JOURNAL OF ENGINEERING
annals OF
FACULTY OF ENGINEERING HUNEDOARA
TOME VI (year 2008), FASCICULE 2, (ISSN 1584 – 2665)

CURVE FITTING ON EMPIRICAL DATA WHEN BOTH VARIABLES ARE LOADED BY ERRORS

[1]András NYÍRI, [2]László KÖNÖZSY

[1]Department of Fluid and Heat Engineering, University of Miskolc, HUNGARY
[2]Christian Doppler Laboratory for Multiphase Modelling of Metallurgical Processes, University of Leoben, AUSTRIA

ABSTRACT:
A method has been developed to fit a curve differentiable up to the r^{th} order derivatives onto a set of empirical data, when both dependent and independent variables are loaded by errors of normal probability distribution. The method purposed can successfully be used in different fields of mechanical/material science and engineering as well as in the field of mesh generation techniques to provide grids for computational fluid dynamics (CFD) simulations.
KEYWORDS:
smoothing procedure, polynomials, curve fitting, continuous functions, mesh generation

1. INTRODUCTION

The importance of the smoothing and curve fitting problem played an important role in Whittaker's work [1] in the middle of the 20th century. Nyíri developed a smoothing procedure and a linear equation system solver method [2,3,4,5], when the empirical data sets have been loaded by random errors. These methods were succesfully built into a second-order continuous mesh generation technique by Könözsy [6] to determine an orthogonal curvilinear coordinate system for computational fluid dynamics (CFD) simulations. The method was further developed by Nyíri [7] to construct Hermite polynomials fitting on to 2, 4, 8, points of a 1D, 2D, 3D functions, respectively up to their r^{th} order derivatives. Using smoothing procedure with an appropriate curve fitting method is one of the most relevant issue currently in the field of mechanical/material science and engineering applications. For example, the discontinuous phase diagram information has to be coupled with the corresponding transport equations for modelling solidification processes using industrial steels [8,9,10]. The purposed method can have beneficial effect on these kinds of problems as well, especially when a discontinuous function has to be substituted by a continuous one.

2. THE EQUATION OF SMOOTHING

The aim of the method proposed is to fit an r times differentiable curve to a set of empirical data loaded by normally distributed errors on both variables. The published papers [2,3,4,5] only the dependent variables in the cases of 1, 2 and 3 dimensions were supposed having errors. The hypothesis will be maintained that the probability distribution of the error follows the normal law, and not any more assumption will be put concerning the class of the exact function from which the values differ, if there is any. The root of the smoothing is the sum of squares of the differences between the empirical data and the obtained values and the r^{th} divided differences of those will be the minimum.

Let the (ξ_k, η_k) empirical data be given in the (x, y) coordinate system $1 \le k \le n$, $\xi_k < \xi_{k+1}$. The minimum of the sum will be sought for

$$S=\sum_{k=0}^{n-r}\left(\delta^r u_k\right)^2+\sum_{k=1}^{n} p_k\left(u_k-\eta_k\right)^2+\sum_{k=1}^{n} q_k\left(x_k-\xi_k\right)^2, \tag{1.1}$$

where p_k and q_k are the smoothing parameters. The r^{th} divided difference is

$$\delta^r u_k=\frac{\delta^{r-1}u_{k+1}-\delta^{r-1}u_k}{x_{k+r}-x_k},\ \delta^0 u_k=u_k. \tag{1.2}$$

Introducing the *Lagrange* function

$$\Psi_{k-i,r}(x)=\prod_{\lambda=0}^{r}\left(x-x_{k-i+\lambda}\right), \tag{1.3}$$

the first derivative of this is

$$\frac{d}{dx}\Psi_{k-i,r}(x)=\Psi'_{k-i,r}(x)=\sum_{\nu=0}^{r}\prod_{\substack{\lambda=0\\ \lambda\neq\nu}}^{r}\left(x-x_{k-i+\lambda}\right),\ 0\le i\le r, \tag{1.4}$$

and

$$\Psi'_{k-i,r}\left(x_{k-i+j}\right)=\prod_{\substack{\lambda=0\\ \lambda\neq j}}^{r}\left(x_{k-i+j}-x_{k-i+\lambda}\right),\ \ 0\le j\le r, \tag{1.5}$$

with this the divided difference can be written as follows

$$\begin{aligned}&\delta^r u_{k-i}=\sum_j u_{k-i+j}\left[\Psi'_{k-i,r}\left(x_{k-i+j}\right)\right]^{-1},\\ &\text{if } 1\le K\le r \text{ then } 0\le i\le K-1,\ 0\le j\le r,\\ &\text{if } r+1\le K\le n-r \text{ then } 0\le i,j\le r,\\ &\text{if } n-r+1\le K\le n \text{ then } 0\le i\le r,\ 0\le j\le \min[r,n-K+i].\end{aligned} \tag{1.6}$$

The numbers $p_k>0$, $q_k>0$ are inversely proportional to the square of the standard deviations. The part sum of the Eq. (1.1) belongs to a point K is

$$S_K=\sum_{i=0}^{r}\left(\delta^r u_{K-i}\right)^2+p_K\left(u_K-\eta_K\right)^2+q_K\left(x_K-\xi_K\right)^2. \tag{1.7}$$

