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Optimization under Uncertainty: Machine Learning Approach

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ABSTRACT

Data is the new oil. From the beginning of the 21st century, data is similar to what oil was in the 18th century, an immensely untapped valuable asset. This paper reviews recent advances in the field of optimization under uncertainty via a modern data lens, highlights key research challenges and promise of data-driven optimization that organically integrates machine learning and mathematical programming for decision-making under uncertainty.
A brief review of classical mathematical programming techniques for hedging against uncertainty is first presented, along with their wide spectrum of applications in Process Systems Engineering.
We provide an introduction to the topic of uncertainty in machine learning as well as an overview of attempts so far at handling uncertainty in general and formalizing this distinction in particular.
In line with the statistical tradition, uncertainty has long been perceived as almost synonymous with standard probability and probabilistic predictions. Yet, due to the steadily increasing relevance of machine learning for practical applications and related issues such as safety requirements, new problems and challenges have recently been identified by machine learning scholars, and these problems may call for new methodological developments.

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1. Introduction

While methods for optimization under uncertainty have been studied intensely over the past decades, the explicit consideration of the interplay between uncertainty and time has gained increasing attention rather recently. Problems requiring a sequence of decisions in reaction to uncertainty realizations are of crucial relevance in real-world applications, e.g., supply chain planning, scheduling, or finance. Several methods emphasizing varying aspects of these problems have been developed, mainly triggered by a particular application. Although these methods all intend to solve a similar underlying problem, they differ strongly with respect to the uncertainty representation, the prescriptive solution information they provide and the means of performance evaluation. Over the last six decades, several pioneers of the industry have worked to steer us in the right direction [1]. Uncertainty and fuzziness are popular phenomena in many application areas such as medicine (medical diagnosis is often not crisp but there exist various degrees of illness e.g. for psychical diseases such as phobia), image processing (areas at object borders or at overlapping regions can seldom uniquely be classified), linguistics (terms such as ‘high’ or ‘small’ are context dependent), etc. Therefore, uncertainty almost automatically occurs in any application of machine learning [2]. An important aspect of these systems is the complete and valid quantification of model uncertainty [3].

From early times people have realized that managing a situation that included many alternatives, is nothing less and nothing more than determining the solution with the more positive and less negative consequences. The procedure to determine the “ideal” solution is called optimization. The oldest optimization technique is the “trial and error” one, according to which the best solution is determined after trying and evaluating a large number, if not all, of possible alternatives. This technique is used even in our days since is the easiest to understand, regardless the fact that it is the most time-consuming. The foundation and establishment of the science of management and optimization was set through time, along with the development of mathematics and the new tools they provided in handling alternative solutions. One of the main problems in applying optimization techniques is the transition between the actual problem and its mathematical model. No natural phenomenon or applied situation can be fully described by mathematical equations. This is because each model incorporates a number of constraints and assumptions that are not applicable in natural systems. Thus, the simulation of natural systems with mathematical models must be applied with extreme caution [4].

As previously discussed in the introduction, uncertainty is a crucial issue in many real-life scenarios. Providing a prediction without the associated uncertainty can be dangerous in cases where the prediction is subsequently used to make important decisions [5]. The sources of uncertainty are often decomposed into two parts—the aleatoric and the epistemic [6]. The first is inherent in the process under study, while the second depends on inadequate knowledge of the model that is most suited to explaining the data. The uncertainty is usually considered as a confidence interval of the point-wise inference. There are many tools for estimating uncertainty, such as bootstrapping, quantile regression, Bayesian inference, and dropout for the neural networks [7, 8, and 9].

2. Uncertainty and Optimization under Uncertainty

Depending on different models, one technique may be more suitable than others; therefore, they will be described in more detail in the subsequent sections, which introduce the tested models. For example, uncertain environments for the SCND problem can be categorized according to the following groups:

Group 1 (G1): Decision-making environments with random parameters in which their probability distributions are known for the decision maker. Here, these parameters are called stochastic parameters. Stochastic parameters in SCND are described by either continuous or discrete scenarios. In a smaller part of Group 1, the stochastic parameters are described using a known continuous probability distribution. This type of SCND problem – except for simple networks with one location layer – engenders intractable optimization models. Additionally, the customers' demand is the most popular stochastic parameter in these studies, which is modeled through the normal distribution with known mean and variance.

