The Data-Weight Duality for Deep Learning Inverse Problems

Christoph Brune[1]

[1] University of Twente
c.brune@utwente.nl

Scientific machine learning combines the approximation power of machine learning with modeling and the numerical analysis of PDEs leading to digital twins where data-driven and model-driven techniques are combined. In this context, deep kernel representations have the potential to form an integral link between scientific computing, inverse problems, uncertainty quantification, and machine learning towards the nonlinear analysis of deep neural operators.

Reproducing Kernel Hilbert spaces (RKHS) have been successful in various areas of machine learning, like kernel SVMs, relating model and feature representations. Recently, Barron spaces have been used to prove bounds on the generalization error for neural networks. Unfortunately, Barron spaces cannot be understood in terms of RKHS due to the strong nonlinear coupling of the weights. This can be solved by using the more general Reproducing Kernel Banach spaces (RKBS).

As a key result, we can show that the dual space of such RKBSs, is again an RKBS where the roles of the data and parameters are interchanged, forming an adjoint pair of RKBSs including a reproducing kernel. This enables the construction of saddle point problems for active learning of neural networks including sparse architecture search, model exploration, model-order reduction, or deep kernel learning following representer theorems.