MA 8020: Numerical Analysis II
Approximating Functions

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Polynomial interpolation

- We are going to solve the following problem: given a table of $n+1$ data points (x_i, y_i),

x	x_0	x_1	x_2	$\cdots$	x_n
y	y_0	y_1	y_2	$\cdots$	y_n

  we seek a polynomial p_n of lowest possible degree for which

$$p_n(x_i) = y_i \quad (0 \le i \le n).$$

- *Such a polynomial $p_n(x)$ is said to interpolate the data.*

Theorem on polynomial interpolation

If $x_0, x_1, \cdots, x_n$ are $n+1$ distinct real (or complex) numbers, then for arbitrary $n+1$ values $y_0, y_1, \cdots y_n$, there exists a unique polynomial p_n of degree at most n such that

$$p_n(x_i) = y_i \quad (0 \le i \le n).$$

Proof: (uniqueness)

Suppose there were two such polynomials p_n and q_n.
Then $(p_n - q_n)(x_i) = 0$ for $0 \le i \le n$.

Since the degree of $p_n - q_n$ can be at most n, this polynomial can have at most n zeros if it is not the 0 polynomial.

Since the x_i are distinct, $p_n - q_n$ has $n+1$ zeros.
Therefore , it must be 0, namely, $p_n \equiv q_n$. $\square$

Theorem on polynomial interpolation (cont'd)

Proof: (existence) We will use the mathematical induction on n.

- For $n = 0$, we take $p_0 \equiv y_0$. Then $p_0(x_0) = y_0$.
- Suppose that it is true for $n = k - 1$, i.e., $\exists$ a polynomial p_{k-1} of degree $\leq k - 1$ with $p_{k-1}(x_i) = y_i$ for $0 \leq i \leq k - 1$. We wish to prove that it is true for $n = k$.

  (i) We try to construct p_k in the form

  $$p_k(x) = p_{k-1}(x) + c(x - x_0)(x - x_1) \cdots (x - x_{k-1}),$$

  where c need to be determined.

  (ii) Note that $deg(p_k) \leq k$ and $p_k(x_i) = p_{k-1}(x_i) = y_i$ for $0 \leq i \leq k - 1$. We can determine c from the condition $p_k(x_k) = y_k$, i.e.,

  $$y_k = p_{k-1}(x_k) + c(x_k - x_0)(x_k - x_1) \cdots (x_k - x_{k-1}).$$

  Therefore, we have

  $$c = \frac{y_k - p_{k-1}(x_k)}{(x_k - x_0)(x_k - x_1) \cdots (x_k - x_{k-1})}.$$

  That is, it is still true for $n = k$. $\square$

Newton form of the interpolation polynomial

- We attempt to translate the constructive existence proof into an algorithm suitable for a computer program.
- Consider the first few cases:

$$
\begin{aligned}
p_0(x) &= c_0 = y_0, \\
p_1(x) &= \underbrace{c_0}_{p_0(x)} + c_1(x - x_0), \\
p_2(x) &= \underbrace{c_0 + c_1(x - x_0)}_{p_1(x)} + c_2(x - x_0)(x - x_1), \\
&\vdots
\end{aligned}
$$

In general, we have

$$p_k(x) = p_{k-1}(x) + c_k(x - x_0)(x - x_1)\cdots(x - x_{k-1}).$$

Thus, we can solve for the coefficients:

$$c_k = \frac{y_k - p_{k-1}(x_k)}{(x_k - x_0)(x_k - x_1)\cdots(x_k - x_{k-1})}.$$

Newton form of the interpolation polynomial (cont'd)

- Notice that each p_k is obtained simply by adding a single term to p_{k-1} and p_k has the form (the interpolation polynomials in Newton's form),

$$\begin{aligned} p_k(x) &= c_0 + c_1(x-x_0) + c_2(x-x_0)(x-x_1) + \cdots \\ &\quad + c_k(x-x_0)(x-x_1)\cdots(x-x_{k-1}), \end{aligned}$$

or expressed in more compact form,

$$p_k(x) = \sum_{i=0}^{k} c_i \prod_{j=0}^{i-1}(x-x_j),$$

where $\prod_{j=0}^{i-1}(x-x_j) := 1$ if $i-1=-1$ and

$$c_k = \frac{y_k - p_{k-1}(x_k)}{(x_k-x_0)(x_k-x_1)\cdots(x_k-x_{k-1})}, \quad k \geq 1.$$

Example

- Consider the polynomial

$$f(x) = 4x^3 + 35x^2 - 84x - 954.$$

Some values of this function are given by

x	5	-7	-6	0
y	1	-23	-54	-954

- The coefficients computed using the above algorithm are:

$c_0 = y_0 = 1, c_1 = 2, c_2 = 3$ and $c_3 = 4 \Longrightarrow$
$p_3(x) = 1 + 2(x-5) + 3(x-5)(x+7) + 4(x-5)(x+7)(x+6),$

which is the Newton form of $f(x) = 4x^3 + 35x^2 - 84x - 954$.

Note that $p_3 \equiv f$.

- *An alternative method is to use divided differences to compute the coefficients (see next section later).*

Lagrange form of the interpolation polynomial

- Consider the alternative form expressing p

$$p_n(x) = y_0\ell_0(x) + y_1\ell_1(x) + \cdots + y_n\ell_n(x) = \sum_{k=0}^{n} y_k\ell_k(x),$$

  where $\ell_0, \ell_1, \cdots \ell_n$ are polynomials that depend on the nodes $x_0, x_1, \cdots, x_n$, but not on the ordinates $y_0, y_1, \cdots, y_n$.

- $\ell_0, \ell_1, \ldots \ell_n$ are cardinal functions with property:

$$\ell_i(x_j) = \delta_{ij}.$$

  Recall that the Kronecker delta is defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

Lagrange form of the interpolation polynomial (cont'd)

- Let's consider ℓ_0. It is a polynomial of degree n that takes the value 0 at $x_1, x_2, \cdots, x_n$ and the value 1 at x_0. It must be of the form:

$$\ell_0(x) = c(x - x_1)(x - x_2)\cdots(x - x_n) = c\prod_{j=1}^{n}(x - x_j).$$

- Setting $x = x_0 \implies 1 = c\prod_{j=1}^{n}(x_0 - x_j)$ or $c = \prod_{j=1}^{n}(x_0 - x_j)^{-1}$.

  So, we have

$$\ell_0(x) = \prod_{j=1}^{n}\frac{x - x_j}{x_0 - x_j}.$$

- Each ℓ_i is obtained by similar reasoning:

$$\ell_i(x) = \prod_{j=0, j\neq i}^{n}\frac{x - x_j}{x_i - x_j}, \quad 0 \le i \le n.$$

Example

x	5	-7	-6	0
y	1	-23	-54	-954

The nodes are 5, −7, −6, 0. So we have

$$
\begin{aligned}
\ell_0(x) &= \frac{(x+7)(x+6)x}{(5+7)(5+6)5} = \frac{1}{660}x(x+6)(x+7), \\
\ell_1(x) &= \frac{(x-5)(x+6)x}{(-7-5)(-7+6)(-7)} = \frac{-1}{84}x(x-5)(x+6), \\
\ell_2(x) &= \frac{(x-5)(x+7)x}{(-6-5)(-6+7)(-6)} = \frac{-1}{66}x(x-5)(x+7), \\
\ell_3(x) &= \frac{(x-5)(x+7)(x+6)}{(0-5)(0+7)(0+6)} = \frac{-1}{210}(x-5)(x+6)(x+7).
\end{aligned}
$$

Thus, the interpolating polynomial is:

$$p_3(x) = 1\ell_0(x) - 23\ell_1(x) - 54\ell_2(x) - 954\ell_3(x).$$

Other algorithm

- Assume that

$$p_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n.$$

- The interpolation conditions, $p_n(x_i) = y_i$ for $0 \le i \le n$, lead to a system of $n+1$ linear equations for determining $a_0, a_1, \cdots, a_n$:

$$\underbrace{\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix}}_{X} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}.$$

- *The coefficient matrix X is called the Vandermonde matrix. It is nonsingular with* $\det X = \prod_{0 \le i < j \le n}(x_j - x_i) \neq 0$*, but is often ill conditioned. Therefore, this approach is not recommended.*

Homework #1

Recall the Vandermonde matrix X in the previous page, and define

$$V_n(x) = \det \begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \ddots & & \vdots \\ 1 & x_{n-1} & x_{n-1}^2 & \cdots & x_{n-1}^n \\ 1 & x & x^2 & \cdots & x^n \end{bmatrix}.$$

- Show $V_n(x)$ is a polynomial of degree n, and that its roots are $x_0, x_1, \cdots, x_{n-1}$. Obtain the formula

  $$V_n(x) = V_{n-1}(x_{n-1})(x - x_0)(x - x_1)\cdots(x - x_{n-1}).$$

  Hint: *expand the last row of $V_n(x)$ by minors to show $V_n(x)$ is a polynomial of degree n and to find the coefficient of the term x^n.*

