Algorithm XXXX: MQSI—Monotone Quintic Spline Interpolation

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MQSI is a Fortran 2003 subroutine for constructing monotone quintic spline interpolants to monotone data. Using sharp theoretical monotonicity constraints, first and second derivative estimates at data provided by a quadratic facet model are refined to produce a C^2 monotone interpolant. Algorithm and implementation details, complexity and sensitivity analyses, usage information, and a brief performance study are included.

Categories and Subject Descriptors: G.1.1 [**Numerical Analysis**]: Interpolation — Spline and piecewise polynomial interpolation; J.2 [**Computer Applications**]: Physical Science and Engineering — *Mathematics*; G.4 [**Mathematics of Computing**]: Mathematical Software

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1. INTRODUCTION

Many domains of science rely on smooth approximations to real-valued functions over a closed interval. Piecewise polynomial functions (splines) provide the smooth approximations for animation in graphics [Herman et al. 2015; Quint 2003], aesthetic structural support in architecture [Brennan 2020], efficient aerodynamic surfaces in automotive and aerospace engineering [Brennan 2020], prolonged effective operation of electric motors [Berglund et al 2009], and accurate nonparametric approximations in statistics [Knott 2012]. While polynomial interpolants and regressors apply broadly, splines are often a good choice because they can approximate globally complex functions while minimizing the local complexity of an approximation.

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It is often the case that the true underlying function or phenomenon being modeled has known properties e.g., convexity, positivity, various levels of continuity, or monotonicity. Given a reasonable amount of data, it quickly becomes difficult to achieve desirable properties in a single polynomial function. In general, the maintenance of function properties through interpolation/regression is referred to as *shape preserving* [Fritsch and Carlson 1980; Gregory 1985]. The specific properties the present algorithm will preserve in approximations are monotonicity and C^2 continuity. In addition to previously mentioned applications, these properties are crucially important in statistics to the approximation of a cumulative distribution function and subsequently the effective generation of random numbers from a specified distribution [Ramsay 1988]. A spline function with these properties could approximate a cumulative distribution function to a high level of accuracy with relatively few intervals. A twice continuously differentiable approximation to a cumulative distribution function (CDF) would produce a corresponding probability density function (PDF) that is continuously differentiable, which is desirable.

The currently available software for monotone piecewise polynomial interpolation includes quadratic [He and Shi 1998], cubic [Fritsch and Carlson 1980], and (with limited application) quartic [Wang and Tan 2004; Piah and Unsworth 2011; Yao and Nelson 2018] cases. In addition, a statistical method for bootstrapping the construction of an arbitrarily smooth monotone fit exists [Leitenstorfer and Tutz 2006], but the method does not take advantage of known analytic properties of quintic polynomials. The code by Fritsch [1982] for C^1 cubic spline interpolation is the predominantly utilized code for constructing monotone interpolants at present. Theory has been provided for the quintic case [Ulrich and Watson 1994; Heß and Schmidt 1994] and that theory was recently utilized in a proposed algorithm [Lux 2020] for monotone quintic spline construction, however no published mathematical software exists.

The importance of piecewise quintic interpolation over lower order approximations can be simply observed. In general, the order of a polynomial determines the number of function (and derivative) values it can interpolate, which in turn determines the growth rate of error away from interpolated values. This work constructs quintic splines in order to match the function value and two derivatives at either end of an interval, which requires six degrees of freedom in an interpolating polynomial. This work provides a Fortran 2003 subroutine `MQSI` based on the necessary and sufficient conditions in Ulrich and Watson [1994] for the construction of monotone quintic spline interpolants of monotone data.

The remainder of this paper is structured as follows: Section 2 provides the algorithms for constructing a C^2 monotone quintic spline interpolant to monotone data, Section 3 outlines the method of spline representation (B-spline basis) and evaluation, Section 4 analyzes the complexity and sensitivity of the algorithms in `MQSI`, and Section 5 presents an empirical performance study and some graphs of constructed interpolants.

2. MONOTONE QUINTIC INTERPOLATION

In order to construct a monotone quintic interpolating spline, two primary problems must be solved. First, reasonable derivative values at data points need to be estimated. Second, the estimated derivative values need to be modified to enforce monotonicity on all polynomial pieces.

Fritsch and Carlson [1980] originally proposed the use of central differences to estimate derivatives, however this often leads to extra and unnecessary *wiggles* in the spline when used to approximate second derivatives. In an attempt to capture the local shape of the data, this package uses a facet model [Haralick and Watson 1981] to estimate first and second derivatives at data. Rather than picking a local linear regressor with minimal residual, this work uses a quadratic facet model that selects the local quadratic interpolant with minimum magnitude curvature.

Algorithm 1: `QUADRATIC_FACET`$\big(X(1{:}n),\, Y(1{:}n),\, i\big)$

where X_j,$Y_j \in \mathbb{R}$ for $j = 1, \ldots, n$, and $1 < i < n$. Returns the slope and curvature at X_i of the local quadratic interpolant with minimum magnitude curvature.

