

# Algorithm XXXX: MQSI—Monotone Quintic Spline Interpolation

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MQSI is a Fortran 2003 subroutine for constructing monotone quintic spline interpolants to univariate 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 univariate  $C^2$  monotone interpolant. Algorithm and implementation details, complexity and sensitivity analyses, usage information, a brief performance study, and comparisons with other spline approaches are included.

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General Terms: Algorithms, Monotonicity, Spline

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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 like 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.

## 1.1 Related Works

These similar works exist.

## 1.2 Available Software

The currently available software for monotone piecewise polynomial interpolation includes quadratic [He and Shi 1998, McAllister and Roulier 1981], 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. Conversely the work on quadratic shape preserving splines by Schumaker [1983] is widely utilized in theory for its conservation of both monotonicity and convexity, but no mathematical software is published.

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 software presented here represents the first published software package for producing  $C^2$  shape preserving splines. This work improves upon the algorithm presented by Lux et al. [2020] by refactoring computations for improved numerical stability, estimating minimum curvature derivatives at breakpoints with a quadratic facet model, and using a binary search to reduce the magnitude of the modifications made to initial derivative estimates when constructing a monotone spline interpolant.

### 1.3 Overview

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. Precisely, the problem is, given a strictly increasing sequence  $X_1 < X_2 < \dots < X_n$  of breakpoints with corresponding monotone increasing function values  $Y_1 \leq Y_2 \leq \dots \leq Y_n$ , find a  $C^2$  monotone increasing quintic spline  $Q(x)$  with the same breakpoints satisfying  $Q(X_i) = Y_i$  for  $1 \leq i \leq n$ . (`MQSI` actually does something slightly more general, producing  $Q(x)$  that is monotone increasing (decreasing) wherever the data is monotone increasing (decreasing).)

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 timing data 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. Modern shape-preserving spline implementations use a weighted harmonic mean to estimate derivative values at breakpoints [Moler 2008], however this method also yields approximations whose second derivative functions often have large  $L^2$  norm (approximations with large *wiggle*). In an attempt to capture the local shape of the data while minimizing wiggle, this package uses a facet model from image processing [Haralick and Watson 1981] to estimate first and second derivatives at breakpoints. Rather than picking a local linear or quadratic fit with minimal residual, this work uses a quadratic facet model that selects the local quadratic interpolant with minimum magnitude curvature.

**Algorithm 1:** `QUADRATIC_FACET`( $X(1:n), Y(1:n), i$ )

where  $X_j, Y_j \in \mathbb{R}$  for  $j = 1, \dots, n$ ,  $1 \leq i \leq n$ , and  $n \geq 3$ . Returns the slope and curvature at  $X_i$  of the local quadratic interpolant with minimum magnitude curvature.

```

if (( $i \neq 1 \wedge Y_i \approx Y_{i-1}$ ) or ( $i \neq n \wedge Y_i \approx Y_{i+1}$ )) then return (0, 0)
else if  $i = 1$  then
   $f_1 :=$  interpolant to  $(X_1, Y_1)$ ,  $(X_2, Y_2)$ , and  $(X_3, Y_3)$ .
  if ( $Df_1(X_1)(Y_2 - Y_1) < 0$ ) then return (0, 0)
  else return ( $Df_1(X_1), D^2f_1$ )

