

Interpolation in general

Given $(n + 1)$ data points $(x_0, y_0), \dots, (x_n, y_n)$ with x_i 's all distinct. (1)

Find a function $f(x) \in \Pi_n \stackrel{\text{def}}{=} \{g : g(x) \text{ is a polynomial with } \deg(g) \leq n\}$
such that f passes through all $(n + 1)$ data points.

Definition 1 (1) called the *interpolation* problem and such f is called the *interpolating function* or *interpolating polynomial*.

Theorem 1 If (1) has a solution, it must be unique.

(pf.) Suppose $f, g \in \Pi_n$, $f \neq g$ both solves $(\star)$. Then $(f - g)(x_i) = 0$ for all $i = 0, \dots, n \Rightarrow (f - g)(x)$ is a polynomial of $\deg(f - g) \geq n + 1$, contradicts $f, g \in \Pi_n$. $\square$

Theorem 2 (1) has a solution.

(pf.) Suppose $f(x) = a_0 + a_1x + \dots + a_nx^n \in \Pi_n$ with
$$\begin{cases} a_0 + a_1x_0 + \dots + a_nx_0^n = y_0, \\ \vdots \\ a_n + a_1x_n + \dots + a_nx_n^n = y_n. \end{cases}$$
 Know x_i 's all distinct, $|\det A| = \left| \prod_{i \neq j} (x_i - x_j) \right| \neq 0 \iff$ the solution $(a_0, \dots, a_n)$, i.e. $f(x)$, exists and is unique. $\square$

Lagrange method

$f(x) = y_0L_0(x) + \dots + y_nL_n(x)$, where $L_i(x) \stackrel{\text{def}}{=} \prod_{j \neq i} \frac{(x - x_j)}{(x_i - x_j)}$ for $i = 0, 1, \dots, n$;

Apparently, $f \in \Pi_n$ and f solves $(\star)$.

Theorem 3 Π_n is a vector space of dimension $(n + 1)$.

$\Pi_n = \langle 1, x, x^2, \dots, x^n \rangle = \langle L_0(x), \dots, L_n(x) \rangle = \dots$, generated by different bases.

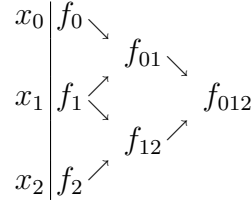
Newton Divided Differences

Suppose $P_{01}(x) = f_0 + f_{01}(x - x_0)$ passing through $(x_0, f_0), (x_1, f_1)$, then $f_{01} = \frac{f_0 - f_1}{x_0 - x_1}$ by point-slope formula.

Suppose $P_{12}(x) = f_1 + f_{12}(x - x_1)$ passing through $(x_1, f_1), (x_2, f_2)$, then $f_{12} = \frac{f_1 - f_2}{x_1 - x_2}$ by point-slope formula.

Suppose $P_{012}(x) = f_0 + f_{01}(x - x_0) + f_{012}(x - x_0)(x - x_1)$ passing through $(x_0, f_0), (x_1, f_1), (x_2, f_2)$, then $\begin{cases} f_{01} = \frac{f_0 - f_1}{x_0 - x_1} \\ f_{012} = \frac{f_{01} - f_{12}}{x_0 - x_2} \end{cases}$.

The dependency of coefficients is shown below:



In general, given $(n+1)$ data points $(x_0, f_0), \dots, (x_n, f_n)$ with all x_i 's distinct, then the interpolating polynomial $f(x) \in \Pi_n$ can be obtained by completing the table of *Newton divided differences*:

$$f_{i_0, \dots, i_k} = \frac{f_{i_1, \dots, i_k} - f_{i_0, \dots, i_{k-1}}}{x_{i_k} - x_{i_0}}, \text{ the } k^{\text{th}} \text{ divided difference, and}$$

$$P_{i_0, \dots, i_k}(x) = f_{i_0} + f_{i_0, i_1}(x - x_{i_0}) + \dots + f_{i_0, \dots, i_k}(x - x_{i_0}) \dots (x - x_{i_{k-1}})$$

is the interpolating polynomial through $(x_{i_0}, f_{i_0}), \dots, (x_{i_k}, f_{i_k})$. Newton's construction of $P_{i_0, \dots, i_k}(x)$ leads to *Neville's Algorithm* as well:

Theorem 4 If $P_{i_0, \dots, i_{k-1}}(x) \in \Pi_{k-1}$ passing through $(x_{i_0}, f_{i_0}), \dots, (x_{i_{k-1}}, f_{i_{k-1}})$, and $P_{i_1, \dots, i_k}(x) \in \Pi_{k-1}$ passing through $(x_{i_1}, f_{i_1}), \dots, (x_{i_k}, f_{i_k})$, then

$$P_{i_0, \dots, i_k}(x) = \frac{(x - x_{i_0})P_{i_1, \dots, i_k}(x) - (x - x_{i_k})P_{i_0, \dots, i_{k-1}}(x)}{x_{i_k} - x_{i_0}} \in \Pi_k$$

passes through $(x_{i_0}, f_{i_0}), \dots, (x_{i_k}, f_{i_k})$.

Note $\Pi_n = \langle 1, (x - x_0), (x - x_0)(x - x_1), \dots, (x - x_0) \dots (x - x_{n-1}) \rangle$ now.

General Hermite Interpolation

Specify

$$\begin{cases} f(x_0), f'(x_0), \dots, f^{(n_0-1)}(x_0), & (n_0 \geq 1) \\ \vdots \\ f(x_m), f'(x_m), \dots, f^{(n_m-1)}(x_m), & (n_m \geq 1) \end{cases} \quad (2)$$

with distance $\{x_i\}_{i=0}^m$ and find $f \in \Pi_n$, where $n+1 = \sum_{i=0}^m n_i = \# \text{conditions}$.

Theorem 5 Hermite interpolating polynomial is unique.

(pf.) (Cannot apply Theorem 1 since these two are different kinds interpolations.)
 Let $f, g \in \Pi_n$ both solve (2). Then $(f - g)^{(i)}(x_j) = 0 \forall i = 0, \dots, n_j - 1, \Rightarrow f - g$ has factors $(x - x_0)^{n_0}, \dots, (x - x_m)^{n_m}$, since x_i 's all distinct, $\deg(f - g) \geq \sum_{i=0}^m n_i = n + 1$, a contradiction. $\square$

Theorem 6 *Solution of (2) exists.*

Question: Can we switch the order like what we do onto the Newton divided difference table?

Piecewise Interpolation

Instead of finding a interpolating polynomial defined explicitly on $\mathbb{R}$, we can loosen this restriction by defining interpolating functions piecewisely, with or without smoothness conditions.

0.1 Splines

Given data points $(x_0, y_0), \dots, (x_m, y_m)$ with all x_i 's distinct, define a corresponding interpolating function $S(x)$ satisfying the following conditions:

$$\begin{cases} S_j(x) \stackrel{\text{def}}{=} S(x) \Big|_{[x_j, x_{j+1}]} \in \Pi_n \quad \forall j = 0, \dots, m-1; \\ S^{(0)}(x), \dots, S^{(n-1)}(x) \text{ all continuous;} \end{cases} \quad (3)$$

Such an $S(x)$ is called an n -spline. Let's take a look at $n = 3$ cubic spline case:

$$\begin{cases} S_j(x) \stackrel{\text{def}}{=} S(x) \Big|_{[x_j, x_{j+1}]} \in \Pi_3 \quad \forall j = 0, \dots, m-1; \\ S(x), S'(x), S''(x) \text{ all continuous;} \end{cases} \quad (4)$$

Let $h_j := x_{j+1} - x_j$, and $M_j := S''(x_j)$, Then $j = 0, \dots, m-1$, and $j = 0, \dots, m$.

$$S_j''(x) = M_j + \frac{M_{j+1} - M_j}{x_{j+1} - x_j}(x - x_j) = M_j + \frac{M_{j+1} - M_j}{h_j}(x - x_j) \quad (5)$$

by point-slope formula, $\Rightarrow$ the continuity of S'' is automatically satisfied.