- Show that

  $$\det X = V_n(x_n) = \prod_{0 \le i < j \le n} (x_j - x_i).$$

Theorem on polynomial interpolation error

Let f be a given real-valued function in $C^{n+1}[a,b]$, and let p_n be the polynomial of degree at most n that interpolates the function f at $n+1$ distinct points (nodes) $x_0, x_1, \cdots, x_n$ in the interval $[a,b]$. To each x in $[a,b]$ there corresponds a point $\xi_x \in (a,b)$ such that

$$f(x) - p_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i).$$

Proof: Let $x \in [a,b]$ be any point other than x_i, $i = 0, 1, \cdots, n$. Define

$$\begin{aligned} w(t) &= \prod_{i=0}^{n} (t - x_i) && \text{(polynomial in } t\text{)}, \\ \varphi(t) &= f(t) - p_n(t) - \lambda w(t) && \text{(function in } t\text{)}, \\ \lambda &= \frac{f(x) - p_n(x)}{w(x)} && \text{(a constant that makes } \varphi(x) = 0\text{)}. \end{aligned}$$

Then $\varphi \in C^{n+1}[a,b]$ and φ vanishes at the $n+2$ points $x, x_0, x_1, \cdots, x_n$. By Rolle's Theorem, φ' has at least $n+1$ distinct zeros in (a,b).

Theorem on polynomial interpolation error (cont'd)

Proof: (continued)

Repeating this process, we conclude eventually that $\varphi^{(n+1)}$ has at least one zero $\xi_x \in (a, b)$.

$$\begin{aligned}\varphi^{(n+1)}(t) &= f^{(n+1)}(t) - p_n^{(n+1)}(t) - \lambda w^{(n+1)}(t) \\ &= f^{(n+1)}(t) - (n+1)!\lambda.\end{aligned}$$

Hence, we have

$$\begin{aligned}0 = \varphi^{(n+1)}(\xi_x) &= f^{(n+1)}(\xi_x) - (n+1)!\lambda \\ &= f^{(n+1)}(\xi_x) - (n+1)!\,\frac{f(x) - p_n(x)}{w(x)}.\end{aligned}$$

This completes the proof. $\square$

Example

If $f(x) = \sin x$ is approximated by a polynomial of degree 9 that interpolates f at 10 points in the interval $[0, 1]$, how large is the error on this interval?

Since

$$|f^{(10)}(\xi_x)| \leq 1 \quad \text{and} \quad \prod_{i=0}^{9} |x - x_i| \leq 1,$$

we have for all x in $[0, 1]$,

$$\left| \sin x - p_9(x) \right| \leq \frac{1}{10!} < 2.8 \times 10^{-7}.$$

Chebyshev polynomials

- The Chebyshev polynomials (of the first kind) are defined recursively as follows:

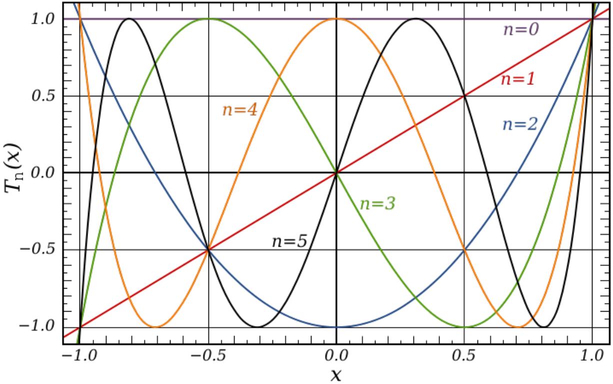
$$\begin{cases} T_0(x) &= 1, \\ T_1(x) &= x, \\ T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x) \quad \textit{for } n \geq 1. \end{cases}$$

- The explicit forms of the next few T_n are:

$$\begin{aligned} T_2(x) &= 2x^2 - 1, \\ T_3(x) &= 4x^3 - 3x, \\ T_4(x) &= 8x^4 - 8x^2 + 1, \\ T_5(x) &= 16x^5 - 20x^3 + 5x, \\ T_6(x) &= 32x^6 - 48x^4 + 18x^2 - 1. \end{aligned}$$

- These polynomials arose when Chebyshev was studying the motion of linkages in a steam locomotive.

Some Chebyshev polynomials: $T_0, T_1, \cdots, T_5$



(quoted from wikipedia.org)

Properties of the Chebyshev polynomials

- **Theorem:** *For x in the interval $[-1, 1]$,*

$$T_n(x) = \cos(n\cos^{-1}x) \quad \textit{for } n \geq 0.$$

Proof: Recall the addition formula for the cosine:

$$\begin{aligned} \cos(n+1)\theta &= \cos\theta\cos n\theta - \sin\theta\sin n\theta, \\ \cos(n-1)\theta &= \cos\theta\cos n\theta + \sin\theta\sin n\theta. \end{aligned}$$

Thus, we have $\cos(n+1)\theta = 2\cos\theta\cos n\theta - \cos(n-1)\theta. \quad (\star)$

Let $\theta = \cos^{-1}x$. Then $x = \cos\theta$. Define

$$f_n(x) = \cos(n\cos^{-1}x) = \cos(n\theta).$$

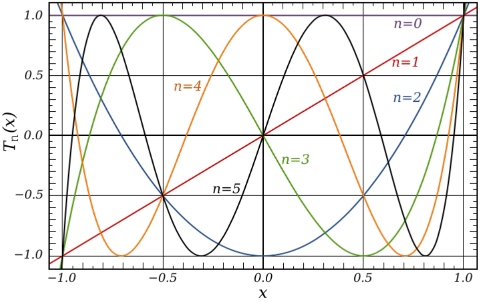
From $(\star)$, we have

$$\begin{cases} f_0(x) = 1, \\ f_1(x) = x, \\ f_{n+1}(x) = 2xf_n(x) - f_{n-1}(x) \quad \textit{for } n \geq 1. \end{cases}$$

Therefore, $f_n = T_n$ for all $n \geq 0$. $\square$

Properties of the Chebyshev polynomials (cont'd)

- $|T_n(x)| \leq 1$ for $-1 \leq x \leq 1$.
- $T_n(\cos\frac{i\pi}{n}) = (-1)^i$ for $0 \leq i \leq n$, where $x_i = \cos\frac{i\pi}{n}$ are the location of absolute extreme points of T_n on $[-1, 1]$.
- $T_n(\cos\frac{2i-1}{2n}\pi) = 0$ for $1 \leq i \leq n$, where $x_i = \cos\frac{2i-1}{2n}\pi$ are the location of zero roots of T_n on $[-1, 1]$ (in fact, on $\mathbb{R}$).



Monic polynomials

- A monic polynomial is one in which the term of highest degree has a coefficient of unity.
- From the definition of the Chebyshev polynomials, we see that in $T_n(x)$ the term of highest degree is $2^{n-1}x^n$ for $n \geq 1$. Therefore, $2^{1-n}T_n$ is a monic polynomial for $n \geq 1$.
- **Theorem:** *If p is a monic polynomial of degree n, then*

$$\|p\|_\infty := \max_{-1\leq x\leq 1} |p(x)| \geq 2^{1-n}.$$

Proof: Suppose that $|p(x)| < 2^{1-n}$ for $-1 \leq x \leq 1$. Let $q(x) = 2^{1-n}T_n(x)$ and $x_i = \cos(\frac{i\pi}{n})$, $0 \leq i \leq n$. Then q is a monic polynomial of degree n. We have

$$\begin{aligned} (-1)^i p(x_i) \leq |p(x_i)| < 2^{1-n} &= (-1)^i q(x_i) \\ \Longrightarrow (-1)^i(q(x_i) - p(x_i)) &> 0, \quad \textit{for } 0 \leq i \leq n. \end{aligned}$$

This shows that $q - p$ oscillates in sign at least $n+1$ times on $[-1, 1]$.
Therefore, $q - p$ have at least n roots in $(-1, 1)$.
This is a contradiction since $q - p$ has degree at most $n - 1$

(Note that x^n will not appear in $q - p$). $\square$

Choosing the nodes

Theorem: *If the nodes x_i are the roots of the Chebyshev polynomial T_{n+1}, then the error formula for the interpolation polynomial p_n yields*

$$|f(x) - p_n(x)| \leq \frac{1}{2^n(n+1)!} \max_{|t|\leq 1} |f^{(n+1)}(t)|, \quad -1 \leq x \leq 1.$$

Proof: By the error formula of the polynomial interpolation p_n of f,

$$\max_{|x|\leq 1} |f(x) - p_n(x)| \leq \frac{1}{(n+1)!} \max_{|t|\leq 1} \left| f^{(n+1)}(t) \right| \max_{|x|\leq 1} \left| \prod_{i=0}^{n} (x - x_i) \right|.$$

