Computational Physics

Interpolation, Extrapolation & Polynomial Approximation

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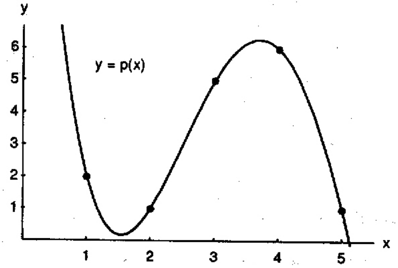
- In many cases, a function $f(x)$ is only known at a set of points $\{x_1, x_2, ..., x_N\}$, and we are interested estimating its value at an arbitrary point.
- Estimating $f(x)$ with $x \in [x_1, x_N]$ is called interpolation.
- Estimating $f(x)$ with $x \notin [x_1, x_N]$ is called extrapolation.



Polynomial Approximations

Polynomial functions are the most popular. Rational and trigonometric functions are also used quite frequently.

We will study the following methods for polynomial approximations:

- Lagrange's Polynomial
- Hermite Polynomial
- Taylor Polynomial
- Cubic Splines

Lagrange Polynomial

Consider the following data:

	x_0	x_1	x_2	x_3
x	3.2	2.7	1.0	4.8
$f(x)$	22.0	17.8	14.2	38.3
	f_0	f_1	f_2	f_3

- A possible interpolating polynomial is :
  $P_3(x) = ax^3 + bx^2 + cx + d$ (i.e. a 3th order polynomial).
- This leads to 4 equations for the 4 unknown coefficients.
- The solutions are $a = -0.5275$, $b = 6.4952$, $c = -16.117$, $d = 24.3499$
- Thus

$$P_3(x) = -0.5275x^3 + 6.4952x^2 - 16.117x + 24.3499$$

Lagrange Polynomial

- For a large number of points, this procedure could be quite laborious.
- Given a set of $n+1$ points $\{x_i, f_i\}_{i=0,\dots,n}$, Lagrange developed a direct way to find the polynomial

$$P_n(x) = f_0 L_0(x) + f_1 L_1(x) + ... + f_n L_n(x) = \sum_{i=0}^{n} f_i \, L_i(x)$$

where $L_i(x)$ are the Lagrange coefficient polynomials

- The coefficients are given by

$$\begin{aligned} L_j(x) &= \frac{(x-x_0)(x-x_1)...(x-x_{j-1})(x-x_{j+1})...(x-x_n)}{(x_j-x_0)(x_j-x_1)...(x_j-x_{j-1})(x_j-x_{j+1})...(x_j-x_n)} \\ &= \prod_{k=0}^{n} \frac{x-x_k}{x_j-x_k} \quad \text{with} \quad k \neq j \end{aligned}$$

- Notice

$$L_j(x_k) = \delta_{jk} = \begin{cases} 0 & \text{if} \quad j \neq k \\ 1 & \text{if} \quad j = k \end{cases}$$

  where δ_{jk} is Kronecker's symbol.
- Therefore,

$$P_n(x_j) = \sum_{i=0}^{n} f_i \, L_i(x_j) = \sum_{i=0}^{n} f_i \, \delta_{ij} = f(x_j)$$

- The error when using Lagrange interpolation is:

$$E_n(x) = f(x) - P_n(x) = (x - x_0)(x - x_1)....(x - x_n)\frac{f^{(n+1)}(\xi)}{(n+1)!}$$

  where $\xi \in [x_0, x_N]$
- Notice that Lagrange polynomial applies to both evenly and unevenly spaced points.

Lagrange Polynomial Formula Derivation

Consider the case of three points.

$$
\begin{aligned}
f(x_1) &= f(x) + (x_1 - x)\, f'(x) + \frac{1}{2}(x_1 - x)^2\, f''(x) + \ldots \\
f(x_2) &= f(x) + (x_2 - x)\, f'(x) + \frac{1}{2}(x_2 - x)^2\, f''(x) + \ldots \\
f(x_3) &= f(x) + (x_3 - x)\, f'(x) + \frac{1}{2}(x_3 - x)^2\, f''(x) + \ldots
\end{aligned}
$$

Is is reasonable to think that $f(x) \approx p(x)$ and $f'(x) \approx p'(x)$. Thus

Lagrange Polynomial Formula Derivation

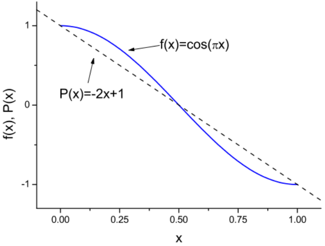
$$
\begin{aligned}
f(x_1) &= p(x) + (x_1 - x)\,p'(x) + \frac{1}{2}(x_1 - x)^2\,p''(x) \\
f(x_2) &= p(x) + (x_2 - x)\,p'(x) + \frac{1}{2}(x_2 - x)^2\,p''(x) \\
f(x_3) &= p(x) + (x_3 - x)\,p'(x) + \frac{1}{2}(x_3 - x)^2\,p''(x)
\end{aligned}
$$

We have a system of three equations for three unknowns $(p(x), p'(x), p''(x))$. Solving for $p(x)$ one gets the desired answer. Notice that one can also get the expression for the derivatives.

