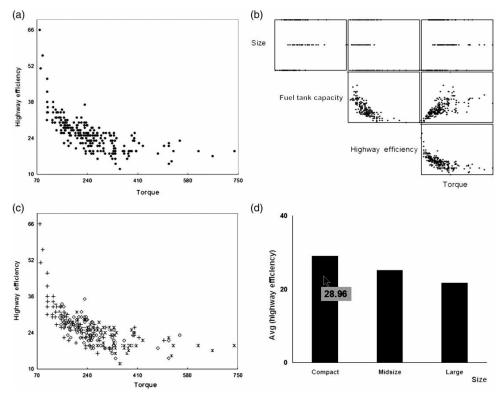


Figure 1. Car design trade-off example. (a) Initial scatter plot. (b) Correlation scatter matrix. (c) Plot glyph coded by size. (d) Average highway efficiency by height.

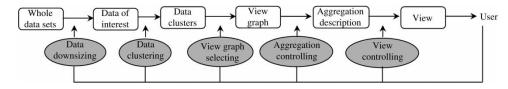


Figure 2. iMSNCA framework for engineering design.

Based on these observations and a visualisation model by Card *et al.* (1999), we propose the iMSNCA framework shown in Figure 2.

This framework elaborates data objects (rounded-squares) and user tasks (ovals) involved in interactive processes of trade space exploration. In the following sections, these tasks are briefly introduced. Detailed descriptions on the algorithms of key task components of this framework can be found in Section 4.

3.2. iMSNCA framework tasks

3.2.1. Data downsizing

There are some benefits to using downsized tables. One of them is to reduce the size of the data that subsequent processes, such as visual mapping and view transformation, have to handle. In particular for large data sets with hundreds or even thousands of dimensions, a downsized

table can dramatically reduce the burden of machine processes and accelerate visualisation speed. Also, with downsized data, unwanted dimensions and information corresponding them can be eliminated on screen, releasing more screen space for important data.

A designer usually relies on data management tools to downsize data. Using a database, for example, the designer has to know how to create tables or index for data subsets. Thus, the designer also needs to master data management tools in trade space exploration. It would be beneficial to integrate interactive tools that can automatically create data subsets based on user actions, with visualisation tools.

3.2.2. Data clustering

Clustering in this case refers to a task that groups data records based on their values in certain dimensions of interest. When a designer is interested in multi-dimensional data, clusters on different dimensions are often needed. Take the aforementioned car design example: the designer wants to know the impact of each design variable, or each dimension of data, on design. It is necessary to examine how different values of a dimension may affect the outcomes of design as well as how these dimensions together may affect designs. Thus, the designer needs tools to cluster data by different design dimensions.

We refer to the clustering of data on multiple dimensions as *multi-dimensional clustering*. Multiple dimensions can be used to cluster the data in different ways. They can be chosen in a *serial* manner, one dimension after the other, or in *parallel*, several dimensions chosen together. For example, suppose two design factors – engine size and the number of cylinders – are of interest in the car design example. With a serial multi-dimensional clustering approach, the designer first clusters design alternatives according to their engine size *or* the number of cylinders first, and then sub-clusters by the other dimension.

The designer often groups data at different scales as well. Larger yet coarser clusters contain more data and can provide a high level of abstraction, while smaller and finer clusters contain less data but provide more accurate information on individual records. Such *multiscale clustering* is important because large clusters can help the designer identify trends and find which clusters to focus on, while small clusters can provide more concrete evidence of trends. With multiscale clustering, the designer can shift between detailed information on individual design alternatives while maintaining a good overall understanding of how alternatives in different clusters may be different from each other. The designer can benefit from tools that support interactive control over data clustering dimensions and if multiple dimensions are involved, the way these dimensions should be linked.

It should be noted that data downsizing and data clustering serve for different purposes in our framework. Both tasks can reduce the amount of data and information users have to deal with, but they achieve this goal in different ways. Data downsizing reduces data amount by eliminating those data dimensions that users are not interested in, while data clustering aggregates data points that share common features so that users will see a small set of data groups rather than a large amount of fragmental data points.

