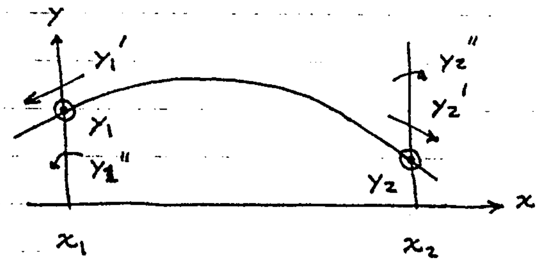
Neil E. Cotter
19 Mar 1994

ref: W.H. Press, B.P. Flannery, S.A. Teukolsky, W.T. Vetterling

derivation:



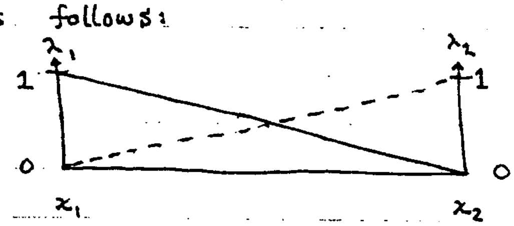
We wish to find a cubic polynomial having values y_1 at x_1, y_1' at x_1, y_2 at x_2, and y_2' at x_2. We assume these values are given. Later we consider the case where y_1, y_2, y_1'', y_2'' are given.

note: We take derivative y_1' in the $-x$ direction so that $y_1' \equiv dy/d(-x)\big|_{x=x_1} = -dy/dx\big|_{x=x_1}$. We do this to simplify our derivation and make our derivation symmetric in x_1 and x_2. Our y_2' is in the $+x$ direction. Thus y_2' is the standard derivative: $y_2' \equiv dy/dx\big|_{x=x_2}$.

For reasons of numerical stability and simplicity, we change our x coordinates to λ_1 and λ_2 defined as follows:

$$\lambda_1 = \frac{x_2 - x}{x_2 - x_1}$$

$$\lambda_2 = \frac{x - x_1}{x_2 - x_1}$$



$\lambda_1(x_1) = 1 \quad \lambda_1(x_2) = 0$

$\lambda_2(x_1) = 0 \quad \lambda_2(x_2) = 1$

These λ's tell us how close we are x_1 or x_2. We use the λ's to split the cubic spline into a piece for x_1 and a piece for x_2.

We also normalize the length of the interval $x_2 - x_1$ by working in terms of derivatives with respect to λ's instead of x.

The chain rule gives us the relationships between derivatives in λ vs derivatives in x.

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$$Y_1' = -\frac{\partial y}{\partial x}\bigg|_{x_1} = -\frac{\partial y}{\partial \lambda_1}\frac{\partial \lambda_1}{\partial x}\bigg|_{x_1}$$

$$\frac{\partial \lambda_1}{\partial x} = \frac{\partial}{\partial x}\frac{x_2 - x}{x_2 - x_1} = \frac{-1}{x_2 - x_1}$$

$$\therefore\ Y_1' = \frac{\partial y}{\partial \lambda_1}\frac{1}{x_2 - x_1}\bigg|_{x_1} \quad \text{or} \quad \mathcal{Y}_1' \equiv \frac{\partial y}{\partial \lambda_1}\bigg|_{x_1} = Y_1'(x_2 - x_1)$$

notn: $\mathcal{Y}' \equiv \frac{\partial y}{\partial \lambda}$ (script $\mathcal{Y}'$ denotes derivatives in λ's)

similarly we get

$$\boxed{\begin{aligned} \mathcal{Y}_1' &= Y_1'(x_2 - x_1) \\ \mathcal{Y}_2' &= Y_2'(x_2 - x_1) \end{aligned}} \qquad \mathcal{Y}_2' \equiv \frac{\partial y}{\partial \lambda_2}\bigg|_{x_2}$$

