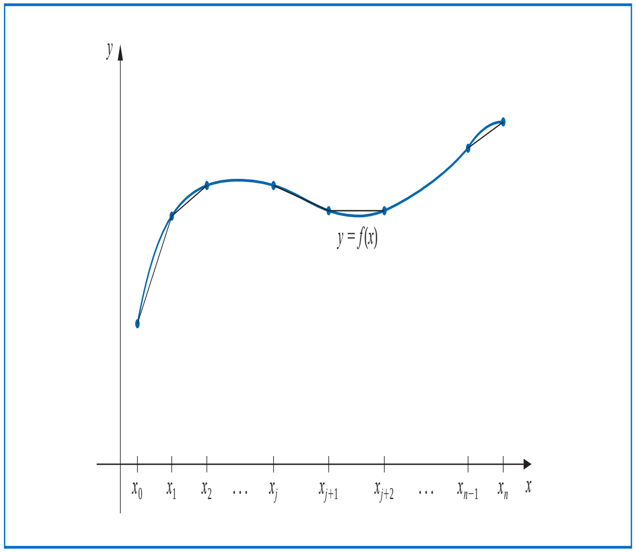
COURSE 5

2.5. Cubic spline interpolation

Lagrange, Hermite, Birkhoff interpolants of large degrees could oscillate widely; a minor fluctuation over a small portion of the interval can induce large fluctuations over the entire interval.

An alternative: to divide the interval into a collection of subintervals and construct a (generally) different approximating polynomial on each subinterval. This is called **piecewise-polynomial approximation.**



Let $f : [a, b] \to \mathbb{R}$ be the approximating function. Examples of piecewise-polynomial interpolation:

- piecewise-linear interpolation: consists of joining a set of data points $\{(x_0, f(x_0)), (x_1, f(x_1)), ..., (x_n, f(x_n))\}$ by a series of straight lines

  Disadvantage: there is likely no differentiability at the endpoints of the subintervals, (the interpolating function is not "smooth"). Often, from physical conditions, that smoothness is required.

- Hermite interpolation when values of f and f' are known at the points $x_0 < x_1 < ... < x_n$;

  Disadvantage: we need to know f' and this is frequently unavailable.

- spline interpolation: piecewise polynomials that require no specific derivative information, except perhaps at the endpoints of the interval.

Definition 1 *The piecewise-polynomial approximation that uses cubic spline polynomials between each successive pair of nodes is called* **cubic spline interpolation.**

(The word "spline" was used to refer to a long flexible strip, generally of metal, that could be used to draw continuous smooth curves by forcing the strip to pass through specified points and tracing along the curve.)

Definition 2 *Let $f : [a, b] \to \mathbb{R}$ and the nodes $a = x_0 < x_1 < ... < x_n = b$, a* **cubic spline interpolant** *S for f is the function that satisfies the following conditions:*

(a) $S(x)$ *is a cubic polynomial, denoted* $S_j(x)$ *on the subinterval* $[x_j, x_{j+1}]$, $\forall j = 0, 1, ..., n-1$, *i.e.,*

$$S(x) = \begin{cases} S_0(x), & x \in [x_0, x_1] \\ S_1(x), & x \in [x_1, x_2] \\ ... & \\ S_{n-1}(x), & x \in [x_{n-1}, x_n] \end{cases}$$

(b) $S_j(x_j) = f(x_j)$ *and* $S_j(x_{j+1}) = f(x_{j+1})$, $\forall j = 0, 1, ..., n-1$;

(c) $S_j(x_{j+1}) = S_{j+1}(x_{j+1})$, $\forall j = 0, 1, ..., n-2$;

(d) $S_j'(x_{j+1}) = S_{j+1}'(x_{j+1})$, $\forall j = 0, 1, ..., n-2$;

(e) $S_j''(x_{j+1}) = S_{j+1}''(x_{j+1})$, $\forall j = 0, 1, ..., n-2$;

(f) *One of the following boundary conditions is satisfied:*

(i) $S''(x_0) = S''(x_n) = 0$ ($\Longleftrightarrow S''_0(x_0) = S''_{n-1}(x_n) = 0$ *natural (or free) boundary)* **natural spline**;

(ii) $S'(x_0) = f'(x_0)$ *and* $S'(x_n) = f'(x_n)$ ($\Longleftrightarrow S'_0(x_0) = f'(x_0)$ *and* $S'_{n-1}(x_n) = f'(x_n)$ *clamped boundary)* **clamped spline**;

(iii) $S_1(x) = S_2(x)$ *and* $S_{n-2} = S_{n-1}$ (**de Boor spline**).

