THE ROLE OF EXPERT KNOWLEDGE IN UNCERTAINTY QUANTIFICATION (ARE WE ADDING MORE UNCERTAINTY OR MORE UNDERSTANDING?)

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Uncertainty quantification can be broadly defined as the process of characterizing, estimating, propagating, and analyzing various kinds of uncertainty for a complex decision problem. In the realm of complex computer and physical models, it is more focused upon computational and modeling uncertainties, e.g., sensitivities of outputs to input values or verification and validation. In either case, sources of uncertainty (including variability) can arise from the two broad categories: epistemic and aleatory. We begin by presenting a brief taxonomy of uncertainties involved in uncertainty quantification of physical and simulation models. Included in this exercise will be some definitions, which remain somewhat non-standard within and between various communities (e.g., artificial intelligence). While listing these sources is relatively straightforward, evaluating uncertainties in complex computer codes presents huge obstacles. In addition, the human enters into the quantification of uncertainty process in much the same way as in any decision process, and that entrée presents both additional obstacles and some solutions. We will discuss how the use of expert judgment and expertise is involved in uncertainty quantification.

1. Definition of Terms. The first term in the title is expert knowledge which is defined as what is known by qualified individuals, responding to complex, difficult (technical) questions, obtained through formal expert elicitation (Meyer and Booker, 2001). It is a snapshot of the expert's state of knowledge at the time, and may be expressed in either qualitative and quantitative form.

Knowledge can be elicited in two distinctive forms: expertise and expert judgment. Expertise refers to that information from experts about the definition and structure of a complex problem. How experts organize and represent their problem solving knowledge and how information flows within a problem are part of expertise. When experts identify relevant data and information sources, including models, experimental results and numerical methods, they are providing expertise. Identification of uncertainties associated with these is also part of expertise. Expertise is used extensively in making everyday decisions; it may not be elicited and documented as such.

Examples of expertise include:

Decisions about what variables to enter into a statistical analysis.

Decision about which data sets should be analyzed.

Assumptions used in model or method selection.

Decisions concerning which forms of uncertainty are appropriate to use (e.g., using a probability density function to represent aleatory uncertainty).

Descriptions of experts' thinking, problem solving, and information sources used in arriving at any of the above.

Expert judgment refers to the contents of the expert's knowledge. When experts provide estimates of phenomena (qualitative or quantitative) or the uncertainties associated with those estimates, they are providing expert judgment. Any assumptions, heuristics, cues, and historical information that experts use in providing estimates is also considered part of expert judgment. Examples of expert judgment include: estimating the occurrence of an event, estimating the uncertainty in a parameter, and predicting the performance of a new product.

Uncertainty quantification is the other major term in the title. In the broadest sense, it refers to the process of characterizing, estimating, propagating and analyzing various types of uncertainty (including variability) for a complex decision or physical problem. In more specific modeling complex and physical communities it focuses upon measurement, computational, parameter (including sensitivities of outputs to input values), and modeling uncertainties leading to verification and validation of the computation and modeling.

Generally speaking, there are two different categories of uncertainty, aleatory and epistemic. Aleatory refers to uncertainty due to random variation or inherent variation. It is irreducible and includes the basic statistical concepts of variability and the definition of probability as describing the uncertainty associated with the outcome of an experiment or event. By contrast, epistemic uncertainty is reducible and stems from a lack of knowledge. There is disagreement on how to classify *error*, which could stem from numerical methods, the process of discretization or simply mistakes. We maintain that error could be either aleatory or epistemic in nature.

2. Uncertainties in the Modeling Process. Using the modeling definition of uncertainty quantification, let us examine the steps involved in modeling and the uncertainties associated with those steps. A complex physical or decision model usually begins with observations of nature. Next models for capturing the observed behavior are conceptualized and then mathematically formulated into computational models. At this point, issues emerge regarding the computational process. Numerical models may be employed to represent the physical model (if one exists). Numerical implementation and evaluation of the model is then implemented. Finally, if physical models and/or numerical models are lacking, surrogate models may be used, such as a statistical response function or a neural network. Implementing and evaluating surrogate models are necessary steps in the surrogate modeling process.

