Tensor product spline interpolation and the TPI package

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I. INTRODUCTION

This document provides a brief summary of the construction and application of tensor product spline interpolants. It accompanies the `TPI` package [1] which provides a `Cython` [2] implementation that can conveniently be used from the `Python` [3] programming language. The TPI implementation also relies on the `NumPy` [4] package for scientific computing with Python. Examples for using the `TPI` package can be found in the tutorial `Jupyter notebook` [5] on github.

A. B-splines

Let the i-th B-spline basis function [6] of degree k with the knots vector $\vec{t}$ evaluated at x be denoted by $B_{i,k,t}(x)$. For distinct knots $t_i, \ldots, t_{i+k+1}$, the B-splines can be defined

$$B_{i,k,t}(x) := (t_{i+k} - t_i)[t_i, \ldots, t_{i+k}](\cdot - x)_+^{k-1} \quad \forall x \in \mathbb{R}, \tag{1}$$

where $[t_i, \ldots, t_{i+k}]f$ is the divided difference of order k of the function f at the sites $t_i, \ldots, t_{i+k}$, and $(x)_+ := \max\{x, 0\}$. The B-splines can also be defined in terms of recurrence relations. The definition can be extended to partially coincident knots which are useful for the specification of boundary conditions.

B. Boundary condition

Cubic splines are C^2 at the knots. To close the linear system additional information is needed at the boundaries. Often a natural boundary condition is used where the second derivative of the basis functions are set to zero at the boundary. If boundary derivatives are not known it is better to use the so-called "not-a-knot" boundary condition. It is defined by demanding that even the 3rd derivative must be continuous at the first and last knots. At the first knot x_1 this is imposed as follows

$$B^{(3)}_{i,k,t}\left(\frac{x_0 + x_1}{2}\right) \stackrel{!}{=} B^{(3)}_{i,k,t}\left(\frac{x_1 + x_2}{2}\right) \tag{2}$$

C. Tensor product spline interpolant

Tensor product spline interpolation is a very useful tool for constructing fast reduced order models (ROM) or surrogate models of time or frequency dependent functions that also depend on a moderate number of parameters $\vec{\lambda}$. For instance, ROMs of the gravitational waves emitted by compact binary coalescences [7–21] have been crucial for the astrophysical detection and inference of parameters characterizing these binaries by LIGO and Virgo [22–32].

Let us assume that we want to model a quantity $A(f; \vec{\lambda})$ and that it has been expanded into a suitable orthonormal basis $A(f; \vec{\lambda}) \approx \sum_l A_l(\vec{\lambda}) \mathcal{B}_l(f)$. The l-th basis coefficient of a ROM evaluated at the parameter space point $\vec{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ for a quantity A can be expressed as an n-dimensional tensor product spline interpolant

$$A_l(\vec{\lambda}) = \sum_{i_1,\ldots,i_n} c^{A,l}_{i_1,\ldots,i_n} \left(B^1 \otimes B^2 \otimes \cdots \otimes B^n\right)_{i_1,\ldots,i_n} (\vec{\lambda}), \tag{3}$$

where we have dropped the degree (usually cubic $k = 3$) and the knots vector of the B-splines and added a superscript number indicating to which parameter space dimension the basis function belongs. The tensor product spline coefficients $c^{A,l}_{i_1,\ldots,i_n}$ and the B-spline tensor product basis form rank n tensors.

D. Partial derivatives

A parameter space partial derivative of an SVD coefficient can then be written

$$\frac{\partial}{\partial \lambda_m} A_l(\vec{\lambda})\big|_{\vec{\lambda}=\vec{\lambda}} = \sum_{i_1,\ldots,i_n} c^{A,l}_{i_1,\ldots,i_n} \frac{\partial}{\partial \lambda_m} \left(B^1 \otimes B^2 \otimes \cdots \otimes B^n\right)_{i_1,\ldots,i_n} (\vec{\lambda})\big|_{\vec{\lambda}=\vec{\lambda}} \tag{4}$$

As an example, consider a partial derivative of a 3D TP interpolant:

$$\frac{\partial}{\partial \lambda_2} A_l(\vec{\lambda})\big|_{\vec{\lambda}=\vec{\lambda}} = \sum_{i,j,k} c^{A,l}_{i,j,k} \frac{\partial}{\partial \lambda_2} \left(B^1 \otimes B^2 \otimes B^3\right)_{i,j,k} (\vec{\lambda})\big|_{\vec{\lambda}=\vec{\lambda}} = \sum_{i,j,k} c^{A,l}_{i,j,k} \left(B^1 \otimes \frac{\partial B^2}{\partial \lambda_2} \otimes B^3\right)_{i,j,k} (\vec{\lambda})\big|_{\vec{\lambda}=\vec{\lambda}} \tag{5}$$

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[1] Tensor product interpolation package for python, `https://github.com/mpuerrer/TPI`.
[2] Cython: C-extensions for python, `http://cython.org/`.
[3] Python programming language, `https://www.python.org/`.
[4] Numpy, `http://www.numpy.org/`.
[5] Jupyter, `https://jupyter.org/`.
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