1. INTRODUCTION TO APPROXIMATION

Approximation is a numerical procedure of calculating fairly accurate values of a function $f(x)$ by using corresponding approximation function suitable for numerical manipulation. For example, a lot of functions, such as logarithmic and trigonometric functions, whose values cannot be calculated directly, are approximated with the corresponding power series. These power series when once determined are forever. The most important ones are included in the standard computers' mathematical libraries and implemented in the hardware of scientific calculators.

Let function $f(x)$ be approximated by *approximation function*

$$\tilde{f}(x,\beta) = \tilde{f}(x, \beta_0, \beta_1, ..., \beta_{N-1}) , \tag{1.1}$$

so that the *approximation error* (usually called *residual*) defined as a difference between function $f(x)$ and its approximation $\tilde{f}(x,\beta)$ is minimised on the chosen domain by the appropriate choice of the coefficients β_n ($n = 0, 1, ..., N-1$).

Depending on whether a domain on which the approximation is provided is continuous or discrete, the approximation is of *continuous type* or *discrete type*.

In the approximation of continuous type the approximated function $f(x)$ and the approximation error

$$E(x,\beta) = E(x, \beta_0, \beta_1, ..., \beta_{N-1}) = f(x) - \tilde{f}(x,\beta) , \tag{1.2}$$

are defined on a continuous domain.

In the approximation of discrete type an approximated function $f(x)$ is defined on a discrete domain by its values $f^k = f(\xi^k)$ in a chosen set of distinct points ξ^k, called *sampling points* or *nodes*[1]. In this case, the approximation error is also defined as the difference between value f^k of approximated function $f(x)$ and its approximation $\widetilde{f}(\xi^k, \beta)$ in the sampling point ξ^k, as

$$E(\xi^k, \beta) = E(\xi^k, \beta_0, \beta_1, ..., \beta_{N-1}) = f^k - \widetilde{f}(\xi^k, \beta) . \tag{1.3}$$

Furthermore, the approximation can be of linear and nonlinear type. In the *approximation of linear type* approximation function $\widetilde{f}(x,\beta)$ is a *linear combination* of so called *coordinate functions* $\phi_n(x)$ and can be expressed by the *approximation formula*:

$$\widetilde{f}(x, \beta) = \sum_{n=0}^{N-1} \beta_n \phi_n(x) = \beta_0 \phi_0(x) + \beta_1 \phi_1(x) + ... + \beta_{N-1} \phi_{N-1}(x) . \tag{1.4}$$

Used set of coordinate functions $\{\phi_n(x)\}$ can be chosen arbitrary as long as it is *complete*[2] and *linearly independent*[3].

If the function $f(x) = f(x(x_1, x_2, ..., x_M))$ depends on *M* arguments x_m, then by substitutions

$$\begin{aligned} & n = n(n_1, n_2, ..., n_M) \quad \text{(unique } n \text{ for each combination of } n_1, n_2, ..., n_M\text{)}, \\ & \beta_n = \beta_{n(n_1 n_2 ... n_M)} = \beta_{n_1 n_2 ... n_M} , \\ & \phi_n(x) = \phi_{n(n_1 n_2 ... n_M)}(x(x_1, x_2, ..., x_M)) = \phi_{n_1}^{[1]}(x_1) \phi_{n_2}^{[2]}(x_2) ... \phi_{n_M}^{[M]}(x_M), \end{aligned} \tag{1.5}$$

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[1] Note that upper index *k* is an index of a function value f^k and sampling point ξ^k and *not* an exponent. Lower index denotes coordinates ξ_1^k, ξ_2^k, … of a sampling point ξ^k.

[2] The set of functions $\{1, x, x^2, ..., x^{N-1}\}$ is *complete* with respect to any approximated function, while the set of functions $\{x, x^2, ..., x^{N-1}\}$ is complete only if $f(0) = 0$, since $\widetilde{f}(x, \beta) = \beta_1 x + \beta_2 x^2 + ... + \beta_{N-1} x^{N-1}$ cannot approximate function that has non zero value at $x = 0$.

