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Knowledge-Assisted Optimization for Large-Scale Design Problems: A Review and Proposition

Practicing design engineers often have certain knowledge about a design problem. However, in the last decades, the design optimization community largely treats design functions as black-boxes. This paper discusses whether and how knowledge can help with optimization, especially for large-scale optimization problems. Existing large-scale optimization methods based on black-box functions are first reviewed, and the drawbacks of those methods are briefly discussed. To understand what knowledge is and what kinds of knowledge can be obtained and applied in a design, the concepts of knowledge in both artificial intelligence (AI) and in the area of the product design are reviewed. Existing applications of knowledge in optimization are reviewed and categorized. Potential applications of knowledge for optimization are discussed in more detail, in hope to identify possible directions for future research in knowledge-assisted optimization (KAO).
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1 Introduction

Current simulation-based optimization strategies usually treat simulation as a black-box function. The assumption of black-box functions is derived from the fact that simulations are used to evaluate design functions, whose mathematical expressions are unknown to the user. One main advantage of treating simulation as a black-box is that the optimization method can be generalized to solve any design problem. The lack of equation is coupled with the unavailable or unreliable gradients of such simulation functions. Hence, nongradient-based (or derivative-free) optimization algorithms have been widely applied in engineering to solve black-box function problems, such as genetic algorithm (GA) [1], simulated annealing method [2], particle swarm optimization (PSO) [3], and so on. One major issue of those algorithms is that the number of function evaluations is normally very large. When the objective function is evaluated via expensive simulation, the computational cost of optimization usually becomes unacceptable.

To reduce the number of expensive black-box function evaluations in the optimization process, an approximation model, known as a metamodel, is developed to replace the expensive simulation in optimization. Different metamodel-based optimization strategies, including efficient global optimization (EGO) [4], mode pursuing sampling (MPS) [5], and so on, are developed to improve the optimization efficiency when dealing with expensive black-box functions. Although those methods perform well for low-dimensional optimization problems, their performances for large-scale optimization problems are less satisfactory. Since metamodels are constructed based on samples, a rapidly increasing number of samples are needed to obtain enough information to construct an effective metamodel in a high-dimensional space. Although different intelligent sampling strategies are developed to improve the efficiency of metamodel-based optimization methods, exploration of a totally blind and high-dimensional space is extremely difficult and costly. To handle the large-scale optimization problems, two types of strategies are developed. One is the space modification strategy to generate new samples in interested subspaces rather than the entire space. One well-known example is the trust-region strategy, which is used in trust-region mode pursuing sampling [6] to solve large-scale problems. Another strategy is based on reducing the dimensionality of the optimization. This kind of strategy can also be categorized into two classes. One is to decompose the problem into several subproblems with lower dimensions, such as optimization on metamodeling-supported iterative decomposition method [7,8]. The other is to perform optimization on several dimensions selected from the whole dimensions, such as dynamic coordinate search using response surface models [9] and partial metamodel-based optimization [10]. Those methods have the capability of solving large-scale optimization problems, but the number of function evaluations is still large.

Generally, either for nongradient-based optimization methods or in metamodel-based optimization methods, the key is how to generate useful samples (offspring or particles) in a high-dimensional space. Generation of new samples needs to balance between exploration and exploitation. Information obtained from previous iterations and existing samples is usually used to help generate better samples. However, the lack of information may lead to low efficiency or even wrong search direction.

In a real-world engineering design, however, practitioners usually have certain knowledge about the design problem such as variables involved in the problem, the input–output relations, or even have some mathematical functions based on physical laws. Such information is largely ignored when solving engineering design problems in current simulation-based optimization strategies. As aforementioned, the black-box assumption demands more computational cost since the optimization is blind to the design problem at hand. This phenomenon is more severe when the dimensionality of the problem is high. Even thousands of sample points are sparse in a 100-dimensional space. Therefore, it becomes difficult to explore and optimize blindly in such a huge space. If existing knowledge of the engineering problem can be incorporated into modeling and optimization, the number of sample points necessary to capture the behavior of such a function and the design space could be reduced. Additionally, by analyzing existing knowledge about an engineering design problem, some hidden valuable information can be extracted, which can help to perform optimization more efficiently. For instance, if one finds that the objective function is monotonic with

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respect to some design variables, values of such design variables can be determined without the need of optimization and the dimensionality of the problem can be reduced. If one knows that the input–output relationship follows a certain trend, it will help in the selection of the most suitable metamodel and reduces the costs of model construction.

To obtain knowledge from problems, different artificial intelligence (AI) methods were applied in the optimization. The application of AI methods can be classified into two categories: knowledge from graph and documents and knowledge from data. The expert system, which belongs to the first category, was used in design problems for decision-making [11,12]. However, there are few applications using experts directly in assisting optimization. For knowledge from the data, multiple data mining (DM) methods [13,14] and classification methods [15–17] were applied in problem formulation and in optimization strategies for generating new samples. Although knowledge and some AI methods have been used in optimization, there still exist limitations. First, researchers only apply a single kind of knowledge in optimization. Additionally, knowledge from graphs and documents are not well utilized in assisting optimization. Therefore, how to systematically incorporate different kinds of knowledge into optimization, rather than ad hoc and problem-specific treatment, becomes an interesting research topic. This issue becomes especially relevant for large-scale design problems in order to break the "curse-of-dimensionality."

