

History Matching for Inverse Modelling in Physical and Biological Systems

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We are often interested in inverse modelling, learning about numerical model inputs from real world observations corresponding to the model outputs. A classical approach to this would use least squares, maximum likelihood or Bayesian calibration. All these methods will overfit as they do not take into account the difference between our numerical model and the real world, the model discrepancy. Although there are methods that perform a Bayesian calibration including a model discrepancy term they suffer from identifiability problems unless there is strong prior information. History matching is an alternative method of inverse modelling. Unlike Bayesian methods history matching does not attempt to find the posterior of the model inputs. Rather we exclude sets of inputs that are implausible given the observations. This is done by setting up an implausibility measure. This is the scaled distance between the observations and the expected value of an emulator. The scaling term is comprised of three variances. The first is the variance of the emulator at this setting of the model inputs. We know this and with every successive wave of the history match we concentrate new model runs in the Not Ruled Out Yet (NROY) space; building a new emulator with each wave. At each wave the emulator has a reduced variance resulting in a smaller NROY. The second term is the discrepancy. This is the distance between the model at its 'best' set of inputs and reality. The final term is the data variance. For a physical system it is reasonable to use the measurement error. But if we think about a biological system this is not the case, this term includes the variability between cases. We can exploit this by looking at hierarchical error structures. The variability in the population, for example, can be split into within and between genders. We discuss these issues and whether biological models should have point estimates at all. For example calibrating to only female subjects will give a much tighter calibration than if we calibrate to the whole population. One of the criticisms of history matching is that it doesn't give point estimates but if we have different calibrations for different groups each of which has an associated variability should we be looking for point estimates or should we rather be looking for ranges of model inputs that reflect this variability. These and other issues will be discussed.