[3] Consider that functions $\phi_n(x)$ are *linearly dependent*, i.e. that at least one of them can be expressed as a linear combination of others as $\phi_L = \sum_{n \neq L} \alpha_n \phi_n$. Substitution of ϕ_L into original approximation formula (1.4) yields to the approximation formula of the same form $\widetilde{f}(x, \overline{\beta}) = \sum_n \overline{\beta}_n \phi_n(x)$ in which $\overline{\beta}_n = \beta_n + \beta_L \alpha_n$ $(n \neq L)$ and $\overline{\beta}_L = 0$, i.e. to the approximation formula in which the linearly depended function ϕ_L is excluded.

the approximation formula $\widetilde{f}(x,\beta)=\sum_{n=0}^{N-1}\beta_n\phi_n(x)$ can also be expressed in the equivalent (but expanded) form

$$\widetilde{f}(x,\beta)=\sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\dots\sum_{n_M=0}^{N_M-1}\beta_{n_1n_2\dots n_M}\phi_{n_1}^{[1]}(x_1)\phi_{n_2}^{[2]}(x_2)\dots\phi_{n_M}^{[M]}(x_M)\,. \tag{1.6}$$

Coordinate functions $\phi_{n_1}^{[1]}(x_1)$, $\phi_{n_2}^{[2]}(x_2)$, … are usually chosen from the same family of functions $\{\phi_n^*\}$. In this case

$$\widetilde{f}(x,\beta)=\sum_{n_1=0}^{N_1-1}\sum_{n_2=0}^{N_2-1}\dots\sum_{n_M=0}^{N_M-1}\beta_{n_1n_2\dots n_M}\,\phi_{n_1}^*(x_1)\,\phi_{n_2}^*(x_2)\dots\phi_{n_M}^*(x_M)\,. \tag{1.7}$$

The approximations of linear type are relatively simple in comparison to the approximations of nonlinear type, and for that reason are frequently used. The approximations of nonlinear type in which nonlinear combinations of coordinate functions are involved, like most nonlinear analysis, are difficult to be formulated and applied and because of that are rarely used. However, the exception is the nonlinear *approximation of real type* which has the form

$$\widetilde{f}(x,a,b)=\frac{\sum_{n_1=0}^{N_1-1}a_{n_1}\phi_{n_1}(x)}{\sum_{n_2=0}^{N_2-1}b_{n_2}\phi_{n_2}(x)}\,, \tag{1.8}$$

where a_{n_1} and b_{n_2} are constant parameters.

Although coordinate functions $\phi_n(x)$ can be chosen arbitrary, it is usually more convenient to expand the function $f(x)$ into infinite series

$$f(x)=\sum_{n=0}^{\infty}\beta_n\phi_n(x)\,, \tag{1.9}$$

such as

1. Taylor series,
2. Maclaurin series (special case of Taylor series),
3. series of orthogonal functions (e.g. Fourier series),
4. series of orthogonal polynomials.

Approximation function $\tilde{f}(x,\beta)$ is then a partial sum of the first *N* elements

$$S_N(x,\beta) = \sum_{n=0}^{N-1} \beta_n \phi_n(x) \tag{1.10}$$

that is compliant with (1.4).

The crux of the approximation problem is a criterion of minimising approximation error that will determine constants β_n. The five major methods of doing this lead to the five main types of approximations which are of the highest importance:

1. *Approximation near the point* in which the approximation and its first derivatives are equal to the approximated function $f(x)$ and its first derivatives $f^{(n)}(x)$ in the single point $x = \xi$:
   a. *Taylor series expansion*: series of powers $(x-\xi)^k$ whose partial sum $S_N(x,\beta) = \beta_0 + \beta_1(x-\xi) + ... + \beta_{N-1}(x-\xi)^{N-1}$ and its first $N-1$ derivatives $S_N^{(n)}(x,\beta)$ are equal to the approximated function $f(x)$ and its first $N-1$ derivatives $f^{(n)}(x)$ in the chosen point $x = \xi$; precisely, $f(\xi) = S_N(\xi,\beta)$ and $f^{(n)}(\xi) = S_N^{(n)}(\xi,\beta)$ for $n = 1,...,N-1$.
   b. *Maclaurin series expansion*: series of powers x^k whose partial sum $S_N(x,\beta) = \beta_0 + \beta_1 x + ... + \beta_{N-1}x^{N-1}$ and its first $N-1$ derivatives $S_N^{(n)}(x,\beta)$ are equal to the approximated function $f(x)$ and its first $N-1$ derivatives $f^{(n)}(x)$ in the point $x = 0$; precisely, $f(0) = S_N(0,\beta)$ and $f^{(n)}(0) = S_N^{(n)}(0,\beta)$ for $n = 1,...,N-1$.
   c. *Padé approximation*: the rational function $R_{nm}(x)$ defined as a quotient of two polynomials $P_n(x)/Q_m(x)$ of orders *n* and *m*, whose value and the values of its first $n+m$ derivatives $R_{nm}^{(k)}(x)$, $k = 1,...,n+m$, equals to the exact values of the approximated function $f(x)$ and its first $n+m$ derivatives $f^{(k)}(x)$ at the point $x = \xi$; precisely, $f(\xi) = R_{nm}(\xi)$ and $f^{(k)}(\xi) = R_{nm}^{(k)}(\xi)$ for $k = 1,...,n+m$.

2. *Exact* or *interpolatory approximation*:
   a. *Interpolation*, in which the constants β_n are chosen so that the approximation $\widetilde{f}(\xi^k,\beta)$ equals to the values of function $f^k = f(\xi^k)$ in the chosen set of *K* distinct points ξ^k, $k = 1,...,K$.
   b. *Hermite interpolation*, in which the approximation $\widetilde{f}(\xi^k,\beta)$ and its first derivatives $\widetilde{f}^{(n)}(\xi^k,\beta)$ (where *n* is positive integer) equals to the values of function $f(\xi^k)$ and its first derivatives $f^{(n)}(\xi^k)$ in the chosen set of *K* distinct points ξ^k, $k = 1,...,K$.

3. *Least-squares approximation*:
   a. *Continuous least-squares approximation,* in which the goal is to minimise the integral of the squared approximation error $[f(x) - \widetilde{f}(x,\beta)]^2$ (optionally multiplied by *weighting function*) over a given continuous domain.
   b. *Discrete least-squares approximation*, in which the goal is to minimise the sum of the squared approximation error $[f(\xi^k) - \widetilde{f}(\xi^k,\beta)]^2$ (optionally multiplied by *weighting coefficients*) over a discrete set of *K* distinct points ξ^k.

   The Fourier series and series of orthogonal functions inherently satisfy *least-squares* criteria.

4. *Uniform or minimum-maximum approximation*:
   a. *Continuous uniform approximation*, in which the aim is to minimise the maximum magnitude of the approximation error $\max|f(x) - \widetilde{f}(x,\beta)|$ (optionally multiplied by *weighting function*) on a continuous domain.
   b. *Discrete uniform approximation*, in which the aim is to minimise the maximum magnitude of the approximation error $\max|f(\xi^k) - \widetilde{f}(\xi^k,\beta)|$ (optionally multiplied by *weighting coefficients*) over a discrete set of *K* distinct points ξ^k.

5. Approximation and interpolation by *splines* consists in splitting an interval into segments on which the approximations or interpolations are provided separately, while the approximation function $\widetilde{f}(\xi^k,\beta)$ and its first derivatives $\widetilde{f}^{(n)}(\xi^k,\beta)$ have equal values on the shared boundary points ξ^k of joined segments.

1.1 APPROXIMATION NEAR THE POINT

In this type of approximations, the values of approximation and its first derivatives are equal to the values of the approximated function and its first derivatives in the single approximation point. Although approximation error is small in the area close to the approximation point, it increases rapidly away from that point.