Remark 3 *A cubic spline function defined on an interval divided into* n *subintervals will require determining* $4n$ *constants.*

We have the following expression of a cubic spline:

$$S_j(x) = a_j + b_j(x - x_j) + c_j(x - x_j)^2 + d_j(x - x_j)^3, \quad \forall j = 0, 1, ..., n-1. \quad (1)$$

Theorem 4 *If* f *is defined at* $a = x_0 < x_1 < ... < x_n = b$, *then* f *has an unique natural spline interpolant* S *on the nodes* $x_0, x_1, ..., x_n$; *that satisfies the natural boundary conditions* $S''(a) = 0$ *and* $S''(b) = 0$.

Theorem 5 *If f is defined at $a = x_0 < x_1 < ... < x_n = b$ and differentiable at a and b, then f has an unique clamped spline interpolant S on the nodes $x_0, x_1, ..., x_n$; that satisfies the clamped boundary conditions $S'(a) = f'(a)$ și $S'(b) = f'(b)$.*

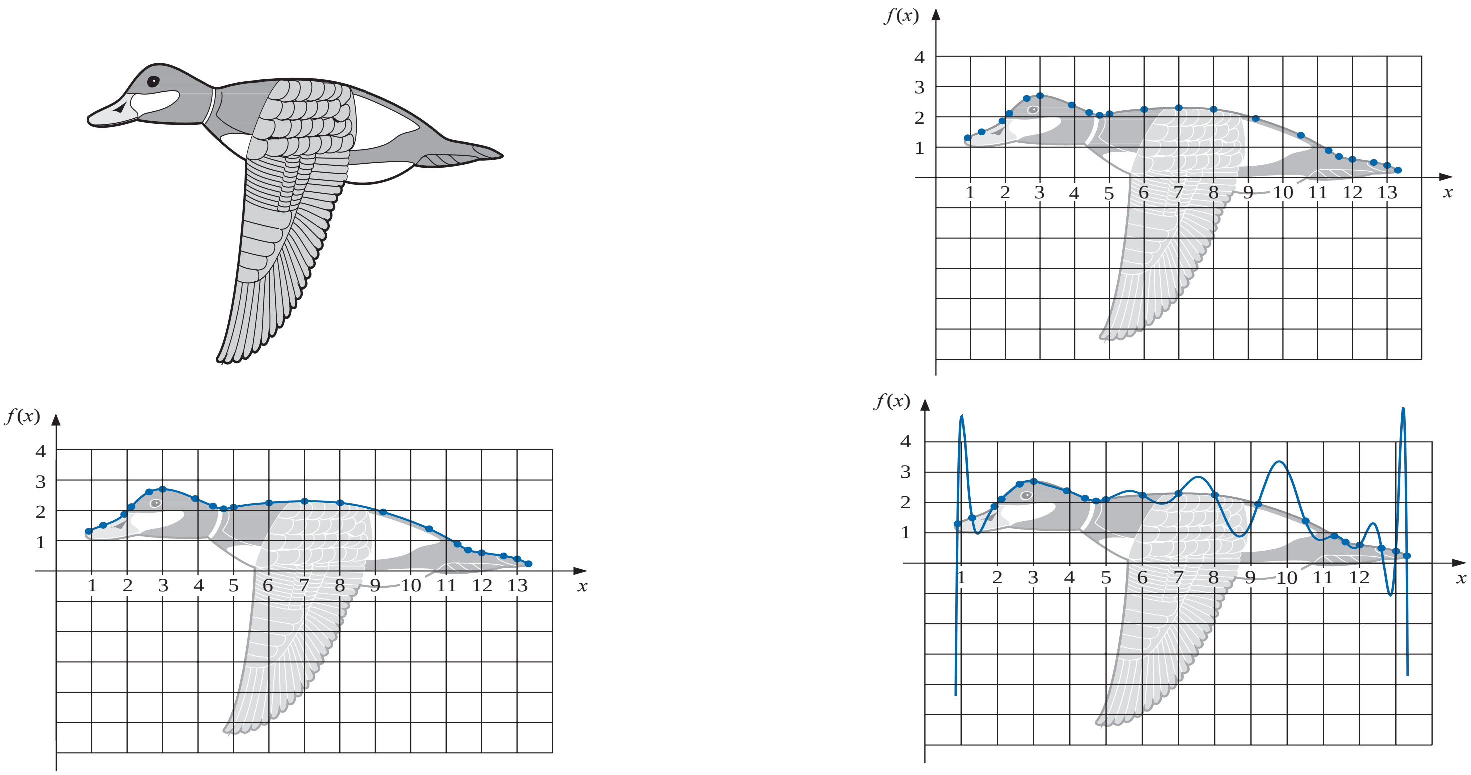
Theorem 6 *Let $f \in C^4[a,b]$ with $\max\limits_{a \le x \le b} |f^{(4)}(x)| = M$. If S is the unique clamped cubic spline interpolant to f with respect to the nodes $a = x_0 < x_1 < \cdots < x_n = b$, then for all x in $[a,b]$,*