Use chain rule and product rule to find $\mathcal{Y}_1''$ and $\mathcal{Y}_2''$:

$$Y_1'' = \frac{\partial}{\partial(-x)}\, -\frac{\partial y}{\partial x}\bigg|_{x_1} = \frac{\partial}{\partial x}\frac{\partial y}{\partial x}\bigg|_{x_1}$$

$$'' = \frac{\partial}{\partial x}\left(\frac{\partial y}{\partial \lambda_1}\cdot\frac{\partial \lambda_1}{\partial x}\right)\bigg|_{x_1} = \left(\frac{\partial}{\partial x}\frac{\partial y}{\partial \lambda_1}\right)\frac{\partial \lambda_1}{\partial x} + \left(\frac{\partial}{\partial x}\frac{\partial \lambda_1}{\partial x}\right)\frac{\partial y}{\partial \lambda_1}\bigg|_{x_1}$$

but $\frac{\partial}{\partial x}\frac{\partial \lambda_1}{\partial x} = \frac{\partial}{\partial x}\frac{-1}{x_2 - x_1} = 0$

$$\therefore\ Y_1'' = \left(\frac{\partial}{\partial x}\frac{\partial y}{\partial \lambda_1}\right)\frac{\partial \lambda_1}{\partial x}\bigg|_{x_1} = \left(\frac{\partial}{\partial \lambda_1}\frac{\partial y}{\partial \lambda_1}\right)\frac{\partial \lambda_1}{\partial x}\cdot\frac{\partial \lambda_1}{\partial x}\bigg|_{x_1}$$

$$'' = \frac{\partial^2 y}{\partial \lambda_1^2}\left(\frac{\partial \lambda_1}{\partial x}\right)^2\bigg|_{x_1} = \mathcal{Y}_1''\left(\frac{-1}{x_2 - x_1}\right)^2$$

Thus,

Similarly,

$$\boxed{\begin{aligned} \mathcal{Y}_1'' &= Y_1''(x_2 - x_1)^2. \\ \mathcal{Y}_2'' &= Y_2''(x_2 - x_1)^2. \end{aligned}}$$

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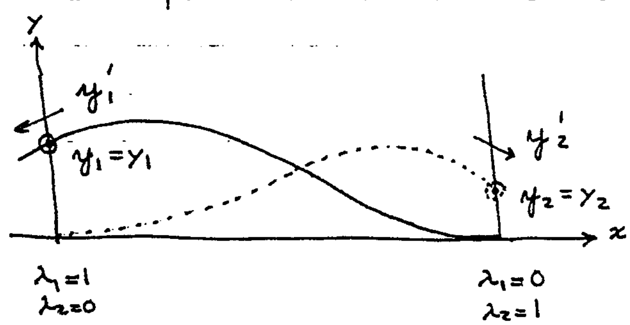
Now split the spline in two and use λ's:



The solid line is the half-spline for matching the value and slope at $\lambda_1 = 1$ and giving value and slope $= 0$ at $\lambda_1 = 0$.

The dashed line is the half-spline for matching the value and slope at $\lambda_2 = 1$ and giving value and slope $= 0$ at $\lambda_2 = 0$.

The solid line + dashed line = desired spline matching value and slope at both ends.

In other words, we solve one end at a time.

Half-prob: So we want to solve the solid line problem. This is equivalent to assuming we have a full problem with $y_2' = 0$, $y_2 = 0$. We assume these values until further notice.

We can now write the cubic polynomial for the spline:

$$y \text{ or } Y = a\lambda_1^3 + b\lambda_1^2 + c\lambda_1 + d$$

given: y_1, y_1', $y_2 = 0$, $y_2' = 0$

Now we find a, b, c, d to match given info. This is where our definition of λ_1 simplifies our derivation.

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$$y_1 \equiv y(\lambda_1=1) = a + b + c + d$$
$$y_2 \equiv y(\lambda_1=0) = d = 0 \quad \text{(given)}$$
$$y_1' \equiv y'(\lambda_1=1) = 3a\lambda_1^2\lambda_1' + 2b\lambda_1\lambda_1' + c\lambda_1'$$
$$= 3a + 2b + c \quad \text{since } \lambda_1' = \partial\lambda_1/\partial\lambda_1 = 1$$
$$y_2' \equiv -y'(\lambda_1=0) = -(3a\lambda_1^2\lambda_1' + 2b\lambda_1\lambda_1' + c\lambda_1')$$
$$= -c = 0 \quad \text{(given)}$$

Thus, $y_1 = a + b$, $y_1' = 3a + 2b$ so

$$3y_1 = 3a + 3b \qquad 2y_1 = 2a + 2b$$
$$y_1' = 3a + 2b \qquad y_1' = 3a + 2b$$
$$3y_1 - y_1' = b \qquad 2y_1 - y_1' = -a.$$

