Surrogate Parametric Metamodel Based On Optimal Transport

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1 Introduction

The description of a physical problem through a model necessarily involves the introduction of parameters. Hence, one wishes to have a solution of the problem that is a function of all these parameters: a parametric solution. However, the construction of such parametric solutions exhibiting localization in space is only ensured by costly and time-consuming tests, for instance numerical simulations. Numerical methodologies used classically imply enormous computational efforts for exploring the design space. Therefore, parametric solutions obtained using advanced nonlinear interpolation are an essential tool to address this challenge.

Interpolation is a mathematical fundamental operation widely used in numerical simulation. However, despite of its simplicity, usual interpolation does not always yield physical meaningful results. Optimal Transport (OT) defines a radically different way to interpolate and calculate distances between functions having disjoint supports. Indeed, while the classical Euclidian interpolation leads to a mixture of the two functions (one which progressively disappears and the other which progressively appears), OT-based interpolation leads to a progressive translation and scaling. Such a numerical solution is much more realistic in several fields, such as, computer graphics or fluid dynamics, justifying its widespread use. In this sense, Optimal Transport quantifies the distance between two functions by considering the cheapest way to move all mass units describing one function to reshape it into the other, taking into account the geometry of the underlying space. Thus, two almost identical functions differing only by a little displacement are considered to be very close by the OT approach while they can be considered as very dissimilar by the usual L1 or L2 norms. Today, Optimal transport has a wide range of applications, such as, computer vision, image processing and machine learning.

However, computing optimal transport is usually numerically expensive and not adapted to online approaches since it is usually performed by sampling from the source and target distributions and solving then a discrete linear programming problem which results numerically costly and statistically inefficient. Indeed, classical linear programming approaches to OT scale roughly with cubic complexity. Some approaches have been developed in order to alleviate such an issue but

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remain very restrictive working only in specific frameworks: e.g., a semi-discrete approach with Laguerre's cells or a dynamical formulation. It can also be noted that entropy regularized approaches to solve OT have been developed. In particular, Sinkhorn's algorithm involves only matrix-vector products and allows the regularized distance to be a smooth function of all its parameters.

Despite of the recent advances to solve OT, the problem remains numerically expensive and not accessible in online applications. Therefore, our goal is to propose a parametric model based on Optimal Transport and accessible in an online manner that allows to interpolate between several simulations of a parametric problem in real time and following the motion-based interpolation that characterizes OT. Based on displacement interpolation, the method developed here approaches the interpolation problem as an optimal mass transport problem where each unit of mass describing the source distribution needs to be transported to the target distribution while minimizing the total cost associated to the transport. For two distributions, the problem can thus be written in terms of bipartite graph matching. The paths taken by each unit of mass are parameterized and an interpolated solution can thus be accessed by partially displacing the mass along the paths at given values of the parameters. To this purpose, a parametric model is built offline relying on Smoothed-Particle Hydrodynamics decomposition and Model Order Reduction.

The approach introduced here proceeds in two stages: an offline non-intrusive training of the parametric OT-based model, followed by an online application of the model in the parametric space. Indeed, high-fidelity simulations of the parametric problem are used to train the model without any need of an insight of the problem equations, hence the non-intrusive terminology.

First, in order to train the model, high-fidelity simulations are used in the offline stage. These simulations belong to a parametric space where our parametric problem is defined. The offline stage proceeds in several steps: first, the high-fidelity simulations of the training set are decomposed into the sum of elementary identical Gaussians. Then, each Gaussian from each simulation is paired with one Gaussian of every other simulation in order to respect Optimal Transport behavior. A Genetic Algorithm is employed in order to approximate the k-Dimensional Matching problem obtained. Next, a sparse Proper Generalized Decomposition (sPGD) regression is applied over the coefficients of the Proper Orthogonal Decomposition (POD) of the matrix of snapshots, which have just been decomposed into Gaussians, in order to create the parametric model.

Then, this model can be evaluated in the parametric space of the problem in the online stage leading to a partial advection of all the Gaussians. Summing all those Gaussians allows to reconstruct, in real-time, the high-fidelity simulation interpolated in this point of the parametric space following the Optimal Transport theory.

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