BP 9: Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)

Time: Friday 11:15–12:30 Location: H2

BP 9.1 Fri 11:15 H2

Tayloring Reservoir Computing Performance via Delay Time Tuning — •Tobias Hülser, Felix Köster, and Kathy Lüdge — Institut für Theoretische Physik, TU Berlin

Reservoir Computing is a versatile, fast-trainable machine learning scheme that utilises the intrinsic information-processing capacities of dynamical systems. In recent years delay-based reservoir computing emerged as a promising, easy to implement alternative to classical reservoir computing. Previous work showed that a mismatch between input time and delay time enhances computational performance significantly[1]. For delays much higher than the input time, it was shown that certain inputs cannot be recalled by the network which lead to gaps in the memory capacity[2]. Via manipulating the delays in a system of ring-coupled Stuart-Landau oscillators, we show that some of the gaps can be closed. Moreover, we can tune the range of previous inputs the reservoir can memorise. Consequently, we find a significant increase in performance for nonlinear memory tasks and the NARMA10 task.

[1] S. Stelzer et al., Neural Networks 124, 158-169 (2020)
[2] F. Köster et al., Cogn. Comput. (2020)

BP 9.2 Fri 11:30 H2

Employing artificial neural networks to find reaction coordinates and pathways for self-assembly — •Jörn Appeldorn, Arash Nikoubashman, and Thomas Speck — Inst. für Physik, Universität Mainz, Germany

We study the spontaneous self-assembly of single-stranded DNA fragments using the coarse-grained oxDNA2 implementation [1]. A successful assembly is a rare event that requires crossing a free energy barrier. Advanced sampling methods like Markov state modeling allow to bridge these long time scales, but they require one or more collective variables (order parameters) that faithfully describe the transition towards the assembled state. Formulating an order parameter typically relies on physical insight, which is then verified, e.g., through a committor analysis. Here we explore the use of autoencoder neural networks to automatize this process and to find suitable collective variables based on structural information. For this step, one still needs to map configurations onto structural descriptors, which is a non-trivial task. Specifically, we investigate the latent space of EncoderMap [2] and how it changes with the amount of information contained in the descriptor. With this approach, we were able to determine the free energy landscape, the locations of the (meta)stable states, and the corresponding transition probabilities.

[1] - Snodin et al., J. Chem. Phys.(2015), 142, 234901 [2] - T. Lemke and and C. Peter,J.Chem.TheoryComput.(2019), 15, 1209-1215

BP 9.3 Fri 11:45 H2

Efficient Bayesian estimation of the generalized Langevin equation from data — •Clemens Willers and Kamps Oliver — Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstr. 2, 48149 Münster, Germany

A recent topic of research attracting broad interest is the modeling of stochastic time series whose dynamics includes memory effects. To cover this non-Markovian case, the Langevin equation, which is frequently used in many fields of science, is extended by a memory kernel, yielding the generalized Langevin equation (GLE). Since a direct derivation of the GLE from basic mechanisms through the well known Mori-Zwanzig formalism is not accessible in many cases, it is a relevant question how to estimate the model solely based on measured data.

In our work we develop a realization of Bayesian estimation of the GLE. The Bayesian approach allows for the determination of both estimates and their credibility in a straightforward manner. To facilitate this method, we consider the GLE with white noise. Although this is an approximation, we still deal with a very general model class representing systems with memory.

Importantly for applications, we realize the method in a numerically efficient manner through a piecewise constant parameterization of the drift and diffusion functions of the model, a reformulation of the likelihood, and an effective initial guess for the estimate.

We illustrate our method by an example from turbulence. Here we are able to reproduce the autocorrelation function of the original data set, which is an essential characteristic of a turbulent flow.

BP 9.4 Fri 12:00 H2

Master memory function for delay-based reservoir computers — •Felix Köster[1], Serhiy Yanchuk[2], and Kathy Lüdge[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, 10623 Berlin — [2]Institut für Mathematik, TU Berlin, Str. des 17. Juni 136, 10587 Berlin

The reservoir computing scheme is a versatile machine learning mechanism, which shows promising results in time-dependent task predictions in comparable fast-training times. Delay-based reservoir computing is a modification in which a single dynamical node under the influence of feedback is used as a reservoir instead of a spatially extended system.

We show that many delay-based reservoir computers considered in the literature can be characterized by a universal master memory function (MMF). Once computed for two independent parameters, this function provides linear memory capacity for any delay-based single-variable reservoir with small inputs. Moreover, we propose an analytical description of the MMF that enables its efficient and fast computation. Our approach can be applied not only to the reservoirs governed by known dynamical rules such as Mackey-Glass or Ikeda-like systems but also to reservoirs whose dynamical model is not available.

BP 9.5 Fri 12:15 H2

Investigating the role of Chaos and characteristic time scales in Reservoir Computing — Marvin Schmidt[1,2], Yuriy Mokrousov[1,3], Stefan Blügel[1,3], Abigail Morrison[2,3,4], and •Daniele Pinna[1,3] — [1]Peter Grünberg Institute (PGI-1), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [2]Institute for Theoretical Neuroscience Institute of Neuroscience and Medicine (INM-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [3]Institute for Advanced Simulation (IAS-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [4]Computational and Systems Neuroscience & JARA-Institut Brain structure-function relationships (INM-10), Wilhelm-Johnen-Straße, 52428 Jülich, Germany

Reservoir Computing (RC) dynamical systems must retain information for long times and exhibit a rich representation of their driving. This talk highlights the importance of matching between input and dynamical timescales in RC systems close to chaos. We compare a chain of Fermi-Pasta-Ulam-Tsingou anharmonic oscillators and a sparsely connected network of spiking excitatory/inhibitory neurons. The first is toy model for magnetic spin-wave reservoirs while the latter that of a biological neural net. Both systems are shown to rely on a close matching of their relaxation timescales with the driving input signal's frequency in order to memorize and make precise use of the information injected. We argue that this is a general property of RC systems.
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