The main motivation of this article is to call for research on how to systematically and methodically extract and incorporate both formal and tacit knowledge about a design problem to help increase the accuracy and efficiency of design optimization. This paper is an enhanced version from the authors' conference paper [18]. To identify what kinds of knowledge can be obtained and applied in an engineering optimization problem, the concept of knowledge is surveyed in Sec. 2. Section 3 reviews existing applications of knowledge in assisting optimization. To overcome the challenges in high-dimensional optimization, Sec. 4 proposes potential applications of knowledge at different optimization stages. Given the fast development of machine learning methods and the close tie between optimization and machine learning, how knowledge can help machine learning is discussed in Sec. 5. Section 6 provides a summary.

2 Concept of Knowledge

Knowledge is defined as familiarity, awareness, or understanding of someone or something [19]. The word "knowledge" is widely used in AI, and the definition of knowledge used in engineering also comes from AI. Hence, the concept of knowledge in AI is reviewed first to give a clear description of knowledge representation and knowledge capture. Then, to define what kinds of knowledge can be obtained from and applied in the engineering world, the knowledge concept in the product design is also surveyed.

2.1 Knowledge in Artificial Intelligence. AI is currently one of the most popular research fields around the world. AI is defined as the study of intelligent agents: any device that perceives its environment and takes actions that maximize its chance of success at some goal [20]. In other words, AI is a technique which can help machines to deal with different problems in an intelligent manner. There are two main problems in AI: learning and problem solving [20]. Knowledge is involved in both problems. In learning, knowledge should be captured and represented in a form that machines can understand. On the other hand, knowledge should be reused to solve problems.

Knowledge representation is central to AI research, which focuses on designing computer representations that capture information about the world to solve complex tasks [20]. As shown in Fig. 1, the earliest knowledge representation work was focused on a general problem solver [21], which was to develop as a universal solver machine. Although the development of a general problem solver is not successful due to its limitation on the problem definition format, this represents the first attempt to regard knowledge as an input to solve problems. Following the idea of a general problem solver, expert systems are developed to represent human knowledge.

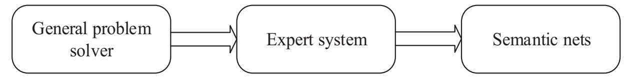

Fig. 1 Knowledge representation methods

Expert systems could match human competence on a specific task [22–24]. Two techniques developed at that time and still used today are the rule-based knowledge representation [25] and the frame-based knowledge representation [26]. Rule-based systems are widely used in domains such as automatic control [27,28], decision support [29,30], and system diagnosis [24]. The frame-based method is used on systems geared toward human interaction for choosing appropriate responses to varied situations. The frame-based knowledge representation focuses on the structure of the concept, while the rule-based knowledge base focuses on logic choices. To combine the properties of the two expert systems, one of the most well-known integrated systems was developed in 1983, named as knowledge engineering environment [31], which contained a complete rule engine with forward and backward chaining and a complete frame-based knowledge base with triggers, slots, inheritance, and message passing. The expert system is a useful knowledge representation tool. By employing the expert system, users can make reasonable decisions. However, the expert system is defined by expert experiences. The effectiveness of expert systems highly depends on the accuracy of the contents in the system. Thus, an incorrect or outdated expert system may lead to wrong decisions. Therefore, how to define an appropriate and evolving expert system remains a main challenge.

Currently, one of the most active areas of knowledge representation research is on semantic net [32,33], which is a network that represents semantic relations between concepts. Different from neural networks, semantic nets are made up of different concepts and semantic relations between concepts. A related concept is ontology [34,35]. In philosophy, ontology is the study of the nature of being, becoming existence, or reality, as well as the basic categories of being and their relations. In computer science, ontology is a formal naming and definition system of properties and interrelationships of entities that fundamentally exist in a particular domain [36]. The main benefit of ontology is that it is not only able to describe different concepts in the domain but also relationships between concepts. By employing ontology mapping [37] and ontology merging [38], similar ontologies can be integrated to include more information, especially relationships between different concepts. The semantic net is a way to create ontologies.

In a general problem solver, knowledge is defined as information of the real world. A problem is solved by employing a knowledge representation method. In AI or computer science, knowledge is represented by language or knowledge graph, which however cannot be directly and automatically used in engineering design. Compared to linguistic knowledge, input–output relationship data are more applicable for engineering design. Based purely on data, machine learning helps to uncover variable relations in a complex system. How to combine the linguistic and graphic knowledge and the knowledge embedded in data is the main question to be addressed in future research.

2.2 Knowledge in Product Design. Although knowledge has been used in product design for a long time, the definition of knowledge is borrowed from AI. In product design, knowledge is understood as the information which is not directly available but is obtained from the analysis of data. In other references, knowledge is also described as the experience, concepts, values, beliefs, and ways of working that can be shared and communicated [39]. Sunnersjö [40] argues that knowledge should include not only the rules that the designer should adhere to but also the background knowledge that makes the design rules possible to review and understand. In summary, the definition of knowledge in product design is varied. But one consensus is that knowledge needs to be captured and represented in an appropriate way.

