Computational Methods Assignment 2 - Interpolation

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1 Question 1

The results outputted by the program to interpolate the following x from the given data are:
(i) $y(x = 0.4) = 0.804498$
(ii) $y(x = -0.128) = 0.967812$
(iii) $y(x = -2.0) = 0.0290775$
(iv) $y(x = 3.2) = 0.000236416$

2 Question2

For natural splines, the second derivatives at the boundaries, denoted $y_1^{''}$ and $y_n^{''}$, are set to zero. This means that they are known and do not need to be solved for, reducing the $N \times N$ matrix to an $N-2 \times N-2$ matrix. However, if we wish to retain the dimensions of the matrix such that they match the square of the number of known data points we have to set the boundary equations such that $F_1 = F_n = c_1 = a_n = 0$ and $b_1 \neq 0$, $b_n \neq 0$ (these can be set to any non-zero constant), giving the boundary equations:

$$b_1 y_1'' = 0, \qquad b_n y_n'' = 0 \tag{1}$$

which satisfy the natural boundary conditions. Additionally, the other equations for the points *next to* the boundaries are:

$$\frac{x_3 - x_1}{3} y_2'' + \frac{x_3 - x_2}{6} y_3'' = \frac{y_3 - y_2}{x_3 - x_2} - \frac{y_2 - y_2}{x_2 - x_1} \tag{2}$$

$$\frac{x_{n-1} - x_{n-2}}{6} y_{n-2}'' + \frac{x_n - x_{n-1}}{3} y_{n-1}'' = \frac{y_n - y_{n-1}}{x_n - x_{n-1}} - \frac{y_{n-1} - y_{n-2}}{x_{n-1} - x_{n-2}} \tag{3}$$

(ii) In the case of estimating the first derivatives at the boundary, we can no longer impose that $y_1'' = y_n'' = 0$ and the system of linear equation includes 2 more unknowns. The 2 extra equations needed for this are provided by specification of the first derivatives. The fundamental master equation is obtain by imposing the continuity of the first derivative at the interface of adjacent segments between known points. At the x_1 and x_n points, this continuity constraint can be written as (for $j = 1$) $\lim_{x \to x_1^+} \frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{x \to x_1^-} \frac{\mathrm{d}y}{\mathrm{d}x}$ where:

$$y = \frac{x_{i+1} - x}{x_{i+1} - x_i} y_i + \frac{x - x_i}{x_{i+1} - x_i} y_{i+1} + \frac{1}{6}(x_{i+1} - x_i)^2 (A_i^3 - A_i) y_i'' + \frac{1}{6}(x_{i+1} - x_i)^2 (B_i^3 - B_i) y_{i+1}'' \tag{4}$$

where $A_i = \frac{x_{i+1} - x}{x_{i+1} - x_i}$ and $B_i = \frac{x - x_i}{x_{i+1} - x_i}$. Since $\lim_{x \to x_1^-} \frac{\mathrm{d}y}{\mathrm{d}x} = \delta_1$, the continuity constraint at $j = 1$ is evaluated as:

$$\frac{y_2 - y_1}{x_2 - x_1} + \frac{1}{6}(x_2 - x_1)\left((3B_1^2 - 1)y_2'' - (3A_1^2 - 1)y_1''\right) = \delta_1; \tag{5}$$

As $x \to x_1^+$, the coefficients are $B_1 \to 0$ and $A_1 \to 1$, meaning that:

$$\frac{y_2 - y_1}{x_2 - x_1} + \frac{1}{6}(x_2 - x_1)\left((-1)y_2'' - 2y_1''\right) = \delta_1 \tag{6}$$

$$\frac{y_2 - y_1}{x_2 - x_1} - \delta_1 = \frac{(x_2 - x_1)}{3} y_1'' + \frac{(x_2 - x_1)}{6} y_2'' \tag{7}$$

as required. Similar treatment can be given to obtaining a second equation to relate the second derivative of y given the first derivative at the boundary ($j = n$) as δ_n:

$$\lim_{x \to x_n^+} \frac{\mathrm{d}y}{\mathrm{d}x} = \lim_{x \to x_n^-} \frac{\mathrm{d}y}{\mathrm{d}x} \tag{8}$$

$$\delta_n = \frac{y_n - y_{n-1}}{x_n - x_{n-1}} + \frac{1}{6}(x_n - x_{n-1})\left((3B_{n-1}^2 - 1)y_n'' - (3A_1^{n-1} - 1)y_{n-1}''\right) \tag{9}$$

