A Comprehensive Review of Machine Learning in Multi-objective Optimization

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***Abstract*— In the real world, it is challenging to calculate a trade-off alternative with traditional classical methods for complex non-linear systems, which always involve multiple conflicting objectives. Such complicated systems urgently desire advanced methods to conquer the multi-objective optimization problems (MOPs). As a promising AI method, the development and application of Machine Learning (ML) attract increasingly more attention from researchers. The natures of ML methods, such as parallel computation possibility, no need for any priori assumptions, etc., ensure the effectiveness and efficiency for solving MOPs. However, as we know, there is no literature related to the comprehensive review of ML in multi-objective optimization domain until now. This literature review aims to provide researchers a global view of mainstream ML methods for MOO in a general domain and a reference for applying ML methods to solve a specific type of MOPs. In this paper, the general ML mainstream methods are summarized, based on which the literature relating to ML on MOPs are retrieved in comprehensive domains. The relevant literature is categorized according to the emphasis of object types, purposes and methods, and the categorization results are finally analyzed and discussed.**

Keywords*— *multi-objective optimization, machine learning, reinforcement learning, neural network

I. Introduction

In the real world, complex systems always involve multiple objectives, and these objectives tend to be inter-dependent and conflict with each other. As a result, how to solve such multi-objective optimization problems (MOPs) attract much attention in the research and engineering areas. Some classic methods, such as Evolutionary Algorithms (EA), play an important role in solving MOPs. However, with the prosperous development of Machine Learning (ML) in recent years, the researches on applying ML to MOPs are increasingly promising. As we know, there is no comprehensive review in the field of ML solving MOPs. This scoping review aims to provide researchers with some ideas about ML for solving MOPs to guide future research directions from a comprehensive perspective.

ML methods are categorized mainly by four types: Supervised Learning, Unsupervised Learning, Semi-supervised Learning and Reinforcement Learning (RL). The mainstream ML methods are summarized in TABLE I [1-7]. The main contributions of this ML review encompass:

- Summarizing mainstream ML methods based on the basic four-category classification. A systematic literature review of ML methods solving MOPs in general domains is committed. As we know, there is no such general review of ML on MOPs published in the recent decade.
- Categorizing ML literature according to different aspects and research emphasis of the application on solving MOPs.
- The category results of ML literature provide researchers an overview graph of utilizing a given ML method solving a certain MOP for a specific purpose. Thus, the results of this literature study can be considered as a reference for researchers for their future research in this domain.
- Providing a logical methodology of establishing the literature pool for the research analysis in a specific domain.

The remaining sections of this paper are organized: in section II, the logical methodology is introduced in detail for building a literature pool of ML on MOPs for the further analysis. The items in the literature pool are categorized based on three aspects and the classification results are proposed in section III. Furthermore, the analysis results are further discussed in section IV. The findings and some recommendations are concluded in section V.

II. Methodology

This section focuses on stating the retrieval methodology for literature on solving MOPs with ML methods. Generally, there are three steps involved during the retrieval process. First, the relevant search strings are created and prioritized based on their relevance to this scoping review topic. The second step is to complete the search process by applying the search-strings in diverse academic databases. Thirdly, some citation management is conducted on the search results to establish the literature pool for further analysis.

A. Create Search Strings

All the keywords that are relevant to the topics of this scoping review are categorized into three groups, which are "object type", "purpose" and "method", according to the emphasis aspects of the keywords. The brief definitions of the groups are:

1) "object type": The "object type" group represents the feature of a "to be optimized" system. These features are described from different aspects, such as the features of the involved multiple-criteria, the participant issues, etc.

The search keywords of "object type" in this review include: multi-objective OR multiobjective OR (multi objective), many-objective OR (many objective), multiple-objective OR (multiple objective), multi-criteria (OR multi criteria OR multicriteria), multiple-criteria OR (multiple criteria), multi-dimension OR multidimension OR (multi dimension), multi-dimensional OR multidimensional OR (multi dimensional).

2) "purpose": The keywords in the group of "purpose" represent what the specific goal is to achieve by a particular optimization method in MOPs, such as "optimization", "decision-making", etc.

The search keywords of "purpose" include optimization OR optimal, decision-making OR (decision making), negotiation OR negotiating, scheduling OR schedule.