By the theorem on the previous page, we have

$$\max_{|x|\leq 1} \left| \prod_{i=0}^{n} (x - x_i) \right| \geq 2^{-n}.$$

Let $x_i = \cos\left(\frac{2i+1}{2n+2}\pi\right)$ for $0 \leq i \leq n$, the roots of T_{n+1}. Then we can show that $2^{-n}T_{n+1}(x) = \prod_{i=0}^{n}(x - x_i)$. Since $|T_n(x)| \leq 1$ for $-1 \leq x \leq 1$, we have

$$\max_{|x|\leq 1} \left| \prod_{i=0}^{n} (x - x_i) \right| = \max_{|x|\leq 1} |2^{-n}T_{n+1}(x)| \leq 2^{-n}. \quad \square$$

(cf. pp. 221-229, E. Isaacson and H. B. Keller, Analysis of Numerical Methods, 1966)

The convergence of interpolating polynomials

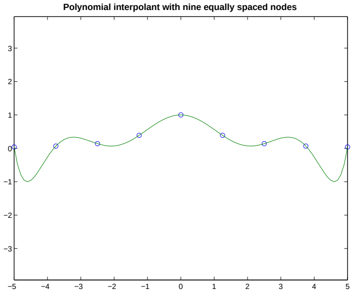
Assume that $f \in C[a,b]$, and if interpolating polynomials p_n of higher and higher degree are constructed for f, then the *natural expectation* is that these polynomials will converge to f uniformly on $[a,b]$. i.e.,

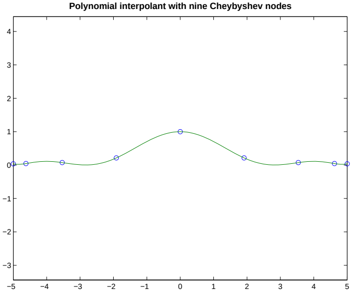
$$\|f - p_n\|_\infty := \max_{a \le x \le b} |f(x) - p_n(x)| \to 0 \text{ as } n \to \infty.$$

- This is true for $f(x) = \sin x$ on $[0,1]$ for any given nodes (p.15).
- **Runge example:** $f(x) = \dfrac{1}{1+x^2}$ on $[-5,5]$. If interpolating polynomials p_n are constructed using equally spaced nodes in $[-5,5]$, the sequence $\{a_n := \|f - p_n\|_\infty\}$ is not bounded.
- **Faber's Theorem:** *For any prescribed,* $a \le x_0^{(n)} < \cdots < x_n^{(n)} \le b$, $n \ge 0$, $\exists f \in C[a,b]$ *s.t. the interpolating polynomials for f using these nodes fail to converge uniformly to f.*
- **Theorem on convergence of interpolants:** *If* $f \in C[a,b]$, *then* $\exists$ $a \le x_0^{(n)} < x_1^{(n)} < \cdots < x_n^{(n)} \le b$, $n \ge 0$, *s.t. the interpolating polynomials* p_n *for f using these nodes satisfy* $\lim_{n\to\infty} \|f - p_n\|_\infty = 0$.

Polynomial interpolants with different sets of nodes

Consider the function $f(x) = \dfrac{1}{1+x^2}$ for $x \in [-5, 5]$.





The technique for choosing points to minimize the interpolating error can be extended to a general closed interval $[a, b]$ by using the *change of variables,*

$$\tilde{x} = \frac{1}{2}\left((b-a)x + a + b\right),$$

to shift the numbers x_i in $[-1, 1]$ into the corresponding numbers $\tilde{x}_i$.

Divided differences (均差)

- Let f be a function whose values are known at points (nodes) $x_0, x_1, \cdots x_n$.
- We assume that these nodes are distinct, but they need not be ordered.
- We know there is a unique polynomial p_n of degree at most n such that

$$p(x_i) = f(x_i) \quad \textit{for } 0 \le i \le n.$$

- p_n can be constructed as a linear combination of $1, x, x^2, \cdots, x^n$.

Divided differences (cont'd)

Instead, we should use the Newton form of the interpolating polynomial:

$$
\begin{aligned}
q_0(x) &= 1, \\
q_1(x) &= (x - x_0), \\
q_2(x) &= (x - x_0)(x - x_1), \\
q_3(x) &= (x - x_0)(x - x_1)(x - x_2), \\
&\vdots \\
q_n(x) &= (x - x_0)(x - x_1)(x - x_2)\cdots(x - x_{n-1}).
\end{aligned}
$$

$$
p_n(x) = \sum_{j=0}^{n} c_j q_j(x).
$$

Divided differences (cont'd)

- The interpolation conditions give rise to a linear system of equations for the unknown coefficients:

$$\sum_{j=0}^{n} c_j q_j(x_i) = f(x_i) \quad \textit{for } 0 \le i \le n.$$

- The elements of the coefficient matrix are

$$a_{ij} = q_j(x_i) \quad \textit{for } 0 \le i, j \le n.$$

- The $(n+1) \times (n+1)$ matrix $A = (a_{ij})$ is lower triangular because

$$q_j(x) = \prod_{k=0}^{j-1} (x - x_k)$$

$$\Longrightarrow \; a_{ij} = q_j(x_i) = \prod_{k=0}^{j-1} (x_i - x_k) = 0 \quad \textit{if } i \le j-1.$$

Divided differences (cont'd)

- For example, consider the case of three nodes with

$$\begin{aligned} p_2(x) &= c_0 q_0(x) + c_1 q_1(x) + c_2 q_2(x) \\ &= c_0 + c_1(x - x_0) + c_2(x - x_0)(x - x_1). \end{aligned}$$

  Setting $x = x_0, x = x_1$, and $x = x_2$, we have a lower triangular system

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & (x_1 - x_0) & 0 \\ 1 & (x_2 - x_0) & (x_2 - x_0)(x_2 - x_1) \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \end{bmatrix}.$$

- Thus, c_n depends on f at $x_0, x_1, \cdots, x_n$, and define the notation

$$c_n := f[x_0, x_1, \cdots, x_n],$$

  which is called a divided difference of f.

- $f[x_0, x_1, \cdots, x_n]$ is the coefficient of q_n when $\sum_{k=0}^{n} c_k q_k$ interpolates f at $x_0, x_1, \cdots, x_n$.

Divided differences (cont'd)

- Note that

$$f[x_0] = f(x_0), \quad f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}.$$

- **Theorem on higher-order divided differences (均差):** *In general, divided differences satisfy the equation:*

$$f[x_0, x_1, \cdots, x_n] = \frac{f[x_1, x_2, \cdots, x_n] - f[x_0, x_1, \cdots, x_{n-1}]}{x_n - x_0}.$$

Proof: Let p_k denote the polynomial of degree $\leq k$ that interpolates f at $x_0, x_1, \cdots, x_k$. Let q denote the polynomial of degree $\leq n-1$ that interpolates f at $x_1, x_2, \cdots, x_n$. Then we can check that

$$p_n(x) = q(x) + \frac{x - x_n}{x_n - x_0}\Big(q(x) - p_{n-1}(x)\Big),$$

because the both sides of the equality have the same values at $x_0, x_1, \cdots, x_n$ and same degree $\leq n$. Examining the coefficient of x^n on the both sides, we arrive at the assertion. □

Table of divided differences

- If a table of function values $(x_i, f(x_i))$ is given, we can construct from it a table of divided differences as follows:

x_0	$f[x_0]$	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$	$f[x_0, x_1, x_2, x_3]$
x_1	$f[x_1]$	$f[x_1, x_2]$	$f[x_1, x_2, x_3]$	
x_2	$f[x_2]$	$f[x_2, x_3]$		
x_3	$f[x_3]$			

- Note that the Newton interpolating polynomial can be written in the form

$$p_n(x) = \sum_{k=0}^{n} f[x_0, x_1, \cdots, x_k] \prod_{j=0}^{k-1} (x - x_j).$$

- The coefficients required in the Newton interpolating polynomial occupy the top row in the divided difference table.