By the continuity of S , we can derive $S_j(x)$ formula in the form

$$a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3$$

in terms of M_* and h_* . Integrating (5) twice:

$$S_j(x) = a_j + b_j(x - x_j) + \underbrace{\frac{M_j}{2}}_{c_j}(x - x_j)^2 + \underbrace{\frac{M_{j+1} - M_j}{6h_j}}_{d_j}(x - x_j)^3 \quad (6)$$

Directly from (6):

$$\begin{aligned} S_j(x_j) &= y_j, \Rightarrow a_j = y_j, \\ S_j(x_{j+1}) &= y_{j+1}, \Rightarrow y_{j+1} = y_j + b_j \cdot h_j + \frac{M_j}{2} h_j^2 + \frac{M_{j+1}-M_j}{6} h_j^2, \\ b_j &= \left((y_{j+1} - y_j) - \left(\frac{2M_j+M_{j+1}}{6} \right) h_j^2 \right) / h_j = \frac{y_{j+1}-y_j}{h_j} - \frac{2M_j+M_{j+1}}{6} h_j. \end{aligned}$$

By the continuity of S' , we can derive a relationship among M_{j-1} , M_j , and M_{j+1} . Differentiate (6):

$$S'_j(x) = \left(\frac{y_{j+1}-y_j}{h_j} \right) - \left(\frac{2M_j+M_{j+1}}{6} \right) h_j + M_j(x - x_j) + \left(\frac{M_{j+1}-M_j}{2h_j} \right) (x - x_j)^2. \quad (7)$$

$S'(x_j^-) = S'(x_j^+)$, i.e. $S'_{j-1}(x_j) = S'_j(x_j)$, $j = 1, \dots, m-1$, if and only if

$$\begin{aligned} \left(\frac{h_{j-1}}{6} \right) M_{j-1} + \left(\frac{h_{j-1}+h_j}{6} \right) M_j + \left(\frac{h_j}{6} \right) M_{j+1} &= \left(\frac{y_{j+1}-y_j}{h_j} \right) - \left(\frac{y_j-y_{j-1}}{h_{j-1}} \right), \\ j &= 1, \dots, m-1 \end{aligned} \quad (8)$$

(8), plus two additional boundary conditions (eg. free B.C.: $S''(x_0) = S''(x_m) = 0$, or, clamped B.C.), becomes a square system in M_* ($m+1$ eqn's and $m+1$ M_j 's). $S_j(x)$ (6) is obtained after a_j, b_j, M_j solved.

Bézier Curves

A parameterized curve $\mathbf{r}(t) = (x(t), y(t))$, $t \in [0, 1]$ with $\begin{cases} \mathbf{r}(0) = (x_0, y_0) \\ \dot{\mathbf{r}}(0) = (u_0, v_0) \end{cases}$ and

$\begin{cases} \mathbf{r}(1) = (x_1, y_1) \\ \dot{\mathbf{r}}(1) = (u_1, v_1) \end{cases}$ specified. If $x, y \in \Pi_3$, then we can uniquely determine $\mathbf{r}(t)$:

For $x(t)$ cubic interpolation (by Hermite's interpolation),

t	0 th	1 st	2 nd	3 rd
0	x_0	u_0		
0	x_0		$\overbrace{x_1-x_0-u_0}^b$	
1	x_1	x_1-x_0		$\overbrace{u_0+u_1-2(x_1-x_0)}^a$
1	x_1	u_1	$u_1-x_1+x_0$	

Then

$$\begin{aligned} x(t) &= x_0 + u_0 t + b t^2 + a t^2 (t-1) \\ &= x_0 + u_0 t + (b-a) t^2 + a t^3 \\ &= x_0 + u_0 t + (3(x_1-x_0)-2u_0-u_1) t^2 + (u_0+u_1-2(x_1-x_0)) t^3. \end{aligned}$$

Similarly,

$$y(t) = y_0 + v_0 t + (3(y_1-y_0)-2v_0-v_1) t^2 + (v_0+v_1-2(y_1-y_0)) t^3.$$

A curve determined by that is called a *Bézier curve*.

