DATA ANALYSIS

Measurements

systematic vs random error
discrete points
smoothing the data
interpolation
extrapolation
difference calculus
numerical integration

→ POLYNOMIALS (Runge's phenomenon)

Errorcontrol:

collocation
osculation
method of least squares
min – max

Collocating polynomials

1.) Vandermonde matrix: $V_{ij} = x_i^{j-1}$

$$\det V = \prod_{1 \le i < j \le n} (x_i - x_j)$$

2.) Newton interpolation (set of $k+1$ data points)

$n_j := \prod_{i=0}^{j-1} (x - x_i) \Rightarrow N(x) := \sum_{j=0}^{k} a_j n_j(x)$
(basis polynomials)

method of divided differences

3.) Lagrange interpolation

$$p_j(x) = y_j \prod_{\substack{i=1 \\ i \neq j}}^{n} \frac{x - x_i}{x_j - x_i}$$

Chapter 2

The Collocation Polynomial

APPROXIMATION BY POLYNOMIALS

Approximation by polynomials is one of the oldest ideas in numerical analysis, and still one of the most heavily used. A polynomial $p(x)$ is used as a substitute for a function $y(x)$, for any of a dozen or more reasons. Perhaps most important of all, polynomials are easy to compute, only simple integer powers being involved. But their derivatives and integrals are also found without much effort and are again polynomials. Roots of polynomial equations surface with less excavation than for other functions. The popularity of polynomials as substitutes is not hard to understand.

CRITERION OF APPROXIMATION

The difference $y(x) - p(x)$ is the error of the approximation, and the central idea is, of course, to keep this error reasonably small. The simplicity of polynomials permits this goal to be approached in various ways, of which we consider

(values coinc) (val+deriv coinc)

1. collocation, 2. osculation, 3. least squares, 4. min.-max.

THE COLLOCATION POLYNOMIAL

The collocation polynomial is the target of this and the next few chapters. It coincides (collocates) with $y(x)$ at certain specified points. A number of properties of such polynomials, and of polynomials in general, play a part in the development.

1. **The existence and uniqueness theorem** states that there is exactly one collocation polynomial of degree n for arguments $x_0, \ldots, x_n$, that is, such that $y(x) = p(x)$ for these arguments. The existence will be proved by actually exhibiting such a polynomial in succeeeding chapters. The uniqueness is proved in the present chapter and is a consequence of certain elementary properties of polynomials.
2. **The division algorithm.** Any polynomial $p(x)$ may be expressed as

$$p(x) = (x - r)q(x) + R$$

where r is any number, $q(x)$ is a polynomial of degree $n - 1$, and R is a constant. This has two quick corollaries.
3. **The remainder theorem** states that $p(r) = R$.
4. **The factor theorem** states that if $p(r) = 0$, then $x - r$ is a factor of $p(x)$.
5. **The limitation on zeros.** A polynomial of degree n can have at most n zeros, meaning that the equation $p(x) = 0$ can have at most n roots. The uniqueness theorem is an immediate consequence, as will be shown.
6. **Synthetic division** is an economical procedure (or algorithm) for producing the $q(x)$ and R of the division algorithm. It is often used to obtain R, which by the remainder theorem equals $p(r)$. This path to $p(r)$ may be preferable to the direct computation of this polynomial value.
7. **The product** $\pi(x) = (x - x_0)(x - x_1) \cdots (x - x_n)$ plays a central role in collocation theory. Note that it vanishes at the arguments $x_0, x_1, \ldots, x_n$ which are our collocation arguments. The error of the collocation polynomial will be shown to be

$$y(x) - p(x) = \frac{y^{(n+1)}(\xi)\pi(x)}{(n+1)!}$$

Chapter 10

Osculating Polynomials

Osculating polynomials not only agree in value with a given function at specified arguments, which is the idea of collocation, but their derivatives up to some order also match the derivatives of the given function, usually at the same arguments. Thus for the simplest osculation, we require

$$p(x_k) = y(x_k) \qquad p'(x_k) = y'(x_k)$$

for $k = 0, 1, \ldots, n$. In the language of geometry, this makes the curves representing our two functions tangent to each other at these $n+1$ points. Higher-order osculation would also require $p''(x_k) = y''(x_k)$, and so on. The corresponding curves then have what is called contact of higher order. The existence and uniqueness of osculating polynomials can be proved by methods resembling those used with the simpler collocation polynomials.

