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SIMULATION METAMODEL ESTIMAITON WITH PENALIZED B-SPLINES: A SECOND-ORDER CONE PROGRAMMING APPROACH

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ABSTRACT

This paper approximates simulation models by B-splines with a penalty on high-order finite differences of the coefficients of adjacent B-splines. The penalty prevents overfitting. The simulation output is assumed to be nonnegative. The nonnegative spline simulation metamodel is casted as a second-order cone programming problem, which can be solved efficiently by modern optimization techniques. The method is implemented in MATLAB.

1 NONNEGATIVE SPLINE METAMODEL

A simulation model can be represented as a function:

$$y = f(x), \tag{1}$$

where x represents the input and y is the response. For complex simulation models, metamodels are often constructed to approximate the input-output functions by simpler functions. Parametric polynomial response surface approximation is the most popular technique for building metamodels (Barton 1998), where the simulation models are approximated by polynomials.

By Weierstrass approximation theorem, every continuous function can be uniformly approximated as closely as desired by a polynomial. Polynomials are easy to compute and have continuous derivatives of all orders. On the other hand, polynomials are inflexible: their values on a complex plane are determined by an arbitrarily small set; they oscillate increasingly with the increase in the order of the polynomials, while high-order is required for suitable accuracy in approximation. A polynomial fits data nicely near one data point a may display repulsive features at parts of the curve not close to a.

Spline metamodels (smooth piecewise polynomials) overcome the inflexibility of polynomial metamodels. In practice, B-Splines are widely used in approximation, as there are good properties associated with B-splines. Particularly, compared with representations by splines in truncated power basis—defined as $\{x^j | j = 0, \dots, d\} \cup \{(x-t_i)_+^d | (i = 1, \dots n)\}$ for knot sequence $(t_i)_{i=1}^n$, B-spline representations are relatively well-conditioned and involve fewer basis functions computationally. Let B_{ik} denote the ith (normalized) B-spline of order k (degree $<$ k) for the knot sequence $\mathbf{t} \equiv (t_i)_{i=1}^n$. The B-Spline metamodel for the simulation model (1) is $y = \sum_{j=1}^n \alpha_j B_{jk}(x)$, where α_j's are parameters commonly determined by the least squares methods for m data points $(x_i; y_i)_{i=1}^m$ is $\min_\alpha \quad \sum_{i=1}^m \left[y_i - \sum_{j=1}^n \alpha_j B_{jk}(x_i)\right]^2$.

The simulation metamodel tool discussed in this paper is the P-spline least squares method (Eilers and Marx 1996). The P-spline least squares model combines B-splines with a penalty on high-order finite differences of the coefficients of adjacent B-splines. The penalty reduces the variation of the fitted curve caused by data error and prevents overfitting. Denote the parameter controlling the smoothness of the fit by λ. The least squares objective function (loss function) of estimating the parameter α for the simulation model on n B-splines of order four with a penalty on second-order differences of the B-spline coefficients based on m data points (x_i, y_i), i.e. the P-spline metamodel studied in this paper, is

$$\min_{\alpha} \quad \sum_{i=1}^{m} \left[y_i - \sum_{j=1}^{n} \alpha_j B_{j4}(x_i) \right]^2 + \lambda \sum_{j=3}^{n} (\alpha_j - 2\alpha_{j-1} + \alpha_{j-2})^2 . \tag{2}$$

In many applications, the model to be fitted is known or required to be nonnegative or above some threshold; for instance, simulations of prices, demand, sales, wages, amount of precipitation, probability mass, etc. Because of the noise or the tendency in the data, quite often, the fitted curve doesn't exhibit nonnegativitiy, even though it should be. To obtain a satisfiable and sometimes meaningful fitted curve, the nonnegativity constraint needs to be integrated into the metamodel. Since the B-spline basis functions are nonnegative, imposing positivity on B-spline coefficients or integrating B-splines with positive coefficients preserves positivity in the model. But this approach excludes some classes of positive splines and thus reduces the accuracy of the model. Because of the approximation and computational advantage of P-splines, this paper focuses on nonnegative P-spline approximation.

2 SECOND-ORDER CONE PROGRAMMING APPROACH

Let ',' denote concatenating vectors row-wise and ';' denote concatenating vectors column-wise; for instance, the adjoining of vectors x, y, and z can be represented as $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \left(x^\top, y^\top, z^\top\right) = (x; y; z)$. Index vectors in $\mathbb{R}^n$ from 0. A *second-order cone* (*quadratic cone*, *Lorentz cone*, or *ice-cream cone*) in $\mathbb{R}^n$ is the set

$$Q_n \equiv \left\{ x = (x_0; \bar{x}) \in \mathbb{R} \times \mathbb{R}^{n-1} : x_0 \geq \|\bar{x}\| \right\}.$$

We omit the subscript n if it is clear from the context. A vector $x \in Q$ is sometimes also represented as $x \succeq_Q 0$, because second-order cone induces a partial order.

Denote $x \equiv (x_1; \ldots; x_r)$. The second-order cone programming in standard form is

$$\begin{array}{ll} \min_x & \sum_{i=1}^r c_i^\top x_i \\ \text{subject to} & \sum_{i=1}^r A_i x_i = b \\ & x_i \succeq_Q 0, \ (i = 1, \ldots, r). \end{array}$$

Second-order cone programming has many applications. A solution to a second-order cone programming problem can be obtained approximately by interior point methods in polynomial time of the problem data size.

Nonnegative univariate polynomials are representable as positive semidefinite matrices (Nesterov 2000), which, in three dimensional cases, can be characterized by second-order cones. We reformulate the P-spline metamodel (2) as a second-order cone programming problem. Finally, we give a numerical example on simulating probability density distributions by the P-spline metamodel in MATLAB.

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