Annales Univ. Sci. Budapest., Sect. Comp. 32 (2010) 103-121

A GENERALIZED SPLINE APPROXIMATION

R. Polgár (Sopron, Hungary)

Abstract. In this paper a new method of spline approximation is given which is continuously differentiable to second order and applicable for robust estimators. The model computations have shown that the method is suitable for the accurate determination of the velocity and acceleration vectors in mechanical problems. Because of the good characteristic of the method, e.g. fast convergence, it seems to be widely applicable in engineering problems and time series analysis, e.g. modeling stock-market and economical processes.

AMS Subject Classification: 41A15, 65D04

1. Introduction

In engineering applications or during the analization of acoustic phenomena and stock-market processes the estimation of the main parameters describing samples with a huge number of data is of great importance. One of the simple methods is the application of regression theory. One chooses a so-called possible regression curve in this model based on the geometrical location of data points. This reveals that the solution is not unique. In this problem there are N points given by coordinates, (x_i, f_i), for $i = 1, 2, \dots, N$, and a regression function $g(x)$. To find the solution for $g(x)$ one solves the equation

$$\sum_{i=1}^{N} (f_i - g(x_i))^2 = \min_g$$

with the method of least squares.

Another possible method is the application of interpolation or approximation functions. During interpolation one reconstructs the function f from its values $f_1, f_2, \dots, f_N$ given in discrete points $x_1, x_2, \dots, x_N$. Again, in general, the solution is not unique. One chooses a suitable polynomial which best approximates the analyzed function on the interval $[x_1, x_N]$ in a given respect. The classical methods are Lagrange (Newton) and Hermite interpolation. Undesirable oscillations and huge computational capacity required to handle polynomials with high degree are characteristics of these approximation methods which can be avoided by the use of spline interpolation. In this case one looks for the m times continuously differentiable function g which is the solution of the equations

$$\delta(g) = \int_{x_0}^{x_N} (\partial^m g)^2 dx = \min_{W_2^m}, \tag{1.1}$$

and

$$g(x_i) = f(x_i) = f_i,\ i = 1, 2, \dots, N$$

Here W_2^m denotes the space of m times continuously differentiable and square-integrable functions. When $m < N$ the solution is unique, see the proof of Sard [1] who uses $(2m-1)$ degree smoothly connecting polynomials defined on intervals.

In most cases, as in our investigations, one is dealing with the solution with $m = 2$. The cubic smoothing spline of Schoenberg [8], Reinsch [9], [10], deBoor [11], [12], Wahba [13], has become the most commonly used and analyzed spline. When the values of f are modified by errors in the points x_i one looks for the best approximating solution in a given respect, namely with the composition of the theory of regression and interpolation curves,

$$\delta(g) = \int_{x_0}^{x_N} (\partial^2 g)^2 dx + \sum_{i=1}^{N} p_i (g(x_i) - f_i)^2 = \min_{W_2^2},$$

where the positive weighting numbers $\{p_i\}_{i=1}^n$ are capable of smoothing the solution when the errors are known.

2. The problem

Here we generalize the above description to the case when there are significantly more points given than the number of spline approximation polynomials

we choose. The weights are fixed by the method of least squares as in the case of robust estimators and the spline approximation is obtained as a result of an iteration process.
Let us take a subdivision $a = x_0 < x_1 < x_2 < \cdots < x_n = b$ of the interval $[a, b]$ of the x axis and the sample (x_{i_j}, f_{i_j}), $j = 1, 2, \ldots, n_i$ be given in the intervals (x_{i-1}, x_i), $i = 1, 2, \ldots, n$ where $\sum_{i=1}^{n} n_i = N$. Using this notation we solve the variation problem

$$\delta_p(g) = \lambda \int_{x_0}^{x_N} (\partial^2 g)^2 dx + \sum_{i=1}^{n} \sum_{j=1}^{n_j} p_{i_j} (g(x_{i_j}) - f_{i_j})^2 = \min_{W_2^2}, \tag{2.1}$$

with the generalized Lagrange multiplicator λ and positive weighting numbers p_{i_j}.

The solution of the problem (1.1) for $m = 2$ results in piecewise cubic polynomials which are continuous in zeroth, first and second order. Let us denote this as

$$g(x) = \begin{cases} g_1(x), & x_0 \le x \le x_1 \\ g_2(x), & x_1 \le x \le x_2 \\ \vdots & \vdots \\ g_n(x), & x_{n-1} \le x \le x_n \end{cases} \tag{2.2}$$

where

$$g_i(x) = a_i(x_i - x)^3 + b_i(x_i - x)^2 + c_i(x_i - x) + d_i$$

for every $i = 1, 2, \ldots, n$. Using (2.2) the problem

$$\begin{aligned} &Func(a_1, a_2, \ldots, a_n, b_1, \ldots, d_n, \Lambda_1, \ldots, \Lambda_{n-1}, \Delta_1, \ldots, \Xi_{n-1}) = \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n_j} p_{i_j} (g(x_{i_j} - f_{i_j})^2 + 2 \sum_{i=1}^{n-1} \Lambda_i (g_{i+1}(x_i) - g_i(x_i)) + \\ &+2 \sum_{i=1}^{n-1} \Delta_i (g'_{i+1}(x_i) - g'_i(x_i)) + \sum_{i=1}^{n-1} \Xi_i (g''_{i+1}(x_i) - g''_i(x_i)) \equiv \\ &\equiv Func \to \min \end{aligned} \tag{2.3}$$

is solved with the help of Lagrange multiplicators as an extremal value problem. A possible solution is found by Prvan [2]. The number of unknowns a_i, b_i, c_i, d_i is $4n$, and the number of multiplicators Λ_i, Δ_i, Ξ_i is $3(n-1)$. For the solution we need $4n + 3(n-1)$ linearly independent equations, which are determined by the solution of the analytic maximization problem. Since the number of unknowns equals to the number of equations of the linear system the problem can be solved in principle. The difficulty of (2.3) is the huge number of unknowns and equations ($7n-3$). We show how the number of equations can be reduced by eliminating $6n-3$ unknowns. The resulting equation system consists of n equations and has n unknowns. The determination of the weights p_{i_j} means additional difficulties. The system of linear equations is solved with unit weights first, then with the help of the solutions and the application of the methods of robust estimators the weights are redefined. These steps are repeated until the condition of iteration holds. The solution of this problem for $n=3$ is given by Závoti (1985) [3].