Hermite's formula, for example, exhibits a polynomial of degree $2n+1$ or less which has first-order osculation. It has the form

$$p(x) = \sum_{i=0}^{n} U_i(x) y_i + \sum_{i=0}^{n} V_i(x) y_i'$$

where y_i and y_i' are the values of the given function and its derivative at x_i. The functions $U_i(x)$ and $V_i(x)$ are polynomials having properties similar to those of the Lagrange multipliers $L_i(x)$ presented earlier. In fact,

$$U_i(x) = [1 - 2L_i'(x_i)(x - x_i)][L_i(x)]^2$$
$$V_i(x) = (x - x_i)[L_i(x)]^2$$

The *error of Hermite's formula* can be expressed in a form resembling that of the collocation error but with a higher-order derivative, an indication of the greater accuracy obtainable by osculation. The error is

$$y(x) - p(x) = \frac{y^{(2n+2)}(\xi)}{(2n+2)!}[\pi(x)]^2$$

A *method of undetermined coefficients* may be used to obtain polynomials having higher-order osculation. For example, taking $p(x)$ in standard form

$$p(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_{3n+2} x^{3n+2}$$

and requiring $p(x_k) = y_k$, $p'(x_k) = y_k'$, $p''(x_k) = y_k''$ for the arguments $x_0, \ldots, x_n$ leads to $3n+3$ equations for the $3n+3$ coefficients c_i. Needless to say, for large n this will be a large system of equations. The methods of a later chapter may be used to solve such a system. In certain cases special devices may be used to effect simplifications.

Solved Problems

10.1. Verify that $p(x) = \sum_{i=0}^{n} U_i(x) y_i + \sum_{i=0}^{n} V_i(x) y_i'$ will be a polynomial of degree $2n+1$ or less, satisfying $p(x_k) = y_k$, $p'(x_k) = y_k'$ provided

(*a*) $U_i(x)$ and $V_i(x)$ are polynomials of degree $2n+1$.

(*b*) $U_i(x_k) = \delta_{ik}$, $V_i(x_k) = 0$.

Osculating polynomials

cubic splines

natural splines

$$\begin{bmatrix} 2 & 1 & & & & \\ 1 & 4 & 1 & & & \\ & 1 & 4 & 1 & & \\ & & & \ddots & & \\ & & & 1 & 4 & 1 \\ & & & & 1 & 2 \end{bmatrix} \begin{bmatrix} D_0 \\ D_1 \\ D_2 \\ \vdots \\ D_{n-1} \\ D_n \end{bmatrix} = \begin{bmatrix} 3(y_1 - y_0) \\ 3(y_2 - y_0) \\ 3(y_3 - y_1) \\ \vdots \\ 3(y_n - y_{n-2}) \\ 3(y_n - y_{n-1}) \end{bmatrix}$$

$$Y_i(t) = a_i + b_i t + c_i t^2 + d_i t^3 \qquad t \in [0,1]$$
$$i = 0, \dots, n-1$$

$(n+1)$ point : $(y_0, y_1, \dots, y_n)$

ith spline is $Y_i(t)$

$$\begin{cases} Y_i(0) = y_i = a_i \\ Y_i(1) = y_{i+1} = a_i + b_i + c_i + d_i \\ Y_i'(0) = D_i = b_i \\ Y_i'(1) = D_{i+1} = b_i + 2c_i + 3d_i \end{cases}$$

Least-squares methods

Objective function: $S = \sum_{i=0}^{N} \left[\left(y_i - (a_0 + a_1 x_i + \dots + a_m x_i^m) \right) \right]^2 \Rightarrow S \geq 0$

Normal equations

Example: $p(x) = Mx + B$, data: (x_i, y_i)

$$S = \sum_{i=0}^{N} (y_i - Mx_i - B)^2$$

$$0 = \frac{\partial S}{\partial B} \;\&\; \frac{\partial S}{\partial M} = 0$$

Chapter 21

Least-Squares Polynomial Approximation

THE LEAST-SQUARES PRINCIPLE

The basic idea of choosing a polynomial approximation $p(x)$ to a given function $y(x)$ in a way which minimizes the squares of the errors (in some sense) was developed first by Gauss. There are several variations, depending on the set of arguments involved and the error measure to be used.

