Geometric Numerical Analysis and Deep Learning (L16)

Non-Examinable (Graduate Level)

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Differential equations are fundamental to mathematically describe physical phenomena and play a crucial role in many disciplines. Finding an exact solution to these equations is generally impossible; thus, reliable numerical approximations are essential. Among the methods providing such approximations, some aim not only to obtain a quantitatively accurate result but also to ensure a qualitatively accurate representation of the underlying dynamics. These methods are generally called *geometric* or *structure-preserving.*

This non-examinable course focuses on a selection of geometric numerical methods for Ordinary Differential Equations (ODEs), including

- Symplectic numerical methods for Hamiltonian systems, and
- Methods reproducing the non-expansive nature of some ordinary differential equations, such as negative gradient flows of convex potentials.

In addition to traditional applications, the numerical approximation of ODE solutions has also demonstrated importance in the analysis and design of neural networks. A neural network $\mathcal{N}_\theta = F_{\theta_L} \circ \cdots \circ F_{\theta_1}$ can be seen as the composition of parametric maps, called layers of the network, where the parameters in $\theta = (\theta_1, ..., \theta_L)$ are chosen so that the resulting function solves sufficiently accurately a task of interest. When the number of network layers is larger than two, $\mathcal{N}_\theta$ is called a *deep neural network*, and *deep learning* is the field studying these deep networks.

Using geometric numerical methods to design neural networks has proven to be a valuable approach to structure them as desired, such as making them less sensitive to input perturbations. This course will include some applications of the presented geometric numerical methods in the context of deep learning, highlighting their direct relevance and importance in the field.

Prerequisites

This course assumes some familiarity with numerical methods for ordinary differential equations, particularly Runge–Kutta methods. The numerical experiments presented in the course will be based on the Python programming language. Some experience with Python is beneficial but not necessary. No knowledge about neural networks is required.

Literature

1. Iserles, A., *A first course in the numerical analysis of differential equations.* Cambridge University Press, 2009
2. Hairer, E., Lubich, C., and Wanner, G., *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, 2006
3. Weinan, E., *A proposal on machine learning via dynamical systems.* Communications in Mathematics and Statistics, 1(5), 1-11, 2017.
4. Celledoni, E., Ehrhardt, M. J., Etmann, C., McLachlan, R. I., Owren, B., Schonlieb, C. B., and Sherry, F., *Structure-preserving deep learning.* European journal of applied mathematics, 32(5), 888-936, 2021.