Cubic Spline
Root Finding

Charles O'Neill

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A need exists for determining a solution to the following cubic spline

$$f(x) = a_i (x - x_i)^3 + b_i (x - x_i)^3 + c_i (x - x_i)^3 + d_i = V$$

The solution is the real root of a cubic spline

$$f(x) = a_i (x - x_i)^3 + b_i (x - x_i)^3 + c_i (x - x_i)^3 + (d_i - V) = 0$$

Part I
Analytical Solution

One-step analytical solutions exist for a cubic polynomial[1]. The history behind this solution is quite interesting and only a few hundred years old. Given an arbitrary cubic polynomial,

$$f(x) = a_i (x - x_i)^3 + b_i (x - x_i)^3 + c_i (x - x_i)^3 + d_i$$

the polynomial is non-dimensionalized by a_i to give

$$F(x) = (x - x_i)^3 + a_2 (x - x_i)^3 + a_1 (x - x_i)^3 + a_0$$

Three intermediate terms are calculated

$$Q = \frac{3a_1 - a_2^2}{9}$$

$$R = \frac{9a_2 a_1 - 27a_0 - 2a_2^3}{54}$$

$$\theta = \arccos\left(\frac{R}{\sqrt{-Q^3}}\right)$$

[1] See `http://mathworld.wolfram.com/CubicFormula.html`

The real solutions are

$$z_1 = 2\sqrt{-Q}\cos\left(\frac{\theta}{3}\right) - \frac{a_2}{3}$$

$$z_2 = 2\sqrt{-Q}\cos\left(\frac{\theta + 2\pi}{3}\right) - \frac{a_2}{3}$$

$$z_3 = 2\sqrt{-Q}\cos\left(\frac{\theta + 4\pi}{3}\right) - \frac{a_2}{3}$$

The roots are selected from the z value calculated above

$$x = \{z_1, z_2, z_3\}$$

0.1 Issues

There are several issues associated with this method.

- Out of Range: θ will not exist if the search value is outside the range of possible function values $f(x)$.
- Picking the correct solution: multiple solutions may exist, you must ensure the calculated x lies in the correct domain.

Part II
Numerical Methods

Quick comments:

- Suggested to avoid Newton-Raphson iterative root finding since division by a near zero derivative causes problems. N-R is however excellent for polishing a root after a prior routine gets "close".
- Simple bisection would likely be the most robust especially if a human can identify a known upper and lower bound.

1 Bisection Root Finding

Bisection Iteration for a set of spline curves

$$f(x) = a_i\hat{x}^3 + b_i\hat{x}^2 + c_i\hat{x} + d_i$$

with a constraint

$$f(x) = V$$

gives a residual equation

$$g(x) = f(x) - V$$

1.1 Search for $f(x) = 0.141531$

Start with an initial bound of $x_b = \{0, 1000\}$with the values

$$g(0) = -0.04937$$

$$g(1000) = 0.0567623$$

Iteration 1 Pick a new point at the midpoint of the boundary

$$x = 500$$

with the value

$$g(500) = 0.0257831$$

Since $g(1000)$ and $g(500)$ are both positive, the right hand side boundary is reduced to $x = 500$. Thus the new boundary is $x_b = \{0, 500\}$.

Iteration 2 Pick a new point at the midpoint of the boundary

$$x = 250$$

with the value

$$g(250) = -0.02103$$

Since $g(0)$ and $g(250)$ are both negative, the left hand side boundary is reduced to $x = 250$. Thus the new boundary is $x_b = \{250, 500\}$.

Iteration 3 Pick a new point at the midpoint of the boundary

$$x = 375$$

with the value

$$g(375) = 0.0037887$$

Thus the new boundary is $x_b = \{250, 375\}$.

Iteration 4 Pick a new point at the midpoint of the boundary

$$x = 312.5$$

with the value

$$g(312.5) = -0.00876$$

Thus the new boundary is $x_b = \{312.5, 375\}$.

Bisection converges *slowly* but at a bounded rate!

1.2 Search for $f(x) = 0.16721$

Start with an initial bound of $x_b = \{0, 1000\}$with the values

$$g(0) = -0.075$$

$$g(1000) = 0.03108$$

Iteration 1 Pick a new point at the midpoint of the boundary

$$x = 500$$

with the value

$$g(500) = 0.0001041$$

Since $g(1000)$ and $g(500)$ are both positive, the right hand side boundary is reduced to $x = 500$. Thus the new boundary is $x_b = \{0, 500\}$.

Iteration 2 Pick a new point at the midpoint of the boundary

$$x = 250$$

with the value

$$g(500) = -0.046$$

Since $g(0)$ and $g(250)$ are both negative, the left hand side boundary is reduced to $x = 250$. Thus the new boundary is $x_b = \{250, 500\}$.

Iteration 3 Pick a new point at the midpoint of the boundary

$$x = 375$$

Since and $g(375)$ and $g(250)$ are both negative, the left hand side boundary is reduced to $x = 375$. Thus the new boundary is $x_b = \{375, 500\}$.

Since $V = 0.16721$ is so close to the value at $x = 500$, almost all boundary reduction will be on the left hand side.

2 Newton-Raphson Root Finding

Newton Raphson Iteration for a set of spline curves

The definition of N-R for a given function f and desired value V is

$$x_{new} = x_{old} - \frac{f(x_{old}) - V}{f'(x_{old})}$$

where

$$\hat{x} = x - x_i$$

$$f(x) = a_i\hat{x}^3 + b_i\hat{x}^2 + c_i\hat{x} + d_i$$

$$f'(x) = 3a_i\hat{x}^2 + 2b_i\hat{x} + c_i$$

2.1 Search for $f(x) = 0.141531$

Start with an initial guess of $x = 500$ at the edge of segment 2 and 3

Iteration 1

$$f(500) = 0.1673141$$

$$f'(500) = 0.000143$$

$$x_{new} = 500 - \frac{0.1673141 - 0.141531}{0.000143} = 320.0$$

Iteration 2

$$f(320.0) = 0.1342735$$

$$f'(320.0) = 0.000202$$

$$x_{new} = 320.0 - \frac{0.1342735 - 0.141531}{0.000202} = 355.99$$

Iteration 3

$$f(355.99) = 0.1415281$$

$$f'(355.99) = 0.000201$$

$$x_{new} = 320.0 - \frac{0.1415281 - 0.141531}{0.000201} = 356$$

This matches a manual search of:

$$f(356) = 0.141531$$

2.2 Search for $f(x) = 0.167314$

Start with an initial guess of $x = 100$ at the edge of segment 1 and 2

Iteration 1

$$f(100) = 0.0982628$$

$$f'(100) = 9.3 \cdot 10^{-5}$$

$$x_{new} = 845.5921$$

Iteration 2

$$f(845.5921) = 0.1673140$$

$$f'(845.5921) = 0.000143$$

$$x_{new} = 251.7$$

Iteration 3

$$f(251.7) = 0.1208250$$

$$f'(251.7) = 0.000189$$

$$x_{new} = 497.6057$$

Iteration 4

$$x_{new} = 499.98$$

Iteration 5

$$x_{new} = 499.9992$$

This is converging on the exact solution of $x = 500$. Notice that NR overshot on the first iteration; this overshoot can for certain "S" shaped curves cause divergence or a limit cycle rather than convergence.