First of all, *when the data are discrete* we may minimize the sum

$$S = \sum_{i=0}^{N} (y_i - a_0 - a_1 x_i - \cdots - a_m x_i^m)^2$$

for given data x_i, y_i, and $m < N$. The condition $m < N$ makes it unlikely that the polynomial

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$$

can collocate at all N data points. So S probably cannot be made zero. The idea of Gauss is to make S as small as we can. Standard techniques of calculus then lead to the *normal equations*, which determine the coefficients a_j. These equations are

$$\begin{aligned}
s_0 a_0 + s_1 a_1 + \cdots + s_m a_m &= t_0 \\
s_1 a_0 + s_2 a_1 + \cdots + s_{m+1} a_m &= t_1 \\
\cdots\cdots\cdots\cdots&\cdots\cdots \\
s_m a_0 + s_{m+1} a_1 + \cdots + s_{2m} a_m &= t_m
\end{aligned}$$

where $s_k = \sum_{i=0}^{N} x_i^k$, $t_k = \sum_{i=0}^{N} y_i x_i^k$. This system of linear equations does determine the a_i uniquely, and the resulting a_j do actually produce the minimum possible value of S. For the case of a linear polynomial

$$p(x) = Mx + B$$

the normal equations are easily solved and yield

$$M = \frac{s_0 t_1 - s_1 t_0}{s_0 s_2 - s_1^2} \qquad B = \frac{s_2 t_0 - s_1 t_1}{s_0 s_2 - s_1^2}$$

In order to provide a unifying treatment of the various least-squares methods to be presented, including this first method just described, a general problem of minimization in a vector space is considered. The solution is easily found by an algebraic argument, using the idea of *orthogonal projection*. Naturally the general problem reproduces our $p(x)$ and normal equations. It will be reinterpreted to solve other variations of the least-squares principle as we proceed. In most cases a duplicate argument for the special case in hand will also be provided.

Except for very low degree polynomials, the above system of normal equations proves to be *ill-conditioned*. This means that, although it does define the coefficients a_j uniquely, in practice it may prove to be impossible to extricate these a_j. Standard methods for solving linear systems (to be presented in Chapter 26) may either produce no solution at all, or else badly magnify data errors. As a result, *orthogonal polynomials* are introduced. (This amounts to choosing an orthogonal basis for the abstract vector space.) For the case of discrete data these are polynomials $P_{m,N}(t)$ of degree $m = 0, 1, 2, \ldots$ with the property

$$\sum_{t=0}^{N} P_{m,N}(t) P_{n,N}(t) = 0$$

Chapter 1

The Difference Calculus

OPERATORS

We are often concerned in mathematics with performing various operations such as squaring, cubing, adding, taking square roots, etc. Associated with these are *operators*, which can be denoted by letters of the alphabet, indicating the nature of the operation to be performed. The object on which the operation is to be performed, or on which the operator is to act, is called the *operand*.

Example 1.

If C or $[\quad]^3$ is the *cubing operator* and x is the operand then Cx or $[\quad]^3 x$ represents the cube of x, i.e. x^3.

Example 2.

If D or $\frac{d}{dx}$ is the *derivative operator* and the operand is the function of x given by $f(x) = 2x^4 - 3x^2 + 5$ then

$$Df(x) \;=\; D(2x^4 - 3x^2 + 5) \;=\; \frac{d}{dx}(2x^4 - 3x^2 + 5) \;=\; 8x^3 - 6x$$

Example 3.

If $\mathcal{J}$ or $\int (\quad)\,dx$ is the *integral operator* then

$$\mathcal{J}(2x^4 - 3x^2 + 5) \;=\; \left[\int (\quad)\,dx\right](2x^4 - 3x^2 + 5) \;=\; \int (2x^4 - 3x^2 + 5)\,dx \;=\; \frac{2x^5}{5} - x^3 + 5x + c$$

where c is an arbitrary constant.

Example 4.

The *doubling operator* can be represented by the ordinary symbol 2. Thus

$$2(2x^4 - 3x^2 + 5) \;=\; 4x^4 - 6x^2 + 10$$

It is assumed, unless otherwise stated, that the class of operands acted upon by a given operator is suitably restricted so that the results of the operation will have meaning. Thus for example with the operator D we would restrict ourselves to the set or class of *differentiable functions*, i.e. functions whose derivatives exist.