In engineering design, knowledge is often used in the concept design phase to help designers come up with better designs [41]. Knowledge used in design can be classified into two categories: formal knowledge and tacit knowledge. Formal knowledge is embedded in product documents, repositories, product function and structure descriptions, problem solving routines, technical and management systems, computer algorithms, and so on [42]. On the other hand, knowledge tied to experience, intuition, unarticulated models, or implicit rules of thumb is regarded as tacit knowledge [43]. It is easier to capture and represent formal knowledge than the latter. On the other hand, tacit knowledge is rather difficult to be expressed, which is generally gained over a long period with learning and experience. One reason is that there is not a common recording method to capture the knowledge in human's brain. Another reason is that such knowledge can only be transferred by willing and articulating people. One main research direction of the knowledge in product design is how to capture and represent tacit knowledge. Either formal knowledge or tacit knowledge should be represented in a way that is easy to be understood [44].

Knowledge representation methods can be classified into five categories [42]: pictorial, symbolic, linguistic, virtual, and algorithmic approaches as shown in Table 1. Pictorial presentation presents knowledge as a picture or a graph, including sketches, detailed drawings, and photographs. The symbolic method represents knowledge by drawing a chart or a network. Decision tables, flowcharts, assembly trees, and ontologies are all symbolic representation methods. The rule-based and frame-based expert systems can be regarded as the symbolic knowledge. Linguistic representation uses document files including customer requirements, design principles, constraints, and so on. Computer-aided design (CAD) models, computer-aided engineering (CAE) simulations, and virtual reality are examples of the virtual representation methods. Finally, the algorithmic methods include the procedural or methodical knowledge used in modeling, analysis, and optimization. The information obtained from AI methods such as data mining methods or machine learning methods can also be classified into algorithmic knowledge.

Different knowledge is used at different stages of product design [36,37]. To start a design, user requirements are needed for requirement modeling. House of quality, falling into the linguistic knowledge category, is often employed to summarize the necessary requirements. In the functional modeling stage, decision trees can be used to determine the function of the product and how to realize those functions. Then, some linguistic methods, such as design principles, will be used to generate concepts whose behaviors are modeled based on the functions of the product. Different ideas are generated in the concept design stage. A rich and well-structured knowledge representation system is needed to support such plenty of concepts and ideas [45]. Ontology is an appropriate method to organize ideas. Ontology, which is a highly structured domain covering processes, objects, and attributes, has the ability to integrate and migrate valuable, unstructured information and knowledge to provide a complex domain that contains rich conceptualization [46,47]. The semantic net is a tool to capture and represent the ontology in a graph with nodes and arcs [48]. In the above three stages, i.e., requirement modeling, functional modeling, and concept design stages, the linguistic and pictorial knowledge plays the main role. The next stage is embodiment design, where symbolic, algorithm, and pictorial methods are highly involved. Information about the product architecture, material, and mathematical equations are applied at this step. Next is the detailed design, where different virtual knowledge, including CAD model, CAE, and virtual reality, are used to generate 3D models of the design. Then, more accurate simulation models are generated and optimization is employed to modify details of the product.

Table 1 Classification of knowledge representation [41]

Representation approaches	Examples
Pictorial	Sketch Detailed drawing Photograph
Symbolic	Decision table Flowchart Assembly tree Semantic net Expert system
Linguistic	Customer requirement Design principles Constraint
Virtual	CAD model CAE simulation Virtual reality
Algorithmic	Mathematical equation Computer algorithm Optimization algorithm Data mining method Machine learning method

Different kinds of knowledge can be utilized for engineering design. The issue is that traditional knowledge is often represented by documents or graph. How to use the knowledge appropriately in forming an engineering design and optimization problem is the main task. An engineering simulation model is one attractive type of virtual knowledge that can help in design. Such model gives input and output relations, based on which one can dig out more hidden information such as monotonic influence of certain inputs on the output. In addition, approximation models can be constructed on simulation models.

To combine the rule-based and frame-based expert systems with engineering design, the knowledge-based engineering (KBE) system was developed [49,50]. Rule-based and frame-based knowledge can be captured, represented, and reused with CAD tools and simulation tools in the KBE system to reduce time and costs of product development. References [50,51] stated that KBE was likely to be the best possible technology at hand to deal with rule-driven, multidisciplinary, and repetitive geometry manipulation problems. In Refs. [52–54], a multimodel generator was created by KBE to develop a distributed design framework to support aircraft multidisciplinary design optimization. A specific family of aircrafts was generated automatically through the KBE system [53]. In each model, discipline abstractions are obtained and used as the input of simulation tools to evaluate the performance of an aircraft. One disadvantage of the KBE system is that it can only deal with revision from existing designs. In other words, before using KBE to design a product, similar products and their design details are required. Another shortcoming is the expert system used in the KBE system. One issue is how to validate the accuracy of the rules and classes in the knowledge base. Another issue is that modeling the knowledge domain is also a burden to developers. Additionally, only an expert system is involved in the KBE system to deal with design problems, which is just one type of knowledge applied in the design. To better assist the design process, different kinds of knowledge need to be involved. Thus, the KBE system needs to be enhanced to include other kinds of knowledge when it is used for optimization.