Associated with these modeling steps are various kinds of uncertainties, some of which are extremely difficult to estimate. Regardless of the difficulty, decisions are made every day by humans, whose mental intervention now enters the modeling process as potentially important sources of uncertainty. Uncertainties of measurement include noise, resolution and processing, many of which could be classified as aleatory. Mathematical modeling uncertainties are found in choices and uses of equations, boundary conditions, initial conditions and inputs. Many of these could be classified as epistemic. For numerical modeling, uncertainties arise in the use of weak formulations, in the choices of discretizations for mesh sizing and time steps, in the use of approximate solution algorithms, and with issues of truncation and roundoff. Statistical or surrogate modeling is listed as distinctly different from physical or mathematical modeling in that interpretability of these models is one step removed from the real world. Neural networks and other dimension reduction models fall into this category. Uncertainties also emerge from errors of approximation, interpolation and extrapolation.

In general modeling uncertainties (whether from mathematical, numerical or surrogate models) are extremely difficult to characterize, understand and estimate. They can be both epistemic and aleatory in nature. We list the issue of model parameters and the uncertainties and sensitivities of inputs to outputs separately from model uncertainty because significant progress has been made in this area (McKay et al., 1999). Beyond modeling issues are uncertainties that might be termed as scenario uncertainties. These would encompass the application realm and the choices made regarding the problem definition (Oberkampf et al., 2001).

Regardless of the source or type of uncertainty involved, decisions made in the modeling process also contain uncertainties. Therefore the "human in the loop" is an additional source of uncertainty, whether specifically acknowledged or not.

3. Uncertainties from Humans. The human decision making contribution to the overall uncertainties in the modeling process can originate in the cognitive and motivational biases that affect human thinking and judgment. By *bias*, we do not imply statistical bias (or shift of the mean value) but instead refer to a skewing from a standard or reference point that can degrade the quality of the information and contribute to uncertainty.

Among the list of various cognitive biases, the most prominent contributor to uncertainty is the *underestimation of uncertainty bias* (or false precision bias). Humans tend to believe and think about the world as having more precision that it really does. Other cognitive biases contributing to uncertainty are:

- *Availability*—how humans account for rare events depends upon whether they have experienced them or not.
- *Anchoring*—humans cannot move from preconceptions, but instead anchor to them even in light of new data/information.
- *Inconsistency*—humans forget what has preceded and hence produce inconsistent conclusions.

The most noted motivational biases that contribute to uncertainty are:

- *Group Think*—following the leader, regardless of the consequence.
- *Impression Management*—being politically correct.
- *Wishful Thinking*—wanting something makes it a reality.
- *Misimpression*—poor, incorrect or bad translation of information.

To top this list of biases as contributors to uncertainty in human thinking and judgment is the well-studied phenomena that humans are poor probability thinkers (Meyer and Booker, 2001). It is so easy to contradict the axioms of probability, even if the person is an expert in probability theory. Human thinking is just not conducive to probabilistic thinking. Therefore asking expert to provide probability estimates for uncertainties is quite dangerous.

4. Countering Human Contributions to Uncertainty. One would hope that experts could offer assistance in understanding and estimating uncertainties in the modeling process, without contributing additional uncertainty. The human brain has a tremendous capacity to integrate complexities, such as uncertainty. Experts should be able to identify sources of uncertainty, provide estimates (quantitative or qualitative) for these, be able to update estimates as new information becomes available and suggest methods of how to propagate uncertainties throughout the modeling process. With the use of some recently developed tools and technologies, it is possible to counter the human contributions to uncertainty enabling us to take advantage of the knowledge that experts are capable of providing.

Formal, structured elicitation of expertise and expert judgment is designed to counter the common biases arising from human cognition and behavior. These techniques (Meyer and Booker, 2001) draw from cognitive psychology, decision analysis, statistics, cultural anthropology and knowledge acquisition. They add rigor and defensibility, and increase the ability to update judgments in light of new knowledge.

In addition to providing bias minimization, formal elicitation provides documentation and utilizes the way people think, work and solve problems. For example, an expert unfamiliar with probability would never be asked to express uncertainties in the form of a probability density function. Instead he might be accustomed to thinking about uncertainty in terms of a range of possible values; therefore, the range would be elicited.