Lagrange Polynomial : Example

Find the Lagrange polynomial that approximates the function $y = \cos(\pi x)$ using the following data.

x_i	0	0.5	1
f_i	1	0.0	-1



The Lagrange coeffiecient polynomials are:

$$L_1(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)} = \frac{(x-0.5)(x-1)}{(0-0.5)(0-1)} = 2x^2 - 3x + 1,$$

$$L_2(x) = \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)} = \frac{(x-0)(x-1)}{(0.5-0)(0.5-1)} = -4x^2 + 4x$$

$$L_3(x) = \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)} = \frac{(x-0)(x-0.5)}{(1-0)(1-0.5)} = 2x^2 - x$$

thus

$$P(x) = (1)(2x^2-3x+1)+(0.0)(-4x^2+4x)+(-1)(2x^2-x) = -2x+1$$

The error from using $P(x) = -2x + 1$ will be:

$$
\begin{aligned}
E(x) &= (x - x_0)(x - x_1)\ldots(x - x_n)\frac{f^{(n+1)}(\xi)}{(n+1)!} \\
&= (x - x_0)(x - x_1)(x - x_2)\frac{f^{(3)}(\xi)}{(3)!} \\
&= x\,(x - 0.5)\,(x - 1)\frac{\pi^3 \sin(\pi\xi)}{3!}
\end{aligned}
$$

for example $E(x = 0.25) \leq 0.24$.

Hermite Polynomial Interpolation

This type of interpolation is very useful when in addition to the values of $f(x)$ one also has its derivative $f'(x)$

$$P_n(x) = \sum_{i=1}^{n} A_i(x) f_i + \sum_{i=1}^{n} B_i(x) f_i'$$

where

$$\begin{aligned} A_i(x) &= [1 - 2(x - x_i) L_i'(x_i)] \cdot [L_i(x)]^2 \\ B_i(x) &= (x - x_i) \cdot [L_i(x)]^2 \end{aligned}$$

and $L_i(x)$ are the Lagrange coefficients.

Hermite Polynomial Interpolation Example

k	x_k	y_k	y'_k
0	0	0	0
1	4	2	0

The Lagrange coefficients are:

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} = \frac{x-4}{0-4} = -\frac{x-4}{4} \quad L_1(x) = \frac{x-x_0}{x_1-x_0} = \frac{x}{4}$$

$$L'_0(x) = \frac{1}{x_0 - x_1} = -\frac{1}{4} \quad L'_1(x) = \frac{1}{x_1 - x_0} = \frac{1}{4}$$

Thus

$$A_0(x) = \left[1 - 2\cdot L'_0(x - x_0)\right]\cdot L_0^2 = \left[1 - 2\cdot\left(-\frac{1}{4}\right)(x-0)\right]\cdot\left(\frac{x-4}{4}\right)^2$$

$$A_1(x) = \left[1 - 2\cdot L'_0(x - x_1)\right]\cdot L_1^2 = \left[1 - 2\cdot\frac{1}{4}(x-4)\right]\cdot\left(\frac{x}{4}\right)^2 = \left(3 - \frac{x}{2}\right)\cdot\left(\frac{x}{4}\right)^2$$

$$B_0(x) = (x-0)\cdot\left(\frac{x-4}{4}\right)^2 = x\left(\frac{x-4}{4}\right)^2 \quad B_1(x) = (x-4)\cdot\left(\frac{x}{4}\right)^2$$

And

$$P(x) = (6 - x)\frac{x^2}{16}.$$

Taylor Polynomial Interpolation

Instead of finding a polynomial $P(x)$ such that $P(x) = f(x)$ at N points (Lagrange) or that both $P(x) = f(x)$ and $P'(x) = f'(x)$ at N points (Hermite), Taylor polynomial interpolation consists of, for a given value x_0, finding a function $P(x)$ that agrees up to the *Nth* derivative at x_0. That is:

$$P^{(i)}(x_0) = f^{(i)}(x_0) \quad \text{for} \quad i = 0, 1, ..., n$$

and the Taylor polynomial is given by

$$P_N(x) = \sum_{i=0}^{N} \frac{f^{(i)}(x_0)}{i!}(x - x_0)^i$$

The error is given by

$$E_N(x) = (x - x_0)^{N+1} \frac{f^{(N+1)}(x_0)}{(N+1)!}$$

Taylor Polynomial Interpolation Example

Find out how many Taylor expansion terms are required for 13-digit approximation of $e = 2.718281828459...$.