3.2.3. View graph selecting

Various kinds of view graphs can be used in data visualisation; however, choosing an appropriate graph type is important for cognition (Card *et al.* 1999). Different view graphs can serve different purposes in knowledge exploration. Figure 3 shows two other types of view graphs to compare the averages of three groups. In addition to the histogram shown in Figure 1(d), the designer can also use a simple line graph (Figure 3(a)) for ratio or scale data. Or if exploring the fuel

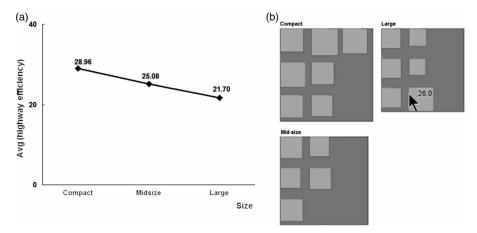


Figure 3. Different view graphs for visual comparison. (a) Line chart for scale or ratio data. (b) Multi-level clustered data as nested boxes.

efficiencies of sub-clusters within three car sizes is needed, the designer can choose a view shown in Figure 3(b) to see how many sub-clusters exist inside each car size and what their average highway efficiencies are based on the relationships of those nesting boxes and their sizes.

3.2.4. Aggregation controlling

To compare clustered data, the designer can use aggregation tools to acquire descriptive information about how clusters differ from one to another. Data can be aggregated in different ways. Often seen aggregation methods include the total count of records, the average, median, and sum of data of interest, the maximum and minimal values of data, etc. It would also be desirable to let the designer choose different data aggregation methods.

3.2.5. View controlling

The designer can control the view of view graphs by panning or zooming. What we are interested in here is the zooming tool that can change the size of viewed objects as well as data clusters. With zooming, the designer can easily move from the glyph-based scatter plot in Figure 1(c), which shows a general pattern but is still cluttered, to a view by which it is easy to compare design options in different clusters side by side (Figure 4).

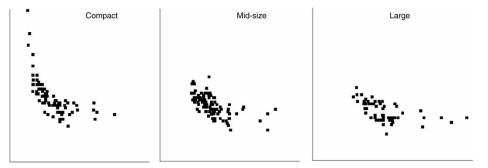


Figure 4. Separated scatter plots of three size clusters.

When data are clustered under two dimensions, the designer can zoom in the graph seen in Figure 1(c) and see scatter plots in two dimensions. Figure 5 shows such two-dimensional scatter plots organised as a spreadsheet (Chi *et al.* 1997), in which the values of car size change horizontally and those of car type change vertically. The designer can compare design options in two dimensions simultaneously.

Changing the view scale from Figure 1(c) to Figure 4 or from Figure 1(c) to Figure 5 also implies a scale change for data clustering since the levels of the data clusters visualised in Figures 4 and 5 are different from that of the data cluster in Figure 1(c). Thus, the notion of scale in our iMSNCA framework differs from the concept of scale in traditional multiscale user interfaces, which is usually regarded as a measure of the rendered size of objects (Bederson *et al.* 1996, Perlin and Fox 1993). Scale in our framework is a measure of interaction activities that include both data clustering and graph viewing. Zooming here is a tool to resize visual objects as well as a means to control the level of data clustering.

Although our research on trade space exploration has studied most of these data manipulation tasks (Stump *et al.* 2003, 2004), it is rare to see systems to support engineering design with interactive data clustering across different scale levels of analysis. This research investigates the design, implementation, and application of the proposed approach.

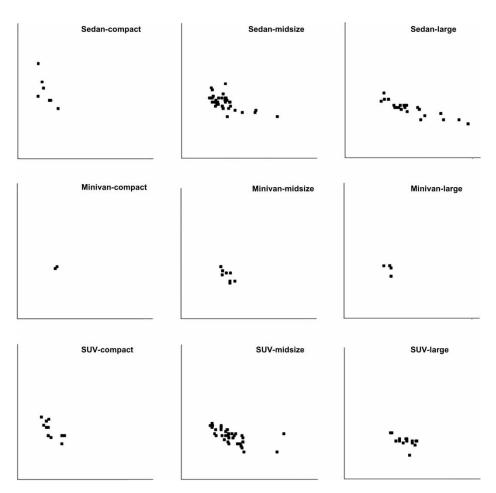


Figure 5. Part of scatter plots matrix on size and type.

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4. Prototype design and implementation

To test the proposed framework, a prototype system is developed. In this section, we introduce the analytical forms of data downsizing, clustering, and aggregating and describe the design and implementation of the system. Analytic forms are developed to provide a formal definition for downsizing, clustering, and aggregating tasks and to guide their implementation.

4.1. Analytic forms for data transform

Let us define a raw data set D with n-dimensions:

$$A = \{a_1, a_2, \dots, a_n\},$$
 (1)

where A is the set of all dimensions; a_i is one dimension; and n is the total number of dimensions. Any data record in the data set is

$$d = (da_1, da_2, \dots, da_n), \tag{2}$$

where da_i is the value of the record on the a_i dimension.

Then, the data set can be written as

$$D = \{d_1, d_2, \dots, d_m\},$$
(3)

where d_i is one record and *m* is the total number of records.