A second major advancement to counter human contributions to uncertainty is the development of alternative mathematical theories for handling different kinds of uncertainty, such as ambiguity and vagueness. Because humans have difficulty with consistent thinking that preserves the axioms of probability, these other theories offer alternatives for characterizing uncertainties which may be more consistent with human thinking. These theories include (Oberkampf, et al. 2001):

Possibility Theory (for crisp or fuzzy sets).
Fuzzy Sets
Dempster-Schafer (Evidence) Theory
Choquet Capacities
Upper and Lower Probabilities
Convex Sets
Interval Analysis Theories
Information Gap Decision Theory (non measure based) (Ben-Haim, 2001)

While most of these theories are measure based, all are set based, using either crisp (classical) or fuzzy set theory. They are all axiomatic and have a calculus (or algebra) with rules for combining sets and implementing the axioms. They are internally consistent and coherent such that one cannot be caught up in a situation of "heads I win and tails you lose." With modern computational methods and computers, they are computationally practical. As seen in Section 5, many have or are in the process of developing metrics for uncertainty.

Having these choices is an advantage, but there may be different kinds of uncertainties within a modeling problem such that these different theories would apply. For combining all uncertainties within a problem, we need bridges and linkages between the various theories. To our knowledge the only developed linkage has been between probability theory and membership functions in fuzzy set theory (Singpurwalla and Booker, 2002). Hierarchical relationships between them have been developed as shown in Figure 1, with more specific theories at the bottom and more general ones at the top.

As noted in Figure 1, probability theory can have more than one interpretation. Historically speaking there are as many as eleven different interpretations of probability, all consistent with its axioms and calculus (Bement, et al, 2002). Two competing interpretations today are Frequentist and Subjective (or Personalistic). The latter encompasses the ever expanding set of Bayesian analysis methods, and it is the interpretation that permits linkage between probability and fuzzy logic (Singpurwalla and Booker, 2002).

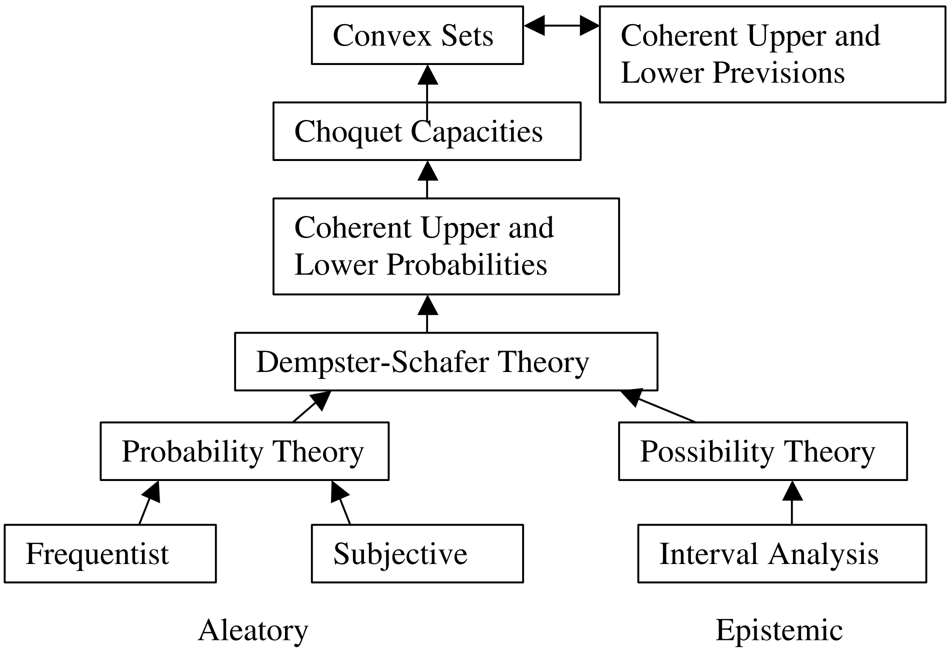

Figure 1. Hierarchy of Theories for Crisp Sets

5. Some Measure Theoretic Approaches to Uncertainty. In this section, we provide brief comparison of three of the measure based, crisp set approaches in Figure 1: Probability Theory, Dempster-Schafer Theory and Possibility Theory.

Probability is based upon a single measure function, *Pr*, and has the property of additivity as noted in equation (5.2) below.

