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Enhancing Engineering Design through Topological Data Analysis (TDA) and Adaptive Clustering Algorithms

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ABSTRACT

This paper explores advanced methodologies for component analysis and clustering in engineering design processes, focusing on generalized Principal Component Analysis (g-PCA) and topological data analysis (TDA). We discuss deep-learning-based methods that minimize information loss (MIL) and adaptive clustering algorithms for equal variance circles and g-circles. Additionally, we review traditional and modern approaches to component analysis, highlighting TDA's role in extracting topological features such as Betti numbers. TDA's integration into engineering design is examined through various applications, demonstrating its ability to manage high-dimensional data and optimize complex systems. Future research directions are proposed to further leverage TDA and machine learning for robust and efficient engineering design optimization.

Keywords: Topological Data Analysis, Generalized Principal Component Analysis, Adaptive Clustering, Information Loss Minimization and Engineering Design

INTRODUCTION

In the era of big data and complex system design, traditional statistical methods often fall short in capturing and interpreting the intricate structures and patterns within high-dimensional datasets. This has led to the emergence of advanced analytical techniques, such as generalized Principal Component Analysis (g-PCA) and Topological Data Analysis (TDA), which offer more nuanced approaches for data simplification and pattern recognition [1-5]. These methods are particularly valuable in engineering design processes, where understanding the underlying structure of data is crucial for optimization and innovation. Generalized PCA extends the conventional PCA by incorporating methods that minimize information loss and consider within-cluster dispersion [6-8]. Deep-learning-based clustering algorithms that leverage g-PCA principles have shown significant promise in enhancing the accuracy and robustness of data clustering. These methods utilize adaptive clustering algorithms to form equal variance circles and g-circles, effectively capturing the variations and patterns in complex datasets [9-10]. In parallel fashion, Topological Data Analysis (TDA) has emerged as a powerful tool for extracting topological features from data, providing insights into the geometric and structural properties that traditional methods often overlook. By computing topological invariants such as Betti numbers, TDA allows for the identification of connected components, loops, and voids, offering a comprehensive view of the data's shape and structure [11-14]. The integration of TDA with other modern techniques, such as machine learning and manifold learning, has opened new avenues for addressing the challenges of high-dimensional data analysis. TDA's ability to handle noisy and outlier-rich datasets makes it particularly effective in various engineering applications, from aerospace and material engineering to electrical and mechanical engineering [15-18]. This paper aims to explore the synergy between TDA and g-PCA, focusing on their application in enhancing engineering design processes [19-20]. This paper discusses the methodologies involved, review the existing literature, and present case studies demonstrating the practical implementations and benefits of these techniques. Furthermore, we will outline future research directions to advance the integration of TDA and machine learning in optimizing complex systems, thereby contributing to the ongoing evolution of engineering design optimization.

Introduction to Topological Data Analysis

Few methods that are also fall into category of generalized Principal Component Analysis (g-PCA) are deep-learning-based method that uses minimization of information loss (MIL) clustering algorithm. The MIL-based method can be classified further based on the methods that consider within cluster minimization of dispersion of the distances of data points of the cluster from the center of the cluster, and another is the methods that besides dispersion of the data points of the clusters from their centers, also minimize the dispersion of distance of the centroid from the centre of the dataset [21-24]. The clustering-based methodology is based on the adaptive clustering algorithm to cluster the equal variance circles and g-circles of the datasets. This approach enhances the accuracy and robustness of the clustering process, allowing for more effective handling and interpretation of complex datasets. By incorporating the adaptive clustering algorithm, the method is able to identify and group similar data points together, leading to the formation of clusters that accurately represent the underlying structure of the dataset [25-28]. Through the utilization of equal variance circles and g-circles, the method is able to capture the variations and patterns present in the data, providing a comprehensive view of the dataset's characteristics. Overall, the clustering-based methodology utilizing adaptive clustering algorithm in combination with g-PCA presents a powerful approach for analyzing and understanding complex datasets. The currently available methods for component analysis includes [29-30]. Classical PCA, probabilistic PCA, ICA, factor analysis, factor analysis models for data consisting of multiple data types simultaneously, multidimensional scaling (MDS), kernel PCA, isomap, and locally linear embedding, and spectral embedding. The method called principal curve analysis are disjointed methods and does not cover all applicable classes of functions. TDA uses topological methods to analyze data and is related to persistent homology [31-35]. In TDA, the main goal is to extract basic topological properties of the underlying spaces. Topological data analysis is one of the leading approaches that bridge the gap between topological methods and data. It has received the spotlight from the research community to analyze the shape of data and find the intrinsic structure of the data. TDA uses topological descriptors like holes, connected components, and high dimensional simplicial homology groups to analyze the shape of the data. The application of TDA is extended to various fields of data science, in particular, to analyze the high-dimensional data efficiently [30]. The importance of geometry in data analysis [36-38]. Indeed, traditional statistical methods often fail to capture and extract information from high-dimensional datasets. Data is often difficult to visualize and the traditional mean and covariance matrix are not computed for the data respectively. A vast amount of information in the structure of the dataset can be extracted using topological methods. In this survey paper, we first clarify the terms of geometry, shape, topology, and analyze to what extent exploring the geometry is useful in data analysis [39-42].

