Learning signals defined on graphs with optimal transport and Gaussian process regression

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Abstract

In computational physics, machine learning has now emerged as a powerful complementary tool to explore efficiently candidate designs in engineering studies. In this context, we would like to be able to easily predict fields defined on meshes corresponding to new geometries without the need for costly simulations. While some methods like Graph Neural Networks [4] are intrinsically designed to predict signals defined on graphs or point clouds, a natural question is the extension of general scalar output regression models to such complex outputs. Changes between input geometries in terms of both size and adjacency structure in particular make this transition non-trivial. Another key challenge is the obtention of predictive uncertainties, which is crucial to certify the quality of results, to assist sequential design of experiments or to plug the models into Bayesian optimization workflows.

In this work, we propose an innovative strategy for Gaussian process regression where inputs are large and sparse graphs with continuous node attributes and outputs are signals defined on the nodes of the associated inputs. The methodology relies on the combination of regularized optimal transport [3], dimension reduction techniques [2], and the use of Gaussian processes [5] indexed by graphs. It extends previous work on Gaussian processes with Sliced Wasserstein Weisfeiler Lehman graph kernels [1] previously limited to scalar outputs. In addition to enabling signal prediction, the main point of our proposal is to come with confidence intervals on node values.

We illustrate the efficiency of the method with regression tasks involving large graphs from mesh-based simulations in computational fluid dynamics and mechanics [1]. Train datasets are made up of a few hundred graphs with their respective 2D/3D coordinates, where adjacency matrices vary between several inputs, and output fields represent physical quantities of interest on the nodes such as the pressure or the temperature. In Figure 1, we show predictions and associated uncertainties for two test samples of a problem in computational mechanics.

[1]Datasets: https://plaid-lib.readthedocs.io/en/latest/source/data_challenges.html

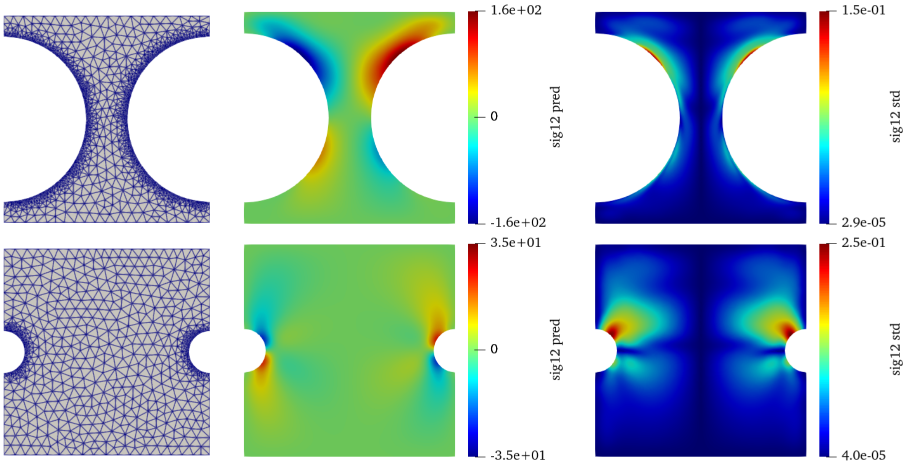

Figure 1: Predictions for two test meshes from the Tensile2d dataset (top and bottom lines). From left to right: the input mesh, the predicted field and the posterior standard deviation of the Gaussian process regression.

Short biography (PhD student)

I have a double Master's degree in Mathematics and Computer Science for Data Science (MIDS) from the University Paris Cité (formerly Diderot).
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