Let $y(x) = e^x$. All the derivatives are $y^{(i)}(x) = e^x$. Thus at $x = 0$, one has $y^{(i)}(x = 0) = 1$. Therefore

$$P_n(x) = \sum_{i=0}^{n} \frac{x^i}{i!} \quad \text{and} \quad E_n(x) = \frac{x^{n+1}}{(n+1)!}$$

Evaluate at $x = 1$

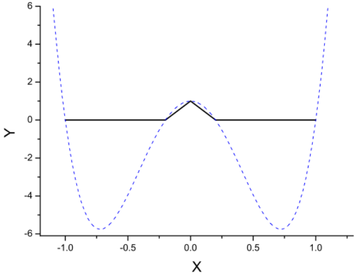
$$P_n(1) = \sum_{i=0}^{n} \frac{1}{i!} \quad \text{and} \quad E_n(1) = \frac{1}{(n+1)!}$$

and you will find that you need $n = 15$ and $E_{15} = 1.433 \times 10^{-13}$

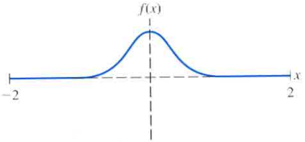
In some cases the typical polynomial approximation cannot smoothly fit certain sets of data. For instance, consider the function

$$f(x) = \begin{cases} 0 & -1 \leq x \leq -0.2 \\ 1 - 5|x| & -0.2 < x < 0.2 \\ 0 & 0.2 \leq x \leq 1.0 \end{cases}$$

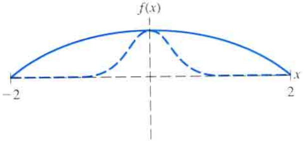
We can easily verify that we cannot fit the above data with any polynomial degree!



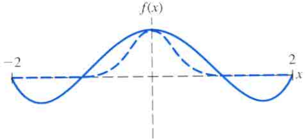
$$P(x) = 1 - 26x^2 + 25x^4$$



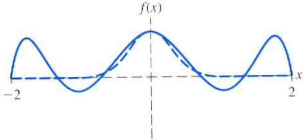
(a) Original function



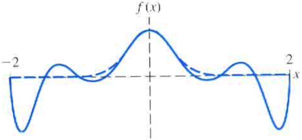
(b) Fitted with quadratic



(c) Fitted with $P_4(x)$



(d) Fitted with $P_6(x)$



(e) Fitted with $P_8(x)$

Spline Fitting

General Idea:

- Consider the tabulated function $y_i = y(x_i)$ with $i = 0, \ldots, N$.
- Split the domain $[x_0, x_N]$ into N intervals $[x_i, x_{i+1}]$ with $i = 0, \ldots, N-1$.
- For each interval construct a cubic polynomial or spline such that neighboring splines have the same slope and curvature at their joining point.
- That is, the essential idea is to fit a piecewise function of the form

$$S(x) = \begin{cases} s_0(x) & \text{if} \quad x_0 \leq x \leq x_1 \\ s_1(x) & \text{if} \quad x_1 \leq x \leq x_2 \\ & \vdots \\ s_{N-1}(x) & \text{if} \quad x_{N-1} \leq x \leq x_N \end{cases}$$

where

$$\begin{aligned} s_i(x) &= a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i \\ s_i'(x) &= 3\, a_i(x - x_i)^2 + 2\, b_i(x - x_i) + c_i \\ s_i''(x) &= 6\, a_i(x - x_i) + 2\, b_i \end{aligned}$$

Cubic Spline Interpolation Properties

- $S(x)$ interpolates all data points. That is, $S(x_i) = y_i$. Since $x_i \in [x_i, x_{i+1}]$, one has that

$$\begin{aligned} y_i &= s_i(x_i) \\ &= a_i(x_i - x_i)^3 + b_i(x_i - x_i)^2 + c_i(x_i - x_i) + d_i \\ &= d_i \end{aligned}$$

