

# MA 8020: Numerical Analysis II

## Approximating Functions



Suh-Yuh Yang (楊肅煜)

Department of Mathematics, National Central University  
Jhongli District, Taoyuan City 320317, Taiwan

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## Polynomial interpolation

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- 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

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

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

## Theorem on polynomial interpolation

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

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

*Proof:* (uniqueness)

Suppose there were two such polynomials  $p_n$  and  $q_n$ .

Then  $(p_n - q_n)(x_i) = 0$  for  $0 \leq i \leq n$ .

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),

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

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:

$$c_0 = y_0 = 1, c_1 = 2, c_2 = 3 \text{ and } c_3 = 4 \implies$$

$$p_3(x) = 1 + 2(x - 5) + 3(x - 5)(x + 7) + 4(x - 5)(x + 7)(x + 6),$$

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

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

- $\ell_0, \ell_1, \dots, \ell_n$  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  $\ell_0$ . It is a polynomial of degree  $n$  that takes the value 0 at  $x_1, x_2, \dots, x_n$  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  $\ell_i$  is obtained by similar reasoning:

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

## Example

$x$	$\parallel$	5		-7		-6		0
$y$	$\parallel$	1		-23		-54		-954

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

$$\ell_0(x) = \frac{(x+7)(x+6)x}{(5+7)(5+6)5} = \frac{1}{660}x(x+6)(x+7),$$

$$\ell_1(x) = \frac{(x-5)(x+6)x}{(-7-5)(-7+6)(-7)} = \frac{-1}{84}x(x-5)(x+6),$$

$$\ell_2(x) = \frac{(x-5)(x+7)x}{(-6-5)(-6+7)(-6)} = \frac{-1}{66}x(x-5)(x+7),$$

$$\ell_3(x) = \frac{(x-5)(x+7)(x+6)}{(0-5)(0+7)(0+6)} = \frac{-1}{210}(x-5)(x+6)(x+7).$$

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 method

- Assume that

$$p_n(x) = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n.$$

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

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

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

## Homework #1

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

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

Then obviously we have  $\det X = V_n(x_n)$ .

- (1) Show that  $V_n(x)$  is a polynomial of degree  $n$  and its roots are  $x_0, x_1, \dots, x_{n-1}$  by deriving 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  $x^n$ .

- (2) Show that

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

## 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)  $x_0, x_1, \dots, x_n$  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  $x_i, i = 0, 1, \dots, n$ . Define

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

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

## Theorem on polynomial interpolation error (cont'd)

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*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

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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:

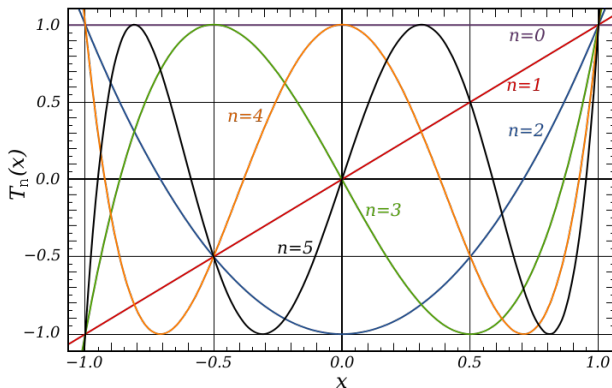
$$\begin{cases} T_0(x) &= 1, \\ T_1(x) &= x, \\ T_{n+1}(x) &= 2xT_n(x) - T_{n-1}(x) \quad \text{for } n \geq 1. \end{cases}$$

- 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: $T_0, T_1, \dots, T_5$



(quoted from wikipedia.org)

## Properties of the Chebyshev polynomials

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

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

*Proof:* Recall the addition formula for the cosine:

$$\cos(n+1)\theta = \cos \theta \cos n\theta - \sin \theta \sin n\theta,$$

$$\cos(n-1)\theta = \cos \theta \cos n\theta + \sin \theta \sin n\theta.$$

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

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

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

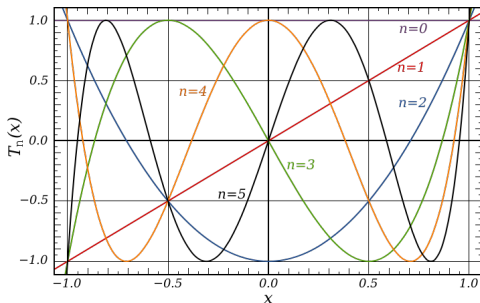
From (★), we have

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

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

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

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  $f$ ,

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

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

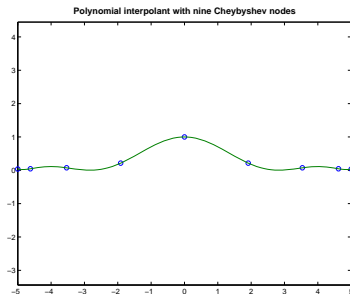
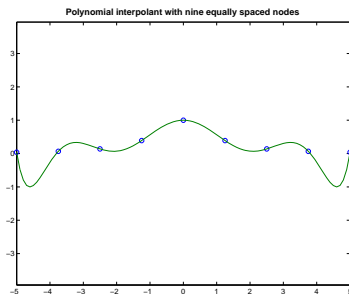
Assume that  $f \in C[a, b]$ , and if interpolating polynomials  $p_n$  of higher and higher degree are constructed for  $f$ , then the *natural expectation* is that these polynomials will converge to  $f$  uniformly on  $[a, b]$ . i.e.,

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

- This is true for  $f(x) = \sin x$  on  $[0, 1]$  for any given nodes (p.15).
- **Runge example:**  $f(x) = \frac{1}{1+x^2}$  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,  $a \leq x_0^{(n)} < \dots < x_n^{(n)} \leq b$ ,  $n \geq 0$ ,  $\exists f \in C[a, b]$  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  $\exists a \leq x_0^{(n)} < x_1^{(n)} < \dots < x_n^{(n)} \leq b$ ,  $n \geq 0$ , s.t. the interpolating polynomials  $p_n$  for  $f$  using these nodes satisfy  $\lim_{n \rightarrow \infty} \|f - p_n\|_\infty = 0$ .*

## Polynomial interpolants with different sets of nodes

Consider the function  $f(x) = \frac{1}{1+x^2}$  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*,

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

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

## Divided differences (均差)

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- Let  $f$  be a function whose values are given at points (nodes)  $x_0, x_1, \dots, x_n$ .
- 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

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

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

## Divided differences (cont'd)

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Instead, we use the Newton form of the interpolating polynomial. Let

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

Then we have

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

for some  $c_j$  given on page 6.

## Divided differences (cont'd)

- The interpolation conditions give rise to a linear system of equations  $Ac = f$  for the unknown coefficients  $c_j$ 's:

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

- The elements of the coefficient matrix  $A = (a_{ij})$  are

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

- The  $(n+1) \times (n+1)$  matrix  $A$  is *lower triangular* because

$$\begin{aligned} q_j(x) &= \prod_{k=0}^{j-1} (x - x_k) \\ \implies a_{ij} &= q_j(x_i) = \prod_{k=0}^{j-1} (x_i - x_k) = 0 \quad \text{if } i \leq j-1. \end{aligned}$$

## Divided differences (cont'd)

- For example, consider the case of three nodes with

$$\begin{aligned}p_2(x) &= c_0q_0(x) + c_1q_1(x) + c_2q_2(x) \\ &= c_0 + c_1(x - x_0) + c_2(x - x_0)(x - x_1).\end{aligned}$$

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  $x_0, x_1, \dots, x_n$ , and define the notation

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

which is called a *divided difference* of  $f$ .

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

## 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:*

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

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

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

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

## 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

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

- 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
$y_i = f(x_i)$	1	-3	2	4

*Solution:*

3	1	2	$-\frac{3}{8}$	$\frac{7}{40}$
1	-3	$\frac{5}{4}$	$\frac{3}{20}$	
5	2	2		
6	4			

- 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  $(z_0, z_1, \dots, z_n)$  is a permutation of  $(x_0, x_1, \dots, x_n)$ , then*

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

- **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  $x_0, x_1, \dots, x_n$ . If  $t \neq x_i, i = 0, 1, \dots, n$ , then*

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

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

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

## Proof of Theorem A

---

- $f[z_0, z_1, \dots, z_n]$  is the coefficient of  $x^n$  in the polynomial of degree  $\leq n$  that interpolates  $f$  at the nodes  $z_0, z_1, \dots, z_n$ .
- $f[x_0, x_1, \dots, x_n]$  is the coefficient of  $x^n$  in the polynomial of degree  $\leq n$  that interpolates  $f$  at the nodes  $x_0, x_1, \dots, x_n$ .
- *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  $x_0, x_1, \dots, x_n, t$ . Then

