Uncertainty Quantification in Mathematics-Embedded Ontologies Using Stochastic Reduced Order Model

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Abstract—To resolve one of uncertainty features, *randomness*, in ontologies, this paper shows how to characterize uncertainty of concepts from a statistical viewpoint. In addition, with a focus on indirect entities, which are computed from direct entities through mathematical models, the uncertainties propagated from those direct entities are important and should be quantified. Thus, a novel algorithm, named *Stochastic Reduced Order Model (SROM)*, is presented to be applied to quantify the ontological uncertainty propagation in presence of multiple input entities. This SROM-based method could approximate the statistics of indirect entities accurately and efficiently by using a very small amount of samples of input entities. The computational cost is considerably reduced while guaranteeing a reasonable degree of accuracy. Furthermore, the predicted statistics of output entities could be regarded as high-level information and be beneficial for other ontological operations, such as ontology filtering and ontology reasoning. The implementation of the SROM algorithm is non-intrusive to the mathematical model; therefore, this algorithm could be applicable to quantify uncertainty in ontologies with any mathematical relationships.

Index Terms—Ontology, statistics, stochastic reduced order models, uncertainty propagation

1 Introduction

There is an increasing need to model information in a formalized manner so that interoperability can be achieved through having a common understanding. Ontology, which originates from the subject of philosophy and studies the nature of being, existence and categories of being, and their relations, has been widely used to rigorously and expressively provide this "specification of a shared conceptualization" [1]. Ontology is formalized in web ontology languages, which are based on expressive description logics [2]. Despite its popularity in modelling information, ontology lacks the ability to deal with uncertain data [3], [4], [5]. The uncertainty inherent to data could be various depending on different applications. Therefore, different understanding of the uncertainty of ontology representation coexists to fit specific interests of applications. The W3C UR3W-XG group[1] proposed an uncertainty ontology, which captures top-level classes and properties for characterizing the uncertainty consideration in ontologies. According to this uncertainty ontology, uncertainty can be classified into five main types, namely, *Ambiguity*, *Randomness*, *Vagueness*, *Inconsistency*, and *Incompleteness*. The uncertainty concern in ontologies comes from mainly two kinds of derivation: objective and subjective. Further, this uncertainty ontology categorizes different mathematical theories for uncertain types including probability, fuzzy sets, belief functions, random sets, rough sets, similarity models, preference models, trust models, and combinations of several models. This uncertainty ontology provides a formal vocabulary to represent different types of uncertainty, but further refinement is needed [6], e.g., inaccuracy should also be subsumed into ontological uncertainty.

Based on this uncertainty ontology, a considerable amount of efforts has been made to resolve different ontological uncertainty concerns defined in the uncertainty ontology. For instance, Bobillo et al. [4] presented their attempts to manage uncertainty by introducing fuzzy logic that drives crisp ontology to a more powerful version, referring to fuzzy ontology. Fuzzy ontology is explained as "it introduces fuzzy logic to extend classical ontology to allow the representation of imprecise and vague knowledge" [4]. However, the fuzzy endowed capability of managing the uncertainty of data does not cover all aspects. In fact, it addresses two main difficulties. This first one, which could be abstracted as ambiguity, is that the referents of terms in the ontology are not clearly specified and therefore it cannot be determined whether an individual is satisfied. The latter is regarded as vagueness, which solves the correspondences in different concepts. However, the randomness feature defined in the uncertainty ontology is comparatively under-researched. Randomness, due to imperfect instruments, noise, partial views, occlusions, etc., is widely inherent to ontological data from the objective sense, particularly

1. https://www.w3.org/2005/Incubator/urw3/

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referring to measurements repeatedly obtained to describe a specific phenomenon. For instance, instances of the concept *Length*, which describes the length of an object, could be random and variable in a scale due to imperfect instruments adopted. This randomness implies that each measurement, which is a potential instance to be populated in *Length*, could not represent the actual length of the observed object. Existing approaches in current literature propose to use degree of certainty or probabilistic theory to resolve the randomness in ontologies [6], [7]. For instance, the population of data in the underwater ontology [8] includes different degrees of certainty in order to represent the uncertainty, such as linking the concept *LengthofObstacle* (1.2 m) with a data property *hasDegreeofCertainty* (0.9). Quantifying uncertainty at an individual level is only one aspect of probability. The statistics (e.g., probability distribution), which takes a history or sequence of instances into account, could also be interesting and important to provide additional useful information to characterize the randomness of the concept. To measure the uncertainty of concepts from a holistic view based on statistics can be applicable in many domain-specific ontologies, which are sensitive to probabilistic research, such as engineering surveying, electromagnetism, and manufacturing industry. In this way, the uncertainty of ontological data could be quantified not only at a low level restricted to individuals but also at a high level aiming to achieve a holistic view of the probabilistic distribution. In addition, the statistics of uncertain ontological entities can be useful to make ontological reasoning based on probabilistic reasoning, such as Bayesian Network (BN) [9] or Multi-Entity Bayesian Network (MEBN) [7] theories.

The ontological uncertainty consideration, from the statistical aspect, would introduce more attention to indirect entities [10]. Indirect entities refer to those computed from direct entities through mathematical models in ontologies. In other words, the accuracy of indirect entities is subject to their corresponding direct entities because of the computational dependencies between them. Thus, it is very valuable to characterize, quantify, and properly address uncertainties propagated from direct entities to the indirect entity.

