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

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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 successfully 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 $(\xi_k, \eta_k)$ empirical data be given in the $(x,y)$ coordinate system $1 \leq k \leq n$, $\xi_k < \xi_{k+1}$. The minimum of the sum will be sought for
\[
S = \sum_{k=0}^{n-r} (\delta^r u_k)^2 + \sum_{k=1}^{n} p_k (u_k - \eta_k)^2 + \sum_{k=1}^{n} q_k (x_k - \xi_k)^2 .
\]

where \( p_k \) and \( q_k \) are the smoothing parameters. The \( r \)th divided difference is
\[
\delta^r u_k = \frac{\delta^{r-1} u_{k+1} - \delta^{r-1} u_{k}}{x_{k+r} - x_k} , \quad \delta^0 u_k = u_k .
\]

Introducing the Lagrange function
\[
\Psi_{k-j,r}(x) = \prod_{\lambda=0}^{r} (x - x_{k+1}) ,
\]
the first derivative of this is
\[
\frac{d}{dx} \Psi_{k-j,r}(x) = \Sigma_{\lambda=0}^{r} \prod_{\lambda \neq v}^{r} (x - x_{k+1}) , \quad 0 \leq i \leq r .
\]

and
\[
\Psi_{k-j,r}(x_{k+1}) = \prod_{\lambda=0}^{r} (x_{k+1} - x_{k+i}) , \quad 0 \leq j \leq r ,
\]
with this the divided difference can be written as follows
\[
\delta^r u_{k-j} = \Sigma_{j} u_{k+i} \left[ \Psi_{k-j,r}(x_{k+i}) \right]^{-1} .
\]
if \( 1 \leq K \leq r \) then \( 0 \leq i \leq K-1 , \quad 0 \leq j \leq r ,
\]
if \( r+1 \leq K \leq n-r \) then \( 0 \leq i,j \leq r ,
\]
if \( n-r+1 \leq K \leq n \) then \( 0 \leq i , j \leq r , \quad 0 \leq j \leq \min[r,n-K+1] .
\]
The numbers \( p_k > 0 , \quad q_k > 0 \) are inversely proportional to the square of the standard deviations. The part sum of the Eq. (1.1) belongs to a point \( K \) is
\[
S_k = \sum_{j=0}^{r} (\delta^r u_k)^2 + p_k (u_k - \eta_k)^2 + q_k (x_k - \xi_k)^2 .
\]
The necessary conditions for the minimum of this sum are
\[
\frac{\partial S_k}{\partial u_k} = 0 , \quad \frac{\partial S_k}{\partial x_k} = 0 .
\]