The necessary conditions for the minimum of this sum are

$$\frac{\partial S_K}{\partial u_K}=0,\ \frac{\partial S_K}{\partial x_K}=0. \tag{1.8}$$

3. THE FIRST CONDITION OF SMOOTHING

Let us differentiate S_K respect to u_K getting

$$\frac{1}{2}\frac{\partial S_K}{\partial u_K}=\sum_{i=0}^{r}\delta^r u_{K-i}\frac{\partial\delta^r u_{K-i}}{\partial u_K}+p_K\left(u_k-\eta_K\right)=0, \tag{2.1}$$

where

$$\delta^r u_{K-i}\frac{\partial\delta^r u_{K-i}}{\partial u_K}=\sum_{j=0}^{r}u_{K-i+j}\left[\Psi'_{K-i,r}\left(x_{K-i+j}\right)\Psi'_{K-i,r}\left(x_K\right)\right]^{-1}.$$

The linear equation system (L.E.S.) has to be solved is as follows

$$\sum_{j=0}^{r}u_{K-i+j}\left[\Psi'_{K-i,r}\left(x_{K-i+j}\right)\Psi'_{K-i,r}\left(x_K\right)\right]^{-1}+p_K u_K=p_K\eta_K. \tag{2.2}$$

The compact form of the system is

$$a_{K,\ell}u_{K+\ell}=p_K\eta_K\ ,\ 1\le K\le n, \tag{2.3}$$

where if $1\le K\le r$, then $1-K\le\ell\le r$,
if $r+1\le K\le n-r$, then $-r\le\ell\le r$,
if $n-r+1\le K\le n$, then $-r\le\ell\le n-K$.

The coefficients are

$$a_{K,0} = p_K + \sum_{i=\mu}^{\nu}\left[\Psi'_{K-i,r}(x_K)\right]^{-2}, \tag{2.3a}$$

if $1 \le K \le r$, then $\mu = 0$, $\nu = K-1$,
if $r+1 \le K \le n$, then $\mu = 0$, $\nu = r$,
if $n-r+1 \le K \le n$, then $\mu = K+r-n$.

$$a_{K,\ell} = \sum_{i=\mu}^{\nu}\left[\Psi'_{K-i,r}(x_{K+\ell})\Psi'_{K-i,r}(x_K)\right]^{-1}, \tag{2.3b}$$

if $1 \le K \le r$, then $1-K \le \ell \le r$,
where if $\ell < 0$, then $\mu = -\ell \le i \le K-1 = \nu$,
if $\ell > 0$, then $\mu = 0 \le i \le \nu = \min\{K-1, r-\ell\}$,
if $r+1 \le K \le n-r$, then $-r \le \ell \le r$,
if $\ell < 0$, then $\mu = -\ell \le i \le r = \nu$,
if $\ell > 0$, then $\mu = 0 \le i \le r-\ell = \nu$,
if $n-r+1 \le K \le n$, then $-r \le \ell \le n-K$,
if $\ell < 0$, then $\mu = \max\{-\ell, K-n+r\}, \nu = r$,
if $\ell > 0$, then $\mu = K-n+r$, $\nu = r-\ell$.

The algorithm for the solution of the banded L.E.S. has been found in paper [4].

4. THE SECOND CONDITION OF SMOOTHING

For satisfying the second condition, let us differentiate the S_K according to x_K

$$\frac{\partial}{\partial x_K}\sum_{i=0}^{r}\left(\delta^r u_{K-i}\right)^2 + q_K(x_K - \xi_K) = 0, \tag{3.1}$$

and denoting this by f_K

$$f_K = \sum_{i=0}^{r}\delta^r u_{K-i}\frac{\partial}{\partial x_K}\delta^r u_{K-i} + q_K(x_K - \xi_K) = 0, \tag{3.2}$$

$$f_K = f_K(x_{K-\mu},\ldots x_{K-1}, x_K, x_{K+1},\ldots x_{K+\nu}),\ \mathbf{x} = \left[x_{K-\mu},\ldots x_{K-1}, x_K, x_{K+1},\ldots x_{K+\nu}\right]^T,\ \mathbf{f} = \left[f_1, f_2, \ldots f_n\right]^T,$$

where

if $1 \le K \le r$, then $\mu = K-1$, $\nu = r$,
if $r+1 \le K \le n-r$, then $\mu = \nu = r$,
if $n-r+1 \le K \le n$, then $\mu = r$, $\nu = n-K$.

The *Jacobian* matrix of $\mathbf{f}$ vector according to $\mathbf{x}$ is

$$\mathbf{D} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \tag{3.3}$$

and the entries of it are

$$D_{K,K+\ell} = \frac{\partial f_K}{\partial x_{K+\ell}} = \sum_{i=0}^{r}\frac{\partial}{\partial x_{K+\ell}}\left[\delta^r u_{K-i}\frac{\partial}{\partial x_K}\delta^r u_{K-i}\right] + q_K\frac{\partial x_K}{\partial x_{K+\ell}}$$

where the intervals for ℓ are as same as in the case of Eq. (2.3). We have obtained a banded structure non-linear system of equations as we have had previously. Furthermore, let us differentiate the Eq. (3.2)

$$\frac{\partial \delta^r u_{K-i}}{\partial x_K} = -\sum_{j=0}^{r}u_{K-i+j}\left[\Psi'_{K-i,r}(x_{K-i+j})\right]^{-2}\frac{\partial}{\partial x_K}\Psi'_{K-i,r}(x_{K-i+j}),\ 0 \le i \le r,$$