`if` $\big((Y_i \approx Y_{i-1})$ `or` $(Y_i \approx Y_{i+1})\big)$ `then; return` $(0, 0)$
`else if` $\big((Y_{i+1} - Y_i)(Y_i - Y_{i-1}) < 0\big)$ `then`
  The point $(X_i,\, Y_i)$ is an extreme point. The quadratic with minimum curvature that has slope 0 at X_i will be returned.
  $f_1 :=$ interpolate $(X_{i-1}$,$Y_{i-1})$, $(X_i$,$Y_i)$, and $Df_1(X_i) = 0$.
  $f_2 :=$ interpolate $(X_i$,$Y_i)$, $(X_{i+1}$,$Y_{i+1})$, and $Df_2(X_i) = 0$.
  `if` $\big(|D^2 f_1| \le |D^2 f_2|\big)$ `then; return` $\big(Df_1,\, D^2 f_1\big)$
  `else;` `return` $\big(Df_2,\, D^2 f_2\big)$
  `endif`
`else`
  The point $(X_i,\, Y_i)$ is in a monotone segment of data. In the following, it is possible that either f_1 or f_3 does not exist because $i = 2$ or $i = n - 1$. In those cases, the minimum curvature among existing quadratics is chosen.
  $f_1 :=$ interpolate $(X_{i-2}$,$Y_{i-2})$, $(X_{i-1}$,$Y_{i-1})$, and $(X_i$,$Y_i)$.
  $f_2 :=$ interpolate $(X_{i-1}$,$Y_{i-1})$, $(X_i$,$Y_i)$, and $(X_{i+1}$,$Y_{i+1})$.
  $f_3 :=$ interpolate $(X_i$,$Y_i)$, $(X_{i+1}$,$Y_{i+1})$, and $(X_{i+2}$,$Y_{i+2})$.
  `if` $\big(|D^2 f_1| \le |D^2 f_2|, |D^2 f_3|\big)$ `then; return` $\big(Df_1,\, D^2 f_1\big)$
  `else if` $\big(|D^2 f_2| \le |D^2 f_1|, |D^2 f_3|\big)$ `then; return` $\big(Df_2,\, D^2 f_2\big)$
  `else;` `return` $\big(Df_3,\, D^2 f_3\big)$
  `endif`
`endif`

The estimated derivative values by the quadratic facet model are not guaranteed to produce monotone quintic polynomial segments. Ulrich and Watson [1994] established tight constraints on the monotonicity of a quintic polynomial piece, while deferring to Heß and Schmidt [1994] for a relevant simplified case. The following algorithm implements a sharp check for monotonicity by considering the nondecreasing case. The nonincreasing case is handled similarly.

Algorithm 2: IS_MONOTONE(x_0, x_1, f)

where x_0, $x_1 \in \mathbb{R}$, $x_0 < x_1$, and f is an order six polynomial defined by $f(x_0)$, $Df(x_0)$, $D^2f(x_0)$, $f(x_1)$, $Df(x_1)$, $D^2f(x_1)$. Returns TRUE if f is monotone increasing on $[x_0, x_1]$.

1. `if` $\big(f(x_0) \approx f(x_1)\big)$ `then`
2.   `return` $\big(0 = Df(x_0) = Df(x_1) = D^2f(x_0) = D^2f(x_1)\big)$
3. `endif`
4. `if` $\big(Df(x_0) < 0$ `or` $Df(x_1) < 0\big)$ `then; return FALSE; endif`
5. $w := x_1 - x_0$
6. $v := f(x_1) - f(x_0)$

The necessity of steps 2 and 4 follows directly from the fact that f is C^2. The following steps 7–13 coincide with a simplified condition for quintic monotonicity that reduces to one of cubic positivity studied by Schmidt and Heß [1988]. Given α, β, γ, and δ as defined by Schmidt and Heß, monotonicity results when $\alpha \geq 0$, $\delta \geq 0$, $\beta \geq \alpha - 2\sqrt{\alpha\delta}$, and $\gamma \geq \delta - 2\sqrt{\alpha\delta}$. Step 4 checked for $\delta < 0$, step 8 checks $\alpha < 0$, step 10 checks $\beta < \alpha - 2\sqrt{\alpha\delta}$, and step 11 checks $\gamma < \delta - 2\sqrt{\alpha\delta}$. If none of the monotonicity conditions were violated, then the order six piece is monotone and step 12 concludes.

7. `if` $\big(Df(x_0) \approx 0$ `or` $Df(x_1) \approx 0\big)$ `then`
8.   `if` $\big(D^2f(x_1)w > 4Df(x_1)$ `then; return FALSE; endif`
9. $t := 2\sqrt{Df(x_0)\,(4Df(x_1) - D^2f(x_1)w)}$
10.   `if` $\big(t + 3Df(x_0) + D^2f(x_0)w < 0\big)$ `then; return FALSE; endif`
11.   `if` $\Big(60v - w\big(24Df(x_0) + 32Df(x_1) - 2t + w(3D^2f(x_0) - 5D^2f(x_1))\big) < 0\Big)$
        `then; return FALSE; endif`
12.   `return TRUE`
13. `endif`

The following code considers the full quintic monotonicity case studied by Ulrich and Watson [1994]. Given τ_1, α, β, and γ as defined by Ulrich and Watson, a quintic piece is proven to be monotone when $\tau_1 > 0$ and $\alpha, \gamma \geq -(\beta + 2)/2$ when $\beta \leq 6$, and $\alpha, \gamma \geq -2\sqrt{\beta - 2}$ when $\beta > 6$. Step 12 checks $\tau_1 <= 0$, steps 18 and 19 determine monotonicity based on α, β, and γ.