2.3 Summary Remarks. Knowledge has been employed in problem solving and engineering design for decades. Knowledge is captured from different resources, including documents, human experiences, previous designs, and so on, and it is represented in a structured way for further usage. The knowledge-based system is first developed in the AI field, and the expert system is one of the most common applications. By employing knowledge, the engineering design process can be executed with little human intervention. However, by employing frames and rules, the generated design through the expert system is only a feasible design but not an optimal one. To reach the best, optimization needs to be performed on the design obtained from KBE. Another issue about the current knowledge base is that it focuses on linguistic knowledge, neglecting knowledge hidden in data obtained from engineering analyses. In addition, knowledge represented in an expert system can be used to help define and solve the optimization problem. Nevertheless, fundamental elements of optimization are still data or numbers. Therefore, how to mine knowledge from data and how to utilize such knowledge in optimization are two research directions of the knowledge-assisted optimization methodology. Moreover, how to combine the linguistic knowledge, such as design principles and customer requirements, with data is another area of interest.

3 Existing Applications of Knowledge in Design Optimization

Large-scale design optimization problems are difficult to solve. There are several techniques that can be used to tackle these problems, including dimension reduction, decomposition, metamodeling, and optimization strategies [55]. Although knowledge is not formally incorporated in optimization methods, there are some techniques employing knowledge to tackle large-scale optimization problems. Table 2 gives a summary of existing optimization methods involving knowledge. Note that the pictorial knowledge is usually used at the beginning of the concept design and only includes rough information of the design. Thus, the pictorial knowledge is rarely applied in optimization. As for the other four kinds of knowledge, the symbolic and algorithmic knowledge are widely used in different solution methods when dealing with high-dimensional optimization problems. The details are reviewed in the following sections.

3.1 Symbolic Knowledge. Symbolic knowledge is knowledge represented through graphs and symbols. Symbolic knowledge is widely employed in optimization methods. To reduce the dimensionality of an optimization problem, causal graph is employed to identify and remove certain design variables. A causal graph is an oriented graph showing the causal relations between variables. Through analyzing causal relationships between design variables and the objective, variables monotonically influencing the objective are identified. The optimal values of these variables can thus be determined without optimization, which means the number of design variables can be reduced. To further decompose the problem, sensitivity values are applied to simplify the causal graph and decompose the original problem into several subproblems with less design variables. This method was applied to solve an aircraft concept design problem and a power converter design with improved optimization efficiency [56]. The shortcoming of this method is that if the monotonic variables cannot be found in the problem or the range of variables is not carefully chosen so that monotonicity is not ensured, this method will be ineffective.

One kind of symbolic knowledge, design structure matrix (DSM), is usually used to show the interdependence of each discipline in decomposition strategies. DSM is a square matrix that has identical row and column listings to represent a single set of objects. The key advantage of DSM is that DSM can show to designers a complete view of the coupling structure within a system [57]. By analyzing DSM, decomposition can be performed and the multidisciplinary design optimization architecture can be constructed. Moreover, different DSM analysis methods are developed to simplify optimization problems. By performing the graph partitioning [58–60], clustering analysis [61], and optimization [62] on DSM, complex problems can be decomposed into subproblems. Then, different decomposition strategies, including concurrent subspace optimization (CSSO) [63], collaborative optimization (CO) [64], and bilevel integrated system synthesis (BLISS) [65], have been developed according to the relations represented in the DSM. The main disadvantage of those decomposition strategies is the large number of function evaluations needed when dealing with high-dimensional optimization problems. In Ref. [66], CO and CSSO were tested with several numerical benchmarks and the results show that even for low-dimensional problems, CO and CSSO need thousands of discipline function calls. For different variations of BLISS methods in solving an aircraft concept design problem, although the number of system analysis was reduced to 10, the total number of discipline calls was around 400 and BLISS/RS2 required more than 1000 discipline calls [65].

Symbolic knowledge was used to determine the structure of an approximation model. In Ref. [67], the intermediate variables in a Bayesian network are used as hidden nodes to construct an artificial neural network (ANN) in a traffic accident prediction. However, the Bayesian network is only used to represent the input–output relations; detailed mathematical relations cannot be captured by the Bayesian network.

In summary, symbolic knowledge usually assists optimizations at the beginning stage of optimization. By employing symbolic knowledge, properties of the problem can be found to reduce the number of dimensions or construct a more accurate metamodel, easing the difficulties of solving high-dimensional optimization problems.

3.2 Linguistic Knowledge. Linguistic knowledge is information represented by documents. This kind of knowledge is difficult to involve in optimization since optimization methods usually focus on the trend of the data. One way to apply linguistic knowledge in optimization is in selecting suitable approximation methods according to the properties of the problem. A response surface method with different orders can be chosen according to the problem. Additionally, different metamodels are fit for different problems. A common conclusion regarding traditional metamodeling methods is that a Kriging method performs better for low-dimensional problems while radial basis function outperforms others for high-dimensional problems [68]. Thus, considering the properties of metamodeling methods and features of the problem, a suitable metamodeling method may be selected for a certain problem.

Other than selecting a metamodeling method, properties of the design problem can be used in selecting operators in optimization methods such as the GA. Reference [69] suggested to use domain knowledge in the three stages of GA, i.e., initial population generation, encoding the genotype, and genetic operations of crossover and mutation. In Ref. [70], knowledge of truss is used to guide the initial sampling in GA. Hu and Yang [71] used the specific knowledge in GA to solve a path planning problem. Piroozfard et al. [72] employed knowledge-based operators to solve job shop scheduling problems. In general, specific property of the problem is applied to generate custom operators for the problem. However, such ad hoc approaches cannot be extended to solve other problems.