The Stochastic Reduced Order Model (SROM) [11] algorithm was proposed very recently and has been proven to be useful to quantify the uncertainty propagated from multiple input variables to the output response with a very low computational cost and a high degree of accuracy. Essentially, this algorithm is to construct an SROM with fewer samples to provide an approximation of an uncertain entity in the statistical sense. It has been applied to solve uncertainty propagation in mechanical engineering [12] and material problems [13], but has not been used for uncertainty considerations for ontologies. To this end, the aim of this paper is to present the first application of the SROM algorithm to quantify uncertainty propagation in mathematics-embedded ontologies, where the output entity is computed from multiple input entities. The SROM algorithm is non-intrusive to the mathematical model. It does not introduce any change to the mathematical model, which shows another advantage, namely, ease of use. Besides, it could accurately predict the uncertainty of entities, which are conclusions drawn from the mathematical model. By using the SROM algorithm, the ontological uncertainty quantification process is able to reduce the computational cost. The exploration of the SROM-based uncertainty quantification in ontologies will be shown by means of a case study.

The remainder of this paper is structured as follows: Section 2 presents related work in the uncertainty research in ontologies. Section 3 introduces the discipline of SROM. A case study on quantifying uncertainty propagation in mathematics-embedded ontologies using SROM is demonstrated in Section 4. Finally, conclusions and future work are presented in Section 5.

2 Related Work

In this section, current research on ontology uncertainty considerations is presented. Specifically, Section 2.1 provides the state of the art in mathematical representations in ontologies. Afterward, Section 2.2 reviews existing work on dealing with different kinds of ontological uncertainty.

2.1 Mathematical Models in Ontologies

Ontologies should support mathematical expressions as some concepts defined in ontologies might be computed through mathematical models by taking other concepts as inputs. For those indirect concepts, their uncertainties are subject to the uncertainty considerations of input concepts. To define concepts that have computational relationships with other concepts clearly, allowance of expressing the underlying mathematical model in ontologies is needed. Mathematical models can be represented as a set of rules encapsulated into ontologies by employing Semantic Web Rule Language (SWRL)[2] math built-ins. Further, Sanches-Macian et al. [14] presented an extension to SWRL to enable advanced mathematical support in SWRL rules. By using this extended SWRL, complex mathematical relationships and formulae can be described and included in ontologies. Gangemi [15] proposed a novel idea to import MathML[3] and OpenMath[4], which are standard XML-based languages for mathematical knowledge, into ontology annotations so that descriptions of mathematical relationships can be enabled.

2.2 Uncertainty Considerations in Ontologies

In current literature, uncertainties at different levels are defined and resolved from different aspects. In order to represent a clear separation between domain concepts [16], the introduction of tolerance for imprecision, through fuzzy logic, into crisp ontology in the uncertainty research field has obtained more and more popularity. Fuzzy logic is a suitable formalism to handle uncertainty in many domains [17], such as machining [18], waste management [19], renewable energy [20], risk assessment [21], and ambient intelligent environments [22]. Encasing fuzzy set (e.g., membership functions) and fuzzy logic, fuzzy ontologies can make a clear definition for vague concepts. Fuzzy ontology has been extensively exploited in many application domains, such as text, image and multimedia objects representation, and semantic query expansion and retrieval in the semantic web [23]. A fuzzy Ontology Generation

2. https://www.w3.org/Submission/SWRL/
3. https://www.w3.org/Math/
4. http://www.openmath.org/overview/technical.html

Framework (FOGA) [24] was presented to automatically generate fuzzy ontology by considering all uncertain input knowledge. In order to support mapping and solving confusions of fuzzy controls defined by different fuzzy applications or legacy environments, Maio et al. [25] created an upper ontology named OWL-FC aiming to provide a common and high-level abstraction of the specification and semantics regarding fuzzy ontology. In addition, extending semantic web languages to support probabilistic, possibilistic, and fuzzy reasoning is another step forward to realize fuzzy ontology. Mazzieri et al. [26] extended syntax and semantics of RDF to support real numbers on the interval [0,1] so as to assign subject and object with a degree of membership to the extension of the predicate. A set of fuzzy extensions of Description Logics (DLs) [3] can also be found in current literature. In addition, some fuzzy DL reasoners have been implemented, such as FuzzyDL [27], DeLorean [28], and FIRE [29]. However, each reasoner uses its own fuzzy DL language, which results in a lack of a standard way to represent fuzzy information. Based on OWL and OWL2, proposals with fuzzy upgrades were presented in [30], [31], [32]. Notably, an approach to representing fuzzy ontology using OWL 2 annotation properties [4] was proposed without imposing any change in OWL 2. Fudholi et al. [33] provided another approach to representing fuzzy ontology by means of rules formulated in SWRL. This approach is easy to be used in spite of increasing the number of rules and limiting the scalability of defined ontology.

To define the incompleteness and inaccuracy of concepts, degree of certainty is widely employed to enable this description. Using the degree of certainty or probability, the belief on a certain object could be expressed. This strategy can be used in many real world applications where data obtained are associated with uncertainty. A data property, such as *hasDegreeOfCertainty*, could be defined to associate individuals with corresponding degrees of certainty. Those certainty degrees can either be calculated by confidence functions or provided by domain experts. To quantify the probability of concept which inherits probabilistic belief from known concepts, Bayesian Networks [9] and Markov Logic Networks [34] are integrated into ontologies.