```

```

endif
else if  $i = n$  then
   $f_1 :=$  interpolant to  $(X_{n-2}, Y_{n-2})$ ,  $(X_{n-1}, Y_{n-1})$ , and  $(X_n, Y_n)$ .
  if  $(Df_1(X_n)(Y_n - Y_{n-1}) < 0)$  then return  $(0, 0)$ 
  else return  $(Df_1(X_n), D^2f_1)$ 
endif
else if  $(1 < i < n \wedge (Y_{i+1} - Y_i)(Y_i - Y_{i-1}) < 0)$  then
  The point  $(X_i, Y_i)$  is an extreme point. The quadratic with minimum magnitude
  curvature that has slope zero at  $X_i$  will be the facet chosen.
   $f_1 :=$  interpolant to  $(X_{i-1}, Y_{i-1})$ ,  $(X_i, Y_i)$ , and  $Df_1(X_i) = 0$ .
   $f_2 :=$  interpolant to  $(X_i, Y_i)$ ,  $(X_{i+1}, Y_{i+1})$ , and  $Df_2(X_i) = 0$ .
  if  $(|D^2f_1| \leq |D^2f_2|)$  then return  $(0, D^2f_1)$ 
  else return  $(0, D^2f_2)$ 
endif
else
  The point  $(X_i, Y_i)$  is in a monotone segment of data. In the following, it is
  possible that  $f_1$  or  $f_3$  do not exist because  $i \in \{2, n-1\}$ . In those cases, the
  minimum magnitude curvature among existing quadratics is chosen.
   $f_1 :=$  interpolant to  $(X_{i-2}, Y_{i-2})$ ,  $(X_{i-1}, Y_{i-1})$ , and  $(X_i, Y_i)$ .
   $f_2 :=$  interpolant to  $(X_{i-1}, Y_{i-1})$ ,  $(X_i, Y_i)$ , and  $(X_{i+1}, Y_{i+1})$ .
   $f_3 :=$  interpolant to  $(X_i, Y_i)$ ,  $(X_{i+1}, Y_{i+1})$ , and  $(X_{i+2}, Y_{i+2})$ .
  if  $(Df_1(X_i)(Y_i - Y_{i-1}) \geq 0 \wedge |D^2f_1| = \min\{|D^2f_1|, |D^2f_2|, |D^2f_3|\})$  then
    return  $(Df_1(X_i), D^2f_1)$ 
  else if  $(Df_2(X_i)(Y_i - Y_{i-1}) \geq 0 \wedge |D^2f_2| = \min\{|D^2f_1|, |D^2f_2|, |D^2f_3|\})$ 
    then return  $(Df_2(X_i), D^2f_2)$ 
  else if  $(Df_3(X_i)(Y_{i+1} - Y_i) \geq 0)$  then
    return  $(Df_3(X_i), D^2f_3)$ 
  else return  $(0, 0)$ 
endif
endif
endif

```

For constructing a quadratic interpolant in  $x$  over the interval  $[L, R]$ , the Chebyshev basis  $1, z, 2z^2 - 1$  is used, where  $z = \frac{x - (L+R)/2}{(R-L)/2}$ . 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( $x_0, x_1, f(x_0), Df(x_0), D^2f(x_0), f(x_1), Df(x_1), D^2f(x_1)$ )

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** ( $f(x_0) \approx f(x_1)$ ) **then**
2.     **return** ( $0 = Df(x_0) = Df(x_1) = D^2f(x_0) = D^2f(x_1)$ )
3. **endif**
4. **if** ( $Df(x_0) < 0$  or  $Df(x_1) < 0$ ) **then return FALSE endif**
5.  $w := x_1 - x_0$
6.  $z := f(x_1) - f(x_0)$
- The necessity of Steps 1–4 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  $\alpha, \beta, \gamma$ , and  $\delta$  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 are violated, then the order six piece is monotone and Step 12 concludes.
7. **if** ( $Df(x_0) \approx 0$  or  $Df(x_1) \approx 0$ ) **then**
8.     **if** ( $D^2f(x_1)w > 4Df(x_1)$ ) **then return FALSE endif**
9.      $t := 2\sqrt{Df(x_0)(4Df(x_1) - D^2f(x_1)w)}$
10.    **if** ( $t + 3Df(x_0) + D^2f(x_0)w < 0$ ) **then return FALSE endif**
11.    **if** ( $60z - w(24Df(x_0) + 32Df(x_1) - 2t + w(3D^2f(x_0) - 5D^2f(x_1))) < 0$ ) **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  $\tau_1, \alpha, \beta$ , and  $\gamma$  as defined by Ulrich and Watson, a quintic piece is proven to be monotone if and only if  $\tau_1 > 0$ , and  $\alpha, \gamma > -(\beta + 2)/2$  when  $\beta \leq 6$ , and  $\alpha, \gamma > -2\sqrt{\beta - 2}$  when  $\beta > 6$ . Step 14 checks  $\tau_1 \leq 0$ , Steps 19 and 20 determine monotonicity based on  $\alpha, \beta$ , and  $\gamma$ .
14. **if** ( $w(2\sqrt{Df(x_0)Df(x_1)} - 3(Df(x_0) + Df(x_1))) - 24z \leq 0$ ) **then return FALSE endif**
15.  $t := (Df(x_0)Df(x_1))^{3/4}$
16.  $\alpha := (4Df(x_1) - D^2f(x_1)w)\sqrt{Df(x_0)}/t$
17.  $\gamma := (4Df(x_0) - D^2f(x_0)w)\sqrt{Df(x_1)}/t$
18.  $\beta := \frac{60z/w + 3(w(D^2f(x_1) - D^2f(x_0)) - 8(Df(x_0) + Df(x_1)))}{2\sqrt{Df(x_0)Df(x_1)}}$
19. **if** ( $\beta \leq 6$ ) **then return** ( $\min\{\alpha, \gamma\} > -(\beta + 2)/2$ )
20. **else return** ( $\min\{\alpha, \gamma\} > -2\sqrt{\beta - 2}$ )
21. **endif**