$$\frac{\partial}{\partial x_{K+\ell}}\frac{\partial u_{K-i}}{\partial x_K}=-\sum_{j=0}^{r}u_{K-i+j}\Big\{-2\left[\Psi'_{K-i,r}\left(x_{K-i+j}\right)\right]^{-3}\cdot\frac{\partial}{\partial x_{K+\ell}}\Psi'_{K-i,r}\left(x_{K-i+j}\right)\cdot\frac{\partial}{\partial x_K}\Psi'_{K-i,r}\left(x_{K-i+j}\right)+$$
$$+\left[\Psi'_{K-i,r}\left(x_{K-i+j}\right)\right]^{-2}\cdot\frac{\partial}{\partial x_{K+\ell}}\frac{\partial}{\partial x_K}\Psi'_{K-i,r}\left(x_{K-i+j}\right)\Big\},$$
$$\frac{\partial\delta^r u_{K-i}}{\partial x_{K+\ell}}=-\sum_{j=0}^{r}u_{K-i+j}\left[\Psi'_{K-i,r}\left(x_{K-i+j}\right)\right]^{-2}\frac{\partial}{\partial x_{K+\ell}}\Psi'_{K-i,r}\,,\ -r\le\ell\le r\,,$$

and the non-linear system of equations

$$\mathbf{D}(\mathbf{x})\mathbf{t}=-\mathbf{f}(\mathbf{x})=\mathbf{b}$$

has to be solved by iteration for $\mathbf{t}$, and $\mathbf{x}^{m+1}=\mathbf{x}^m+\mathbf{t}^m$. The elements of the $\mathbf{D}(\mathbf{x})$ matrix can be approximated as

$$D_{K,K+\ell}\approx\frac{f_K(\mathbf{x}+\mathbf{t})-\mathbf{f}(\mathbf{x})}{\Delta x_{K+\ell}}.$$

5. THE CHOICE OF THE SMOOTHING PARAMETERS

For the sake of simplicity, let us choose the parameters independent of K, i.e. $p_K=p$ and $q_K=q$. Let us define the following vectors

$$\mathbf{x}=\left[x_1,\ldots xn\right]^T,\ \mathbf{u}=\left[u_1,\ldots,u_n\right]^T,\ \xi=\left[\xi_1,\ldots,\xi_n\right]^T$$

introducing the following

$$D(\mathbf{x},\mathbf{u},\xi,\eta;p,q)=\sum_{K=1}^{n-r}\left(\delta^r u_K\right)^2,\ \mathrm{K}_u(\mathbf{u},\eta;p)=\sum_{K=1}^{n}\left(u_K-\eta_K\right)^2,\ \mathrm{K}_x(\mathbf{x},\xi;q)=\sum_{K=1}^{n}\left(x_K-\xi_K\right)^2, \tag{4.1}$$

functions which give the expression for Eq. (1.1) as

$$S=D+p\mathrm{K}_u+q\mathrm{K}_x\,, \tag{4.2}$$

and the conditions for getting the minimum value are

$$\frac{\partial S}{\partial u_K}=\frac{\partial S}{\partial x_K}=0\,.$$

Let us nominate $\mathbf{x}_e$ and $\mathbf{u}_e$ at which the minimum is reached, then

$$S=S^*\left(\mathbf{u}_e,\mathbf{x}_e;p,q\right).$$

Choosing arbitrary numbers like $\kappa,\rho>0$ and examining the following

$$\overline{S}\left(\mathbf{u}_e,\mathbf{x}_e;\kappa,\rho\right)=D\left(\mathbf{u}_e,\mathbf{x}_e;p,q\right)+\kappa\mathrm{K}_u\left(\mathbf{u}_e;p\right)+\rho\mathrm{K}_x\left(\mathbf{x}_e;q\right)$$

sum-total which agrees with S^* if $\kappa=p$ and $\rho=q$. In order to search the minimum of $\overline{S}$ as the function of p and q, we have to calculate the derivatives

$$\frac{\partial\overline{S}}{\partial p}=\frac{\partial D}{\partial p}+\kappa\frac{\partial\mathrm{K}_u}{\partial p},\ \frac{\partial\overline{S}}{\partial q}=\frac{\partial D}{\partial q}+\rho\frac{\partial\mathrm{K}_x}{\partial q}\,.$$

If $\kappa=\overline{\kappa}$ and $\rho=\overline{\rho}$, then the derivatives will be zero

$$\overline{\kappa}=-\frac{\dfrac{\partial D}{\partial p}}{\dfrac{\partial\mathrm{K}_u}{\partial p}}\ \text{and}\ \overline{\rho}=-\frac{\dfrac{\partial D}{\partial q}}{\dfrac{\partial\mathrm{K}_x}{\partial q}}\,.$$

Choosing $p^*=\overline{\kappa}$ and $q^*=\overline{\rho}$, then

$$S^*\left(p^*,q^*\right)=\overline{S}\left(\overline{\kappa},\overline{\rho}\right)$$

and $\overline{S}$ has its minimum. At first let us consider the case when the ordinates are smoothed only

$$S=\sum_{k=1}^{n-r}\left(\delta^r u_K\right)^2+p\sum_{K=1}^{n}\left(u_K-\eta_K\right)^2.$$

If $p=0$ then the solution will correspond to the conditions $\delta^r u_K = 0$, i.e. it is an $r-1$ degree parabola which minimizes the sum $\sum (u_K - \eta_K)^2$. This is a *Gaussian* least square polynomial, and this method is an extension of it. In this case, D_0 and K_{u0} denotes the corresponding values. K_{x0} belongs to $q=0$. There will be no smoothing in the second case, then $\mathrm{K}_{u\infty} = 0$ and $D_\infty = \sum (\delta^r u_K)^2$.