However, research work on characterization of the uncertainty of ontological concepts from a holistic view attracts less focus. In some specific domains, such as engineering surveying and material analysis, acquisition of the statistics of random concepts is significant to obtain an overall view of the variation range. In this way, the usage of the historical data could be maximized. Besides, with regard to mathematical models encased in ontologies, none of the existing work put their focus on researching how uncertainty is propagated from input entities to output entity through those models. Therefore, in this paper, a novel algorithm, called SROM, is presented to solve the uncertainty quantification for ontologies with mathematical considerations. To the best of our knowledge, uncertainty propagation through ontological computational models is investigated from a statistical aspect for the first time in this paper. Using this algorithm, the uncertainty of concepts can be viewed from a high level, which refers to a holistic probability distribution. In addition, this algorithm introduces a lower computational cost. The propagated uncertainty, which is regarded as high-level information, is very useful for further use, such as ontological filtering and inference.

3 Stochastic Reduced Order Model (SROM)

The principle of the Stochastic Reduced Order Model (SROM) method is presented in this section. Assuming that $\boldsymbol{X}$ is an N-dimensional random variable ($N \geq 1$), being $\boldsymbol{X}$ jointly described by N independent variables. Then, $\boldsymbol{X}$ can be represented as $[X_1,\ X_2,\ X_3,\ \cdots,\ X_N]$. The statistical properties of $\boldsymbol{X}$ are assumed to be fully known with marginal distributions, moments of order q, and correlation matrix specified as in [35]:

$$F_i(x) = P(X_i \leq x) \tag{1}$$

$$u_i(q) = E\big(X_i^q\big) \tag{2}$$

$$\boldsymbol{r} = E\big[XX^T\big] \tag{3}$$

where i varies from 1 to N.

3.1 The Definition of SROMs

In essence, an SROM $\tilde{X}$ is a simplified random element that approximates the statistical properties of the random variable $\boldsymbol{X}$. $\tilde{X}$ is composed of two components: a finite set of samples $\{\tilde{x}^{(1)},\ \ldots,\ \tilde{x}^{(m)}\}$ and a corresponding set of probabilities $p = \{p^{(1)}, \ldots,\ p^{(m)}\}$. Any element $p^{(l)}$ $(1 \leq l \leq m)$ of the set of probabilities is required to meet two laws: $p^{(l)} \geq 0$ and $\sum_{l=1}^{m} p^{(l)} = 1$. The range of $\tilde{X}$, also referred to as model size m, is determined under the consideration of accuracy and computational cost. A large model size m is more likely to accurately approximate the statistics of $\boldsymbol{X}$, but the computational load increases [11]. With fulfilling the aforementioned conditions, $\tilde{X}$, represented as sample-probability pairs $(\tilde{x}^{(l)},\ p^{(l)}), l = 1, \ldots,\ m$, is able to have similar statistics as $\boldsymbol{X}$. Similar to $\boldsymbol{X}$, the distributions and moments of $\tilde{X}$ can be given as follows:

$$\tilde{F}_i(x) = P(\tilde{x}_i \leq x) \sum_{l=1}^{m} p^{(l)} I\Big(\tilde{x}_i{}^{(l)} \leq x\Big) \tag{4}$$

$$\tilde{u}_i(q) = E\big(\tilde{x}_i^q\big) \sum_{l=1}^{m} p^{(l)} \Big(\tilde{x}_i^{(l)}\Big)^q \tag{5}$$

$$\tilde{r}_{ij} = E\big[\tilde{X}_i \tilde{X}_j\big] \sum_{l=1}^{m} p^{(l)} \tilde{x}_i^{(l)} \tilde{x}_j^{(l)} \tag{6}$$

where $I(S)$ is an indicator function and has two possible values: 1 if S is true and 0 if S is false. Different SROMs can be generated with different sample-probability pairs $(\tilde{x}^{(l)},\ p^{(l)}), l = 1, \ldots,\ m$. Nevertheless, they differ from each other with regard to the degree of approximation to the real statistics of $\boldsymbol{X}$. How to achieve a trade-off between accuracy and computation complexity and therefore produce an optimal candidate SROM are a key point and will be discussed in next section.

3.2 Building SROMs

As stressed in Section 3.1, there could exist many different SROMs to approximate the statistics of $\boldsymbol{X}$. Construction of SROM alternatives can be achieved by different algorithms. Grigoriu [11] introduced the usefulness of three algorithms including *Dependent thinning*, *Integer optimization*, and *Pattern classification* in SROM construction. Furthermore, Warner et al. [12] proposed a new algorithm to construct SROMs that is stated to be improved considerably with respect to efficiency and accuracy. In this paper, the commonly used algorithm in building SROMs, which refers to pattern classification, is briefly outlined as follows:

Algorithm 1. Pattern Classification

1. Collect a set of n finite independent samples $\{\delta_1, \ldots, \delta_n\}$ from the random variable $\boldsymbol{X}$. The sample size n should be large enough to characterize the statistics of $\boldsymbol{X}$ accurately.
2. The set $\{\delta_1, \ldots, \delta_n\}$ becomes the raw source to generate SROMs. From $\{\delta_1, \ldots, \delta_n\}$, randomly extract subsets $\{\tilde{x}^{(1)}(\gamma), \ldots, \tilde{x}^{(m)}(\gamma)\}$, where m$\leq n$ and $1 \leq \gamma \leq C_n^m$. It could obtain C_n^m different kinds of SROM candidates.
3. Taking each trial subset $\{\tilde{x}^{(1)}(\gamma), \ldots, \tilde{x}^{(m)}(\gamma)\}$ as generator seeds [36], the uncertain space of $\boldsymbol{X}$ could be divided into m partitions $\mathcal{L}_l(\gamma)(1 \leq l \leq m)$ centered at $\tilde{x}^{(l)}(\gamma)$. Each region $\mathcal{L}_l(\gamma)$ contains $n_{(l)}$ points, where $\sum_{l=1}^{m} n_{(l)} = n$.
4. Let $d^{(l)}$ denote the sum of euclidean distances between $n_{(l)}$ points located in $\mathcal{L}_l(\gamma)$ to the corresponding center point $\tilde{x}^{(l)}(\gamma)$.
5. Accumulate $d^{(l)}$ $(1 \leq l \leq m)$ to get the overall distance $d = \sum_{l=1}^{l=m} d^{(l)}$.
6. Select the subset $\{\tilde{x}^{(1)}, \ldots, \tilde{x}^{(m)}\}$ with the minimum d as the most potential SROM $\tilde{X}_{(opt)}$.
7. The probability for $\tilde{x}^{(l)}$ is determined by the law $p^{(l)} = n_{(l)}/n$ such that the sum of $p^{(l)}$ could be 1.