3. The equations

We introduce the following notation: $h_{i+1}=x_{i+1}-x_i$; $i=1,\dots,n-1$. Using these quantities for the partial derivatives of the function $Func$ by Λ_i, Δ_i, Ξ_i the following relations hold

$$a_{i+1}h_{i+1}^3+b_{i+1}h_{i+1}^2+c_{i+1}h_{i+1}+d_{i+1}-d_i=0, \tag{3.1}$$

$$3a_{i+1}h_{i+1}^2+2b_{i+1}h_{i+1}+c_{i+1}-c_i=0, \tag{3.2}$$

$$3a_{i+1}h_{i+1}+b_{i+1}-b_i=0 \tag{3.3}$$

for every $i=1,\dots,n-1$. For a simpler notation of the partial derivatives we use the following expressions

$$\begin{aligned}
\Phi_i &= \sum_{j=1}^{n_j} p_{i_j}(f_{i_j}-g(x_{i_j})),\\
\Psi_i &= \sum_{j=1}^{n_j} p_{i_j}(f_{i_j}-g(x_{i_j}))(x_i-x_{i_j}),\\
\Gamma_i &= \sum_{j=1}^{n_j} p_{i_j}(f_{i_j}-g(x_{i_j}))(x_i-x_{i_j})^2,\\
\Theta_i &= \sum_{j=1}^{n_j} p_{i_j}(f_{i_j}-g(x_{i_j}))(x_i-x_{i_j})^3
\end{aligned}$$

for $i=1,\dots,n$. In this way the partial derivatives of $Func$ by $d_1,\dots,d_n$ are

$$-\Phi_1-\Lambda_1=0, \tag{3.4}$$

$$-\Phi_i-\Lambda_i+\Lambda_{i-1}=0,\quad i=2,\dots,n-1, \tag{3.5}$$

$$-\Phi_n + \Lambda_{n-1} = 0. \tag{3.6}$$

The partial derivatives of $Func$ by $c_1, \ldots\ldots, c_n$ are

$$-\Psi_1 - \Delta_1 = 0, \tag{3.7}$$

$$-\Psi_i - \Delta_i + \Delta_{i-1} + h_i\Lambda_{i-1} = 0, \quad i = 2, \ldots, n-1, \tag{3.8}$$

$$-\Psi_n + \Delta_{n-1} + h_n\Lambda_{n-1} = 0. \tag{3.9}$$

The partial derivatives of $Func$ by $b_1, \ldots, b_n$ are

$$-\Gamma_1 - \Xi_1 = 0, \tag{3.10}$$

$$-\Gamma_i - \Xi_i + \Xi_{i-1} + 2h_i\Delta_{i-1} + h_i^2\Lambda_{i-1} = 0, \quad i = 2, \ldots, n-1, \tag{3.11}$$

$$-\Gamma_n + \Xi_{n-1} + 2h_n\Delta_{n-1} + h_n^2\Lambda_{n-1} = 0. \tag{3.12}$$

The partial derivatives of $Func$ by $a_1, \ldots, a_n$ are

$$\Theta_1 = 0, \tag{3.13}$$

$$-\Theta_i + 3h_i\Xi_{i-1} + 3h_i^2\Delta_{i-1} + h_i^3\Lambda_{i-1} = 0, \quad i = 2, \ldots, n. \tag{3.14}$$

To obtain the solution of the system of linear equations (3.4)-(3.14) we eliminate the Λ_i, Δ_i, Ξ_i, $i = 1, \ldots, n-1$ factors first. The sum of Eqs. (3.4)-(3.6) gives

$$\sum_{i=1}^{n} \Phi_i = 0, \tag{3.15}$$

and

$$\begin{aligned} \Lambda_1 &= -\Phi_1, \\ \Lambda_j &= -\sum_{i=1}^{j} \Phi_i, \quad j = 2, \ldots, n-1, \\ \Lambda_{n-1} &= \Phi_n. \end{aligned} \tag{3.16}$$

From the sum of Eqs. (3.7)-(3.9) there follows

$$\sum_{i=1}^{n} \Psi_i = \sum_{i=2}^{n} h_i\Lambda_{i-1}.$$

Using Eqs. (3.15) and (3.16) and the definition of h_i the resummation of $\sum_{i=2}^{n} h_i \Lambda_{i-1}$ gives

$$\begin{aligned}\sum_{i=2}^{n} h_i\Lambda_{i-1} &= -\sum_{i=2}^{n}\Big(h_i\sum_{j=1}^{i-1}\Phi_j\Big) = -\sum_{i=1}^{n-1}\Big(\Phi_i\sum_{j=i+1}^{n}h_j\Big) = \\ &= -\sum_{i=1}^{n-1}\big(\Phi_i(x_n - x_i)\big) = -\sum_{i=1}^{n}\big(\Phi_i(x_n - x_i)\big) = \\ &= -x_n\sum_{i=1}^{n}\Phi_i + \sum_{i=1}^{n}x_i\Phi_i = \sum_{i=1}^{n}x_i\Phi_i,\end{aligned}$$

which can be written as

$$\sum_{i=1}^{n}(\Psi_i - x_i\Phi_i) = 0, \tag{3.17}$$

and

$$\begin{aligned}&\Delta_1 = -\Psi_1,\\ &\Delta_j = -\sum_{i=1}^{j}\Psi_i - \sum_{i=1}^{j-1}(\Phi_i(x_j - x_i)), \quad j = 2,\ldots,n-1,\\ &\Delta_{n-1} = \Psi_n - h_n\Phi_n.\end{aligned} \tag{3.18}$$