Next examination will be the case, when p and q are variables, and let us consider to the following function

$$U(p,q) = \frac{D(p,q)}{D_\infty} + \frac{\mathrm{K}_u(p)}{\mathrm{K}_{u0}} + \frac{\mathrm{K}_x(q)}{\mathrm{K}_{x0}},$$

where K_{x0} is belonging to $q=0$. For $\bar{S}$, we obtain

$$\bar{S} = D_\infty U, \text{ and } \kappa = \frac{D_\infty}{\mathrm{K}_{u0}}, \ \rho = \frac{D_\infty}{\mathrm{K}_{x0}},$$

consequently

$$p^* = \frac{D_\infty}{\mathrm{K}_{u0}}, \ q^* = \frac{D_\infty}{\mathrm{K}_{x0}}, \tag{4.3}$$

and

$$S(p^*, q^*) = D_\infty U(p^*, q^*),$$

$$\frac{\partial U(p^*, q^*)}{\partial p} + \frac{\partial U(p^*, q^*)}{\partial q} = 0.$$

Choosing these parameters accordingly the sum S will be minimized so that the sums of $(u_K - \eta_K)^2$ and $(x_K - \xi_K)^2$ will be the smallest. If the errors of the empirical data are known, i.e. $\mathrm{K}_{ug} = \sum_{K=1}^{n} (u_K - \eta_K)^2$, $\mathrm{K}_{xg} = \sum_{K=1}^{n} (x_K - \xi_K)^2$ are given, then computing the functions $\mathrm{K}_u(p)$, $\mathrm{K}_x(q)$ with proper p and q can be determined.

6. THE CURVE FITTING

After being completed to the smoothing procedure, the obtained set of values can be used by applying the forward and backward *Newtonian I. and II. m^th* order polynomials. One can fit onto $m+1$ points of one of the polynomials

$$P_{K,m} = u_K + \sum_{i=1}^{m} \delta^i u_K \Psi_{K,i-1}(x), \tag{5.1}$$

or

$$Q_{K,m}(x) = u_K + \sum_{i=1}^{m} \delta^i_{K-i} \Psi_{K+1-i,i-1}(x). \tag{5.2}$$

Using the derivatives of those polynomials at every neighbouring point, one can fit a *Hermite* polynomials [7] joining smoothly up to the required order of differential quotients [2,7]. Finally, the $(r-\mu)^{th}$ derivative of the function Ψ is

$$\Psi^{(r-\mu)}_{K,r} = (r-\mu)!\, p_{\mu+1}[x - x_K, x - x_{K+1}, \ldots, x - x_{K+r}], \tag{5.3}$$

where

$$p_\nu[\ell] = p_\nu[a_1, a_2, \ldots, a_\ell] \tag{5.4}$$

means the sum of all the possible ν elements products of a_i.

$$p_\nu(\ell) = \sum_{\lambda_\nu=\nu}^{\ell} a_{\lambda_\nu} \sum_{\lambda_{\nu-1}=\nu-1}^{\lambda_\nu - 1} a_{\lambda_{\nu-1}} \ldots \sum_{\lambda_2=2}^{\lambda_3-1} a_{\lambda_2} \sum_{\lambda_1=1}^{\lambda_2-1} a_{\lambda_1}. \tag{5.5}$$

7. THE ALGORITHM OF SMOOTHING PROCEDURE

For the following example, we suppose that there are two upper and lower bands exist compared to the main diagonal of the linear equation system $(r = 2)$, therefore $0 \le i, j \le 2$, $-2 \le \ell \le 2$ and $3 \le K \le n-2$. First of all, the divided differences will be computed, and each step can be found in **Tables** 1-3.

$$\delta^2 u_K = \sum_{j=0}^{2} u_{K+j}\left[\Psi'_{K,2}\left(x_{K+j}\right)\right]^{-1};$$

$$\delta^2 u_{K-1} = \sum_{j=0}^{2} u_{K-1+j}\left[\Psi'_{K-1,2}\left(x_{K+1+j}\right)\right]^{-1};$$

$$\delta^2 u_{K-2} = \sum_{j=0}^{2} u_{K-2+j}\left[\Psi'_{K-2,2}\left(x_{K+2+j}\right)\right]^{-1}$$

