Predictive Computational Science

by
J. Tinsley Oden
The University of Texas at Austin

The last decade has seen great interest and activity in a subject some call predictive science: the scientific discipline concerned with the forecast of events that take place in the physical universe -- the prediction of the future including the prediction of the behavior of engineered systems under design conditions.

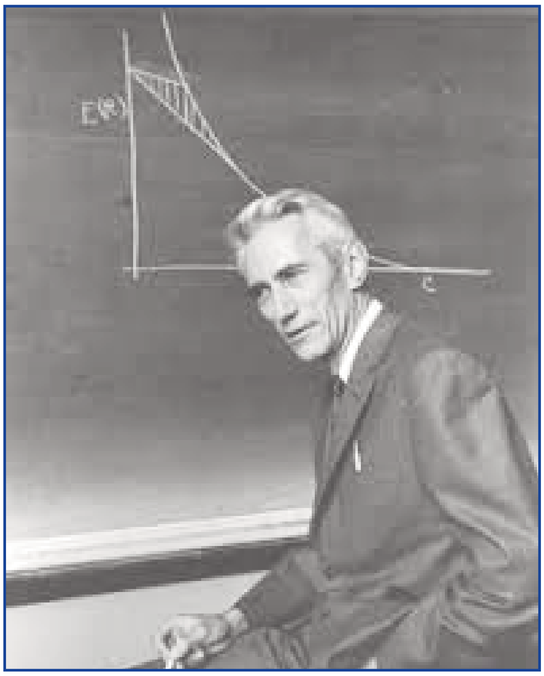
One's first reaction to predictive science is to ask "Why?" – has not the purpose of science always been to explain physical phenomena and, once explained, to use the knowledge to predict the occurrence of related events in the future? Predictivity is at the heart of inductive reasoning – a foundational pillar of science itself, involving the development of hypotheses to explain physical observations and then extrapolating those explanations to similar events happening in the future, or in the past. Prediction of the response of engineered systems under design conditions has been undertaken for centuries.

" Predictivity is at the heart of inductive reasoning ... "

But what has happened in recent times, say within the last three decades or so, is that dramatic advances in computational science have enabled the scientific community to push its predictive capabilities to the limit, and the result has often been disappointing, humbling, and even disastrous. Not only have we found that our favorite theories of mechanics cannot be applied with brute-force to prediction, but also that every phase of prediction faces overpowering uncertainties – in the models, their parameters, the physical observational data, and in numerical implementations. Another factor is that advances in algorithms and computing capabilities have gradually moved computer modeling from a qualitative endeavor, designed to only determine trends and qualitative features of the response of a system, to a quantitative science in which specific answers are needed to make important and sometimes life and death decisions. This is at a time when the great promise of the predictive power of computational sciences has been heralded as a boon to mankind, making possible tremendous advances in such areas as climate prediction, predictive medicine, the design of new materials, manufacturing processes, drug design, and many other subjects.

Predictive science has emerged in an attempt to dissect, formalize and understand all the aspects of science and engineering that truly influence the reliability of predictions. The anatomy of predictions is well known: one first has a model of the event in question that is generally represented by a mathematical characterization of a theory or a surrogate of a theory generated by special assumptions and approximations. Then, there are physical observations that supply data that bring the model into closer touch with reality by calibrating model parameters. Then, there is the discretization of the model to render it into a form that can be processed on a computer, and, finally, there is the prediction itself, which must be made in a way that takes into account all of the uncertainties met at every phase of the process.

To address these uncertainties, we choose to embed predictive science in the framework of probability theory and, therefore, to seek probabilistic characterizations of answers to what is to be predicted: the quantities of interest, which are the target goals of the simulation. Now we must face the fact that these quantities of interest are not numbers. They are, within the framework of probability theory, random variables or probability distributions. There are, of course, other ways to quantify uncertainty outside of probability, but we subscribe to the widely held view that the logic of science indeed finds a comfortable fit within the framework of logical probability.