Note that if A is an operator and f is the operand then the result of the operation is indicated by Af. For the purposes of this book f will generally be some function belonging to a particular class of functions.

SOME DEFINITIONS INVOLVING OPERATORS

1. **Equality of operators.** Two operators are said to be *equal*, and we write $A = B$ or $B = A$, if and only if for an arbitrary function f we have $Af = Bf$.

2. **The identity or unit operator.** If for arbitrary f we have $If = f$ then I is called the *identity* or *unit operator*. For all practical purposes we can and will use 1 instead of I.

3. **The null or zero operator.** If for arbitrary f we have $Of = 0$ then O is called the *null* or *zero operator*. For all practical purposes we can and will use 0 instead of O.

4. Sum and difference of operators. We define

$$(A+B)f = Af + Bf, \qquad (A-B)f = Af - Bf \tag{1}$$

and refer to the operators $A+B$ and $A-B$ respectively as the *sum* and *difference* of operators A and B.

Example 5. $(C+D)x^2 = Cx^2 + Dx^2 = x^6 + 2x, \quad (C-D)x^2 = Cx^2 - Dx^2 = x^6 - 2x$

5. Product of operators. We define

$$(A \cdot B)f = (AB)f = A(Bf) \tag{2}$$

and refer to the operator AB or $A \cdot B$ as the *product* of operators A and B. If $A = B$ we denote AA or $A \cdot A$ as A^2.

Example 6. $(CD)x^2 = C(Dx^2) = C(2x) = 8x^3, \quad C^2x^2 = C(Cx^2) = C(x^6) = x^{18}$

6. Linear operators. If operator A has the property that for arbitrary functions f and g and an arbitrary constant α

$$A(f+g) = Af + Ag, \qquad A(\alpha f) = \alpha A f \tag{3}$$

then A is called a *linear operator*. If an operator is not a linear operator it is called a *non-linear operator*. See Problem 1.3.

7. Inverse operators. If A and B are operators such that $A(Bf) = f$ for an arbitrary function f, i.e. $(AB)f = f$ or $AB = I$ or $AB = 1$, then we say that B is an *inverse* of A and write $B = A^{-1} = 1/A$. Equivalently $A^{-1}f = g$ if and only if $Ag = f$.

ALGEBRA OF OPERATORS

We will be able to manipulate operators in the same manner as we manipulate algebraic quantities if the following laws of algebra hold for these operators. Here A, B, C denote any operators.

I-1.	$A + B = B + A$	Commutative law for sums
I-2.	$A + (B + C) = (A + B) + C$	Associative law for sums
I-3.	$AB = BA$	Commutative law for products
I-4.	$A(BC) = (AB)C$	Associative law for products
I-5.	$A(B + C) = AB + AC$	Distributive law

Special care must be taken in manipulating operators if these do not apply. If they do apply we can prove that other well-known rules of algebra also hold, for example the *index law* or *law of exponents* $A^mA^n = A^{m+n}$ where A^m denotes repeated application of operator A m times.

THE DIFFERENCE OPERATOR

Given a function $f(x)$ we define an operator Δ, called the *difference operator*, by

$$\Delta f(x) = f(x+h) - f(x) \tag{4}$$

where h is some given number usually positive and called the *difference interval* or *differencing interval*. If in particular $f(x) = x$ we have

$$\Delta x = (x+h) - x = h \quad \text{or} \quad h = \Delta x \tag{5}$$

Successive differences can also be taken. For example

$$\Delta^2 f(x) = \Delta[\Delta f(x)] = \Delta[f(x+h) - f(x)] = f(x+2h) - 2f(x+h) + f(x) \tag{6}$$

We call Δ^2 the *second order difference operator* or *difference operator of order 2*. In general we define the nth *order difference operator* by

$$\Delta^n f(x) = \Delta[\Delta^{n-1} f(x)] \tag{7}$$

THE TRANSLATION OR SHIFTING OPERATOR

We define the *translation* or *shifting operator* E by

$$Ef(x) = f(x+h) \tag{8}$$

By applying the operator twice we have

$$E^2 f(x) = E[Ef(x)] = E[f(x+h)] = f(x+2h)$$

In general if n is any integer [or in fact, any real number], we define

$$E^n f(x) = f(x+nh) \tag{9}$$

We can show [see Problem 1.10] that operators E and Δ are related by

$$\Delta = E - 1 \quad \text{or} \quad E = 1 + \Delta \tag{10}$$

using 1 instead of the unit operator I.