Definition and Principles

The first step in topological data analysis is often the construction of the cubical or simplicial complexes, and then the determination of the homology of it to extract the topological features that can be reconstructed through connected lines, i.e. they are not distorted. The main output of this first step is the computation of the Betti numbers which count the number of connected components, loops and voids counted with their corresponding number of holes. These invariants do not depend on the parameters of the complexes and give a determination of the topological features [43-45]. TDA is algebraic in nature but purely combinatorial. It is built upon defining a sequence of approximations to data structures through a discrete family of topological spaces: the α-skeletons. These spaces inherit certain abstract algebraic structures, which can then be analyzed in order to discern the shapes of the α-skeletons. In particular, Betti numbers from the homology of the α-skeletons give information about the number and kinds of connected components, holes, and voids in the collection of points sampled by the dataset [phi], all of which can be considered as special forms of shapes of interest. Besides appearing in the triangle-inequality, and hence also in analysis of that kind, such notions are used throughout mathematics [43-45]. Topological Data Analysis (TDA) is a modern method of extracting and analyzing the relevant structures, shapes, and spatial relationships that can be transformed (deformed) continuously from complex data. It approaches the target of simplifying data by mapping the data into a continuous space, transforming the data, and then mapping it back without loss of relevant structural information. As such, TDA is building on the idea that dimensionality reduction and feature extraction are crucial steps in many complex data analysis tasks. However, with its emphasis on problems presented in the context of geometric and topological regularity, TDA differs in focus from popular spectral and variational problems of classical dimensionality reduction [46-47].

Engineering Design Processes in Complex Systems

Our previous simulation work mostly focused on using topological summaries in time invariant graphs, because of the need to merge data from different repetitions, e.g., a tradeoff with short filtering time yields little topological features. Using those graphs to predict system behavior, where the needed topological summaries are generically unclear. But many industrial designs can be better represented by dynamic graphs as the interconnections, manufacturing rules and management laws could change over time. Such structural changes are not necessarily due to malfunctions, as they can also reflect adaptive, self healing, or reconfiguring processes [5-8]. Dynamical changes are then allowed to be part of the design strategies if they do not lead to more dangerous conditions. Devices prohibiting transmission, rather than interfering with the structure, are decisions that block detouring once routes all become part of overlapping cycles. Consequently, we could tackle design challenges using topological data analysis (TDA) techniques, which could effectively guide design processes by tapping on the structure of those coupling relations. Persistent homology assigns topological summaries (Betti numbers) to a family of increasingly filtered “proximity graphs” created from data. These elementary materials allow us to build connectivity summaries with a low-dimensional order, which we rearrange into more abstract and powerful concepts to assign topological characteristics – such as cavities or loops – for an array of diverse datasets. Such global industrial networks implement various control and protection mechanisms, where these constraints are maintained at most times and are allowed to change as the system adapts or responds to external stimuli. This structuring – particularly considering the hierarchies – endows the framework with robustness and resiliency, where the utility of these assumptions can be assessed from the topologically driven industrial design processes [10-14]. Engineers are frequently required to design complex systems that are interconnected, multi-scale, and subject to uncertainties. In the digital age, modern design frequently drives systems into operation through distributed and autonomous processes rather than centralized logic [16-19]. As a result, the design insights emerge from complex, adaptive, and self-organizing behavior of sub-systems [20-26]. As small-scale complexity compounds into emergent global behaviors that cannot be organized, treated nor understood, control engineering neither offers a sufficient direction to guide design processes [27-29]. One alternative is to recognize that complex systems produce topological structures that are robust under perturbations; particularly in the presence of hierarchies, constraints, and feedback mechanisms.