The sum of Eqs. (3.10)-(3.12) is

$$\sum_{i=1}^{n}\Gamma_i = \sum_{i=2}^{n}h_i^2\Lambda_{i-1} + 2\sum_{i=2}^{n}h_i\Delta_{i-1}.$$

Substituting (3.16) and (3.18) into this equation, gives

$$\sum_{i=1}^{n}\Gamma_i = -2\sum_{i=2}^{n}\Big(h_i\sum_{j=1}^{i-1}\Psi_j\Big) - \sum_{i=2}^{n}\Big(h_i^2\sum_{j=1}^{i-1}\Phi_j\Big) - 2\sum_{i=3}^{n}\Big(h_i\sum_{j=2}^{i-1}\Big(h_j\sum_{k=1}^{j-1}\Phi_k\Big)\Big).$$

With the use of Eq. (3.17) the term containing Φ can be reformulated as

$$\begin{aligned}-\sum_{i=2}^{n}\Big(h_i\sum_{j=1}^{i-1}\Psi_j\Big) &= -\sum_{i=1}^{n-1}\Big(\Psi_i\sum_{j=i+1}^{n}h_j\Big) = -\sum_{i=1}^{n-1}\Psi_i(x_n - x_i) = \\ &= -\sum_{i=1}^{n}\Psi_i(x_n - x_i) = -x_n\sum_{i=1}^{n}\Psi_i + \sum_{i=1}^{n}x_i\Psi_i = \\ &= -x_n\sum_{i=1}^{n}x_i\Psi_i + \sum_{i=1}^{n}x_i\Phi_i,\end{aligned}$$

The remaining terms on the right-hand side are

$$\begin{aligned}
-\sum_{i=2}^{n}\Big(h_i^2\sum_{j=1}^{i-1}\Phi_j\Big)-2\sum_{i=3}^{n}\Big(h_i\sum_{j=2}^{i-1}\Big(h_j\sum_{k=1}^{j-1}\Phi_k\Big)\Big) &= -\sum_{i=1}^{n-1}\Big(\Phi_i\Big(\sum_{j=2}^{n}h_j\Big)^2\Big)= \\
&= -\sum_{i=1}^{n-1}\Phi_i(x_n-x_i)^2 = -\sum_{i=1}^{n}\Phi_i(x_n-x_i)^2 = \\
&= -x_n^2\sum_{i=1}^{n}\Phi_i + 2x_n\sum_{i=1}^{n}x_i\Phi_i - \sum_{i=1}^{n}x_i^2\Phi_i = \\
&= 2x_n\sum_{i=1}^{n}x_i\Phi_i - \sum_{i=1}^{n}x_i^2\Phi_i
\end{aligned}$$

using Eq. (3.15). Finally we have

$$\sum_{i=1}^{n}\Gamma_i = -2x_n\sum_{i=1}^{n}x_i\Phi_i + 2\sum_{i=1}^{n}x_i\Psi_i + 2x_n\sum_{i=1}^{n}x_i\Phi_i - \sum_{i=1}^{n}x_i^2\Phi_i,$$

or equivalently

$$\sum_{i=1}^{n}(\Gamma_i - 2x_i\Psi_i + x_i^2\Phi_i) = 0. \tag{3.19}$$

Moreover, we obtain

$$\begin{aligned}
\Xi_1 &= -\Gamma_1, \\
\Xi_j &= -\sum_{i=1}^{j}\Gamma_i - \sum_{i=1}^{j-1}\Psi_i(x_j-x_i) - \sum_{i=1}^{j-1}\Phi_i(x_j-x_i)^2, \quad j=2,\ldots,n-1, \\
\Xi_{n-1} &= \Gamma_n - 2h_n\Psi_n + h_n^2\Phi_n.
\end{aligned} \tag{3.20}$$

We can write Eq. (3.14) for $i = n$ by Eqs. (3.16), (3.18) and (3.20) as

$$\Theta_n - 3h_n\Gamma_n + 3h_n^2\Psi_n - h_n^3\Phi_n = 0, \tag{3.21}$$

since we have

$$\begin{aligned}
-\Theta_n + 3h_n\Xi_{n-1} + 3h_n^2\Delta_{n-1} + h_n^3\Lambda_{n-1} &= \\
= -\Theta_n + 3h_n(\Gamma_n - 2h_n\Psi_n + h_n^2\Phi_n) + 3h_n^2(\Psi_n - h_n\Phi_n) + h_n^3\Phi_n &= \\
= -\Theta_n + 3h_n\Gamma_n - 3h_n^2\Psi_n + h_n^3\Phi_n.&
\end{aligned}$$

After inserting Eqs. (3.16), (3.18) and (3.20) into Eq. (3.14) for $i = 2,\ldots,n-1$ there follows

$$\begin{aligned}
&\Theta_i + 3\sum_{j=1}^{i-1}\Big(\Gamma_j(x_i-x_{i-1}) + \Psi_j\left[(x_i-x_j)^2-(x_{i-1}-x_j)^2\right]\Big) + \\
&\quad + \sum_{j=1}^{i-1}\Phi_j\left[(x_i-x_j)^3-(x_{i-1}-x_j)^3\right] = 0.
\end{aligned} \tag{3.22}$$

Note that we have an equation equivalent to Eq. (3.22). This equivalent equation arises if we add (3.13) to (3.14) and then in the resulting new equation we add the terms up to the index i. This gives

$$\Theta_i + \sum_{j=1}^{i-1} \Big(\Theta_j + 3\Gamma_j \sum_{k=j+1}^{i} h_k + 3\Psi_j \Big(\sum_{k=j+1}^{i} h_k\Big)^2 + \Phi_j \Big(\sum_{k=j+1}^{i} h_k\Big)^3\Big) = 0, \tag{3.23}$$

for $i = 2, \ldots, n-1$.