At this point, an SROM with a set of sample-probability pairs $\{(\tilde{x}^{(1)},\ p^{(1)}), \ldots, (\tilde{x}^{(m)}, p^{(m)})\}$ is generated by the *pattern classification* algorithm. Likewise, other SROMs can be constructed by using other algorithms, such as the aforementioned ones: *Dependent thinning* and *Integer optimization*.

With a set of SROM candidates available, an optimal SROM should be found by imposing the condition that $\tilde{X}$ should have a similar probability law as $\boldsymbol{X}$. Discrepancy between statistics of $\tilde{\boldsymbol{X}}$ and $\boldsymbol{X}$ is considered as the primary factor to evaluate the performance of different SROMs. The essential discipline is to select an SROM, which minimizes the discrepancy from a set of alternative SROMs. The discrepancy is measured by an objective function with three components that express differences of the marginal distributions, the marginal moments, and the correlation matrices between $\tilde{X}$ and $\boldsymbol{X}$, respectively. The definitions for the objective function are as follows:

$$e_1(\tilde{x}, \boldsymbol{p}) = \sum_{i=1}^{n}\sum_{l=1}^{m} (\tilde{F}_i(\tilde{x}_i^{(l)}) - F_i(\tilde{x}_i^{(l)}))^2 \tag{7}$$

$$e_2(\tilde{x}, \boldsymbol{p}) = \sum_{i=1}^{n}\sum_{q=1}^{\bar{q}} (\tilde{u}_i(q) - u_i(q))^2 \tag{8}$$

$$e_3(\tilde{x}, \boldsymbol{p}) = \sum_{i,j=1,\ldots,n; j>i} \left(\tilde{r}_{ij} - r_{ij}\right)^2 \tag{9}$$

$$e(\tilde{x},\ \boldsymbol{p}) = \boldsymbol{\alpha}_1 e_1(\tilde{x}, \boldsymbol{p}) + \boldsymbol{\alpha}_2 e_2(\tilde{x}, \boldsymbol{p}) + \boldsymbol{\alpha}_3 e_3(\tilde{x}, \boldsymbol{p}) \tag{10}$$

where $\alpha_1,\ \alpha_2,$ and α_3 are weighting factors to define the relative importance of differences between marginal distributions, marginal moments and correlations in the overall discrepancy between $\tilde{X}$ and $\boldsymbol{X}$. Coefficients $\alpha_1,\ \alpha_2,$ and α_3 can be set with different constants in particular applications, to ensure that each error component has the same importance, or to emphasize the SROM's ability to represent a particular statistic of $\boldsymbol{X}$ over other statistics.

3.3 SROM-Based Uncertainty Quantification

This section describes the procedures how the SROM algorithm is used to quantify the uncertainty propagation from multiple uncertain variables to the output with the deterministic solver known. The statistics of the output variable, which is jointly affected by multiple uncertain variables, can be approximated with low computational cost and high accuracy by using the SROM-based method. The SROM-based uncertainty quantification method is outlined as follows:

Algorithm 2. The SROM-based Uncertainty Quantification

1. The mathematical relation between multiple input variables and the output variable Y is modelled by a deterministic solver, which could be a set of mathematical relations. Multiple input variables can be merged to construct the random input variable $\boldsymbol{X}$ (described by $\varepsilon_1, \varepsilon_1, \ldots, \varepsilon_n$).
2. The statistics of the input variable $\boldsymbol{X}$ are known beforehand. The method introduced in Section 3.2 is applied to generate its SROM $\tilde{X}$, with sample-prability pairs $\{(\tilde{x}^{(1)}, {p_x}^{(1)}), (\tilde{x}^{(2)}, {p_x}^{(2)}), \ldots, (\tilde{x}^{(m)}, {p_x}^{(m)})\}$, where $m \leq n$.
3. The SROM of the output variable $\tilde{y}^{(i)}$ $(1 \leq i \leq m)$ is obtained through m deterministic calculations with $\tilde{x}^{(i)}$.
4. Sequentially, the probabilities of $\tilde{y}^{(i)}$, denoted as ${p_y}^{(i)}$, can be obtained using ${p_y}^{(i)} = {p_x}^{(i)}$ because the acquisition of $\tilde{y}^{(i)}$ is subject to the occurrence of $\tilde{x}^{(i)}$.
5. Then the SROM of the output variable $\tilde{Y}$ is completely defined.