THE DERIVATIVE OPERATOR

From (4) and (5) we have

$$\frac{\Delta f(x)}{\Delta x} = \frac{f(x+h) - f(x)}{h} \tag{11}$$

where we can consider the operator acting on $f(x)$ to be $\Delta/\Delta x$ or Δ/h. The *first order derivative* or briefly *first derivative* or simply *derivative* of $f(x)$ is defined as the limit of the quotient in (11) as h or Δx approaches zero and is denoted by

$$Df(x) = f'(x) = \lim_{\Delta x \to 0} \frac{\Delta f(x)}{\Delta x} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{12}$$

if the limit exists. The operation of taking derivatives is called *differentiation* and D is the *derivative* or *differentiation operator*.

The *second derivative* or *derivative of order two* is defined as the derivative of the first derivative, assuming it exists, and is denoted by

$$D^2 f(x) = D[Df(x)] = f''(x) \tag{13}$$

We can prove that the second derivative is given by

$$D^2 f(x) = \lim_{\Delta x \to 0} \frac{\Delta^2 f(x)}{(\Delta x)^2} = \lim_{h \to 0} \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} \tag{14}$$

and can in fact take this as a definition of the second derivative. Higher ordered derivatives can be obtained similarly.

THE DIFFERENTIAL OPERATOR

The *differential of first order* or briefly *first differential* or simply *differential* of a function $f(x)$ is defined by

$$df(x) = f'(x)\,\Delta x = f'(x)h \tag{15}$$

In particular if $f(x) = x$ we have $dx = \Delta x = h$ so that (15) becomes

$$df(x) = f'(x)\,dx = f'(x)h \quad \text{or} \quad df(x) = Df(x)\,dx = hDf(x) \tag{16}$$

We call d the *differential operator.* The second order differential of $f(x)$ can be defined as

$$d^2f(x) = f''(x)(\Delta x)^2 = f''(x)(dx)^2 \tag{17}$$

and higher ordered differentials are defined similarly.

Note that $df(x)$, $dx = \Delta x = h$, $d^2f(x)$, $(dx)^2 = (\Delta x)^2 = h^2$ are numbers which are not necessarily zero and not necessarily small.

It follows from (*16*) and (*17*) that

$$f'(x) = \frac{df(x)}{dx} = Df(x), \quad f''(x) = \frac{d^2f(x)}{dx^2} = D^2f(x), \quad \ldots \tag{18}$$

where in the denominator of (*18*) we have written $(dx)^2$ as dx^2 as indicated by custom or convention. It follows that we can consider the operator equivalence

$$D = \frac{d}{dx}, \quad D^2 = \frac{d^2}{dx^2}, \quad \ldots \tag{19}$$

Similarly we shall write $\quad \dfrac{\Delta^2}{(\Delta x)^2}f(x) \quad$ as $\quad \dfrac{\Delta^2}{\Delta x^2}f(x)$

RELATIONSHIP BETWEEN DIFFERENCE, DERIVATIVE AND DIFFERENTIAL OPERATORS

From (*16*) we see that the relationship between the derivative operator D and the differential operator d is

$$D = \frac{d}{dx} = \frac{d}{h} \quad \text{or} \quad d = hD \tag{20}$$

Similarly from (*12*) and (*16*) we see that the relationship between the difference operator Δ and the derivative operator D is

$$D = \lim_{\Delta x \to 0} \frac{\Delta}{\Delta x} = \lim_{h \to 0} \frac{\Delta}{h} = \frac{d}{dx} \tag{21}$$

with analogous relationships among higher ordered operators.

Because of the close relationship of the difference operator Δ with the operators D and d as evidenced by the above we would feel that it should be possible to develop a *difference calculus* or *calculus of differences* analogous to *differential calculus* which would give the results of the latter in the special case where h or Δx approaches zero. This is in fact the case as we shall see and since h is taken as some given constant, called *finite,* as opposed to a variable approaching zero, called *infinitesimal,* we refer to such a calculus as the *calculus of finite differences.*

To recognize the analogy more clearly we will first review briefly some of the results of differential calculus.

GENERAL RULES OF DIFFERENTIATION

It is assumed that the student is already familiar with the elementary rules for differentiation of functions. In the following we list some of the most important ones.