$$|f(x) - S(x)| \le \frac{5M}{384} \max_{0 \le j \le n-1} (x_{j+1} - x_j)^4.$$

Remark 7 *A fourth-order error-bound result also holds in the case of natural boundary conditions, but it is more difficult to express.*

Remark 8 *The natural boundary conditions will generally give less accurate results than the clamped conditions near the ends of the interval $[x_0, x_n]$ unless the function f happens to nearly satisfy $f''(x_0) = f''(x_n) = 0$.*

Illustration. To approximate the top profile of a duck, we have chosen 21 points along the curve through which we want the approximating curves to pass.



1) The duck in flight. 2) The points. 3) The natural cubic spline.
4) The Lagrange interpolation polynomial.

Example 9 *Construct* **a natural cubic spline** *that passes through the points* $(1,2)$, $(2,3)$ *and* $(3,5)$.

Sol. (Sketch of the solution) *We follow Definition 2:*

Here $S(x)$ *consists of two cubic splines,* $S_j(x)$ *on the subinterval* $[x_j, x_{j+1}]$, $\forall j = 0, 1$, *i.e.,*

$$S(x) = \begin{cases} S_0(x), & x \in [x_0, x_1] \\ S_1(x), & x \in [x_1, x_2] \end{cases}$$

given by (*1*),

$$S_0(x) = a_0 + b_0(x-1) + c_0(x-1)^2 + d_0(x-1)^3,$$
$$S_1(x) = a_1 + b_1(x-2) + c_1(x-2)^2 + d_1(x-2)^3.$$

There are 8 constants ($a_i, b_i, c_i, d_i,\ i = 0, 1$) *to be determined, which requires 8 conditions, that come from (b),(c),(d),(e),(i).*

Example 10 *Construct* **a clamped spline** S *that passes through the points* $(1,2)$, $(2,3)$ *and* $(3,5)$ *and that has* $S'(1) = 2$ *and* $S'(3) = 1$.

2.6. Least squares approximation

• It is an extension of the interpolation problem.

• More desirable when the data are contaminated by errors.

• To estimate values of parameters of a mathematical model from measured data, which are subject to errors.

When we know $f(x_i)$, $i = 0, ..., m$, an interpolation method can be used to determine an approximation φ of the function f, such that

$$\varphi(x_i) = f(x_i), \ i = 0, ..., m.$$

If only approximations of $f(x_i)$ are available or the number of interp. conditions is too large, instead of requiring that the approx. function reproduces $f(x_i)$ exactly, we ask only that it fits the data "as closely as possible".

It seems that the least squares method was first introduced by C. F. Gauss in 1795. In 1801 he used it for making the best prediction for the orbital position of the planet Ceres (dwarf planet, lies between Mars and Jupiter, first considered planet and further reclassified as an asteroid) using the measurements of G. Piazzi (who was the first that discovered it).

The first clear and concise exposition of the method of least squares was first published by A. M. Legendre in 1805. P. S. Laplace and R. Adrain have also contributed to the development of this theory.