After obtaining the SROM-based output $(\tilde{y}^{(i)}, {p_y}^{(i)})$ $(1 \leq i \leq m)$, the statistics of the output variable Y can be studied by the approximation result $\tilde{Y}$. Therefore, the statistics of Y, estimated by $\tilde{Y}$, can be measured by means of the marginal distributions, moments of order q and the standard deviation σ,

$$F(\theta) = P(\tilde{y} \leq \theta) = \sum_{i=1}^{i=m} {p_y}^{(i)} I(\tilde{y}^{(i)} \leq \theta) \tag{11}$$

$$E(\tilde{y}^q) = \sum_{i=1}^{i=m} {p_y}^{(i)} (\tilde{y}^{(i)})^q \tag{12}$$

$$\sigma(\tilde{y}) = \sum_{i=1}^{i=m} {p_y}^{(i)} (\tilde{y}^{(i)} - E(\tilde{y}^1))^2 \tag{13}$$

Concisely, the SROM-based method can accurately approximate the statistics of an uncertain output variable in presence of multiple input variables and in the meanwhile simplify the uncertainty quantification process with a lower computational load. It is also noted that the SROM solution is guaranteed to converge to the theoretical statistics of the output variable when the model size of input variable approaches infinity [37].

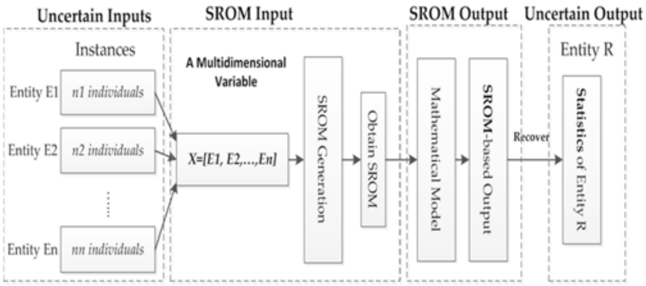

Fig. 1. SROM-based uncertainty propagation in ontologies.

4 Application of SROM in Mathematics-Embedded Ontologies

In this section, the first application of SROM to quantify uncertainty propagation in mathematics-embedded ontologies is presented. In addition, a specific case study is provided to show the usefulness of SROM in ontologies with regard to characterizing the uncertainty propagation.

4.1 Workflow of Using SROM in Ontologies

Data obtained from specific domains are encapsulated in ontologies as instances under relevant entities. In general, data that is going to be constructed in ontologies is classified into two categories: direct and indirect [10]. The differentiation of direct and indirect information is related to the complexity to obtain it. Indirect information is more complex to acquire and needs additional computation or inference. Therefore, a variety of entities in ontologies is obtained as outcomes of computational models, which involve a set of direct entities as inputs. Thus, uncertainties existing in input entities will jointly affect the accuracy of the output entity through the computational model. The characterization of uncertainties is significant in such kind of mathematical and computational models of complex processes and data. In this sense, the SROM algorithm can be employed to address this problem in ontologies from a statistical aspect. The process of SROM to propagate uncertainty in ontologies is illustrated in Fig. 1.

Assuming that entity R is a concept representing an abstraction of a class of individuals with similar attributes in an ontology, R is determined as conclusions drawn from a mathematical model. The mathematical model, also referred to as a deterministic solver, describes the relationship between the input entities and the output entity. Instances of R could be variable and random affected by the uncertainties and randomness of input entities. From this point, different entities defined in the ontology could be regarded as independent variables in the SROM-based consideration. The SROM algorithm can be used to construct an SROM, which represents an approximation of statistics of multiple input variables. Instances of different input entities form the raw source to generate an SROM. The core principle is to integrate multiple inputs as a multidimensional variable. As a result, the uncertainties of different input concepts are modelled by the multidimensional variable. An optimal SROM of the input variable could be produced by using the method introduced in Section 3.2. Afterward, following the steps introduced in Section 3.3, this SROM, which contains similar statistics of input entities, is applied in the mathematical model to generate the SROM of output entity. Therefore, the statistical law of the output entity can be approximated and recovered by applying its SROM in Equations (11), (12), (13). Based on the obtained statistics, the uncertainty of output entity (*e.g.*, mean, standard deviation, and the variation range) can be extracted.

The application of SROM in quantifying uncertainty in ontologies can bring three benefits: 1) considerably reducing the computational cost, 2) accurately obtaining the statistics of the uncertain and random output entity, and 3) generally suiting ontological uncertainty propagation with any kind of mathematical models because of its non-intrusive feature. In the following section, a case study will be given to demonstrate the usefulness of the SROM algorithm in quantifying uncertainty propagation in mathematics-embedded ontologies.

4.2 A Case Study

In this section, the proposed SROM-based uncertainty quantification method will be shown through a case study. The concept of *Body Mass Index (BMI)*, which is an important index for evaluating health, has been included in many biomedical ontologies. For instance, Lee et al. [38] proposed an ontology-based context-awareness information model to gather and formalize information in home healthcare scenarios. In this proposed ontology, the concept *BMI* is regarded as a combined concept, which is inferred from two concepts *Height* and *Weight*. Height and weight are easily obtainable by height and weight measurement instruments. This *BMI* class is explicitly defined by a rule written in SWRL, which essentially describes the mathematical relationship between *BMI* and *Weight* and *Height*,

$$BMI = \frac{Weight}{Height^2}. \tag{14}$$

The SWRL rule to specify the mathematical relationship between *BMI* and *Weight* & *Height* encased in ontologies is as follows:

$$Height(?y),\ Weight(?x),\ divide(?b,\ ?x,\ ?z),$$
$$multiply(?z,\ ?y,\ ?y)- >\ BMI(?b).$$

In a home healthcare scenario, the patient's weight and height are periodically measured and recorded in a specific time span because those two parameters are important criteria to monitor the patient's health. Different measurements of weight and height are treated as instances of class *Weight* and *Height*, respectively. All this weight and height data can be populated into the ontology and kept in an ontology-based database. Due to a variety of reasons, such as imperfect instruments adopted, the *Weight* and *Height* classes are associated with uncertainty, particularly referring to randomness. Thus, the concept *BMI* inferred from them could be variable in a specific scale. It is necessary to make the uncertainty analysis on the *BMI* as its statistics, such as the variation range in a specific period of time, could provide merits for further use, like predicting trends [39] and making decisions.