Numerical Integration (quadrature about $\int_a^b f(x) dx$)

Trapezoidal Rule (2 point interpolation) Let $h := x_0 - x_1$,

$$f(x) = \underbrace{\frac{(x-x_1)}{(x_0-x_1)}f(x_0) + \frac{(x-x_0)}{(x_1-x_0)}f(x_1)}_{\text{interpolating polynomial}} + \underbrace{(x-x_0)(x-x_1)\frac{f''(\xi_1)}{2!}}_{\text{error term}}$$

for some $\xi_1 \in [x_0, x_1]$, then

$$\int_{x_0}^{x_1} f(x) dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12}f''(\bar{\xi}_1)$$

for some $\bar{\xi}_1 \in [x_0, x_1]$.

Composite Trapezoidal Rule: divide $[a, b]$ into n equal pieces $a = x_0 < x_1 < \dots < x_{n-1} < x_n = b$, $h := \frac{b-a}{n}$, then

$$\int_a^b f(x) dx = \frac{h}{2} \left\{ f(x_0) + 2f(x_1) + \dots + 2f(x_{n-1}) + f(x_n) \right\} - \frac{b-a}{12} f''(\bar{\xi}) \cdot h^2$$

for some $\bar{\xi} \in [a, b]$. If f'' is continuous on $[a, b]$, then f is integrable on $[a, b]$ and the above converges as $h \rightarrow 0^+$.

Notice that **composite trapezoidal rule is an order 2 method**.

Simpson's Rule (3 point interpolation) Let $h := x_{i+1} - x_i$,

$$f(x) = \underbrace{\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)}_{\text{interpolating polynomial}} + \underbrace{(x-x_0)(x-x_1)(x-x_2)\frac{f'''(\xi_2)}{3!}}_{\text{error term}}$$

for some $\xi_2 \in [x_0, x_2]$, then

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) - \frac{h^5}{90}f^{(4)}(\bar{\xi}_2)$$

for some $\bar{\xi}_2 \in [x_0, x_2]$.

Composite Simpson's Rule: divide $[a, b]$ into $2n$ equal pieces $a = x_0 < x_1 < \dots < x_{2n-1} < x_{2n} = b$, $h := \frac{b-a}{2n}$, then

$$\int_a^b f(x) dx = \frac{h}{3} \left\{ f(x_0) + 4f(x_1) + 2f(x_2) + \dots + 4f(x_{2n-2}) + 2f(x_{2n-1}) + f(x_{2n}) \right\} - \frac{b-a}{90} f^{(4)}(\bar{\xi}) \cdot h^4$$

for some $\bar{\xi} \in [a, b]$. If $f^{(4)}$ is bounded on $[a, b]$, then f is integrable on $[a, b]$ and the above converges as $h \rightarrow 0^+$.

Notice that **composite Simpson's rule is an order 4 method**.

Richardson Extrapolation

Let $F(0) = \lim_{h \rightarrow 0} F(h)$ and $F(h) = F(0) + Kh^p + \mathcal{O}(h^r)$ ($r > p$) be an order p method which approximates $F(0)$. *Richardson Extrapolation* is a way to derive a new method F^* of higher precision order:

$$F^*(h) := F(h) - \frac{F(qh) - F(h)}{q^p - 1}$$

is an order r method, i.e. $F^*(h) = F(0) + \mathcal{O}(h^r)$.

Corollary 1 If $F(h) = F(0) + K_1 h^{p_1} + K_2 h^{p_2} + \dots + K_n h^{p_n} + \dots$, $0 < p_1 < p_2 < \dots$, define $F_1(h) := F(h)$, $F_2(h) := F_1^*(h)$, $F_3 := F_2^*$, $\dots$, then for $j \geq 1$,

$$F_{j+1}(h) := F_j^*(h) = F_j(h) - \frac{F_j(qh) - F_j(h)}{q^{p_j} - 1} \quad (\star)$$

is of order p_{j+1} .