(5.1) $Pr: 2^X \rightarrow [0,1] \quad Pr(\varnothing) = 0 \quad Pr(X) = 1$

(5.2) $Pr(\cup_i A_i) = \Sigma_i Pr(A_i) - \Sigma_{j>k} Pr(A_j \cap A_k) + \ldots + (-1)^{n+1} Pr(\cap_i A_i)$

$Pr(\cap_i A_i) = \Sigma_i Pr(A_i) - \Sigma_{j>k} Pr(A_j \cup A_k) + \ldots + (-1)^{n+1} Pr(\cup_i A_i)$

Dempster-Schafer is based upon two measure functions, belief (*Bel*) and plausibility (*Pl*). Non additivity is illustrated in equation (5.4) below.

(5.3) $Bel: 2^X \rightarrow [0,1] \quad Bel(\varnothing) = 0 \quad Bel(X) = 1$

$Pl: 2^X \rightarrow [0,1] \quad Pl(\varnothing) = 0 \quad Pl(X) = 1$

(5.4) $Bel(\cup_i A_i) = \Sigma_i Bel(A_i) - \Sigma_{j>k} Bel(A_j \cap A_k) + \ldots + (-1)^{n+1} Bel(\cap_i A_i)$

$Pl(\cap_i A_i) = \Sigma_i Pl(A_i) - \Sigma_{j>k} Pl(A_j \cup A_k) + \ldots + (-1)^{n+1} Pl(\cup_i A_i)$

Possibility is also based upon two measure functions, possibility (*Pos*) and necessity (*Nec*). Non additivity is illustrated in equation (5.6) below.

(5.5) $Pos: 2^X \rightarrow [0,1] \quad Pos(\varnothing) = 0 \quad Pos(X) = 1$

$Nec: 2^X \rightarrow [0,1] \quad Nec(\varnothing) = 0 \quad Nec(X) = 1$

(5.6) $Pos(\bigcup_i A_i) = \sup_i Pos(A_i)$

$Nec(\bigcap_i A_i) = \inf_i Nec(A_i)$

Applications of Dempster-Schafer are conspicuously lacking in the literature, especially regarding the important issue of how this theory might be useful for capturing how some experts think about uncertainties. Perhaps the most applicability can be found using fuzzy membership functions and possibility theory (Ross, 1995).

Some metrics for uncertainty have been developed under these alternative theories. Information theory based concepts such as entropy provide the foundation for some, as noted below.

Hartley measure for nonspecificity:

$H(A) = \log_2|A|$, where $|A|$ is the cardinality of A.

Generalized Hartley measure for nonspecificity in Dempster-Schafer:

$N(m) = \Sigma_{A\in 2^X}\, m(A) \log_2|A|$, where m: $2^X \rightarrow [0,1]$, $m(\emptyset) = 0$, and $\Sigma_{A\in 2^X}\, m(A) = 1$.

U-uncertainty measure for nonspecificity in possibility theory:

$U(r) = \Sigma_{j=2}\, (r_j - r_{j+1})\log_2 j$, where $r(x) = Pos(\{x\})$, for $r_j = r_{j+1}$, for all j.

Shannon entropy for total uncertainty in probability theory:

$S(p) = -\,\Sigma_{x\in X}\, p(x)\log_2 p(x)$

Generalized Shannon entropy for total uncertainty in Demspter-Schafer theory:

$AU(Bel) = \max_{p_x} (-\Sigma_{x\in X}\, p_x \log 2 p_x)$, where $Bel(A) = \Sigma_{x\in X}\, p(x)$, for all $A\in 2^X$.

Hamming distance for fuzzy sets:

$f(A) = \Sigma_{x\in X}\, [1-|2A(x)-1|]$, where $A(x)$ is a membership function.

6. Role of Expert Knowledge in Uncertainty Quantification. Experts and the knowledge they provide can be valuable in the processes of understanding, estimating and propagating different kinds of uncertainties within a complex model. However, the experts are human, subjected to the cognitive and motivational biases which also contribute to the overall uncertainties within that problem. There is hope for minimizing these contributions by utilizing bias minimization elicitation techniques and by offering experts alternative (to probability) theories for handling uncertainties.

Two major areas of research are necessary to fulfill the usefulness of these alternative theories. First, continued study is required to be able to link the various theories for handling different types of uncertainties within the same modeling problem. Second, more study is needed to determine the usefulness of these alternative theories as better methods (than probability) for capturing the way experts think and problem solve.

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