3. THE FIRST CONDITION OF SMOOTHING

Let us differentiate \( S_k \) respect to \( u_k \) getting
\[
\frac{1}{2} \frac{\partial^2 S_k}{\partial u_k^2} = \sum_{j=0}^{r} \frac{\partial^2 u_{k-j}}{\partial u_k^2} + p_k (u_k - \eta_k) = 0 ,
\]
where
\[
\frac{\partial^2 u_{k-j}}{\partial u_k^2} = \sum_{j=0}^{r} u_{k+i} \left[ \Psi_{k-j,r}(x_{k+i}) \right]^{-1} .
\]
The linear equation system (L.E.S.) has to be solved is as follows
\[
\sum_{j=0}^{r} u_{k+1} \left[ \Psi_{k-j,r}(x_{k+i}) \right]^{-1} + p_k u_k = p_k \eta_k .
\]
The compact form of the system is
\[
a_k u_{k+r} = p_k \eta_k , \quad 1 \leq K \leq n ,
\]
where if \( 1 \leq K \leq r \), \( \ell - K \leq \ell \leq r ,
\]
if \( r+1 \leq K \leq n-r \), \( -r \leq \ell \leq r ,
\]
if \( n-r+1 \leq K \leq n \), \( -r \leq \ell \leq n-K ,
\]
The coefficients are
\[ a_{K,0} = p_K + \sum_{i=1}^{\nu} \left[ \psi'_{K-i,r}(x_k) \right]^2, \] (2.3a)
if \( 1 \leq K \leq r \), then \( \mu = 0 \), \( v = K-1 \).
if \( r + 1 \leq K \leq n \), then \( \mu = 0 \), \( v = r \).
if \( n - r + 1 \leq K \leq n \), then \( \mu = K + r - n \).
\[ a_{K,i} = \sum_{i=1}^{\nu} \left[ \psi'_{K-i,r}(x_k) \psi'_{K-i-1,r}(x_k) \right]^2, \] (2.3b)
if \( 1 \leq K \leq r \), then \( 1 - K \leq \ell \leq r \),
where
- if \( \ell < 0 \), then \( \mu = -\ell, \leq i \leq K - 1 = v \),
- if \( \ell > 0 \), then \( \mu = 0 \leq i \leq v = \min \{ K - 1, r - \ell \} \),
- if \( r + 1 \leq K \leq n - r \), then \( -r \leq \ell \leq r \),
- if \( \ell < 0 \), then \( \mu = -\ell, \leq i \leq r = v \),
- if \( \ell > 0 \), then \( \mu = 0 \leq i \leq r - \ell = v \),
- if \( n - r + 1 \leq K \leq n \), then \( -r \leq \ell \leq n - K \),
- if \( \ell < 0 \), then \( \mu = \max \{ -\ell, K - n + r \}, v = r \),
- if \( \ell > 0 \), then \( \mu = K - n + r, v = r - \ell \).

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 \( x_K \)
\[ \frac{\partial}{\partial x_K} \sum_{i=0}^{r} \left( \delta^r u_{K-i} \right)^2 + q_K(x_k - \xi_K) = 0, \] (3.1)
and denoting this by \( f_K \)
\[ f_K = \sum_{i=0}^{r} \delta^r u_{K-i} \frac{\partial}{\partial x_K} \delta^r u_{K-i} + q_K(x_k - \xi_K) = 0, \] (3.2)
\[ f_K = f_k(x_{K-n}, \ldots, x_{K}, x_{K+1}, \ldots, x_{K+n}), \ x = [x_{K-n}, \ldots, x_{K-1}, x_{K}, x_{K+1}, \ldots, x_{K+n}]^T, \ f = [f_1, f_2, \ldots, f_f]^T, \]
where
- if \( 1 \leq K \leq r \), then \( \mu = K - 1 \), \( v = r \),
- if \( r + 1 \leq K \leq n - r \), then \( \mu = v = r \),
- if \( n - r + 1 \leq K \leq n \), then \( \mu = r, v = n - K \).

The Jacobian matrix of \( f \) vector according to \( x \) is
\[ D = \frac{\partial f}{\partial x} \] (3.3)
and the entries of it are
\[ D_{K,i} = \frac{\partial f_K}{\partial x_K} = \sum_{i=0}^{r} \frac{\partial}{\partial x_K} \left[ \delta^r u_{K-i} \frac{\partial}{\partial x_K} \delta^r u_{K-i} \right] + q_K \frac{\partial x_K}{\partial x_K}, \]
where the intervals for \( \ell \) 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)
\[ \frac{\partial \delta^r u_{K-i}}{\partial x_K} = -\sum_{i=0}^{r} u_{K-i} \left[ \psi'_{K-i-1,r}(x_{K-i+1}) \right]^2 \frac{\partial}{\partial x_K} \psi'_{K-i-1,r}(x_{K-i+1}), \ 0 \leq i \leq r, \]
\[ \frac{\partial}{\partial x_{k,i'}} \frac{\partial u_{K-1}}{\partial x_k} = - \sum_{j=0}^{r} u_{K-1,j} \left\{ -2 \left[ \psi_{K-1,r}(x_{K-1,j}) \right]^3 \cdot \frac{\partial}{\partial x_{k,i'}} \psi_{K-1,r}(x_{K-1,j}) + \left[ \psi_{K-1,r}(x_{K-1,j}) \right]^2 \cdot \frac{\partial}{\partial x_k} \psi_{K-1,r}(x_{K-1,j}) \right\}, \]
\[ \frac{\partial^2 u_{K-1}}{\partial x_{k,i'}} = - \sum_{j=0}^{r} u_{K-1,j} \left[ \psi_{K-1,r}(x_{K-1,j}) \right]^2 \frac{\partial}{\partial x_k} \psi_{K-1,r}(x_{K-1,j}), \right\} \]
and the non-linear system of equations
\[ D(x) = -f(x) = b \]
has to be solved by iteration for \( t \), and \( x^{m+1} = x^m + t^m \). The elements of the \( D(x) \) matrix can be approximated as
\[ D_{K,K'} \approx \frac{f_k(x + t) - f(x)}{\Delta x_{K,K'}}. \]

