Diffeomorphism-based feature learning using Poincaré inequalities on augmented input space

Romain Verdière*[1], Clémentine Prieur†[1], and Olivier Zahm‡[1]

[1]Université Grenoble Alpes – L'Institut National de Recherche en Informatique et e n Automatique (INRIA), Laboratoire Jean Kuntzmann (LJK) – France

Résumé

Modern computational models for scientific and engineering applications typically involve a large number of input parameters and are expensive-to-evaluate both in time and resources. Replacing the model with an accurate and fast-to-evaluate surrogate (or approximation) offers a viable workaround in many applications. Approximating such high-dimensional functions with classical approximation tools such as polynomials, wavelets or neural networks is, however, a difficult task. This is even aggravated in the small sample regime where one only has access to a little number of model evaluations. To address this challenge, we propose a gradient-enhanced algorithm which proceeds in two steps: firstly, we reduce the input dimension by learning the relevant input features from gradient evaluations, and secondly, we regress the function output against the pre-learned features. To ensure theoretical guarantees, we construct the feature map as the first components of a diffeomorphism, which we learn by minimizing an error bound obtained using Poincaré Inequality applied either in the input space or in the feature space. This leads to two different strategies, which we compare both theoretically and numerically and relate to existing methods in the literature. In addition, we propose a dimension augmentation trick to increase the approximation power of feature detection while preserving the theoretical guarantees. In practice, we construct the diffeomorphism using coupling flows, a particular class of invertible neural networks. Numerical experiments on various high-dimensional functions show that the proposed algorithm outperforms state-of-the-art competitors, especially with small datasets.

Mots-Clés: high, dimensional function approximation, nonlinear feature learning, augmented space, Poincaré Inequality, invertible neural networks

*Intervenant

†Auteur correspondant: clementine.prieur@univ-grenoble-alpes.fr

‡Auteur correspondant: olivier.zahm@inria.fr