In 1809 C. F. Gauss applied the method in calculating the orbits of some celestial bodies. In that work he claimed and proved that he have been in possession of the method since 1795. The least squares approximation φ is determined such that:

- in the discrete case:

$$\left(\sum_{i=0}^{m}\left[f\left(x_i\right)-\varphi\left(x_i\right)\right]^2\right)^{1/2} \rightarrow \min,$$

- in the continuous case:

$$\left(\int_a^b [f(x) - \varphi(x)]^2 \, dx \right)^{1/2} \to \min,$$

Remark 11 *Notice that the interpolation is a particular case of the least squares approximation, with*

$$f(x_i) - \varphi(x_i) = 0, \quad i = 0, ..., m.$$

Linear least square. Consider the data

x	1	2	3	4	5
$f(x)$	1	1	2	2	4

The problem consists in finding a function φ that "best" represents the data.

Plot the data and try to recognize the shape of a "guess function φ" such that $f \approx \varphi$.

For this example, a resonable guess may be a linear one, $\varphi(x) = ax + b$. The problem: find a and b that makes φ the best function to fit the data. The least squares criterion consists in minimizing the sum

$$E(a,b) = \sum_{i=0}^{4} \left[f\left(x_i\right) - \varphi\left(x_i\right)\right]^2 = \sum_{i=0}^{4} \left[f\left(x_i\right) - \left(ax_i + b\right)\right]^2 .$$

The minimum of the sum is obtained when

$$\frac{\partial E(a,b)}{\partial a} = 0$$
$$\frac{\partial E(a,b)}{\partial b} = 0.$$

We get

$$55a + 15b = 37$$
$$15a + 5b = 10$$

and further $\varphi(x) = 0.7x - 0.1$.

Consider a more general problem with the data from the table

x	x_0	x_1	...	x_m
$f(x)$	y_0	y_1	...	y_m

and the approximating linear function $\varphi(x) = ax + b$. We have to find a and b.

We have to minimize the sum

$$E(a,b) = \sum_{i=0}^{m} [f(x_i) - \varphi(x_i)]^2 = \sum_{i=0}^{m} [f(x_i) - (ax_i + b)]^2 . \qquad (2)$$

The minimum of the sum is obtained by

$$\frac{\partial E(a,b)}{\partial a} = 2 \sum_{i=0}^{m} [f(x_i) - (ax_i + b)] \cdot (-x_i) = 0$$
$$\frac{\partial E(a,b)}{\partial b} = 2 \sum_{i=0}^{m} [f(x_i) - (ax_i + b)] \cdot (-1) = 0$$

These are called **normal equations**. Further,

$$\sum_{i=0}^{m} x_i f(x_i) = a \sum_{i=0}^{m} x_i^2 + b \sum_{i=0}^{m} x_i$$
$$\sum_{i=0}^{m} f(x_i) = a \sum_{i=0}^{m} x_i + (m+1)b.$$

The solution is

$$a = \frac{(m+1)\sum\limits_{i=0}^{m} x_i f(x_i) - \sum\limits_{i=0}^{m} x_i \sum\limits_{i=0}^{m} f(x_i)}{(m+1)\sum\limits_{i=0}^{m} x_i^2 - (\sum\limits_{i=0}^{m} x_i)^2} \tag{3}$$

$$b = \frac{\sum\limits_{i=0}^{m} x_i^2 \sum\limits_{i=0}^{m} f(x_i) - \sum\limits_{i=0}^{m} x_i f(x_i) \sum\limits_{i=0}^{m} x_i}{(m+1)\sum\limits_{i=0}^{m} x_i^2 - (\sum\limits_{i=0}^{m} x_i)^2}.$$

Example 12 *Having the data*

x	0	1	2	3
$f(x)$	-4	0	4	-2

find the corresponding least squares polynomial of the first degree.

Sol. We have

$$E(a,b)=\sum_{i=0}^{3}\left[f\left(x_i\right)-\varphi\left(x_i\right)\right]^2=\sum_{i=0}^{3}\left[f\left(x_i\right)-\left(ax_i+b\right)\right]^2 \tag{4}$$

and we have to find a and b from the system

$$\begin{cases} \frac{\partial E(a,b)}{\partial a}=2\sum\limits_{i=0}^{3}\left[f\left(x_i\right)-\left(ax_i+b\right)\right]\cdot x_i=0 \\ \frac{\partial E(a,b)}{\partial b}=2\sum\limits_{i=0}^{3}\left[f\left(x_i\right)-\left(ax_i+b\right)\right]=0 \end{cases}$$

$$\begin{cases} \sum\limits_{i=0}^{3}\left[f\left(x_i\right)-\left(ax_i+b\right)\right]\cdot x_i=0 \\ \sum\limits_{i=0}^{3}\left[f\left(x_i\right)-\left(ax_i+b\right)\right]=0 \end{cases}$$

Polynomial least squares. In many experimental results the data are not linear or can be better estimated by a polynomial. Suppose that

$$\varphi(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0.$$

Consider $m+1$ points (x_i, y_i), $i = 0, \ldots, m$.