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
\[ x = [x_1, \ldots, x_n]^T, \quad u = [u_1, \ldots, u_n]^T, \quad \xi = [\xi_1, \ldots, \xi_n]^T \]
introducing the following
\[ D(x, u, \xi, p, q) = \sum_{K=1}^{n} (\psi_{K} u_{K}^p)^2, \quad K_u(u, \eta; p) = \sum_{K=1}^{n} (u_{K} - \eta_{K} p)^2, \quad K_x(x, \xi; q) = \sum_{K=1}^{n} (x_{K} - \xi_{K} q)^2, \]
functions which give the expression for Eq. (1.1) as
\[ S = D + pK_u + qK_x, \]
and the conditions for getting the minimum value are
\[ \frac{\partial S}{\partial u_k} = 0. \]

Let us nominate \( x_e \) and \( u_e \) at which the minimum is reached, then
\[ S = S(u_e, x_e; p, q). \]
Choosing arbitrary numbers like \( \kappa, \rho > 0 \) and examining the following
\[ \tilde{S}(u_e, x_e; \kappa, \rho) = D(u_e, x_e; p, q) + \kappa K_u(u_e; p) + \rho K_x(x_e; q) \]
sum-total which agrees with \( S \) if \( \kappa = p \) and \( \rho = q \). In order to search the minimum of \( \tilde{S} \) as the function of \( p \) and \( q \), we have to calculate the derivatives
\[ \frac{\partial \tilde{S}}{\partial \rho} = \frac{\partial D}{\partial \rho} + \kappa \frac{\partial K_u}{\partial \rho}, \quad \frac{\partial \tilde{S}}{\partial q} = \frac{\partial D}{\partial q} + \rho \frac{\partial K_x}{\partial q}. \]
If \( \kappa = \kappa^* \) and \( \rho = \rho^* \), then the derivatives will be zero
\[ \rho^* = - \frac{\partial D}{\partial K_u} \quad \text{and} \quad \rho^* = - \frac{\partial D}{\partial K_x}. \]
Choosing \( p^* = \kappa^* \) and \( q^* = \rho^* \), then
\[ S(p^*, q^*) = \tilde{S}(\kappa, \rho) \]
and \( \tilde{S} \) has its minimum. At first let us consider the case when the ordinates are smoothed only
\[ S = \sum_{K=1}^{n} (\psi_{K} u_{K}^p)^2 + p \sum_{K=1}^{n} (u_{K} - \eta_{K} p)^2. \]
If \( p = 0 \) then the solution will correspond to the conditions \( \delta^i u_k = 0 \), 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 \( K_{ux} = 0 \) and \( D_{x} = \sum (\delta^i u_k)^2 \).