- $S(x)$ is continuous on the interval $[x_0, x_N]$, thus $s_i(x_i) = s_{i-1}(x_i)$ with

$$\begin{aligned} s_i(x_i) &= d_i \\ s_{i-1}(x_i) &= a_{i-1}(x_i - x_{i-1})^3 + b_{i-1}(x_i - x_{i-1})^2 + c_{i-1}(x_i - x_{i-1}) + d_{i-1} \\ &= a_{i-1}h_{i-1}^3 + b_{i-1}h_{i-1}^2 + c_{i-1}h_{i-1} + d_{i-1} \end{aligned}$$

where $h_{i-1} = x_i - x_{i-1}$. Therefore

$$d_i = a_{i-1}h_{i-1}^3 + b_{i-1}h_{i-1}^2 + c_{i-1}h_{i-1} + d_{i-1}$$

Cubic Spline Interpolation Properties

- $S'(x)$ is continuous on the interval $[x_0, x_N]$, thus $s'_i(x_i) = s'_{i-1}(x_i)$ with

$$\begin{aligned} s'_i(x_i) &= c_i \\ s'_{i-1}(x_i) &= 3\,a_{i-1}(x_i - x_{i-1})^2 + 2\,b_{i-1}(x_i - x_{i-1}) + c_{i-1} \\ &= 3\,a_{i-1}h_{i-1}^2 + 2\,b_{i-1}h_{i-1} + c_{i-1} \end{aligned}$$

Therefore

$$c_i = 3\,a_{i-1}h_{i-1}^2 + 2\,b_{i-1}h_{i-1} + c_{i-1}$$

Cubic Spline Interpolation Properties

- $S''(x)$ is continuous on the interval $[x_0, x_N]$, thus $s_i''(x_i) = s_{i-1}''(x_i)$ with

$$\begin{aligned} s_i''(x_i) &= 2\,b_i \\ s_{i-1}''(x_i) &= 6, a_{i-1}(x_i - x_{i-1}) + 2\,b_{i-1} \\ &= 6\,a_{i-1}h_{i-1} + 2\,b_{i-1} \end{aligned}$$

Therefore

$$2\,b_i = 6\,a_{i-1}h_{i-1} + 2\,b_{i-1}$$

In Summary

$$s_i''(x_i) = s_{i-1}''(x_i) \quad \Rightarrow \quad b_i = 3\,a_{i-1} h_{i-1} + b_{i-1}$$

$$s_i'(x_i) = s_{i-1}'(x_i) \quad \Rightarrow \quad c_i = 3\,a_{i-1} h_{i-1}^2 + 2\,b_{i-1} h_{i-1} + c_{i-1}$$

$$s_i(x_i) = s_{i-1}(x_i) \quad \Rightarrow \quad d_i = a_{i-1} h_{i-1}^3 + b_{i-1} h_{i-1}^2 + c_{i-1} h_{i-1} + d_{i-1}$$

Let's define $M_i \equiv s_i''(x_i)$. Then from $s_i''(x_i) = 2\, b_i$ and $2\, b_{i+1} = 6\, a_i h_i + 2\, b_i$, we have that

$$b_i = \frac{M_i}{2}\,, \quad a_i = \frac{M_{i+1} - M_i}{6 h_i}$$

Also, from

$$s_i(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i$$

and $s_i(x_i) = y_i, s_i(x_{i+1}) = y_{i+1}$ and , we have that

$$y_{i+1} = \frac{M_{i+1} - M_i}{6 h_i} h_i^3 + \frac{M_i}{2} h_i^2 + c_i h_i + y_i$$

Therefore

$$c_i = \frac{y_{i+1} - y_i}{h_i} - \frac{h_i}{6}(2M_i + M_{i+1}) \quad \text{and} \quad d_i = y_i$$

Recall the condition that the slopes of the two cubics joining at (x_i, y_i) are the same. That is $s'_i(x_i) = s'_{i-1}(x_i)$, which yielded

$$c_i = 3\,a_{i-1} h_{i-1}^2 + 2\,b_{i-1} h_{i-1} + c_{i-1}$$

Substitution of a, b, c and d yields:

$$\begin{aligned} \frac{y_{i+1} - y_i}{h_i} - \frac{2h_i M_i + h_i M_{i+1}}{6} &= 3\left(\frac{M_i - M_{i-1}}{6h_{i-1}}\right) h_{i-1}^2 \\ +2\frac{M_{i-1}}{2} h_{i-1} + \frac{y_i - y_{i-1}}{h_{i-1}} &- \frac{2h_{i-1} M_{i-1} + h_{i-1} M_i}{6} \end{aligned}$$

and by simplifying we get:

$$h_{i-1} M_{i-1} + 2\,(h_{i-1} + h_i)\, M_i + h_i M_{i+1} = 6\left(\frac{y_{i+1} - y_i}{h_i} - \frac{y_i - y_{i-1}}{h_{i-1}}\right)$$

- If we have $n+1$ points, the relationship

$$h_{i-1}M_{i-1} + 2\left(h_{i-1} + h_i\right)M_i + h_i M_{i+1} = 6\left(\frac{y_{i+1} - y_i}{h_i} - \frac{y_i - y_{i-1}}{h_{i-1}}\right)$$

  can be applied to the $n-1$ internal points.
- Thus we create a system of $n-1$ equations for the $n+1$ unknown M_i.
- This system can be solved if we specify the values of M_0 and M_n.