Group 2 (G2): Decision-making environments with random parameters in which the decision maker has no information about their probability distributions. Under this setting, robust optimization models are usually developed for SCND with the purpose of optimizing the worst-case performance of SC network. The random parameters in this decision-making group are divided into either continuous or discrete. To model discrete uncertain parameters, the scenario approach has been used. However, for continuous uncertain parameters, some pre-specified intervals are defined. This approach is also called interval-uncertainty modeling.

Group 3 (G3): Fuzzy decision-making environments. In general, there exist two types of uncertainties including ambiguity and vagueness under the fuzzy decision-making environment. Ambiguity denotes the conditions in which the choice among multiple alternatives is undetermined. However vagueness states the situations in which sharp and precise boundaries for some domains of interest are not delineated. In this context, fuzzy mathematical programming handles the planner's expectations about the level of objective function, the uncertainty range of coefficients, and the satisfaction level of constraints by using membership functions [10].

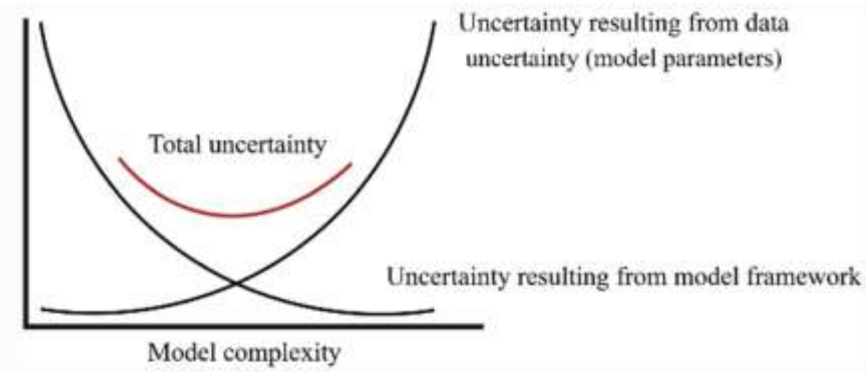

Fig. 1. The Trade-Off between data and model uncertainty [11]

Optimization applications abound in many areas of science and engineering. In real practice, some parameters involved in optimization problems are subject to uncertainty due to a variety of reasons, including estimation errors and unexpected disturbance. Such uncertain parameters can be product demands in process planning, kinetic constants in reaction-separation-recycling system design, and task durations in batch process scheduling, among others. The issue of uncertainty could unfortunately render the solution of a deterministic optimization problem (i.e. the one disregarding uncertainty) suboptimal or even infeasible. The infeasibility, i.e. the violation of constraints in optimization problems, has a disastrous consequence on the solution quality. Motivated by the practical concern, optimization under uncertainty has attracted tremendous attention from both academia and industry [12]. A large number of problems in production planning and scheduling, location, transportation, finance, and engineering design require that decisions be made in the presence of uncertainty. Uncertainty, for instance, governs the prices of fuels, the availability of electricity, and the demand for chemicals. A key difficulty in optimization under uncertainty is in dealing with an uncertainty space that is huge and frequently leads to very large-scale optimization models. Decision-making under uncertainty is often further complicated by the presence of integer decision variables to model logical and other discrete decisions in a multi-period or multi-stage setting [13]. Design optimization of structural and multidisciplinary systems under uncertainty has been an active area of research due to its evident advantages over deterministic design optimization. In deterministic design optimization, the uncertainties of a structural or multidisciplinary system are taken into account by using safety factors specified in the regulations or design codes. This uncertainty treatment is a subjective and indirect way of dealing with uncertainty. On the other hand, design under uncertainty approaches provide an objective and direct way of dealing with uncertainty [14].

3. Machine Learning

Since their evolution, humans have been using many types of tools to accomplish various tasks in a simpler way. The creativity of the human brain led to the invention of different machines. These machines made the human life easy by enabling people to meet various life needs, including travelling, industries, and computing. And Machine learning is the one among them. According to Arthur Samuel Machine learning is defined as the field of study that gives computers the ability to learn without being explicitly programmed. Arthur Samuel was famous for his checkers playing program. Machine learning (ML) is used to teach machines how to handle the data more efficiently. Sometimes after viewing the data, we cannot interpret the extract information from the data. In that case, we apply machine learning. With the abundance of datasets available, the demand for machine learning is in rise. Many industries apply machine learning to extract relevant data. The purpose of machine learning is to learn from the data. Many studies have been done on how to make machines learn by themselves without being explicitly programmed. Many mathematicians and programmers apply several approaches to find the solution of this problem which are having huge data sets [15]. Figure 2 shows that machine learning is a subset of artificial intelligence.