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

\[
U(p, q) = \frac{D(p, q)}{D_{x}} + \frac{K(u(p) + K_x(q))}{K_{x0}},
\]

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

\[
S = D_{x} U, \quad \kappa = \frac{D_{x0}}{K_{u0}}, \quad \rho = \frac{D_{x0}}{K_{x0}},
\]

consequently

\[
p^* = \frac{D_{x0}}{K_{u0}}, \quad q^* = \frac{D_{x0}}{K_{x0}}.
\]

and

\[
S(p^*, q^*) = D_{x} U(p^*, q^*).
\]

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

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. \( K_{ug} = \sum (u_k - \eta_k)^2, \quad K_{xg} = \sum (x_k - \xi_k)^2 \) are given, then computing the functions \( K_u(p), \quad K_x(q) \) 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

\[
P_{k,m} = u_k + \sum_{i=1}^{m} \delta^i u_k \Psi_{k,i-1}(x),
\]

or

\[
Q_{k,m}(x) = u_k + \sum_{i=1}^{m} \delta^i u_k \Psi_{k,i-1}(x).
\]

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 \( \Psi \) is

\[
\Psi^{(r-\mu)}_{k,r} = (r-\mu) p_{\mu+1} [x - x_k, x - x_{k+1}, ..., x - x_{k+r}],
\]

where

\[
p_{r} (\varepsilon) = p_{r} [a_1, a_2, ..., a_r]
\]

means the sum of all the possible \( \nu \) elements products of \( a_1 \).

\[
p_{r} (\varepsilon) = \sum_{\lambda_1 + \lambda_2 + ... + \lambda_r = \nu} a_{1}^{\lambda_1} a_{2}^{\lambda_2} ... a_{r}^{\lambda_r}
\]

\[
= \sum_{\lambda_1 + \lambda_2 + ... + \lambda_r = \nu} a_{1}^{\lambda_1} a_{2}^{\lambda_2} ... a_{r}^{\lambda_r}
\]

\[
= \sum_{\lambda_1 + \lambda_2 + ... + \lambda_r = \nu} a_{1}^{\lambda_1} a_{2}^{\lambda_2} ... a_{r}^{\lambda_r}
\]
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 \(0 \leq i, j \leq 2\), \(-2 \leq \ell \leq 2\) and \(3 \leq K \leq n - 2\). First of all, the divided differences will be computed, and each step can be found in Tables 1-3.

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

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

\[
a_{K,0} = p_K + \sum_{j=0}^{2} \left[ \psi_{K-1,2} (x_K) \right]^{2}; \\
a_{K,\ell} = \sum_{j=0}^{2} \left[ \psi_{K-1,2} (x_{K+1}) \psi_{K-1,2} (x_K) \right]^{-1},
\]

if \(\ell = -2, -1\) then \(\mu = -\ell \leq i \leq 2 = \nu\),

if \(\ell = 1, 2\) then \(\mu = 0 \leq i \leq 2 - \ell = \nu\).

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

\[
D_{K,K+\ell} = \frac{\partial f_K}{\partial x_{K+\ell}} = \sum_{i=0}^{2} \frac{\partial}{\partial x_{K+\ell}} \left[ \delta^2 u_{K-1} \frac{\partial \delta^2 u_{K-1}}{\partial x_K} \right] + q_K \frac{\partial x_K}{\partial x_{K+\ell}}
\]

where

\[
f_K = \sum_{i=0}^{2} \delta^2 u_{K-1} \frac{\partial \delta^2 u_{K-1}}{\partial x_K} + q_K (x_K - \xi_K) = 0,
\]

and the necessary derivatives are

\[
\frac{\partial}{\partial x_{K+\ell}} \delta^2 u_{K-1} = -\sum_{j=0}^{2} u_{K-j+1} \left[ \psi_{K,2}^r (x_{K+1}) \right]^{-2} \frac{\partial}{\partial x_{K+\ell}} \psi_{K,2}^r (x_{K+1}), \\
\frac{\partial}{\partial x_K} \delta^2 u_{K-1} = -\sum_{j=0}^{2} u_{K-j+1} \left[ \psi_{K,2}^r (x_{K+1}) \right]^{-2} \frac{\partial}{\partial x_K} \psi_{K,2}^r (x_{K+1}) \psi_{K,2}^r (x_{K+1}).
\]