II-1. $D[f(x) + g(x)] = Df(x) + Dg(x)$

II-2. $D[\alpha f(x)] = \alpha Df(x) \qquad \alpha = \text{constant}$

II-3. $D[f(x)\,g(x)] = f(x)\,Dg(x) + g(x)\,Df(x)$

II-4. $D\left[\dfrac{f(x)}{g(x)}\right] = \dfrac{g(x)\,Df(x) - f(x)\,Dg(x)}{[g(x)]^2}$

II-5. $D[f(x)]^m = m[f(x)]^{m-1}\,Df(x) \qquad m = \text{constant}$

Interpolation with simple forward differences

Taylor-expansion about $x \neq 0$

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \dots$$

$$Ef(x) = \left[1 + hD + \frac{h^2D^2}{2!} + \dots\right] f(x) = e^{hD} f(x)$$

$$\varphi_k'(x) = \varphi_{k-1}(x)$$

$$\Downarrow$$

$$\varphi_k(x) = \frac{x(x-h)(x-2h)\dots(x-kh+h)}{k!} \text{; thus } \varphi_k(x) = \frac{x^{(k)}}{k!}$$

Gregory–Newton interpolation formula:

$$f(x) = f(0) + \Delta f(0)\, x + \Delta^2 f(0) \frac{x(x-1)}{2!} + \dots + \Delta^k f(0) \frac{x(x-1)\dots(x-k+1)}{k!} + \dots$$

Interpolation with central differences

Stirling:

$$y(x) = y_0 + (\delta y)_0 x + (\delta^2 y)_0 \frac{x^2}{2} + (\delta^3 y)_0 \frac{x(x^2-1)}{6} + (\delta^4 y)_0 \frac{x^2(x^2-1)}{24} + \dots$$

Bessel

$$y(x) = y_0 + (\delta y)_0 x + (\delta^2 y)_0 \frac{x^2 - \frac{1}{4}}{2} + (\delta^3 y)_0 \frac{x(x^2 - \frac{1}{4})}{6} + (\delta^4 y)_0 \frac{(x^2 - \frac{1}{4})(x^2 - \frac{9}{4})}{24} + \dots$$

Data smoothing: via fourth-order differences

$$y = a + bx + cx^2 \longleftrightarrow 5 \text{ data points}$$

$\downarrow$ least-squares

$$a = y_0 - \frac{3}{35}\delta^4 y_0$$

Differentiation of tabulated functions

Gregory – Newton (forward difference)

$$D = \Delta - \Delta^2/2 + \Delta^3/3 - \dots = \ln(1+\Delta)$$

$$D^2 = \frac{1}{h^2}\left(\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \dots\right)$$

Central difference

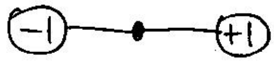
Stirling: $D = \delta - \delta^3/6 + \delta^5/30 - \dots$

Bessel: $D = \delta - \frac{1}{24}\delta^3 + \frac{3}{640}\delta^5 - \dots$

XII. CENTRÁLIS DIFFERENCIA FORMULÁK

1-D

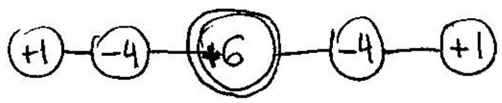
$(2h)\dfrac{\partial}{\partial x}$



$(h^2)\dfrac{\partial^2}{\partial x^2}$

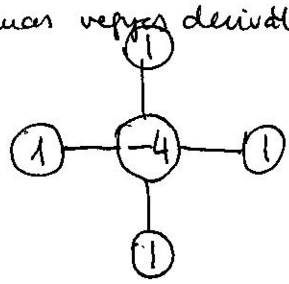
$(2h^3)\dfrac{\partial^3}{\partial x^3}$