Challenges and Opportunities

A few noteworthy opportunities and challenges of TDA techniques that are attributed to optimization, approximation, and performance of engineering design processes in complex system based on TDA are listed below. With the fast development of TDA, it has been applied across engineering design tasks to directly analyze the data spaces by including both the functional relationships [30-37]. The main attractive property of TDA is that it can convert the complicated data spaces into simple meaningful shapes that inform the characteristics of the data. While there have been successful demonstrations as a preliminary step towards this direction, it has been recently argued that to consider TDA as a mature approach across all engineering design tasks in complex systems, more robust TDA tools and guidelines are necessary [31-36]. At present, engineering design problems are increasingly more complex in any field - from manufacturing, structure design to network optimization. The design processes are generally driven by optimization strategies, and the design areas are represented through multidimensional data obtained from different sources depending on the problem at hand. The main goal of design process is to tailor some of these data points towards the desired objectives. The challenge is that in many difficult-to-model engineered systems, the function of some design parameters is unknown or too complicated to model. Today, engineers directly optimize over large data spaces, either through non-parametric modeling or by using computationally expensive physics-based simulators [37-40].

Integration of TDA in Engineering Design

TDA opened a new page in state-of-the-art engineering systems analysis – through the adjustment of its algorithms, it is now seen as a potent tool for dealing with a host of different engineering topics, a lot beyond contemporary manual, most popular uses in machine learning. The embedded logic and control flow for utilizing TDA in engineering systems are at present inchoate and are currently mostly familiar to only a limited number of scientists or engineers [25-30]. In this effort, we hope to bring the technologies to a much broader audience and to show that TDA is of direct applicability in many sophisticated engineering systems, because it provides a range of computational analysis methods to solve sophisticated, and often, very high-dimensional design-related problems. Topological data analysis (TDA) represents an innovative strategy for the simplification, compression, and then analysis of large datasets by identifying non-linear patterns within them, thus building on - and often improving over - information gained from existing analysis approaches. TDA in future systems engineering requires the slotting together of the various abstract and rigorous or formal mathematical methods (e.g. from computational algebraic topology, from statistics and statistical geometry, from machine learning and clustering, from manifold learning, and from a collection of recent new directions involving, for instance, persistent topology and as homology) emphasizing the coordination of data (and data analytics) and mathematical structures and tools, thereby leading to the new, hybrid branch of systems analysis known as TDA [30-32]. Methods for optimizing complex systems design weighted heuristics more heavily than data [20-25]. Not until recently has the ascension of complex system simulation and data acquisition and storage capability obliged a reversal to evolve engineering design back toward a bottom-up or analysis problem. Understanding the form and meaningfulness of large datasets has become a significant challenge for complex systems design optimization (CSDO) [26-30].

Benefits and Applications

There are several significant benefits and applications of TDA, especially for complex systems. Let us summarize. Firstly, TDA can flexibly transform various data types (e.g., images, meshes, feature vectors, signals) into topological abstracts. Therefore, it can be naturally introduced into multi-model, heterogeneous data analysis [6]. Secondly, TDA has low-dimensional and so-called injective representations of high-dimensional datasets. It was provided with relatively high-level computation efficiency in some datasets [8]. Thirdly, TDA is a model-free method, and it is especially effective in complex datasets with a big outlier or noising data. TDA and TDA-based machine learning methods have demonstrated great success in some medical datasets, where traditional methods fail, with the introduction of penalty or shrinkage. Fourthly, similar to other "math knowledge", the topological structures are also stable under certain conditions. That is to say, the insight of TDA results generalizes well to the related dataset or unseen data [9]. Fifthly, TDA was intrinsically statistical and machine learning method pure in some sense. Therefore, the existing iterative improvements of tree, filtration and persistence can be further delivered and developed. For example, Rips sheaves introduced in graph sheaf can be further introduced and improved in TDA at the level of ridge sheafs, which is missing in the existing library. Finally, assessing TDA may be helpful for nature and society. Sequential behaviors of complex systems can be linked to following categories, safe, risk, and failure. Ideal, less adsorbable methods, are always preferred to approach the boundary of data revolution [10]. Topological Data Analysis (TDA) is a collection of tools for studying the shape and geometry of data 15-19]. As an efficient and flexible data method, TDA has been introduced into traditional dimension reduction and pattern analysis fields. TDA can summarize high-dimensional datasets based on topological structures, and it can be used to recognize patterns and clusters that are not evident in traditional statistical diagram and bivariate graphs.