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

<table>
<thead>
<tr>
<th>(\psi_{K,i}^r (x_{K+1}))</th>
<th>(j = 0)</th>
<th>(1)</th>
<th>(2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i = 0)</td>
<td>((x_K - x_{K+1})(x_K - x_{K+2}))</td>
<td>((x_{K+1} - x_K)(x_{K+1} - x_{K+2}))</td>
<td>((x_{K+2} - x_K)(x_{K+2} - x_{K+1}))</td>
</tr>
<tr>
<td>(1)</td>
<td>((x_{K+1} - x_K)(x_{K+1} - x_{K+1}))</td>
<td>((x_K - x_{K+1})(x_K - x_{K+1}))</td>
<td>((x_{K+1} - x_K)(x_{K+1} - x_K))</td>
</tr>
<tr>
<td>(2)</td>
<td>((x_{K+2} - x_{K+1})(x_{K+2} - x_K))</td>
<td>((x_{K+1} - x_{K+2})(x_{K+1} - x_K))</td>
<td>((x_K - x_{K+2})(x_K - x_{K+1}))</td>
</tr>
</tbody>
</table>
### Table 2. First Derivatives for Satisfying the Conditions of Smoothing Procedure

<table>
<thead>
<tr>
<th>i</th>
<th>j</th>
<th>( \Psi'<em>{k-1,2}(x</em>{k-i+1}) )</th>
<th>( \frac{\partial}{\partial x_{k-i}} )</th>
<th>( \frac{\partial}{\partial x_k} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>j = 0</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>( \ell = -2 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>( -1 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>( (x_k - x_{k-1}) + (x_{k-1} - x_{k+2}) )</td>
<td>( - (x_{k-1} - x_{k+2}) )</td>
<td>( - (x_{k+2} - x_k) )</td>
</tr>
<tr>
<td>1</td>
<td>( \ell = -2 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>( -1 )</td>
<td>( (x_{k-1} - x_k) )</td>
<td>( (x_{k-1} - x_{k+1}) )</td>
<td>( - (x_{k+1} - x_k) )</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>( - (x_{k+1} - x_k) )</td>
<td>( (x_k - x_{k+1}) )</td>
<td>( - (x_{k+1} - x_k) )</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>( (x_k - x_{k+1}) )</td>
<td>( (x_k - x_{k+1}) )</td>
<td>( (x_{k+1} - x_k) )</td>
</tr>
<tr>
<td>i = 1</td>
<td>( \ell = -2 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>( -1 )</td>
<td>( (x_{k-1} - x_k) )</td>
<td>( (x_{k-1} - x_{k+2}) )</td>
<td>( - (x_{k+1} - x_k) )</td>
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<tr>
<td></td>
<td>0</td>
<td>( (x_{k-1} - x_{k+2}) )</td>
<td>( (x_{k-1} - x_{k+2}) )</td>
<td>( - (x_{k+1} - x_k) )</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>( (x_{k-1} - x_{k+2}) )</td>
<td>( (x_{k-1} - x_{k+2}) )</td>
<td>( - (x_{k+1} - x_k) )</td>
</tr>
<tr>
<td>i = 2</td>
<td>( \ell = -2 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>( -1 )</td>
<td>( (x_{k-2} - x_{k-1}) )</td>
<td>( -(x_{k-2} - x_k) )</td>
<td>( - (x_{k-2} - x_k) )</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>( (x_{k-2} - x_{k-1}) )</td>
<td>( (x_{k-2} - x_{k-1}) )</td>
<td>( - (x_{k-2} - x_k) )</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>( (x_{k-2} - x_{k-1}) )</td>
<td>( (x_{k-2} - x_{k-1}) )</td>
<td>( - (x_{k-2} - x_k) )</td>
</tr>
</tbody>
</table>