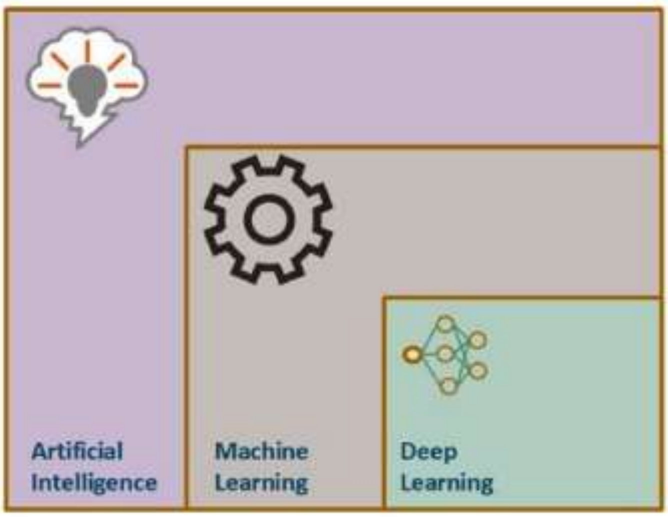

Fig. 2. Machine Learning Subset [16]

Machine learning is a tool for transforming information into knowledge. In the previous 50 years, there has been a blast of information/ data. This mass of information is pointless except if we investigate it and discover the examples covered up inside. Machine learning techniques are utilized to consequently locate the significant fundamental examples inside complex information that we would somehow battle to find. Hidden patterns and information about the problem can be used to predict future events and to make all sorts of complex decisions [16]. Traditionally, uncertainty is modeled in a probabilistic way, and indeed, in fields like statistics and machine learning, probability theory has always been perceived as the ultimate tool for uncertainty handling. Without questioning the probabilistic approach in general, one may argue that conventional approaches to probabilistic modeling, which are essentially based on capturing knowledge in terms of a single probability distribution, fail to distinguish two inherently different sources of uncertainty, which are often referred to as aleatoric and epistemic uncertainty. Machine learning is essentially concerned with extracting models from data, often (though not exclusively) using them for the purpose of prediction. As such, it is inseparably connected with uncertainty. Indeed, learning in the sense of generalizing beyond the data seen so far is necessarily based on a process of induction, i.e., replacing specific observations by general models of the data-generating process. Such models are never provably correct but only hypothetical and therefore uncertain, and the same holds true for the predictions produced by a model. In addition to the uncertainty inherent in inductive inference, other sources of uncertainty exist, including incorrect model assumptions and noisy or imprecise data [17]. Nowadays, a wide array of emerging machine learning tools can be leveraged to analyze data and extract accurate, relevant, and useful information to facilitate knowledge discovery and decision-making. Deep learning, one of the most rapidly growing machine learning subfields, demonstrates remarkable power in deciphering multiple layers of representations from raw data without any domain expertise in designing feature extractors. More recently, dramatic progress of mathematical programming [18], coupled with recent advances in machine learning, especially in deep learning over the past decade, sparks a flurry of interest in data-driven optimization. In the data-driven optimization paradigm, uncertainty model is formulated based on data, thus allowing uncertainty data “speak” for themselves in the optimization algorithm. In this way, rich information underlying uncertainty data can be harnessed in an automatic manner for smart and data-driven decision making [12].

Machine learning is widely used in academia and industry to analyze big and complex datasets to uncover the hidden patterns and reach conclusive insights. It is well known that the performance of machine learning models has a close relationship not only with the selected algorithms but also depends on the nature of data [19]. Machine learning algorithms that can model uncertainty to reveal beneficial information for a better decision-making process will be of great use. Generally, uncertainty may be due to two reasons: data (noise) uncertainty and model uncertainty (also called epistemic uncertainty). It is likely to have noise among labels due to measurement imprecision which may lead to aleatoric uncertainty. Meanwhile, model uncertainty can be divided into two main types: structure uncertainty and uncertainty in model parameters. In structural uncertainty, we find out the type of model structure to be used and to specify our proposed model for either extrapolating and/or interpolating. In the second type, i.e. uncertainty in model parameters, optimal model parameters are selected for more accurate predictions [20]. Different types of uncertainty can be observed: (i) Input data are subject to noise, outliers, and errors. A machine learning method has to deal with this type of fuzzy information, showing robustness with respect to such disturbances. Thereby, input noise can have a positive effect on the generalization behavior of the machine learning method since the method is forced to develop some form of invariance and to abstract from the noise. (ii) Output decisions should be accompanied by a measure which allows to judge the certainty or belief of the output. This is particularly important in critical domains such as clinical diagnosis, in safety critical areas, or in semiautomatic systems where human expert knowledge is accompanied by automatic inference. (iii) Representation of information within a machine learning system is distributed and fuzzy. This is the standard situation for classical neural network models and it is difficult to assign a crisp meaning to specific parts of a neural model. For a deeper insight into the network behavior, an interpretation of the fuzzy information in the internal representation is required [2].

