Algorithm for Constructing Piecewise Quintic Monotone Interpolating Splines

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Forward

When provided data that has no assigned first and second derivative values, the derivative data is filled by a linear fit of neighboring data points. End points are set to be the slope between the end and its nearest neighbor.

The method for finding the transition point of a boolean function on a line is the Golden Section search. This will be referred to in pseudo code as `line_search(`$g,\ a,\ b$`)` where $a,\, b \in S$ for S closed under convex combination, $g : S \to \{0, 1\}$ is a boolean function, and $g(b) = 1$. If $g(a) = 1$ then a is returned, otherwise the smallest $c \in [0, 1]$ such that $g\big(a(1 - c) + cb\big) = 1$ is returned.

After assigning function values and derivative values, an interpolating function is constructed from a quintic B-spline basis.

1 Verifying Monotonicity of a Quintic Polynomial

Let f be a quintic polynomial over a closed interval $[x_0, x_1] \subset \mathbb{R}$. Now f is uniquely defined by the evaluation tuples $\big(x_0,\ f(x_0),\ f'(x_0),\ f''(x_0)\big)$ and $\big(x_1,\ f(x_1),\ f'(x_1),\ f''(x_1)\big)$. Assume without loss of generality that $f(x_0) < f(x_1)$, where the case of monotonic decreasing f would consider the negated the function values. The following algorithm will determine whether or not f is monotone increasing on the interval $[x_0, x_1]$.

Algorithm 1a: `is_monotone`

0: `if` $\big(f'(x_0) = 0$ `or` $f'(x_1) = 0\big)$ `return is_monotone_simplified`

1: `if` $\big(f'(x_0) < 0$ `or` $f'(x_1) < 0\big)$ `return FALSE`

This can be seen clearly from the fact that f is analytic; there will exist some nonempty ball about x_0 or x_1 on which f is decreasing.

2: $A = f'(x_0)\frac{x_1 - x_0}{f(x_1) - f(x_0)}$

3: $B = f'(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)}$

The variables A and B correspond directly to the theoretical foundation for positive quartic polynomials established in [3], first defined after equation 18.

8: $\gamma_0 = 4\frac{f'(x_0)}{f'(x_1)}(B/A)^{3/4}$
9: $\gamma_1 = \frac{x_1-x_0}{f'(x_1)}(B/A)^{3/4}$
4: $\alpha_0 = 4(B/A)^{1/4}$
5: $\alpha_1 = -\frac{x_1-x_0}{f'(x_1)}(B/A)^{1/4}$
6: $\beta_0 = 30 - \frac{12\left(f'(x_0)+f'(x_1)\right)(x_1-x_0)}{\left(f(x_1)-f(x_0)\right)\sqrt{A}\sqrt{B}}$
7: $\beta_1 = \frac{-3(x_1-x_0)^2}{2\left(f(x_1)-f(x_0)\right)\sqrt{A}\sqrt{B}}$

The γ, α, and β terms with subscripts 0 and 1 are algebraic reductions of the simplified conditions for satisfying Theorem 2 in [3] (equation 16). These terms with subscripts 0 and 1 give the computation of α, β, and γ the form seen in lines 10-12 below.

10: $\gamma = \gamma_0 + \gamma_1 f''(x_0)$
11: $\alpha = \alpha_0 + \alpha_1 f''(x_1)$
12: $\beta = \beta_0 + \beta_1\left(f''(x_0) - f''(x_1)\right)$
13: `if` $(\beta \leq 6)$ `then return` $\alpha > -(\beta+2)/2$
14: `else return` $\gamma > -2\sqrt{\beta-2}$

Given the same initial conditions there are special circumstances which allow for the usage of simpler monotonicity conditions. In this case, consider when the quintic function has either $f'(x_0) = 0$ or $f'(x_1) = 0$, which can be tested for monotonicity via the cubic positivity conditions established by [2].

Algorithm 1b: `is_monotone_simplified`

0: $\alpha = 30 - \frac{(x_1-x_0)\left(14f'(x_0)+16f'(x_1)-\left(f''(x_1)-f''(x_0)\right)(x_1-x_0)\right)}{2\left(f(x_1)-f(x_0)\right)}$
1: $\beta = 30 - \frac{(x_1-x_0)\left(2f'(x_0)+24f'(x_1)-\left(f''(x_0)+3f''(x_1)\right)(x_1-x_0)\right)}{2\left(f(x_1)-f(x_0)\right)}$
2: $\gamma = \frac{(x_1-x_0)\left(7f'(x_0)+f''(x_0)(x_1-x_0)\right)}{f(x_1)-f(x_0)}$
3: $\delta = \frac{f'(x_0)(x_1-x_0)}{f(x_1)-f(x_0)}$

The variables above are algebraic expansions of the coefficients for the cubic derivative function in [2].