4.1.1. Downsizing

Downsizing is a task to generate a subset, D_s , out of D. D_s is written as

$$A^{s} = \{a_{i}^{s} | a_{i}^{s} \in A, i = 1, 2, ..., k\}$$

$$d^{s} = (da_{1}^{s}, da_{2}^{s}, ..., da_{k}^{s})$$

$$D_{s} = \{d_{1}^{s}, d_{2}^{s}, ..., d_{k}^{s}\},$$
(4)

where A^s is the set of all dimension chosen for a data table; a_i^s is its member; k is the total number of its members; d^s is a data record of the subset D_s ; and da_i^s is its value on the a_i^s dimension.

4.1.2. Clustering

Assume all possible values of a dimension a_i make up a set, Va_i . k clusters can be created on the dimension, and the value ranges of each cluster are defined as sets V_i , $i = 1 \dots k$.

Assume a_c is the clustering dimension. Then, a cluster is

$$C_{i} = \{d^{s} | d^{s} a_{c} \in V_{i}\}i = 1, \dots, k,$$

$$V_{i} \subset V a_{c}, \Sigma V_{i} \subset V a_{c} \quad i = 1, \dots, k,$$

$$V_{l} \cap V_{m} = \phi l, m = 1, \dots, k, l \neq m,$$
(5)

where C_i is a cluster.

4.1.3. Multi-dimensional clustering

Multi-dimensional clustering chooses different a_c . For *parallel* multi-dimensional clustering, multiple dimensions are applied at once. Assume two clustering dimensions are a_{c1} and a_{c2} and the numbers of data clusters on each individual dimension are k^1 and k^2 , respectively. A cluster C_l under this parallel multi-dimensional clustering is

$$C_{l} = \{d^{s} | d^{s}_{a_{c_{1}}} \in V^{1}_{i} \text{ and } d^{s}_{a_{c_{2}}} \in V^{2}_{j}\} \quad i = 1, \dots, k^{1}, \ j = 1, \dots, k^{2}, l = 1, \dots, k^{1} \times k^{2}, V^{1}_{i} \subset Va_{c1}, \qquad \sum V^{1}_{i} \subset Va_{c1} \ i = 1, \dots, k^{1}, V^{1}_{l} \cap V^{1}_{m} = \varphi \quad l, m = 1, \dots, k^{1}, \ l \neq m, V^{2}_{i} \subset Va_{c2}, \sum V^{2}_{i} \subset Va_{c2} \quad i = 1, \dots, k^{2}, V^{2}_{l} \cap V^{2}_{m} = \varphi \quad l, m = 1, \dots, k^{2}, \ l \neq m.$$

$$(6)$$

Multi-dimensional clustering with more clustering dimensions can be defined similarly.

As shown, how many data clusters should be created in our method is based on a given number. For discrete variables, such as categorical variables, this number can be determined by the number of all possible values and data clusters can be created by group data with similar values. For continues variables, this number can be specified by users and then clusters can be created with k-mean algorithms.

4.1.4. Multiscale clustering

For multiscale clustering, a cluster may have sub-clusters. Assume a cluster C_i is further divided into q sub-clusters according to a clustering dimension a'_c , and the value ranges of each sub-cluster are defined as sets V'_i , j = 1, ..., q. Then, all of the sub-clusters of C_i can be written as

$$C_{i,j} = \{d^{s} | d^{s}_{a'_{c}} \in V'_{i}\} \quad i = 1, ..., q,$$

$$V'_{i} \subset Va'_{c}, \qquad \sum V'_{j} \subset Va'_{c} \ i = 1, ..., k,$$

$$V'_{l} \cap V'_{m} = \varphi \quad l, m = 1, ..., k, \ l \neq m,$$
(7)

where $C_{i,j}$ is a sub-cluster within the cluster C_i . In this multiscale clustering, clustering dimensions at different scales, a'_c and a_c , could be the same or different.

4.1.5. Aggregating

With data clusters, aggregation can be done easily as long as the dimension(s) that would be aggregated and the aggregation functions are known or specified. Assuming the dimension to aggregate a_g , for a particular cluster C_i , its aggregated description is

$$G_i = F(d_{1|a_p}^c, \ d_{2|a_p}^c, \dots, d_{p|a_p}^c),$$
(8)

where G_i is the aggregated value of C_i ; F is the specified aggregation function; $d_{i|a_g}^c$ is the value of the *i*th member of C_i on the dimension of a_g ; and p is the total number of elements in C_i .