After knowing the divided differences, the first derivative of the *Lagrange* polynomial and the other derivatives for satisfying the conditions of smoothing procedure, we have to solve the linear equation system according to Eqs. (2.3a)-(2.3b). The coefficients of the linear equation system for satisfying the first condition of smoothing procedure are as follows

$$a_{K,0} = p_K + \sum_{i=0}^{2}\left[\Psi'_{K-1,2}\left(x_K\right)\right]^{-2}$$

$$a_{K,\ell} = \sum_{i=\mu}^{\nu}\left[\Psi'_{K-i,2}\left(x_{K+\ell}\right)\Psi'_{K-i,2}\left(x_K\right)\right]^{-1},$$

$$\text{if } \ell = -2,-1 \text{ then } \mu = -\ell \le i \le 2 = \nu,$$

$$\text{if } \ell = 1,2 \quad \text{then } \mu = 0 \le i \le 2-\ell = \nu.$$

For satisfying the second condition of smoothing, we have to solve a non-linear system of equation, therefore the elements of the *Jacobian* matrix Eq. (3.3) has to be constructed according to

$$D_{K,K+\ell} = \frac{\partial f_K}{\partial x_{K+\ell}} = \sum_{i=0}^{2}\frac{\partial}{\partial x_{K+\ell}}\left[\delta^2 u_{K-i}\frac{\partial \delta^2 u_{K-i}}{\partial x_K}\right] + q_K\frac{\partial x_K}{\partial x_{K+\ell}}$$

where

$$f_K = \sum_{i=0}^{2}\delta^2 u_{K-i}\frac{\partial \delta^2 u_{K-i}}{\partial x_K} + q_K\left(x_K - \xi_K\right) = 0,$$

and the necessary derivatives are

$$\frac{\partial}{\partial x_{K+\ell}}\delta^2 u_{K-i} = -\sum_{j=0}^{2} u_{K-i+j}\left[\Psi'_{K-i,2}\left(x_{K-i+j}\right)\right]^{-2}\frac{\partial}{\partial x_{K+\ell}}\Psi'_{K-i,2}\left(x_{K-i+j}\right),$$

$$\frac{\partial}{\partial x_{K+\ell}}\frac{\partial}{\partial x_K}\delta^2 u_{K-i} = -\sum_{j=0}^{2} u_{K-i+j}\left\{\left[\Psi'_{K-i,2}\left(x_{K-i+j}\right)\right]^{-2}\frac{\partial}{\partial x_K}\Psi'_{K-i,2}\Psi'_{K-i,2}\left(x_{K-i+j}\right)\right\}.$$

TABLE 1. THE FIRST DERIVATIVE OF THE LANGRANGE FUNCTION USING EQUATION (1.5)

$\Psi'_{K-i,r}\left(x_{K-i+j}\right)$			
	j = 0	1	2
i = 0	$(x_K - x_{K+1})(x_K - x_{K+2})$	$(x_{K+1} - x_K)(x_{K+1} - x_{K+2})$	$(x_{K+2} - x_K)(x_{K+2} - x_{K+1})$
1	$(x_{K-1} - x_K)(x_{K-1} - x_{K+1})$	$(x_K - x_{K-1})(x_K - x_{K+1})$	$(x_{K+1} - x_{K-1})(x_{K+1} - x_K)$
2	$(x_{K-2} - x_{K-1})(x_{K-2} - x_K)$	$(x_{K-1} - x_{K-2})(x_{K-1} - x_K)$	$(x_K - x_{K-2})(x_K - x_{K-1})$

TABLE 2. FIRST DERIVATIVES FOR SATISFYING THE CONDITIONS OF SMOOTHING PROCEDURE

$\frac{\partial}{\partial x_{K+\ell}} \Psi'_{K-i,2}\left(x_{K-i+j}\right)$				
		$j=0$	1	2
$i=0$	$\ell=-2$	0	0	0
	-1	0	0	0
	0	$(x_K - x_{K+1})+(x_K - x_{K+2})$	$-(x_{K+1} - x_{K+2})$	$-(x_{K+2} - x_{K+1})$
	1	$-(x_K - x_{K+2})$	$(x_{K+1} - x_K)+(x_{K+1} - x_{K+2})$	$-(x_{K+2} - x_K)$
	2	$-(x_K - x_{K+1})$	$-(x_{K+1} - x_K)$	$(x_{K+2} - x_K)+(x_{K+2} - x_{K+1})$
$i=1$	$\ell=-2$	0	0	0
	-1	$(x_{K-1} - x_K)+(x_{K-1} - x_{K+1})$	$-(x_K - x_{K+1})$	$-(x_{K+1} - x_K)$
	0	$-(x_{K-1} - x_{K+1})$	$(x_K - x_{K-1})+(x_K - x_{K+1})$	$-(x_{K+1} - x_{K-1})$
	1	$-(x_{K-1} - x_K)$	$-(x_K - x_{K-1})$	$(x_{K+1} - x_K)+(x_{K+1} - x_{K-1})$
	2	0	0	0
$i=2$	$\ell=-2$	$(x_{K-2} - x_{K-1})+(x_{K-2} - x_K)$	$-(x_{K-1} - x_K)$	$-(x_K - x_{K-1})$
	-1	$-(x_{K-2} - x_K)$	$(x_{K-1} - x_{K-2})+(x_{K-1} - x_K)$	$-(x_K - x_{K-2})$
	0	$-(x_{K-2} - x_{K-1})$	$-(x_{K-1} - x_{K-2})$	$(x_K - x_{K-2})+(x_K - x_{K-1})$
	1	0	0	0
	2	0	0	0

TABLE 3. SECOND DERIVATIVES FOR SATISFYING THE CONDITIONS OF SMOOTHING PROCEDURE

$\frac{\partial}{\partial x_{K+\ell}} \frac{\partial}{\partial x_K} \Psi'_{K-i,2}\left(x_{K-i+j}\right)$				
		$j=0$	1	2
$i=0$	$\ell=-2$	0	0	0
	-1	0	0	0
	0	2	0	0
	1	-1	-1	1
	2	-1	1	-1
$i=1$	$\ell=-2$	0	0	0
	-1	-1	-1	1
	0	0	2	0
	1	1	-1	-1
	2	0	0	0
$i=2$	$\ell=-2$	-1	1	-1
	-1	1	-1	-1
	0	0	0	2
	1	0	0	0
	2	0	0	0

8. NUMERICAL EXAMPLE FOR SMOOTHING PROCEDURE

A complete numerical example had been found in **Tables** 4-12.

