Computational Mathematics/Information Technology

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Introduction

The basic problem is:

Given a set of data points $\{(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)\}$ how can we best construct a function, $f(x)$, that in some way approximates this information.

This function is then used to

- approximate y between the data points interpolation
- approximate y outside the range of the data points extrapolation

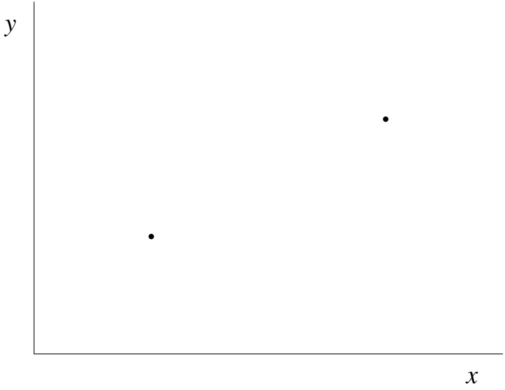
We can extend this problem to the case where y depends on more than one variable x.

We will find that there are two basically different cases that we consider:

- The points (x_n, y_n) are accurate — we want a curve that goes through these points.
- The is some statistical scatter in the points (x_n, y_n) — we want some curve that approximates the underlying curve.

Linear Fit

If we only have two points



you can approximate by a straight line.

Linear Fit

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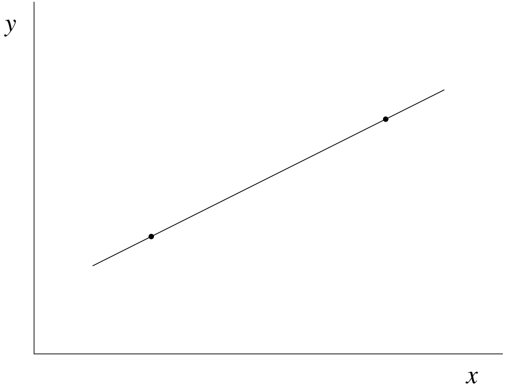
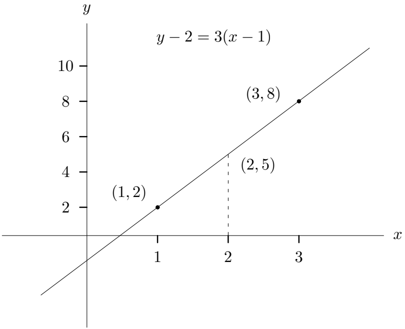


you can approximate by a straight line.

Example: Fit a straight line through the points $\{(1,2),(3,8)\}$ and use this to approximate $f(x)$ at $x = 2$.



How do you find the line? There is only one line, so all methods should produce the same answer!

- Use equation of line $y = mx + c$, substitute in points and solve the resulting pair of equations:

$$2 = m \times 1 + c, \qquad 8 = m \times 3 + c$$

giving

$$m = 3, \qquad c = -1$$

- Find gradient

$$m = \frac{y_2 - y_1}{x_2 - x_1} = \frac{8 - 2}{3 - 1} = 3$$

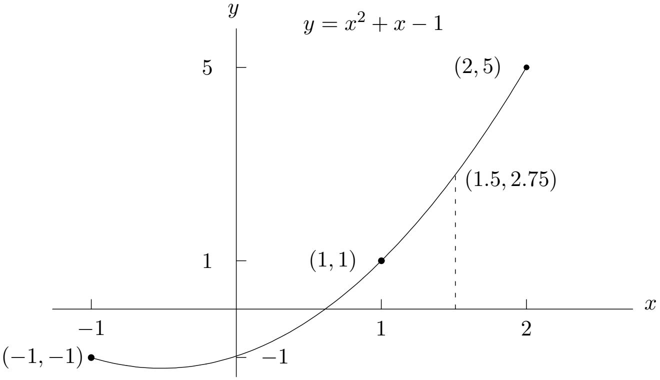
Use the fact you have to pass through, say, (x_1, y_1):

$$y - y_1 = m(x - x_1) \qquad \text{or} \qquad y - 2 = 3(x - 1) \qquad \text{or} \qquad y = 3x - 1$$

- Construct an equation for a straight line that passes through the points
$$y = y_1 \frac{x - x_2}{x_1 - x_2} + y_2 \frac{x - x_1}{x_2 - x_1}$$
Note that $(x - x_2)/(x_1 - x_2)$ is 1 at x_1 and zero at x_2.
$$y = 2 \times \frac{x-3}{1-3} + 8 \times \frac{x-1}{3-1} = 2 \times \frac{x-3}{-2} + 8 \times \frac{x-1}{2} = 3x - 1$$

Quadratic Fit

We can fit a quadratic through 3 data points:



Higher Order polynomial Fits

We can extend this to fitting a cubic through 4 points, a quartic through 5 points, etc.