3.3 Virtual Knowledge. Virtual knowledge, such as CAD, CAE, and virtual reality models, allows users to get insight into problems, find key trends and relationships among variables in a problem, and make decisions by interacting with the data. A visual design steering method [73,74] was developed as an aid in

Table 2 Existing applications of knowledge in optimization

	Dimension reduction	Decomposition	Metamodeling	Optimization strategy
Pictorial				
Symbolic	◎	◎	◎	
Linguistic			◎	
Virtual				◎
Algorithmic	◎	◎	◎	◎

multidisciplinary design optimization, which helped a designer to make decisions before, during, or after an analysis or optimization via a visual environment to effectively steer the solution process. Virtual knowledge is helpful when little is known about the data and the exploration goals are implicit, since users are able to directly participate in the exploration processes, shift and adjust the exploration goals if necessary. However, currently there lacks direct translation of such knowledge into formulation for optimization problems.

3.4 Algorithmic Knowledge. Algorithmic knowledge is the most popular knowledge used in optimization since this knowledge has the closest relation with data. As mentioned in Sec. 2.2, equations, procedural models, and information obtained from machine learning algorithms can all be categorized as algorithmic knowledge.

Equations, which widely exist in different optimization problems, can be used at different stages of optimization. Note that the equations may not be the accurate model of the design problem, but the mathematical relations provided in the equations can help in solving the optimization problem. Empirical equations with lower fidelity can be employed in multifidelity models to reduce the number of function evaluations of the expensive simulation models. The co-Kriging method can be employed to generate metamodels based on multifidelity models [75]. In Ref. [76], empirical equations are used to construct a knowledge layer in the ANN to solve a microwave design problem. Physical theories, empirical data, and historical data are treated as white-box models, which may be employed in constructing a grey-box metamodel [77]. The residual between the white-box prediction and the simulation data is estimated by a metamodel. The grey-box method is applied in prediction in two manufacturing problems, and the results show that the metamodel is sufficiently accurate with small amount of sample points. Equations can make the optimization easier, but the inaccuracy of equations may negatively impact the optimization results.

Data of historic designs can also be employed in optimization. Kurek et al. [78] developed a novel approach for automatic optimization of reconfigurable design parameters based on knowledge transfer. Solutions and historic data of related previous design are treated as prior knowledge and will be transferred to the new design and optimization. The autotransfer algorithm is developed based on Bayesian optimization to determine which design will be transferred, when it will be transferred, and how it will be transferred [79]. The efficiency improvement of the optimization method based on knowledge transfer algorithm is significant.

Recently, more and more machine learning methods are employed in assisting optimization. The screening methods and mapping methods were employed to reduce the dimensionality of the problem [80,81]. But there is information loss either in screening or mapping. The influences of those lost information on the optimization results are difficult to quantify. If key information was lost due to screening or mapping, the optimization would fail. The classification method is also employed in optimization to help with sampling. A classifier-guided sampling method is developed to generate samples toward the area with a high probability of yielding preferred performance [15]. Instead of random sampling, the samples are generated based on the information obtained from the classification results. Compared with traditional optimization methods such as GA, the rate of convergence of the method was improved significantly. In many cases, users tend to specify an excessive number of, and often redundant, constraints. Methods were developed to find the redundant constraints for the mathematical problems [82]. Cutbill and Wang [14] introduced a novel method based on association analysis to detect redundant black-box constraints.

3.5 Summary Remarks. Knowledge has been used in solving optimization problems although the concept of knowledge is not widely applied in the optimization field. In current optimization methods, algorithmic knowledge is still the most used type of knowledge. On the other hand, symbolic knowledge, such as causal graph and DSM, are also employed in optimization methods. However, employing specific knowledge may help to improve effectiveness and efficiency of optimization for one problem but it may not be suitable for different problems. The issue of the current knowledge-assisted optimization method is that there is no systematic way to employ different kinds of knowledge together to deal with one problem. Besides, because of the property of the linguistic knowledge and virtual knowledge, they are difficult to use in optimization. Therefore, how to combine the linguistic/virtual knowledge and data is one of the research directions for knowledge-assisted optimization methods.

4 Potential Applications of Knowledge for Optimization

Potential applications of knowledge to assist optimization are summarized in this section. As shown in Table 3, we list five main tasks in optimization, including problem formulation, dimension reduction, decomposition, metamodeling, and optimization

Table 3 Potential applications of knowledge in optimization

Optimization tasks	Challenges	Knowledge
Problem formulation	• Constraints definition • Determining feasible space	Linguistic knowledge Expert system Ontologies (semantic nets)
Dimension reduction	• Determining omittable variables	Equations Expert system Causal graphs Design principles Ontologies (semantic nets)
Decomposition	• Relations between disciplines • Correlations between variables	Equations Linguistic knowledge Causal/Bayesian graphs
Metamodeling	• Selecting a metamodeling method • Accuracy of the metamodel	Equations Historical data/designs Causal/Bayesian graphs Expert system
Optimization strategy	• How to generate new samples	Equations Causal/Bayesian graph Flowcharts

strategy/algorithm. These tasks can also be viewed as different stages of an optimization process. Then, we map the challenges of each task with possible applications of knowledge in addressing these challenges. Here, the knowledge entails linguistic knowledge, pictorial/symbolic knowledge, and data knowledge.