Thus,

$$\boxed{y_{left} = [-2\lambda_1^3 + 3\lambda_1^2]\, y_1 + [\lambda_1^3 - \lambda_1^2]\, y_1'.}$$

check:

$$y_1 = y(\lambda_1=1) = (-2+3)\, y_1 + (1-1)\, y_1' = y_1 \checkmark$$
$$y_2 = y(\lambda_1=0) = (0+0)\, y_1 + (0-0)\, y_1' = 0 \checkmark$$
$$y_1' = y'(\lambda_1=1) = (-6\lambda_1^2\lambda_1' + 6\lambda\lambda_1')\, y_1 + (3\lambda_1^2\lambda_1' - 2\lambda_1\lambda_1')\, y_1'$$
$$= (-6+6)\, y_1 + (3-2)\, y_1' = y_1' \checkmark$$
$$y_2' = y'(\lambda_1=0) = (-6\lambda_1^2\lambda_1' + 6\lambda_1\lambda_1')\, y_1 + (3\lambda_1^2\lambda_1' - 2\lambda_1\lambda_1')\, y_1'$$
$$= (-6\cdot 0 + 6\cdot 0)\, y_1 + (3\cdot 0 - 2\cdot 0)\, y_1' = 0 \checkmark$$

For the other half-spline on the right we get, by symmetry,

$$\boxed{y_{right} = [-2\lambda_2^3 + 3\lambda_2^2]\, y_2 + [\lambda_2^3 - \lambda_2^2]\, y_2'.}$$

Add the y_{left} and y_{right} to get the total y:

$$\boxed{y = y_{left} + y_{right}}$$

note: This y uses two different coordinates, λ_1 and λ_2 for x. This is redundant but gives us symmetry and reduces the likelihood of numerical problems.

comment: We use the above formulation for y when we know y and y' values.

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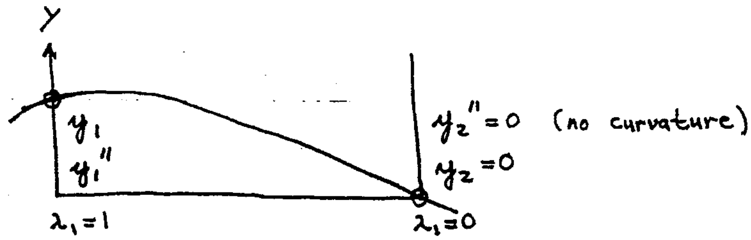
For the typical case where we want to solve for y' by requiring continuity of both y' and y'' we need a * formula for y in terms of y''.

As before, we solve the half-spline problem for the left side by setting $y_2 = 0$, $y_2'' = 0$.



note: We can only specify two conditions on right side since this gives us four conditions on our cubic polynomial having four coefficients. Thus, we may and probably do have $y_2' \neq 0$.

We have y or $y = a\lambda_1^3 + b\lambda_1^2 + c\lambda_1 + d$

given: $y_1,\ y_1'',\ y_2 = 0,\ y_2'' = 0$

Differentiate twice: (with respect to λ_1)

$$y' = 3a\lambda_1^2\lambda_1' + 2b\lambda_1\lambda_1' + c\lambda_1'$$
$$= 3a\lambda_1^2 + 2b\lambda_1 + c \qquad \lambda_1' = 1 \text{ everywhere}$$

$$y'' = 6a\lambda_1\lambda_1' + 2b\lambda_1'$$
$$= 6a\lambda_1 + 2b$$

$$y_1 = a + b + c + d \qquad (\lambda_1 = 1)$$
$$y_1'' = 6a + 2b \qquad ''$$
$$y_2 = d = 0 \qquad (\lambda_1 = 0)$$
$$y_2'' = 2b = 0 \qquad ''$$

$$\therefore\ y_1 = a + c$$
$$y_1'' = 6a \qquad y_1 - \frac{y_1''}{6} = c \qquad \frac{y_1''}{6} = a$$

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$$y_{\text{left}} = \lambda_1 y_1 + \frac{\lambda_1^3 - \lambda_1}{6} y_1''$$

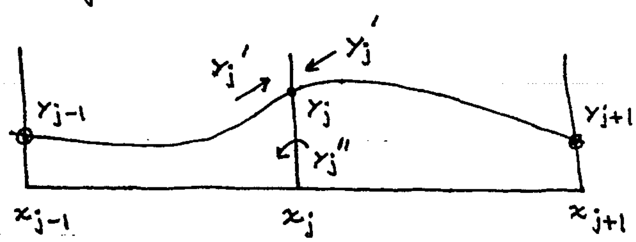
By symmetry

$$y_{\text{right}} = \lambda_2 y_2 + \frac{\lambda_2^3 - \lambda_2}{6} y_2''$$

$$y = y_{\text{left}} + y_{\text{right}}$$

note: Recall from 4 pages earlier that $y_1'' = Y_1''(x_2 - x_1)^2$
$y_2'' = Y_2''(x_2 - x_1)^2$.