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 (in magnitude) initial derivative estimates until a monotone spline is achieved and outlines the core routine in the accompanying package.

**Algorithm 3:** MQSI( $X(1:n), Y(1:n)$ )

where  $(X_i, Y_i) \in \mathbb{R} \times \mathbb{R}$ ,  $i = 1, \dots, n$  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 monotone increasing (decreasing).

Approximate first and second derivatives at  $X_i$  with QUADRATIC\_FACET.

for  $i := 1$  step 1 until  $n$  do

$(u_i, v_i) := \text{QUADRATIC\_FACET}(X, Y, i)$

enddo

Identify and store all intervals where  $Q$  is nonmonotone in a queue  $\mathcal{Q}$ .

for  $i := 1$  step 1 until  $n - 1$  do

    if not IS\_MONOTONE( $X_i, X_{i+1}, Y_i, u_i, v_i, Y_{i+1}, u_{i+1}, v_{i+1}$ ) then

        Add interval  $(X_i, X_{i+1})$  to queue  $\mathcal{Q}$ .

    endif

enddo

do while ( queue  $\mathcal{Q}$  of intervals is nonempty )

    Shrink (in magnitude)  $DQ$  (in  $u$ ) and  $D^2Q$  (in  $v$ ) that border intervals where  $Q$  is nonmonotone.

    Identify and store remaining intervals where  $Q$  is nonmonotone in queue  $\mathcal{Q}$ .

enddo

Construct and return a  $B$ -spline representation of  $Q(x)$ .

Since IS\_MONOTONE can handle both nondecreasing and nonincreasing simultaneously by taking into account the sign of  $z$ , Algorithm 3 produces  $Q(x)$  that is monotone increasing (decreasing) over exactly the same intervals that the data  $(X_i, Y_i)$  is monotone increasing (decreasing).

Given the minimum magnitude 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 binary search for the boundary of monotonicity is used in place of solely shrinking  $DQ$  and  $D^2Q$  at breakpoints adjoining *active* intervals: intervals over which  $Q$  is nonmonotone at least once during the search. The binary search considers a Boolean function  $B_i(s)$ , for  $0 \leq s \leq 1$ , that is true if the order six polynomial piece of  $Q(x)$  on  $[X_i, X_{i+1}]$  matching derivatives  $Q(X_i) = Y_i$ ,  $DQ(X_i) = s u_i$ ,  $D^2Q(X_i) = s v_i$  at  $X_i$ , and derivatives  $Q(X_{i+1}) = Y_{i+1}$ ,  $DQ(X_{i+1}) = s u_{i+1}$ ,  $D^2Q(X_{i+1}) = s v_{i+1}$  at  $X_{i+1}$  is monotone, and false otherwise. The binary search is only applied at those breakpoints adjoining intervals  $[X_i, X_{i+1}]$  over which  $Q$  is nonmonotone and hence  $B_i(1)$  is false. It is further assumed that there exists  $0 \leq s^* \leq 1$  such that  $B_i(s)$

is true for  $0 \leq s \leq s^*$  and false for some  $1 > s > s^*$ . Since the derivative conditions at interior breakpoints are shared by intervals left and right of the breakpoint, the binary search is performed at all breakpoints simultaneously. Specifically, the monotonicity of  $Q$  is checked on all active intervals in each step of the binary search to determine the next derivative modification at each breakpoint. The goal of this search is to converge on the boundary of the monotone region in the  $(\tau_1, \alpha, \beta, \gamma)$  space (described in Ulrich and Watson [1994]) for all intervals. This multiple-interval binary search allows the value zero to be obtained for all (first and second) derivative values in a fixed maximum number of computations, hence has no effect on computational complexity order. This binary search algorithm is outlined below.