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

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

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

Therefore,

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



## Proof of Theorem C

---

Let  $p_{n-1}$  be the polynomial of degree  $\leq n-1$  that interpolates  $f$  at  $x_0, x_1, \dots, x_{n-1}$ . 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

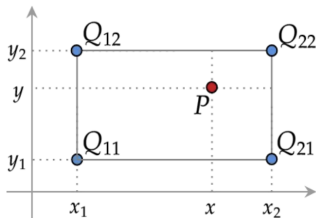
$$f(x_n) - p_{n-1}(x_n) = f[x_0, x_1, \dots, x_n] \prod_{j=0}^{n-1} (x_n - x_j).$$

Therefore, we have

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

## Bilinear interpolation

Assume that the function values of  $f$  are given at four points:  
 $Q_{11} = (x_1, y_1)$ ,  $Q_{12} = (x_1, y_2)$ ,  $Q_{21} = (x_2, y_1)$ , and  $Q_{22} = (x_2, y_2)$ .



*(cited from “omni calculator”)*

Then by the Lagrange linear interpolation, we have

$$f(x, y_1) \approx \frac{x - x_2}{x_1 - x_2} f(Q_{11}) + \frac{x - x_1}{x_2 - x_1} f(Q_{21}),$$

$$f(x, y_2) \approx \frac{x - x_2}{x_1 - x_2} f(Q_{12}) + \frac{x - x_1}{x_2 - x_1} f(Q_{22}).$$

## Bilinear interpolation (cont'd)

Let  $P = (x, y)$  be a given point in the rectangular region enclosed by  $Q_{11}$ ,  $Q_{12}$ ,  $Q_{21}$ , and  $Q_{22}$ . By the Lagrange linear interpolation again,

$$\begin{aligned} f(x, y) &\approx p_{11}(x, y) = \frac{y - y_2}{y_1 - y_2} f(x, y_1) + \frac{y - y_1}{y_2 - y_1} f(x, y_2) \\ &= \frac{y - y_2}{y_1 - y_2} \left( \frac{x - x_2}{x_1 - x_2} f(Q_{11}) + \frac{x - x_1}{x_2 - x_1} f(Q_{21}) \right) \\ &\quad + \frac{y - y_1}{y_2 - y_1} \left( \frac{x - x_2}{x_1 - x_2} f(Q_{12}) + \frac{x - x_1}{x_2 - x_1} f(Q_{22}) \right) \\ &= \frac{1}{(x_1 - x_2)(y_1 - y_2)} \left( f(Q_{11})(x - x_2)(y - y_2) \right. \\ &\quad \left. + f(Q_{21})(x - x_1)(y_2 - y) + f(Q_{12})(x_2 - x)(y - y_1) \right. \\ &\quad \left. + f(Q_{22})(x - x_1)(y - y_1) \right) \\ &= \frac{1}{(x_1 - x_2)(y_1 - y_2)} \begin{bmatrix} x_2 - x \\ x - x_1 \end{bmatrix}^T \begin{bmatrix} f(Q_{11}) & f(Q_{12}) \\ f(Q_{21}) & f(Q_{22}) \end{bmatrix} \begin{bmatrix} y_2 - y \\ y - y_1 \end{bmatrix}. \end{aligned}$$

## A direct approach: bilinear and bicubic interpolations

---

- For bilinear interpolation, a direct approach is given by

$$f(x, y) \approx p_{11}(x, y) = a + bx + cy + dxy,$$

where the four coefficients are determined from the four equations in four unknowns  $a, b, c, d$ :

$$f(Q_{11}) = a + bx_1 + cy_1 + dx_1y_1,$$

$$f(Q_{12}) = a + bx_1 + cy_2 + dx_1y_2,$$

$$f(Q_{21}) = a + bx_2 + cy_1 + dx_2y_1,$$

$$f(Q_{22}) = a + bx_2 + cy_2 + dx_2y_2.$$

- For bicubic interpolation, a direct approach is given by

$$f(x, y) \approx p_{33}(x, y) = \sum_{i=0}^3 \sum_{j=0}^3 a_{ij} x^i y^j,$$

where the 16 coefficients  $a_{ij}$ ,  $0 \leq i, j \leq 3$  are determined from the 16 equations with 16 unknowns, using the function values of the 16 nearest neighboring points in the rectangular region.