3) "method": The group "method" includes not only the general keywords in the review domain, such as "Machine Learning" or "ML", etc., and the titles of the categories and sub-categories, such as "Unsupervised Learning", "Neural Network", etc., but also containing the specific ML methods, such as "Feedforward Neural Network", etc. The involved ML methods in the group "method" refer to Table I.

For improving searching effectiveness and accuracy, the search strings are prioritized according to the relevance to the topic in each group. For instance, in terms of the "method" group, the keywords that represent an explicit ML method are with high priority, while the keywords of general concepts, categories and sub-categories of ML are with low priority. The retrieval process starts with searching the keyword combinations with high priority. If the search results of high-priority keywords are not adequate as expected, the keywords with low-priority will be used for further search. In this review, the keywords with high and low priorities are all involved in the literature retrieval phase.

During the literature retrieval, each search string is a combination of keywords from the three groups, respectively. For instance, one of the search strings can be "multi-criteria" AND "negotiation" AND "Neural Network".

B. Apply the Search Strings in Databases

With the search methods in the last sector, each search-string combination's retrieval results are imported into EndNote. After analyzing the titles and the abstracts, it is found that NN and RL are the most widely used ML methods for

TABLE I. SUMMARY OF ML MAINSTREAM METHODS

Category	Sub-Category	ML methods	Reference
Supervised Learning	Neural Network	Deep Learning	[1]
		Convolutional Neural Network	[2]
		Back propagation	[3]
		Recurrent Neural Network	[4]
		Hopfield Network	[5]
		Multi-layer Perceptron	[6]
		Radial Basis Function Network	[7]
		Restricted Boltzmann Machine	[8]
		Self-organizing Map	[9]
		Spiking Neural Network	[10]
	Bayesian	Naive Bayes	[11]
		Gaussian Naive Bayes	[12]
		Bayesian Belief Network (BBN)	[13]
		Multinomial Naive Bayes	[14]
		Averaged One-Dependence Estimators	[15]
	Decision Tree	Decision Tree	[16]
		Random Forest	[17]
		Classification and Regression Tree (CART)	[18]
		Iterative Dichotomies	[19]
		C4.5 Algorithm	[20]
		C5.0 Algorithm	[21]
		Chi-squared Automatic Interaction Detection	[22]
		Decision Stump	[23]
		Supervised Learning in Quest	[24]
	Linear Classifier	Linear Regression	[25]
		Logistic Regression	[26]
		Naive Bayes Classifier	[27]
		Support Vector Machine	[28]

Category	Sub-Category	ML methods	Reference
Supervised Learning	Linear Classifier	Fisher's Linear Discriminant	[29]
		Multinomial Logistic Regression	[30]
Unsupervised Learning	Neural Network	Feedforward Neural Network	[31]
		Logic Learning Machine	[32]
		Generative Adversarial Networks	[33]
	Association Rule Learning	Priori Algorithm	[34]
		Eclat Algorithm	[35]
		FP-Growth Algorithm	[36]
	Hierarchical Clustering	Single-linkage Clustering	[37]
		Conceptual Clustering	[38]
	Cluster analysis	K-means	[39]
		K-means Clustering	[40]
		Expectation-maximization	[41]
		BIRCH Algorithm	[42]
		DBSCAN Algorithm	[43]
		Fuzzy Clustering	[44]
		K-medians Clustering	[45]
		Mean-shift	[46]
		OPTICS Algorithm	[47]
	Anomaly detection	K-nearest Neighbor	[48]
		Local Outlier Factor	[49]
Semi-supervised Learning	Generative Models		[50]
	Low-density Separation		[51]
	Graph-based Methods		[52]
	Co-training		[53]
Reinforcement Learning	Q-learning		[54]
	Temporal Different Learning (TD-learning)		[55]
	Deep Q learning (DQN)		[56]
	State Action Reward State Action (SARSA)		[57]
	Policy Gradients		[58]
	Model Based RL		[59]

solving MOPs. Therefore, this paper focuses on the analysis of NN and RL applied to MOPs. Table II shows the retrieval results by searching literature titles in databases.