**Algorithm 4:** `BINARY_SEARCH`( $X(1:n), Y(1:n), u(1:n), v(1:n)$ )

where  $(X_i, Y_i) \in \mathbb{R} \times \mathbb{R}$ ,  $i = 1, \dots, n$  are data points, and  $Q(x)$  is a quintic spline interpolant such that  $Q(X_i) = Y_i$ ,  $DQ(X_i) = u_i$ ,  $D^2Q(X_i) = v_i$ . Modifies derivative values ( $u$  and  $v$ ) of  $Q$  at data points to ensure `IS_MONOTONE` is true for all intervals defined by adjacent data points, given a desired precision  $\mu \in \mathbb{R}$ .  $\text{proj}(w, \text{int}(a, b))$  denotes the projection of  $w$  onto the closed interval with endpoints  $a$  and  $b$ .

Initialize the step size  $s$ , make a copy of data defining  $Q$ , and construct three queues necessary for the multiple-interval binary search.

```

s := 1
( $\hat{u}, \hat{v}$ ) := ( $u, v$ )
searching := TRUE
checking := empty queue for holding left indices of intervals
growing := empty queue for holding indices of data points
shrinking := empty queue for holding indices of data points
for  $i := 1$  step 1 until  $n - 1$  do
    if not IS_MONOTONE( $X_i, X_{i+1}, Y_i, u_i, v_i, Y_{i+1}, u_{i+1}, v_{i+1}$ ) then
        Add data indices  $i$  and  $i + 1$  to queue shrinking.
    endif
enddo
do while (searching or (shrinking is nonempty))
    Compute the step size  $s$  for this iteration of the search.
    if searching then  $s := \max\{\mu, s/2\}$  else  $s := 3s/2$  endif
    if ( $s = \mu$ ) then searching := FALSE; clear queue growing endif
    Increase in magnitude  $u_i$  and  $v_i$  for all data indices  $i$  in growing such that
    the points  $X_i$  are strictly adjoining intervals over which  $Q$  is monotone.
    for ( $i \in \text{growing}$ ) and ( $i \notin \text{shrinking}$ ) do
         $u_i := \text{proj}(u_i + s \hat{u}_i, \text{int}(0, \hat{u}_i))$ 
         $v_i := \text{proj}(v_i + s \hat{v}_i, \text{int}(0, \hat{v}_i))$ 
        Add data indices  $i - 1$  (if not 0) and  $i$  (if not  $n$ ) to queue checking.
    enddo
enddo

```

```

Decrease in magnitude  $u_i$  and  $v_i$  for all data indices  $i$  in shrinking and
ensure those data point indices are placed into growing when searching.
for  $i \in \text{shrinking}$  do
  If searching, then add index  $i$  to queue growing if not already present.
   $u_i := \text{proj}(u_i - s \hat{u}_i, \text{int}(0, \hat{u}_i))$ 
   $v_i := \text{proj}(v_i - s \hat{v}_i, \text{int}(0, \hat{v}_i))$ 
  Add data indices  $i - 1$  (if not 0) and  $i$  (if not  $n$ ) to queue checking.
enddo
Empty queue shrinking, then check all intervals left-indexed in queue
checking for monotonicity with IS_MONOTONE, placing data endpoint in-
dices of intervals over which  $Q$  is nonmonotone into queue shrinking.
Clear queue shrinking.
for  $i \in \text{checking}$  do
  if not IS_MONOTONE( $X_i, X_{i+1}, Y_i, u_i, v_i, Y_{i+1}, u_{i+1}, v_{i+1}$ ) then
    Add data indices  $i$  and  $i + 1$  to shrinking.
  endif
enddo
Clear queue checking.
enddo

```

In the subroutine MQSI,  $\mu = 2^{-26}$ , which results in 26 guaranteed search steps for all intervals that are initially nonmonotone. An additional 43 steps could be required to reduce a derivative magnitude to zero with step size growth rate of  $3/2$ . This can only happen when  $Q$  becomes nonmonotone on an interval for the first time while the step size equals  $\mu$ , but for which the only viable solution is a derivative value of zero. The maximum number of steps is due to the fact that  $\sum_{i=0}^{42} \mu(3/2)^i > 1$ . In total BINARY\_SEARCH search could require 69 steps.