3.1. Types of Machine Learning

The development of algorithms that enable computers to automatically process text and natural language has always been one of the great challenges in Artificial Intelligence [1]. Several types of ML can be distinguished. Well-known ones are supervised, unsupervised and reinforcement learning.

3.1.1 Supervised Learning

Supervised learning accounts for a lot of research activity in machine learning and many supervised learning techniques have found application in the processing of multimedia content. The defining characteristic of supervised learning is the availability of annotated training data. The name invokes the idea of a ‘supervisor’ that instructs the learning system on the labels to associate with training examples. Typically these labels are class labels in classification problems. Supervised learning algorithms induce models from these training data and these models can be used to classify other unlabeled data [21]. Traditional supervised learning approaches rely heavily on the amount of annotated training data available. Even though there is a plethora of data available, the lack of annotations has pushed researchers to find alternative approaches that can leverage them. This is where self-supervised methods play a vital role in fueling the progress of deep learning without the need for expensive annotations and learn feature representations where data provide supervision. Supervised learning not only depends on expensive annotations, but also suffers from issues such as generalization error, spurious correlations, and adversarial attacks [22]. Recently, self-supervised learning methods have integrated both generative and contrastive approaches that have been able to utilize unlabeled data to learn the underlying representations. A popular approach has been to propose various pretext tasks that help in learning features using pseudo labels. Tasks such as image-in painting, colorizing grayscale images, jigsaw puzzles, super-resolution, video frame prediction, audio-visual correspondence, etc. have proven to be effective for learning good representations [23]. Supervised Learning is schematically demonstrated in Figure 3.

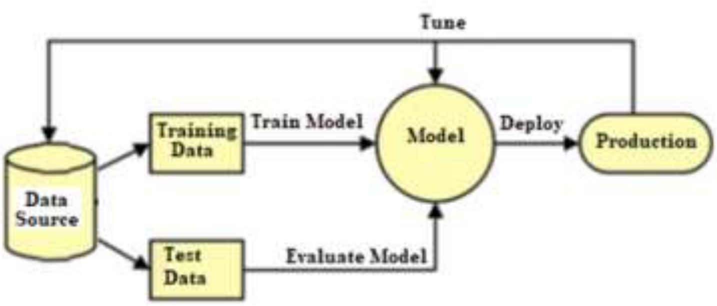

Fig. 3. Supervised Learning

3.1.2. Unsupervised Learning

For a given problem we often have access to a large dataset of unlabeled data [2]. While deep learning strategies achieve outstanding results in computer vision tasks, one issue remains: The current strategies rely heavily on a huge amount of labeled data. In many real-world problems, it is not feasible to create such an amount of labeled training data. Therefore, it is common to incorporate unlabeled data into the training process to reach equal results with fewer labels. Due to a lot of concurrent research, it is difficult to keep track of recent developments [24]. The key idea behind the unsupervised learning of disentangled representations is that real-world data is generated by a few explanatory factors of variation which can be recovered by unsupervised learning algorithms [25]. Taxonomy of Unsupervised Learning Techniques is shown in figure 4.

