Estimating hidden components in kinetic systems using functional data analysis

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Mass action kinetic systems are defined by linear interactions between different signal functions. Including unobserved players into such systems, the so-called hidden influences, is an important task in this field and can significantly improve the model fit. Common approaches in modeling such systems use differential equations in order to describe the observed signals in terms of their (unobserved) time-derivatives.
Our approach focuses on the approximation of these derivatives. To that end, we use the observed signals and approximate the time course through smoothing spline functions. This approach allows fast computation of the derivative which can then be utilized for the estimation of the hidden quantities. The specification of an error distribution in the model allows statistical inference techniques to be applied to the data: likelihood computation as well as model selection and regularization methods will be presented on this poster. In order to evaluate robustness of the procedure, multiple kinetic toy models are considered with varying numbers of observed signals, noise intensities, as well as different types of hidden influences.
First results show that the estimation procedure is able to handle heavy noise and still produce good estimation of the hidden components.

Figure 1: schematic representation of mass action kinetic system and ordinary differential equations

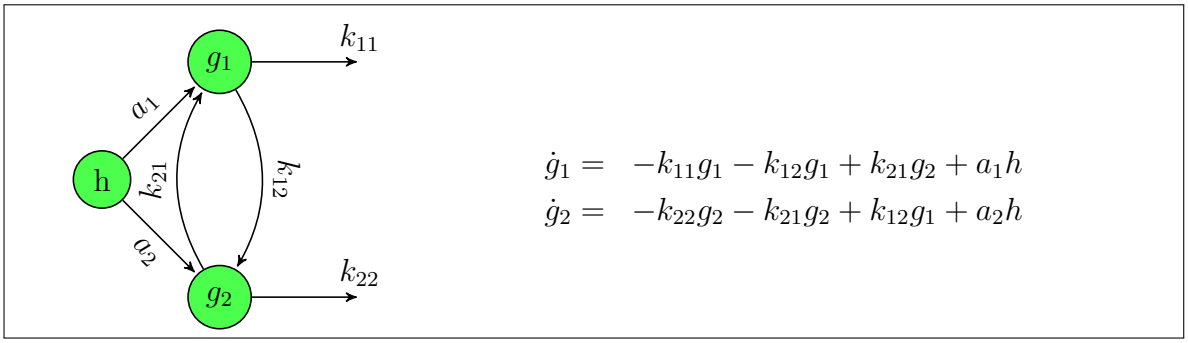

Figure 2: demonstration of hidden influence estimation by using information from both the noisy input functions and the estimated derivatives