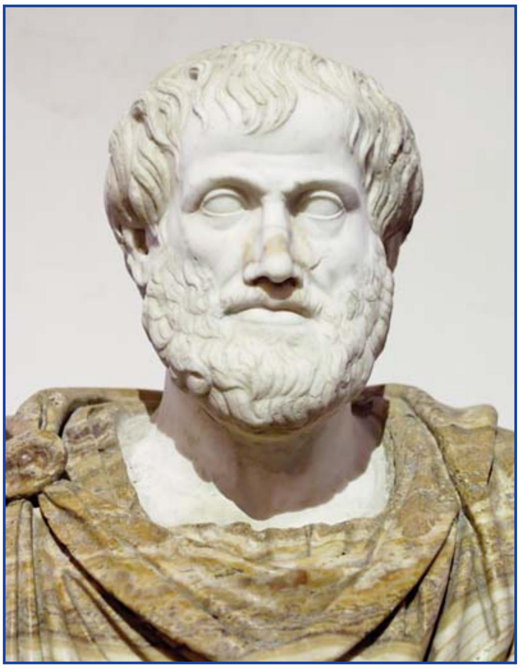


Figures 1:
Claude Shannon

One approach to predictive science is to embark on a very basic journey going back to the primitive foundations of logic, human reasoning and philosophy, that attempts to make clear how scientific knowledge is obtained, and how one copes with uncertainties as epistemic uncertainty, randomness due to ignorance. At the very beginning of scientific thought, one finds deductive logic, top-down reasoning, the establishment of rules to distinguish truth in propositions. These form the rules of mathematics; they are infallible and exact (modulo concerns in closedness and consistency embedded in Gödel's Theorem). But inductive logic, which is bottom-up reasoning, is, according to some, the basis of all scientific discovery. So, the next question is: what fundamental logical system can be developed that naturally extends Aristotelian deductive logic and accounts for uncertainties, and lays the foundations that underline predictive science?

I believe that a fundamental component of the answer is the theory of logical probability advanced by R.T. Cox in 1946 and expanded by E.T. Jaynes in his treatise, Probability Theory: The Logic of Science and formalized and interpreted by K.S. van Horn and others. The basic result is this: the natural extension of Aristotelian logic that includes uncertainty is Bayesian. By accounting for prior knowledge in constructing plausibilities and employing at the outset rules for conditional probability, the Bayes application domain far exceeds that of classical Kolmogorov probability and frequency-based statistics, while providing results in agreement with these approaches when they are applicable. The debate on Bayesian approaches has gone on for 250 years and still persists. Sharon McGrayne calls Bayes' rule "The Theory That Would Not Die", while recent literature calls attention to the paradoxes that may infect infinite parametric spaces and underline the so-called the brittleness of Bayesian approaches in extreme cases. Jaynes dispenses with such paradoxes by saying, "they cannot arise from correct application of our basic rules".

Bayes rule, which actually predates the work of Bayes himself, is now known to be a fundamental axiom of logical probability emanating from the product rule of the conjunction of two propositions, where, for the random events A and B, we have $P(A|B)= P(B|A)\ (P(A))/(P(B).\ )$ Bayes himself appreciated the chilling power of this simple formula. To him, it captured "cause and effect": given information from past experiences, thrusting forward with a theory of physical behavior informed by experimental observations, now deduce new information about the phenomena under study—a remarkable process. To Bayes, a clergyman, it undoubtedly had a spiritual aura.



Figures 2
Aristotle

What does it take to make a science-based prediction taking into account uncertainty? The prediction cannot be done without experimental data or without a model based on inductive hypotheses. To this we add prior information on the model parameters calibrated statistically by direct use of Bayes' rule for the probability of the likelihood function and the prior, with the likelihood measuring the discrepancy between the parameter-to-observation map provided by the model.

With this done, we sample the product distributions to determine the posterior distributions for the parameters. In this step, we call on an appropriate sampling algorithm such as the Metropolis Hastings version of the Markov-Chain Monte Carlo method. We use the model to solve the forward problem, projecting the particular parameters into a prediction of a quantity of interest, which itself is a probability distribution. Along the way, we must ask the question of whether or not the model is a valid model for this purpose, and this requires intermediate experimental observations to determine if the model can predict, with sufficient accuracy, the behavior of subsystems relevant to the quantity of interest.

"...it will provide the guidance to construct very useful models and their calibration and validation ..."

Figure 1:
Edwin T. Jaynes

The most important components of these steps are: 1) calculation of priors, 2) calculation of likelihoods, which embrace the model used for the predictions, and 3) the design of the validation experiment that best informs the user of the model's ability to predict the quantities of interest. All these steps are discussed in the literature, even though exactly how each of these steps is interpreted and implemented is still under debate.

One thing is certain; the Bayesian framework is not, in itself, sufficient to perform model validation. Additional tools are needed. One important tool is the notion of information entropy and other information theoretic ideas that are fundamental to decision theory and experimental design. For example, it can be argued that the optimal quantification of uncertainty in a probability distribution is the information entropy first introduced by Claude Shannon. The principle of maximum entropy can be used to generate priors in many cases. The Intellectual process of constructing likelihoods is still an area of active research and in current applications is most typically based on Gaussian approximations of experimental noise and model inadequacy. Beyond that, how does one design the validation experiment? The key, once again, is information theory: design the experiment so that there is a high enough information gain between the calibration posteriors and the posteriors in the validation experiments. The design of those validation tests to best reflect the influence of the choice of the quantity of interest is an illusive issue and is very much a topic of current research.

What does predictive science hold for the field of computational mechanics in the future? I believe it will provide the guidance to construct very useful models and their calibration and validation so that the field will, indeed, move towards a more truly quantitative science, in which predictions can be made with a measureable level of confidence and, based on model prediction, decision makers can make the right decisions about natural events or about the behavior of engineered systems. ●