$(h^4)\dfrac{\partial^4}{\partial x^4}$

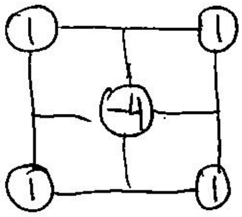


2-D → alkalmas vegyes derivált meghatározására is

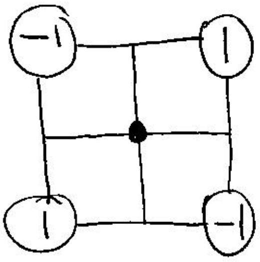
$h^2\nabla^2$



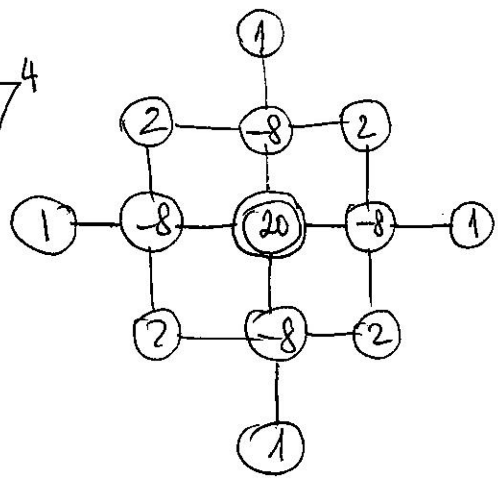
$(2h^2)\nabla^2$



$(4h^2)\dfrac{\partial^2}{\partial x\,\partial y}$



$(h^4)\nabla^4$



__Megjegyzések:__

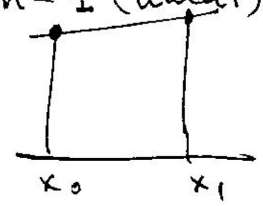
- $\Delta x = \Delta y = h$
- Szátalizos hibák h^2 rendűek
- minél magasabb rendű differencia, annál pontosabb fv-értékek kellenek
- h optimális nagysága probléma függő:
  kis h => kis szátalizos hiba
  $y_{+1} - y_{-1}$ numerikus hiba jelentősödik

Numerical integration

Polynomial approximations

1.) Newton forward difference

$n = 1$ (linear)



$$\int_{x_0}^{x_1} p(x)\,dx = \frac{h}{2}(y_0 + y_1)$$

since

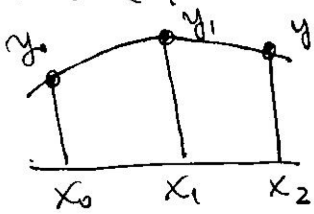
$$p_k = y_0 + k\Delta y_0$$

$$x_k = x_0 + kh \longrightarrow dx = h\,dk$$

$$\int_{x_0}^{x_1} p(x)\,dx = h\int_0^1 p_k\,dk = h\int_0^1 (y_0 + k\Delta y_0)\,dk =$$

$$= h\left[y_0 + \frac{1}{2}\Delta y_0\right] = \frac{h}{2}(y_0 + y_1)$$

$n = 2$ (quadratic)



$$\int_{x_0}^{x_2} p(x)\,dx = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

since

$$p_k = y_0 + k\Delta y_0 + \frac{1}{2}k(k-1)\Delta^2 y_0$$

$n = 1$: trapezoidal rule

$n = 2$: Simpson rule

Newton – Cotes coefficients

Method of Romberg:

$$I^* = I_{h/2} + \frac{1}{2^n - 1}\left(I_{h/2} - I_h\right)$$

Chapter 15

Gaussian Integration

CHARACTER OF A GAUSSIAN FORMULA

The main idea behind Gaussian integration is that in the selection of a formula

$$\int_a^b y(x)\,dx \simeq \sum_{i=1}^{n} A_i y(x_i)$$

it may be wise not to specify that the arguments x_i be equally spaced. All the formulas of the preceding chapter assume equal spacing, and if the values $y(x_i)$ are obtained experimentally this will probably be true. Many integrals, however, involve familiar analytic functions which may be computed for any argument and to great accuracy. In such cases it is useful to ask what choice of the x_i and A_i together will bring maximum accuracy. It proves to be convenient to discuss the slightly more general formula

$$\int_a^b w(x)y(x)\,dx \simeq \sum_{i=1}^{n} A_i y(x_i)$$

in which $w(x)$ is a weighting function to be specified later. When $w(x) = 1$ we have the original, simpler formula.

One approach to such Gaussian formulas is to ask for perfect accuracy when $y(x)$ is one of the power functions $1, x, x^2, \ldots, x^{2n-1}$. This provides $2n$ conditions for determining the $2n$ numbers x_i and A_i. In fact,

$$A_i = \int_a^b w(x)L_i(x)\,dx$$

where $L_i(x)$ is the Lagrange multiplier function introduced in Chapter 8. The arguments $x_1, \ldots, x_n$ are the zeros of the nth-degree polynomial $p_n(x)$ belonging to a family having the orthogonality property

δ_{mn}

$$\int_a^b w(x)p_n(x)p_m(x)\,dx = 0 \qquad \text{for } m \neq n$$

These polynomials depend upon $w(x)$. The weighting function therefore influences both the A_i and the x_i but does not appear explicitly in the Gaussian formula.