So far we have eliminated the variables Λ_i, Δ_i and Ξ_i from the equations. The remaining unknowns are $a_1, \ldots, a_n, b_1, \ldots, d_n$, the determination of which is our task, since Θ_i, Γ_i, Ψ_i and Φ_i are depending on these variables, too.

Now we turn to our equations expressed in terms of the unknown variables $a_1, \ldots, d_n$. For the sake of simplicity we introduce the notation

$$X_{ik} = \sum_{j=1}^{n_i} p_{i_j} (x_i - x_{i_j})^k, \quad k = 0, 1, \ldots, 6, \tag{3.24}$$

and

$$F_{ik} = \sum_{j=1}^{n_i} p_{i_j} f_{i_j} (x_i - x_{i_j})^k, \quad k = 0, 1, 2, 3. \tag{3.25}$$

In terms of these expressions the equations containing Φ_i, Ψ_i, Γ_i, and Θ_i have the following form.
From Eq. (3.13) we have

$$\sum_{j=1}^{n_i} p_{i_j} \left(f_{i_j} - a_{i_j}(x_i - x_{i_j})^3 - b_{i_j}(x_i - x_{i_j})^2 - c_{i_j}(x_i - x_{i_j}) - d_{i_j}\right) = 0,$$

which is

$$X_{ik+3} a_i + X_{ik+2} b_i + X_{ik+1} c_i + X_{ik} d_i = F_{ik}, \tag{3.26}$$

for $i = 1, \ldots, n$ and $k = 0, 1, 2, 3$.
To obtain a more compact form of Eq. (3.21) let us denote

$$\begin{aligned} \xi_k &= X_{nk+3} - 3h_n X_{nk+2} + 3h_n^2 X_{nk+1} - h_n^3 X_{nk}, \quad k = 0, 1, 2, 3, \\ \xi_4 &= F_{n3} - 3h_n F_{n2} + 3h_n^2 F_{n1} - h_n^3 F_{n0}. \end{aligned} \tag{3.27}$$

Using these quantities we have

$$\xi_3 a_n + \xi_2 b_n + \xi_1 c_n + \xi_0 d_n = \xi_4. \tag{3.28}$$

For a simple form of Eq. (3.22) let be

(3.29)
$$Y_{ijk} = 3X_{jk+2}(x_i - x_{i-1}) + 3X_{jk+1}\big((x_i - x_j)^2 - (x_{i-1} - x_j)^2\big) + \\ + X_{jk}\big((x_i - x_j)^3 - (x_{i-1} - x_j)^3\big),$$

where $k = 0, 1, 2, 3$.
In this case we have
(3.30)
$$X_{i6}a_i + X_{i5}b_i + X_{i4}c_i + X_{i3}d_i + \\ + \sum_{j=1}^{i-1} \big(Y_{ij3}a_j + Y_{ij2}b_j + Y_{ij1}c_j + Y_{ij0}d_j\big) = \\ = F_{i3} + \sum_{j=1}^{i-1} \Big(F_{j2}(x_i - x_{i-1}) + 3F_{j1}\big((x_i - x_j)^2 - (x_{i-1} - x_j)^2\big) + \\ + F_{j0}\big((x_i - x_j)^3 - (x_{i-1} - x_j)^3\big)\Big)$$

for $i = 2, \ldots, n-1$.
Inserting Eqs. (3.24) and (3.25) into Eqs. (3.15), (3.17) and (3.19) we get the following expressions

(3.31)
$$\sum_{i=1}^{n}(X_{i3}a_i + X_{i2}b_i + X_{i1}c_i + X_{i0}d_i) = \sum_{i=1}^{n} F_{i0},$$

(3.32)
$$\sum_{i=1}^{n} \Big((X_{i4} - x_iX_{i3})a_i + (X_{i3} - x_iX_{i2})b_i + \\ + (X_{i2} - x_iX_{i1})c_i + (X_{i1} - x_iX_{i0})d_i\Big) = \\ = \sum_{i=1}^{n}(F_{i1} - x_iF_{i0}),$$

(3.33)
$$\sum_{i=1}^{n} \Big((X_{i5} - 2x_iX_{i4} + x_i^2X_{i3})a_i + (X_{i4} - 2x_iX_{i3} + x_i^2X_{i2})b_i + \\ + (X_{i3} - 2x_iX_{i2} + x_i^2X_{i1})c_i + (X_{i2} - 2x_iX_{i1} + x_i^2X_{i0})d_i\Big) = \\ = \sum_{i=1}^{n}(F_{i2} - 2x_iF_{i1} + x_i^2F_{i0}).$$

Matrix representation

With the help of the equations derived in the previous section we determine the quantities $a_1, \ldots, d_n$.