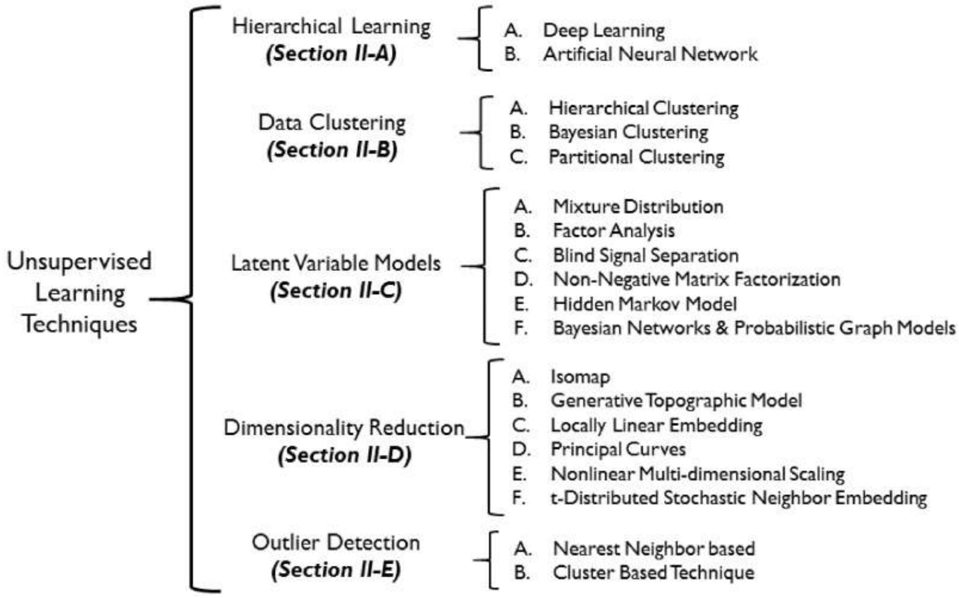

Fig. 4. Taxonomy of Unsupervised Learning Techniques [26]

3.1.3. Reinforcement Learning

As an area of Artificial Intelligence and Machine Learning, Reinforcement learning (RL) deals with the problem of a learning agent placed in an environment to achieve a goal. Contrary to supervised learning, where the learner structure gets examples of good and bad behavior, the RL agent must discover by trial and error how to behave to get the most reward [12]. For this task, the agent must percept the state of the environment at some level and based on this information, and it needs to take actions that result in a new state. As a result of its action, the agent receives a reward, which aids in the development of future behavior [27]. RL, unlike other machine learning techniques, can learn the environment by having minimum information about the parameters to be learned. It solves the optimization problem by interacting with the environment adapting the parameters on the fly [28].

4. Conclusion

Optimization applications abound in many areas of science and engineering. Over the second half of the 20th century, optimization found widespread applications in the study of physical and chemical systems, production planning and scheduling systems, location and transportation problems, resource allocation in financial systems, and engineering design. From the very beginning of the application of optimization to these problems, it was recognized that analysts of natural and technological systems are almost always confronted with uncertainty. Model uncertainty, and directly linked to it model sensitivity, are the most fundamental features and characteristics of a model. The uncertainty refers to the result of measurement that reflects a lack of exact knowledge of the value of the measurand. In order to understand the model's accuracy and reliability, it is important to estimate the uncertainty. Four types of uncertainties are typically evaluated in the models: structural, functional, parameter and data uncertainty. Approaches to optimization under uncertainty have followed a variety of modeling philosophies, including expectation minimization, minimization of deviations from goals, minimization of maximum costs, and optimization over soft constraints. Decision-making based on machine learning systems, especially when this decision-making can affect human lives, is a subject of maximum interest in the Machine Learning community. It is, therefore, necessary to equip these systems with a means of estimating uncertainty in the predictions they emit in order to help practitioners make more informed decisions. Although conventional stochastic programming, robust optimization, and chance constrained optimization are the most recognized modeling paradigms for hedging against uncertainty, it is foreseeable that in the near future data-driven mathematical programming frameworks would experience a rapid growth fueled by big data and deep learning. Depending on the decision variables, objectives, and constraints, the problems were classified as LP, NLP, IP, MILP, or MINLP. However, as stated above, the future cannot be perfectly forecast but instead should be considered random or uncertain. Optimization under uncertainty refers to this branch of optimization where there are uncertainties involved in the data or the model, and is popularly known as stochastic programming or stochastic optimization problems. Design research is important for understanding and interrogating how emerging technologies shape human experience. However, design research with Machine Learning is relatively underdeveloped. Crucially, designers have not found a grasp on ML uncertainty as a design opportunity rather than an obstacle. The technical literature points to data and model uncertainties as two main properties of ML.

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Conflicts of Interest

All co-authors have seen and agree with the contents of the manuscript and there is no financial interest to report. We certify that the submission is original work and is not under review at any other publication.

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