Example

- Compute a divided difference table from

x_i	3	1	5	6
$f(x_i)$	1	-3	2	4

Solution:

$$\begin{array}{cc|ccc} 3 & 1 & 2 & -\frac{3}{8} & \frac{7}{40} \\ 1 & -3 & \frac{5}{4} & \frac{3}{20} & \\ 5 & 2 & 2 & & \\ 6 & 4 & & & \end{array}$$

- The Newton interpolating polynomial can be written as

$$p_3(x) = 1 + 2(x-3) - \frac{3}{8}(x-3)(x-1) + \frac{7}{40}(x-3)(x-1)(x-5).$$

Properties of divided differences

- **Theorem A:** *If* $(z_0, z_1, \cdots z_n)$ *is a permutation of* $(x_0, x_1, \cdots x_n)$, *then*

$$f[z_0, z_1, \cdots, z_n] = f[x_0, x_1, \cdots, x_n].$$

- **Theorem B (Theorem on the interpolation error):** *Let* p_n *be the polynomial of degree* $\leq n$ *that interpolates* f *at* $n+1$ *distinct nodes* $x_0, x_1, \cdots, x_n$. *If* $t \neq x_i$, $i = 0, 1 \cdots, n$, *then*

$$f(t) - p_n(t) = f[x_0, x_1, \cdots, x_n, t] \prod_{j=0}^{n} (t - x_j).$$

- **Theorem C (Theorem on derivatives and divided differences):** *If* $f \in C^n[a,b]$ *and* $x_0, x_1, \cdots, x_n$ *are distinct points in* $[a,b]$, *there exists a point* $\xi \in (a,b)$ *such that*

$$f[x_0, x_1, \cdots, x_n] = \frac{1}{n!} f^{(n)}(\xi).$$

Proof of Theorem A

- $f[z_0, z_1, \cdots, z_n]$ is the coefficient of x^n in the polynomial of degree $\leq n$ that interpolates f at the nodes $z_0, z_1, \cdots, z_n$.
- $f[x_0, x_1, \cdots, x_n]$ is the coefficient of x^n in the polynomial of degree $\leq n$ that interpolates f at the nodes $x_0, x_1, \cdots, x_n$.
- *These two polynomials are the same. This leads to the conclusion.* $\square$

Proof of Theorem B

Let q be the polynomial of degree $\leq n+1$ that interpolates f at the nodes $x_0, x_1, \cdots, x_n, t$. Then

$$q(x) = p_n(x) + f[x_0, x_1, \cdots, x_n, t] \prod_{j=0}^{n} (x - x_j).$$

Since $q(t) = f(t)$, we obtain

$$f(t) = q(t) = p_n(t) + f[x_0, x_1, \cdots, x_n, t] \prod_{j=0}^{n} (t - x_j).$$

Therefore,

$$f(t) - p_n(t) = f[x_0, x_1, \cdots, x_n, t] \prod_{j=0}^{n} (t - x_j).$$

□

Proof of Theorem C

Let p_{n-1} be the polynomial of degree $\leq n-1$ that interpolates f at $x_0, x_1, \cdots, x_{n-1}$. By the *Theorem on Polynomial Interpolation Error* on page 13, $\exists\, \xi \in (a, b)$ such that

$$f(x_n) - p_{n-1}(x_n) = \frac{1}{n!} f^{(n)}(\xi) \prod_{j=0}^{n-1} (x_n - x_j).$$

On the other hand, by Theorem B with $t = x_n$, we have

$$f(x_n) - p_{n-1}(x_n) = f[x_0, x_1, \cdots, x_n] \prod_{j=0}^{n-1} (x_n - x_j).$$

Therefore, we have

$$f[x_0, x_1, \cdots, x_n] = \frac{1}{n!} f^{(n)}(\xi). \quad \Box$$

Hermite interpolation

- **Regular interpolation (Lagrange interpolation)** refers to the interpolation of a function at a set of nodes:

$$f(x_i), i = 0, 1, \cdots, n, \quad \textit{are given.}$$

- **Hermite interpolation** refers to the interpolation of a function and some of its derivatives at a set of nodes:

$$f(x_i), i = 0, 1, \cdots, n, \quad \textit{are given,}$$

and

$$\textit{some of } f'(x_i), i = 0, 1, \cdots, n, \quad \textit{are given.}$$

Basic concepts

- Given f and its derivative f' at two distinct points, say x_0 and x_1, find a polynomial with the lowest degree such that

$$p(x_i) = f(x_i) \quad \textit{and} \quad p'(x_i) = f'(x_i) \quad \textit{for } i = 0, 1.$$

- What degree? Since there are four conditions, a polynomial of degree 3 seems reasonable; i.e., find a, b, c, d such that

$$p(x) = a + bx + cx^2 + dx^3$$

satisfies all the four conditions. Notice that

$$p'(x) = b + 2cx + 3dx^2.$$

- (a, b, c, d) is the solution of the following system:

$$\begin{aligned} p(x_0) &= a + bx_0 + cx_0^2 + dx_0^3 = f(x_0), \\ p(x_1) &= a + bx_1 + cx_1^2 + dx_1^3 = f(x_1), \\ p'(x_0) &= b + 2cx_0 + 3dx_0^2 = f'(x_0), \\ p'(x_1) &= b + 2cx_1 + 3dx_1^2 = f'(x_1). \end{aligned}$$

- *Does this have a solution? Unique? How to solve it?*

Basic concepts (cont'd)

- A better form of a polynomial of degree 3

$$p(x) = a + b(x - x_0) + c(x - x_0)^2 + d(x - x_0)^2(x - x_1)$$

and

$$p'(x) = b + 2c(x - x_0) + 2d(x - x_0)(x - x_1) + d(x - x_0)^2.$$

- The four conditions on p can now be written in the form

$$\begin{aligned} f(x_0) &= a, \\ f'(x_0) &= b, \\ f(x_1) &= a + bh + ch^2, \\ f'(x_1) &= b + 2ch + dh^2, \end{aligned}$$

where $h := x_1 - x_0$.

Some difficulties

- *How general is this linear system approach?*
- An example: find a polynomial p that assumes these values: $p(0) = 0, p(1) = 1, p'(\frac{1}{2}) = 2$.

$$p(x) = a + bx + cx^2.$$

(1) $p(0) = 0$ leads to $a = 0$.
(2) the other two conditions lead to

$$\begin{aligned} 1 &= p(1) = b + c, \\ 2 &= p'(\frac{1}{2}) = b + c. \end{aligned}$$

- *It doesn't work!*

Birkhoff interpolation

- Let us try a cubic polynomial

$$p(x) = a + bx + cx^2 + dx^3.$$

We discover that a solution exists but not unique.

(1) notice that $a = 0$ $\quad (\because\ p(0) = 0)$.
(2) the remaining conditions are

$$\begin{aligned} 1 &= b + c + d & (\because p(1) = 1), \\ 2 &= b + c + \frac{3}{4}d & (\because p'(\frac{1}{2}) = 2). \end{aligned}$$

- The solution of this system is $d = -4$ and $b + c = 5$ *(infinitely many solution)*.

Hermite interpolation

- In a Hermite interpolation, it is assumed that whenever a derivative $p^{(j)}(x_i)$ is prescribed at note x_i, then $p^{(j-1)}(x_i)$, $p^{(j-2)}(x_i), \cdots, p'(x_i)$ and $p(x_i)$ will also be prescribed.

  That is at node x_i, $k_i := j + 1$ interpolation conditions are prescribed. Notice that k_i may vary with i.

- Let nodes be $x_0, x_1, \cdots, x_n$. Suppose that at node x_i these interpolation conditions are given:

$$p^{(j)}(x_i) = c_{ij} \quad \textit{for } 0 \leq j \leq k_i - 1 \textit{ and } 0 \leq i \leq n.$$

- The total number of conditions on p denoted by $m + 1$, i.e.,

$$m + 1 := k_0 + k_1 + \cdots + k_n.$$

Theorem on Hermite interpolation

There exists a unique polynomial $p \in \Pi_m$ fulfilling the Hermite interpolation conditions, where Π_m is the space containing all polynomials of degree less than or equal to m.

Sketch of the proof:

From the interpolation conditions, we have an associated linear system problem, say $Ax = b$, where A is an $(m+1) \times (m+1)$ matrix.

To prove that A is nonsingular, it suffices to prove that $Ax = 0$ has only the 0 solution.

That is, we need to show that if $p \in \Pi_m$ such that

$$p^{(j)}(x_i) = 0 \quad \textit{for } 0 \le j \le k_i - 1 \textit{ and } 0 \le i \le n,$$

then $p(x) \equiv 0$. Such polynomial has a zero of multiplicity k_i at x_i for $0 \le i \le n$. Therefore, p must be a multiple of $q(x) := \prod_{i=0}^{n}(x - x_i)^{k_i}$.