From Eq. (3.3) we have

$$a_{i+1} = \frac{1}{3h_{i+1}}(b_i - b_{i+1}), \quad i = 1, \ldots, n-1. \tag{3.34}$$

We multiply Eq. (3.2) by h_{i+1}, subtract Eq. (3.1) and then we subtract Eq. (3.34) from this:

$$c_i = \frac{h_{i+1}}{3}(2b_i + b_{i+1}) + \frac{1}{h_{i+1}}(d_i - d_{i+1}), \quad i = 1, \ldots, n-1. \tag{3.35}$$

Substituting Eq. (3.34) into Eq. (3.1) we have

$$c_{i+1} = -\frac{h_{i+1}}{3}(b_i + 2b_{i+1}) + \frac{1}{h_{i+1}}(d_i - d_{i+1}), \quad i = 1, \ldots, n-1. \tag{3.36}$$

We express c_1 from Eq. (3.35) and insert it into Eq. (3.26),

$$\begin{aligned} a_1 = -\frac{1}{X_{1,6}}\Big(&\big(-X_{1,5} - \frac{2h_2}{3}X_{1,4}\big)b_1 + \big(-\frac{h_2}{3}X_{1,4}\big)b_2 + \\ &+\big(-X_{1,3} - \frac{1}{h_2}X_{1,4}\big)d_1 + \big(\frac{1}{h_2}X_{1,4}\big)d_2 + F_{1,3}\Big), \end{aligned} \tag{3.37}$$

which is expressed as

$$a_1 = \alpha_1 b_1 + \alpha_2 b_2 + \alpha_3 d_1 + \alpha_4 d_2 + \alpha_5. \tag{3.38}$$

Let be

$$\overline{a} = (a_1, \ldots, a_n)^T,\ \overline{b} = (b_1, \ldots, b_n)^T,\ \overline{c} = (c_1, \ldots, c_n)^T,\ \overline{d} = (d_1, \ldots, d_n)^T.$$

This way Eqs. (3.34) and (3.37) can be written in matrix form as

$$\overline{a} = A_b\overline{b} + A_d\overline{d} + \overline{v}_a, \tag{3.39}$$

where we have

$$A_b = \begin{bmatrix} \alpha_1 & \alpha_2 & & \\ \frac{1}{3h_2} & -\frac{1}{3h_2} & & \\ & \ddots & \ddots & \\ & & \frac{1}{3h_n} & -\frac{1}{3h_n} \end{bmatrix},$$

$$A_d = \begin{bmatrix} \alpha_3 & \alpha_4 & & \\ & & & \\ & & & \end{bmatrix}, \qquad \overline{v}_a = \begin{bmatrix} \alpha_5 \\ \\ \\ \end{bmatrix} \tag{3.40}$$

and we have also introduced the following notation: for matrices and vectors the elements, which are not specified, are 0.
Substituting a_n from Eq. (3.34) into Eq. (3.28) we have

$$c_n = \frac{1}{\xi_1}\Big(\big(-\frac{1}{3h_n}\xi_3\big)b_{n-1} + \big(\frac{1}{3h_n}\xi_3 - \xi_2\big)b_n + (-\xi_0)d_n + \xi_4\Big) \tag{3.41}$$

which is written as

$$c_n = \beta_1 b_{n-1} + \beta_2 b_n + \beta_3 d_n + \beta_4. \tag{3.42}$$

With the help of Eqs. (3.35) and (3.41) the matrix equation for $\overline{c}$ is

$$\overline{c} = C_b^* \overline{b} + C_d^* \overline{d} + \overline{c}^*, \tag{3.43}$$

where

$$C_b^* = \begin{bmatrix} \frac{2h_2}{3} & \frac{h_2}{3} & & \\ & \ddots & \ddots & \\ & & \frac{2h_n}{3} & \frac{h_n}{3} \\ & & \beta_1 & \beta_2 \end{bmatrix},$$

$$C_d^* = \begin{bmatrix} \frac{1}{h_2} & -\frac{1}{h_2} & & \\ & \ddots & \ddots & \\ & & \frac{1}{h_n} & -\frac{1}{h_n} \\ & & & \beta_3 \end{bmatrix}, \qquad \overline{c}_v^* = \begin{bmatrix} \\ \\ \\ \beta_4 \end{bmatrix}. \tag{3.44}$$

We substitute a_1, a_2 from Eq. (3.39) and c_2 from Eq. (3.36) into Eq. (3.30) if $i = 2$. This way we obtain

$$\begin{aligned} c_1 = \frac{1}{Y_{2,1,1}}\Big(&\big(-\alpha_1 Y_{2,1,3} - Y_{2,1,2} - \frac{X_{2,6}}{3h_2} + \frac{h_2 X_{2,4}}{3}\big)b_1 + \\ &+\big(-\alpha_2 Y_{2,1,3} + \frac{X_{2,6}}{3h_2} - X_{2,5} + \frac{2h_2}{3}X_{2,4}\big)b_2 + \\ &+\big(-\alpha_3 Y_{2,1,3} - Y_{2,1,0} - \frac{X_{2,4}}{h_2}\big)d_1 + \\ &+\big(-\alpha_4 Y_{2,1,3} + \frac{X_{2,4}}{h_2} - X_{2,3}\big)d_2 + \\ &+\big(F_{2,3} + 3h_2 F_{1,2} + 3h_2^2 F_{1,1} + h_2^3 F_{1,0}\big)\Big) \end{aligned} \tag{3.45}$$

which is written as

$$c_1 = \gamma_1 b_1 + \gamma_2 b_2 + \gamma_3 d_1 + \gamma_4 d_2 + \gamma_5. \tag{3.46}$$