### Table 3. Second Derivatives for Satisfying the Conditions of Smoothing Procedure

<table>
<thead>
<tr>
<th>i</th>
<th>j</th>
<th>( \Psi'<em>{k-1,2}(x</em>{k-i+1}) )</th>
<th>( \frac{\partial}{\partial x_{k-i}} )</th>
<th>( \frac{\partial}{\partial x_k} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>j = 0</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>( \ell = -2 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>( -1 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>( -1 )</td>
<td>( -1 )</td>
<td>( 1 )</td>
</tr>
<tr>
<td>2</td>
<td>( -1 )</td>
<td>1</td>
<td>( -1 )</td>
<td></td>
</tr>
<tr>
<td>i = 1</td>
<td>( \ell = -2 )</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>( -1 )</td>
<td>( -1 )</td>
<td>( -1 )</td>
<td>( 1 )</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>( 1 )</td>
<td>( -1 )</td>
<td>( -1 )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>i = 2</td>
<td>( \ell = -2 )</td>
<td>( -1 )</td>
<td>( 1 )</td>
<td>( -1 )</td>
</tr>
<tr>
<td></td>
<td>( -1 )</td>
<td>1</td>
<td>( -1 )</td>
<td>( -1 )</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

### 8. Numerical Example for Smoothing Procedure

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

### Table 4. The \((\xi_k, \eta_k)\) Set of Empirical Data

<table>
<thead>
<tr>
<th>K</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \xi_k )</td>
<td>0</td>
<td>1.0</td>
<td>1.5</td>
<td>2.0</td>
<td>2.5</td>
</tr>
<tr>
<td>( \eta_k )</td>
<td>10.2</td>
<td>8.4</td>
<td>8.1</td>
<td>7.5</td>
<td>7.9</td>
</tr>
</tbody>
</table>
TABLE 5. ELEMENTS OF THE LINEAR EQUATION SYSTEM FOR THE FIRST CONDITION

<table>
<thead>
<tr>
<th></th>
<th>$\Psi'<em>{3-1,2}(x</em>{3-i+1})$</th>
<th>$\frac{\partial}{\partial x_3} \Psi'<em>{3-1,2}(x</em>{3-i+1})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$j = 0$</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>$i = 0$</td>
<td>0.5</td>
<td>-0.25</td>
</tr>
<tr>
<td></td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>-1.5</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>-0.5</td>
<td>-0.5</td>
</tr>
<tr>
<td>1</td>
<td>1.5</td>
<td>-0.5</td>
</tr>
<tr>
<td></td>
<td>0.75</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>-1.0</td>
</tr>
</tbody>
</table>

The divided differences

$$\delta^2 u_3 = \sum_{j=0}^{2} u_{3+j} \left[ \Psi'_{3,2}(x_{3+j}) \right] = 2.00000,$$
$$\delta^2 u_2 = \sum_{j=0}^{2} u_{2+j} \left[ \Psi'_{2,2}(x_{2+j}) \right] = -0.60000,$$
$$\delta^2 u_1 = \sum_{j=0}^{2} u_{1+j} \left[ \Psi'_{1,2}(x_{1+j}) \right] = 0.80000.$$

and the diagonal elements of the linear equation system

$a_{3,0} = p_3 + \sum_{i=0}^{2} \left[ \Psi'_{3-1,2}(x_3) \right] = 21.77778,$

$a_{3,-2} = \sum_{i=0}^{2} \left[ \Psi'_{3-1,2}(x_1) \Psi'_{3-1,2}(x_3) \right] = 0.88889,$

$a_{3,-1} = \sum_{i=0}^{2} \left[ \Psi'_{3-1,2}(x_2) \Psi'_{3-1,2}(x_3) \right] = -10.66667,$

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

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

TABLE 6. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

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

TABLE 7. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

<table>
<thead>
<tr>
<th>$\frac{\partial^2 u_{3-1}}{\partial x_{3+i}}$</th>
<th>$\sum_{i=0}^{2} \frac{\partial^2 u_{3-1}}{\partial x_3} \frac{\partial^2 u_{3-1}}{\partial x_{3+i}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\ell = -2$</td>
<td>1.73333</td>
</tr>
<tr>
<td>-1</td>
<td>-2.0</td>
</tr>
<tr>
<td>0</td>
<td>0.26667</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>
### TABLE 8. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