In general we can fit a polynomial of order n through $n + 1$ data points.

Example: Given the points:

$$\{(-2,3),\ (-1,5),\ (0,4),\ (1,6),\ (3,7),\ (4,8)\}$$

construct a polynomial that passes through all the points.

Example: Given the points:

$$\{(-2,3),\ (-1,5),\ (0,4),\ (1,6),\ (3,7),\ (4,8)\}$$

construct a polynomial that passes through all the points.

There are six points so we construct a polynomial of degree five:

$$p(x) = a_5x^5 + a_4x^4 + a_3x^3 + a_2x^2 + a_1x + a_0$$

The polynomial must pass through the six points:

$$
\begin{aligned}
p(-2) = 3 = &\quad a_0 - 2a_1 + 4a_2 - 8a_3 + 16a_4 - 32a_5 \\
p(-1) = 5 = &\quad a_0 - a_1 + a_2 - a_3 + a_4 - a_5 \\
p(0) = 4 = &\quad a_0 \\
p(1) = 6 = &\quad a_0 + a_1 + a_2 + a_3 + a_4 + a_5 \\
p(3) = 7 = &\quad a_0 + 3a_1 + 9a_2 + 27a_3 + 81a_4 + 243a_5 \\
p(4) = 8 = &\quad a_0 + 4a_1 + 16a_2 + 64a_3 + 256a_4 + 1024a_5
\end{aligned}
$$

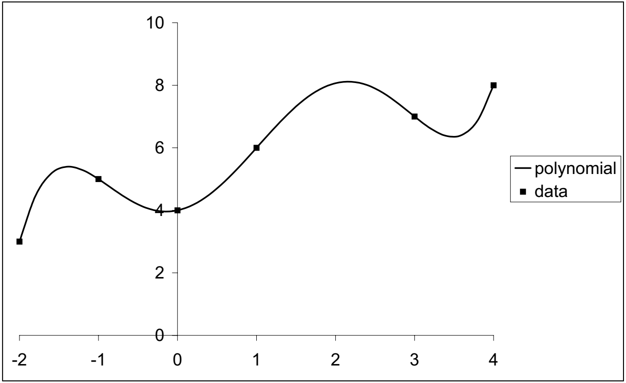
Write this in the standard matrix form $A\mathbf{a} = \mathbf{b}$

$$\begin{pmatrix} 3 \\ 5 \\ 4 \\ 6 \\ 7 \\ 8 \end{pmatrix} = \begin{pmatrix} 1 & -2 & 4 & -8 & 16 & -32 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 9 & 27 & 81 & 243 \\ 1 & 4 & 16 & 64 & 256 & 1024 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix}$$

$$\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} 1 & -2 & 4 & -8 & 16 & -32 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 3 & 9 & 27 & 81 & 243 \\ 1 & 4 & 16 & 64 & 256 & 1024 \end{pmatrix}^{-1} \begin{pmatrix} 3 \\ 5 \\ 4 \\ 6 \\ 7 \\ 8 \end{pmatrix} = \begin{pmatrix} 4 \\ 0.533 \\ 1.872 \\ -0.106 \\ -0.372 \\ 0.072 \end{pmatrix}$$

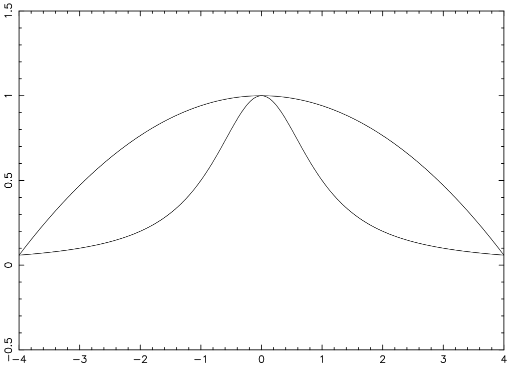
The polynomial through the six points is given by:

$$p(x) = 4 + 0.533x + 1.872x^2 - 0.106x^3 - 0.372x^4 + 0.072x^5$$

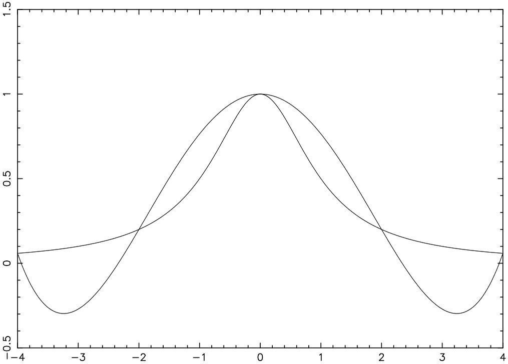


However, if you try to fit a polynomial through too many points things can go very wrong...