It should be noted that in our framework, how individual data sets are generated is less of a concern. Data clusters can be created by conventional methods (e.g. *k*-mean clustering and

hierarchical clustering), database queries (e.g. using aggregation functions to create data groups), or other advanced statistic approaches. What really matters here is the capability that designers need to interact with a clustering method in determining what data dimension should be chosen to cluster data, what different scales should be applied in clustering, and how to aggregate clustered data. In this sense, the clustering concept we discuss here emphasises interactive data clustering that involves both raw data and user interests in data analysis. Massive research has been done on data clustering algorithms, but little attention has been given to user interaction with such clustering methods. The focus on this framework is on integrating the user factor with advanced data analysis methods in knowledge discovery, rather than on the development of clustering methods.

4.2. User interface design

Figure 6 shows the overall user interface of the prototype system after a designer provides information about the database and table where the data of interest are stored. The user interface has eight panels. Panels 1–4 are for data control. When raw data is ported into the system, the names of all data dimensions are displayed in Panels 1 and 3 for the designer to choose what dimensions to observe (Panel 1) and to what dimensions data are clustered (Panel 3). In Panel 2, the designer can choose aggregation methods (e.g. simple count, average, sum). Panel 4 allows the designer to choose data filtering.

Panels 5–7 are for results display and interactive view control. Panel 5 shows view graphs and allows the designer to zoom and pan workspace as well as to choose different graphs. Panel 6 is a scale canvas that shows the viewing scale and allows the designer to manipulate the clustering order when multiple clustering dimensions are involved, of which we will provide more details later. Panel 7 displays the data results in text corresponding different analysis operations.

4.2.1. Choosing dimensions to observe and aggregate

The designer can choose one or two dimensions to observe simultaneously. When two dimensions are selected, a scatter plot is generated and displayed in the primary view, as shown in Figure 6. When the designer chooses one dimension to observe and another dimension to cluster, visualisation results show different clusters and their aggregated values. Based on the data from the car

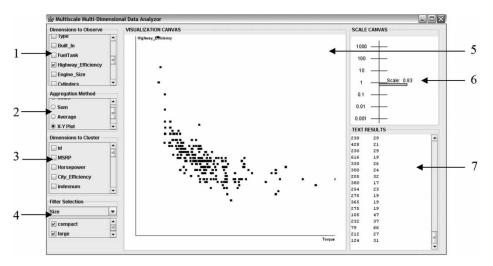


Figure 6. User interface of the prototype system.

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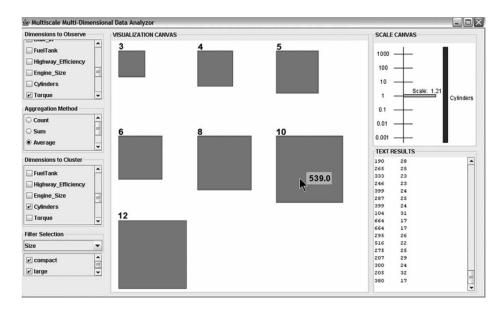


Figure 7. Example of four clusters based on different observing and clustering dimensions.

design example, Figure 7 shows a view with torque as the dimension to observe and the number of cylinders as the clustering dimension. The seven boxes indicate seven clusters and box size corresponds to the aggregation result, which is the average torque, of each cluster. It is easy to compare different clusters based on the box sizes.

4.2.2. Choosing multiple clustering dimensions

The designer can also choose different dimensions to observe the same data set. Different dimensions can be observed either independently or combined simultaneously. Keeping multiple dimensions independently, the designer can switch from one clustering dimension to another. Figure 8 is a view under the same aggregation method as in Figure 7, but with a different clustering dimension (car size here). As seen, different clusters are produced under different clustering dimensions.

Combining different clustering dimensions together creates multiscale and multi-dimensional clustering. Figure 9 shows the view results of choosing both car size and the number of cylinders as clustering dimensions. Figure 9(a) is the clustering result under car size only. Zooming in, the designer sees each size cluster has several sub-clusters on the number of cylinders (Figure 9(b)). Zooming in further, the designer finds details of individual clusters on car size and the number of cylinders (Figure 9(c)). The nesting boxes show the relationship between these two clustering dimensions and provide contextual information about individual clusters and their parent or child clusters. The transition from Figure 9(a) to (c) is continuous and smooth through semantic zooming (Furnas and Bederson 1995, Bederson *et al.* 1996).