(pf.) (Induction) $(\star)$ is true for $j = 1$. Suppose $(\star)$ is also true for $j = n - 1$, i.e. $F_n(h) = F(0) + \mathcal{O}(h^{p_n}) = F(0) + a_n h^{p_n} + a_{n+1} h^{p_{n+1}} + \dots$, then

$$\begin{aligned} F_{n+1}(h) &:= F_n(h) - \frac{F_n(qh) - F_n(h)}{q^{p_n} - 1} \\ &= F(0) + \underbrace{b_n}_{\parallel 0?} h^{p_n} + b_{n+1} h^{p_{n+1}} + \dots \end{aligned}$$

Look at h^{p_n} term: $a_n h^{p_n} - \frac{a_n h^{p_n} q^{p_n} - a_n h^{p_n}}{q^{p_n} - 1} = h^{p_n} (a_n - a_n \frac{q^{p_n} - 1}{q^{p_n} - 1}) = 0$,
 $\therefore b_n = 0$, i.e. F_{n+1} is of order p_{n+1} . $\square$

Let $F_1(h_i) := R_{i,1}$, $R_{i,j} := F_j(h_i)$, and $h_i = \frac{h_{i-1}}{q}$. Then $R_{i,j}$ is a new approximation method improved from $R_{i,j-1}$, i.e. $\begin{matrix} R_{i,j} = R_{i,j-1}^* \\ \parallel \\ F_j(h_i) = F_{j-1}^*(h_i) \end{matrix}$, and $R_{i,j}$ formula can be written in terms of $R_{*,j-1}$:

$$\begin{aligned} R_{i,j} &= F_{j-1}(h_i) - \frac{F_{j-1}(qh_i) - F_{j-1}(h_i)}{q^{p_{j-1}} - 1} \\ &= R_{i,j-1} - \frac{R_{i-1,j-1} - R_{i,j-1}}{q^{p_{j-1}} - 1} \end{aligned}$$

i.e. the dependency of $R_{i,j}$ is shown in the following table:

$$\begin{array}{ccccccc} & & R_{1,1} & \searrow & & & \\ & & & R_{2,2} & \searrow & & \\ R_{2,1} & \swarrow & & & R_{3,3} & \searrow & \\ & & & R_{3,2} & \swarrow & \vdots & \ddots \\ R_{3,1} & \swarrow & & & & \vdots & \\ & & & & & \vdots & \end{array}$$

Romberg Integration

If $F_1(h_i) := R_{i,1}$ is the quadrature of $\int_a^b f(x) dx$ by means of *composite trapezoidal rule* with $[a, b]$ being sub-divided into 2^{i-1} equal pieces, i.e. $\begin{cases} q = 2, \\ h_i := \frac{b-a}{q^{i-1}}, \end{cases}$ Then, by *Euler-Maclaurin expansion formula*, we can show that $R_{i,1} = F_1(h_i) = F_1(0) + K_1 h_i^2 + K_2 h_i^4 + \dots + K_n h_i^{2n} + \dots$, i.e. $p_j = 2j$, and the above $R_{i,j}$ formula becomes

$$R_{i,j} = R_{i,j-1} - \frac{R_{i-1,j-1} - R_{i,j-1}}{4^{j-1} - 1}$$

To complete $R_{i,j}$ table, we need to compute the first column $R_{*,1}$, and $R_{i,1}$ can be derived in terms of $R_{i-1,1}$ and f :