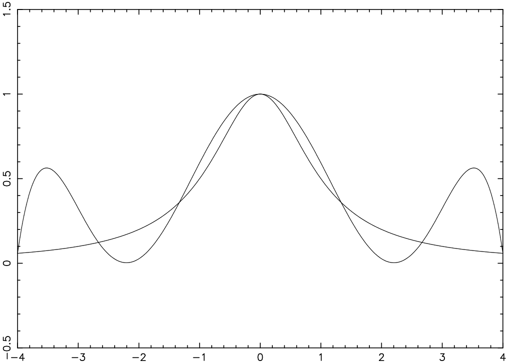
Approximating $y = 1/(1+x^2)$ with a polynomial of order 2 between -4 and 4 with 3 evenly spaced data points:



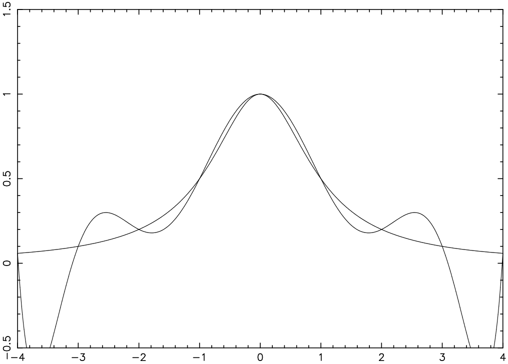
Approximating $y = 1/(1 + x^2)$ with a polynomial of order 4 between -4 and 4 with 5 evenly spaced data points:



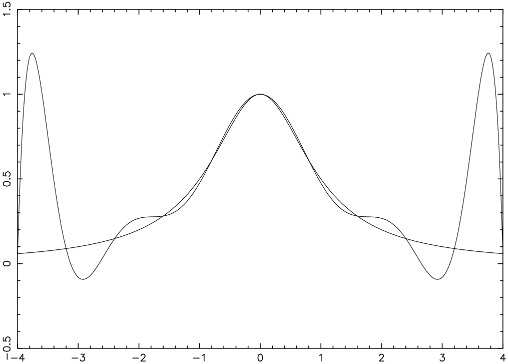
Approximating $y = 1/(1 + x^2)$ with a polynomial of order 6 between -4 and 4 with 7 evenly spaced data points:



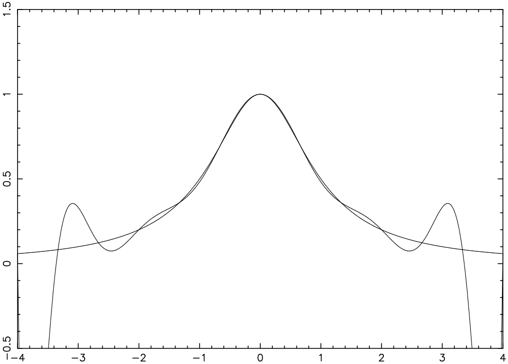
Approximating $y = 1/(1+x^2)$ with a polynomial of order 8 between -4 and 4 with 9 evenly spaced data points:



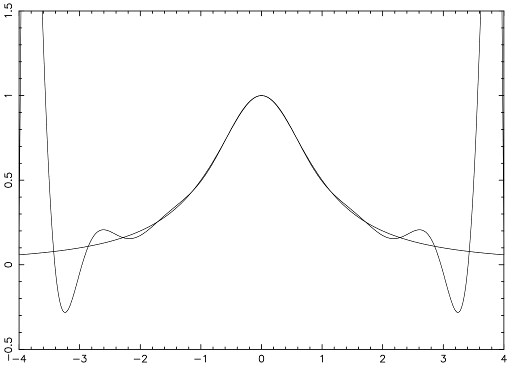
Approximating $y = 1/(1+x^2)$ with a polynomial of order 10 between -4 and 4 with 11 evenly spaced data points:



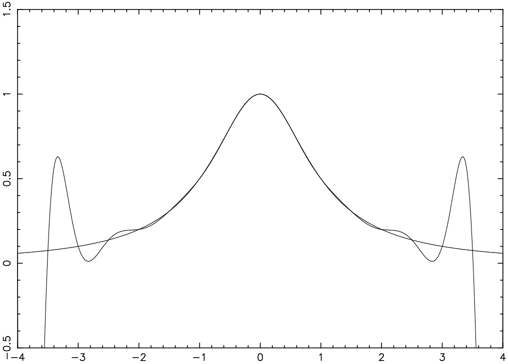
Approximating $y = 1/(1 + x^2)$ with a polynomial of order 12 between -4 and 4 with 13 evenly spaced data points:



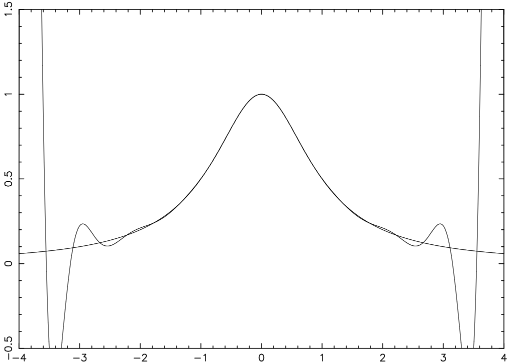
Approximating $y = 1/(1+x^2)$ with a polynomial of order 14 between -4 and 4 with 15 evenly spaced data points:



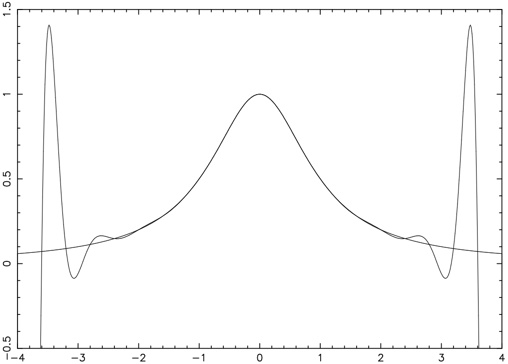
Approximating $y = 1/(1+x^2)$ with a polynomial of order 16 between -4 and 4 with 17 evenly spaced data points:



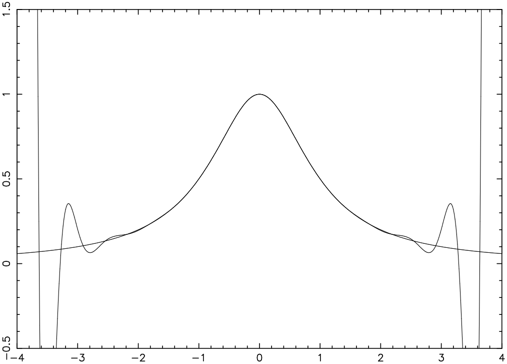
Approximating $y = 1/(1+x^2)$ with a polynomial of order 18 between -4 and 4 with 19 evenly spaced data points:



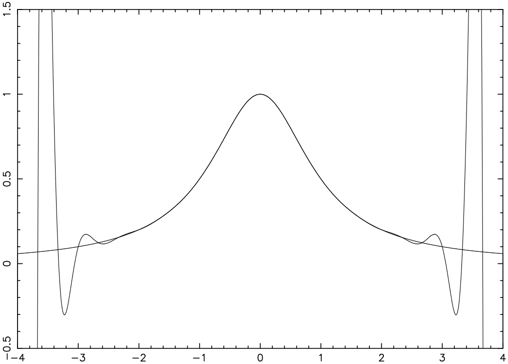
Approximating $y = 1/(1+x^2)$ with a polynomial of order 20 between -4 and 4 with 21 evenly spaced data points:



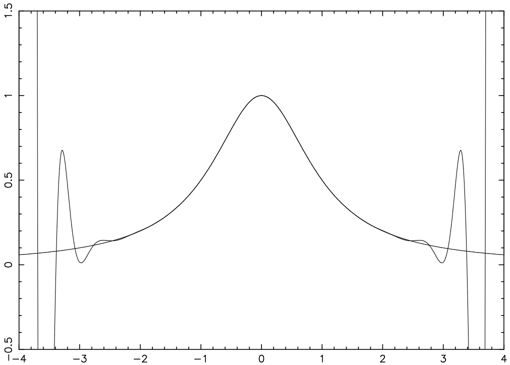
Approximating $y = 1/(1+x^2)$ with a polynomial of order 22 between -4 and 4 with 23 evenly spaced data points:



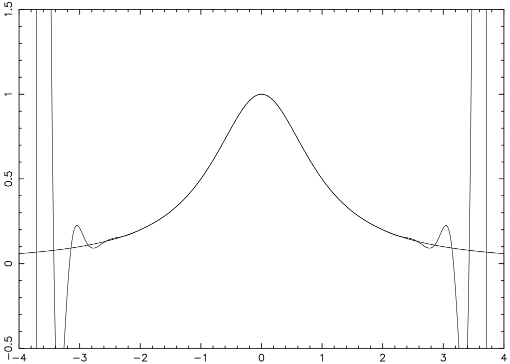
Approximating $y = 1/(1+x^2)$ with a polynomial of order 24 between -4 and 4 with 25 evenly spaced data points:



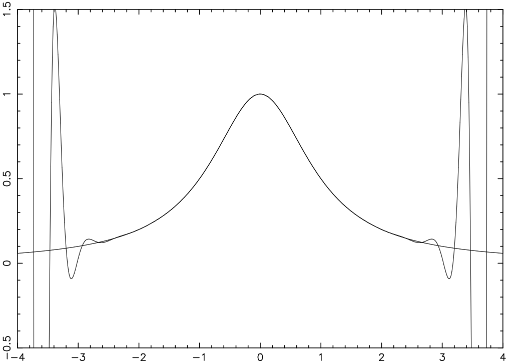
Approximating $y = 1/(1 + x^2)$ with a polynomial of order 26 between -4 and 4 with 27 evenly spaced data points:



Approximating $y = 1/(1+x^2)$ with a polynomial of order 28 between -4 and 4 with 29 evenly spaced data points:



Approximating $y = 1/(1+x^2)$ with a polynomial of order 30 between -4 and 4 with 31 evenly spaced data points:



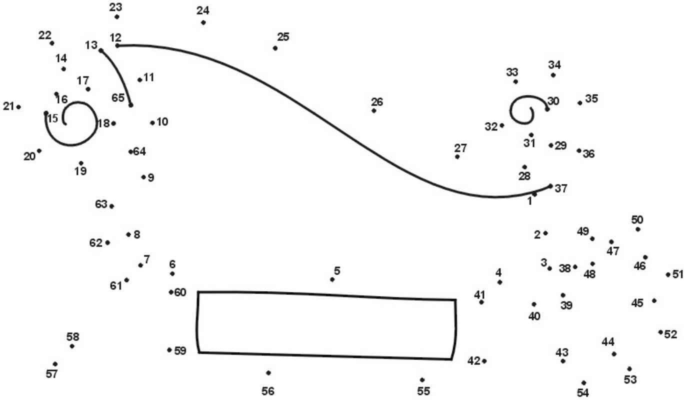
If we were to sketch a graph through the end few points by hand we would do much better than this!

Is there another approach we can use?

If we were to sketch a graph through the end few points by hand we would do much better than this!

Is there another approach we can use?

There is one method you probably learned 10 years or so ago....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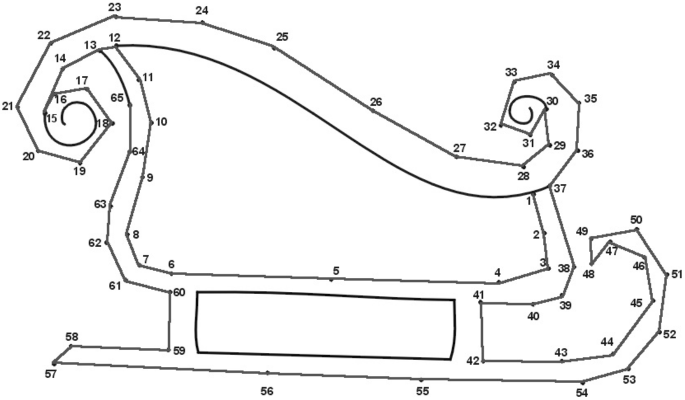
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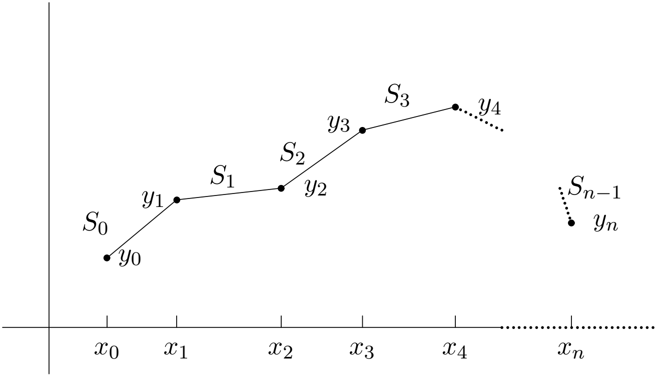
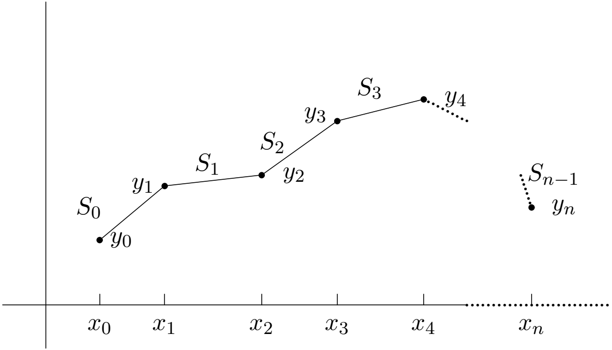
Linear Spline

