Technische Universität Braunschweig

TU Delft

Master thesis: Separating longtime behavior and learning of mechanisms

Mathematical modeling of complex systems is challenging and becomes even harder if the underlying principles are partly unknown. Life-science application are examples of such processes, where the role of individual particles is often unclear. Furthermore, experiments are expensive or even impossible because the interactions are strongly coupled processes. As many of the processes take place inside the body, observations are even more difficult. Therefore, mathematical models are useful for gaining insight in the underlying mechanisms of the complex processes and for testing hypothetical treatments of diseases. Viral liver inflammations like hepatitis B and C are a prominent example for such complex processes with unknown mechanisms leading to either healing or chronic infection courses.

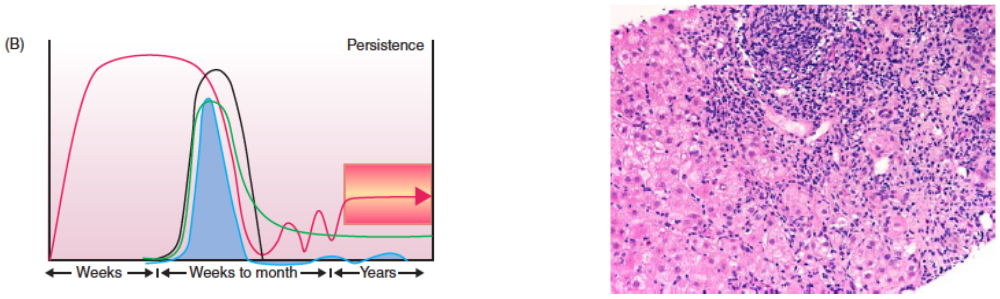

Figure 1: Left: Development of chronic inflammation after a transient phase (Bowen & Walker, 2005). Right: Pathological image of a chronic liver inflammation with spatial heterogenous spead of immune cells (Kanel 2018)

The infection courses show a transient phase in the beginning, cf. Figure 1: The human body reacts on the virus in the tissue and tries to eliminate it. After this active battle, the infection is either eliminated or remains as a chronic disease. From the mathematical point of view, the interaction of the virus and the immune cells of the body can be described by differential equations

$$\dot{u} = f(u) = \sum_i f_i(u). \tag{1}$$

The occurrence of an infection courses is the tendency to a stationary state of the system after a transient phase.

By means of machine learning algorithms, we want to discover the model mechanisms f_i behind the dynamical processes which are responsible for the shifting behavior, compare [1]. Therefore, we propose a set of functions f_i, including for example polynomials of the system states, and aim to select those functions f_i fitting the transient phase and the longtime behavior best. The selected functions f_i may explain the dynamics of the hidden processes.

This master thesis explores the possibility of learning mechanisms f_i with physics-informed neural network (PINN) [4] algorithms if the system behavior takes place on several time scales; for instance, if the longtime behavior depends only weakly on short-time effects. In the PINN approach, the idea to employ a neural network u_θ to discretize the differential equation eq. (1) by optimizing the loss function

$$\sum_{t_j} \left\| \dot{u}_\theta(x_j) - \sum_i f_i(u_\theta)(t_j) \right\|^2.$$

Our idea is to impose specific structures into the network function. For instance, in the case of two temporal scales, we want to construct

$$u_\theta = g(\bar{u}_{\bar{\theta}}, \hat{u}_{\hat{\theta}}),$$

where $\bar{u}_{\bar{\theta}}$ is a model that describes the behavior on a macroscale and $\hat{u}_{\hat{\theta}}$ describes the microscale behavior; then, $\theta = (\bar{\theta}, \hat{\theta})$. The function g is a generic function that represents the coupling of the time scales. We will consider and/or design different types of coupling approaches during the thesis project; one example is to use a multi-level domain decomposition approach as in [2].

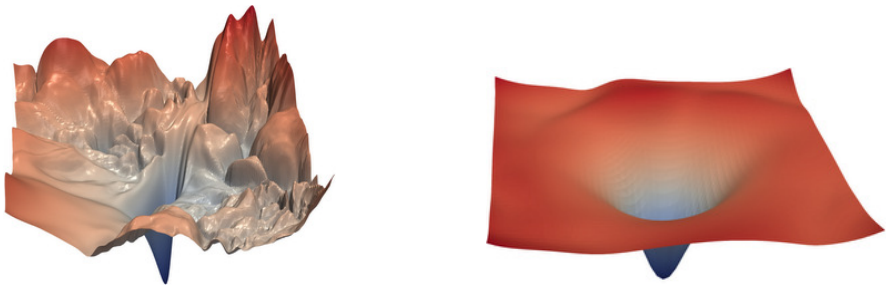

Figure 2: Visualization of a projection of the loss landscape based on [3]: network without (left) and with (right) skip connections. Images taken from `https://github.com/tomgoldstein/loss-landscape`.

A first toy problem is the equation for saturated growth

$$\dot{u} = u(C - u)$$

which tends towards C for initial values $u(0) = u_0 > 0$. In the introduced example of liver inflammation, this equation models the growth of the virus population in the liver tissue.

A second model is the competition between two species u_1 and u_2 with dynamics

$$\dot{u_1} = u_1(C_1 - \alpha_1 u_1 - \alpha_2 u_2)$$
$$\dot{u_2} = u_2(C_2 - \beta_1 u_1 - \beta_2 u_2)$$

which tends for certain parameter values α_i, β_i to a stationary co-existence state. Interpreting u_1 and u_2 as virus and immune cells, this is a model for chronic inflammation courses.

We are also interested in the question of how this multiscale approach influences the loss landscape of the neural network model compared against a simple PINN model cf. Figure 2.

For implementation, we will employ state-of-the-art deep learning libraries, such as tensorflow (`https://www.tensorflow.org/`) or PyTorch (`https://pytorch.org/`). Programming experience in Python is beneficial. Good communication skills in English or German are required.

The project is in collaboration of TU Braunschweig (Germany) and TU Delft (the Netherlands). We will try to enable research visit(s) during the time of the project (e.g. by using PROMOS grants at TU Braunschweig).

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References

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