With the search methods in the last sector, each search-string combination's retrieval results are imported into EndNote. After analyzing the titles and the abstracts, it is found that NN and RL are the most widely used ML methods for solving MOPs. Therefore, this paper focuses on the analysis of NN and RL applied to MOPs. Table II shows the retrieval results by searching literature titles in databases.

Considering the relevant engineering domains, four databases are selected for this literature retrieval, that are Scopus, IEEE Xplore, Web of Science (WoS) and for Computing Machinery (ACM). During the literature retrieval, each search string is a combination of keywords from the three groups, respectively. For instance, one of the search strings is: "multi-criteria" AND "negotiation" AND "Neural Network".

TABLE II. SEARCH STRINGS AND SEARCH RESULTS IN DATABASES

ML method	Databases			
	Scopus	***IEEE***	***WoS***	***ACM***
(Machine Learning) OR ML	70	16	290	136
(Neural Network) OR ANN OR NN	298	52	247	226
(Reinforcement Learning) OR RL	27	19	77	179
Total (each database)	**395**	**87**	**614**	**541**
Total				**1,637**

C. Citation Management

Citation management is applied to the literature items identified above to obtain the final literature pool for further detailed analysis. The management process for this literature review is shown in Fig. 1. The purpose of the citation management is to ensure the literature pool is highly relevant to the topic so that the analysis results of the literature pool can be accurate.

There are 1,637 literature items in the literature pool at the beginning. Firstly, after removing the duplicates automatically by EndNote and manually in the original pool, 1,015 literature is left. The next step is to ensure the content of the literature can be searched, which is committed by the function "find full text" of EndNote. As a result, there are 775 pieces of literature can be found in full papers or URLs. Finally, by analyzing the titles, keywords and abstracts of the literature, there is 410 literature left in the literature pool for the literature analysis in the next section.

III. RESULTS

In this section, the filter results in the literature pool are categorized and analyzed. Firstly, the literature is categorized by "purpose" in section Methodology, which are optimization, decision-making, negotiation and scheduling. Next, the literature items in each "purpose" group are further categorized by "ML method" and "object type". The category results are analyzed according to the relevant research aspects, respectively.

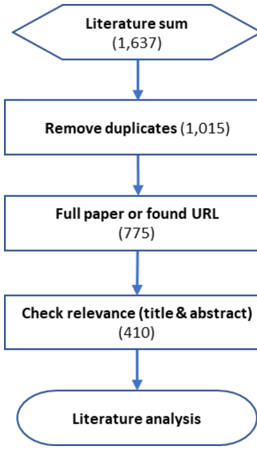

Fig. 1. Literature management process

In Table III, a summary of the numbers of literature according to "object type" and "purpose" is proposed. The overall numbers of the items in the literature pool based on "object type" and "ML method" are depicted in TABLE IV. In these two tables, the total sum of all categories is larger than the paper number in the literature pool. The reason is some papers exist overlapping search-string keywords in different categories so that these papers are counted in more than one category.

TABLE III. SUMMARY OF LITERATURE NUMBER ACCORDING TO OBJECT TYPE AND PURPOSE

Object type / Purpose	multi-objective	multi-criteria	multi-dimension	multi-issue	multi-agent	others	SUM
Note: The sum of all the literature in this table is larger than the actual total item number in the literature pool, because some literature includes hybrid key search strings in the specific group. Same in TABLE IV.							
Optimization	305	4	2	0	5	36	**351**
Decision-making	9	7	0	0	2	0	**18**
Negotiation	1	0	0	5	1	0	**7**
Scheduling	19	1	0	0	7	10	**37**
SUM	**334**	**12**	**2**	**5**	**15**	**46**	**413**

TABLE IV. SUMMARY OF LITERATURE NUMBER ACCORDING TO ML METHODS AND PURPOSE

Purpose / ML method	Optimization	Decision-making	Negotiation	Scheduling	SUM
NN	271	11	0	8	**290**
RL	74	6	7	28	**115**
Other ML	6	1	0	1	**8**
SUM	351	18	7	37	**413**

A. Optimization

The research category on solving MOPs using ML methods with the "purpose" of optimization is shown in TABLE V. In the domain of "optimization" in the "purpose", 351 papers are involved in the literature pool. Among them, there are 271 literature items on the application of NN, 74 literature are related to RL. Six literature items are related to some other ML methods for solving MOPs.