TABLE 4. THE (ξ_k, η_k) SET OF EMPIRICAL DATA

K	1	2	3	4	5
ξ_K	0	1.0	1.5	2.0	2.5
η_K	10.2	8.4	8.1	7.5	7.9

TABLE 5. ELEMENTS OF THE LINEAR EQUATION SYSTEM FOR THE FIRST CONDITION

	$\Psi'_{3-i,2}(x_{3-i+j})$			$\frac{\partial}{\partial x_3}\Psi'_{3-i,2}(x_{3-i+j})$		
	$j=0$	1	2	0	1	2
$i=0$	0.5	−0.25	0.5	−1.5	0.5	−0.5
1	0.5	−0.25	0.5	1.0	0	−1.0
2	1.5	−0.5	0.75	1.0	−1.0	3.0

The divided differerences

$$\delta^2 u_3 = \sum_{j=0}^{2} u_{3+j}\left[\Psi'_{3,2}(x_{3+j})\right]^{-1} = 2.00000,$$

$$\delta^2 u_2 = \sum_{j=0}^{2} u_{2+j}\left[\Psi'_{2,2}(x_{2+j})\right]^{-1} = -0.60000,$$

$$\delta^2 u_1 = \sum_{j=0}^{2} u_{1+j}\left[\Psi'_{1,2}(x_{1+j})\right]^{-1} = 0.80000,$$

and the diagonal elements of the linear equation system

$$a_{3,0} = p_3 + \sum_{i=0}^{2}\left[\Psi'_{3-i,2}(x_3)\right]^{-2} = 21.77778,$$

$$a_{3,-2} = \sum_{i=2}^{2}\left[\Psi'_{3-i,2}(x_1)\Psi'_{3-i,2}(x_3)\right]^{-1} = 0.88889,$$

$$a_{3,-1} = \sum_{i=1}^{2}\left[\Psi'_{3-i,2}(x_2)\Psi'_{3-i,2}(x_3)\right]^{-1} = -10.66667,$$

$$a_{3,1} = \sum_{i=0}^{1}\left[\Psi'_{3-i,2}(x_4)\Psi'_{3-i,2}(x_3)\right]^{-1} = -16.00000,$$

$$a_{3,2} = \sum_{i=0}^{0}\left[\Psi'_{3-i,2}(x_5)\Psi'_{3-i,2}(x_3)\right]^{-1} = 4.00000.$$

TABLE 6. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

	$\frac{\partial}{\partial x_{3+\ell}}\Psi'_{3-i,2}(x_{3-i+j})$								
	$i=0$			1			2		
	$j=0$	1	2	$j=0$	1	2	$j=0$	1	2
$\ell=-2$	0	0	0	0	0	0	−2.5	0.5	−0.5
−1	0	0	0	−1.5	0.5	−0.5	1.5	0.5	−1.5
0	−1.5	0.5	−0.5	1.0	0	−1.0	1.0	−1.0	2.0
1	1.0	0	−1.0	0.5	−0.5	1.5	0	0	0
2	0.5	−0.5	1.5	0	0	0	0	0	0

TABLE 7. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

	$\frac{\partial\delta^2 u_{3-i}}{\partial x_{3+\ell}}$			$\sum_{i=0}^{2}\frac{\partial\delta^2 u_{3-i}}{\partial x_3}\frac{\partial\delta^2 u_{3-i}}{\partial x_{3+\ell}}$
	$i=0$	1	2	
$\ell=-2$	1.73333	0	0	0.46222
−1	−2.0	0.6	0	−2.69333
0	0.26667	−3.6	4.4	32.39111
1	0	3.0	−0.8	−14.32000
2	0	0	−3.6	−15.84000

TABLE 8. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

		$\frac{\partial}{\partial x_{3+\ell}}\left[\Psi'_{3-i,2}\left(x_{3-i+j}\right)\right]^{-2}\cdot\frac{\partial}{\partial x_3}\Psi'_{3-i,2}\left(x_{3-i+j}\right)$		
		$j=0$	1	2
$i=0$	$\ell=-2$	0	0	0
	-1	0	0	0
	0	-36.0	32.0	-4.0
	1	24.0	0	-8.0
	2	12.0	-32.0	12.0
$i=1$	$\ell=-2$	0	0	0
	-1	24.0	0	-8.0
	0	-16.0	0	-16.0
	1	-8.0	0	24.0
	2	0	0	0
$i=2$	$\ell=-2$	1.48148	-8.0	4.74074
	-1	-0.88889	-8.0	14.22222
	0	-0.59259	16.0	-18.96296
	1	0	0	0
	2	0	0	0