$$\begin{aligned} R_{i,1} &= \sum_{j=0}^{2^{i-1}-1} \frac{f(a + jh_i) + f(a + (j+1)h_i)}{2} h_i = \frac{h_i}{2} \left(f(a) + f(b) + 2 \sum_{j=1}^{2^{i-1}-1} f(a + jh_i) \right) \\ &= \frac{1}{2} \frac{h_{i-1}}{2} \left(f(a) + f(b) + 2 \sum_{\substack{j=1 \\ j \text{ is even}}}^{2^{i-1}-1} f(a + jh_i) + 2 \sum_{\substack{j=1 \\ j \text{ is odd}}}^{2^{i-1}-1} f(a + jh_i) \right) \\ &= \frac{1}{2} \left[R_{i-1,1} + h_{i-1} \sum_{\substack{j=1 \\ j \text{ is odd}}}^{2^{i-1}-1} f(a + jh_i) \right] = \frac{1}{2} \left[R_{i-1,1} + h_{i-1} \sum_{k=1}^{2^{i-2}} f(a + (2k-1)h_i) \right] \\ &= \frac{1}{2} \left[R_{i-1,1} + h_{i-1} \sum_{k=1}^{2^{i-2}} f(a + (k-0.5)h_{i-1}) \right] \end{aligned}$$

The so-called **Romberg integration** is the $j = 3$ (order 6 method) quadrature $R_{i,3}$'s

Trapzodial	Simpson	Romberg	
$R_{1,1} \searrow$			
$R_{2,1} \swarrow \searrow$	$R_{2,2} \searrow$	$R_{3,3} \searrow$	
$R_{3,1} \nearrow \swarrow$	$R_{3,2} \nearrow$	$\vdots$	$\ddots$
$\vdots$	$\vdots$		

Numerical Differentiation

Given $n + 1$ data points $(x_0, f(x_0)), \dots, (x_n, f(x_n))$ (with $x_0, \dots, x_n$ all distinct) from $f(x)$ and if Lagrange interpolation is taken:

$$f(x) = \underbrace{\sum_{i=0}^n f(x_i) L_{n,i}(x)}_{\text{interpolating polynomial } p(x)} + \underbrace{\frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))}_{\text{error } \epsilon(x)},$$

where $L_{n,i}(x) := \prod_{\substack{j \neq i \\ j=0}}^n \frac{(x-x_j)}{(x_i-x_j)}$, Lagrange polynomials.

$$f'(x) = \underbrace{\sum_{i=0}^n f(x_i) L'_{n,i}(x)}_{p'(x)} + \underbrace{\frac{d}{dx} \left[\frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} \right] f^{(n+1)}(\xi(x)) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} \frac{d}{dx} [f^{(n+1)}(\xi(x))]}_{\epsilon'(x)},$$

If $f^{(n+1)}$ is bounded and $x_0, \dots, x_n$ are “pretty close”, then $\begin{cases} f(x) \approx p(x), \\ f'(x) \approx p'(x). \end{cases}$

In particular, if $x := x_j$, then $f'(x_j) = \sum_{i=0}^n f(x_i) L'_{n,i}(x_j) + \prod_{\substack{i \neq j \\ i=0}}^n (x_j - x_i) \cdot \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!}$,

$$\text{i.e. } f'(x_j) \approx p'(x_j) = \sum_{i=0}^n f(x_i) L'_{n,i}(x_j) :$$

$n = 1$ (two-point formula) $f'(x_0) = f'(x_1) \approx \frac{f(x_0) - f(x_1)}{x_0 - x_1}$, i.e. slope of secant line.

$n = 2$ (three-point formula) $f'(x_j) \approx f(x_0) \frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1) \frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} + f(x_2) \frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$

Let $\begin{cases} x_1 := x_0 - h, \\ x_2 := x_0 + h, \end{cases}$ then $f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h}$, $\xrightarrow{h \rightarrow 0} f'(x_0)$.

$n = 4$ (five-point formula) Let $\begin{cases} x_1 := x_0 - h, & x_2 := x_0 + h, \\ x_3 := x_0 - 2h, & x_4 := x_0 + 2h, \end{cases}$ then

$$f'(x_0) \approx \sum_{i=0}^n f(x_i) L'_{n,i}(x_0) = \frac{4}{3} \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{1}{3} \frac{f(x_0+2h) - f(x_0-2h)}{4h}.$$