4.2.3. Control multiple clustering dimensions

The designer can manipulate the ordering of the dimensions for clustering when multiple clustering dimensions are involved (e.g. cylinder number clusters within car size clusters or vice versa). Controlling the ordering allows exploring data from various aspects. The ordering of clustering

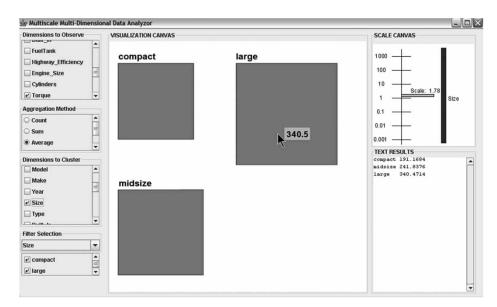


Figure 8. Different clustering dimensions.

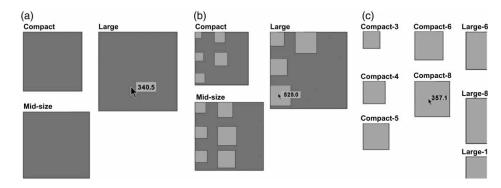


Figure 9. Multiscale clustering. (a) Clusters on car size. (b) Sub-clusters on cylinder number within size clusters. (c) Clusters on car size and cylinder number.

dimensions is achieved in the scale canvas through direct manipulation. Each clustering dimension is represented as a bar in the canvas (Figure 10). These bars are stacked together and can be dragged and dropped. Figure 10 shows the process adjusting the two clustering dimensions in the example of Figure 9. Consequently, the nesting relationship between clusters in these two dimensions is reversed.

4.3. Implementation

The prototype is implemented with Java and the Piccolo toolkits (Bederson *et al.* 2004). It has three layers. The bottom layer processes raw data and converts the data from other formats (e.g. tab or comma-delimited raw data) into a MySQL database. The middle layer is a module to connect the user interface with the database. The responsibilities of this layer include formulating SQL queries based on user preferences (e.g. data dimension, aggregation method, and filtering method), sending queries to the database, receiving query results, and constructing data tables. As discussed previously, the focus of this framework is on integrating the user factor with advanced

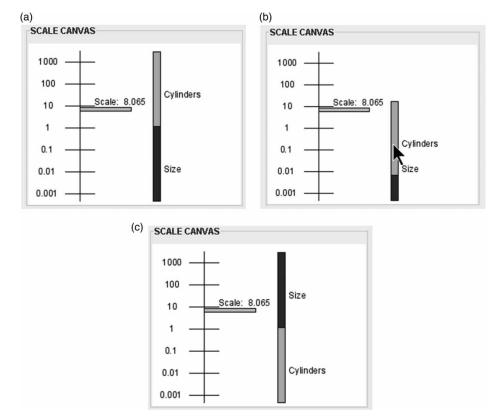


Figure 10. Adjusting the ordering of clustering dimensions. (a) Initial order, (b) adjusting the order, and (c) final order.

data analysis methods in knowledge discovery, rather than on the development of clustering methods. One of the assumptions here is that users can choose any appropriate clustering method for targeted data type. Thus, this layer also includes a module that can plug in other data clustering methods. Finally, the top layer includes a user interaction module and a visualisation module. The interaction module takes and processes the user's inputs and sends information to the middle layer or the visualisation module. The visualisation module presents graphs based on data tables from the middle layer and user preferences.

5. Evaluation study: morphing wing design

To better understand how the iMSNCA framework can help engineering design, we conducted a preliminary study to evaluate the use of our prototype system in a real design scenario. The study involved two doctoral students, both with an engineering background, and used an engineering task involving the design of morphing wings for aircraft.

The study was based on focus group observation and interviews. The reason for choosing this method was due to our interest in knowing how our visualisation system would be used and what the advantages and disadvantages our system may have, compared with other tools. We did not use lab experiments for two reasons. First, we could not find other comparable tools that can offer similar support for multi-dimensional and multiscale data clustering and aggregation. Without such tools for comparison, a controlled lab experiment was less meaningful. Second, it was not our interest to measure user performances (e.g. task completion time) when using our system as a

stand-along tool. Our ultimate goal is to integrate this multi-dimensional and multiscale clustering and aggregation tool with other visualisation systems, such as ATSV (Stump *et al.* 2003, 2004).

5.1. Design task and design data

Recently, there has been military and commercial interest in designing a wing that can 'morph' from one configuration to another to improve aircraft performance during each phase of its mission (Lesieutre *et al.* 2006). A potential drawback of such a morphing wing is the added weight due to the actuators and structural supports that it would require. This requires trade-offs during their design, namely maximising the change in wing shape while minimising the added structural weight.