As (I hope) you found out many years ago, the simplest way to construct an underlying function is to just join adjacent data points with straight lines.





Given the data points $\{(x_0, y_0), (x_1, y_1), \ldots (x_n, y_n)\}$ we join adjacent points with a straight line. The straight line between (x_k, y_k) and (x_{k+1}, y_{k+1}) is denoted by $y = S_k(x)$ and the complete set of all line segments by $S(x)$. It is this complete set of all line segments that is referred to as the **linear spline** through the points.

Notationally we write:

$$S(x) = \begin{cases} S_0(x) & x_0 \le x \le x_1 \\ S_1(x) & x_1 \le x \le x_2 \\ \vdots & \vdots \\ \vdots & \vdots \\ S_{n-1} & x_{n-1} \le x \le x_n \end{cases}$$

Since the components $S_k(x)$ of $S(x)$ are straight lines their equations are given by:

$$S_k(x) = y_k + \left(\frac{y_{k+1} - y_k}{x_{k+1} - x_k}\right)(x - x_k)$$

Example: Construct the linear spline through the given points. Hence obtain an approximation to the function at $x = 0.3$.

x_k	0.1	0.2	0.4
$f(x) = \dfrac{1}{x \ln x}$	-4.343	-3.107	-2.728

For $x \in [0.1, 0.2]$

$$S_0(x) = -4.343 + \frac{(-3.107 + 4.343)}{(0.2 - 0.1)}(x - 0.1) \quad = \quad 12.36x - 5.579$$

For $x \in [0.2, 0.4]$

$$S_1(x) = -3.107 + \frac{(-2.728 + 3.107)}{(0.4 - 0.2)}(x - 0.2) \quad = \quad 1.895x - 3.486$$

For $x \in [0.1, 0.2]$

$$S_0(x) = -4.343 + \frac{(-3.107 + 4.343)}{(0.2 - 0.1)}(x - 0.1) \quad = \quad 12.36x - 5.579$$

For $x \in [0.2, 0.4]$

$$S_1(x) = -3.107 + \frac{(-2.728 + 3.107)}{(0.4 - 0.2)}(x - 0.2) \quad = \quad 1.895x - 3.486$$

Thus we can write:

$$S(x) = \begin{cases} 12.36x - 5.579 & 0.1 \leq x \leq 0.2 \\ 1.895x - 3.486 & 0.2 \leq x \leq 0.4 \end{cases}$$

Since $x = 0.3$ is between 0.2 and 0.4 we have:

$$S(0.3) = S_1(0.3) = 1.895(0.3) - 3.486 = -2.918$$

Comparing this with the exact value of $f(0.3)$ we have:

$$f(0.3) = \frac{1}{(0.3)\ln(0.3)} = -2.79 \quad \Rightarrow \quad |\text{error}| \; = 2.918 - 2.769 = 0.149$$

which represents around a 5% error.

Advantages:

- Simple and robust.
- Looks OK if you have enough points.

Disadvantages:

- Curve has kinks in it — not differentiable.
- Approximation is only affected by the nearest points on either side.

Cubic Spline

Something to look forward to for next term....

We can improve things by having a cubic between adjacent points. As well as passing through the points we will also require the curves to have continuous first and second derivatives at the data points.