AN EVOLUTIONARY APPROACH TO KINETIC MODELLING INSPIRED BY LAMARCKIAN INHERITANCE

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Key Words: process-model mismatch, diagnosis, information, Lagrange multipliers.

The mechanistic description of kinetic phenomena requires the construction of systems of differential and algebraic equations where a high number of parameters and state variables may be involved. The complexity associated with kinetic phenomena frequently leads to the construction of kinetic models characterised by some degree of approximation. Whenever an approximated model is falsified by observations, its mathematical structure should be evolved embracing the available experimental evidence [1]. Nonetheless, improving a model is a time and resource intensive task that heavily relies on the presence of experienced researchers. An evolutionary approach to kinetic modelling is proposed in this work which is inspired by the theory of evolution proposed by Jean-Baptiste Lamarck, namely the theory of Lamarckian inheritance [2]. The approach is illustrated qualitatively in the sketch in Figure 1. Lamarck states that the evolution of living beings is directly driven by their interaction with the environment. The use/disuse of an organ determines the evolution of that organ towards higher/lower complexity. The long neck of the giraffe is frequently reported as an example to explain Lamarck's theory. Primitive giraffes with a short neck would strive to reach the highest leaves. This behaviour, driven by necessities of adaptation, would lead to an elongation of the neck during the giraffe's lifetime and the characteristic of the long neck is inherited by the offspring. Lamarck's theory is now widely dismissed. Nonetheless, the field of epigenetics stemmed directly from Lamarck's philosophy and aims at explaining the complex mechanisms behind the hereditability of environment-driven phenotype changes [3]. In this work, the principles of Lamarckian inheritance are translated into a framework for kinetic model building. In the proposed framework, the evolution of model structures is data-driven. When the model is over-fitting, model parameters that are irrelevant for representing the data are removed from the model structure. When the model is under-fitting, relevant model parameters are evolved into more complex state-dependent expressions. A statistical index, namely a Model Modification Index (MMI), based on the Lagrange multipliers statistic [4], is proposed as a measure of model misspecification to support the evolution of approximated kinetic models towards higher levels of complexity. The use of the MMI is demonstrated in a simulated case study to diagnose misspecification in an approximated kinetic model of baker's yeast growth [5].

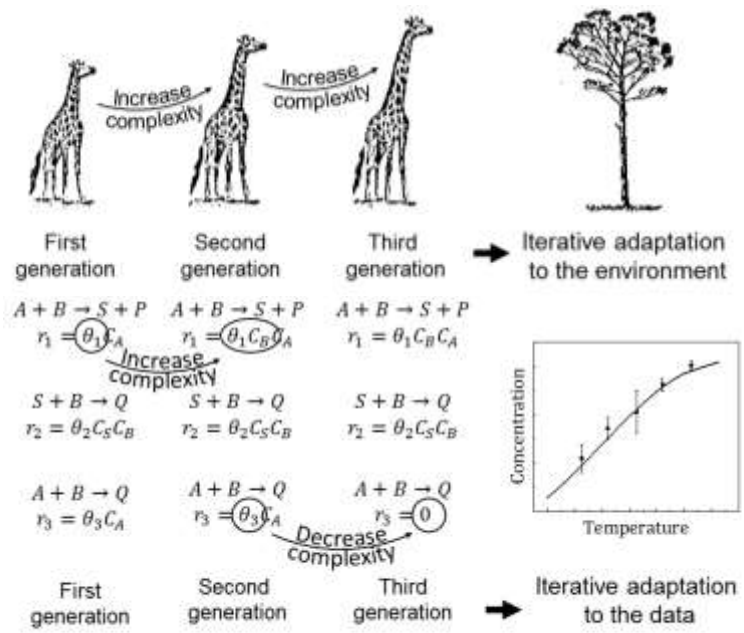

Figure 1 – Analogy between the evolution of a giraffe and the evolution of a kinetic model in a Lamarckian framework.

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