In this case study, the studied variable concept *BMI* is affected by two variables *Weight* and *Height*. The SROM-

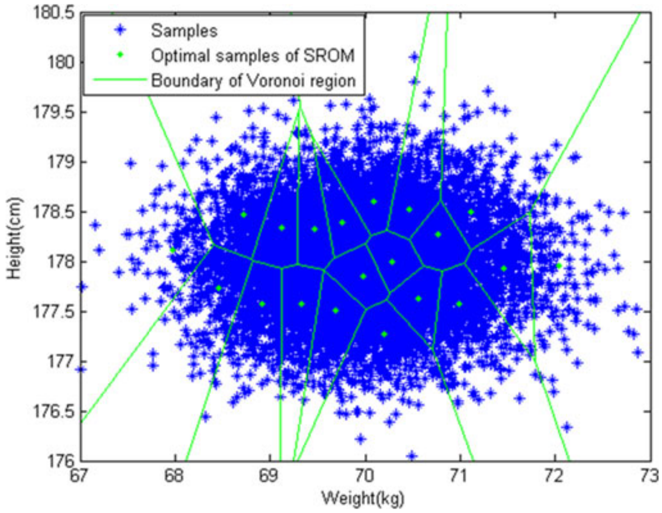

Fig. 2. The distribution of 10^4 instances of *Weight* and *Height*.

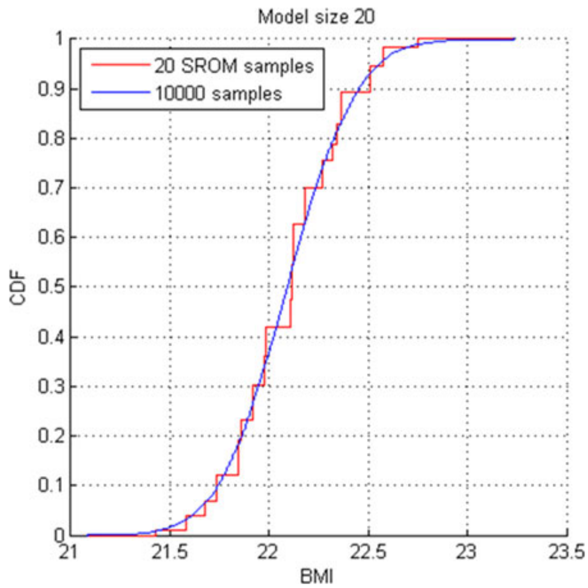

Fig. 3. The CDF of *BMI* obtained by the SROM-based method ($m = 20$) and the benchmark.

based method can construct a reduced model, which consists of fewer samples from *Weight* and *Height* with the capability to represent the similar statistics of the original database of *Weight* and *Height*.

To deal with two uncertain input variables with the SROM method, the idea is to integrate these uncertainty sources into a bidimensional variable and then construct an SROM to globally approximate the overall uncertain input space. In this case, two variables *Weight* and *Height* are merged into a bivariate variable $X = [Weight, Height]$, where cardinality D equals 2. Instances of *Weight* and *Height* are filled into the input variable and treated as samples of X. Up to this point, the input variable X is completely defined. It is noted that in real home healthcare scenarios, a history of weight and height data can be acquired by instruments. Here, for the demonstration purpose, uncertain *Weight* and *Height* concepts are assumed to have Gaussian distributions and a series of instances are randomly selected from the known distribution. However, it is worth noting that the SROM method can be applicable for any type of probability distribution.

More specifically, it can be assumed that class *Weight* contains 10^4 instances and the dataset is randomly selected from a Gaussian distribution with mean $E(w) = 70\ kg$ and standard deviation $\sigma(w) = 0.8\ kg$. Similarly, class *Height* has a historical dataset that contains 10^4 instances randomly selected from a Gaussian distribution with mean $E(h) = 1.78\ m$ and standard deviation $\sigma(h) = 0.005\ m$. Then, the input variable X has 10^4 samples of weight and height values. As can be seen in Fig. 2, each sample of X can be represented as a blue star marker in a plane, which sets *Weight* as the x-axis and *Height* as the y-axis. The coordinates of the blue star marker show a pair of possible values for *Weight* and *Height* to calculate *BMI*.

With the raw source of the input variable X, the SROM-based method could be used to extract a suitable SROM that contains a small amount of samples and is able to reflect the original distribution of X. By applying the algorithm introduced in Section 3.2, a SROM $\tilde{X}$ can be produced to globally approximate the statistics of *Weight* and *Height*. For instance, the model size is set with a very small number: 20 samples to generate a SROM of uncertain inputs *Weight* and *Height*. Twenty green points, which are scattered in Fig. 2 to ensure the exploration of the entire uncertain region X, are selected by applying the algorithm introduced in Section 3.2. These twenty samples and their corresponding probabilities form the optimal SROM $\tilde{X}$. Each SROM sample is able to maximize the similarities between other samples, which are located in the same Voronoi region and itself. Thus, the produced SROM $\tilde{X}$ can be guaranteed to have similar statistics as X to a certain extent.