1.1.1 Taylor series expansion

The function $f(x)$ of single argument x can be expanded into infinite power series

$$f(x)=\sum_{n=1}^{\infty}\beta_n(x-\xi)^n=\beta_0+\beta_1(x-\xi)+\beta_2(x-\xi)^2+\beta_3(x-\xi)^3+\dots. \qquad (1.11)$$

If the function $f(x)$ has derivatives of all orders on an interval containing the points x and ξ, the coefficients $\beta_0, \beta_1, \dots$ can be determined by the conditions

$$\begin{aligned} &f(\xi)=\beta_0, \\ &\frac{\mathrm{d}^n f(\xi)}{\mathrm{d}x^n}=n!\beta_n, \quad n\geq 1. \end{aligned} \qquad (1.12)$$

So obtained power series in ($x-\xi$) of the form

$$f(x)=f(\xi)+\sum_{n=1}^{\infty}\frac{\mathrm{d}^n f(\xi)}{\mathrm{d}x^n}\frac{(x-\xi)^n}{n!}, \qquad (1.13)$$

is called the *Taylor series expansion* of function $f(x)$ in the point ξ [1].

By introducing notation

$$\begin{aligned} &f^{(0)}(\xi)=f(\xi), \\ &f^{(n)}(\xi)=\frac{d^n f(\xi)}{dx^n}, \quad n\geq 1, \end{aligned} \qquad (1.14)$$

the Taylor formula (1.13) can be expressed in a simpler form

$$f(x)=\sum_{n=0}^{\infty}f^{(n)}(\xi)\frac{(x-\xi)^n}{n!}. \qquad (1.15)$$

Example 1.1. Taylor series expansion of the function $\ln(x)$ in the point $\xi = 1$

$$\ln(x) = (x-1) - \frac{(x-1)^2}{2} + \frac{(x-1)^3}{3} - \frac{(x-1)^4}{4} + \ldots, \quad 0 < x \le 2. \tag{1.16}$$

Function $f(x)$ can be approximated by the first N terms of the Taylor series as

$$\tilde{f}(x) = S_N(x) = \sum_{n=0}^{N-1} f^{(n)}(\xi) \frac{(x-\xi)^n}{n!}. \tag{1.17}$$

This formula is equivalent to the approximation formula (1.4). Precisely

$$\tilde{f}(x, \beta) = \sum_{n=0}^{N-1} \beta_n \phi_n(x, \xi), \tag{1.18}$$

where

$$\begin{aligned} \beta_n &= \frac{f^{(n)}(\xi)}{n!}, \qquad n \ge 0, \\ \phi_n(x,\xi) &= (x-\xi)^n, \quad n \ge 0. \end{aligned} \tag{1.19}$$

The approximation error in the integral form is [2]:

$$\begin{aligned} E_N(x) = f(x) - S_N(x) &= \frac{1}{(N-1)!} \int_{\xi}^{x} f^{(N)}(\xi)(x-\xi)^{N-1} \mathrm{d}\xi \\ &= N \int_{\xi}^{x} \beta_N(\xi)\, \phi_{N-1}(x,\xi)\, \mathrm{d}\xi. \end{aligned} \tag{1.20}$$

By the use of a mean theorem of calculus which says

$$\int_{\xi}^{x} f^{(N)}(\xi)(x-\xi)^{N-1} \mathrm{d}\xi = f^{(N)}(\zeta) \int_{\xi}^{x} (x-\xi)^{N-1} \mathrm{d}\xi, \tag{1.21}$$

where ζ is a point between ξ and x, otherwise unknown, the approximation error can be obtained in the Lagrange form

$$E_N(x) = \frac{f^{(N)}(\zeta)}{N!}(x-\xi)^N \quad \text{or} \quad E_N(x) = \beta_N(\zeta)\, \phi_N(x,\xi). \tag{1.22}$$

This form of the error is very popular because of its close similarity to the terms of the Taylor polynomial. Except for a ζ in the place of a ξ it would be a term which produces the Taylor polynomial of the next higher degree.