### 3. SPLINE REPRESENTATION

The monotone quintic spline interpolant  $Q(x)$  is represented in terms of a B-spline basis. The routine FIT\_SPLINE in this package computes the B-spline coefficients  $\alpha_i$  of  $Q(x) = \sum_{i=1}^{3n} \alpha_i B_{i,6,t}(x)$  to match the piecewise quintic polynomial values and (first two) derivatives at the breakpoints  $X_i$ , where the spline order is six and the knot sequence  $t$  has the breakpoint multiplicities  $(6, 3, \dots, 3, 6)$ . The routine EVAL\_SPLINE evaluates a spline represented in terms of a B-spline basis. A Fortran 2003 implementation EVAL\_BSPLINE of the B-spline recurrence relation evaluation code by C. de Boor [1978] for the value, derivatives, and integral of a B-spline is also provided.

### 4. COMPLEXITY AND SENSITIVITY

Algorithms 1, 2, and 4 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 the time, still  $\mathcal{O}(n)$ , is spent solving the banded linear system of



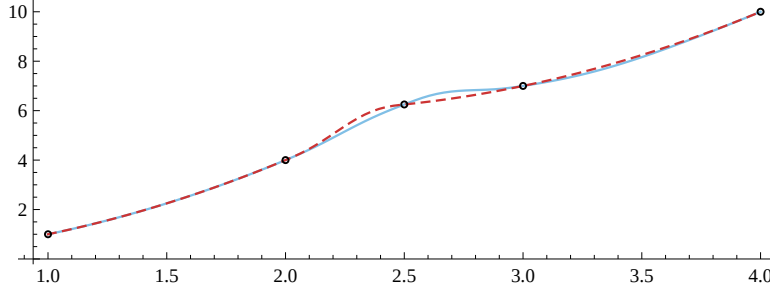


Fig. 1. A demonstration of the quadratic facet model's sensitivity to small data perturbations. This example is composed of two quadratic functions  $f_1(x)=x^2$  over points  $\{1, 2, 5/2\}$ , and  $f_2(x)=(x-2)^2+6$  over points  $\{5/2, 3, 4\}$ . Notably,  $f_1(5/2)=f_2(5/2)$  and  $f_1, f_2$  have the same curvature. Given the exact five data points seen above, the quadratic facet model produces the slope seen in the solid blue line at  $x=5/2$ . However, by subtracting the value of  $f_3 = \epsilon(x-2)^2$  from points at  $x=3, 4$ , where  $\epsilon$  is the machine precision ( $2^{-52}$  for an IEEE 64-bit real), the quadratic facet model produces the slope seen in the dashed red line at  $x=5/2$ . This is the nature of a facet model and a side effect of associating data with local facets.

equations for the B-spline coefficients. Thus for  $n$  data points, the overall execution time is  $\mathcal{O}(n)$ .

The quadratic facet model produces a unique sensitivity to input perturbation, as small changes in input may cause different quadratic facets to be associated with a breakpoint, and thus different initial derivative estimates can be produced. This phenomenon is depicted in Figure 1. Despite this sensitivity, the quadratic facet model is still preferred because it exactly captures local linear and quadratic behavior while empirically producing final approximations with less wiggle ( $L^2$  norm of the second derivative) than other methods. A weighted harmonic mean estimate of first derivatives may be more accurate when the underlying function changes at a rate greater than a quadratic, but that method increases the second derivative sensitivity to small perturbations in data and empirically results in quintic splines with greater wiggle.