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

### TABLE 9. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

\[
\begin{array}{cccc}
\left[ \psi'_{3-i,2} \left( x_{3-i+j} \right) \right]^2 \cdot \frac{\partial}{\partial x_{3+l}} \frac{\partial}{\partial x_3} \psi'_{3-i,2} \left( x_{3-i+j} \right) \\
\hline
i = 0 & j = 0 & 1 & 2 \\
\ell = -2 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 8.0 & 0 & 0 \\
1 & -4.0 & -16.0 & -4.0 \\
2 & -4.0 & 16.0 & -4.0 \\
\ell = -1 & 0 & 0 & 0 \\
-1 & -4.0 & -16.0 & 4.0 \\
0 & 0 & 32.0 & 0 \\
1 & 4.0 & -16.0 & -4.0 \\
2 & 0 & 0 & 0 \\
\ell = 0 & -0.44444 & 4.0 & -1.77778 \\
-1 & -0.44444 & -4.0 & -1.77778 \\
0 & 0 & 0 & 3.55556 \\
1 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 \\
\end{array}
\]

### TABLE 10. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

\[
\frac{\partial}{\partial x_{3+l}} \frac{\partial}{\partial x_3} s^2 u_{3-i} \\
\hline
i = 0 & 1 & 2 \\
\ell = -2 & 0 & 0 & 0.977778 \\
-1 & 0 & 37.2 & -4.53339 \\
0 & -49.2 & -24.0 & 3.55564 \\
1 & 37.2 & -13.2 & 0 \\
2 & 12.0 & 0 & 0 \\
\end{array}
\]

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### TABLE 11. DERIVATIVES FOR CONSTRUCTING THE JACOBIAN MATRIX

\[
\sum_{i=0}^{2} \delta^2 u_{3-i} \frac{\partial}{\partial x_{3, i}} \frac{\partial}{\partial x_3} \delta^2 u_{3-i}
\]

<table>
<thead>
<tr>
<th>( \ell )</th>
<th>( \delta^2 u_{3-i} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2</td>
<td>0.78222</td>
</tr>
<tr>
<td>-1</td>
<td>-25.94667</td>
</tr>
<tr>
<td>0</td>
<td>-81.15549</td>
</tr>
<tr>
<td>1</td>
<td>82.32000</td>
</tr>
<tr>
<td>2</td>
<td>24.00000</td>
</tr>
</tbody>
</table>

### TABLE 12. DIAGONAL ELEMENTS OF THE JACOBIAN MATRIX

\[
D_{3,3+\ell} = \frac{\partial f_3}{\partial x_{3, \ell}} = \sum_{i=0}^{2} \frac{\partial^2 u_{3-i}}{\partial x_{3, i}} \frac{\partial^2 u_{3-i}}{\partial x_3} + \frac{\partial^2 u_{3-i}}{\partial x_{3, i}} \frac{\partial^2 u_{3-i}}{\partial x_3} \frac{\partial}{\partial x_3} \partial^2 u_{3-i}
\]

<table>
<thead>
<tr>
<th>( \ell )</th>
<th>( D_{3,3+\ell} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-2</td>
<td>1.24444</td>
</tr>
<tr>
<td>-1</td>
<td>-28.64000</td>
</tr>
<tr>
<td>0</td>
<td>-48.76438 + q_3</td>
</tr>
<tr>
<td>1</td>
<td>68.00000</td>
</tr>
<tr>
<td>2</td>
<td>81.60000</td>
</tr>
</tbody>
</table>