TABLE 9. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

		$\left[\Psi'_{3-i,2}\left(x_{3-i+j}\right)\right]^{-2}\cdot\frac{\partial}{\partial x_{3+\ell}}\frac{\partial}{\partial x_3}\Psi'_{3-i,2}\left(x_{3-i+j}\right)$		
		$j=0$	1	2
$i=0$	$\ell=-2$	0	0	0
	-1	0	0	0
	0	8.0	0	0
	1	-4.0	-16.0	-4.0
	2	-4.0	16.0	-4.0
$i=1$	$\ell=-2$	0	0	0
	-1	-4.0	-16.0	4.0
	0	0	32.0	0
	1	4.0	-16.0	-4.0
	2	0	0	0
$i=2$	$\ell=-2$	-0.44444	4.0	-1.77778
	-1	0.44444	-4.0	-1.77778
	0	0	0	3.55556
	1	0	0	0
	2	0	0	0

TABLE 10. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

	$\frac{\partial}{\partial x_{3+\ell}}\frac{\partial}{\partial x_3}\delta^2 u_{3-i}$		
	$i=0$	1	2
$\ell=-2$	0	0	0.977778
-1	0	37.2	-4.53339
0	-49.2	-24.0	3.55564
1	37.2	-13.2	0
2	12.0	0	0

TABLE 11. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

	$\sum_{i=0}^{2} \delta^2 u_{3-i} \frac{\partial}{\partial x_{3+\ell}} \frac{\partial}{\partial x_3} \delta^2 u_{3-i}$
$\ell = -2$	0.78222
-1	-25.94667
0	-81.15549
1	82.32000
2	24.00000

TABLE 12. DIAGONAL ELEMENTS OF THE JACOBIAN MATRIX

	$D_{3,3+\ell} = \frac{\partial f_3}{\partial x_{3+\ell}} = \sum_{i=0}^{2} \frac{\partial \delta^2 u_{3-i}}{\partial x_3} \frac{\partial \delta^2 u_{3-i}}{\partial x_{3+\ell}} + \delta^2 u_{3-i} \frac{\partial}{\partial x_{3+\ell}} \frac{\partial \delta^2 u_{3-i}}{\partial x_3}$
$\ell = -2$	1.24444
-1	-28.64000
0	$-48.76438 + q_3$
1	68.00000
2	81.60000

9. NUMERICAL EXAMPLE FOR CHOOSING THE SMOOTHING PARAMETERS

TABLE 13. THE SET OF EMPIRICAL AND SMOOTHED DATA SYSTEM

K	ξ_K	η_K	x_K^*	u_K^*
1	0.0	10.2	-0.44301	9.79926
2	1.0	8.4	0.86080	8.56901
3	1.5	8.1	1.46634	8.20335
4	2.0	7.5	2.05231	7.98061
5	2.5	7.9	2.56754	7.91858
6	3.0	7.8	3.04186	7.96851
7	3.7	8.6	3.83898	8.16074
8	5.0	8.3	4.83828	8.06250
9	6.5	6.0	6.68653	6.07335
10	8.0	3.4	8.23354	3.47118
11	1.0	0.2	10.05684	0.19294
	$D_\infty = 7.93984$		$q^* = 0.18974$	$p^* = 0.55334$

TABLE 14. QUANTITIES FOR CHOOSING THE SMOOTHING PARAMETER

p	K_u	D	$\frac{K_u}{K_{u0}} + \frac{D}{D_\infty}$
10.0	0.09519	1.63643	0.21257
$10.0^{0.5}$	0.16648	1.24534	0.16831
p^*	0.71943	0.61642	0.12767
$10.0^{-0.5}$	1.19108	0.42017	0.13582
10.0^{-1}	2.62681	0.15847	0.20286
10.0^{-5}	$K_{u0} = 14.36061$	0.00000	1.00000

TABLE 15. QUANTITIES FOR CHOOSING THE SMOOTHING PARAMETER

q	K_x	D	$\frac{K_u}{K_{u0}}+\frac{K_x}{K_{x0}}+\frac{D}{D_\infty}$
10.0	0.00102	0.59246	0.12466
1.0	0.04610	0.49391	0.12327
q^*	0.36385	0.37265	0.10569
10.0^{-1}	0.72650	0.32376	0.10820
10.0^{-2}	7.08487	0.15582	0.23902
10.0^{-3}	$K_{x0} = 41.84478$	0.05197	1.05664