Hermite's formula for an osculating polynomial provides another approach to Gaussian formulas. Integrating the osculating polynomial leads to

$$\int_a^b w(x)y(x)\,dx \simeq \sum_{i=1}^{n} [A_i y(x_i) + B_i y'(x_i)]$$

but the choice of the arguments x_i as the zeros of a member of an orthogonal family makes all $B_i = 0$. The formula then reduces to the prescribed type. This suggests, and we proceed to verify, that a simple collocation polynomial at these unequally spaced arguments would lead to the same result.

Orthogonal polynomials therefore play a central role in Gaussian integration. A study of their main properties forms a substantial part of this chapter.

The *truncation error* of the Gaussian formula is

$$\int_a^b w(x)y(x)\,dx - \sum_{i=1}^{n} A_i y(x_i) = \frac{y^{(2n)}(\xi)}{(2n)!}\int_a^b w(x)[\pi(x)]^2\,dx$$

where $\pi(x) = (x - x_1)\cdots(x - x_n)$. Since this is proportional to the $(2n)$th derivative of $y(x)$, such formulas are exact for all polynomials of degree $2n - 1$ or less. In the formulas of the previous chapter it is $y^{(n)}(\xi)$ which appears in this place. In a sense our present formulas are *twice as accurate* as those based on equally spaced arguments.

PARTICULAR TYPES OF GAUSSIAN FORMULAS

Particular types of Gaussian formulas may be obtained by choosing $w(x)$ and the limits of integration in various ways. Occasionally one may also wish to impose constraints, such as specifying certain x_i in advance. A number of particular types are presented.

1. **Gaussian–Legendre formulas** occur when $w(x) = 1$. This is the prototype of the Gaussian method and we discuss it in more detail than the other types. It is customary to normalize the interval (a, b) to $(-1, 1)$. The orthogonal polynomials are then the Legendre polynomials

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$$

with $P_0(x) = 1$. The x_i are the zeros of these polynomials and the coefficients are

$$A_i = \frac{2(1 - x_i^2)}{n^2[P_{n-1}(x_i)]^2}$$

Tables of the x_i and A_i are available to be substituted directly into the Gauss–Legendre formula

$$\int_a^b y(x)\,dx \simeq \sum_{i=1}^{n} A_i y(x_i)$$

Various properties of Legendre polynomials are required in the development of these results, including the following:

$$\int_{-1}^{1} x^k P_n(x)\,dx = 0 \qquad \text{for } k = 0, \ldots, n-1$$ 15.9

$$\int_{-1}^{1} x^n P_n(x)\,dx = \frac{2^{n+1}(n!)^2}{(2n+1)!}$$ 15.10

$$\int_{-1}^{1} [P_n(x)]^2\,dx = \frac{2}{2n+1}$$ 15.11

$$\int_{-1}^{1} P_m(x) P_n(x)\,dx = 0 \qquad \text{for } m \neq n$$ 15.12

$P_n(x)$ has n real zeros in $(-1, 1)$ 15.13

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$$ 15.17

$$(t - x)\sum_{i=0}^{n} (2i+1)P_i(x)P_i(t) = (n+1)[P_{n+1}(t)P_n(x) - P_n(t)P_{n+1}(x)]$$ 15.19

$$\int_{-1}^{1} \frac{P_n(x)}{x - x_k}\,dx = \frac{-2}{(n+1)P_{n+1}(x_k)}$$

$$(1 - x^2)P_n'(x) + nxP_n(x) = nP_{n-1}(x)$$ 15.21

Lanczos' estimate of truncation error for Gauss–Legendre formulas takes the form

$$E \simeq \frac{1}{2n+1}\left[y(1) + y(-1) - I - \sum_{i=1}^{n} A_i x_i y'(x_i)\right]$$

where I is the approximate integral obtained by the Gaussian n-point formula. Note that the $\sum$ term involves applying this same formula to the function $xy'(x)$. This error estimate seems to be fairly accurate for smooth functions.