## Hermite interpolation

---

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

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

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

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

and

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

## 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

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

- 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:

$$p(x_0) = a + bx_0 + cx_0^2 + dx_0^3 = f(x_0),$$

$$p(x_1) = a + bx_1 + cx_1^2 + dx_1^3 = f(x_1),$$

$$p'(x_0) = b + 2cx_0 + 3dx_0^2 = f'(x_0),$$

$$p'(x_1) = b + 2cx_1 + 3dx_1^2 = f'(x_1).$$

- 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

$$1 = p(1) = b + c,$$

$$2 = p'(\frac{1}{2}) = b + c.$$

- *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  $a = 0$  ( $\because p(0) = 0$ ).
- (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 node  $x_i$ , then  $p^{(j-1)}(x_i)$ ,  $p^{(j-2)}(x_i), \dots, p'(x_i)$  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  $x_0, x_1, \dots, x_n$ . Suppose that at node  $x_i$  these interpolation conditions are given:

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

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

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

## Theorem on Hermite interpolation

---

*There exists a unique polynomial  $p \in \Pi_m$  fulfilling the Hermite interpolation conditions, where  $\Pi_m$  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

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

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

Since  $\text{degree}(q) = \sum_{i=0}^n k_i = m+1$ , 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

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

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:

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

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  $\lim_{x \rightarrow x_0} f[x_0, x] = \lim_{x \rightarrow x_0} \frac{f(x) - f(x_0)}{x - x_0} = f'(x_0)$ , 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:

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

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),

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

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

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

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 takes these values:

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

$$\begin{array}{cc|ccc} 1 & 2 & 3 & ? & ? & ? \\ 1 & 2 & ? & ? & ? & \\ 2 & 6 & 7 & 8/2 & & \\ 2 & 6 & & & & \\ 2 & 6 & & & & \end{array}$$

$$\begin{array}{cc|cccc} 1 & 2 & 3 & 1 & 2 & -1 \\ 1 & 2 & 4 & 3 & 1 & \\ 2 & 6 & 7 & 4 & & \\ 2 & 6 & & & & \\ 2 & 6 & & & & \end{array}$$

- 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

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

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:

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

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

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

## 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

$$A_0(x) = (1 - 2(x - x_0)\ell'_0(x_0))\ell_0^2(x),$$

$$A_1(x) = (1 - 2(x - x_1)\ell'_1(x_1))\ell_1^2(x),$$

$$B_0(x) = (x - x_0)\ell_0^2(x),$$

$$B_1(x) = (x - x_1)\ell_1^2(x),$$

and

$$\ell_0(x) = \frac{x - x_1}{x_0 - x_1},$$

$$\ell_1(x) = \frac{x - x_0}{x_1 - x_0},$$

$$\ell'_0(x) = \frac{1}{x_0 - x_1},$$

$$\ell'_1(x) = \frac{1}{x_1 - x_0}.$$

## Theorem on Hermite interpolation error estimate

Let  $x_0, x_1, \dots, x_n$  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

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

then to each  $x$  in  $[a, b]$  there corresponds a point  $\xi$  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  $x_i, i = 0, 1, \dots, n$ . Define

$$w(t) = \prod_{i=0}^n (t - x_i)^2 \quad (\text{polynomial in } t),$$

$$\varphi(t) = f(t) - p_{2n+1}(t) - \lambda w(t) \quad (\text{function in } t),$$

$$\lambda = \frac{f(x) - p_{2n+1}(x)}{w(x)} \quad (\text{a constant that makes } \varphi(x) = 0). \quad \square$$

## 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)  $t_0, t_1, \dots, t_n$  have been specified and satisfy  $t_0 < t_1 < \dots < t_n$ .
- **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:

$$S(x) = \begin{cases} S_0(x) = a_0x + b_0 & x \in [t_0, t_1), \\ S_1(x) = a_1x + b_1 & x \in [t_1, t_2), \\ \vdots & \vdots \\ S_{n-1}(x) = a_{n-1}x + b_{n-1} & x \in [t_{n-1}, t_n]. \end{cases}$$

- 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

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

## 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  $[t_0, t_1], [t_1, t_2], \dots, [t_{n-1}, t_n]$ ,  $S$  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

