TECHNISCHE UNIVERSITÄT DARMSTADT

Learning Sequential Chemical Reactions

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Industrial chemical processes are often composed of a number of stages. For each stage, chemical reactions happen until equilibrium. Next the products are extracted and serve as input for the following stage. Given the input of individual stages, the output concentration is given by an ordinary differential equation (ODE). Consider for example the reaction $A + B \xrightarrow{k} C$ and let c denote the concentrations of C. The concentration c obeys the ODE

$$\dot{c}(t) = k(a_0 - c(t))(b_0 - c(t))) \,,$$

where a_0 and b_0 are initial concentrations. The equilibrium concentration c_∞ is obtained by setting the l.h.s. to zero. For more complex reaction system, the same approach leads to a non-linear equation system of the form

$$0 = F(x, x_0)$$

with concentration vector x and initial concentration x_0. Combining the individual stages allows to predict the output up to the last stage, as illustrated in Fig. 1 a). While similar sequential processes are used in biology experiments, the concentrations of the substances are much lower. This requires to take noise into account. Prototypical examples for procedures where noise can have a large effect are the polymerase chain reaction (PCR) and the SELEX method for selecting aptamers with desired properties [1]. An additional challenge is that reaction parameters (such as k in the above example) are unknown.

The goal of this project is to extend the ODE-based simulation of sequential reaction networks to incorporate noise (cf. Fig. 1 b)). In a second step, this simulator will be used in combination with simulation-based inference to learn reaction parameters from noisy measurements [2].

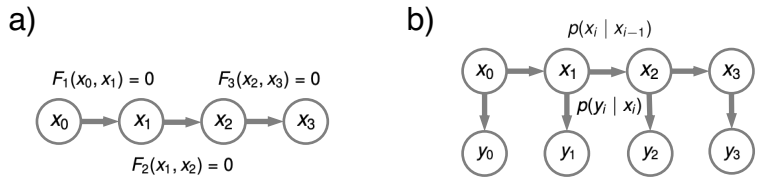

Figure 1: a) Illustration of a deterministic sequential reaction system. Stage i takes input x_{i-1} and is run to equilibrium. The product is then passed as input to stage $i + 1$. b) A probabilistic version in which the output of each reaction is noisy due to low concentrations. Additionally measuring the concentrations after each step leads to a a hidden Markov model structure.

Requirements:

- Background in statistical machine learning, applied probability or an interest in mathematical modeling
- Basic Python programming

For further information, please contact Christian Wildner.

References

[1] Fabian Spill, Zohar B. Weinstein, Atena Irani Shemirani, Nga Ho, Darash Desai, and Muhammad H. Zaman. Controlling uncertainty in aptamer selection. *Proceedings of the National Academy of Sciences*, 2016.

[2] Kyle Cranmer, Johann Brehmer, and Gilles Louppe. The frontier of simulation-based inference. *Proceedings of the National Academy of Sciences*, 2020.