Since $degree(q) = \sum_{i=0}^{n} k_i = m + 1$, we have $p(x) \equiv 0$. $\square$

Remark

What happens in Hermite interpolation when there is only one node? In this case, we require a polynomial p of degree k, for which

$$p^{(j)}(x_0) = c_{0j} \quad \textit{for } 0 \le j \le k.$$

The solution is the Taylor polynomial:

$$p(x) = c_{00} + c_{01}(x - x_0) + \frac{c_{02}}{2!}(x - x_0)^2 + \cdots + \frac{c_{0k}}{k!}(x - x_0)^k.$$

Newton form of Hermite interpolation

Suppose that we are going to find a quadratic polynomial of the form

$$p(x) = c_0 + c_1(x - x_0) + c_2(x - x_0)^2,$$

which satisfies the requirements:

$$p(x_0) = f(x_0), \quad p'(x_0) = f'(x_0) \quad \textit{and} \quad p(x_1) = f(x_1).$$

Then

$$p'(x) = c_1 + 2c_2(x - x_0)$$

and we have a lower triangular system

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & (x_1 - x_0) & (x_1 - x_0)^2 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f'(x_0) \\ f(x_1) \end{bmatrix}.$$

Thus, $c_0 = f(x_0) = f[x_0]$, c_1 depends on $f'(x_0)$, and c_2 depends on $f(x_0), f'(x_0)$, and $f(x_1)$.

Newton form of Hermite interpolation (cont'd)

- Since $\lim_{x\to x_0} f[x_0,x] = \lim_{x\to x_0} \frac{f(x)-f(x_0)}{x-x_0} = f'(x_0)$, we define

$$f[x_0,x_0] := f'(x_0).$$

Then $c_1 = f'(x_0) = f[x_0,x_0]$. From

$$f[x_0,x_1] = \frac{f(x_1)-f(x_0)}{x_1-x_0},$$

we have

$$f[x_0,x_0,x_1] = \frac{f[x_0,x_1]-f[x_0,x_0]}{x_1-x_0} = \frac{f(x_1)-f(x_0)}{(x_1-x_0)^2} - \frac{c_1}{x_1-x_0} = c_2.$$

- We can check that

$$p(x) = f(x_0) + f[x_0,x_0](x-x_0) + f[x_0,x_0,x_1](x-x_0)^2.$$

(see Problem 6.3.5)

Remarks

- We write the divided difference table in this form:

$$\begin{array}{cc|cc} x_0 & f[x_0] & f[x_0,x_0] & ? \\ x_0 & f[x_0] & ? & \\ x_1 & f[x_1] & & \end{array}$$

  The question marks stand for entries that are not yet computed. Observe that x_0 appears twice and the prescribed value of $f'(x_0)(= f[x_0,x_0])$ has been placed in the column of first-order divided differences.

- From Theorem C (page 31),

$$f[x_0, x_1, \cdots, x_k] = \frac{1}{k!} f^{(k)}(\xi),$$

  where ξ belongs to the open interval containing $x_0, x_1, \cdots, x_k$. Hence, we define

$$f[x_0, x_0, \cdots, x_0] := \frac{1}{k!} f^{(k)}(x_0).$$

  Notice that when $k \geq 2$ need to include $1/k!$ in the table.

Example

- Use the extended Newton divided difference algorithm to determine a polynomial that that takes these values:

$$p(1) = 2, \quad p'(1) = 3, \quad p(2) = 6, \quad p'(2) = 7, \quad \text{and} \quad p''(2) = 8.$$

1	2	3	?	?	?
1	2	?	?	?	
2	6	7	8/2		
2	6				
2	6				

1	2	3	1	2	−1
1	2	4	3	1	
2	6	7	4		
2	6				
2	6				

- The interpolating polynomial is

$$p(x) = 2 + 3(x-1) + (x-1)^2 + 2(x-1)^2(x-2) - (x-1)^2(x-2)^2.$$

Lagrange form of Hermite interpolation

Let us try to satisfy

$$p(x_i) = c_{i0} \quad \textit{and} \quad p'(x_i) = c_{i1}, \quad 0 \le i \le n$$

by a polynomial of the form

$$p(x) = \sum_{i=0}^{n} c_{i0} A_i(x) + \sum_{i=0}^{n} c_{i1} B_i(x).$$

Similar to the Lagrange formula, we wish the following properties:

$$\begin{cases} A_i(x_j) &= \delta_{ij}, \\ A_i'(x_j) &= 0; \end{cases} \qquad \begin{cases} B_i(x_j) &= 0, \\ B_i'(x_j) &= \delta_{ij}. \end{cases}$$

Recall the notation

$$\ell_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}.$$

Then, A_i and B_i can be defined as follows

$$\begin{cases} A_i(x) &= [1 - 2(x - x_i)\ell_i'(x_i)]\ell_i^2(x) \quad 0 \le i \le n, \\ B_i(x) &= (x - x_i)\ell_i^2(x) \quad 0 \le i \le n. \end{cases}$$

Lagrange form of Hermite interpolation (cont'd)

Take a two-point case:

$$p(x) = f(x_0)A_0(x) + f(x_1)A_1(x) + f'(x_0)B_0(x) + f'(x_1)B_1(x),$$

where

$$\begin{aligned} A_0(x) &= \left(1 - 2(x - x_0)\ell_0'(x_0)\right)\ell_0^2(x), \\ A_1(x) &= \left(1 - 2(x - x_1)\ell_1'(x_1)\right)\ell_1^2(x), \\ B_0(x) &= (x - x_0)\ell_0^2(x), \\ B_1(x) &= (x - x_1)\ell_1^2(x), \end{aligned}$$

and

$$\begin{aligned} \ell_0(x) &= \frac{x - x_1}{x_0 - x_1}, \\ \ell_1(x) &= \frac{x - x_0}{x_1 - x_0}, \\ \ell_0'(x) &= \frac{1}{x_0 - x_1}, \\ \ell_1'(x) &= \frac{1}{x_1 - x_0}. \end{aligned}$$

Theorem on Hermite interpolation error estimate

Let $x_0, x_1, \cdots, x_n$ be distinct nodes in $[a, b]$ and let $f \in C^{2n+2}[a, b]$. If p_{2n+1} is the polynomial of degree at most $2n + 1$ such that

$$p_{2n+1}(x_i) = f(x_i), \quad p'_{2n+1}(x_i) = f'(x_i) \quad \text{for } 0 \le i \le n,$$

then to each x in $[a, b]$ there corresponds a point ξ in (a, b) such that

$$f(x) - p_{2n+1}(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!} \prod_{i=0}^{n} (x - x_i)^2.$$

Sketch of the proof: The proof is similar to the proof of Theorem on Lagrange interpolation error estimate, pp. 13-14.

Let $x \in [a, b]$ be any point other than x_i, $i = 0, 1, \cdots, n$. Define

$$\begin{aligned} w(t) &= \prod_{i=0}^{n} (t - x_i)^2 && \text{(polynomial in } t\text{)}, \\ \varphi(t) &= f(t) - p_{2n+1}(t) - \lambda w(t) && \text{(function in } t\text{)}, \\ \lambda &= \frac{f(x) - p_{2n+1}(x)}{w(x)} && \text{(a constant that makes } \varphi(x) = 0\text{)}. \quad \square \end{aligned}$$

Spline interpolation (樣條插值)

- **A spline function** consists of polynomial pieces on subintervals joined together with certain continuity conditions. Formally, suppose that $n+1$ points (knots) $t_0, t_1, \cdots, t_n$ have been specified and satisfy $t_0 < t_1 < \cdots < t_n$.
- **A spline function of degree** k is a function S such that
  (1) on each interval $[t_{i-1}, t_i)$, S is a polynomial of degree $\leq k$.
  (2) S has a continuous $(k-1)$st derivative on $[t_0, t_n]$.
- **Example:** A spline of degree 0 is a piecewise constant function. A spline of degree 0 can be given explicitly in the form:

$$S(x) = \begin{cases} S_0(x) = c_0 & x \in [t_0, t_1), \\ S_1(x) = c_1 & x \in [t_1, t_2), \\ \vdots & \vdots \\ S_{n-1}(x) = c_{n-1} & x \in [t_{n-1}, t_n]. \end{cases}$$

A spline of degree 1

A spline function of degree 1 takes the following form:

$$S(x) = \begin{cases} S_0(x) = a_0 x + b_0 & x \in [t_0, t_1), \\ S_1(x) = a_1 x + b_1 & x \in [t_1, t_2), \\ \vdots & \vdots \\ S_{n-1}(x) = a_{n-1} x + b_{n-1} & x \in [t_{n-1}, t_n]. \end{cases}$$

- Note that when $k = 1$, the $k - 1$ derivative has to be continuous, i.e., $S(x)$ has to be continuous on $[t_0, t_n]$.
- The pieces are not independent. They have to satisfy the conditions

$$S_i(t_{i+1}) = S_{i+1}(t_{i+1}) \quad \textit{for } i = 0, 1, \cdots, n-2.$$

Cubic splines $(k = 3)$

- Cubic splines are most famous and often used in practice.
- We assume that a table of value has been given

x	t_0	t_1	$\cdots$	t_n
y	y_0	y_1	$\cdots$	y_n

  On each interval $[t_0, t_1], [t_1, t_2], \cdot, [t_{n-1}, t_n]$, S is given by a different cubic polynomial.