We have a matrix equation obtained from Eqs. (3.36) and (3.45)

$$\overline{c} = C_b\overline{b} + C_d\overline{d} + \overline{c}_v, \tag{3.47}$$

where

$$C_b = \begin{bmatrix} \gamma_1 & \gamma_2 & & & \\ -\frac{h_2}{3} & -\frac{2h_2}{3} & & & \\ & \ddots & \ddots & & \\ & & & -\frac{h_n}{3} & -\frac{2h_n}{3} \end{bmatrix},$$
$$C_d = \begin{bmatrix} \gamma_3 & \gamma_4 & & & \\ \frac{1}{h_2} & -\frac{1}{h_2} & & & \\ & \ddots & \ddots & & \\ & & \frac{1}{h_n} & -\frac{1}{h_n} & \end{bmatrix}, \qquad \overline{c}_v = \begin{bmatrix} \gamma_5 \\ \\ \\ \\ \end{bmatrix}. \tag{3.48}$$

With the use of the matrix equations (3.39), (3.43) and (3.47) we have expressed the vectors $\overline{a}$ and $\overline{c}$ in terms of $\overline{b}$ and $\overline{d}$. To determine the relation between $\overline{b}$ and $\overline{d}$ it is enough to subtract Eq. (3.47) form Eq. (3.43)

$$(C_b^* - C_b)\overline{b} + (C_d^* - C_d)\overline{d} + \overline{c}_v^* - \overline{c}_v = \overline{0}, \tag{3.49}$$

which is written as

$$B\overline{b} + D\overline{d} + \overline{v} = \overline{0}, \tag{3.50}$$

where

(3.51)

$$B = \begin{bmatrix} \frac{2h_2}{3}-\gamma_1 & \frac{h_2}{3}-\gamma_2 & & & \\ \frac{h_2}{3} & -\frac{2(h_2+h_3)}{3} & \frac{h_3}{3} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{h_{n-1}}{3} & -\frac{2(h_{n-1}+h_n)}{3} & \frac{h_n}{3} \\ & & & \beta_1+\frac{h_n}{3} & \beta_2+\frac{2h_n}{3} \end{bmatrix},$$

$$D = \begin{bmatrix} \frac{1}{h_2}-\gamma_3 & -\frac{1}{h_2}-\gamma_4 & & & \\ \frac{1}{h_2} & \frac{1}{h_2}+\frac{1}{h_3} & -\frac{1}{h_3} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{h_{n-1}} & \frac{1}{h_{n-1}}+\frac{1}{h_n} & -\frac{1}{h_n} \\ & & & -\frac{1}{h_n} & \beta_3+\frac{1}{h_n} \end{bmatrix},$$

$$\overline{v} = \begin{bmatrix} -\gamma_5 \\ \\ \\ \beta_4 \end{bmatrix}.$$

From Eq. (3.50) there follows

$$D\overline{d} = -B\overline{b} - \overline{v}, \tag{3.52}$$

and finally $\overline{d}$ can be expressed in terms of $\overline{b}$ as

$$\overline{d} = -D^{-1}B\overline{b} - D^{-1}\overline{v}. \tag{3.53}$$

As a consequence of the above result, with the use of Eq. (3.53) $\overline{a}$ and $\overline{c}$ can also be expressed in terms of $\overline{b}$ in Eqs. (3.39) and (3.47). We note that to obtain Eq. (3.53) one has to compute the inverse D^{-1}, which can be done by Gaussian elimination, since D is tridiagonal (see e.g. [4], p. 71.).

From Eq. (3.30) for $i = 3, \ldots, n-1$ and Eqs. (3.31)-(3.33) we construct the following equation:

$$M_3\overline{a} + M_2\overline{b} + M_1\overline{c} + M_0\overline{d} = \overline{m}_v, \tag{3.54}$$

where

$$M_k = \begin{bmatrix} Y_{3,1,k} & Y_{3,2,k} & X_{3,k+3} & & & \\ \vdots & \vdots & \ddots & \ddots & & \\ Y_{n-1,1,k} & Y_{n-1,2,k} & \cdots & Y_{n-1,n-2,k} & X_{n-1,k+3} & \\ X_{1,k} & X_{2,k} & & \cdots & & X_{n,k} \\ X^*_{1,k} & X^*_{2,k} & & \cdots & & X^*_{n,k} \\ X^{**}_{1,k} & X^{**}_{2,k} & & \cdots & & X^{**}_{n,k} \end{bmatrix},$$

$$X^*_{i,k} = X_{i,k+1} - x_i X_{i,k} \text{ and } X^{**}_{i,k} = X_{i,k+2} - 2x_i X_{i,k+1} + x_i^2 X_{i,k},$$

for $i = 1, ..., n$, $l = 0, 1, 2, 3$ and

$$\overline{m} = \begin{bmatrix} F_{3,3} + \sum\limits_{j=1}^{2}\sum\limits_{k=0}^{2}\binom{3}{k} F_{j,k}\left((x_3 - x_j)^{3-k} - (x_2 - x_j)^{3-k}\right) \\ \vdots \\ F_{n-1,3} + \sum\limits_{j=1}^{n-2}\sum\limits_{k=0}^{2}\binom{3}{k} F_{j,k}\left((x_{n-1} - x_j)^{3-k} - (x_{n-2} - x_j)^{3-k}\right) \\ \sum\limits_{i=1}^{n} F_{i,0} \\ \sum\limits_{i=1}^{n} (F_{i,1} - x_i F_{i,0}) \\ \sum\limits_{i=1}^{n} \left(F_{i,2} - 2x_i F_{i,1} + x_i^2 F_{i,0}\right) \end{bmatrix}.$$