4.1 Problem Formulation. There are three elements in an optimization problem, design variables, objectives, and constraints. The number of design variables, number of constraints, and strictness of these constraints will influence the efficiency and effectiveness of optimization. One of the challenges in problem formulation is constraint specification. The number of constraints will influence the efficiency of optimization. A large number of constraints will increase the computational cost of an optimization problem. Additionally, a very strict set of constraints may cause the optimization to fail since it is difficult to find a feasible solution, while a loose set of constraints may lead to a design failure in the real world. Another task related to problem formulation is to detect the feasible area. If the feasible space can be determined, it will be much easier for optimization algorithms to find the optimum. To deal with these two challenges, different kinds of knowledge can be applied including linguistic knowledge and symbolic knowledge.

Symbolic knowledge can be used for constraint specification to avoid redundant constraints. The expert system can become one of the useful tools for problem formulation. KBE systems were widely used in engineering design problems to represent rules and requirements in a structured manner [49], through which a more complete and accurate set of constraints could be defined according to different design scenarios [83]. By employing the structured representation of rules and frames, the constraints and relations between different constraints can be obtained and the definition of the problem can be generated through the expert system.

For constrained optimization, some data-based methods were developed to find the feasible space in black-box constrained optimization problems [84–86]. The expert system has the capability to generate feasible design considering different rules, and it can also be used to detect the feasible area of one design problem [49,51,87,88]. The expert system can also be used to determine the constraints that must not be violated, and the constraints can be mildly violated.

Semantic nets model not only a single concept but also relations between different concepts. If one treats the design variables, constraints, and objectives as nodes in semantic nets and generates semantic nets among those nodes, designers may have a clearer and deeper understanding of the problem and the optimization problem formulation may be more targeted. Similar to expert systems, ontology can help to make judgements. In Refs. [89,90], ontology was used to represent the requirements in engineering design. The relationships between different concepts in the ontology can give a clearer insight of the design problem at the problem formulation stage. For example, similar requirements can be detected through analyzing the ontology. Then, the constraints of the optimization problem can be defined more appropriately by employing knowledge. Additionally, ontology can be used to validate system requirements early on Ref. [91]. Thus, using ontology to guide formulation is a future research direction.

4.2 Dimension Reduction. Dimensionality of an optimization problem often determines the computational cost, especially when choosing metamodel-based optimization methods. Dimension reduction is a common way to improve the optimization efficiency. There are two kinds of methods, one is screening to select the important variables and the other is mapping high-dimensional data to a low-dimensional space. However, how to determine the omittable variables in screening and how to determine the dimensionality of the lower-dimensional space in mapping methods are two challenges for dimension reduction.

As mentioned in Sec. 3.1, dimensionality of the optimization problem can be reduced through analyzing the causal graph of the problem [92]. Some design variables are removed from the variable set due to their monotonic influences on the objective. The monotonic influences can also be obtained from other knowledge, such as equations or design principles/guidelines.

In screening methods, sensitivity analysis is performed to determine the importance of variables. The screening process can also be performed based on rules and frames in an expert system. In this case, sensitivity analysis can be employed as a validation method by checking the screening results with the expert system.

In the traditional mapping method, the dimensionality of low-dimensional space is always a question. Usually, the dimensionality is determined by the user and often fixed at an arbitrary small number. The ontology knowledge may be used to find out such dimensionality and latent variables. By analyzing relations between design variables, the dimensionality of the lower-dimensional space may be defined. In Ref. [93], a mapping method named as generative topographic mapping is used to solve 30-dimensional airfoil design optimization problems and different lower-dimensional spaces were tested. It is found that the optimized result of two-dimensional lower spaces is the best. One reason is that for the airfoil design problem, the naive 30 non-uniform rational basis spline (NURBS) variables might have a more sensible dimension of two. If the designers can find out through knowledge that the 2D spaces are the best, the optimization results may be more accurate.

Various dimension reduction methods are developed in the data mining field. Feature selection is one of the dimension reduction methods by removing irrelevant and redundant features to reduce dimensionality [94]. Two categories of feature selection methods, filter methods and wrapper methods, were developed to select features [95]. In filter methods, variables are ranked according to different principle criteria, such as correlation criteria [96] and mutual information [97]. Wrapper methods use the prediction performance of different subsets of variables to reduce the dimensionality [98,99]. Compared with wrapper methods, filter methods have lower computational costs as the expense of accuracy.

4.3 Decomposition. There are two categories of commonly used decomposition methods, one is based on relations of disciplines and the other is based on correlations among variables. One multidisciplinary design optimization problem is usually decomposed according to relations among disciplines. A common problem in decomposition is that there is no general method in generating the decomposition framework. In other words, a new framework needs to be constructed for every different problem. For the variable-based decomposition method, the main challenge is detecting the correlations of the variables with low computational cost.

As mentioned in Sec. 3.2, a problem can be decomposed according to variables rather than disciplines. The causal graph or Bayesian networks constructed based on variables and their relationships can be used to help find out where the coupling is in the problem. In Ref. [92], three coupled loops can be reduced to one when breaking the discipline-based DSM to the variable-based DSM. Thus, the graphic knowledge representation methods have the capability in generating more efficient decomposition results. A group of decomposition methods based on variables is rooted in the high-dimensional model representation (HDMR) method [7,100]. High-dimensional problems are decomposed into several subproblems based on the sensitivity information of different component functions in the HDMR model.