- Let S_i be the cubic polynomial that represent S on $[t_i, t_{i+1}]$. Thus,

$$S(x) = \begin{cases} S_0(x) & x \in [t_0, t_1], \\ S_1(x) & x \in [t_1, t_2], \\ \vdots & \vdots \\ S_{n-1}(x) & x \in [t_{n-1}, t_n]. \end{cases}$$

Cubic splines (cont'd)

- The polynomials S_{i-1} and S_i interpolate the same value at the point t_i and therefore

$$S_{i-1}(t_i) = y_i = S_i(t_i) \quad \textit{for } 1 \le i \le n-1.$$

  This implies that $S(x)$ is continuous.

- Now, since $k = 3$, we also need to have both $S'(x)$ and $S''(x)$ to be continuous.

- *How do we satisfy these conditions?*

  (1) we have $4n$ coefficients for n cubic polynomials.
  (2) on each subinterval $[t_i, t_{i+1}]$, we have 2 interpolation conditions: $S(t_i) = y_i$ and $S(t_{i+1}) = y_{i+1} \Longrightarrow 2n$ conditions.
  (3) continuity of $S' \Longrightarrow$ one condition at each knot: $S'_{i-1}(t_i) = S'_i(t_i) \Longrightarrow n-1$ conditions.
  (4) similarly for $S'' \Longrightarrow n-1$ conditions.
  (5) total: $4n-2$ conditions, $4n$ coefficients. $\Longrightarrow$ *two degrees of freedom.*

Derive the equation for $S_i(x)$ on $[t_i, t_{i+1}]$

- Let $z_i := S''(t_i)$ for $0 \le i \le n$. $S''(x)$ is continuous everywhere including the nodes

$$\lim_{x \downarrow t_i} S''(x) = z_i = \lim_{x \uparrow t_i} S''(x) \quad \textit{for } 1 \le i \le n-1.$$

- Since S_i is a cubic polynomial on $[t_i, t_{i+1}]$, $S_i''(x)$ is a degree 1 polynomial (linear function) satisfying $S_i''(t_i) = z_i$ and $S_i''(t_{i+1}) = z_{i+1}$. Then

$$S_i''(x) = \frac{z_i}{h_i}(t_{i+1} - x) + \frac{z_{i+1}}{h_i}(x - t_i),$$

  where $h_i = t_{i+1} - t_i$.

- Taking the integral twice to obtain S_i itself,

$$S_i(x) = \frac{z_i}{6h_i}(t_{i+1} - x)^3 + \frac{z_{i+1}}{6h_i}(x - t_i)^3 + C(x - t_i) + D(t_{i+1} - x),$$

  where C and D are integration constants.

Derive the equation for $S_i(x)$ on $[t_i, t_{i+1}]$ (cont'd)

- We need to use other conditions to determine C and D.
- Using the interpolation conditions

$$S_i(t_i) = y_i \quad \textit{and} \quad S_i(t_{i+1}) = y_{i+1},$$

we obtain

$$\begin{aligned} S_i(x) &= \frac{z_i}{6h_i}(t_{i+1} - x)^3 + \frac{z_{i+1}}{6h_i}(x - t_i)^3 \\ &+ \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}h_i}{6}\right)(x - t_i) + \left(\frac{y_i}{h_i} - \frac{z_i h_i}{6}\right)(t_{i+1} - x). \end{aligned}$$

- **Note:** We still do not know the values of z_i and z_{i+1}.

Derive the equation for $S_i(x)$ on $[t_i, t_{i+1}]$ (cont'd)

- Let us use the condition that S' is continuous. This means

$$
\begin{aligned}
S'_{i-1}(t_i) &= S'_i(t_i), \\
S'_i(t_i) &= -\frac{h_i}{3}z_i - \frac{h_i}{6}z_{i+1} - \frac{y_i}{h_i} + \frac{y_{i+1}}{h_i}, \\
S'_{i-1}(t_i) &= \frac{h_{i-1}}{6}z_{i-1} + \frac{h_{i-1}}{3}z_i - \frac{y_{i-1}}{h_{i-1}} + \frac{y_i}{h_{i-1}}.
\end{aligned}
$$

- Hence, we have

$$
h_{i-1}z_{i-1} + 2(h_i + h_{i-1})z_i + h_i z_{i+1} = \frac{6}{h_i}(y_{i+1} - y_i) - \frac{6}{h_{i-1}}(y_i - y_{i-1}),
$$

  where z_{i-1}, z_i and z_{i+1} are the unknowns, everything else is known.

- The above equation is valid only for points $t_1, t_2, \cdots, t_{n-1}$. Why?
- **Boundary conditions:** For z_0 and z_n, we can pick any values. *natural cubic spline:* $z_0 = z_n = 0$.

A linear system

- Putting all the conditions togethers, for $i = 1, 2, \cdots, n-1$, we have

$$\begin{bmatrix} u_1 & h_1 & & & & \\ h_1 & u_2 & h_2 & & & \\ & h_2 & u_3 & h_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & h_{n-1} & u_{n-2} & h_{n-2} \\ & & & & h_{n-2} & u_{n-1} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_{n-2} \\ z_{n-1} \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{n-2} \\ v_{n-1} \end{bmatrix},$$

where

$$h_i = t_{i+1} - t_i, \quad u_i = 2(h_i + h_{i-1}),$$
$$b_i = \frac{6}{h_i}(y_{i+1} - y_i), \quad v_i = b_i - b_{i-1}.$$

- The matrix is strictly diagonally dominant, therefore it is nonsingular!

Smoothness properties

- **Theorem on optimality of natural cubic splines:** *If f'' is continuous in $[a, b]$, then*

$$\int_a^b (S''(x))^2 dx \le \int_a^b (f''(x))^2 dx.$$

Proof: See Textbook, page 355. $\square$

- Recall, the curvature of a smooth function $f : \mathbb{R} \to \mathbb{R}$ is

$$|f''(x)|(1 + (f'(x))^2)^{-3/2} \approx |f''(x)| \quad \text{if } f'(x) \text{ is small.}$$

- The natural cubic spline function has a curvature *"smaller"* than that of f over an interval $[a, b]$.

A classical problem in best approximation

- **Problem:** A continuous function f is defined on an interval $[a,b]$. For a fixed n, we ask for a polynomial p of degree at most n such that

$$\max_{a \le x \le b} |f(x) - p(x)| \quad \textit{is minimized.}$$

- **Remarks:**
  - Interpolations use pointwise values, e.g., Lagrange interpolation: $p(x_i) = f(x_i)$.
  - Approximations use global information.

Some backgrounds

Consider a normed linear space $(E, \|\cdot\|)$ and a subspace G in E.

- For any $f \in E$, the distance from f to G is defined as

$$dist(f, G) = \inf_{g \in G} \|f - g\|.$$

- If an element $g^* \in G$ has the property

$$\|f - g^*\| = dist(f, G) = \inf_{g \in G} \|f - g\|,$$

  then g^* achieves this minimum deviation. It is a best approximation of f from G.

  The meaning of best approximation thus depends on the norm chosen for the problem.

Some backgrounds (cont'd)

- In the classic problem mentioned on page 59, the normed space is $E := C[a,b]$, the space of all continuous functions defined on $[a,b]$, and the norm is defined by

$$\|f\|_\infty := \max_{a\le x\le b} |f(x)| \quad for\, f \in C[a,b].$$

The subspace G is the space Π_n of all polynomials of degree $\le n$.

- In general, best approximations are not unique. For example, let $f(x) = \cos x$ on $[0,\pi/2]$. Then $f \in C[0,\pi/2]$. Let $G = span\{x\}$, then G is a finite-dimensional subspace of $C[0,\pi/2]$. Then $g(x) = \lambda x$ are best approximations for all $0 \le \lambda \le 2/\pi$ in $\|\cdot\|_\infty$.

Solution: By definition, we have

$$\begin{aligned} dist(f,G) &= \inf_{g\in G}\|f-g\|_\infty = \inf_{g\in G}\max_{0\le x\le \pi/2}|f(x)-g(x)| \\ &= \inf_{\lambda\in\mathbb{R}}\max_{0\le x\le \pi/2}|\cos x - \lambda x| = 1, \end{aligned}$$

and $\|f-\lambda x\|_\infty = 1, \forall\, 0 \le \lambda \le 2/\pi$.

Theorem on existence of best approximation

If G is a finite-dimensional subspace in a normed linear space E, then each point of E possesses at least one best approximation in G.

Sketch of the proof:

Let $f \in E$. If $g \in G$ is a best approximation of f, then
$\|f - g\| \le \|f - 0\| = \|f\|$ (since $0 \in G$).

Define $K = \{h \in G : \ \|f - h\| \le \|f\|\}$. Then K is closed and bounded.

Since G is a finite-dimensional space and $K \subseteq G$, K is compact.