Inserting Eqs. (3.39) and (3.47) into Eq. (3.54) we have

$$M_3(A_b\overline{b} + A_d\overline{d} + \overline{a}_v) + M_2\overline{b} + M_1(C_b\overline{b} + C_d\overline{d} + \overline{c}_v) = \overline{m}_v,$$

that is

$$(M_3A_b + M_2 + M_1C_b)\overline{b} + (M_3A_d + M_0 + M_1C_d)\overline{d} + M_3\overline{a}_v + M_1\overline{c}_v = \overline{m}_v,$$

into which we insert Eq. (3.53):

$$\begin{aligned}(M_3A_b + M_2 + M_1C_b)\overline{b} + (M_3A_d + M_0 + M_1C_d)(-D^{-1})(B\overline{b} - \overline{v}) = \\ = \overline{m}_v - M_3\overline{a}_v - M_1\overline{c}_v,\end{aligned}$$

which equals to

$$\begin{aligned}(M_3A_b + M_2 + M_1C_b - (M_3A_d + M_0 + M_1C_d)D^{-1}B)\overline{b} = \\ = \overline{m}_v - M_3\overline{a}_v - M_1\overline{c}_v + (M_3A_d + M_0 + M_1C_d)D^{-1}\overline{v},\end{aligned} \tag{3.55}$$

and is written as

$$L\overline{b} = \overline{w}, \tag{3.56}$$

where L is not a sparse matrix, yet.
To determine the coefficients of the spline functions we have to solve Eq. (3.56) for $\overline{b}$, then Eq. (3.53) for $\overline{d}$, and finally Eqs. (3.39) and (3.47) for $\overline{a}$ and $\overline{c}$.

The Algorithm

The main steps of the iteration are:

1. choose suitable values for the initial weights p_{i_j}, $i = 1, \dots, n, j = 1, \dots, n_i$. At start use unit weights;
2. compute the values of the auxiliary variables (3.24), (3.25), (3.27), (3.29), (3.37), α_1, α_2, α_3, α_4, α_5, (3.41), β_1, β_2, β_3, β_4, (3.45), γ_1, γ_2, γ_3, γ_4, γ_5;
3. initialize the matrices $A_b, A_d, C_b, C_d, B, D, M_0, M_1, M_2, M_3$ and vectors $\overline{a}_v$, $\overline{c}_v$, $\overline{v}$, $\overline{m}_v$;
4. from Eq. (3.52) compute the form of $\overline{d}$ as given in Eq. (3.53).
5. initialize L and $\overline{w}$ figuring in Eqs. (3.55) and (3.56);
6. solve the system of linear equations $L\overline{b} = \overline{w}$;
7. with the solution $\overline{b}$ calculate $\overline{d}$ from Eq. (3.53), then $\overline{a}$ and $\overline{c}$ from Eqs. (3.39) and (3.47);
8. stop if the stop condition is satisfied. Otherwise with the use of the spline function g calculate the weights p_{i_j} and repeat from step 2.

Remarks on step 8:

- one of the possible stop condition is the following: compute the summed square of the difference of the samples and the approximating spline function (at the k^{th} iteration step it is denoted by S_k). At startup set $\varepsilon > 0$ and compare ε with the value of $\dfrac{|S_{k-1} - S_k|}{S_{k-1}}$.
- the larger the difference between point (x_{i_j}, f_{i_j}) and the spline function the smaller the value of p_{i_j} is advisable to choose, e.g.:

$$p_{i_j} = \begin{cases} \dfrac{1}{|f_{i_j} - g_i(x_{i_j})|} & \text{ha } |f_{i_j} - g_i(x_{i_j})| > \varepsilon', \\ \frac{1}{\varepsilon'} & \text{ha } |f_{i_j} - g_i(x_{i_j})| \le \varepsilon', \end{cases}$$

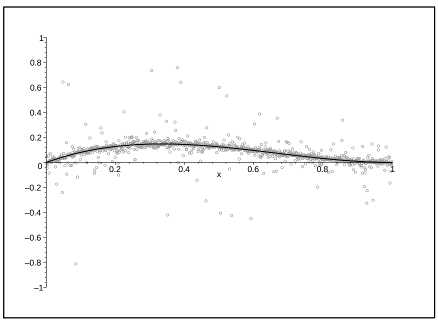
  where the number $\varepsilon' > 0$ is sufficiently small.

4. Example

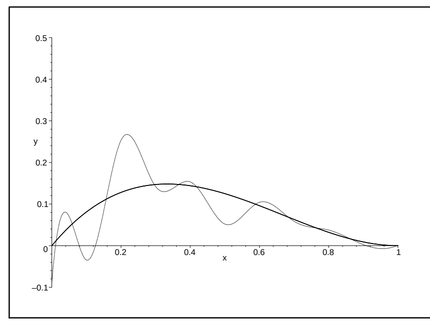
We check the applicability of the solution with the so-called stochastic simulation method: a known solution is polluted with a random variable of normal or Cauchy distribution. The method is then applied to the polluted sample.
In the first example (Figure 1) we have modified the values of the function $f(x) = x^3 - 2x^2 + x$ with a random variable of Cauchy distribution. The interval $[0, 1]$ is divided into 1000 equal parts and the data are collected into 10

groups with equal size. The iteration is done with the help of the Maple V Rel. 5 computer algebra system according to the algorithm presented in the previous section.