At the point $x = \xi$, the approximation $\tilde{f}(\xi) = f(\xi)$ has no error, since $(x-\xi)^n = 0$ for $x = \xi$ and $n \geq 1$.

The Taylor series expansion can also be applied in multiple dimension domains.

In a two dimensional domain the function $f(x)$ depends on two coordinates x_1 and x_2 of the point $x(x_1, x_2)$. The function $f(x) = f(x_1, x_2)$ of two arguments x_1 and x_2 can be expanded into infinite power series

$$f(x) = \sum_{n_1=1}^{\infty}\sum_{n_2=1}^{\infty} \beta_{n_1 n_2} (x_1 - \xi_1)^{n_1} (x_2 - \xi_2)^{n_2} \ . \tag{1.23}$$

If the function $f(x)$ has derivatives of all orders on a domain containing the points $x(x_1, x_2)$ and $\xi(\xi_1, \xi_2)$, the coefficients $\beta_{n_1 n_2}$ can be determined by the conditions

$$\begin{aligned}
& f(\xi) = \beta_{0,0}, \\
& \frac{\partial^{n_1} f(\xi)}{\partial x_1^{n_1}} = n_1! \beta_{n_1,0}, \qquad n_1 \geq 1, \\
& \frac{\partial^{n_2} f(\xi)}{\partial x_2^{n_2}} = n_2! \beta_{0,n_2}, \qquad n_2 \geq 1, \\
& \frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2}} = n_1! n_2! \beta_{n_1 n_2}, \quad n_1 \geq 1, n_2 \geq 1.
\end{aligned} \tag{1.24}$$

Therefore, the expansion at the point $\xi(\xi_1, \xi_2)$ can be done by

$$\begin{aligned}
f(x) = f(\xi) &+ \sum_{n_1=1}^{\infty} \frac{\partial^{n_1} f(\xi)}{\partial x_1^{n_1}} \frac{(x_1-\xi_1)^{n_1}}{n_1!} + \sum_{n_2=1}^{\infty} \frac{\partial^{n_2} f(\xi)}{\partial x_2^{n_2}} \frac{(x_2-\xi_2)^{n_2}}{n_2!} + \\
&+ \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} \frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2}} \frac{(x_1-\xi_1)^{n_1}}{n_1!} \frac{(x_2-\xi_2)^{n_2}}{n_2!}.
\end{aligned} \tag{1.25}$$

It is convenient to define zero-derivative that is only formally a derivative as it leaves functions unchanged. I.e., if it is assumed that

$$\frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2}} = \begin{cases} f(\xi) & n_1 = 0,\ n_2 = 0, \\ \dfrac{\partial^{n_1}}{\partial x_1^{n_1}} f(\xi) & n_1 \geq 1,\ \ n_2 = 0, \\ \dfrac{\partial^{n_2}}{\partial x_2^{n_2}} f(\xi) & n_1 = 0,\ \ n_2 \geq 1, \end{cases} \tag{1.26}$$

then the Taylor formula for two arguments can be written in the short form

$$f(x) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2}} \frac{(x_1-\xi_1)^{n_1}}{n_1!} \frac{(x_2-\xi_2)^{n_2}}{n_2!}. \tag{1.27}$$

The approximation can be made by using the approximation formula

$$\tilde{f}(x) = \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \frac{\partial^{n_1+n_2} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2}} \frac{(x_1-\xi_1)^{n_1}}{n_1!} \frac{(x_2-\xi_2)^{n_2}}{n_2!}. \tag{1.28}$$

N_1 is a constant, while N_2 can be either a constant (usually $N_2 = N_1$) or a function of n_1. If N_2 is a constant, the approximation formula (1.28) has $N = N_1 N_2$ elements. If N_2 is a function of n_1, so that $N_2 = N_1 - n_1$, the approximation formula (1.28) has $N = N_1(N_1+1)/2$ elements.