Gradient descent is applied in [60, 61] on MOO in the domains of discharging process and bioprinting, respectively. Bayesian optimization is used for approximating the Pareto Front set in [62]. [63] presents the application of . Extreme Learning Machine [64], which is categorized as "other ML" in spite it is a special variant of Feedforward Neural Network. In [65], an ML package "scikit-learn" is utilized for selecting a mathematical framework in order to surrogate objective the functions.

From Table V, the most popular research object type is multi-objective in the "optimization" area, and the number of the relevant literature items is 305, which accounts for approximately 86.9% of the total literature in this purpose. In the multi-objective object type, the number of researches on NN is 243, followed by 56 literature on RL. All six pieces of literature of other ML methods focus on the object type of multi-objective.

Aparting from the five proposed object types in TABLE V, there are 36 papers related to "others" of "object types" in the "optimization" area in the literature pool.

Regarding to the "others" of "object type" that NN is applied on, "multi-core" accounts for six literature items, which is the most widely researched "object type". Among the six literature, [66] focuses on the hybrid object types of multilayer and multi-core, and [67] hybrids multigrid and multi-core. In addition, "multi-layer" accounts for 2 papers [68, 69] and each of the remaining "object type" is mentioned for once in the literature pool, that include multi-processor[70], multi-goal[71], multioutput[72], multi-constrained path[73], feature-rich[74], multi-phase[75], multiple Indexes[76], multi-echelon[76], multi-heuristic[77], multi-Level[78], multi-view [79], multi-class[80], multigrid[81], many-field[82], multiple access[81], multi-population[64], multiple voltage regulators[83], multiple Smartphones[84].

With respect to RL, there are ten different object types. Among them, the relatively popular object type is multi-policy (two papers). There is one paper in each "object type" of "high-dimensional [85], many-core [86], multi-area [87], multiple sequence [88], multi-access [89], multi-armed [90], multi-hop [91], multiple time-points [92], multiple embedding candidates [55].

B. Decision-making

There are 18 papers related to the "decision-making" of "purpose" in the literature pool in total.

The literature number sum of NN is 11 in this area, approximately twice of RL (six papers). An "other ML" is proposed in [93], in which k-Nearest Neighbor (kNN) and K-Star (KS) algorithms are utilized in the "multi-criteria" of flash-flood susceptibility assessment. "decision-making" in the literature pool. The most widely researched "object type" area is "multi-objective" (nine papers), which is followed by "multi-criteria" (seven papers). Besides, "multi-agent" is discussed in two papers.

TABLE V. CATEGORY OF ML METHODS IN OPTIMIZATION

object type / purpose	multi-objective	multi-criteria	multi-dimension	multi-issue	multi-agent	others	SUM
NN	243	2	2	0	0	24	**271**
RL	56	2	0	0	5	12	**74**
Other ML	6	0	0	0	0	0	**6**
SUM	**305**	**4**	**2**	**0**	**5**	**36**	**351**

Note:
(1) The title of each column is only a representative of a specific category of "object type". For example, the statistic result of "multi-objective" also involves the literature statics with "multiple objective", "many objective" and so on.
(2) The literature number sums of each "object type" are listed in the last row, and the literature number sums of each method are listed in the last column. The sum of literature items with purpose "optimization" is in the lower right cell.

Although NN on "multi-criteria" is the area that is researched most in the decision-making domain, the relevant literature number (six papers) is very close to the applications of RL on multi-objective (five papers) and NN on multi-objective (four papers). In addition, there is one paper in each area of NN on "multi-agent" [94], RL on "multi-agent" [95] and "other ML" on "multi-criteria" [93].

C. Negotiation

Only seven relevant papers related to ML solving the MOPs with "negotiation" are involved in the literature pool, and the application of RL contributes to all the seven literature.

Here, the predominant "object type" is "multi-issue" with five items in this area. Besides, there is one paper in each of the domain of "multi-objective"[96] and "multi-agent"[97], respectively.

D. Scheduling

In total 37 literature items were identified in the "scheduling" category.

RL is the most utilized ML method for solving MOPs with the "purpose" of "scheduling". The literature related to RL (28 papers) is more than three times of NN (eight papers) in this domain. Besides, [98] proposes a hybrid method of estimation of distribution algorithm and ML, which is considered as "other ML" in "scheduling".