The system of $n-1$ equations with $n+1$ unknown will be written as:

$$\begin{pmatrix} & & & \cdots\cdots & & & \\ h_0 & 2(h_0+h_1) & h_1 & & & & \\ & h_1 & 2(h_1+h_2) & h_2 & & & \\ & & h_2 & 2(h_2+h_3) & h_3 & & \\ & & & \cdots\cdots & \cdots\cdots & & \\ & & & & h_{n-2} & 2(h_{n-2}+h_{n-1}) & h_{n-1} \end{pmatrix} \begin{pmatrix} M_0 \\ M_1 \\ M_2 \\ \vdots \\ M_{n-2} \\ M_{n-1} \\ M_n \end{pmatrix}$$

$$= 6 \begin{pmatrix} \cdots \\ \frac{y_2-y_1}{h_1} - \frac{y_1-y_0}{h_0} \\ \frac{y_3-y_2}{h_2} - \frac{y_2-y_1}{h_1} \\ \cdots \\ \frac{y_n-y_{n-1}}{h_{n-1}} - \frac{y_{n-1}-y_{n-2}}{h_{n-2}} \\ \cdots \end{pmatrix}$$

Recall

$$h_{i-1}M_{i-1} + 2\left(h_{i-1}+h_i\right)M_i + h_iM_{i+1} = 6\left(\frac{y_{i+1}-y_i}{h_i} - \frac{y_i-y_{i-1}}{h_{i-1}}\right)$$

From the solution of this linear systems we get the coefficients a_i, b_i, c_i and d_i via the relations:

$$
\begin{aligned}
a_i &= \frac{M_{i+1} - M_i}{6h_i} \\
b_i &= \frac{M_i}{2} \\
c_i &= \frac{y_{i+1} - y_i}{h_i} - \frac{2h_i M_i + h_i M_{i+1}}{6} \\
d_i &= y_i
\end{aligned}
$$

Let's define

$$\vec{Y} \equiv 6 \begin{pmatrix} \frac{y_2 - y_1}{h_1} - \frac{y_1 - y_0}{h_0} \\ \frac{y_3 - y_2}{h_2} - \frac{y_2 - y_1}{h_1} \\ \dots . \\ \frac{y_n - y_{n-1}}{h_{n-1}} - \frac{y_{n-1} - y_{n-2}}{h_{n-2}} \end{pmatrix}$$

and

$$\vec{M} \equiv \begin{pmatrix} M_1 \\ M_2 \\ : \\ M_{n-2} \\ M_{n-1} \end{pmatrix}$$

Choice I

Take, $M_0 = 0$ and $M_n = 0$. This will lead to the solution of the $(n-1) \times (n-1)$ linear system:

$$\mathbf{H} \cdot \vec{M} = \vec{Y}$$

where

$$\mathbf{H} \equiv \begin{pmatrix} 2(h_0 + h_1) & h_1 & & \\ h_1 & 2(h_1 + h_2) & h_2 & \\ & h_2 & 2(h_2 + h_3) & h_3 \\ & & .... & \\ & & h_{n-2} & 2(h_{n-2} + h_{n-1}) \end{pmatrix}$$

Choice II

Take, $M_0 = M_1$ and $M_n = M_{n-1}$. This will lead to the solution of the $(n-1) \times (n-1)$ linear system:

$$\mathbf{H} \cdot \vec{M} = \vec{Y}$$

where

$$\mathbf{H} \equiv \begin{pmatrix} 3h_0 + 2h_1 & h_1 & & & \\ h_1 & 2(h_1 + h_2) & h_2 & & \\ & h_2 & 2(h_2 + h_3) & h_3 & \\ & & \cdots & \cdots & \\ & & & h_{n-2} & 2h_{n-2} + 3h_{n-1} \end{pmatrix}$$

Choice III

Use linear extrapolation

$$\frac{M_1 - M_0}{h_0} = \frac{M_2 - M_1}{h_1} \Rightarrow M_0 = \frac{(h_0 + h_1)M_1 - h_0 M_2}{h_1}$$

$$\frac{M_n - M_{n-1}}{h_{n-1}} = \frac{M_{n-1} - M_{n-2}}{h_{n-2}} \Rightarrow M_n = \frac{(h_{n-2} + h_{n-1})M_{n-1} - h_{n-1} M_{n-2}}{h_{n-2}}$$