The binary search for a point on the monotone boundary in  $(\tau_1, \alpha, \beta, \gamma)$  space is performed because it results in monotone quintic spline interpolants with derivative values that are absolutely nearer to initial estimates than a search that strictly shrinks derivative values. Given that the initial derivative estimates have desirable properties (capture low-order phenomena and are low wiggle), this search results in an approximation that is both monotone and has derivative values similar to the initial estimates.

## 5. PERFORMANCE AND APPLICATIONS

This section contains graphs of sample MQSI results given various data configurations. Execution times for Algorithms 1 and 4 are given; the total execution time of MQSI is utterly dominated by the time for a banded linear system solve computing the  $3n$  B-spline coefficients, which is  $\mathcal{O}(n)$ . The files `sample_main.f90` and `sample_main.dat` accompanying the subroutine MQSI illustrate Fortran 2003

subroutine usage with optional arguments and data points from a file. Compilation instructions and the full package contents are specified in the `README` file.

Throughout, all visuals have points that are stylized by local monotonicity conditions. Blue circles denote extreme points, purple squares are in *flat* regions with no change in function value, red down triangles are monotone decreasing, and green up triangles are monotone increasing.

Figure 2 offers examples of the interpolating splines produced by the routine `MQSI` on various hand-crafted sets of data. These same data sets are used for testing local installations in the provided program `test_all.f90`. Notice that the quadratic facet model perfectly captures the local linear segments of data in the piecewise polynomial test for Figure 2. Figure 3 depicts an approximation of a cumulative distribution function made by `MQSI` on a computer systems application by Cameron et al. [2019] that studies the distribution of throughput (in bytes per second) when reading files from a storage medium. Figure 4 provides a particularly difficult monotone interpolation challenge using randomly generated monotone data.

On a computer running MacOS 10.15.5 with a 2 GHz Intel Core i5 CPU, the quadratic facet (Algorithm 1) takes roughly one microsecond ( $10^{-6}$  seconds) per breakpoint, while the binary search (Algorithm 4) takes roughly four microseconds per breakpoint; these times were generated from 100 repeated trials averaged over 14 different testing functions. The vast majority of execution time is spent solving the banded linear system of equations in the routine `FIT_SPLINE` for the  $B$ -spline coefficients. For large problems ( $n > 100$ ) it would be faster to construct splines over intervals independently (each interval requiring a  $6 \times 6$  linear system to be solved for a local  $B$ -spline representation, or the construction of the Newton form of the interpolating polynomial from the derivative information at the endpoints), however the single linear system is chosen here for the decreased redundancy in the spline description. An optional argument to `MQSI` returns the derivative information at the breakpoints (interval endpoints) for the Newton form of the interpolating polynomial (piece of  $Q(x)$ ) over each interval.

Comparisons between this work and lower order methods are problematic, especially with sparse data. For exact data from smooth functions, comparing derivative values, higher order methods always win (all other things being equal) as the data density increases. For sparse or synthetic data, what constitutes a better fit is either subjective or dependent on the specific problem. If an application demands  $C^2$  continuity and monotonicity, the target of `MQSI`, then this package provides such interpolants while no existing published spline software suffices.

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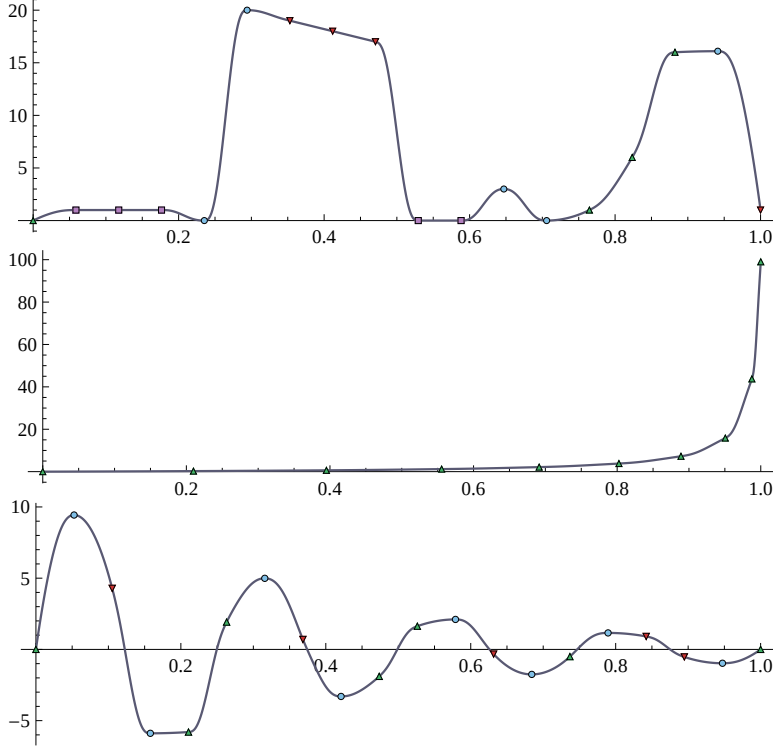