4: `if` $\left(\min(\alpha,\delta) < 0\right)$ `return FALSE`
5: `else if` $\left(\beta < \alpha - 2\sqrt{\alpha\delta}\right)$ `return FALSE`
6: `else if` $\left(\gamma < \delta - 2\sqrt{\alpha\delta}\right)$ `return FALSE`
7: `else return TRUE`

Next the modification of a quintic spline to enforce monotonicity will be discussed.

2 Enforcing Monotonicity of a Quintic Polynomial

Algorithm 2a: `make_monotone`

0: $\texttt{if}\ \big(f(x_1) - f(x_0) = 0\big)\ \ \texttt{return}\ \ f'(x_0) = f'(x_1) = f''(x_0) = f''(x_1) = 0$

1: $f'(x_0) = \texttt{median}\big(0, f'(x_0), 14\frac{f(x_1)-f(x_0)}{x_1-x_0}\big)$

2: $f'(x_1) = \texttt{median}\big(0, f'(x_1), 14\frac{f(x_1)-f(x_0)}{x_1-x_0}\big)$

This selection of value for $f'(x_0)$ and $f'(x_1)$ is suggested by [3] (originally from [1]), and quickly enforces upper and lower bounds on derivative values to allow for quintic monotonicity.

3: $A = f'(x_0)\frac{x_1-x_0}{f(x_1)-f(x_0)}$

4: $B = f'(x_1)\frac{x_1-x_0}{f(x_1)-f(x_0)}$

5: $\texttt{if}\ AB \leq 0\ \texttt{return make\_monotone\_simplified}$

6: $\texttt{if}\ \big(\texttt{max}(A, B) > 6\big)$
$f'(x_0) = 6f'(x_0)\ /\ \texttt{max}(A, B)$
$f'(x_1) = 6f'(x_1)\ /\ \texttt{max}(A, B)$

This simple box bound ensures that (A, B) remains within a viable region of monotonicity (satisfying Theorem 4, seen in Fig. 6 of [3]).

7: $\hat{f}''(x_0) = -\sqrt{A}\big(7\sqrt{A} + 3\sqrt{B}\big)\frac{f(x_1)-f(x_0)}{(x_1-x_0)^2}$
$\hat{f}''(x_1) = \sqrt{B}\big(3\sqrt{A} + 7\sqrt{B}\big)\frac{f(x_1)-f(x_0)}{(x_1-x_0)^2}$

This selection of values of f'' is guaranteed to satisfy Theorem 4 from [3] and is chosen because it is (reasonably) the average of the two endpoints of the interval of monotonicity for second derivative values.

8: $\eta = \big(f''(x_0), f''(x_1)\big)$
$\eta_0 = \big(\hat{f}''(x_0), f''(x_1)\big)$
$f''(x_0), f''(x_1) = \texttt{line\_search}\big(\texttt{is\_monotone},\ \eta,\ \eta_0\big)$

Similar to the simplified check for monotonicity, when the derivative value at one endpoint of the interval is 0, a simplified set of steps can be taken to enforce monotonicity.

Algorithm 2b: `make_monotone_simplified`

0: $f''(x_0) = \texttt{max}\left(f''(x_0), \frac{-6f'(x_0)}{x_1-x_0}\right)$

Considering the α, γ, β, and δ defined in [2], this first step enforces $\gamma > \delta$. It is already guaranteed that $\delta = \frac{f'(x_0)(x_1-x_0)}{f(x_1)-f(x_0)} > 0$. Only two conditions remain to guarantee monotonicity.

1: $f''(x_1) = \max\left(f''(x_1), f''(x_0) + \frac{14f'(x_0)+16f'(x_1)+60(f(x_1)-f(x_0))/(x_1-x_0)}{x_1-x_0}\right)$

Now it is guaranteed that $\alpha \geq 0$.

2: $f''(x_1) = \max\left(f''(x_1), 6f'(x_0) - 4f'(x_1) - f''(x_0)\right)$

Lastly, this guarantees that $\beta \geq \alpha$. All conditions are met to satisfy proposition 2 of [2] and ensure monotonicity.

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3 Constructing a Piecewise Quintic Monotone Spline

Finally, the construction of a full piecewise quintic spline is outlined using the above algorithms.

Let $f : \mathbb{R} \to \mathbb{R}$ be a function in $\mathcal{C}^2$. Proceed given evaluation tuples $\big(x_i, f(x_i), f'(x_i), f''(x_i)\big)$ for $i = 0, \ldots, N$ such that $x_i < x_{i+1}$ and (without loss of generality) $f(x_i) \leq f(x_{i+1})$ for $i = 1, \ldots, N-1$.

Algorithm 3: `monotone_spline`

- Compute

References

[1] Huynh, H.T.: Accurate monotone cubic interpolation. SIAM Journal on Numerical Analysis **30**(1), 57–100 (1993)

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[3] Ulrich, G., Watson, L.T.: Positivity conditions for quartic polynomials. SIAM Journal on Scientific Computing **15**(3), 528–544 (1994)