Model Uncertainty in "Stochastic" and "Deterministic" Systems

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Abstract: In this paper I explore a categorization of sources of uncertainty arising in predictive modeling based on "stochastic" and "deterministic" systems. The ingredients in this categorization are {past and future observables} and **scenario**, **structural**, **parametric**, and **predictive** uncertainty. I use examples from physics and nuclear waste disposal risk assessment to illustrate topics in problem formulation and computation, and argue that the distinction—often made in the physical sciences—between "stochastic" and "deterministic" models is not useful: all models (even ones with deterministic outputs) are best treated as stochastic in order to realistically account for model uncertainty.

Keywords: Bayes factors, Bayesian prediction, Forbes' Law, GESAMAC, Hooke's Law, Laplace approximations, (Markov chain) Monte Carlo integration, predictive calibration.

1 Introduction

Prediction of observable quantities is a central activity in science and decision-making. Indeed, it is arguably *the* central activity in both of these fields: (a) good (bad) theories in science make testable predictions that turn out to be (in)accurate, and (b) what more is there to decision-making beyond (i) predicting the future under different sets of conditions, partially under your control, and (ii) choosing your favorite future?

Prediction almost always involves a **model** embodying facts and assumptions about how past observables (data) will relate to future observables, and how future observables will relate to each other. Full deterministic understanding of these relationships is the causal goal, rarely achieved at fine levels of measurement: if I stand on the roof of my house and drop a hammer, it will always fall down, but the time it will take to hit the ground is something that I will have to treat stochastically if I want to measure it carefully enough.

Thus we are often led in statistics to models that blend determinism and chance: many (most?) of our models have the form

$$\begin{array}{rcccl} y_i = & f(x_i) & + & e_i, & i = 1, \ldots, n, \\ \text{observable} = & \text{“deterministic” bit} & + & \text{“stochastic” bit}, & \end{array} \qquad (1)$$

where x is often a vector, and we may or may not pretend that f is known. The hope is that successive refinements of causal understanding over time will add more components to x, shifting the bulk of the variation in y from e to f, so to speak, until (for the problem currently under study, at least) our services as statisticians are no longer required.

In the (typically long) period in which causal understanding is only partial, however, a number of uncertainties are recognizable in attempts to apply equation (1) in practice. In Sections 2 and 3 below I argue that these uncertainties may usefully be organized into four types—**scenario, structural, parametric,** and **predictive**—and I explore issues arising in the quantification of these four types of uncertainty in examples from physics and nuclear waste disposal risk assessment. Section 4 details how to make the relevant model uncertainty calculations, Section 5 gives results from such calculations in the examples of Sections 2 and 3, and Section 6 contains some concluding comments on the distinction between "stochastic" and "deterministic" models.

2 Physics: Hooke's Law and Forbes' Law

To begin with two simple examples that illustrate the ideas, let's say that you are an inquisitive sort of person with an empirical bent, and (among other things) you have become interested in two particular relationships: between the length of a springy piece of metal (such as piano wire) and the load placed upon it, and between barometric pressure and the boiling point of water. You gather some data relevant to each of these relationships and begin to construct predictive models without much knowledge of the theory underlying either relationship.

In the case of the springy metal your experiment might consist of attaching a length of piano wire to the ceiling of a tall room, hanging weights from the free end of the wire ranging in mass from 1kg to 11kg (one replication per mass), under conditions that are as close to identical as you can make them, and measuring the length of the wire under each load. With a room (say) 5m in height or more you might get data like those in Table 1.

Table 1: Experimental data, modified slightly from the data set in FREEDMAN et al. (1978), relating the length of a spring to the amount of mass hanging from it.

Mass (kg)	1	3	5	7	9	11
Length(cm)	439.05	439.17	439.26	439.36	439.45	439.55

As for the relationship between barometric pressure and the boiling point of water, this was investigated in the middle 19th century by the Scottish physicist Forbes, who was interested in developing an easy and reliable method for travelers in mountainous regions of the world to estimate the altitude of their present position. He knew that altitude could be determined with a fairly high degree of accuracy from atmospheric pressure, measured with a barometer, with lower pressures corresponding to higher altitudes, but the barometers of his day were quite fragile and hard to transport. He decided to try to experimentally relate barometric