12. `if` $\Big(w\big(2\sqrt{Df(x_0)Df(x_1)} - 3(Df(x_0) + Df(x_1))\big) - 24v \leq 0\Big)$
    `then; return FALSE; endif`
14. $t := \sqrt[3/4]{Df(x_0)Df(x_1)}$
15. $\alpha := (4Df(x_1) - D^2f(x_1)w)\sqrt{Df(x_0)}/t$
16. $\gamma := (4Df(x_0) - D^2f(x_0)w)\sqrt{Df(x_1)}/t$

```
β := (60v/w + 3(w(D²f(x₁) − D²f(x₀)) − 8(Df(x₀) + Df(x₁)))) / (2√(Df(x₀)Df(x₁)))
if (β ≤ 6) then; return min(α, γ) > −(β + 2)/2
else;            return min(α, γ) > −2√(β − 2)
endif
```

$$\beta := \frac{60v/w + 3\big(w(D^2f(x_1) - D^2f(x_0)) - 8(Df(x_0) + Df(x_1))\big)}{2\sqrt{Df(x_0)Df(x_1)}}$$

It is shown by Ulrich and Watson [1994] that when $0 = DQ(X_i) = DQ(X_{i+1}) = D^2Q(X_i) = D^2Q(X_{i+1})$, the quintic polynomial over $[X_i,\ X_{i+1}]$ is guaranteed to be monotone. Using this fact, the following algorithm shrinks initial derivative estimates until a monotone spline is achieved and outlines the core routine in the accompanying package.

Algorithm 3: `MQSI`$\big(X(1{:}n), Y(1{:}n)\big)$

where $(X_i, Y_i) \in (\mathbb{R}, \mathbb{R})$ $i = 1, \ldots, n$ are data points. Returns monotone quintic spline interpolant $Q(x)$ such that $Q(X_i) = Y_i$ and is monotone increasing (decreasing) on all intervals that Y_i is increasing (decreasing).

```
Approximate first and second derivatives at all Xᵢ with QUADRATIC_FACET.
do i = 1,... n − 1
    DQ(Xᵢ), D²Q(Xᵢ) := QUADRATIC_FACET(X, Y, i)
enddo
Identify and store all nonmonotone intervals in a queue.
do i = 1,... n − 1
    if not IS_MONOTONE(Xᵢ, Xᵢ₊₁, Q) then
        Add interval (Xᵢ, Xᵢ₊₁) to queue.
    endif
enddo
do while ( queue of nonmonotone intervals is nonempty )
    Shrink DQ and D²Q that border nonmonotone intervals.
    Identify and store all remaining nonmonotone intervals in queue.
enddo
```

Given the minimum curvature nature of the initial derivative estimates, it is desirable to make the smallest necessary changes to the initial interpolating spline Q while enforcing monotonicity. In practice a quasi-bisection search is used in place of solely shrinking DQ and D^2Q, adding an additional step that increases previously shrunken derivative values by a smaller step. As long as a step size schedule is set that allows the value 0 to be obtained in a fixed number of computations, this has no effect on computational complexity. Notably, Algorithm 3 is equally capable of ensuring a *piecewise* monotone quintic spline interpolates piecewise monotone data.

3. SPLINE REPRESENTATION

The monotone quintic spline interpolant is represented in terms of a B-spline basis. Two routines in this package are provided, `FIT_SPLINE` and `EVAL_SPLINE` that compute the B-spline coefficients to match the piecewise quintic polynomial values and derivatives, and evaluate a spline represented in terms of a B-spline basis. A Fortran 95 implementation of the B-spline recurrence relation evaluation code by C. deBoor for the value, derivatives, and integral of a B-spline is also provided.

4. COMPLEXITY AND SENSITIVITY

Both Algorithms 1 and 2 have $\mathcal{O}(1)$ runtime. Given a fixed schedule for shrinking derivative values, Algorithm 3 has a $\mathcal{O}(n)$ runtime for n data points. In execution, the majority of time is spent solving the banded linear system of equations for B-spline coefficients. The quadratic facet model produces a unique sensitivity to input perturbation, as small changes in input may cause data points to be associated with different local quadratic interpolants. While this makes the technique susceptible to random perturbations, it generally produces high quality monotone quintic splines and is preferred for that reason.

5. PERFORMANCE AND APPLICATIONS

This section contains graphs of sample `MQSI` results given various sources of data. Tables of computation times for various problems sizes are also provided.

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