With different model size m, the approximation of statistics of *Weight* and *Height* could be different and therefore, the uncertainty quantification of output *BMI* could be different. To validate the performance of the SROM-based method, the result after 10^4 deterministic calculations is set as the benchmark. The benchmark Cumulative Distribution Function (CDF) of *BMI* is drawn in a blue curve in fig. 3. The comparison of the SROM-based *BMI* ouput ($m = 20$) with the benchmark in terms of constructing *BMI* CDF is also presented in Fig. 3.

The SROM-based method, here with 20 samples, is able to approximate the statistics of *BMI* with a slight difference. As shown in Fig. 3, the predicted CDF by the SROM method with model size 20 can reflect the general shape of the reference CDF. The computational cost is dramatically reduced by a factor of $10^4/20 = 500$. The model size 20 is reasonable as the approximated CDF matches the reference CDF in good agreement and the computational cost is kept low. When changing the model size, the difference between SROM-based results with benchmark will change accordingly. Fig. 4 depicts the SROM-based approximation of CDF of *BMI* with model size 40, 60, 80, and 100.

As can be seen from Fig. 4, introducing more samples can steadily converge the reference CDF and get a better approximation. At the size of 60, the CDF of *BMI* can be very accurately recovered, while it still requires less computational load than the benchmark. The rate of acceleration in computation is still notable which is $10^4/60 \approx 166.7$. When the model size reaches 100, the recovered CDF is almost identical as the benchmark result that shows that the

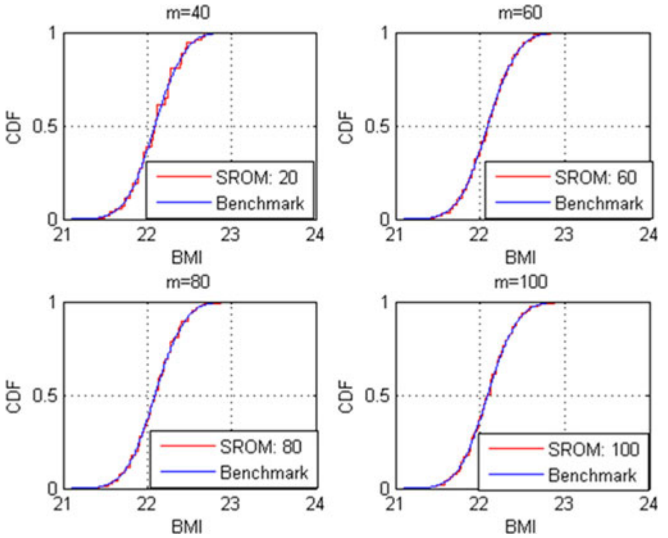

Fig. 4. The CDF of *BMI* obtained by the SROM-based method ($\mathrm{m} = 40, 60, 80,$ and 100) and the benchmark.

SROM-based method has a very fast convergence rate to recover the benchmark result.

In addition to providing the distribution information, the SROM method can also obtain a very accurate prediction of the mean and standard deviation of *BMI*. As Fig. 5 shows, even at the model side of 5, the mean of *BMI* can be approximated with an error of mean below 0.003%. The predicted mean of *BMI* is identical to the reference mean of *BMI* using 45 samples. In terms of predicting the mean of the *BMI*, the SROM method converges very fast to the benchmark.

With regard to the approximation to the reference standard deviation of *BMI*, the convergence rate is slower. As can be seen in Fig. 6, an increasing model size makes it converge to the benchmark. Using the same amount of samples, the performance of predicting standard deviation of the *BMI* is not as ideal as predicting the mean *BMI*. However, at the small size of 10, the error of standard deviation of the *BMI* is still below 10 percent.

To show the performance of predicting the mean and standard deviation of the *BMI* using more samples, Table 1 presents different SROM-based results obtained by 20, 40, 60, 80 and 100 samples, accordingly.

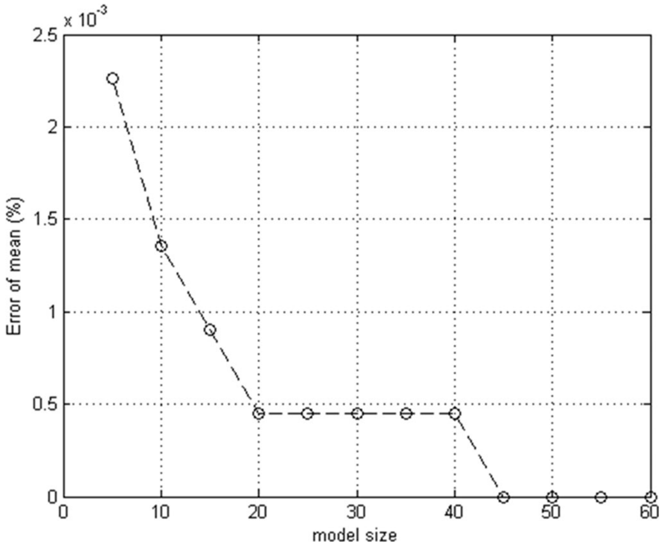

Fig. 5. The error of mean of *BMI*.

