Learning Interactions in Reaction Diffusion Equations by Neural Networks

Sichen Chen[1], Nicolas J-B Brunel[2,3], Xin Yang[4], Xinping Cui[1]

[1]Department of Statistics, University of California, Riverside, U.S.A.
[2]ENSIIE & Laboratoire de Mathématiques et Modélisation d'Evry, Université Paris Saclay, France
[3]Quantmetry, France
[4]Department of Mathematics, University of California, Riverside, U.S.A.

Abstract

Partial differential equations are common models in biology for predicting and explaining complex behaviors. Nevertheless, deriving the equations and estimating the corresponding parameters remains challenging from data. In particular, the fine description of the interactions between species requires care for considering various regimes such as saturation effects. We apply a method based on neural networks to discover the underlying PDE systems, which involve fractional terms and may also contain integration terms based on observed data. Our proposed framework, called Frac-PDE-Net, adapts the PDE-Net 2.0 by adding layers that are designed to learn fractional and integration terms. The key technical challenge of this task is the identifiability issue. More precisely, one needs to identify the main terms and combine similar terms among a huge number of candidates in fractional form generated by the neural network scheme due to the division operation. To overcome this barrier, we set up certain assumptions according to realistic biological behavior. Additionally, we use an $L2$-norm based term selection criterion and the sparse regression to obtain a parsimonious model. It turns out that the method of Frac-PDE-Net can recover the main terms with accurate coefficients, allowing for effective long-term prediction. We demonstrate the interest of the method on a biological PDE model proposed to study the pollen tube growth problem.

Keywords: neural networks; deep learning; non-linear reaction–diffusion equations; model discovery; sparse regression; multiple testing