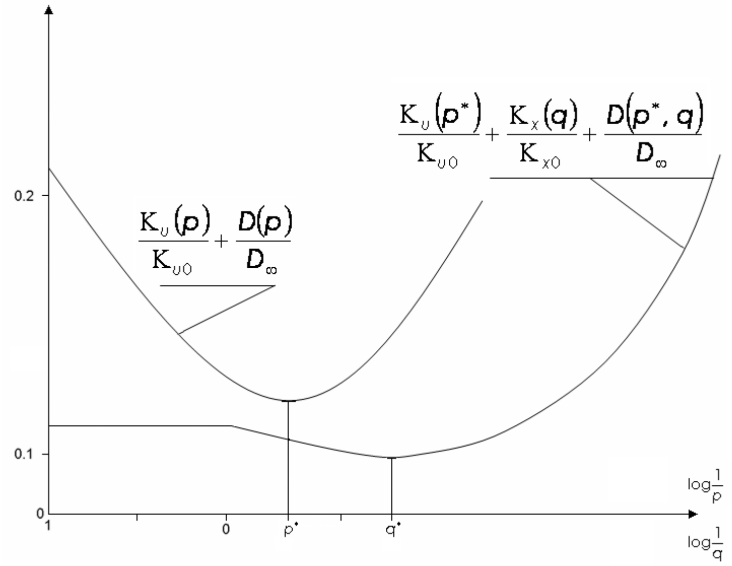

FIGURE 1. CHOOSING THE SMOOTHING PAREMETERS

10. NUMERICAL EXAMPLE FOR MESH GENERATION

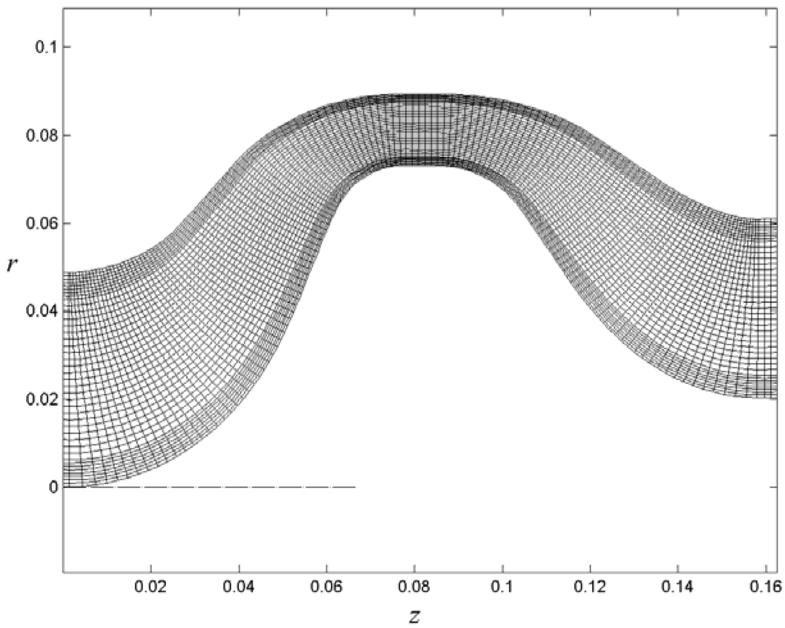

FIGURE 2. A GRID FOR COMPUTATIONAL FLUID DYNAMICS (CFD) SIMULATIONS

11. CONCLUSIONS

The idea of the presented method has been based on an extension of *Gaussian* least square polynomial. It is applicable to smooth empirical data system which is loaded by errors of normal probability distribution, and to fit a curve differentiable up to the r^{th} order derivatives onto a set of smoothed empirical data system. The method purposed can be used in different fields of mathematical and engineering sciences as well as in the field of mesh generation techniques, especially when a discontinuous function has to be substituted by a continuous one.

REFERENCES/BIBLIOGRAPHY

[1] E. Whittaker: The Calculus of Observation, Blackie & Son Ltd., London, 1954.

[2] A. Nyíri: Solution of the Three-Dimensional Flow in the Bladed Space of a Hydraulic Machine based on Potential Theory (in Hungarian), Doctoral Thesis of the Hungarian Academy of Sciences, University of Miskolc, Department of Fluid- and Heat Engineering, Miskolc, Hungary, 1990.

[3] A. Nyíri: A Method of Smoothing Empirical Function at Non-Equidistant Points, Proceedings of the 9th Conference on Fluid Machinery, Budapest, Hungary, 1991. pp. 338-345.

[4] A. Nyíri: Surface Fitting and a New Direct Method for Solving Block Band Linear System, An International Journal Computers & Mathematics with Application, Vol. 38, 1999, pp. 161-173.

[5] A. Nyíri: Smoothing Three-Dimensional Set of Empirical Data, Manuscript, University of Miskolc, Department of Fluid- and Heat Engineering, Miskolc, Hungary, 2002.

[6] L. Könözsy: Computation of Two-Dimensional Shear Flows with the Solution of Turbulent Vorticity Transport Equation (in Hungarian), Ph.D. thesis, University of Miskolc, Department of Fluid and Heat Engineering, Miskolc, 2004.

[7] A. Nyíri: Hermite Interpolating Polynomials, Miskolc Mathematical Notes, Vol. 6, No. 2, Miskolc, Hungary, 2005, pp. 225-240.

[8] A. Ludwig, M. Gruber-Pretzler, F. Mayer, A. Ishmurzin, M. Wu: A Way of Coupling Ternary Phase Diagram Information with Multiphase Solidification Simulations, *Mat. Sci. Eng. A*, *413-414*, 2005, pp. 485-489.

[9] A. Ludwig, A. Ishmurzin, M. Gruber-Pretzler, F. Mayer, M. Wu, R. Tanzer, W. Schützenhöfer: How To Combine Ternary Phase Diagram Information with Multiphase Solidification Simulations, *Proceedings of the 5th Decenial International Conference on Solidification Processing*, *Sheffield*, UK, 2007, pp. 493-496.

[10] A. Ishmurzin, M. Gruber-Pretzler, F. Mayer, M. Wu, A. Ludwig: Multiphase Multicomponent Modeling of Solidification Processes: Coupling Solidification Kinetics with Thermodynamics, International Journal of Materials Research, 2008. (*in printing*)