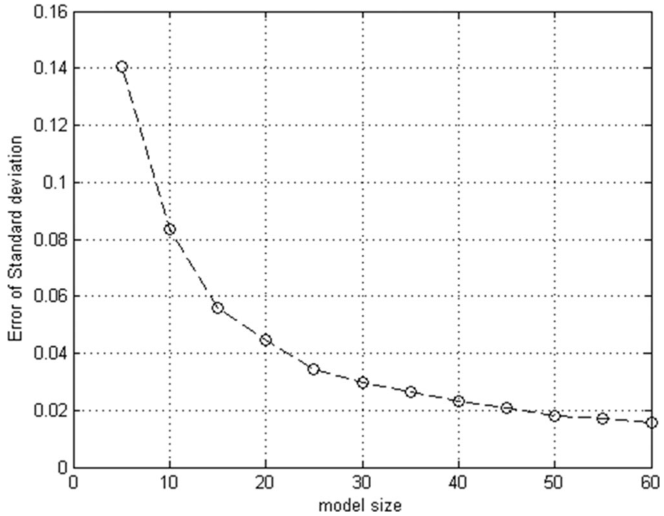

Fig. 6. The error of standard deviation of *BMI*.

As can be seen in Table 1, even with a very small model size of 20, the mean of *BMI* can be very accurately approximated. The slight difference existing in the SROM-based results and the benchmark is affordable compared with the significant acceleration in computations. Besides, the standard deviation by the SROM method is still accurate to a certain extent. Taking the SROM-based result with model size 20 as an example, the SROM-based standard deviation is within the error of 5 percent.

Based on the mean and standard deviation of *BMI* obtained by the SROM method ($m = 20$), *BMI* can be predicted to likely vary within this interval: [21.2965, 22.8919]. This variation range predicted by the SROM-based method with model size 20 has very small difference compared to the benchmark, which bounds the variation range as [21.2594, 22.9292]. With a bigger model size, the SROM-based prediction on statistics of the output variable can be refined and get a better convergence to the benchmark. It is worth noting that even with a small sized SROM, the uncertainty propagated from input entities to the output entity can be quantified with a reasonable degree of accuracy and a low computational cost. Since the increase of model size could guarantee a very good approximation to the reference result, a trade-off between accuracy and computational complexity should be figured out to suit different requirements of applications.

By using the SROM-based method, the uncertainty of the output entity is quantified from a statistical aspect to obtain the holistic variation range. This method can be used in the phase of ontology reasoning, which aims to deduce more

TABLE 1
Comparisons of the SROM-Based Results and the Benchmark

Attributes of *BMI*	SROM Model Size					Reference
	20	40	60	80	100	10000
Mean	22.0942	22.0942	22.0943	22.0943	22.0943	22.0943
Standard deviation	0.2659	0.2719	0.2740	0.2751	0.2756	0.2783

useful information from raw data. In this case study, instances of entities *Weight* and *Height* are low-level information. After applying the SROM-based method, the statistics of *BMI* are achieved as high-level information.

According to the previous case study, it has been proven that the SROM-based method can considerably reduce the computational cost while guaranteeing a good prediction of statistics of the output variable. The predicted uncertainty information of *BMI*, mainly referring to the mean, standard deviation, and CDF, can be very useful to quantify the statistics of *BMI*. In addition, the statistics of *BMI* can be regarded as high-level information for other usages. For example, newly obtained instances of *BMI* could be removed as outliers based on its statistics. The change of *BMI* within a period of time, estimated by the variation range, can be considered as an index to evaluate the patient's health.

The SROM-based method is non-intrusive to the mathematical model, which results in its compatibility and usability in all kinds of mathematical models regardless of different complexities. The selection of model size could be flexible, but it mainly should be based on considerations of computational cost and accuracy to fit in different needs of applications. The SROM-based method has been demonstrated using a bivariate case study. This method could be also applicable to multiple variables. But the convergence rate could be different with regard to the number of input variables.

5 Conclusions and Future Work

This paper has shown how to characterize the uncertainty of ontology entities from a statistical viewpoint. Analysis of the historical statistics of uncertain entities as the obtained high-level information could be used for further purposes. The study on the holistic probability distribution of uncertain concepts is able to compensate existing efforts on resolving uncertainty, particularly referring to randomness, in ontologies. Thus, the understanding and study of different uncertainty features in ontologies could be complete and profound. In addition, with a particular focus on indirect entities that have mathematical dependencies on direct entities defined in ontologies, the first application of a novel algorithm SROM to quantify the uncertainty propagation has been presented. This SROM-based method is non-intrusive to the mathematical model so that it could be applicable to predict uncertainty propagation in any kind of mathematics-embedded ontology models. This proposed method is able to approximate the statistics of output entity accurately by using a few samples from input entities. Thus, the computational cost in predicting the uncertainty propagation is reduced considerably. By using this SROM-based method, the uncertainty of the indirect entity is accurately quantified based on its statistics recovered from the SROM-based result.

Furthermore, the uncertainty analysis on a concept *BMI* in biomedical ontologies has been presented as a case study to validate the usefulness of the SROM-based method. The results have shown that the SROM-based method can be efficient and accurate in characterizing the uncertainty propagation from two variables *Weight* and *Height* to the concept *BMI*. The uncertainty information of *BMI* has been accurately obtained including the mean, standard deviation, and CDF of *BMI*, which could be regarded as high-level information to be used in other ontological operations, such as ontology filtering and ontology reasoning.

Though the SROM algorithm has been stated to be able to deal with uncertainty propagation in presence of multiple variables, future work should focus on including more case studies with more variables to justify how the number of input variables might affect the performance. Besides, applying the SROM-based method to deal with uncertainty propagation in real world ontological applications is a step forward, which is intended as future work.

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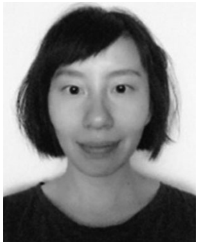

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