With this derivation we have guaranteed the continuity of Y'' at the data points. Now we differentiate y and make y' continuous for adjacent intervals:



In interval $[x_{j-1}, x_j]$ we have

$$y = \lambda_1 Y_{j-1} + \frac{\lambda_1^3 - \lambda_1}{6}(x_j - x_{j-1})^2 Y_{j-1}'' + \lambda_2 Y_j + \frac{\lambda_2^3 - \lambda_2}{6}(x_{j+1} - x_j)^2 Y_j''$$

$$\lambda_1 = \frac{x_j - x}{x_j - x_{j-1}} \qquad \lambda_2 = \frac{x - x_{j-1}}{x_j - x_{j-1}}$$

In interval $[x_j, x_{j+1}]$ we have

$$\tilde{y} = \Lambda_1 Y_j + \frac{\Lambda_1^3 - \Lambda_1}{6}(x_{j+1} - x_j)^2 Y_j'' + \Lambda_2 Y_{j+1} + \frac{\Lambda_2^3 - \Lambda_2}{6}(x_{j+1} - x_j)^2 Y_{j+1}''$$

$$\Lambda_1 = \frac{x_{j+1} - x}{x_{j+1} - x_j} \qquad \Lambda_2 = \frac{x - x_j}{x_{j+1} - x_j}$$

After differentiation, setting $y' = \tilde{y}'$, and rearranging we get:

Example

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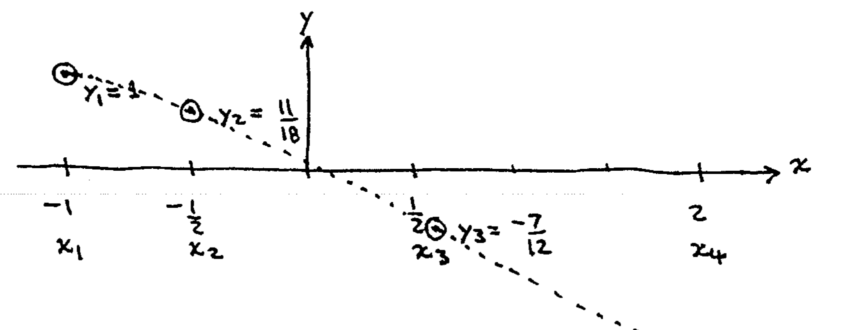
$$\frac{x_j - x_{j-1}}{6} y''_{j-1} + \frac{x_{j+1} - x_{j-1}}{3} y''_j + \frac{x_{j+1} - x_j}{6} y''_{j+1} = \frac{y_{j+1} - y_j}{x_{j+1} - x_j} - \frac{y_j - y_{j-1}}{x_j - x_{j-1}}$$

We get $N-2$ such equations for N data points. We get 2 more equations by setting $y''_1 = 0$ and $y''_N = 0$ for a natural spline. Alternatively, we give values for y'_0 and y'_1 to get 2 more eqn's.

We solve these simultaneous equations to find the values of the y''_j. We then use the equation for y from the previous page to evaluate our spline fit for arbitrary x.

ex:



data: $(x_1, y_1) = (-1, 1)$

$(x_2, y_2) = (-\frac{1}{2}, \frac{11}{18})$

$(x_3, y_3) = \left(\frac{1}{2}, -\frac{7}{12}\right)$

$(x_4, y_4) = (2, -2)$

$j =$	1	2	3	4
$x_j =$	-1	$-\frac{1}{2}$	$\frac{1}{2}$	2
$x_j - x_{j-1} =$		$\frac{1}{2}$	1	$\frac{3}{2}$
$x_{j+1} - x_j =$	$\frac{1}{2}$	1	$\frac{3}{2}$	
$x_{j+1} - x_{j-1} =$		$\frac{3}{2}$	$\frac{5}{2}$	
$y =$	1	11/18	−7/12	−2

Use a natural spline: $y''_1 = 0$, $y''_4 = 0$.