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

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  $S(t_{i+1}) = y_{i+1} \implies 2n$  conditions.
  - (3) continuity of  $S' \implies$  one condition at each knot:  
 $S'_{i-1}(t_i) = S'_i(t_i) \implies n-1$  conditions.
  - (4) similarly for  $S'' \implies n-1$  conditions.
  - (5) total:  $4n-2$  conditions,  $4n$  coefficients.  $\implies$  *two degrees of freedom.*

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

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

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

- 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

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

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

$$S'_{i-1}(t_i) = S'_i(t_i),$$

$$S'_i(t_i) = -\frac{h_i}{3}z_i - \frac{h_i}{6}z_{i+1} - \frac{y_i}{h_i} + \frac{y_{i+1}}{h_i},$$

$$S'_{i-1}(t_i) = \frac{h_{i-1}}{6}z_{i-1} + \frac{h_{i-1}}{3}z_i - \frac{y_{i-1}}{h_{i-1}} + \frac{y_i}{h_{i-1}}.$$

- 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  $t_1, t_2, \dots, t_{n-1}$ . 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 together, for  $i = 1, 2, \dots, n-1$ , 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

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

- 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*

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

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

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

$$\max_{a \leq x \leq b} |f(x) - p(x)| \text{ is minimized.}$$

- **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

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

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

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

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 62, the normed space is  $E := C[a, b]$ , the space of all continuous functions defined on  $[a, b]$ , and the norm is defined by

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

The subspace  $G$  is the space  $\Pi_n$  of all polynomials of degree  $\leq n$ .

- 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  $G = \text{span}\{x\}$ , then  $G$  is a finite-dimensional subspace of  $C[0, \pi/2]$ . Then  $g(x) = \lambda x$  are best approximations for all  $0 \leq \lambda \leq 2/\pi$  in  $\|\cdot\|_{\infty}$ .

*Solution:* By definition, we have

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

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

## 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  $\|f - g\| \leq \|f - 0\| = \|f\|$  (since  $0 \in G$ ).

Define  $K = \{h \in G : \|f - h\| \leq \|f\|\}$ . 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”)**

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

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

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

## Inner product spaces

---

- A real inner product space is a real linear space  $E$  with an inner product  $\langle \cdot, \cdot \rangle : E \times E \rightarrow \mathbb{R}$  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

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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).
- $|\langle f, g \rangle| \leq \|f\| \|g\|$  (Schwarz inequality).
- $\|f + g\|^2 + \|f - g\|^2 = 2\|f\|^2 + 2\|g\|^2.$

*Proof:* see Textbook, page 395.  $\square$

## 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  $\lambda \rightarrow 0^+$ , 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  $g(x) = c_1x + c_2x^3 + c_3x^5$  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  $i = 1, 2, 3$ .

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

- 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  $3 \times 3$  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  $\{u_1, u_2, \dots, u_n\}$  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 69).
- An equivalent condition is that  $\langle u - f, u_i \rangle = 0$  for  $1 \leq i \leq n$ . Setting  $u = \sum_{j=1}^n c_j u_j$ , we find

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

- These are the normal equations:  $n$  linear equations in the  $n$  unknowns  $c_1, c_2, \dots, c_n$ . 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  $\{u_1, u_2, \dots, u_n\}$  is linearly independent, then its Gram matrix is nonsingular* (see page 403).

## Orthonormal systems

- A sequence of vectors  $f_1, f_2, \dots$  in an inner product space is
  - (1) orthogonal if  $\langle f_i, f_j \rangle = 0$  for  $i \neq j$ .
  - (2) orthonormal if  $\langle f_i, f_j \rangle = \delta_{ij}$  for all  $i, j$ .
- **Theorem on constructing best approximation:** *Let  $\{g_1, \dots, g_n\}$  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  $G = \text{span}\{g_1, g_2, \dots, g_n\}$ . Then

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

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

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

## Example

---

We reconsider the previous example:  $\sin x \approx c_1x + c_2x^3 + c_3x^5$ . 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  $c_i = \langle f, g_i \rangle$ .

$$c_1 = \sqrt{3/2} \int_{-1}^1 x \sin x dx = 2\sqrt{3/2}(\alpha - \beta),$$

$$c_2 = \frac{1}{2}\sqrt{7/2} \int_{-1}^1 \sin x (5x^3 - 3x) dx = \sqrt{7/2}(-18\alpha + 28\beta),$$

