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A smoothing stochastic simulated annealing method for localized shapes approximation

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ABSTRACT

In B-splines approximation setting, it is known that monotony and convexity (or concavity) shapes can easily be controlled by the spline coefficients. In this paper we deal with the general context of combinations of localized shape constraints. We prove that unimodality constraint is fulfilled simply by an increasing and decreasing sequence of the spline coefficients by using the Descartes' sign rule. Then, the local support property of B-splines is used to locate each constraint on a given interval. We formulate a smoothing spline approximation under inequality constraints in function of the spline coefficients. We also give a simulated annealing algorithm to solve the optimization problem and we establish the almost sure convergence of the efficient solution.

1. Introduction

In various fields, some information on a function f that we aim to approximate may be known. This information may be related to the shape of f. The literature on approximation under shape constraints usually focus on a single shape restriction on the whole definition domain of f. Consider the following problem: given a number of observation points, find an approximation for f which is unimodal on $[a, b]$, concave only on $[c, b]$ ($c \in]a, b[$) and twice continuously differentiable everywhere. It is worth noting that such a combination of constraints has never been considered in the literature on B-spline approximation though it seems of practical interest and realistic. In this paper we provide such an approximation. By using the fact that any straight line crosses the spline no more often than it crosses the control polygon, de Boor [4] has illustrated the property says that a spline has the same shape as its control polygon. However, the above works only on monotonicity and concavity (or convexity) shape constraints and cannot be applied to other shapes like unimodality or more sophisticated shapes. Motivated by the above idea, we generalize the shape preservation property to unimodality thanks to the Descartes' sign rule. Then, by using the local support property of B-splines, combinations of several localized shape constraints follows immediately. The

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present work is a contribution in which controlled mathematical localized shape constrained approximations are obtained for the usual constraints for a class of B-splines bases encompassing the Bernstein basis.

Furthermore, we formulate a smoothing spline approximation under inequality constraints in terms of the shape constraints to illustrate the idea. In a practical viewpoint, we propose a Monte Carlo simulated annealing scheme as a tool to solve the optimization problem. The almost sure convergence of the simulated annealing algorithm is proved for an inversely logarithmic temperature parameter by checking the sufficient conditions given by [2].

The outline of this paper is as follows: In Section 2, we give some basic definitions and results which will be used in the paper. In Section 3, we establish the preservation of the unimodality shape and we explain the concept of combinations of localized shape constraints by using the local support property of B-splines. In Section 4, we derive an optimization problem involving smoothing constrained spline function and we establish the efficient solution thanks to a simulated annealing algorithm. In Section 5, the convergence of the simulated annealing is proved by assuming the compactness and by taking the uniform probability measure. In Section 6, we conclude the results of this paper.

2. Notations and preliminaries

Some notation in this paper is as follows: we use $D^r f$ (instead of $f^{(r)}$) to denote the r-th derivative of the function f. Let us briefly recall the definition and some properties of B-splines. The intent is to give a simple and direct development and for this reason B-splines will be defined via the recurrence relations. Let the integer $(k-1)$ denote the degree of the B-spline (i.e., the order is k). Given a nondecreasing sequence of points $\{t_i \in \mathbb{R} | t_i \leq t_{i+1}\}$ called knots. The vector $\mathbf{t} := (t_i)$ is called the knot vector and some of these knots can be equal. In the case where ℓ knots are equal to a real α, i.e. $\ell_i = \#t_i = \#\{t_j : t_i = t_j = \alpha\}$, we say that α has multiplicity ℓ_i. The B-spline function of order 1 is given by: $B_{i1}(x) := 1$ if $t_i \leq x < t_{i+1}$ and $B_{i1}(x) := 0$ otherwise. From this first-order B-spline, we obtain higher-order B-splines by recurrence:

$$B_{ik}(x) := \omega_{ik}(x)\, B_{i,k-1}(x) + \Big(1 - \omega_{i+1,k}(x)\Big)\, B_{i+1,k-1}(x), \tag{1}$$

with

$$\omega_{ik}(x) := \begin{cases} \frac{x - t_i}{t_{i+k-1} - t_i}, & \text{if } t_i < t_{i+k-1} \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

From definitions of B-splines, a spline of order k with knot sequence $\mathbf{t}$ is by definition a linear combination of the B-splines B_{ik}, i.e., a function of the form

$$f_{k,\infty} = \sum_i \beta_i B_{ik}; \qquad \beta_i \in \mathbb{R}, \tag{3}$$

which is a piecewise polynomial of degree $(k-1)$ with breakpoints t_i and which is $(k-1-\ell_i)$-times continuously differentiable at t_i. We highlight the bi-infinite knot sequence of the B-splines by noting $f_{k,\infty}$ instead of f_k as we assume until now that $\lim_{i\to\pm\infty} t_i = \pm\infty$. This assumption is convenient since it ensures that every $x \in \mathbb{R}$ is in the support of some B-spline.

From now on, without loss of generality, we fix the order $k > 1$ and the knot sequence $\mathbf{t}$. In this sense, we consider a finite sequence of coefficients β_i, for $i = 1, \dots, m$. We aim to control the shape of the function $f_I = \sum_{i=1}^m \beta_i B_{i,k}$ defined on an interval $I = [a, b] \subseteq \mathbb{R}$. To avoid any confusion in the sequel, the spline is denoted by f_I to highlight its domain of definition I. Regarding shape constrained approximation problem, the B-spline basis approach turn out to be quite useful; since the B-splines $B_{1,k}, \dots, B_{m,k}$ are positive functions, then one can model a positive function as $\sum_{i=1}^m \beta_i B_{i,k}$ where $\beta_i \geq 0$ for all i. Having a model