Evaluate the equation at the top of this page for $j = 2$ and $j = 3$.

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j=2: $\frac{\frac{1}{2}}{6}\cancel{(0)}^{0} + \frac{\frac{3}{2}}{3} y_2'' + \frac{1}{6} y_3'' = \frac{\left(\frac{-7}{12} - \frac{11}{18}\right)}{1} - \frac{\left(\frac{11}{18} - 1\right)}{\frac{1}{2}}$

j=3: $\frac{1}{6} y_2'' + \frac{\frac{5}{2}}{3} y_3'' + \frac{\frac{3}{2}}{6}\cancel{(0)}^{0} = \frac{\left(-2 - -\frac{7}{12}\right)}{\frac{3}{2}} - \frac{\left(-\frac{7}{12} - \frac{11}{18}\right)}{1}$

multiply by 18 to clear fractions

$$6 \cdot \frac{3}{2} y_2'' + 3 y_3'' = \left(-7\frac{3}{2} - 11\right) - 2(11 - 18)$$

$$3 y_2'' + 15 y_3'' = (-24 + 7) + \left(\frac{3}{2} \cdot 7 + 11\right)$$

$$9 y_2'' + 3 y_3'' = -\frac{43}{2} + \frac{28}{2} = -\frac{15}{2}$$

$$3 y_2'' + 15 y_3'' = -\frac{\cancel{28}\,34}{2} + \frac{43}{2} = \frac{9}{2}$$

$$45 y_2'' + 15 y_3'' = -\frac{5 \cdot 15}{2}$$

$$3 y_2'' + 15 y_3'' = \frac{9}{2}$$

$$42 y_2'' = \frac{-75 - 9}{2} = -\frac{84}{2} = -42$$

$$\therefore \boxed{y_2'' = -1}$$

$$9 y_2'' + 3 y_3'' = -\frac{15}{2}$$

$$9 y_2'' + 45 y_3'' = \frac{27}{2}$$

$$-42 y_3'' = -\frac{42}{2}$$

$$\therefore \boxed{y_3'' = \frac{1}{2}}$$

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Now evaluate the spline at $x=0$.

$x=0$ lies in the interval $[x_2, x_3] = \left[-\frac{1}{2}, \frac{1}{2}\right]$

$$y = y_{\text{left}} + y_{\text{right}} \quad \text{(see spline derivation)}$$

$$= \lambda_1 y_2 + \frac{\lambda_1^3 - \lambda_1}{6} y_2'' (x_3 - x_2)^2$$

$$+ \lambda_2 y_3 + \frac{\lambda_2^3 - \lambda_2}{6} y_3'' (x_3 - x_2)^2$$

where $\lambda_1 = \dfrac{x_3 - x}{x_3 - x_2}$ $\qquad \lambda_2 = \dfrac{x - x_2}{x_3 - x_2}$

At $x=0$ we have $\lambda_1 = \dfrac{\frac{1}{2} - 0}{\frac{1}{2} - -\frac{1}{2}} = \frac{1}{2}$

$$\lambda_2 = \frac{0 - -\frac{1}{2}}{\frac{1}{2} - -\frac{1}{2}} = \frac{1}{2}$$

note: We expect $\lambda_1 = \lambda_2 = \frac{1}{2}$ since $x=0$ is halfway between $x_2 = -\frac{1}{2}$ and $x_3 = \frac{1}{2}$.

$$(x_3 - x_2)^2 = \left(\frac{1}{2} - -\frac{1}{2}\right)^2 = 1^2 = 1 \qquad \lambda_1^3 - \lambda_1 = -\frac{7}{8}$$

Thus $y(x=0) = \frac{1}{2} y_2 + \frac{-7/8}{6} y_2''$

$$+ \frac{1}{2} y_3 + \frac{-7/8}{6} y_3''$$

$$= \frac{1}{2} \cdot \frac{11}{18} + \frac{-7/8}{6}(-1)$$

$$+ \frac{1}{2}\left(\frac{-7}{12}\right) + \frac{-7/8}{6}\left(\frac{1}{2}\right)$$

$$= \frac{11}{36} + \frac{7}{48} - \frac{7}{24} - \frac{7}{96} = \frac{88}{288} + \frac{42}{288} - \frac{84}{288} - \frac{21}{288}$$

$$= \frac{25}{288} \approx .087$$ Agrees with picture at start of example. ✓

note: See Numerical Recipes in C for spline computer code.