For this study, we varied six input (design) variables to generate 716 different design alternatives (note: several input combinations are not feasible designs). These six variables and their possible values are:

- (1) Gross weight (Wo): 4 levels (1, 10, 100, 1000)
- (2) Cell material (Mat): 2 levels (Mat 1 or Mat 2)
- (3) Number of rows (NR): 4 levels (2, 4, 8, 10)
- (4) Aspect ratio (AR): 3 levels (2, 3.5, 5)
- (5) Cell fraction (Cf): 3 levels (0.5, 0.75, 0.9)
- (6) Goal weight (Goal): 3 levels (0.65, 0.75, 0.85)

For each design alternative, we recorded the predicted change in span (dSpan) and structural weight (Wst). The design objective was to find the best design that maximises dSpan while minimising Wst, i.e. the design that offers the best compromise between these two competing objectives. While this type of problem is traditionally solved using multi-objective optimisation techniques (Browne *et al.* 2006), our intent was to examine whether the iMSNCA framework can help designers to identify trends and discover new knowledge about this complex structure that would otherwise be missed if relying solely on optimisation. Given the uniqueness of the structure, these insights are more useful and important at this conceptual stage of development than is finding the 'best' design, which will certainly change as we learn more about the capabilities of such a morphing wing.

5.2. Procedure

In a study session, a subject was first informed about the design task – maximising dSpan while minimising Wst – and was asked to identify the values of design variables that could lead to the best wing. The subject was given time to study a set of 10 sample designs in a spreadsheet and to ask questions about the task. The sample designs had the same six design variables and the two outputs (dSpan and Wst). Among these sample points, two were optimal with maximum dSpan and minimum Wst, two were unacceptable with minimum dSpan and maximum Wst, and the remaining were in between these two extremes. To make sure the subject understood the design task, the subject was asked to identify all possible optimal designs as well as all possible unacceptable ones before using the visualisation tools. If any design was wrongfully identified, the subject was given more time to study the data and the objectives until correct identifications were made.

Two student subjects participated in two separated sessions of the study. In each session, a subject was first provided with four tools: our prototype system, ATSV, Matlab, and Excel. ATSV is a system that supports the exploration of a multi-dimensional trade space with a set of visualisation tools (Stump *et al.* 2003, 2004). We used its latest version (V 4.6.4, 2008) in the

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study. Matlab and Excel also offer tools for multi-dimensional data visualisation and analysis. One subject rejected Matlab and chose Microsoft Excel instead because the subject thought the graphing tools in Excel were sufficient to the task. The other subject declined Excel. Each subject was provided training on the use of our prototype system and the multi-dimensional visualisation tools in ATSV. No training on Matlab or Excel was provided because subjects were already familiar with these tools.

After training, the subject was given 716 design alternatives and asked to solve the design task. The subject was told that any of the tools—our prototype, ATSV, Matlab, and Excel—could be used to optimise the wing and that the activities associated with the use of these tools would be observed. After finishing the task, the subject was interviewed about the experience in the study.

Both subjects finished the task. One session lasted about 2 h (the subject who used Excel), and the other session was about 2.5 h (the subject who used Matlab).

5.3. Results

Both subjects correctly identified the values of the four design variables that could lead to the best wing design. Although two subjects used all three tools in exploring data, their final decisions were primarily based on the visualisation with our prototype system. Our observations show that both subjects extensively used the following tools provided by our prototype system:

- choosing individual data dimensions for data clustering and aggregation;
- switching between different aggregation methods to understand the size of data cluster, and the average value of a dimension of interest;
- combining two or more dimensions in data clustering and aggregation;
- changing the granularity of data clusters in exploration, either along one data dimension or switch between different dimensions.

Figures 11–14 show some visual results of a subject who relied on our prototype system to analyse various design variable combinations. Figure 11 is a 2D scatter plot of the outputs – Wst on the x-axis and dSpan on the y-axis – of all 716 design alternatives.

Figure 12 is a view that shows output data clusters based on a design dimension, namely cell material (Mat). As shown in the figure, the Mat 2 option (Figure 12(b)) provides noticeably lower Wst as seen by the points residing close to the *y*-axis, while for Mat 1 (Figure 12(a)), there are 'gaps' along the *y*-axis for very low values of Wst. This difference implies that the Mat2 option is probably a better choice.

Figure 13 was used to examine two variables, AR and Wo, at once to identify interesting correlations between these two dimensions. As shown, when Wo is low (the first row), the impact of AR on the outputs is less significant, compared with designs with high Wo designs (the second and third rows). This implies that lower values of AR and Wo are much more preferable since they yield higher dSpan values for lower Wst. The worst case would be high Wo and high AR at the lower-right corner, which leads to high Wst and low dSpan – the complete opposite of the design task given to the subjects.