### 9. NUMERICAL EXAMPLE FOR CHOOSING THE SMOOTHING PARAMETERS

#### TABLE 13. THE SET OF EMPIRICAL AND SMOOTHED DATA SYSTEM

<table>
<thead>
<tr>
<th>( K )</th>
<th>( \xi_K )</th>
<th>( \eta_K )</th>
<th>( X_K )</th>
<th>( U_K )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0</td>
<td>10.2</td>
<td>-0.44301</td>
<td>9.79926</td>
</tr>
<tr>
<td>2</td>
<td>1.0</td>
<td>8.4</td>
<td>0.86080</td>
<td>8.56901</td>
</tr>
<tr>
<td>3</td>
<td>1.5</td>
<td>8.1</td>
<td>1.46634</td>
<td>8.20335</td>
</tr>
<tr>
<td>4</td>
<td>2.0</td>
<td>7.5</td>
<td>2.05231</td>
<td>7.98061</td>
</tr>
<tr>
<td>5</td>
<td>2.5</td>
<td>7.9</td>
<td>2.56754</td>
<td>7.91858</td>
</tr>
<tr>
<td>6</td>
<td>3.0</td>
<td>7.8</td>
<td>3.04186</td>
<td>7.98851</td>
</tr>
<tr>
<td>7</td>
<td>3.7</td>
<td>8.6</td>
<td>3.83988</td>
<td>8.16074</td>
</tr>
<tr>
<td>8</td>
<td>5.0</td>
<td>8.3</td>
<td>4.83828</td>
<td>8.06250</td>
</tr>
<tr>
<td>9</td>
<td>6.5</td>
<td>6.0</td>
<td>6.68653</td>
<td>6.07335</td>
</tr>
<tr>
<td>10</td>
<td>8.0</td>
<td>3.4</td>
<td>8.23354</td>
<td>3.47118</td>
</tr>
<tr>
<td>11</td>
<td>1.0</td>
<td>0.2</td>
<td>10.05684</td>
<td>0.19294</td>
</tr>
</tbody>
</table>

\[
D_\alpha = 7.93984 \quad q^* = 0.18974 \quad p^* = 0.55334
\]

#### TABLE 14. QUANTITIES FOR CHOOSING THE SMOOTHING PARAMETER

<table>
<thead>
<tr>
<th>( p )</th>
<th>( K_u )</th>
<th>( D )</th>
<th>( \frac{K_u}{K_u} + \frac{D}{D_\alpha} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>0.09519</td>
<td>1.63643</td>
<td>0.21257</td>
</tr>
<tr>
<td>10.0^{0.5}</td>
<td>0.16648</td>
<td>1.24534</td>
<td>0.16831</td>
</tr>
<tr>
<td>( p^* )</td>
<td>0.71943</td>
<td>0.61642</td>
<td>0.12767</td>
</tr>
<tr>
<td>10.0^{-0.5}</td>
<td>1.19108</td>
<td>0.42017</td>
<td>0.13582</td>
</tr>
<tr>
<td>10.0^{-1}</td>
<td>2.62681</td>
<td>0.15847</td>
<td>0.20286</td>
</tr>
<tr>
<td>10.0^{-5}</td>
<td>14.36061</td>
<td>0.00000</td>
<td>1.00000</td>
</tr>
</tbody>
</table>
TABLE 15. QUANTITIES FOR CHOOSING THE SMOOTHING PARAMETER

<table>
<thead>
<tr>
<th>q</th>
<th>K_x</th>
<th>D</th>
<th>( \frac{K_u}{K_u0} + \frac{K_x}{K_x0} + \frac{D}{D_m} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>0.00102</td>
<td>0.59246</td>
<td>0.12466</td>
</tr>
<tr>
<td>1.0</td>
<td>0.04610</td>
<td>0.49391</td>
<td>0.12327</td>
</tr>
<tr>
<td>q*</td>
<td>0.39385</td>
<td>0.37265</td>
<td>0.10569</td>
</tr>
<tr>
<td>10.0^{-1}</td>
<td>0.72650</td>
<td>0.32376</td>
<td>0.10820</td>
</tr>
<tr>
<td>10.0^{-2}</td>
<td>7.08487</td>
<td>0.15582</td>
<td>0.23902</td>
</tr>
<tr>
<td>10.0^{-3}</td>
<td>K_x0 = 41.84478</td>
<td>0.05197</td>
<td>1.05664</td>
</tr>
</tbody>
</table>

FIGURE 1. CHOOSING THE SMOOTHING PARAMETERS

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