For engineering problems, correlations between different variables can be determined through equations, documented (linguistic) knowledge, or the analysis of the graphic knowledge. Then, decomposition can be performed according to the obtained knowledge.

4.4 Metamodeling. Metamodels are widely employed to replace expensive simulation models. Different metamodels have different properties. Therefore, how to select a suitable metamodeling method is one of the tasks. Second, the accuracy of the metamodel is another issue when approximating high-dimensional problems. The basic idea of improving the model accuracy is to generate more samples in the space when treating the problem as a black-box. However, thousands of samples are still extremely scarce for a 100-dimensional problem. Moreover, sometimes adding more samples may lead to over-fitting. To overcome this problem, other information should be considered rather than simply regarding the problem as a black-box.

ANN is one effective metamodeling method for nonlinear problems [101]. Increasing the number of nodes and the number of layers can improve the accuracy of the ANN model to a certain extent. In a fully connected ANN with plenty of nodes, the number of weights needed to be estimated is very large and often thousands of sample points are needed to generate an accurate set of weights. Thus, how to reduce the number of nodes and the number of links, or in other words, how to determine the structure of a neural network is one of the issues for ANN approximation. Similar with ANN, the causal graph or Bayesian network is also a structure based on nodes and links. Those graphic knowledge representation methods can be used as a guide in generating the ANN structure. Another potential improvement of ANN is to consider values of intermediate variables. Even in a black-box function model, actual values of some intermediate variables can be obtained by simulation. However, such information is not considered in metamodel construction. After employing a causal graph to determine the structure of an ANN, values of intermediate variables can be determined to improve the approximation accuracy. In other words, some hidden layers in ANN can be taken to the surface as actual values and the links related to them can be obtained.

In Ref. [10], a partial metamodel is employed to deal with high-dimensional problems. In that case, only selected component functions are constructed in the HDMR model instead of constructing the complete model to reduce the function evaluations. A component function is selected based on the importance of the design variables via estimated sensitivity information. By using knowledge of the engineering problems, such as causal graph or empirical equations, the important component functions may be predetermined.

Fuzzy logic knowledge can be used to construct the prediction model. In fuzzy expert systems, continuous inputs and outputs are transferred to fuzzy sets and they are linked together by if-then rules. In prediction, the predicted fuzzy output will be converted back to the continuous output. In Ref. [102], fuzzy logic knowledge was used to forecast energy demand. A type-2 fuzzy rule-based expert system model was constructed to estimate the stock prices [103].

Previous knowledge in constructing metamodels for similar problems can also be utilized. The response of the metamodel may be different from the actual model, but the trend of the problems or some interesting design spaces may be found through the metamodel. Multitask regression is a method to construct a regression model for different but related tasks by analyzing data from all the tasks instead of constructing an individual regression model for each task [104]. Thus, combining the data from previous design problems, a multitask regression model can be constructed on all the related designs. Additionally, with the increase of the number of design, the multitask models can be updated.

4.5 Optimization Strategy. How to generate new samples is the main question for metamodel-based optimization strategies. Some strategies generate samples in the area with the highest uncertainty [4], some generate samples uniformly in the desired space [105–107], and others generate samples according to the probability distribution calculated from the previous metamodel [5,6]. Those methods are all based on the data captured from the analysis of the black-box model.

Knowledge can also be employed to guide the sampling in the design space. Bayesian network is a method that represents not only the graphic structure of the problem but also the probability distribution of different variables [101]. Bayesian network can also be used to estimate the probability distribution for input variables when given a certain value of the output. This distribution is named as likelihood. By predicting the likelihood and generating samples following the likelihood trend, more improvements are expected in the metamodel-based optimization. Additionally, if the prior probability distribution in the Bayesian network is known before optimization, the initial sampling and the updating can be performed following the knowledge of the prior probability distribution.

Equation is another kind of information that can be used in the optimization. The optimization results of the empirical equations may not be accurate, but equations can be used in helping generating new samples in the optimization iterations.

Evolutionary and metaheuristic optimization algorithms have been widely used for optimization on inexpensive problems. In those algorithms, new samples at each iteration are generated following the evolution theory or other crowd behavior. The properties of the design problem can be captured and involved in the algorithm to guide the generation of new sample points to improve the search efficiency of those optimization algorithms. Most of the current knowledge-based operators in evolutionary algorithm are developed for special cases. Therefore, general-applicable methods of employing knowledge in assisting generating offspring (new samples) should be developed.

4.6 Summary Remarks and Challenges. To overcome the limitation of assuming black-box functions in metamodel-based design optimization, knowledge is involved to help in solving large-scale optimization problems. Knowledge can be applied to assist different optimization tasks. At the beginning, knowledge is very useful in defining a reasonable and effective optimization problem, either in dimension reduction or in constraint specification. During optimization, knowledge can help in metamodel construction and to guide generation of new samples.

In assisting optimization, equations tend to be most useful information. Graphic knowledge such as causal graph and Bayesian networks can also be used in problem formulation, metamodel construction, new sample generation, and other processes of optimization. Additionally, ontology knowledge base tends to be useful in the problem formulation stage to determine the constraints and design variables. Another important piece of information which is not considered yet is data records from previous similar optimizations. In practice, sample points in similar optimizations can potentially be employed for the current problem through modifications.