Based on these trends, the subject constructed a plot to 'zoom in' on promising design alternatives. Figure 14 is a view that shows alternatives with the Mat 2 option and Wo = 1 (square) and Wo = 10 (cross), where the data are clustered based on NR and AR. In the figure, AR increases from left to right, and NR increases from top to bottom. As shown, if low Wst values are chosen, then lower NR values are more desired and that lower AR values tend to yield higher values of dSpan, which satisfy the design goal. The figure also shows that as AR increases, higher NR values tend to yield lower Wst values, which is an interesting interaction that would be missed without this multi-dimensional clustering. Finally, the figure shows that Mat 2 is a better option,

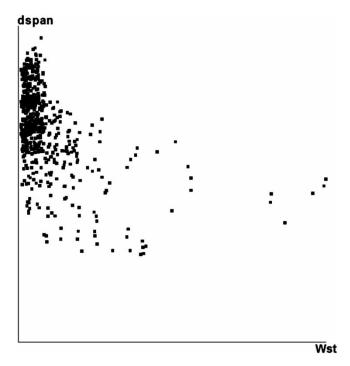


Figure 11. Scatter plot on outputs.

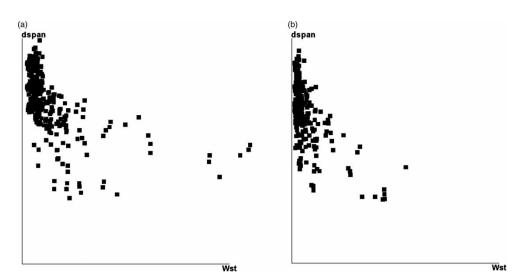


Figure 12. Scatter plots of two data clusters based on cell material (Mat). (a) Cluster on the Mat 1 option. (b) Cluster on the Mat 2 option.

and that NR and AR are highly correlated at the upper end of their respective ranges, which poses unique opportunities for resolving this trade-off while also creating the potential to yield a poor wing design as well.

A couple of interesting user behaviours were observed during the study. First, both subjects abandoned the tools in Excel and Matlab quickly. The subject who chose Excel actually started the task in Excel but got frustrated with its graphing tools and switched to ATSV and then our

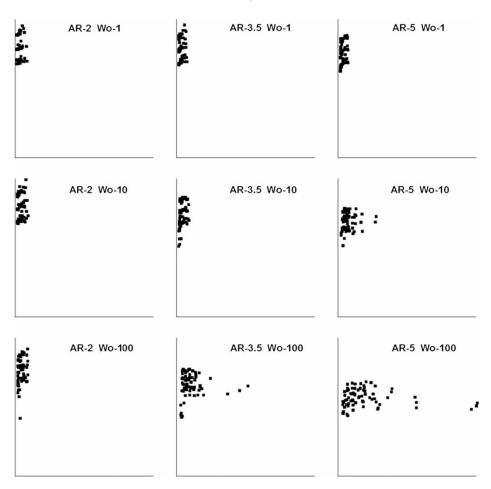


Figure 13. X-Y plot matrix under two clustering dimensions.

prototype system. The other subject first used all three tools – our prototype, Matlab, and ATSV – to generate a scatter plot similar to Figure 11. However, after moving to multiscale clustering views in our prototype, the subject failed to duplicate these views in Matlab and then gave up Matlab. Interestingly, the subject returned to Matlab after completing the task and used it for about 15 min.

When both subjects were asked in the post-task interview about why they stopped using Excel or Matlab, they cited the significant amount of work required to generate the necessary figures when using the graphing tools in Excel or Matlab as the primary reason. The subject using Matlab indicated that after finishing the task, Matlab was used to try and replicate the spreadsheet-like multi-dimensional and multiscale clustering graphs similar to Figure 14 from the prototype system. The attempt was unsuccessful, however, because it was 'tedious' to generate 'many intermediate data matrix needed to create similar views' and to 'arrange these views in a reasonable way' for comparison.

Second, although subjects checked data with ATSV every now and then, they spent most of their time on our prototype system. One subject often used the 3D scatter plots in ATSV, and the other used the brush tool in ATSV; however, such use was relatively brief, as subjects usually spent much longer using our prototype system to cluster and aggregate data. In the post-task interview, subjects said that they used ATSV primarily for the purpose of confirming their findings they