Then

$$\mathbf{M} \equiv \begin{pmatrix} \frac{(h_0+h_1)(h_0+2h_1)}{h_1} & \frac{h_1^2-h_0^2}{h_1} & & \\ h_1 & 2(h_1+h_2) & h_2 & \\ & h_2 & 2(h_2+h_3) & h_3 \\ & & \dots & \dots \\ & & \frac{h_{n-2}^2-h_{n-1}^2}{h_{n-2}} & \frac{(h_{n-1}+h_{n-2})(h_{n-1}+2h_{n-2})}{h_{n-2}} \end{pmatrix}$$

Choice IV

Force the slopes at the end points to assume certain values. If $f'(x_0) = A$ and $f'(x_n) = B$ then

$$\begin{aligned} 2h_0 M_0 + h_1 M_1 &= 6\left(\frac{y_1 - y_0}{h_0} - A\right) \\ h_{n-1} M_{n-1} + 2h_n M_n &= 6\left(B - \frac{y_n - y_{n-1}}{h_{n-1}}\right) \end{aligned}$$

Then

$$\mathbf{H} \equiv \begin{pmatrix} 2h_0 & h_1 & & & \\ h_0 & 2(h_0 + h_1) & h_1 & & \\ & h_1 & 2(h_1 + h_2) & h_2 & \\ & & .... & & \\ & & & h_{n-2} & 2h_{n-1} \end{pmatrix}$$

Interpolation with Cubic Splines : Example

Fit a cubic spline in the data ($y = x^3 - 8$):

x	0	1	2	3	4
y	-8	-7	0	19	56

- **Condition I** : $M_0 = 0$, $M_4 = 0$

$$\begin{pmatrix} 4 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 4 \end{pmatrix} \cdot \begin{pmatrix} M_1 \\ M_2 \\ M_3 \end{pmatrix} = \begin{pmatrix} 36 \\ 72 \\ 108 \end{pmatrix} \Rightarrow \begin{array}{l} M_1 = 6.4285 \\ M_2 = 10.2857 \\ M_3 = 24.4285 \end{array}$$

- **Condition II** : $M_0 = M_1$, $M_4 = M_3$

$$\begin{pmatrix} s & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & s \end{pmatrix} \cdot \begin{pmatrix} M_1 \\ M_2 \\ M_3 \end{pmatrix} = \begin{pmatrix} 36 \\ 72 \\ 108 \end{pmatrix} \Rightarrow \begin{array}{l} M_1 = M_0 = 4.8 \\ M_2 = 1.2 \\ M_3 = 19.2 = M_4 \end{array}$$

- **Condition III** :

$$\begin{pmatrix} 6 & 0 & 0 \\ 1 & 4 & 1 \\ 0 & 0 & 6 \end{pmatrix} \cdot \begin{pmatrix} M_1 \\ M_2 \\ M_3 \end{pmatrix} = \begin{pmatrix} 36 \\ 72 \\ 108 \end{pmatrix} \Rightarrow \quad \begin{matrix} M_0 = 0 \;\; M_1 = 6 \\ M_2 = 12 \; M_3 = 18 \\ M_4 = 24 \end{matrix}$$

- **Condition IV** :

$$\begin{pmatrix} 2 & 1 & 0 & 0 & 0 \\ 1 & 4 & 1 & 0 & 0 \\ 0 & 1 & 4 & 1 & 0 \\ 0 & 0 & 1 & 4 & 1 \\ 0 & 0 & 0 & 1 & 2 \end{pmatrix} \cdot \begin{pmatrix} M_0 \\ M_1 \\ M_2 \\ M_3 \\ M_4 \end{pmatrix} = \begin{pmatrix} 6 \\ 36 \\ 72 \\ 108 \\ 66 \end{pmatrix} \quad \begin{matrix} M_0 = 0 \\ M_1 = 6 \\ M_2 = 12 \\ M_3 = 18 \\ M_4 = 24 \end{matrix}$$

Tri-diagonal Matrix

The system of equations in the cubic spline fitting method has the following form:

$$
\begin{pmatrix}
b_1 & c_1 & 0 & \dots & & & \\
a_2 & b_2 & c_2 & \dots & & & \\
0 & a_3 & b_3 & \dots & & & \\
 & & & \dots & & & \\
 & & & \dots & b_{N-2} & c_{N-2} & 0 \\
 & & & \dots & a_{N-1} & b_{N-1} & c_{N-1} \\
 & & & \dots & 0 & a_N & b_N
\end{pmatrix}
\cdot
\begin{pmatrix}
x_1 \\ x_2 \\ x_3 \\ \dots \\ x_{N-2} \\ x_{N-1} \\ x_N
\end{pmatrix}
=
\begin{pmatrix}
d_1 \\ d_2 \\ d_3 \\ \dots \\ d_{N-2} \\ d_{N-1} \\ d_N
\end{pmatrix}
$$