The challenge of employing knowledge in assisting optimization is still huge. The first challenge is how to validate knowledge. The expert system is useful in optimization formulation, but the accuracy of the expert system highly depends on qualities of the expert and the knowledge that could possibly be extracted from the expert. Causal graph is in the same situation. To validate knowledge, different sources of knowledge can be used. For instance, the experimental data can be used to validate knowledge obtained from experiences while the experience can be used to judge the validity of data.

The second challenge is how to employ different kinds of knowledge to support various tasks of optimization. As proposed in Secs. 4.1–4.5, knowledge can be applied to support different optimization tasks, from problem formulation to optimization strategy. Moreover, different kinds of knowledge can be applied together to one optimization task. How to organize different knowledge for one task is a challenge. How to manage different kinds of knowledge? When and where to involve knowledge, and what kinds of knowledge can be involved? All these questions needed to be answered in order to develop a systematic approach of applying knowledge in optimization, instead of falling into convenient ad hoc solutions. Therefore, a systematical methodology of organizing different kinds of knowledge is needed to concertedly assist optimization.

The third challenge is knowledge updating. During optimization, new knowledge can be obtained as more samples are generated. Then, how to update the current knowledge base and how to apply the newly obtained knowledge in optimization are research questions. Moreover, another related challenge in knowledge updating is error correction. When errors are found in the current knowledge base, these errors should be corrected through certain methodologies. How to correct errors in knowledge is also a key research direction for knowledge updating.

5 Machine Learning, Optimization, and Knowledge

There exists close ties between sample-based optimization and machine learning. One of the issues in sample-based optimization is to determine the next samples without or with less expensive function evaluations. In heuristic optimization algorithms (e.g., GA, PSO, etc.), the expensive function is evaluated at all sample points, which increases the computational cost significantly. Instead of using expensive functions, metamodels are employed to predict the responses and only the interesting points are evaluated by the expensive functions to improve the efficiency of metamodel-based optimization (e.g., MPS, EGO, etc.). Similar to optimization, machine learning methods also try to learn from data (or samples). ANN, one of the machine learning models, is widely used as prediction and classification models in manufacturing [108]. ANN essentially plays the same role as a metamodel and it is in fact a commonly used metamodel in design optimization community. The ability of ANNs (especially deep ANNs) in dealing with high-dimensional spaces and large amount of data has been noticed [109]. For example, convolutional neural networks can be used to deal with pictures with thousands or even millions of pixels as inputs [110]. Instead of estimating the actual responses of samples, judging the performance of samples via classification is another way to guide sampling, which has been used in optimization algorithms by employing Bayesian network classifier [15,17] or support vector machine [111]. Another application of classification models is found in heuristic optimization algorithms, where classification is used to determine whether the next generation of sample positions improves the search or not. Some other ANNs can also be employed to assist optimization. Autoencoder can be used to reduce dimensionality [112]. Recurrent neural networks (RNNs) are usually used to learn from sequential data as the circular architecture of RNN [113]. An optimization process also has a loop structure that the current optimal point and samples can determine the next optimal solutions. Thus, there is a potential to use RNN to learn the optimization process.

DM, also known as knowledge discovery from data, is a method to help find knowledge from existing data [114]. Regression and classification are also employed in DM to find the trend of the data. Another benefit obtained from DM is the ability of preprocessing. As mentioned in Sec. 4.2, feature selection methods can be used to reduce the dimensionality. Additionally, feature selection methods can also be used in determining redundant constraints according to the data of constraints. If data of intermediate variables can be obtained from simulations, feature selection can also be applied in input-intermediate and intermediate-output pairs to identify the structure of engineering problems.

Both machine learning methods and data mining methods, however, are also based on samples, similar to sample-based optimization. Wu et al. suggested that domain and application knowledge should be applied to design big data mining algorithms and systems [115]. In machine learning, deep learning methods are developed to improve the effectiveness of learning without engineering skills and domain expertise [116], but the amount of training data and computational costs are large. Therefore, knowledge can help both optimization and machine learning. In Refs. [117,118], fuzzy rules were employed to predict the flying ash and the performance of a gasoline engine and the results were similar to or outperformed the ANN predictions. Bayesian networks came into sights of researchers, as they contain the structures of problems (knowledge) and the probability distributions of variables (data). By combining knowledge and data together, Bayesian networks have the potential to be applied in optimization to guide sampling.

6 Summary

To overcome the challenge of search blindly in design optimization, the application of knowledge to assist optimization is discussed in this paper. The concepts of knowledge in AI and product design are reviewed. In those fields, knowledge is captured, represented, and reused to solve decision-making or design problems. Next, some existing applications of knowledge assisting optimization are described and categorized. Although the concept of knowledge may not explicitly appear in these methods, the idea of involving knowledge in improving the efficiency of optimization is employed in these works. Finally, multiple future potential applications of knowledge in optimization, as well as its relation to machine learning, are discussed.

To summarize, to tackle challenging optimization problems and to further improve the efficacy of design optimization, it seems imperative to let go the assumption of black-box functions, but rather incorporating existing knowledge in optimization. It is not only because that it is a waste not using these valuable knowledge but also necessary if we want to ultimately break the "curse-of-dimensionality" for simulation-based optimization. This paper reviews on this very topic and proposes many possible ways to develop knowledge-assisted optimization approaches.

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