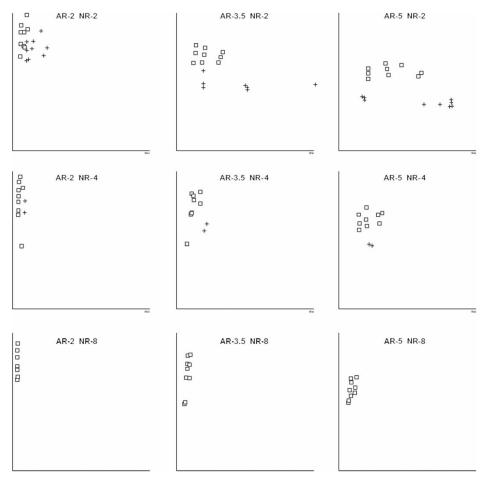


Figure 14. Three-dimensional clustering. (Clusters on the third dimension are glyph coded.)

got from our prototype system. They also indicated that although the visualisation tools in ATSV (e.g. brushing, 3D scatter plots) could present different data clusters, it was not easy to compare clusters of design variables, because (a) data were 'cluttered within one view', and (b) no tool was available to control the size and level of data clusters.

When asked about their opinions on the prototype system and their experience in using it, both subjects gave positive comments on our prototype system. They believed the design was 'very effective' in assisting information exploration and knowledge discovery in multi-dimensional data. In particular, the flexibility in 'combining different design variables at different granularities' was seen as novel and beneficial. Both subjects regarded the continuous zooming tool as very useful and provided contexts in understanding the relationship among different data clusters. The subject using Matlab wanted to replicate our tools in Matlab for future use. Furthermore, one subject indicated that arranging multiple views side by side based on different data dimensions had greatly helped the decision-making by simplifying the comparison of different design results.

Some issues were also raised during the post-task interview. First, it was suggested that the current views, which are still 2D-based, limit the data dimensions that can be combined and compared. Although our prototype system used glyphs and colour coding to address this issue, subjects felt that the system should support 3D views. Second, a subject pointed out that view transitions in changing the level of clustering and switching clustering dimension were abrupt,

making it difficult to understand how views before and after switching were connected. Furthermore, both subjects mentioned that our multiscale clustering and aggregation tools would benefit from being integrated into a visualisation tool like ATSV.

6. Discussion

The preliminary evaluation study results are encouraging. It shows that the proposed framework and the multi-dimensional, multiscale data clustering tools can benefit knowledge exploration of engineering data. Our tools allow designers to compare different design alternatives from different dimensions and at different scales and to identify how individual design variables may affect design outcome and how they may be correlated. Designers can identify some 'best' designs from a given data set and the corresponding value regions of design variables. The tool also helps identify regions that lead to bad (i.e. non-competitive) designs.

The contributions of our multiscale-nested clustering and aggregation framework include the following. First, our framework outlines a practical method in analysing multi-dimensional data visually and provides formalised definitions of this method. These definitions can guide the design and implementation of visualisation tools to analyse multi-dimensional data in engineering design at different levels of granularity. Second, the user tasks that we discussed in our framework may shed some light on visual analytics tasks in designer-driven engineering design methods, such as trade space exploration. Visual analytics becomes increasingly important to tasks like engineering design that deal with large data sets. However, many challenges still exist in developing general visual analytics tools, including identifying basic analytical tasks and reducing the complexity of information displayed on workspace (Thomas and Cook 2005). Our multiscale-nested clustering and aggregating approach will not only enrich the repertoire of analytical tasks but also help to control the amount of information to visualise. Furthermore, our research advocates a multidisciplinary approach to support engineering design. This approach involves the analyses of a designer's diverse tasks in manipulating and understanding complicated data, the use of advanced computational tools to assist data feature detections, and the design of visualisation tools to present data characteristics that are critical to design. We believe that when the interactions among designers, design data, data processing algorithms, and design support systems become more and more important, as seen in trade space exploration, a good design support system must integrate human factors (e.g. design tasks) and information factors (e.g. data dimensions or data values).

Some limitations exist in this research. For the theoretical framework, the key tasks are incomplete as they are based largely on our empirical observation of engineering design. To improve and validate the framework, we need to consider more diverse user tasks. On the aspect of system design and implementation, our prototype can also be enhanced in many ways. For example, we need better tools for selecting the dimensions of interest. Currently, users need to specify these dimensions one by one using checkboxes. For large data sets with hundreds, or even thousands, of dimensions, going through all dimensions to identify interesting ones is a daunting task for users.

Future research efforts will proceed in several directions. First, we will refine our framework by investigating what other interaction tasks should be included, such as cluster-size manipulation. Second, we will explore the integration of advanced statistics methods on data clustering and dimension reduction, as discussed in (Unwin *et al.* 2006, Cook and Swayne 2007), into our iMSNCA framework to offer designers more comprehensive data analysis tools. Furthermore, we plan to validate our framework and system with industry data (e.g. corporate marketing data) and research data (e.g. physiology data) by soliciting data from engineering designers and making our prototype system public for downloading.

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