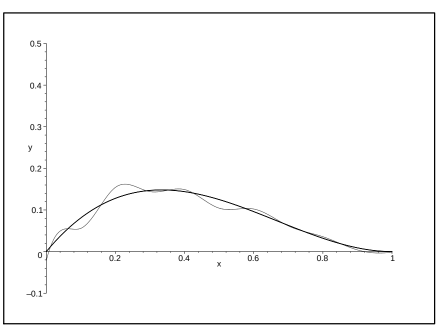
Figure 1:



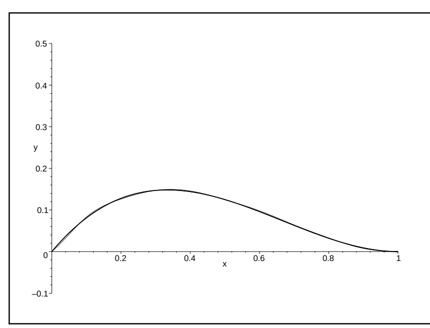
(a) The initial sample



(b) Iteration, step 1



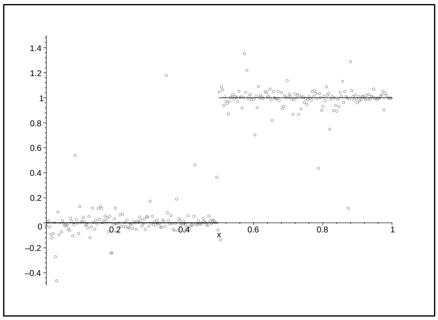
(c) Iteration, step 2



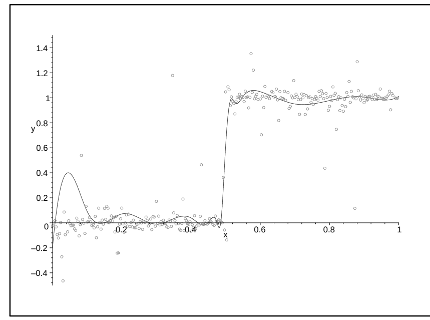
(d) End of iteration, step 8

A discontinuity example is $f(x) := 0$, if $0 \leq x < 1/2$ and 1, if $1/2 \leq x \leq 1$. The interval $[0, 1]$ is divided into 300 equal parts and the data are collected into 10 groups (Figure 2).

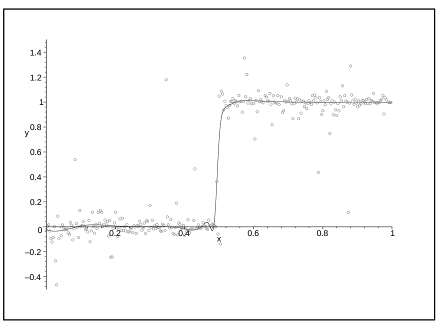
Figure 2:



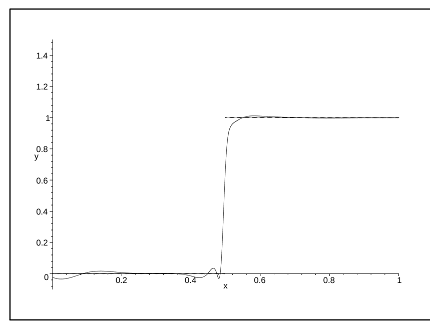
(a) The initial sample



(b) Iteration, step 2



(c) End of iteration, step 8



(d) End of iteration, step 9

5. Conclusion

We have modeled a function approximating a large number of samples with piecewise third-degree spline polynomials. The solution is a twice continuously differentiable spline function which gives the minimum of the variational problem according to the method of least squares and approximates the data in a similar manner as robust estimators.

The novelty of the method is that it makes global equalization with piecewise approximation on a large number of samples. Contrary to the current spline approximation methods, where a third-order polynomial is defined between every point, in this treatment the points are grouped together. After that we search for curves which approximate these groups well according to specific conditions and, moreover, give a good approximation of the data points globally.

The method can be applied to analyze dynamical properties and determine the velocity and acceleration vectors with the use of the location of the bodies as data points. In the model calculations fast convergence is apparent and large oscillations, known in the Newtonian interpolation method, do not appear.

References

[1] **Sard A.,** *A book of splines*, John Wiley and Sons, Mc., New York, 1971.

[2] **Prvan T.,** Smoothing splines with variable continuity properties and degree, *Appl. Math. Lett.,* **10** (2) (1997), 75-80. `http://www.ingentaconnect.com/content/els/08939659/1997/00000010/00000002/art00014`

[3] **Závoti J.,** *A DTM matematikai alapjai és geodéziai alkalmazásai*, kandidátusi értekezés, MTA GGKI, Sopron, 1985.

[4] **Stoyan G. 'es Takó G.,** *Numerikus módszerek 1.,* ELTE-Typotex, Budapest, 1993. (Stoyan G. and Takó G., *Numerical methods 1.*, (in Hungarian))

[5] **Marcsuk G.I.,** *A gépi matematika numerikus módszerei (Parciális differenciál egyenletek)*, Műszaki könyvkiadó, Budapest, 1976. (Marchuk G.I., *Numerical methods for computerized mathematics (Partial differential equations)* (in Hungarian))

[6] **Utreras F.,** Natural spline functions, their associated eigenvalue problem, *Numer. Math.* **42** (1983), 107-117.

[7] **Meise M.,** *Residual based selection of smoothing parameters*, Dissertation, Universität Duisburg-Essen, 2004.

[8] **Schoenberg I.J.,** Spline functions and the problem of graduation, *Proc. Amer. Math. Soc.,* **52** (1964), 947-950.

[9] **Reinsch C.H.,** Smoothing by spline functions, *Numer. Math.,* **10** (1967), 177-183.

[10] **Reinsch C.H.,** Smoothing by spline functions II., *Numer. Math.,* **16** (1971), 451-454.

[11] **de Boor C.,** *A practical guide to splines*, Springer-Verlag, New York, 1978.

[12] **de Boor C.,** Calculation of the smoothing spline with weighted roughness measure, *Math. Models Methods Appl. Sci.,* **11** (1) (2001), 33-41.

[13] **Wahba G.,** Smoothing noisy data with spline functions, *Numer. Math.,* **24** (1975), 383-393.

(*Received June 26, 2008*)

R. Polgár
Institute of Mathematics
University of West Hungary
H-9400 Sopron, Ady E. u. 5.
polgar@emk.nyme.hu