Case Studies and Practical Implementations

In aerospace engineering, a TDA technique called Mapper has been used in a multi-disciplinary design optimization of an Air Vehicle Concept. Mapper has been also used in the optimization of the actuation system of aircraft wings, with the specific goal of identifying interf to minimize the influence of BVI (Boundary Layer Ingestion fiber compositions for composite wings [20-21]. Broadband Noise) on the SINFAC In Material engineering, a TDA analysis using the Mapper algorithm has been used to design new materials for additive manufacturing. The task of the optimization was minimizing the solidification length at the bond line of adhesively bonded joints, thus trying to promote greater interfacial adhesion. In electrical engineering, Topological Data Analysis (TDA) has been applied to the Power System Planning (PPS) optimization. TDA has been used to analyze the data resulting from an optimization of the electrical systems, particularly to reduce the dimensionality of the solution space [22-26]. TDA has also been employed in Electrical Science and Engineering to optimize the material compositions used for thermoelectric. All the above examples provide evidence of the applicability, and effectiveness, of TDA techniques in mechanical engineering for reducing the dimensionality of the optimization problem, enabling the optimization of complex problems. In mechanical engineering, TDA has been used to design and optimize mechanical parts. As an example, Gu et al. used a TDA technique called Mapper to reduce the number of design variables in the optimization process. [1-5], implemented in their work a TDA analysis to support mechanical design against wind-induced vibrations. TDA has also been employed in the optimization of composite materials with particular attention to pore distribution [8-12]. In this section, we provide examples of how TDA techniques have been employed in engineering fields to optimize complex systems. We divide the applications in mechanical engineering, electrical engineering, aerospace engineering and material engineering.

Future Directions and Conclusion

The work is a starting point for understanding the topological data analysis method in the context of optimization process. However, there are many research areas that have not been considered. First, Researchers could focus on finding frequent patterns for complex systems in optimization process using topological data analysis methods like Persistent homology, local neighborhood information or cohomology, and multi-scale local geometric regression through optimization. Second, they can also focus on combining the TDA and the machine learning approach for the optimization of problem of new application areas [9]. Third, many complex systems for optimization process such as Architecture, Environmental, or Digital Twin have different features that should be captured in this optimization process. The choice of TDA methods and its modeling configurations may vary depending on the problem, and much research is still needed and open for complex optimization systems in the future study. We anticipate future work in TDA applications in optimizing engineering design processes in complex systems. Use of data-sets in parameterization of high-dimensional models, arises naturally in engineering design optimization methods, such as in Product design, Systems design, Supply chain, industrial processes, Structural and material design, Multi-scale simulation, Automotive engineering, Aerospace applications, Civil, environmental, and energy engineering, Networking and communication, Cloud and machine learning systems, 5G, Machine learning models, Robotics operational design and Simulation, Additive and Subtractive Manufacturing. It's also become important in Architecture and smart buildings, in Simulating and control of pandemics, and lastly, in Digital Twins. Through systematic research on optimization process, TDA common application domains in engineering is already supported based on a literature review. Engineering design processes in complex systems require a large multidimensional data set, necessitating a statistical approach for validation of data quality [8-12]. Furthermore, engineering teams must continuously refine design parameters, thereby necessitating an iterative optimization process [12]. To this end, a novel topology-based statistical approach named Topological Data Analysis (TDA) has found applications in various fields and has been utilized for automatic detection of quality faults in data, like high-dimensional, or complex data sets wherein traditional statistical methods are impractical [15].

CONCLUSION

Topological Data Analysis (TDA) represents a transformative approach to engineering design, providing a robust framework for analyzing high-dimensional and complex datasets. By integrating TDA with generalized Principal Component Analysis (g-PCA) and adaptive clustering algorithms, this methodology offers enhanced accuracy and robustness in clustering and component analysis. The use of TDA allows for the extraction of meaningful topological features, facilitating a deeper understanding of data structures and improving the optimization processes in various engineering domains. Future research should focus on expanding the application of TDA in combination with machine learning to address the unique challenges of complex system design, thereby advancing the field of engineering design optimization.

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