The matrix has the so-called tri-diagonal form. That is, each equations has the form

$$a_i\, x_{i-1} + b_i\, x_i + c_i\, x_{i+1} = d_i$$

Method to Solve a Tri-diagonal System

Redefine

$$c_i' = \begin{cases} \frac{c_i}{b_i} & i = 1 \\ \frac{c_i}{b_i - c_{i-1}' a_i} & i = 2, 3, \ldots, n-1 \end{cases}$$

and

$$d_i' = \begin{cases} \frac{d_i}{b_i} & i = 1 \\ \frac{d_i - d_{i-1}' a_i}{b_i - c_{i-1}' a_i} & i = 2, 3, \ldots, n \end{cases}$$

With these new coefficients the systems takes the form

$$\begin{pmatrix} 1 & c'_1 & 0 & \dots & & & \\ 0 & 1 & c'_2 & \dots & & & \\ 0 & 0 & 1 & \dots & & & \\ & & & \dots & & & \\ & & & \dots & 1 & c'_{N-2} & 0 \\ & & & \dots & 0 & 1 & c'_{N-1} \\ & & & \dots & 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \dots \\ x_{N-2} \\ x_{N-1} \\ x_N \end{pmatrix} = \begin{pmatrix} d'_1 \\ d'_2 \\ d'_3 \\ \dots \\ d'_{N-2} \\ d'_{N-1} \\ d'_N \end{pmatrix}$$

The systems can be solved using back substitution

$$x_n = d'_n \qquad\qquad i = n$$

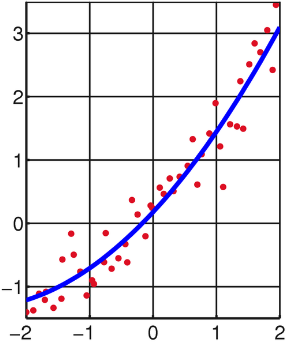
$$x_i = d'_i - c'_i\, x_{i+1} \qquad i = n-1, n-2, n-3, \dots, 1$$

Chi-Square Fitting

- Consider a set of N data points $\{x_i, y_i\}_{i=0,\ldots,N-1}$ with standard deviations σ_i.
- The objective is to find a model function $f(x;\vec{\beta})$ with $\vec{\beta} = \{\beta_0, \ldots, \beta_M\}$ a set of M adjustable parameters.
- Such that

$$\chi^2 \equiv \sum_{i=0}^{N-1} \left(\frac{y_i - f(x_i;\vec{\beta})}{\sigma_i} \right)^2$$

  is a minumum.
- Notice that $r_i \equiv y_i - f(x_i;\vec{\beta})$ are the residuals.



Fitting Data to a Straight Line

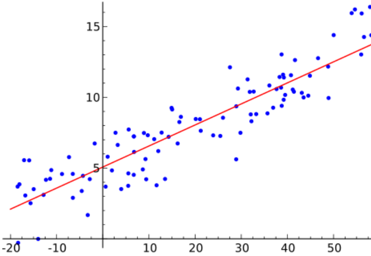
- Consider the case $f(x;\vec{\beta}) = a + b\,x$. Therefore

$$\chi^2 \equiv \sum_{i=0}^{N-1} \left(\frac{y_i - a - b\,x_i}{\sigma_i} \right)^2$$

- To minimize χ^2 with respect to a and b, we need to solve

$$0 = \frac{\partial \chi^2}{\partial a} = -2 \sum_{i=0}^{N-1} \frac{y_i - a - b\,x_i}{\sigma_i^2}$$

$$0 = \frac{\partial \chi^2}{\partial b} = -2 \sum_{i=0}^{N-1} \frac{x_i\,(y_i - a - b\,x_i)}{\sigma_i^2}$$



Define

$$S \equiv \sum_{i=0}^{N-1} \frac{1}{\sigma_i^2} \qquad S_x \equiv \sum_{i=0}^{N-1} \frac{x_i}{\sigma_i^2} \qquad S_y \equiv \sum_{i=0}^{N-1} \frac{y_i}{\sigma_i^2}$$

$$S_{xx} \equiv \sum_{i=0}^{N-1} \frac{x_i^2}{\sigma_i^2} \qquad S_{xy} \equiv \sum_{i=0}^{N-1} \frac{x_i\, y_i}{\sigma_i^2}$$

Then

$$\begin{aligned} a\,S + b\,S_x &= S_y \\ a\,S_x = b\,S_{xx} &= S_{xy} \end{aligned}$$