In this area, twelve categories of "object type" are involved. Among these categories of "object type", 19 papers in "multi-objective" and seven papers in "multi-agent" are included in the literature pool, respectively, which are the most widely researched in this domain. There are two papers related to each of the "object type" of "multi-stage"[68, 69] and "multi resource" [99, 100] respectively. Additionally, there is one paper for each "object type", they are multi-criteria[98], multiple machines[68], multi-user[101], multihop[102], multi-core[103], multiphase[104], multi-task[105] and multilevel[106]. For example, in [105], RL is used to solve a routing scheduling for multi-task; in [99], an object type of multi-resource fairness is introduced; there are two relevant papers of multi-stage and multi-resource, respectively relating to RL on MOPs; two object types, multi-stage and multiple machines, are involved in [68].

The most widely researched sub-field of "scheduling" is applying RL on "multi-objective" problems, which is followed by the areas of NN on "multi-objective" and RL on "multi-agent", including eight and seven papers, respectively.

IV. Discussion

In conclusion, there is 410 literature relating to ML methods solving MOPs in the literature pool. Due to some papers have hybrid keywords in one of the three groups of "object type", "purpose" and "ML method", the total sum in TABLE III and TABLE IV is 413, which is slightly larger than the actual size of the literature pool.

In TABLE III, among the four groups of "purpose", 351 literature items are related to the research on "optimization" problems, accounting for approximately 85% of the literature pool. However, there are only seven papers related to "negotiation". Concerning the five "object types", "multi-objective", containing 334 literature items, is the dominating one. By contrast, "multi-dimension" problems only attracts two relevant papers in the literature pool.

The problem of "multi-objective" "optimization", with totally 306 papers in the literature, is the combination of "purpose" and "object type" that receives most research attention. The number of papers focusing on this domain accounts for approximately 86.7% in the "optimization" of group "purpose", approximately 91.3% in the "multi-objective" of group "object type" and approximately 74.6% of the literature pool.

From TABLE IV, concerning ML methods corresponding to "object type", the literature that utilizes NN (290 papers) is more than twice of RL (115 papers) in the literature pool. There are eight papers apply other ML methods expecting NN or RL, which are analyzed in detail in section III. Therefore, the application of NN and RL is the dominant research direction of utilizing ML methods on MOPs.

Among the papers related to NN, the most widely researched "object type" is "optimization" (271 papers), which accounts for approximately 93.4% of total 290 papers in MOO domain. Besides, eleven and eight papers focus on "decision-making" and "scheduling", respectively. Concerning RL, "optimization" is also the most popular research domain, with 74 papers, which covers around 64.3% of the papers that apply RL (115 papers). Additionally, there are 28 literature items focus on "scheduling" problems, which is followed by "negotiation" (seven papers) and "decision-making" (six papers).

V. Conclusion

In this paper, a comprehensive scoping review on the application of ML methods in solving MOPs is proposed. A citation management methodology containing strategies to categorize search-strings into groups and prioritize them was applied to ensure effective retrieval of literature items. This methodology also ensured that only literature items with relevant topics were included. Therefore, all the papers in the literature pool are relevant to the review topic. A total of 410 literature items were added to a literature pool covering comprehensive respects of ML on solving MOPs. All the literature is categorized into groups from the three emphasis aspects, and the category results are analyzed accordingly.

Compared with other classical algorithms, such as Evolutionary Algorithms, Fussy Logic, etc., for solving MOPs, ML is a new method in this domain, and the number of relevant researches that focus on ML for MOO is much smaller than them. However, the development of ML on MOO is increasing rapidly due to its outstanding performance for solving highly non-linear problems. Besides, ML is a prospecting method for solving complex MOPs because the development of parallel computing capacity of computers benefits the nature advantage of computation efficiency of some ML methods, such as NN.

The aim of this literature review is to provide researchers a reference for their research on solving MOPs with ML methods. The analysis results in this paper provide an overview graph of the application of ML methods for solving a given type of MOP, which can be analyzed from the aspects of "object type" and "purpose". Therefore, researchers can determine the direction of the application of methods for solving a type of MOPs in future researches.

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