where the coefficient A and B are labelled by the jth interval, of which there are $n-1$ between the n points. Since $\lim_{x \to x_n^-} A_{n-1} = 0$ $\lim_{x \to x_n^-} B_{n-1} = 1$ this becomes:

$$\delta_n = \frac{y_n - y_{n-1}}{x_n - x_{n-1}} + \frac{1}{6}(x_n - x_{n-1})\left(2y_n'' - (-1)y_{n-1}''\right) \tag{10}$$

$$\delta_n - \frac{y_n - y_{n-1}}{x_n - x_{n-1}} = \frac{(x_n - x_{n-1})}{6}y_{n-1}'' + \frac{(x_n - x_{n-1})}{3}y_n'' \tag{11}$$

$$\frac{y_n - y_{n-1}}{x_n - x_{n-1}} - \delta_n = \frac{(x_{n-1} - x_n)}{6}y_{n-1}'' + \frac{(x_{n-1} - x_n)}{3}y_n'' \tag{12}$$

3 Question 3

For this program, the routine **tridag** from Numerical Recipes was studied and used for diagonalising the matrix necessary to obtain the second derivatives. In the case of natural boundary conditions, the elements b_1 (the first element of b) and b_n (last element of b) set to 1 and $a_2 = c_1 = a_n = c_{n-1} = 0$. This means an $N \times N$ matrix is still solved but with 2 of the decoupled equations corresponding to $y_1'' = y_n'' = 0$ included as part of the matrix. For first-derivative specified boundary conditions, the values of the first derivative are used in the above equations to include in the matrix, solving the $N \times N$ problem.

4 Question 4

The results from the cubic spline interpolation for both natural splines and zero-first-derivative boundary conditions for the given data are as follow:
(i) Natural spline: $y(x = 0.4) = 0.85085$, Zero first derivative: $y(x = 0.4) = 0.85085$
(ii) Natural spline: $y(x = -0.128) = 0.982731$, Zero first derivative: $y(x = -0.128) = 0.982751$
(iii) Natural spline: $y(x = -2) = 0.0206424$, Zero first derivative: $y(x = -2) = 0.0145888$
(iv) Natural spline: $y(x = 3.2) = 0.00476971$, Zero first derivative: $y(x = 3.2) = 0.00308786$

5 Question 5

See Figure 1.

6 Question 6

The cubic spline interpolation appears to give a better representation of the function, being smooth in both value and first derivative. The reason why is would be a better choice over the linear interpolation is that the gradient smoothly varies, and is not piecewise, meaning it is more likely to be a true representation of a function in nature.
If this function were known to be a probability function, then it would be better to use the linear interpolation scheme. This is because for cubic spline interpolation, the rapid change in gradient towards the right hand side of the graph as the data smooths to zero, results in "ringing" to occur, in which the interpolated function overshoots and as a result there is a portion of the graph which has negative y values. A probability function cannot have negative values as this is unphysical, and hence the linear interpolation, albeit less accurate, will be a better estimate of the function to use, as we can tabulate it for all x within the range of the data without running into negative probabilities.