Fig. 2. MQSI results for three of the functions in the included test suite. The *piecewise polynomial* function (top) shows the interpolant capturing local linear segments, local flats, and alternating extreme points. The *large tangent* (middle) problem demonstrates outcomes on rapidly changing segments of data. The *signal decay* (bottom) alternates between extreme values of steadily decreasing magnitude.

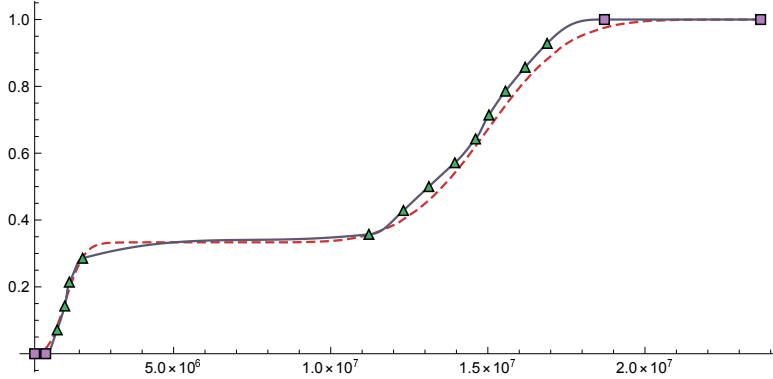


Fig. 3. MQSI results when approximating the cumulative distribution function of system throughput (bytes per second) data for a computer with a 3.2 GHz CPU performing file read operations from Cameron et al. [2019]. The empirical distribution of 30 thousand throughput values is shown in the red dashed line, while the solid line with stylized markers denotes the approximation made with MQSI given equally spaced empirical distribution points from a sample of size 100.

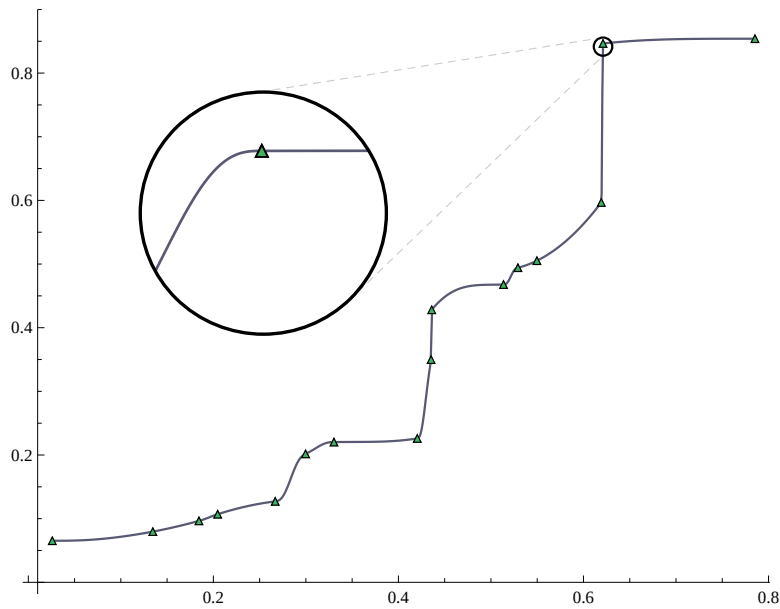


Fig. 4. The *random monotone* test poses a particularly challenging problem with large variations in slope. Notice that despite drastic shifts in slope, the resulting monotone quintic spline interpolant provides smooth and reasonable estimates to function values between data.

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