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

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

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

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

*Proof:* see Textbook, page 399.  $\square$

## Theorem on orthogonal polynomials

---

*The sequence of polynomial defined inductively as following is orthogonal:*

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

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

$$a_n = \langle xp_{n-1}, p_{n-1} \rangle / \langle p_{n-1}, p_{n-1} \rangle \quad \text{for } n \geq 1,$$

$$b_n = \langle xp_{n-1}, p_{n-2} \rangle / \langle p_{n-2}, p_{n-2} \rangle \quad \text{for } n \geq 2,$$

*where  $\langle \cdot, \cdot \rangle$  is any inner product provided it has the property:*

$$\langle fg, h \rangle = \langle f, gh \rangle, \text{ e.g., } \langle f, g \rangle = \int_a^b f(x)g(x)w(x)dx.$$

*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

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

$$n = 1 : \quad \langle p_1, p_0 \rangle = \langle (x - a_1)p_0, p_0 \rangle = \langle xp_0, p_0 \rangle - a_1 \langle p_0, p_0 \rangle = 0.$$

## 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  $i = 0, 1, \dots, n - 3$ , 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  $n \neq m$ ,

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

## Least squares approximation

- Given a data set  $\{(x_i, y_i), i = 1, 2, \dots, m\}$ . We would like to approximate the data set using functions in the following space:  $F = \text{span}\{\phi_1, \phi_2, \dots, \phi_n\}$ , where  $\phi_1, \phi_2, \dots, \phi_n$  are the basis functions of the function space  $F$ . In general,  $m \gg n$ . Functions in  $F$  take the form  $\phi(x) = c_1\phi_1(x) + \dots + c_n\phi_n(x)$ .
- Question:** can we find a  $\phi(x) \in F$ , such as all conditions in the data set are satisfied:

$$\phi(x_i) = y_i, i = 1, 2, \dots, m,$$

which is the same as saying the following

$$c_1\phi_1(x_1) + c_2\phi_2(x_1) + \dots + c_n\phi_n(x_1) = y_1,$$

$$c_1\phi_1(x_2) + c_2\phi_2(x_2) + \dots + c_n\phi_n(x_2) = y_2,$$

...

$$c_1\phi_1(x_m) + c_2\phi_2(x_m) + \dots + c_n\phi_n(x_m) = y_m.$$

- We obtain  $A_{m \times n} c_{n \times 1} = y_{m \times 1}$ . This is not a square system, and usually has no solution.

## Least squares approximation (cont'd)

- No solution in the classical sense, but we can define a least squares solution.
- Define  $d_i = y_i - (c_1\phi_1(x_i) + c_2\phi_2(x_i) + \cdots + c_n\phi_n(x_i))$  for  $1 \leq i \leq m$ . That is,  $\mathbf{d} := \mathbf{y} - A\mathbf{c}$ , where  $\mathbf{d} = (d_1, d_2, \dots, d_m)^\top$ ,  $\mathbf{y} = (y_1, y_2, \dots, y_m)^\top$ ,  $\mathbf{c} = (c_1, c_2, \dots, c_n)^\top$ , and

$$A = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_n(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \cdots & \phi_n(x_2) \\ & & \vdots & \\ \phi_1(x_m) & \phi_2(x_m) & \cdots & \phi_n(x_m) \end{bmatrix}_{m \times n}.$$

- If we can't make all  $d_i = 0$ , can we make all of them small?  
We then consider the least squares problem:

$$\min_{\mathbf{c}} \|\mathbf{d}\|_2^2 = \min_{\mathbf{c}} \|\mathbf{y} - A\mathbf{c}\|_2^2.$$

## Least squares approximation (cont'd)

- Define

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

- We want to find  $c_1, c_2, \dots, c_n$  such that  $\Psi(c_1, c_2, \dots, c_n)$  is minimized:

$$\frac{\partial \Psi}{\partial c_k} = 0, \quad \text{for } k = 1, 2, \dots, n.$$

This leads to a linear system problem:

$$A^\top A c = A^\top y,$$

where  $A^\top A$  is an  $n \times n$  Gram matrix.

- In general, the column vectors of matrix  $A$  are linearly independent, provided  $\phi_1, \phi_2, \dots, \phi_n$  are linearly independent and data points  $x_1, x_2, \dots, x_m$  are sufficiently numerous and well-distributed. *In that case,  $A^\top A$  is nonsingular.*