Example 1.2. Double Taylor series expansion. For $N_1 = N_2 = 4$, the approximation formula (1.28) has 16 summation elements,

1	$(x_2-\xi_2)$	$(x_2-\xi_2)^2$	$(x_2-\xi_2)^3$
$(x_1-\xi_1)$	$(x_1-\xi_1)(x_2-\xi_2)$	$(x_1-\xi_1)(x_2-\xi_2)^2$	$(x_1-\xi_1)(x_2-\xi_2)^3$
$(x_1-\xi_1)^2$	$(x_1-\xi_1)^2(x_2-\xi_2)$	$(x_1-\xi_1)^2(x_2-\xi_2)^2$	$(x_1-\xi_1)^2(x_2-\xi_2)^3$
$(x_1-\xi_1)^3$	$(x_1-\xi_1)^3(x_2-\xi_2)$	$(x_1-\xi_1)^3(x_2-\xi_2)^2$	$(x_1-\xi_1)^3(x_2-\xi_2)^3$

while for $N_1 = 4$ and $N_2 = N_1 - n_1$ the approximation formula (1.28) has 10 summation elements

1	$(x_2-\xi_2)$	$(x_2-\xi_2)^2$	$(x_2-\xi_2)^3$
$(x_1-\xi_1)$	$(x_1-\xi_1)(x_2-\xi_2)$	$(x_1-\xi_1)(x_2-\xi_2)^2$	
$(x_1-\xi_1)^2$	$(x_1-\xi_1)^2(x_2-\xi_2)$		
$(x_1-\xi_1)^3$			

The Taylor formula (1.27) for expansion of a function of two arguments can be generalised to the formula for expansion of a function which has *M* arguments $x_1, x_2, \ldots x_M$

$$f(x) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \ldots \sum_{n_M=0}^{\infty} \frac{\partial^{n_1+n_2+\ldots+n_M} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2} \ldots \partial x_M^{n_M}} \frac{(x_1-\xi_1)^{n_1}}{n_1!} \frac{(x_2-\xi_2)^{n_2}}{n_2!} \ldots \frac{(x_M-\xi_M)^{n_M}}{n_M!}. \tag{1.29}$$

This formula is equivalent to

$$f(x) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \ldots \sum_{n_M=0}^{\infty} \beta_{n_1 n_2 \ldots n_M} \phi_{n_1}^{*}(x_1) \phi_{n_1}^{*}(x_1) \ldots \phi_{n_M}^{*}(x_M), \tag{1.30}$$

where

$$\begin{aligned} \beta_{n_1 n_2 \ldots n_M} &= \frac{1}{n_1! n_2! \ldots n_M!} \frac{\partial^{n_1+n_2+\ldots+n_M} f(\xi)}{\partial x_1^{n_1} \partial x_2^{n_2} \ldots \partial x_M^{n_M}}, \\ \phi_{n_m}^{*}(x_m) &= (x_m - \xi_m)^{n_m}, \quad n_m \geq 1, \quad m = 1, 2, \ldots, M. \end{aligned} \tag{1.31}$$

The approximation can be made by using the formula (1.7) with $N = N_1 N_2 \ldots N_M$ elements.

1.1.2 Maclaurin series expansion

Maclaurin series can be obtained from the Taylor series by putting point ξ on the origin of the coordinate system ($\xi = 0$). The series in *x* of the form

$$f(x) = f(0) + \sum_{n=1}^{\infty} f^{(n)}(0) \frac{x^n}{n!} \tag{1.32}$$

is called the *Maclaurin series expansion* of the function $f(x)$ (upper index of x^n is an exponent).

Example 1.3. Few examples of *Maclaurin series expansion*:

$$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \ldots, \tag{1.33}$$

$$\sin x = \frac{x}{1!} - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots, \tag{1.34}$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots, \tag{1.35}$$