(**Note:** A normed linear space is finite-dimensional if and only if every bounded subset is "relatively compact")

$\because$ The function $F : G \to \mathbb{R}$ defined by $F(h) := \|f - h\|$ is continuous.

$\therefore$ F attains minimum on the compact set K.

$\therefore \exists\, g \in K$ such that $\|f - g\| = \min_{h \in K} \|f - h\| (\underbrace{=}_{(why?)} \inf_{h \in G} \|f - h\|)$. $\Box$

Inner product spaces

- A real inner product space is a real linear space E with an inner product $\langle \cdot, \cdot \rangle : E \times E \to \mathbb{R}$ satisfying the following properties: for any $f, g \in E$,
  (1) $\langle f,f \rangle \geq 0$ and $\langle f,f \rangle = 0$ *if and only if* $f = 0$.
  (2) $\langle f,h \rangle = \langle h,f \rangle$.
  (3) $\langle f, \alpha h + \beta g \rangle = \alpha \langle f, h \rangle + \beta \langle f, g \rangle$, for any $\alpha, \beta \in \mathbb{R}$.
- A natural norm associated with the inner product is defined as $\|f\| = \sqrt{\langle f,f \rangle}$.
- We write $f \perp g$ if $\langle f, g \rangle = 0$. We write $f \perp G$ if $f \perp g$ for all $g \in G$.

Examples

Two important inner-product spaces are

- $\mathbb{R}^n$ with

$$\langle x, y \rangle = \sum_{i=1}^{n} x_i y_i.$$

- $C_w[a, b]$, the space of continuous functions on $[a, b]$, with

$$\langle f, g \rangle = \int_a^b f(x) g(x) w(x) dx,$$

where $w(x)$ is a fixed continuous positive function (for example, $w(x) \equiv 1$).

Lemma on inner product space properties

In an inner product space, we have

- $\left\langle \sum_{i=1}^{n} a_i f_i, g \right\rangle = \sum_{i=1}^{n} a_i \langle f_i, g \rangle$.
- $\|f+g\|^2 = \|f\|^2 + 2\langle f, g\rangle + \|g\|^2$.
- If $f \perp g$, then $\|f+g\|^2 = \|f\|^2 + \|g\|^2$ (Pythagorean law).
- $|\langle f, g\rangle| \le \|f\| \|g\|$ (Schwarz inequality).
- $\|f+g\|^2 + \|f-g\|^2 = 2\|f\|^2 + 2\|g\|^2$.

Proof: see Textbook, page 395. □

Theorem on characterizing best approximation

Let G be a subspace in an inner product space E. For $f \in E$ and $g \in G$, the following two properties are equivalent:

1. *g is a best approximation to f in G.*
2. *$(f-g) \perp G$.*

Proof: (2) $\Rightarrow$ (1): If $f - g \perp G$, then for any $h \in G$ we have, by the Pythagorean law,

$$\|f-h\|^2 = \|(f-g)+(g-h)\|^2 = \|f-g\|^2 + \|g-h\|^2 \geq \|f-g\|^2.$$

$\therefore$ we have (1).

(1) $\Rightarrow$ (2): Let $h \in G$ and $\lambda > 0$. Then

$$\begin{aligned} 0 &\leq \|f-g+\lambda h\|^2 - \|f-g\|^2 \\ &= \|f-g\|^2 + 2\lambda\langle f-g, h\rangle + \lambda^2\|h\|^2 - \|f-g\|^2 \\ &= \lambda\{2\langle f-g, h\rangle + \lambda\|h\|^2\}. \end{aligned}$$

Letting $\lambda \to 0^+$, we obtain $\langle f-g, h\rangle \geq 0$. Replacing h by $-h$, we have $\langle f-g, -h\rangle \geq 0$. Therefore $\langle f-g, h\rangle = 0$. Since h is arbitrary in G, $(f-g)\perp G$. $\square$

Example

- Determine the best approximation of the function $f(x) = \sin x$ by a polynomial $g(x) = c_1 x + c_2 x^3 + c_3 x^5$ on the interval $[-1, 1]$ using the inner product:

$$\langle f, g \rangle := \int_{-1}^{1} f(x) g(x) dx, \quad \forall f, g \in L^2(-1, 1).$$

- The optimal function g has the property $(f - g) \perp G$. G is the space generated by $g_1(x) = x$, $g_2(x) = x^3$, and $g_3(x) = x^5$. Thus, $\langle g - f, g_i \rangle = 0$ is required for $i = 1, 2, 3$.

$$c_1 \langle g_1, g_i \rangle + c_2 \langle g_2, g_i \rangle + c_3 \langle g_3, g_i \rangle = \langle f, g_i \rangle \quad \textit{for } i = 1, 2, 3.$$

- These are called the normal equations.

Example (cont'd)

- Putting in the details, we have

$$\begin{cases} c_1 \int_{-1}^{1} x^2 dx + c_2 \int_{-1}^{1} x^4 dx + c_3 \int_{-1}^{1} x^6 dx & = & \int_{-1}^{1} x \sin x dx, \\ c_1 \int_{-1}^{1} x^4 dx + c_2 \int_{-1}^{1} x^6 dx + c_3 \int_{-1}^{1} x^8 dx & = & \int_{-1}^{1} x^3 \sin x dx, \\ c_1 \int_{-1}^{1} x^6 dx + c_2 \int_{-1}^{1} x^8 dx + c_3 \int_{-1}^{1} x^{10} dx & = & \int_{-1}^{1} x^5 \sin x dx. \end{cases}$$

- Results in a 3×3 linear system:

$$\begin{bmatrix} \frac{1}{3} & \frac{1}{5} & \frac{1}{7} \\ \frac{1}{5} & \frac{1}{7} & \frac{1}{9} \\ \frac{1}{7} & \frac{1}{9} & \frac{1}{11} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} \alpha - \beta \\ -3\alpha + 5\beta \\ 65\alpha - 101\beta \end{bmatrix},$$

  where $\alpha = \sin 1$ and $\beta = \cos 1$. Solving this system, we obtain $c_1 \approx -0.99998$, $c_2 \approx -0.16652$, and $c_3 \approx 0.00802$.

- This coefficient matrix is an example of the ill-conditioned *Hilbert matrix.*

The Gram matrix

- Let $\{u_1, u_2, \cdots, u_n\}$ be any basis for a subspace U. In order that an element $u \in U$ be the best approximation to f, it is necessary and sufficient that $u - f \perp U$ by the *Theorem on characterizing best approximation* (cf. page 66).
- An equivalent condition is that $\langle u - f, u_i \rangle = 0$ for $1 \le i \le n$. Setting $u = \sum_{j=1}^{n} c_j u_j$, we find

$$\sum_{j=1}^{n} c_j \langle u_j, u_i \rangle = \langle f, u_i \rangle \quad \textit{for } 1 \le i \le n.$$

- These are the normal equations: n linear equations in the n unknowns $c_1, c_2, \cdots, c_n$. The coefficient matrix G is called a Gram matrix, where $G_{ij} = \langle u_i, u_j \rangle = \langle u_j, u_i \rangle$.
- **Lemma on Gram matrix:** *If $\{u_1, u_2, \cdots, u_n\}$ is linearly independent, then its Gram matrix is nonsingular* (see page 403).

Orthonormal systems

- A sequence of vectors $f_1, f_2, \cdots$ in an inner product space is
  (1) orthogonal if $\langle f_i, f_j \rangle = 0 \quad$ for $i \neq j$.
  (2) orthonormal if $\langle f_i, f_j \rangle = \delta_{ij} \quad$ for all i, j.

- **Theorem on constructing best approximation:** *Let $\{g_1, \cdots, g_n\}$ be an orthonormal system in an inner product space E. The best approximation of f by an element $\sum_{i=1}^{n} c_i g_i$ is obtained if and only if $c_i = \langle f, g_i \rangle$.*

  Proof: Let $G = span\{g_1, g_2, \cdots, g_n\}$. Then

$$\sum_{i=1}^{n} c_i g_i \textit{ is a best approximation of } f \textit{ in } G$$

$$\iff (f - \sum_{i=1}^{n} c_i g_i) \perp G \iff (f - \sum_{i=1}^{n} c_i g_i) \perp g_j \textit{ for } j = 1, 2, \cdots, n.$$

$$\iff 0 = \left\langle f - \sum_{i=1}^{n} c_i g_i, g_j \right\rangle = \langle f, g_j \rangle - \sum_{i=1}^{n} c_i \langle g_i, g_j \rangle = \langle f, g_j \rangle - c_j. \qquad \square$$

Example

We reconsider the previous example: $\sin x \approx c_1 x + c_2 x^3 + c_3 x^5$. It is known that an orthonormal basis for our three-dimensional subspace is provided by three Legendre polynomials as follows:

$$\begin{aligned} g_1(x) &= \frac{x}{\sqrt{2/3}}, \\ g_2(x) &= \frac{5x^3 - 3x}{2\sqrt{2/7}}, \\ g_3(x) &= \frac{63x^5 - 70x^3 + 15x}{8\sqrt{2/11}}. \end{aligned}$$

Example (cont'd)

The solution is then the polynomial $\sum_{i=1}^{3} c_i g_i$, where $c_i = \langle f, g_i \rangle$.

$$
\begin{aligned}
c_1 &= \sqrt{3/2}\int_{-1}^{1} x \sin x dx = 2\sqrt{3/2}(\alpha - \beta), \\
c_2 &= \frac{1}{2}\sqrt{7/2}\int_{-1}^{1} \sin x(5x^3 - 3x)dx = \sqrt{7/2}(-18\alpha + 28\beta), \\
c_3 &= \frac{1}{8}\sqrt{11/2}\int_{-1}^{1} \sin x(63x^5 - 70x^3 + 15x)dx \\
&= \frac{1}{4}\sqrt{11/2}(4320\alpha - 6728\beta),
\end{aligned}
$$

where $\alpha = \sin 1$ and $\beta = \cos 1$. The approximate solution is $c_1 \approx 0.738$, $c_2 \approx -3.37 \times 10^{-2}$, and $c_3 \approx 4.34 \times 10^{-4}$.