We have to find $a_i, i = 0, ..., n$, that minimize the sum

$$\begin{aligned} E(a_0, ..., a_n) &= \sum_{i=0}^{m} \left[f\left(x_i\right) - \varphi\left(x_i\right)\right]^2 \qquad (5) \\ &= \sum_{i=0}^{m} \left[f\left(x_i\right) - \sum_{k=0}^{n} a_k x_i^k\right]^2. \end{aligned}$$

Denoting $y_i = f(x_i)$ we have

$$E(a_0, ..., a_n) = \sum_{i=0}^{m} y_i^2 - 2\sum_{i=0}^{m} y_i \varphi(x_i) + \sum_{i=0}^{m} (\varphi(x_i))^2$$
$$= \sum_{i=0}^{m} y_i^2 - 2\sum_{i=0}^{m} \left(\sum_{j=0}^{n} a_j x_i^j\right) y_i + \sum_{i=0}^{m} \left(\sum_{j=0}^{n} a_j x_i^j\right)^2$$
$$= \sum_{i=0}^{m} y_i^2 - 2\sum_{j=0}^{n} a_j \left(\sum_{i=0}^{m} x_i^j y_i\right) + \sum_{j=0}^{n}\sum_{k=0}^{n} a_j a_k \left(\sum_{i=0}^{m} x_i^{j+k}\right).$$

The minimum is obtained when

$$\frac{\partial E(a_0, ..., a_n)}{\partial a_j} = 0, \quad j = 0, ...n,$$

which are **the normal equations** and have a unique solution.

It is obtain

$$\frac{\partial E}{\partial a_j} = -2\sum_{i=0}^{m} x_i^j y_i + 2\sum_{k=0}^{n} a_k \left(\sum_{i=0}^{m} x_i^{j+k}\right) = 0$$

which gives $n+1$ unknowns $a_j,\ j \in \{0, 1, \ldots, n\}$ and $n+1$ equations

$$\sum_{i=0}^{m} x_i^j y_i = \sum_{k=0}^{n} a_k \left(\sum_{i=0}^{m} x_i^{j+k} \right), \quad \text{for each } j \in \{0, 1, \ldots, n\}. \qquad (6)$$

We have the system

$$a_0 \sum_{i=0}^{m} x_i^0 + a_1 \sum_{i=0}^{m} x_i^1 + a_2 \sum_{i=0}^{m} x_i^2 + \cdots + a_n \sum_{i=0}^{m} x_i^n = \sum_{i=0}^{m} x_i^0 y_i,$$

$$a_0 \sum_{i=0}^{m} x_i^1 + a_1 \sum_{i=0}^{m} x_i^2 + a_2 \sum_{i=0}^{m} x_i^3 + \cdots + a_n \sum_{i=0}^{m} x_i^{n+1} = \sum_{i=0}^{m} x_i^1 y_i$$

$$\ldots$$

$$a_0 \sum_{i=0}^{m} x_i^n + a_1 \sum_{i=0}^{m} x_i^{n+1} + a_2 \sum_{i=0}^{m} x_i^{n+2} + \cdots + a_n \sum_{i=0}^{m} x_i^{2n} = \sum_{i=0}^{m} x_i^n y_i$$

General case. Solution of the least squares problem is

$$\varphi(x) = \sum_{i=1}^{n} a_i g_i(x),$$

where $\{g_i,\ i = 1, ..., n\}$ is a basis of the space and the coefficients a_i are obtained solving **the normal equations**:

$$\sum_{i=1}^{n} a_i \langle g_i, g_k \rangle = \langle f, g_k \rangle \,, \qquad k = 1, ..., n.$$

In the discrete case

$$\langle f, g \rangle = \sum_{k=0}^{m} w\left(x_k\right) f\left(x_k\right) g\left(x_k\right)$$

and in the continuous case

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

where w is a weight function.

Example 13 *Fit the data in table*

x	-3	-1	2
$f(x)$	-4	-2	3

a) with the best least squares line;

b) with the best least squares polynomial of degree at most 2.