Finally

$$\begin{aligned} \Delta &\equiv S\,S_{xx} - S_x^2 \\ {\color{red}a} &= \frac{S_{xx}\,S_y - S_x\,S_{xy}}{\Delta} \\ {\color{red}b} &= \frac{S\,S_{xy} - S_x\,S_y}{\Delta} \end{aligned}$$

Propagation of errors

$$\sigma_{f=a,b}^2 = \sum_{i=0}^{N-1} \sigma_i^2 \left(\frac{\partial f}{\partial y_i} \right)^2$$

with

$$\begin{aligned} \frac{\partial a}{\partial y_i} &= \frac{S_{xx} - S_x\, x_i}{\sigma_i^2\, \Delta} \\ \frac{\partial b}{\partial y_i} &= \frac{S\, x_i - S_x}{\sigma_i^2\, \Delta} \end{aligned}$$

Thus

$$\begin{aligned} \sigma_a^2 &= S_{xx}/\Delta \\ \sigma_b^2 &= S/\Delta \end{aligned}$$

Variance, Covariance and Correlation

Consider the case in which $\sigma_i = 1$. Then

$$S \equiv \sum_{i=0}^{N-1} \frac{1}{\sigma_i^2} = N \qquad S_x \equiv \sum_{i=0}^{N-1} \frac{x_i}{\sigma_i^2} = N\,\overline{x} \qquad S_y \equiv \sum_{i=0}^{N-1} \frac{y_i}{\sigma_i^2} = N\,\overline{y}$$

$$S_{xx} \equiv \sum_{i=0}^{N-1} \frac{x_i^2}{\sigma_i^2} = N\,\overline{x^2} \qquad S_{xy} \equiv \sum_{i=0}^{N-1} \frac{x_i\,y_i}{\sigma_i^2} = N\,\overline{x\,y}$$

where the over line denotes average. Thus

$$\Delta \equiv S\,S_{xx} - S_x^2 = N^2\,\overline{x^2} - N^2\,\overline{x}^2 = N^2\,(\overline{x^2} - \overline{x}^2)$$

$$a = \frac{S_{xx}\,S_y - S_x\,S_{xy}}{\Delta} = \frac{\overline{x^2}\,\overline{y} - \overline{x}\,\overline{xy}}{\overline{x^2} - \overline{x}^2}$$

$$b = \frac{S\,S_{xy} - S_x\,S_y}{\Delta} = \frac{\overline{xy} - \overline{x}\,\overline{y}}{\overline{x^2} - \overline{x}^2}$$

Notice

$$\begin{aligned} a &= \frac{\overline{x^2}\,\overline{y} - \overline{x}\,\overline{xy}}{\overline{x^2} - \overline{x}^2} = \frac{\overline{x^2}\,\overline{y} - \overline{x}^2\,\overline{y} + \overline{x}^2\,\overline{y} - \overline{x}\,\overline{xy}}{\overline{x^2} - \overline{x}^2} \\ &= \overline{y} - \overline{x}\left(\frac{\overline{xy} - \overline{x}\,\overline{y}}{\overline{x^2} - \overline{x}^2}\right) = \overline{y} - \overline{x}\,b \\ b &= \frac{\overline{xy} - \overline{x}\,\overline{y}}{\overline{x^2} - \overline{x}^2} \end{aligned}$$

where

$$\begin{aligned} \text{Var[x]} &= \overline{x^2} - \overline{x}^2 \qquad \text{Variance} \\ \text{Cov[x,y]} &= \overline{xy} - \overline{x}\,\overline{y} \qquad \text{Covariance} \end{aligned}$$

Finally, from $y = a + b\,x$ with

$$
\begin{aligned}
a &= \overline{y} - \overline{x}\, b \\
b &= \frac{\overline{xy} - \overline{x}\,\overline{y}}{\overline{x^2} - \overline{x}^2}
\end{aligned}
$$

we have that

$$
\begin{aligned}
y - \overline{y} &= (x - \overline{x}) \left(\frac{\overline{xy} - \overline{x}\,\overline{y}}{\overline{x^2} - \overline{x}^2} \right) \\
\frac{y - \overline{y}}{\sqrt{\overline{y^2} - \overline{y}^2}} &= \frac{x - \overline{x}}{\sqrt{\overline{x^2} - \overline{x}^2}}\, r_{xy}
\end{aligned}
$$

where

$$
r_{xy} = \frac{\overline{xy} - \overline{x}\,\overline{y}}{\sqrt{\overline{x^2} - \overline{x}^2}\sqrt{\overline{y^2} - \overline{y}^2}}
$$

Correlation