Theorem on Gram-Schmidt process

Let $\{v_1, v_2, \cdots, v_n\}$ *be a basis for a subspace* U *in an inner-product space. Define recursively*

$$u_i = \left\| v_i - \sum_{j=1}^{i-1} \langle v_i, u_j \rangle u_j \right\|^{-1} \left(v_i - \sum_{j=1}^{i-1} \langle v_i, u_j \rangle u_j \right) \quad \text{for } i = 1, 2, \cdots, n.$$

Then $\{u_1, u_2, \cdots, u_n\}$ *is an orthonormal base for* U.

Proof: see Textbook, page 399. □

Theorem on orthogonal polynomials

The sequence of polynomial defined inductively as following is orthogonal:

$$p_n(x) = (x - a_n)p_{n-1}(x) - b_n p_{n-2}(x) \quad \textit{for } n \geq 2,$$

with $p_0(x) = 1$, $p_1(x) = x - a_1$, *and*

$$\begin{aligned} a_n &= \langle x p_{n-1}, p_{n-1} \rangle / \langle p_{n-1}, p_{n-1} \rangle \quad \textit{for } n \geq 1, \\ b_n &= \langle x p_{n-1}, p_{n-2} \rangle / \langle p_{n-2}, p_{n-2} \rangle \quad \textit{for } n \geq 2, \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ *is any inner product provided it has the property:* $\langle fg, h \rangle = \langle f, gh \rangle$, *e.g.,* $\langle f, g \rangle = \int_a^b f(x) g(x) w(x) dx$.

Proof: Since each p_i is a monic polynomial of degree i, $\langle p_i, p_i \rangle \neq 0$ for all i. We show by induction on n that

$$\langle p_n, p_i \rangle = 0, \quad \text{for } i = 0, 1, \cdots, n-1.$$

$$n = 1: \quad \langle p_1, p_0 \rangle = \langle (x - a_1) p_0, p_0 \rangle = \langle x p_0, p_0 \rangle - a_1 \langle p_0, p_0 \rangle = 0.$$

Proof of the theorem on orthogonal polynomials (cont'd)

Suppose that the assertion holds for $n-1$. We wish to prove that it is still true for n.

$$
\begin{aligned}
\langle p_n, p_{n-1}\rangle &= \langle xp_{n-1}, p_{n-1}\rangle - a_n\langle p_{n-1}, p_{n-1}\rangle - b_n\langle p_{n-2}, p_{n-1}\rangle = 0, \\
\langle p_n, p_{n-2}\rangle &= \langle xp_{n-1}, p_{n-2}\rangle - a_n\langle p_{n-1}, p_{n-2}\rangle - b_n\langle p_{n-2}, p_{n-2}\rangle = 0.
\end{aligned}
$$

For $i = 0, 1, \cdots, n-3$, we have

$$
\begin{aligned}
\langle p_n, p_i\rangle &= \langle xp_{n-1}, p_i\rangle - a_n\langle p_{n-1}, p_i\rangle - b_n\langle p_{n-2}, p_i\rangle = \langle p_{n-1}, xp_i\rangle \\
&= \langle p_{n-1}, p_{i+1} + a_{i+1}p_i + b_{i+1}p_{i-1}\rangle = 0.
\end{aligned}
$$

Legendre polynomials

Combining the inner product $\langle f, g\rangle := \int_{-1}^{1} f(x)g(x)dx$ with the theorem above, we have the Legendre polynomials:

$p_0(x) = 1.$

$$a_1 = \langle xp_0, p_0\rangle / \langle p_0, p_0\rangle = 0.$$

$p_1(x) = x.$

$$a_2 = \langle xp_1, p_1\rangle / \langle p_1, p_1\rangle = 0.$$

$$b_2 = \langle xp_1, p_0\rangle / \langle p_0, p_0\rangle = \frac{1}{3}.$$

$p_2(x) = x^2 - \frac{1}{3}.$

Similarly, we have

$p_3(x) = x^3 - \frac{3}{5}x.$

$p_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}.$

$p_5(x) = x^5 - \frac{10}{9}x^3 + \frac{5}{21}x.$

Chebyshev polynomials

The Chebyshev polynomials form an orthogonal system on $[-1,1]$ using the following inner product:

$$\langle f,g\rangle := \int_{-1}^{1} f(x)g(x)\frac{dx}{\sqrt{1-x^2}}.$$

Solution: Changing of variable $x = \cos\theta$, we have

$$\langle f,g\rangle := \int_0^{\pi} f(\cos\theta)g(\cos\theta)d\theta.$$

Since $T_n(x) = \cos(n\cos^{-1}x)$, we have for $n \neq m$,

$$\begin{aligned}\langle T_n, T_m\rangle &= \int_0^{\pi}\cos(n\theta)\cos(m\theta)d\theta = \frac{1}{2}\int_0^{\pi}\cos(n+m)\theta + \cos(n-m)\theta d\theta \\ &= \frac{1}{2}\Big[\frac{\sin(n+m)\theta}{n+m} + \frac{\sin(n-m)\theta}{n-m}\Big]_0^{\pi} = 0.\end{aligned}$$

Least squares problems

- Given a data set $\{(x_i, f_i), i = 1, 2, \cdots, m\}$. We would like to approximate the data set using functions in the following space: $F = span\{\phi_1(x), \phi_2(x), \cdots, \phi_n(x)\}$, where $\phi_1(x), \phi_2(x), \cdots, \phi_n(x)$ are the basis functions. In general, $m \gg n$.

  Functions in F take the form $\phi(x) = c_1\phi_1(x) + \cdots + c_n\phi_n(x)$.

- **Question:** can we find a $\phi(x) \in F$, such as all conditions in the data set are satisfied:

$$\phi(x_i) = f_i, i = 1, 2, \cdots, m,$$

  which is the same as saying the following

$$\begin{aligned} c_1\phi_1(x_1) + c_2\phi_2(x_1) + \cdots + c_n\phi_n(x_1) &= f_1, \\ c_1\phi_1(x_2) + c_2\phi_2(x_2) + \cdots + c_n\phi_n(x_2) &= f_2, \\ &\cdots \\ c_1\phi_1(x_m) + c_2\phi_2(x_m) + \cdots + c_n\phi_n(x_m) &= f_m. \end{aligned}$$

- This is not a square system, and usually has no solution.

Least squares problems (cont'd)

- No solution in the classical sense, but we can define a least squares solution.
- Define $d_i = f_i - (c_1\phi_1(x_i) + c_2\phi_2(x_i) + \cdots + c_n\phi_n(x_i))$, $i = 1, 2, \cdots, m$.
- If we can't make all $d_i = 0$, can we make all of them small?
- Define a vector $d = (d_1, d_2, \cdots, d_m)^\top$, and

$$\min \|d\|^2.$$

  Using the 2-norm, we have

$$\min(d_1^2 + d_2^2 + \cdots + d_m^2).$$

Least squares problems (cont'd)

- Define

$$\Psi(c_1, c_2, \cdots, c_n) := \|d\|_2^2 = \sum_{i=1}^{m} \left(f_i - \sum_{j=1}^{n} c_j \phi_j(x_i) \right)^2.$$

- Want to find $c_1, c_2, \cdots, c_n$ such that $\Psi(c_1, c_2, \cdots, c_n)$ is minimized.

$$\frac{\partial \Psi}{\partial c_\ell} = 0, \quad \textit{for } \ell = 1, 2, \cdots, n.$$

  This leads to a linear system problem:

$$Gc = b.$$

  Here G is an $n \times n$ Gram matrix.