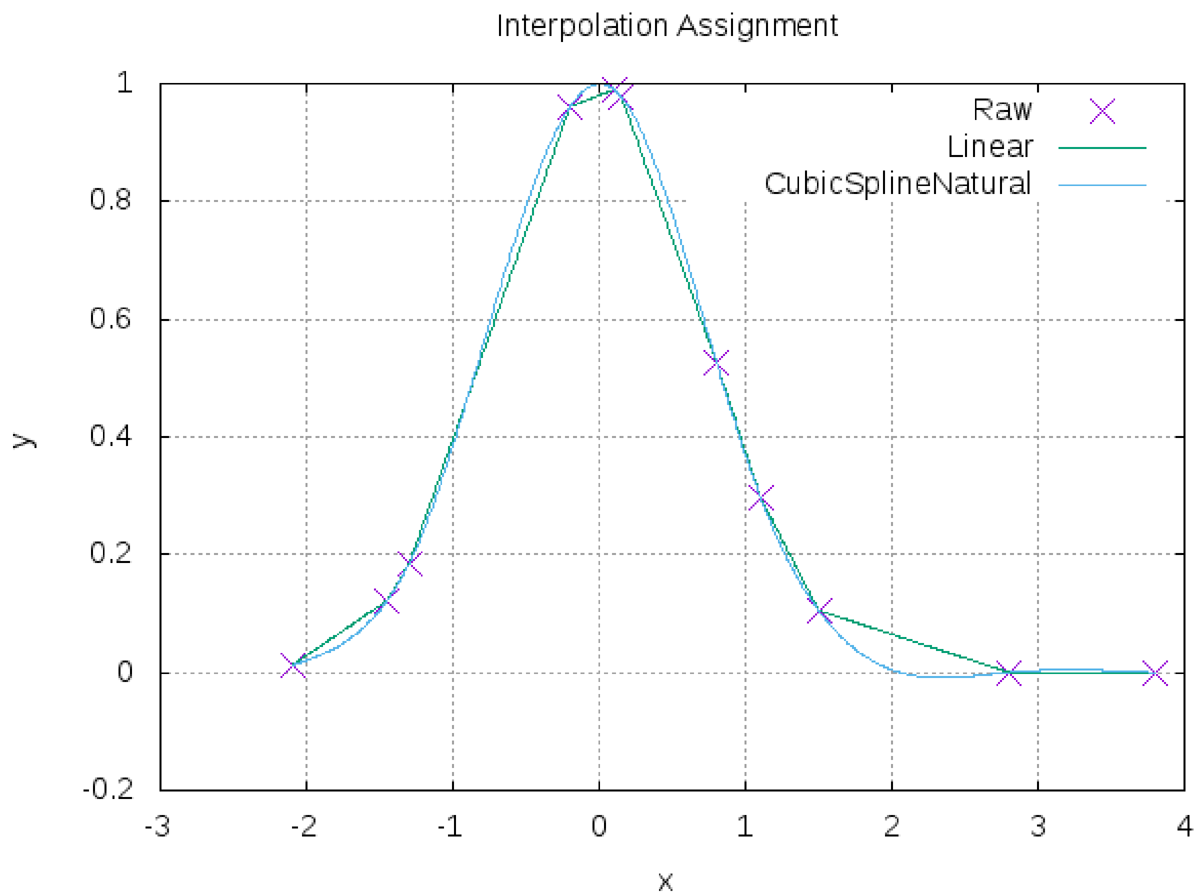

Figure 1: Linear interpolation, and cubic interpolation with natural boundary conditions implemented.

7 Question 7

For a function that is non-single valued, interpolation through splines may lead to a highly oscillating estimated function as the fitted solution attempts to pass through all points. One possible solution to this would be to switch the independent variable from x_j to y_j and perform a cubic spline interpolation to determine first the second derivatives of x with respect to y and find all values of x for a range of values of y. This only works if the function $x(y)$ is a single-valued function, but does not require that $y(x)$ be a single-valued function. Another short coming of this is that we cannot estimate any exact x that we want, and rather find a y for which the resulting interpolated x is close to.

Alternatively, a function $y(x)$ that is not single-valued for all x, can be written down as a parametric representation $x(t)$, $y(t)$ such that to interpolate this values, a set of data (x_i, y_i, t_i) for $i = 1, \cdots, N$, would be needed and the functions $x(t)$ and $y(t)$ are individually interpolated. The t_i can be generated via a linearly spaced array (e.g. using a linspace function or otherwise) and the functions. A good choice of t_i proved to be optimal for parameterisation is by choosing the independent variable t_i to increase with each step by an amount proportional to the arc length between data points (Ref: E. B. Kuznetsov, A. Y. Yakimovich, *Journal of Applied Computational and Applied Mathematics*, Volume 191, Issue 2, July 2006, pg 239-245). This provides a direct representation of $y(x)$ so that the derivative can be found through $\lim_{t\to t_j^+} \frac{\mathrm{d}y}{\mathrm{d}t}\frac{\mathrm{d}t}{\mathrm{d}x} = \lim_{t\to t_j^-} \frac{\mathrm{d}y}{\mathrm{d}t}\frac{\mathrm{d}t}{\mathrm{d}x}$. However in arranging the data points (t_i, x_i), there will be points where the derivative is zero since the value of x will not change with t due to the fact there may be several values of y_i for the same x_i (say if x_i's with identical values are mapped to from consecutive t_i's). This results in the first derivative of $y(x)$ with respect to x comprising of a division by zero since $y'(x) = \frac{\mathrm{d}y}{\mathrm{d}t}\frac{\mathrm{d}t}{\mathrm{d}x}$.