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Linear least squares problems involving fixed knots polynomial splines and their singularity study

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ABSTRACT

In this paper, we study a class of approximation problems appearing in data approximation and signal processing. The approximations are constructed as combinations of polynomial splines (piecewise polynomials) whose parameters are subject to optimisation and so called prototype functions whose choice is based on the application rather than optimisation. We investigate two types of models, namely Model 1 and Model 2 in order to analyse the singularity of their system matrices. The main difference between these two models is that in Model 2, the signal is shifted vertically (signal biasing) by a polynomial spline function. The corresponding optimisation problems can be formulated as Linear Least Squares Problems (LLSPs). If the system matrix is non-singular, then, the corresponding problem can be solved inexpensively and efficiently, while for singular cases, slower (but more robust) methods have to be used. To choose a better suited method for solving the corresponding LLSPs we have developed a singularity verification rule. In this paper, we develop necessary and sufficient conditions for non-singularity of Model 1 and sufficient conditions for non-singularity of Model 2. These conditions can be verified much faster than the direct singularity verification of the system matrices. Therefore, the algorithm efficiency can be improved by choosing a suitable method for solving the corresponding LLSPs.

1. Introduction

We consider two optimisation problems (Model 1 and Model 2) frequently appearing in approximation and signal processing. The signal approximations are constructed as products of two functions: one of them is a polynomial spline (piecewise polynomial) and another one is a prototype (also called basis) function, defined by the application. Common examples of prototype functions are sine and cosine functions. In Model 1, the wave oscillates around “zero level” while Model 2 admits a vertical shift (signal biasing). We model this shift as another polynomial spline.

The choice of polynomial splines is due to the fact that these functions combine the simplicity of polynomials and the flexibility, which is achieved by switching from one polynomial to another. Therefore, on the one hand, the corresponding optimisation problems can be solved efficiently and, on the other hand, the approximation inaccuracy (evaluated as the sum of the corresponding deviation squares) is low.

Model 1 and Model 2 are formulated as Linear Least Squares Problems (LLSPs). There are a variety of methods to solve such problems [1–3]. If it is known that the system matrix is non-singular, then, the most popular approach for solving the

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corresponding LLSP is based on the direct solving of the normal equations (unique solution for non-singular systems). This method is very efficient (fast and accurate) when working with non-singular matrices. If the matrix is singular, one needs to apply more robust methods, for example, QR decomposition or Singular Value Decomposition (SVD). These methods are much more computationally expensive.

In most applications, the number of columns of the corresponding system matrix is lower than the number of rows. Therefore, for singularity verification one needs to verify that the number of linearly independent rows is the same as the number of columns.

We use truncated power basis functions to define splines. Another way to construct basis functions is through B-splines. B-splines have several computational advantages when running numerical experiments (have smallest possible support, see [4]). However, truncated power functions are very common when theoretical properties of the models are the objectives (see [4]).

The reminder of this paper is organised as follows. In Section 2.2, we formulate the optimisation problems (both models). In Section 3, we develop necessary and sufficient conditions for non-singularity verification of Model 1, sufficient non-singularity conditions and sufficient singularity conditions for Model 2 and leave some situations undefined (remain open, listed in our future research directions). In Section 4, we provide two detailed examples from signal processing to demonstrate how our conditions can be applied. In Section 5, we summarise the results and indicate further research directions.

2. Approximation models

In this section, we formally introduce polynomial splines and explain why these functions are used in our models. Then, we formulate the models as mathematical programming problems, demonstrate that these problems are LLSPs and explain how these problems can be solved.

2.1. Polynomial splines

A polynomial spline is a piecewise polynomial. The points where the polynomial pieces join each other called spline knots. Polynomial splines combine the simplicity of polynomials and an additional flexibility property that enables them to change abruptly at the points of switching from one polynomial to another (spline knots). These attributes are essential since, on the one hand, the corresponding optimisation problems are relatively inexpensive to solve and, on the other hand, the obtained approximations are accurate enough for reflecting the essential characteristics of the original signal (raw data). Therefore, polynomial splines are commonly used in approximation problems [4–6].

There are many ways to construct polynomial splines. One possibility is through a truncated power function [4]:

$$S(\mathbf{x}, \boldsymbol{\tau}, t) = x_0 + \sum_{j=1}^{m} x_{1j} t^j + \sum_{l=2}^{n} \sum_{j=1}^{m} x_{lj} ((t - \tau_{l-1})_+)^j, \quad (1)$$

where m is the spline degree, n is the number of subintervals, N is the number of recordings in a time segment $[t_1, t_N]$ when the original signal is recorded, $\mathbf{x} = (x_0, x_{11}, \ldots, x_{mn}) \in \mathbb{R}^{mn+1}$ are the spline parameters and $\boldsymbol{\tau} = (\tau_1, \ldots, \tau_{n-1})$ are the spline knots such that

$$t_1 \le \tau_1 \le \tau_2 \le \cdots \le t_N.$$

In some cases, the border points $\tau_0 = t_1$ and $\tau_n = t_N$ are also considered as knots. Furthermore, for simplicity, we refer to segments $[\tau_0, \tau_n]$ as intervals and to subsegments $[\tau_{i-1}, \tau_i], i = 1, 2, \ldots, n$ as subintervals. The truncated power function is

$$(t - \tau_{l-1})_+ = \max\{0, (t - \tau_{l-1})\} = \begin{cases} t - \tau_{l-1}, & \text{if} \quad t > \tau_{l-1}, \\ 0, & \text{if} \quad t \le \tau_{l-1}, \end{cases} \quad (2)$$

note that this presentation implies that the polynomial splines are continuous. This is achieved by omitting the constant terms in the polynomial presentations for all the subintervals starting from the second one. In general, polynomial splines can be discontinuous at their knots [4]. However, we only consider continuous polynomial splines.

The spline knots can be free or fixed. If the knots are free, then they are considered as additional variables in the corresponding optimisation problem and thus, $\mathbf{x} = (x_0, x_{11}, \ldots, x_{nm}, \boldsymbol{\tau})$. In this case, the corresponding optimisation problem becomes more complex [4,7–10]. In particular, it becomes non-convex. Generally, it is much easier to solve a higher dimension fixed knots problem (with a considerably larger number of subintervals) than a free knots one.

In most applications, we have been working with the signal that is recorded at the same sampling frequency (for example, 100 Hz means 100 recordings per second). The knots split the original interval into subintervals and a simple equidistant knots distribution is used. In this case,

$$\tau_{l-1} = t_0 + (t_N/n)(l-1), \quad l = 2, \ldots, n. \quad (3)$$

In this situation, each subinterval contains the same number of signal recordings. However, in some applications different number of recordings per subinterval can be used. This flexibility is incorporated in the singularity conditions developed further in this paper.